

Anhang zur Dissertation - Ralf Tonner

Zweiwertige Kohlenstoff(0)-Verbindungen:

Quantenchemische Studien zur Bindungssituation und Reaktivität von Carbodiphosphoranen und Analoga

Gegeben sind kartesische Koordinaten und SCF-Energien der berechneten Verbindungen.

Zur Nomenklatur sei auf die Dissertation verwiesen.

Das theoretische Niveau der Optimierung und mögliche Symmetrievorgaben sind ebenfalls gegeben.

Verzeichnisnamen beziehen sich auf elektronische Form, die als CD-ROM beiliegt

Molekuele/1R/BP86_TZ2P

	1H	BP86/TZ2P	
9			
E(SCF) =	-1.346762		
C	0.000000	0.000000	0.691163
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P	0.000000	-1.467861	-0.071679
H	0.000000	2.551528	0.845049
H	-1.080494	1.906674	-0.921843
H	1.080494	1.906674	-0.921843
H	0.000000	-2.551528	0.845049
H	-1.080494	-1.906674	-0.921843
H	1.080494	-1.906674	-0.921843

	1Me	BP86/TZ2P	
27			
E(SCF) =	-5.023395		
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P	0.000000	1.534860	-0.109470
P	0.000000	-1.534860	-0.109470
C	0.000000	2.772830	-1.470430
C	1.431080	2.113630	0.923120
C	-1.431080	2.113630	0.923120
C	0.000000	-2.772830	-1.470430
C	-1.431080	-2.113630	0.923120
C	1.431080	-2.113630	0.923120
H	-0.889700	2.609280	-2.092830
H	0.889700	2.609280	-2.092830
H	0.000000	3.803080	-1.086400
H	2.363160	1.931080	0.371270
H	1.352240	3.184420	1.162820
H	1.462350	1.538860	1.859620
H	-2.363160	1.931080	0.371270

H	-1.352240	3.184420	1.162820
H	-1.462350	1.538860	1.859620
H	-0.889700	-2.609280	-2.092830
H	0.889700	-2.609280	-2.092830
H	0.000000	-3.803080	-1.086400
H	-2.363160	-1.931080	0.371270
H	-1.352240	-3.184420	1.162820
H	-1.462350	-1.538860	1.859620
H	1.462350	-1.538860	1.859620
H	2.363160	-1.931080	0.371270
H	1.352240	-3.184420	1.162820

	1Ph	BP86/TZ2P	
69			
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C	1.432920	2.549046	0.874097
C	0.000000	1.856249	-1.552182
C	1.432920	-2.549046	0.874097
C	-1.432920	-2.549046	0.874097
C	0.000000	-1.856249	-1.552182
C	-1.766664	3.803662	0.342379
C	-2.834170	4.533441	0.866322
C	-3.573332	4.024805	1.937261
C	-3.241791	2.781097	2.478562
C	-2.179435	2.047564	1.946464
C	2.179435	2.047564	1.946464
C	3.241791	2.781097	2.478562
C	3.573332	4.024805	1.937261
C	2.834170	4.533441	0.866322
C	1.766664	3.803662	0.342379
C	-1.209000	1.910733	-2.264207
C	-1.207972	2.045530	-3.653091
C	0.000000	2.117407	-4.350589
C	1.207972	2.045530	-3.653091
C	1.209000	1.910733	-2.264207
C	2.179435	-2.047564	1.946464
C	3.241791	-2.781097	2.478562
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C	2.834170	-4.533441	0.866322
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C	-1.766664	-3.803662	0.342379
C	-2.834170	-4.533441	0.866322

C	-3.573332	-4.024805	1.937261
C	-3.241791	-2.781097	2.478562
C	-2.179435	-2.047564	1.946464
C	1.209000	-1.910733	-2.264207
C	1.207972	-2.045530	-3.653091
C	0.000000	-2.117407	-4.350589
C	-1.207972	-2.045530	-3.653091
C	-1.209000	-1.910733	-2.264207
H	2.156630	-1.855821	-1.727702
H	2.154591	-2.093217	-4.191180
H	0.000000	-2.223625	-5.435695
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H	-2.156630	-1.855821	-1.727702
H	-1.202769	-4.211247	-0.496241
H	-3.090336	-5.501216	0.435036
H	-4.406097	-4.597280	2.346311
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H	-1.908384	-1.072286	2.349152
H	1.908384	-1.072286	2.349152
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H	3.090336	-5.501216	0.435036
H	1.202769	-4.211247	-0.496241
H	1.202769	4.211247	-0.496241
H	3.090336	5.501216	0.435036
H	4.406097	4.597280	2.346311
H	3.813701	2.380148	3.315431
H	1.908384	1.072286	2.349152
H	-3.090336	5.501216	0.435036
H	-1.202769	4.211247	-0.496241
H	-1.908384	1.072286	2.349152
H	-3.813701	2.380148	3.315431
H	-4.406097	4.597280	2.346311
H	-2.156630	1.855821	-1.727702
H	2.156630	1.855821	-1.727702
H	2.154591	2.093217	-4.191180
H	0.000000	2.223625	-5.435695
H	-2.154591	2.093217	-4.191180

Molekuele/1R/RI-BP86_SVP

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C	0.000251	0.000000	0.834150
P	0.000010	-1.497573	0.196506
P	0.000010	1.497573	0.196506

Cl	-0.000037	2.940180	1.649657
Cl	-1.607173	2.079157	-0.988260
Cl	1.607075	2.079496	-0.988184
Cl	-0.000037	-2.940180	1.649657
Cl	-1.607173	-2.079157	-0.988260
Cl	1.607075	-2.079496	-0.988183

	1Cy	RI-BP86/SVP	
105			
E(SCF) =	-2131.229592		
C	-0.053843	0.018054	0.083834
P	1.579429	-0.139058	0.033604
P	-1.677655	0.176660	-0.092719
C	-2.394366	-0.357351	-1.778463
C	-2.049955	-0.212768	-4.317770
C	-3.055993	-2.301373	-3.311209
C	-2.195495	-1.735298	-4.449397
C	-2.519658	-1.889572	-1.927515
C	-1.524761	0.194416	-2.929256
H	-3.040211	0.266599	-4.493183
H	-4.100866	-1.931451	-3.422577
H	-1.185873	-2.203508	-4.411202
H	-1.514501	-2.341681	-1.773886
H	-0.493067	-0.196375	-2.782476
H	-3.413966	0.091411	-1.833232
H	-1.372367	0.182420	-5.105052
H	-3.111098	-3.409302	-3.377925
H	-2.627391	-2.004396	-5.437142
H	-3.174535	-2.313007	-1.141009
H	-1.439329	1.296390	-2.871380
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C	-2.311235	3.956262	1.752095
C	-3.044075	4.248052	-0.652132
C	-2.332404	4.901176	0.541488
C	-2.427247	2.882181	-1.011465
C	-1.703909	2.587838	1.394756
H	-3.352149	3.813604	2.122521
H	-4.120757	4.107000	-0.403305
H	-1.285856	5.148619	0.252128
H	-1.385285	3.038825	-1.368215
H	-0.629015	2.703214	1.135622
H	-3.473816	1.731993	0.477090
H	-1.743908	4.413056	2.591363
H	-3.016165	4.918703	-1.537835
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H	-2.991846	2.439200	-1.857063

H	-1.728181	1.921650	2.282802
C	-2.686595	-0.745284	1.243686
C	-4.899008	-1.428383	2.296580
C	-2.770352	-2.689363	2.875662
C	-4.295349	-2.783554	2.700267
C	-2.090960	-2.113495	1.620887
C	-4.214084	-0.845548	1.043513
H	-4.782208	-0.710191	3.139687
H	-2.541929	-2.035244	3.747913
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H	-2.221479	-2.828141	0.779184
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H	-2.513648	-0.075532	2.119068
H	-5.991973	-1.526964	2.121103
H	-2.346510	-3.687975	3.116733
H	-4.774083	-3.157129	3.630699
H	-0.997103	-2.002642	1.767148
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C	2.180571	-1.791750	-0.719939
C	4.032680	-3.432895	-1.331541
C	1.633168	-4.237489	-1.154343
C	3.114068	-4.615082	-0.985667
C	1.276890	-2.980448	-0.342757
C	3.667248	-2.162469	-0.536469
H	3.949243	-3.212179	-2.420035
H	1.422688	-4.050641	-2.232327
H	3.293605	-4.920463	0.070461
H	1.386673	-3.208164	0.740076
H	3.876470	-2.338461	0.542327
H	2.013295	-1.594395	-1.805917
H	5.096020	-3.700216	-1.150093
H	0.980468	-5.084772	-0.852703
H	3.367916	-5.497564	-1.611159
H	0.216837	-2.689651	-0.488317
H	4.330041	-1.331559	-0.851847
C	2.499877	1.116535	-1.098872
C	2.296918	3.292713	-2.403233
C	4.591764	2.377499	-1.825673
C	3.759217	3.643206	-2.082932
C	3.957370	1.483296	-0.740860
C	1.676637	2.399420	-1.315601
H	2.253266	2.760600	-3.380909
H	4.676170	1.795130	-2.771351
H	3.788635	4.288698	-1.175648
H	3.974393	2.030358	0.227321
H	1.621307	2.969254	-0.360779

H	2.520441	0.574106	-2.073784
H	1.694967	4.218685	-2.526751
H	5.629509	2.647888	-1.533950
H	4.207833	4.241875	-2.904427
H	4.583136	0.579421	-0.596259
H	0.632546	2.123463	-1.565437
C	2.440654	0.019488	1.716431
C	2.747173	1.544943	3.753138
C	2.710378	-0.965049	4.064851
C	2.369348	0.392776	4.695530
C	2.068197	-1.130274	2.674981
C	2.101084	1.377482	2.366257
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H	3.816633	-1.056116	3.970468
H	1.276224	0.435026	4.903756
H	0.960123	-1.154785	2.774159
H	0.994544	1.442260	2.453821
H	3.534517	-0.025247	1.512935
H	2.448040	2.520823	4.192774
H	2.387271	-1.795166	4.729341
H	2.878941	0.506186	5.676330
H	2.364945	-2.109038	2.245892
H	2.405609	2.215988	1.706104

1F

RI-BP86/SVP

9

E(SCF) = -1319.369804

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F	-2.763371	1.135633	-0.032122
P	1.368669	1.125935	-0.309900
F	2.231236	1.279400	1.018924
F	1.576445	2.587164	-0.905252
F	2.431043	0.345212	-1.199775
F	-1.985887	-0.716127	1.314033
F	-2.195282	-0.966044	-1.079758

1H

RI-BP86/SVP

9

E(SCF) = -724.115527

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P	0.000000	-1.466791	-0.073006
H	0.000000	2.574721	0.834194
H	-1.088629	1.904551	-0.940296
H	1.088629	1.904551	-0.940296

H	0.000000	-2.574721	0.834194
H	-1.088629	-1.904551	-0.940296
H	1.088629	-1.904551	-0.940296

	1H2Me	RI-BP86/SVP	
15			
E(SCF) =	-802.714263		
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P	1.479867	-0.414140	0.000088
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H	-1.885682	-1.296016	1.088929
C	-2.876720	0.779882	0.000166
C	2.876671	0.779908	0.000000
H	1.885753	-1.295828	1.089246
H	1.886225	-1.296449	-1.088404
H	3.850591	0.251210	0.000465
H	2.790833	1.419758	-0.899246
H	2.790292	1.420335	0.898787
H	-3.850625	0.251165	0.000776
H	-2.790194	1.420180	0.899038
H	-2.791036	1.419871	-0.898989

	1HMe2	RI-BP86/SVP	
21			
E(SCF) =	-881.307417		
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P	1.478794	-0.113108	0.240879
P	-1.478845	-0.113175	-0.240958
C	2.758187	1.131885	0.691582
H	1.700603	-1.087790	1.307970
C	2.270375	-1.049524	-1.159161
C	-2.758331	1.131774	-0.691486
H	-1.700912	-1.087977	-1.307891
C	-2.270115	-1.049490	1.159335
H	-3.743726	0.658942	-0.875240
H	-2.835094	1.867210	0.133280
H	-2.420265	1.663422	-1.601487
H	3.273581	-1.432711	-0.880615
H	1.620871	-1.902793	-1.437390
H	2.353500	-0.373641	-2.033123
H	3.743532	0.659064	0.875646
H	2.835167	1.867223	-0.133250
H	2.419888	1.663643	1.601433
H	-3.273321	-1.432813	0.880970
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H	-2.353182	-0.373530	2.033241
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1Me	RI-BP86/SVP
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27

E(SCF) =	-959.897236		
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C	0.781897	1.438670	2.524949
C	0.761018	-1.451257	2.519766
C	0.305852	0.009159	-2.878714
C	2.268663	-1.448951	-1.337828
C	2.282188	1.441143	-1.330470
H	-2.257284	-0.879119	1.942082
H	-2.244055	0.912808	1.946071
H	-1.733896	0.009735	3.434319
H	0.332680	2.375557	2.141215
H	0.643942	1.385827	3.624783
H	1.866385	1.454184	2.297211
H	0.298047	-2.380115	2.132867
H	0.624287	-1.400288	3.619839
H	1.845054	-1.481810	2.291395
H	-0.344473	-0.883625	-2.956615
H	-0.336087	0.908365	-2.952204
H	1.048842	0.007689	-3.701525
H	1.667607	-2.378899	-1.365392
H	2.912772	-1.398027	-2.240044
H	2.911957	-1.477219	-0.435812
H	2.925627	1.458961	-0.428295
H	1.689905	2.376819	-1.353591
H	2.925920	1.388554	-2.232860

1Mes	RI-BP86/SVP
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123

E(SCF) =	-2816.601713		
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P	1.586330	0.400878	0.018830
P	-1.586883	-0.400925	0.051871
C	2.278062	2.002208	-0.784261
C	2.788628	-0.831632	-0.885619
C	-2.293894	-2.007234	-0.727489
C	1.959172	0.498780	1.882618
C	-2.806167	0.825930	-0.837387
C	-1.923999	-0.486996	1.923070
C	1.436074	2.967003	-1.418743

C	2.012476	3.988161	-2.204299
C	3.397386	4.134833	-2.368388
C	4.214148	3.233448	-1.667805
C	2.606831	-0.902808	-2.311064
C	3.272422	-1.893284	-3.057751
C	3.694923	2.183128	-0.883540
C	4.144484	-2.829179	-2.478185
C	4.377790	-2.696822	-1.105402
C	3.749686	-1.716318	-0.300945
C	-1.464357	-2.976169	-1.371912
C	-2.055869	-4.002400	-2.139470
C	-3.443668	-4.150023	-2.275695
C	-4.246722	-3.243982	-1.565293
C	-3.712430	-2.188647	-0.798120
C	2.274731	1.704783	2.591724
C	2.417617	1.654369	3.997975
C	2.253858	0.482717	4.749095
C	1.893188	-0.676482	4.044016
C	1.728607	-0.692108	2.647387
C	-2.651634	0.887832	-2.266481
C	-3.330827	1.873964	-3.006642
C	-4.191066	2.814216	-2.416536
C	-4.398257	2.690734	-1.038745
C	-3.755529	1.714876	-0.240193
C	-1.679078	0.708745	2.675817
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C	-2.164221	-0.452818	4.794470
C	-2.342117	-1.629125	4.054032
C	-2.225894	-1.688456	2.645634
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H	-1.641270	1.644661	4.619400
H	-1.386289	-4.721691	-2.639862
H	-5.343153	-3.362602	-1.592100
H	-3.178559	1.896077	-4.098668
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H	5.309838	3.351891	-1.716696
H	1.333233	4.704207	-2.696257
H	3.099355	-1.922483	-4.146514
H	5.103653	-3.371403	-0.619948
H	1.727359	-1.615649	4.597263
H	2.668049	2.591056	4.522830
C	-4.261096	1.694879	1.192836
H	-3.867313	0.874318	1.808144
H	-5.367381	1.607075	1.184024
H	-4.024678	2.645376	1.712958
C	-1.840213	-0.092881	-3.086302

H	-0.920660	-0.414962	-2.569292
H	-1.559800	0.358610	-4.057974
H	-2.435691	-1.005033	-3.298919
C	-4.861594	3.892736	-3.233927
H	-4.153564	4.717626	-3.465788
H	-5.722267	4.338389	-2.697384
H	-5.225892	3.501094	-4.205575
C	1.779217	0.072209	-3.121415
H	0.869715	0.397341	-2.588794
H	1.480306	-0.385711	-4.084521
H	2.370022	0.983181	-3.351485
C	4.282177	-1.687219	1.122129
H	4.055396	-2.634268	1.652735
H	3.900152	-0.862611	1.739436
H	5.388108	-1.599811	1.091936
C	4.800232	-3.912398	-3.301336
H	5.670806	-4.354597	-2.778078
H	5.146450	-3.526487	-4.281856
H	4.088369	-4.738852	-3.515197
C	-4.733143	-1.359410	-0.045676
H	-4.334058	-0.924873	0.886851
H	-5.598952	-1.995934	0.227293
H	-5.120528	-0.523764	-0.662064
C	0.036232	-3.024335	-1.245001
H	0.486293	-3.598533	-2.077146
H	0.328921	-3.533937	-0.301645
H	0.477710	-2.013058	-1.205589
C	-4.046615	-5.231361	-3.140638
H	-3.371640	-6.105152	-3.234332
H	-4.240294	-4.856808	-4.169383
H	-5.016969	-5.584473	-2.737561
C	-2.338224	-0.421503	6.294377
H	-1.487665	0.088255	6.791900
H	-2.424001	-1.440857	6.718858
H	-3.255617	0.137001	6.579670
C	-1.260844	2.023889	2.059087
H	-0.156764	2.078459	2.024905
H	-1.618664	2.870278	2.678502
H	-1.616766	2.169934	1.026941
C	-2.407153	-3.073114	2.052634
H	-2.411484	-3.823578	2.866862
H	-1.602178	-3.347529	1.346615
H	-3.355503	-3.184660	1.493172
C	2.444686	3.085611	1.986540
H	3.382194	3.193395	1.408357
H	2.464650	3.841250	2.795730

H	1.626389	3.355696	1.294309
C	1.298793	-2.011101	2.047021
H	1.635077	-2.163728	1.009271
H	0.194269	-2.065689	2.034002
H	1.668214	-2.853588	2.664944
C	2.457968	0.460813	6.245379
H	2.532405	1.483344	6.664396
H	3.391990	-0.078098	6.514219
H	1.627918	-0.063688	6.761700
C	4.730076	1.358852	-0.145509
H	5.106234	0.519683	-0.764068
H	4.348871	0.929726	0.796956
H	5.600508	1.997399	0.107253
C	-0.061753	3.016053	-1.262884
H	-0.502259	2.005061	-1.208465
H	-0.528035	3.584949	-2.089707
H	-0.336002	3.531635	-0.317236
C	3.983214	5.210491	-3.251973
H	4.964102	5.561837	-2.873659
H	3.309169	6.086273	-3.333184
H	4.150819	4.831109	-4.283521

	1NH2	RI-BP86/SVP	
21			
E(SCF) =	=		
C	0.000001	0.000255	-1.042828
P	1.421067	-0.022383	-0.184295
P	-1.421046	0.022515	-0.184273
N	-2.739503	-0.005980	-1.266095
N	-1.950961	1.272348	0.914794
N	-1.596239	-1.261910	0.960070
N	2.739483	0.005848	-1.266162
N	1.596552	1.261964	0.960048
N	1.950684	-1.272374	0.914722
H	-3.577539	0.503663	-0.970706
H	-2.458572	0.205716	-2.227480
H	-2.533136	-1.315821	1.382652
H	-1.370861	-2.160487	0.516835
H	-1.271630	1.339029	1.687943
H	-1.934837	2.179485	0.427459
H	2.533452	1.315732	1.382635
H	1.371218	2.160596	0.516911
H	3.577540	-0.503732	-0.970734
H	2.458531	-0.205926	-2.227522
H	1.271211	-1.339086	1.687744
H	1.934585	-2.179453	0.427280

-----	1NMe2	RI-BP86/SVP	
57			
E(SCF) =	-1527.472282		
C	-0.042701	0.065526	1.002479
P	0.000585	-0.053330	2.621166
P	-0.010740	0.070403	-0.620724
N	-1.378527	-0.710808	-1.334531
N	1.269714	-0.751063	-1.474657
N	0.202219	1.649792	-1.309163
N	0.274729	-1.600201	3.380053
N	1.289033	0.849444	3.339779
N	-1.506101	0.338987	3.388935
C	1.473987	0.938758	4.778092
H	1.030240	1.864662	5.220519
H	2.560609	0.948039	5.026115
H	1.027201	0.061763	5.281071
C	1.996554	1.858497	2.573354
H	1.796836	1.694535	1.496803
H	3.095120	1.785405	2.749533
H	1.685276	2.898526	2.839593
C	-1.753646	0.160852	4.811500
H	-1.589323	1.093905	5.404965
H	-1.099818	-0.632954	5.216561
H	-2.811490	-0.148218	4.978368
C	-2.381865	1.312049	2.759089
H	-3.447488	1.014349	2.888085
H	-2.157014	1.353852	1.676357
H	-2.268982	2.339190	3.187188
C	-0.750545	-2.611505	3.127580
H	-0.670755	-3.053138	2.103662
H	-1.758390	-2.169040	3.230363
H	-0.650760	-3.437429	3.864887
C	1.619928	-2.153284	3.243254
H	1.798143	-2.604634	2.235638
H	1.775704	-2.949271	4.003602
H	2.374829	-1.361503	3.399562
C	-2.553929	-1.011058	-0.538178
H	-2.924368	-2.039695	-0.757732
H	-3.398005	-0.304821	-0.733414
H	-2.283700	-0.951403	0.533789
C	-1.587450	-0.765712	-2.771194
H	-2.280937	0.028142	-3.143719
H	-2.031897	-1.746834	-3.058311
H	-0.625243	-0.669197	-3.306385
C	1.245146	-2.210611	-1.418826

H	1.623782	-2.609521	-0.445045
H	1.885120	-2.626178	-2.227329
H	0.213059	-2.579979	-1.559051
C	2.614498	-0.226802	-1.241119
H	3.024658	-0.532589	-0.247080
H	2.607142	0.877887	-1.281245
H	3.304788	-0.604134	-2.026560
C	0.412782	1.885824	-2.729333
H	-0.529746	2.134897	-3.276614
H	0.868381	0.996121	-3.200964
H	1.108598	2.744543	-2.873596
C	-0.321217	2.801663	-0.595182
H	-0.410416	2.551682	0.479143
H	-1.323428	3.126604	-0.970540
H	0.369699	3.669036	-0.700632

	1Ph	RI-BP86/SVP	
69			
E(SCF) =	-2109.155405		
C	0.000424	0.006143	-0.924794
P	1.529509	-0.139629	-0.288775
P	-1.529197	0.144046	-0.288293
C	2.355124	1.464839	0.195433
C	2.661730	-0.824569	-1.594086
C	-2.355592	-1.466395	0.174206
C	1.848164	-1.240439	1.181391
C	-2.660119	0.846265	-1.585512
C	-1.848906	1.225603	1.195856
C	1.797102	2.650941	-0.331758
C	2.380844	3.912154	-0.053268
C	3.538702	3.990257	0.767727
C	4.098802	2.798403	1.303648
C	2.099961	-1.147933	-2.847809
C	2.910403	-1.659570	-3.892325
C	3.507026	1.543523	1.014242
C	4.302784	-1.849935	-3.678238
C	4.869468	-1.523722	-2.415155
C	4.047601	-1.012459	-1.380194
C	-1.797233	-2.645683	-0.367701
C	-2.381413	-3.910295	-0.106051
C	-3.540071	-3.998800	0.712751
C	-4.100529	-2.813868	1.263442
C	-3.508292	-1.555455	0.990822
C	1.658296	-0.746794	2.496148
C	1.761299	-1.610067	3.614803
C	2.050566	-2.989336	3.425616

C	2.231981	-3.490008	2.107615
C	2.128701	-2.616175	0.996589
C	-2.097261	1.185552	-2.834532
C	-2.906694	1.711014	-3.872953
C	-4.299148	1.899238	-3.657454
C	-4.866928	1.556983	-2.399115
C	-4.046068	1.031995	-1.370243
C	-2.129107	2.603681	1.028837
C	-2.233288	3.462889	2.151129
C	-2.053113	2.944965	3.462617
C	-1.764165	1.563299	3.633982
C	-1.660265	0.714746	2.504204
H	-1.430811	-0.347561	2.659575
H	-1.623492	1.155131	4.644160
H	-2.133966	3.606987	4.335712
H	-2.453505	4.529705	2.009211
H	-2.271597	3.023782	0.024868
H	-0.896368	-2.571194	-0.992620
H	-1.939714	-4.821365	-0.531845
H	-3.997577	-4.975754	0.921431
H	-4.991978	-2.876947	1.902372
H	-3.952674	-0.658895	1.439752
H	-1.018209	1.028353	-2.981911
H	-2.461499	1.970851	-4.842881
H	-4.933916	2.303652	-4.458018
H	-5.942892	1.697644	-2.228309
H	-4.509030	0.773089	-0.410614
H	3.951117	0.641301	1.451982
H	4.989617	2.853362	1.944209
H	3.995862	4.964502	0.989419
H	1.939418	4.828576	-0.467708
H	0.896851	2.584403	-0.958458
H	2.466046	-1.907046	-4.865864
H	1.020952	-0.989288	-2.993966
H	4.509731	-0.765769	-0.416953
H	5.945371	-1.666082	-2.245376
H	4.938334	-2.243673	-4.483489
H	1.428559	0.313350	2.665226
H	2.272156	-3.023062	-0.012667
H	2.452466	-4.554844	1.951920
H	2.130715	-3.662730	4.290036
H	1.619670	-1.215183	4.630116

Molekuele/1R/RI-BP86_TZVP

1Cl

RI-BP86/TZVP

E(SCF) =	-3482.526114		
C	0.002434	0.000000	0.824712
P	0.000410	-1.500194	0.189096
P	0.000410	1.500194	0.189096
Cl	-0.001064	2.926977	1.670607
Cl	-1.621482	2.093662	-0.992595
Cl	1.620919	2.097237	-0.992669
Cl	-0.001064	-2.926977	1.670607
Cl	-1.621482	-2.093662	-0.992595
Cl	1.620919	-2.097237	-0.992669

1F Σ -BP86/TZVP

9			
E(SCF) =	-1320.347744		
C	-0.100565	0.547092	-0.207288
P	-1.593148	0.057296	-0.020566
F	-2.763035	1.138656	-0.046174
P	1.368148	1.125955	-0.309430
F	2.233104	1.265123	1.021462
F	1.571157	2.593916	-0.894244
F	2.423932	0.347807	-1.212118
F	-1.984546	-0.704749	1.322493
F	-2.186147	-0.976611	-1.075998

1H Σ -BP86/TZVP

9			
E(SCF) =	-724.379231		
C	0.000000	0.000000	0.744772
P	0.000000	1.460216	-0.077928
P	0.000000	-1.460216	-0.077928
H	0.000000	2.562889	0.825386
H	-1.088649	1.881103	-0.945391
H	1.088649	1.881103	-0.945391
H	0.000000	-2.562889	0.825386
H	-1.088649	-1.881103	-0.945391
H	1.088649	-1.881103	-0.945391

1Me Σ -BP86/TZVP

27			
E(SCF) =	-960.419046		
C	0.000001	0.000115	0.779044
P	-1.526363	0.000018	0.117456
P	1.526363	0.000031	0.117451
C	-2.793405	-0.004146	1.464324
C	-2.069411	-1.444949	-0.940715
C	-2.071648	1.449092	-0.933843

C	2.793420	0.000537	1.464314
C	2.070568	1.446691	-0.937791
C	2.070477	-1.447377	-0.936764
H	-2.636222	0.884044	2.089449
H	-2.635104	-0.895236	2.085019
H	-3.818010	-0.003782	1.066244
H	-1.885246	-2.372246	-0.382811
H	-3.134817	-1.383644	-1.208230
H	-1.469273	-1.465085	-1.860541
H	-1.889223	2.373930	-0.371308
H	-3.136859	1.387279	-1.202012
H	-1.471196	1.474805	-1.853321
H	2.635634	0.890377	2.086937
H	2.635722	-0.888904	2.087523
H	3.818022	0.000469	1.066229
H	1.886887	2.372985	-0.378062
H	3.135981	1.385243	-1.205245
H	1.470582	1.469055	-1.857664
H	1.470392	-1.470450	-1.856552
H	1.886863	-2.373250	-0.376321
H	3.135863	-1.386101	-1.204354

	1NH2	RI-BP86/TZVP	
21			
E(SCF) =	-1056.819592		
C	-0.000024	-0.000160	-0.970078
P	1.449924	-0.015964	-0.157535
P	-1.449934	0.015885	-0.157455
N	-2.709096	0.039869	-1.319713
N	-2.035930	1.236482	0.950622
N	-1.705336	-1.304212	0.932377
N	2.709070	-0.039685	-1.319833
N	1.705163	1.304102	0.932392
N	2.036165	-1.236511	0.950474
H	-3.555442	0.542377	-1.059902
H	-2.367742	0.274504	-2.249221
H	-2.658415	-1.360432	1.298708
H	-1.446233	-2.188181	0.493891
H	-1.462658	1.253043	1.798251
H	-1.989451	2.161594	0.517425
H	2.658265	1.360428	1.298647
H	1.445934	2.188059	0.493954
H	3.555394	-0.542294	-1.060138
H	2.367669	-0.274182	-2.249363
H	1.463037	-1.253095	1.798200
H	1.989640	-2.161627	0.517292

	1NMe2	3I-BP86/TZVP	
57			
E(SCF) =	-1528.585005		
C	-0.441349	0.136434	1.014736
P	-0.101992	-0.053780	2.601342
P	-0.100157	0.061627	-0.581956
N	-1.340592	-0.783811	-1.444728
N	1.300135	-0.729301	-1.268478
N	0.172643	1.643409	-1.262136
N	0.202405	-1.616761	3.323738
N	1.339411	0.755094	3.149195
N	-1.481407	0.393716	3.552530
C	1.779590	0.721696	4.541078
H	1.387737	1.571848	5.133757
H	2.882116	0.773038	4.579936
H	1.464545	-0.213819	5.016888
C	1.770504	1.955597	2.444243
H	1.413070	1.917948	1.408241
H	2.873179	2.007710	2.438079
H	1.392231	2.883879	2.918020
C	-1.477379	0.338536	5.008946
H	-1.200031	1.305015	5.474776
H	-0.782305	-0.434211	5.356736
H	-2.487490	0.076685	5.370756
C	-2.460416	1.321042	3.003767
H	-3.475019	1.026774	3.325614
H	-2.405381	1.281807	1.908571
H	-2.289496	2.364411	3.337164
C	-0.911644	-2.566806	3.235699
H	-1.015402	-2.997974	2.220449
H	-1.851617	-2.068365	3.498005
H	-0.736493	-3.392021	3.944378
C	1.470120	-2.261599	2.973865
H	1.441902	-2.725484	1.967620
H	1.685346	-3.056045	3.706725
H	2.286046	-1.530715	2.993951
C	-2.636881	-1.007039	-0.820293
H	-3.006352	-2.017413	-1.071087
H	-3.396487	-0.274262	-1.157991
H	-2.521076	-0.922955	0.267502
C	-1.368394	-0.836411	-2.900932
H	-1.998524	-0.040248	-3.344545
H	-1.781834	-1.806060	-3.230208
H	-0.353722	-0.748057	-3.306023
C	1.312769	-2.193130	-1.241039

H	1.598122	-2.595755	-0.248935
H	2.044543	-2.560561	-1.978833
H	0.321984	-2.582929	-1.498727
C	2.596700	-0.177667	-0.863051
H	2.882832	-0.485825	0.161620
H	2.569251	0.917366	-0.899932
H	3.373849	-0.534411	-1.558139
C	0.556533	1.857635	-2.654592
H	-0.315572	2.020858	-3.318224
H	1.126827	0.998778	-3.025723
H	1.196250	2.755092	-2.724877
C	-0.575862	2.763687	-0.703495
H	-0.826566	2.542154	0.341008
H	-1.513062	2.965461	-1.260590
H	0.039740	3.679142	-0.739427

	1Ph	RI-BP86/TZVP	
69			
E(SCF) =	-2111.208485		
C	0.000000	-0.000019	0.938031
P	1.538922	-0.029123	0.288723
P	-1.538924	0.029118	0.288728
C	2.125983	-1.676640	-0.373565
C	2.748792	0.352453	1.649742
C	-2.125977	1.676654	-0.373521
C	1.997568	1.176975	-1.061093
C	-2.748789	-0.352485	1.649745
C	-1.997581	-1.176953	-1.061109
C	1.451263	-2.821549	0.072088
C	1.861338	-4.090786	-0.344343
C	2.948019	-4.227165	-1.214139
C	3.621568	-3.088869	-1.668467
C	2.237766	0.761204	2.887528
C	3.104505	1.063488	3.942331
C	3.213872	-1.818108	-1.250150
C	4.487700	0.955437	3.766174
C	5.002189	0.542519	2.532152
C	4.136555	0.240711	1.476858
C	-1.451185	2.821540	0.072079
C	-1.861244	4.090790	-0.344328
C	-2.947983	4.227205	-1.214045
C	-3.621598	3.088930	-1.668330
C	-3.213918	1.818157	-1.250037
C	1.690103	0.887844	-2.401550
C	1.905048	1.841124	-3.400262
C	2.424803	3.098114	-3.072462

C	2.726987	3.396087	-1.740293
C	2.515231	2.442098	-0.740279
C	-2.237755	-0.761163	2.887551
C	-3.104488	-1.063456	3.942355
C	-4.487687	-0.955491	3.766178
C	-5.002186	-0.542659	2.532132
C	-4.136558	-0.240836	1.476838
C	-2.515157	-2.442111	-0.740281
C	-2.726931	-3.396094	-1.740294
C	-2.424842	-3.098087	-3.072478
C	-1.905181	-1.841064	-3.400294
C	-1.690223	-0.887785	-2.401581
H	-1.287800	0.091944	-2.666761
H	-1.669632	-1.600703	-4.439019
H	-2.592739	-3.842314	-3.852963
H	-3.134505	-4.374204	-1.477194
H	-2.758660	-2.680819	0.296596
H	-0.598783	2.695829	0.743888
H	-1.328563	4.975889	0.008661
H	-3.266868	5.218371	-1.542046
H	-4.465099	3.188974	-2.354413
H	-3.737193	0.936188	-1.623794
H	-1.151246	-0.827210	2.992325
H	-2.698501	-1.381657	4.904692
H	-5.165333	-1.188692	4.589749
H	-6.080948	-0.451297	2.391674
H	-4.549307	0.086321	0.521207
H	3.737108	-0.936122	-1.623921
H	4.465019	-3.188884	-2.354615
H	3.266916	-5.218321	-1.542157
H	1.328709	-4.975902	0.008680
H	0.598912	-2.695868	0.743968
H	2.698524	1.381749	4.904651
H	1.151260	0.827307	2.992292
H	4.549294	-0.086530	0.521251
H	6.080947	0.451094	2.391708
H	5.165349	1.188626	4.589745
H	1.287603	-0.091858	-2.666716
H	2.758804	2.680782	0.296587
H	3.134640	4.374168	-1.477205
H	2.592675	3.842349	-3.852944
H	1.669423	1.600791	-4.438976

Molekuele/1R/RI-MP2-SVP

1Cl

RI-MP2/SVP

E(SCF) =	-3475.220905		
C	0.000059	0.000000	0.960345
P	0.000009	-1.440438	0.227079
P	0.000009	1.440438	0.227079
Cl	-0.000125	2.971369	1.540746
Cl	-1.578259	1.914588	-0.980673
Cl	1.578346	1.914736	-0.980529
Cl	-0.000125	-2.971369	1.540746
Cl	-1.578259	-1.914588	-0.980673
Cl	1.578346	-1.914736	-0.980529

	1F	RI-MP2/SVP	
9			
E(SCF) =	-1315.338409		
C	-0.119666	0.602798	-0.197707
P	-1.584658	0.070319	-0.021008
F	-2.780988	1.085569	-0.156075
P	1.353975	1.129427	-0.307433
F	2.255685	1.143210	0.984119
F	1.595280	2.610827	-0.784058
F	2.348171	0.398218	-1.285622
F	-1.992283	-0.598556	1.345748
F	-2.106616	-1.047329	-0.999827

	1H	rimp.SVP	
9			
E(SCF) =	-722.429973		
C	-0.002268	0.000000	0.762373
P	-0.000350	1.431490	-0.061463
P	-0.000350	-1.431490	-0.061463
H	0.001134	2.561643	0.779019
H	-1.068774	1.815780	-0.930605
H	1.069125	1.812692	-0.930626
H	0.001134	-2.561643	0.779019
H	-1.068774	-1.815780	-0.930605
H	1.069125	-1.812692	-0.930626

	1Me	RI-MP2/SVP	
27			
E(SCF) =	-956.539380		
C	-0.175868	0.005638	-0.068580
P	-0.032934	0.001435	1.574586
P	1.041779	0.001958	-1.181129
C	-1.680064	0.011353	2.359549
C	0.802789	1.418240	2.407925
C	0.782675	-1.430580	2.401756

C	0.360938	0.008927	-2.873971
C	2.204535	-1.428124	-1.236243
C	2.218539	1.420749	-1.230160
H	-2.229670	-0.873700	2.011257
H	-2.217009	0.905771	2.015457
H	-1.619369	0.008323	3.457554
H	0.340044	2.349781	2.052821
H	0.721572	1.361507	3.504101
H	1.865874	1.430046	2.127055
H	0.306622	-2.353891	2.042778
H	0.702504	-1.377369	3.498187
H	1.845402	-1.456353	2.120470
H	-0.277683	-0.877441	-2.988901
H	-0.268879	0.902055	-2.985079
H	1.148972	0.006661	-3.640982
H	1.612761	-2.352570	-1.292825
H	2.887391	-1.374910	-2.097809
H	2.796701	-1.451554	-0.309973
H	2.810057	1.435200	-0.303301
H	1.635916	2.351144	-1.284107
H	2.901622	1.363751	-2.091302

	1NH2	RI-MP2/SVP	
21			
E(SCF) =	-1052.523246		
C	0.000008	0.000191	-1.082298
P	1.388352	-0.022427	-0.199722
P	-1.388261	0.022496	-0.199633
N	-2.728067	-0.017521	-1.223046
N	-1.865123	1.271497	0.884360
N	-1.525344	-1.237010	0.951009
N	2.728116	0.017425	-1.223181
N	1.525541	1.236924	0.951004
N	1.864945	-1.271472	0.884294
H	-3.562127	0.464895	-0.904290
H	-2.493027	0.180325	-2.189816
H	-2.432049	-1.266580	1.416521
H	-1.338034	-2.137599	0.514138
H	-1.163258	1.357105	1.621890
H	-1.893999	2.163465	0.389839
H	2.432240	1.266521	1.416522
H	1.338034	2.137549	0.514307
H	3.562212	-0.464951	-0.904464
H	2.493031	-0.180380	-2.189946
H	1.163003	-1.357031	1.621759
H	1.893806	-2.163422	0.389751

	1NMe2	RI-MP2/SVP	
57			
E(SCF) =	-1520.472697		
C	-0.042701	0.065526	1.002479
P	0.000585	-0.053330	2.621166
P	-0.010740	0.070403	-0.620724
N	-1.378527	-0.710808	-1.334531
N	1.269714	-0.751063	-1.474657
N	0.202219	1.649792	-1.309163
N	0.274729	-1.600201	3.380053
N	1.289033	0.849444	3.339779
N	-1.506101	0.338987	3.388935
C	1.473987	0.938758	4.778092
H	1.030240	1.864662	5.220519
H	2.560609	0.948039	5.026115
H	1.027201	0.061763	5.281071
C	1.996554	1.858497	2.573354
H	1.796836	1.694535	1.496803
H	3.095120	1.785405	2.749533
H	1.685276	2.898526	2.839593
C	-1.753646	0.160852	4.811500
H	-1.589323	1.093905	5.404965
H	-1.099818	-0.632954	5.216561
H	-2.811490	-0.148218	4.978368
C	-2.381865	1.312049	2.759089
H	-3.447488	1.014349	2.888085
H	-2.157014	1.353852	1.676357
H	-2.268982	2.339190	3.187188
C	-0.750545	-2.611505	3.127580
H	-0.670755	-3.053138	2.103662
H	-1.758390	-2.169040	3.230363
H	-0.650760	-3.437429	3.864887
C	1.619928	-2.153284	3.243254
H	1.798143	-2.604634	2.235638
H	1.775704	-2.949271	4.003602
H	2.374829	-1.361503	3.399562
C	-2.553929	-1.011058	-0.538178
H	-2.924368	-2.039695	-0.757732
H	-3.398005	-0.304821	-0.733414
H	-2.283700	-0.951403	0.533789
C	-1.587450	-0.765712	-2.771194
H	-2.280937	0.028142	-3.143719
H	-2.031897	-1.746834	-3.058311
H	-0.625243	-0.669197	-3.306385
C	1.245146	-2.210611	-1.418826

H	1.623782	-2.609521	-0.445045
H	1.885120	-2.626178	-2.227329
H	0.213059	-2.579979	-1.559051
C	2.614498	-0.226802	-1.241119
H	3.024658	-0.532589	-0.247080
H	2.607142	0.877887	-1.281245
H	3.304788	-0.604134	-2.026560
C	0.412782	1.885824	-2.729333
H	-0.529746	2.134897	-3.276614
H	0.868381	0.996121	-3.200964
H	1.108598	2.744543	-2.873596
C	-0.321217	2.801663	-0.595182
H	-0.410416	2.551682	0.479143
H	-1.323428	3.126604	-0.970540
H	0.369699	3.669036	-0.700632

	1Ph	RI-MP2/SVP	
69			
E(SCF) =	-2098.018926		
C	0.000345	0.009510	-1.246437
P	1.425991	-0.246871	-0.424639
P	-1.425791	0.253953	-0.421884
C	2.090728	1.144389	0.570896
C	2.752940	-0.554013	-1.636713
C	-2.090284	-1.150598	0.554966
C	1.551639	-1.692020	0.698040
C	-2.752521	0.576350	-1.630183
C	-1.552438	1.684052	0.719827
C	1.654990	2.430080	0.196044
C	2.132494	3.578724	0.880686
C	3.060836	3.425309	1.950374
C	3.505883	2.122099	2.318558
C	2.417756	-0.521986	-2.999908
C	3.420746	-0.727872	-3.986760
C	3.017690	0.986148	1.621161
C	4.765439	-0.965734	-3.583868
C	5.095837	-0.995975	-2.195830
C	4.081125	-0.788255	-1.227317
C	-1.655873	-2.431186	0.161430
C	-2.133136	-3.589034	0.830521
C	-3.059878	-3.450112	1.903598
C	-3.503582	-2.151959	2.290689
C	-3.015682	-1.006594	1.608608
C	1.132834	-1.590834	2.040150
C	1.038361	-2.748128	2.855512
C	1.360973	-4.024191	2.309383

C	1.779259	-4.124386	0.950755
C	1.867249	-2.953077	0.153095
C	-2.416531	0.564957	-2.993504
C	-3.419338	0.783674	-3.977780
C	-4.764646	1.013312	-3.572178
C	-5.095867	1.022487	-2.184034
C	-4.081328	0.802222	-1.218117
C	-1.870748	2.951809	0.192319
C	-1.783233	4.112469	1.005482
C	-1.362752	3.994708	2.362008
C	-1.037443	2.711911	2.890512
C	-1.131402	1.565542	2.059836
H	-0.879258	0.581527	2.459833
H	-0.708535	2.612177	3.929819
H	-1.288156	4.885318	2.994882
H	-2.035120	5.093491	0.589989
H	-2.179423	3.036343	-0.854330
H	-0.942383	-2.509768	-0.665507
H	-1.789552	-4.581087	0.521564
H	-3.433236	-4.336708	2.426847
H	-4.220361	-2.038282	3.110302
H	-3.354300	-0.011814	1.908445
H	-1.368704	0.379511	-3.259739
H	-3.157545	0.772956	-5.040384
H	-5.544534	1.179786	-4.322667
H	-6.129061	1.196081	-1.867204
H	-4.331034	0.807544	-0.153865
H	3.357251	-0.012535	1.906573
H	4.223889	1.997391	3.135489
H	3.434398	4.304684	2.485528
H	1.787783	4.574788	0.586228
H	0.940354	2.519813	-0.628771
H	3.159565	-0.701036	-5.049229
H	1.370387	-0.330897	-3.263947
H	4.330237	-0.809885	-0.163148
H	6.128532	-1.176097	-1.881021
H	5.545455	-1.122531	-4.336305
H	0.882897	-0.611897	2.453751
H	2.174263	-3.023988	-0.895060
H	2.029061	-5.100129	0.521793
H	1.286008	-4.923093	2.930377
H	0.711211	-2.661839	3.896576

Molekuele/1R/RI-MP2-TZVP

1Cl

RI-MP2/TZVP

E(SCF) =	-3476.401325		
C	0.001949	0.000000	0.995457
P	0.000231	-1.428632	0.224660
P	0.000231	1.428632	0.224660
Cl	-0.000906	2.966640	1.541389
Cl	-1.588461	1.902006	-0.988455
Cl	1.588162	1.904401	-0.988527
Cl	-0.000906	-2.966641	1.541389
Cl	-1.588461	-1.902006	-0.988455
Cl	1.588162	-1.904401	-0.988527

1F RI-MP2/TZVP

9			
E(SCF) =	-1316.326781		
C	0.036979	0.018522	-0.758893
P	-1.426375	0.041574	-0.117299
F	-2.346719	1.310973	-0.255172
P	1.239578	0.994937	-0.366524
F	1.826162	1.004293	1.094043
F	1.117206	2.549712	-0.578925
F	2.562619	0.742276	-1.160595
F	-1.637585	-0.234299	1.417857
F	-2.402965	-1.033505	-0.696355

1H RI-MP2/TZVP

9			
E(SCF) =	-722.687738		
C	-0.000113	0.000000	0.844609
P	0.000019	1.404679	-0.058850
P	0.000019	-1.404679	-0.058850
H	-0.000060	2.551828	0.750605
H	-1.070730	1.743071	-0.938315
H	1.070828	1.743059	-0.938233
H	-0.000060	-2.551828	0.750605
H	-1.070730	-1.743071	-0.938315
H	1.070828	-1.743059	-0.938233

1Me RI-MP2/TZVP

27			
E(SCF) =	-957.046667		
C	-0.205020	0.006712	-0.080069
P	-0.041540	-0.029582	1.570970
P	1.033679	0.033566	-1.184097
C	-1.673371	0.150659	2.376208
C	0.964736	1.265023	2.427530
C	0.614240	-1.565982	2.360709

C	0.376159	-0.130810	-2.882451
C	2.338685	-1.276866	-1.139165
C	2.069204	1.558398	-1.313870
H	-2.330128	-0.630559	1.995849
H	-2.090925	1.118417	2.101519
H	-1.595514	0.075249	3.461674
H	0.641281	2.244515	2.075936
H	0.856284	1.211378	3.512596
H	2.016010	1.130970	2.169365
H	-0.001923	-2.406541	2.042145
H	0.606199	-1.497186	3.450354
H	1.635545	-1.736568	2.019315
H	-0.128619	-1.092217	-2.967633
H	-0.355279	0.659970	-3.043598
H	1.169357	-0.061348	-3.628103
H	1.850982	-2.250811	-1.104175
H	2.994297	-1.226834	-2.010760
H	2.938919	-1.154258	-0.236678
H	2.591530	1.718293	-0.370300
H	1.410143	2.407721	-1.492667
H	2.800286	1.484738	-2.121470

	1NH2	RI-MP2/TZVP	
21			
E(SCF) =	-1053.162069		
C	-0.000046	-0.000766	-1.064151
P	1.399862	-0.024928	-0.186099
P	-1.399945	0.024631	-0.186079
N	-2.717163	-0.009934	-1.252250
N	-1.910705	1.271614	0.888697
N	-1.567130	-1.243034	0.954293
N	2.716982	0.010343	-1.252287
N	1.566262	1.243031	0.954209
N	1.911538	-1.271647	0.888640
H	-3.541324	0.500838	-0.971452
H	-2.441071	0.170269	-2.206305
H	-2.476641	-1.270022	1.401774
H	-1.363525	-2.138542	0.528028
H	-1.277420	1.336870	1.679523
H	-1.922928	2.168507	0.415448
H	2.475628	1.270229	1.401969
H	1.362754	2.138502	0.527786
H	3.541408	-0.500001	-0.971484
H	2.440899	-0.170195	-2.206291
H	1.278374	-1.337148	1.679519
H	1.924190	-2.168619	0.415510

	1NMe2	RI-MP2/TZVP	
57			
E(SCF) =	-1521.552416		
C	-0.042701	0.065526	1.002479
P	0.000585	-0.053330	2.621166
P	-0.010740	0.070403	-0.620724
N	-1.378527	-0.710808	-1.334531
N	1.269714	-0.751063	-1.474657
N	0.202219	1.649792	-1.309163
N	0.274729	-1.600201	3.380053
N	1.289033	0.849444	3.339779
N	-1.506101	0.338987	3.388935
C	1.473987	0.938758	4.778092
H	1.030240	1.864662	5.220519
H	2.560609	0.948039	5.026115
H	1.027201	0.061763	5.281071
C	1.996554	1.858497	2.573354
H	1.796836	1.694535	1.496803
H	3.095120	1.785405	2.749533
H	1.685276	2.898526	2.839593
C	-1.753646	0.160852	4.811500
H	-1.589323	1.093905	5.404965
H	-1.099818	-0.632954	5.216561
H	-2.811490	-0.148218	4.978368
C	-2.381865	1.312049	2.759089
H	-3.447488	1.014349	2.888085
H	-2.157014	1.353852	1.676357
H	-2.268982	2.339190	3.187188
C	-0.750545	-2.611505	3.127580
H	-0.670755	-3.053138	2.103662
H	-1.758390	-2.169040	3.230363
H	-0.650760	-3.437429	3.864887
C	1.619928	-2.153284	3.243254
H	1.798143	-2.604634	2.235638
H	1.775704	-2.949271	4.003602
H	2.374829	-1.361503	3.399562
C	-2.553929	-1.011058	-0.538178
H	-2.924368	-2.039695	-0.757732
H	-3.398005	-0.304821	-0.733414
H	-2.283700	-0.951403	0.533789
C	-1.587450	-0.765712	-2.771194
H	-2.280937	0.028142	-3.143719
H	-2.031897	-1.746834	-3.058311
H	-0.625243	-0.669197	-3.306385
C	1.245146	-2.210611	-1.418826

H	1.623782	-2.609521	-0.445045
H	1.885120	-2.626178	-2.227329
H	0.213059	-2.579979	-1.559051
C	2.614498	-0.226802	-1.241119
H	3.024658	-0.532589	-0.247080
H	2.607142	0.877887	-1.281245
H	3.304788	-0.604134	-2.026560
C	0.412782	1.885824	-2.729333
H	-0.529746	2.134897	-3.276614
H	0.868381	0.996121	-3.200964
H	1.108598	2.744543	-2.873596
C	-0.321217	2.801663	-0.595182
H	-0.410416	2.551682	0.479143
H	-1.323428	3.126604	-0.970540
H	0.369699	3.669036	-0.700632

	1Ph	RI-MP2/TZVP	
69			
E(SCF) =	-2100.353475		
C	0.000091	0.009864	-1.404472
P	1.398398	-0.238744	-0.508772
P	-1.398332	0.246478	-0.505710
C	1.987532	1.157866	0.533421
C	2.799643	-0.546210	-1.630762
C	-1.987610	-1.163947	0.517624
C	1.445948	-1.699061	0.606138
C	-2.799427	0.568936	-1.623672
C	-1.446007	1.691760	0.628620
C	1.611459	2.440520	0.114952
C	2.022633	3.558565	0.833496
C	2.730055	3.402652	2.026484
C	3.121749	2.129300	2.437215
C	2.563378	-0.652997	-3.001609
C	3.621955	-0.937887	-3.862827
C	2.724840	1.004724	1.712726
C	4.922179	-1.029746	-3.367144
C	5.154167	-0.930445	-1.994378
C	4.100845	-0.644812	-1.129905
C	-1.611444	-2.440887	0.082108
C	-2.022657	-3.568443	0.785610
C	-2.730311	-3.428506	1.980441
C	-3.122033	-2.160759	2.408135
C	-2.725079	-1.026594	1.698772
C	0.937088	-1.636585	1.909686
C	0.807613	-2.791075	2.677585
C	1.102140	-4.034738	2.120282

C	1.624600	-4.106360	0.828926
C	1.755526	-2.951228	0.060797
C	-2.562985	0.694025	-2.992941
C	-3.621453	0.990381	-3.850416
C	-4.921740	1.075616	-3.353717
C	-5.153909	0.957974	-1.982432
C	-4.100696	0.660830	-1.121714
C	-1.755450	2.951111	0.099995
C	-1.624595	4.095880	0.883494
C	-1.102339	4.007004	2.173860
C	-0.807948	2.756001	2.714557
C	-0.937354	1.611869	1.931297
H	-0.710556	0.645417	2.360947
H	-0.417503	2.676407	3.722616
H	-0.998213	4.899279	2.779816
H	-1.874241	5.064450	0.465677
H	-2.138429	3.030286	-0.911979
H	-1.036595	-2.533643	-0.833347
H	-1.731755	-4.553530	0.440112
H	-3.038331	-4.306269	2.536433
H	-3.688131	-2.049440	3.325901
H	-3.034973	-0.044636	2.037349
H	-1.542043	0.603646	-3.349553
H	-3.442490	1.085875	-4.914905
H	-5.743204	1.299587	-4.023638
H	-6.164144	1.027239	-1.596768
H	-4.282608	0.547493	-0.058687
H	3.034710	0.018326	2.038164
H	3.687624	2.005706	3.353547
H	3.038153	4.272908	2.594112
H	1.731695	4.548180	0.501218
H	1.036806	2.545519	-0.799302
H	3.443134	-1.019131	-4.928523
H	1.542478	-0.557891	-3.357112
H	4.282613	-0.545715	-0.065432
H	6.164354	-1.004847	-1.609544
H	5.743726	-1.244773	-4.039887
H	0.710190	-0.675961	2.352161
H	2.138668	-3.016873	-0.952083
H	1.874357	-5.069256	0.398258
H	0.997970	-4.935024	2.714262
H	0.417001	-2.724960	3.686553

Molekuele/1R-Isomere/RI-BP86_SVP

diPhos_h RI-BP86/SVP

E(SCF) =	-724.242826		
C	0.130158	0.011201	-0.322649
H	0.572565	-0.006166	0.695906
H	-0.969664	0.068407	-0.190509
P	0.513997	-1.661542	-1.097434
H	0.043691	-1.350733	-2.426121
H	1.883932	-1.378509	-1.453854
P	0.840756	1.499881	-1.230033
H	-0.057824	1.450027	-2.356492
H	0.057090	2.522993	-0.574065

	diPhos_Me	RI-BP86/SVP	
27			
E(SCF) =	-959.960562		
C	-0.352542	0.050687	-0.171301
P	0.302544	-0.038339	1.639526
P	1.200083	-0.329941	-1.242781
C	-1.278248	-0.302951	2.609816
C	0.558772	1.758463	2.100507
C	0.615338	0.178239	-2.951021
C	2.333282	1.121948	-0.918132
H	-1.634778	-1.345118	2.499697
H	-2.097671	0.394203	2.332814
H	-1.037158	-0.146656	3.681088
H	-0.344851	2.388479	1.968735
H	0.848743	1.784931	3.170891
H	1.391850	2.199776	1.521424
H	-0.217627	-0.473649	-3.282684
H	0.295560	1.238327	-3.025700
H	1.456350	0.016063	-3.655905
H	2.802274	1.019654	0.080296
H	1.839864	2.113827	-0.997226
H	3.148480	1.080700	-1.669335
C	-1.275613	-1.171328	-0.383226
H	-0.800677	-2.112928	-0.037213
H	-1.521918	-1.299605	-1.459089
H	-2.239047	-1.048229	0.153293
C	-1.094323	1.346090	-0.519907
H	-0.433678	2.236378	-0.517651
H	-1.919132	1.543895	0.199635
H	-1.561559	1.280314	-1.525370

	diPhos_Ph	RI-BP86/SVP	
69			
E(SCF) =	-2109.207531		
C	0.024081	0.241349	-1.686006

P	1.531462	-0.352750	-0.539867
P	-1.423729	0.170000	-0.349326
C	2.150768	1.153714	0.359718
C	2.958370	-0.736733	-1.686922
C	-2.981121	0.704204	-1.236789
C	-1.258680	1.495834	0.950767
C	0.275525	1.499803	-2.517850
C	-0.334422	-0.979335	-2.565633
C	2.520974	2.397063	-0.213537
C	3.028271	3.445318	0.592341
C	3.180645	3.260274	1.994120
C	2.817551	2.016491	2.576069
C	2.881984	-1.907988	-2.490037
C	3.978694	-2.329072	-3.279642
C	2.306344	0.977290	1.758126
C	5.197441	-1.597475	-3.260612
C	5.294913	-0.445053	-2.437150
C	4.184712	-0.023833	-1.663159
C	-3.553019	-0.186265	-2.184361
C	-4.798806	0.099399	-2.794400
C	-5.514450	1.276288	-2.443658
C	-4.963407	2.156716	-1.474735
C	-3.708461	1.869363	-0.883405
C	-0.694253	2.790881	0.852359
C	-0.696328	3.671991	1.962506
C	-1.275931	3.270803	3.196303
C	-1.840550	1.971716	3.307588
C	-1.818963	1.096396	2.193953
H	-2.241107	0.088192	2.304493
H	-2.283837	1.643594	4.257822
H	-1.279132	3.953856	4.056929
H	-0.242501	4.667708	1.869382
H	-0.226580	3.132509	-0.076262
H	-3.044557	-1.121101	-2.448560
H	-5.219210	-0.599378	-3.530491
H	-6.485921	1.495881	-2.907331
H	-5.511647	3.062978	-1.183069
H	-3.313975	2.565858	-0.132481
H	2.020640	0.025226	2.224229
H	2.926883	1.862696	3.658223
H	3.576083	4.071311	2.621324
H	3.308395	4.403557	0.133493
H	2.418223	2.569291	-1.291611
H	3.890510	-3.232835	-3.898031
H	1.969198	-2.514228	-2.506345
H	4.301843	0.865757	-1.034335

H	6.234638	0.122592	-2.397321
H	6.054782	-1.926908	-3.863556
C	0.786867	3.808885	-4.157012
C	-0.580389	2.625342	-2.490346
C	1.381497	1.543603	-3.411091
C	1.644139	2.676019	-4.215802
C	-0.335124	3.769773	-3.291079
H	-1.481149	2.617522	-1.870728
H	2.054469	0.682191	-3.492404
H	2.509228	2.676005	-4.892894
H	-1.025397	4.623096	-3.247418
H	0.982650	4.691323	-4.781302
C	-1.102318	-3.250252	-4.146873
C	-0.572811	-0.854271	-3.955027
C	-0.501186	-2.264451	-1.976806
C	-0.876928	-3.387276	-2.749595
C	-0.948447	-1.972363	-4.743137
H	-0.485974	0.119406	-4.448900
H	-0.344949	-2.396005	-0.898637
H	-0.998116	-4.366871	-2.267627
H	-1.127735	-1.843425	-5.819021
H	-1.395078	-4.118486	-4.752971

	hc_p2h5	RI-BP86/SVP	
9			
E(SCF) =	-724.175017		
C	-0.205794	-0.015352	-0.406732
P	0.652918	-1.536087	-0.859752
P	0.348793	1.422789	-1.100792
H	1.720038	1.313318	-1.473856
H	-1.188740	0.027389	0.091921
H	-0.381925	-2.334440	-1.490380
H	0.537553	-2.271516	0.378908
H	-0.171513	2.048161	-2.319559
H	0.266776	2.593224	-0.269503

	hc_p2Me4ch2	RI-BP86/SVP	
27			
E(SCF) =	-959.879340		
C	-0.127535	0.063387	-0.084275
P	0.012200	-0.149827	1.598427
P	1.068229	-0.010265	-1.387179
C	-1.627963	0.165675	2.353622
C	1.181019	0.963164	2.508728
C	0.503287	-1.821531	2.228876
C	0.341810	-0.499941	-2.836079

C	2.539227	-0.942855	-0.630349
C	1.887125	1.626393	-1.695286
H	-2.364097	-0.539784	1.922766
H	-1.943174	1.200016	2.117848
H	-1.587380	0.031603	3.451746
H	0.886712	2.013652	2.320046
H	1.185321	0.760088	3.598928
H	2.205351	0.813391	2.113820
H	-0.209511	-2.568365	1.828892
H	0.510118	-1.858974	3.337182
H	1.514217	-2.070291	1.852582
H	-0.291804	-1.400203	-2.798005
H	-1.139552	0.331139	-0.426382
H	0.905418	-0.323215	-3.766934
H	2.242478	-1.999089	-0.473941
H	3.363912	-0.929038	-1.371518
H	2.926965	-0.518996	0.323762
H	2.444543	1.972004	-0.802167
H	1.106267	2.364811	-1.957082
H	2.592369	1.535526	-2.546800

	Mec_p2Me5	RI-BP86/SVP	
27			
E(SCF) =	-959.930339		
C	-0.026727	0.105486	0.001424
P	0.460630	0.564379	1.680143
P	1.265729	-0.314500	-1.041535
C	-0.421080	-0.673084	2.789792
C	-0.622856	2.053949	2.049104
C	0.821069	-0.113789	-2.819869
C	2.760029	0.713173	-0.768516
H	0.033143	-1.675105	2.651169
H	-1.509990	-0.746983	2.582316
H	-0.287699	-0.381575	3.852473
H	-1.701510	1.870505	1.855289
H	-0.505212	2.343556	3.114054
H	-0.290178	2.902914	1.419414
H	0.016288	-0.822282	-3.095637
H	0.461706	0.919320	-2.989527
H	1.702105	-0.314914	-3.460246
H	2.994448	0.694739	0.313707
H	2.538478	1.757592	-1.058967
H	3.616165	0.325661	-1.355335
C	-1.457124	-0.254776	-0.376020
H	-1.800665	-1.253270	-0.011897
H	-1.633383	-0.243422	-1.474143

H	-2.169918	0.488903	0.043890
C	1.949539	-2.057086	-1.022814
H	1.117141	-2.766492	-1.202507
H	2.742835	-2.224993	-1.780956
H	2.358772	-2.256146	-0.012384

	Phc_p2Ph5	RI-BP86/SVP	
69			
E(SCF) =	-2109.196760		
C	0.135359	1.051533	-0.899918
P	1.475701	0.003502	-0.534769
P	-1.476027	0.311856	-0.496586
C	-2.540735	0.687024	-1.978422
C	-2.234966	1.347877	0.857896
C	0.335947	2.240484	-1.764177
C	1.059642	-1.215449	0.781871
C	2.146627	-1.014604	-1.946769
C	2.941322	0.874272	0.186014
C	4.056673	0.117335	0.624549
C	5.144518	0.751654	1.272941
C	5.120035	2.156903	1.490658
C	3.994813	2.912674	1.063430
C	2.908512	2.268149	0.418559
C	3.457248	-0.889233	-2.464201
C	3.848925	-1.616671	-3.617096
C	2.924960	-2.481433	-4.262462
C	1.603454	-2.603145	-3.748568
C	1.220151	-1.865290	-2.603037
C	-3.870368	1.164316	-1.884118
C	-4.680476	1.300847	-3.039472
C	-4.166153	0.962062	-4.318927
C	-2.828507	0.491017	-4.421810
C	-2.031532	0.355098	-3.260386
C	-3.443182	0.900987	1.454745
C	-4.004168	1.579121	2.564630
C	-3.346316	2.714744	3.111680
C	-2.122404	3.151712	2.536353
C	-1.577222	2.467520	1.421489
C	1.491726	2.411897	-2.583779
C	1.680162	3.561258	-3.385161
C	0.699233	4.587458	-3.411974
C	-0.472351	4.424557	-2.623699
C	-0.645310	3.275020	-1.820929
C	1.325418	-2.596266	0.646225
C	1.064438	-3.484177	1.721729
C	0.544657	-2.987233	2.945946

C	0.293628	-1.593336	3.086314
C	0.555028	-0.714514	2.008301
H	-3.946585	0.000660	1.077700
H	-4.941676	1.221592	3.012423
H	-3.774648	3.242314	3.974794
H	-1.602090	4.023780	2.955624
H	-0.627455	2.811327	0.991186
H	-0.994906	0.011447	-3.369398
H	-2.409493	0.241940	-5.406214
H	-4.788902	1.070938	-5.217018
H	-5.707475	1.679206	-2.945326
H	-4.292974	1.453910	-0.914544
H	4.085861	-0.972041	0.493235
H	6.002969	0.158345	1.616544
H	5.961433	2.653236	1.994075
H	3.964179	3.997436	1.233995
H	2.044240	2.863539	0.099707
H	0.878924	-3.262059	-4.246885
H	0.187381	-1.953648	-2.235470
H	4.188612	-0.221453	-1.992230
H	4.867018	-1.508139	-4.015500
H	3.224647	-3.044674	-5.157212
H	-1.568245	3.183482	-1.237753
H	2.256973	1.627741	-2.636802
H	2.583091	3.651745	-4.004109
H	-1.254699	5.195400	-2.641289
H	0.834440	5.477951	-4.039451
H	0.350881	0.356278	2.137049
H	-0.109053	-1.198169	4.028906
H	0.338102	-3.672782	3.779584
H	1.262227	-4.558433	1.605623
H	1.727233	-3.006905	-0.287521

Molekuele/2R/BP86_TZ2P

2H

BP86/TZ2P

9

E(SCF) =	-2.054462		
C	0.131714	2.303039	1.558319
N	1.228412	2.793838	0.901024
H	2.167464	2.551368	1.186563
N	-0.867672	2.896980	0.834390
H	-1.842306	2.747714	1.057649
C	0.932890	3.641718	-0.163587
H	1.682879	4.109456	-0.787508
C	-0.423519	3.708509	-0.206638
H	-1.082838	4.243912	-0.876845

-----	2H.c2v	BP86/TZ2P	
9			
E(SCF) =	-2.054472		
C	0.000000	0.000000	-0.196720
N	1.049894	0.000000	-1.076088
H	2.008076	0.000000	-0.754259
N	-1.049894	0.000000	-1.076088
H	-2.008076	0.000000	-0.754259
C	0.679481	0.000000	-2.418612
H	1.385254	0.000000	-3.238679
C	-0.679481	0.000000	-2.418612
H	-1.385254	0.000000	-3.238679

Molekuele/2R/RI-BP86_SVP

	2Ad	RI-BP86/SVP	
57			
E(SCF) =	-1004.551227		
N	-0.676147	5.304397	19.804687
N	-1.443137	5.245019	21.809643
C	-0.260219	5.264488	21.112679
C	-2.068161	5.309901	19.687926
C	-2.558015	5.272038	20.968383
C	0.301863	5.336312	18.684457
C	1.200312	6.591756	18.823811
C	2.250617	6.623847	17.693382
C	3.131159	5.356916	17.772882
C	2.244099	4.101921	17.615800
C	1.193779	4.070000	18.746263
C	-0.408071	5.380298	17.313165
C	0.642564	5.412506	16.177818
C	1.530661	6.667147	16.327840
C	1.524093	4.146298	16.250339
C	-1.462375	5.201139	23.296294
C	-0.725872	3.926445	23.781335
C	-0.698412	3.880808	25.323810
C	0.036128	5.128578	25.862630
C	-0.703733	6.402852	25.398241
C	-0.731219	6.448096	23.855717
C	-2.906741	5.181909	23.844107
C	-2.882210	5.136289	25.390368
C	-2.151687	6.383511	25.934806
C	-2.146344	3.862299	25.860522
H	-2.608261	5.339091	18.738158
H	-3.594309	5.262966	21.315672
H	0.561594	7.501254	18.791572

H	1.678540	6.565263	19.824151
H	2.884959	7.528767	17.811740
H	3.907015	5.379483	16.976790
H	3.667557	5.325561	18.745609
H	2.873674	3.188134	17.678265
H	1.672011	4.032639	19.746190
H	0.550298	3.167597	18.658119
H	-1.061716	4.489181	17.193592
H	-1.057283	6.280326	17.248584
H	0.111379	5.443861	15.202162
H	2.272208	6.708504	15.500634
H	0.911324	7.587342	16.250132
H	2.265504	4.152032	15.422043
H	0.899872	3.235944	16.116491
H	-1.241656	3.030740	23.371804
H	0.297953	3.935986	23.355360
H	-0.165373	2.962059	25.651040
H	1.084958	5.141620	25.495781
H	0.082572	5.095926	26.973020
H	-0.174564	7.302952	25.779156
H	0.292689	6.467955	23.430154
H	-1.250772	7.364279	23.499648
H	-3.455455	6.087180	23.504844
H	-3.451728	4.296072	23.451646
H	-3.929186	5.123152	25.762740
H	-2.152156	6.368891	27.046382
H	-2.687511	7.307553	25.625700
H	-2.678273	2.955782	25.497543
H	-2.146654	3.811466	26.971057

	2Cl	RI-BP86/SVP	
9			
E(SCF) =	-1144.948113		
C	0.000001	-1.299232	0.000015
N	-1.035117	-0.420376	0.000430
Cl	-2.695548	-0.920841	0.000257
N	1.035121	-0.420370	0.000134
Cl	2.695558	-0.920831	0.000018
C	-0.686688	0.931436	0.000677
H	-1.413460	1.749473	0.000825
C	0.686694	0.931444	-0.000344
H	1.413460	1.749490	-0.000430

	2F	RI-BP86/SVP	
9			
E(SCF) =	-424.208366		

C	0.000000	0.000000	1.036570
N	0.000000	1.011830	0.154491
F	0.000000	2.327590	0.552205
N	0.000000	-1.011830	0.154491
F	0.000000	-2.327590	0.552205
C	0.000000	0.690650	-1.193138
H	0.000000	1.427114	-2.002167
C	0.000000	-0.690650	-1.193138
H	0.000000	-1.427114	-2.002167

	2Me	RI-BP86/SVP	
15			
E(SCF) =	-304.593789		
C	-0.190705	0.000004	1.561935
N	-0.011457	1.068693	2.412261
C	-0.105388	2.449941	1.966737
N	-0.011594	-1.068699	2.412283
C	-0.105634	-2.449950	1.966772
C	0.265079	-0.685634	3.724975
H	0.436718	-1.397472	4.539996
C	0.265162	0.685625	3.724955
H	0.436881	1.397458	4.539957
H	-0.914085	2.989134	2.502118
H	0.850437	2.989259	2.130548
H	-0.332972	2.434027	0.886163
H	-0.914168	-2.989156	2.502391
H	-0.333531	-2.434029	0.886261
H	0.850249	-2.989262	2.130296

2Me.ungesaettigt		RI-BP86/SVP	
17			
E(SCF) =	-305.792346		
C	-0.192851	0.026959	-0.098449
N	-0.883998	0.688928	-1.057192
C	-0.289289	0.636491	-2.413527
C	0.976062	-0.211106	-2.176289
N	0.885564	-0.500860	-0.725767
C	-2.116063	1.406443	-0.830010
C	1.903617	-1.292564	-0.076834
H	1.915663	0.335964	-2.414086
H	0.985470	-1.152608	-2.769723
H	-0.993920	0.170832	-3.138350
H	-0.062422	1.659729	-2.787741
H	1.974463	-2.313715	-0.517239
H	2.909186	-0.819726	-0.160722
H	1.639039	-1.382110	0.992242

H	-2.016969	2.486582	-1.085443
H	-2.952383	0.992314	-1.438982
H	-2.374143	1.314732	0.240467

	2Mes	RI-BP86/SVP	
47			
E(SCF) =	-923.546526		
N	-1.077250	0.007241	0.605453
C	-2.449270	0.023133	0.166103
N	1.061233	-0.010853	0.608175
C	-3.189800	1.223825	0.258458
C	-4.535676	1.206879	-0.160338
H	-5.120447	2.139195	-0.096855
C	-5.145688	0.045050	-0.666552
C	-4.368013	-1.127353	-0.755926
H	-4.822730	-2.047515	-1.158640
C	-3.022403	-1.165613	-0.348355
C	-2.553685	2.497875	0.763297
H	-1.588732	2.689559	0.251486
H	-2.331081	2.452295	1.850123
H	-3.218280	3.366515	0.593899
C	-6.590798	0.044938	-1.111305
H	-6.686531	-0.261300	-2.174086
H	-7.051968	1.045922	-1.005154
H	-7.196550	-0.670920	-0.516535
C	-2.205858	-2.428699	-0.472649
H	-2.821343	-3.266138	-0.853108
H	-1.349511	-2.269975	-1.159994
H	-1.772885	-2.731533	0.503529
C	-0.006905	-0.001621	-0.265048
C	-0.694054	0.003206	1.953733
H	-1.414204	0.001205	2.778366
C	0.674597	-0.007284	1.955476
H	1.392634	-0.005525	2.781948
C	2.434329	-0.026226	0.172189
C	3.008364	1.162920	-0.340300
C	4.355287	1.125523	-0.743644
H	4.811062	2.046309	-1.143728
C	5.133184	-0.046575	-0.652595
C	4.522621	-1.208547	-0.147331
H	5.108160	-2.140165	-0.080704
C	3.175476	-1.226349	0.267270
C	2.191866	2.425921	-0.465730
H	2.808137	3.263770	-0.844007
H	1.337365	2.267486	-1.155433
H	1.756267	2.727961	0.509527

C	6.576523	-0.048559	-1.103101
H	6.658454	0.149750	-2.192801
H	7.162649	0.741785	-0.589433
H	7.067319	-1.020323	-0.901164
C	2.539174	-2.500417	0.771860
H	3.204312	-3.368882	0.603687
H	2.315161	-2.454509	1.858391
H	1.574970	-2.692686	0.258874

2Mes.ungesaettigt RI-BP86/SVP

49

E(SCF) = -924.745075

C	9.908499	17.256425	11.947195
C	9.756328	18.677528	13.873739
H	9.252910	19.657405	13.720288
C	11.210059	18.671090	13.382000
H	11.900871	18.153462	14.083491
C	7.753420	17.281809	13.137685
C	7.348839	16.503733	14.250749
C	5.982318	16.185628	14.390996
H	5.667929	15.573150	15.252375
C	5.017836	16.606312	13.459575
C	5.455424	17.366015	12.355404
H	4.718811	17.701606	11.606504
C	6.804211	17.718362	12.173618
C	8.350490	15.992749	15.260434
H	9.312146	15.732538	14.775728
H	7.966156	15.092923	15.778914
H	8.572153	16.746508	16.047905
C	3.556514	16.254120	13.622573
H	3.174038	15.694827	12.743072
H	2.928964	17.165306	13.719127
H	3.383570	15.630099	14.520885
C	7.230251	18.528809	10.973354
H	7.761944	19.456044	11.274041
H	6.356712	18.819349	10.358490
H	7.942362	17.953673	10.346851
C	12.242160	17.666891	11.277932
C	12.844996	16.380044	11.237248
C	13.979472	16.197974	10.427231
H	14.446054	15.199349	10.392940
C	14.537885	17.245707	9.666812
C	13.914553	18.503800	9.724806
H	14.320719	19.334118	9.123568
C	12.769463	18.737449	10.513816
C	12.277182	15.228728	12.031643

H	12.899081	14.320211	11.916150
H	11.240249	15.004755	11.707584
H	12.218183	15.468941	13.114092
C	15.763344	17.010153	8.813054
H	15.589097	16.206217	8.067398
H	16.630635	16.691601	9.429237
H	16.059958	17.923512	8.261557
C	12.115029	20.099552	10.510133
H	11.012635	20.015498	10.581522
H	12.363719	20.655707	9.585511
H	12.453043	20.728219	11.363370
N	9.132798	17.642740	12.991619
N	11.097545	17.889844	12.111277
H	11.611331	19.687509	13.201936
H	9.659740	18.412696	14.944799

2NH2

RI-BP86/SVP

13

E(SCF) = -336.603822

C	0.000000	0.000000	0.987455
N	0.000122	1.054953	0.113596
N	0.000175	2.416188	0.493468
N	-0.000122	-1.054953	0.113596
N	-0.000175	-2.416188	0.493468
C	0.000000	0.685941	-1.231581
H	-0.000083	1.422304	-2.040637
C	0.000000	-0.685941	-1.231581
H	0.000083	-1.422304	-2.040637
H	0.814471	-2.545951	1.111886
H	-0.818642	-2.547730	1.106419
H	-0.814471	2.545951	1.111886
H	0.818642	2.547730	1.106419

2NMe2

RI-BP86/SVP

25

E(SCF) = -493.720725

C	0.000000	0.000000	0.489047
N	0.000035	1.054772	-0.383517
N	0.000259	2.419566	-0.005867
N	-0.000035	-1.054772	-0.383517
N	-0.000259	-2.419566	-0.005867
C	0.000000	0.685363	-1.731647
H	-0.000001	1.423391	-2.539341
C	0.000000	-0.685363	-1.731647
H	0.000001	-1.423391	-2.539341
C	1.219799	-2.757921	0.729166

C	-1.221523	-2.758071	0.727100
C	-1.219799	2.757921	0.729166
C	1.221523	2.758071	0.727100
H	1.226562	3.850759	0.912147
H	1.307597	2.222116	1.702359
H	2.104182	2.507869	0.106697
H	-1.224621	3.850674	0.914079
H	-2.103468	2.507587	0.110285
H	-1.304131	2.222101	1.704609
H	1.224621	-3.850674	0.914079
H	2.103468	-2.507587	0.110285
H	1.304131	-2.222101	1.704609
H	-1.226562	-3.850759	0.912147
H	-1.307597	-2.222116	1.702359
H	-2.104182	-2.507869	0.106697

	2Ph	RI-BP86/SVP	
29			
E(SCF) =	-687.822466		
C	0.336735	-0.060509	0.000000
N	-0.509739	0.122080	1.073132
C	-0.071288	0.013766	2.430414
N	-0.509739	0.122080	-1.073132
C	-0.071288	0.013766	-2.430414
C	-1.825537	0.411048	0.682799
H	-2.633959	0.634362	1.384571
C	-1.825537	0.411048	-0.682799
H	-2.633959	0.634362	-1.384571
C	-0.988395	-0.260641	3.463837
C	-0.539149	-0.351365	4.791403
C	0.820471	-0.181692	5.096185
C	1.732885	0.079591	4.058314
C	1.295448	0.181362	2.731009
H	-2.050938	-0.428721	3.237337
H	-1.263018	-0.568408	5.591680
H	1.168900	-0.256127	6.137277
H	2.801922	0.212523	4.284816
H	1.988445	0.380921	1.902214
C	-0.988395	-0.260641	-3.463837
C	-0.539149	-0.351365	-4.791403
C	0.820471	-0.181692	-5.096185
C	1.732885	0.079591	-4.058314
C	1.295448	0.181362	-2.731009
H	-2.050938	-0.428721	-3.237337
H	-1.263018	-0.568408	-5.591680
H	1.168900	-0.256127	-6.137277

H	2.801922	0.212523	-4.284816
H	1.988445	0.380921	-1.902214

	2H	RI-BP86/SVP	
9			
E(SCF) =	-226.030912		
C	-0.000008	-1.286975	0.000059
N	-1.053597	-0.404208	0.000332
H	-2.020495	-0.728898	0.000923
N	1.053592	-0.404226	-0.000409
H	2.020505	-0.728881	-0.000483
C	-0.685606	0.941510	-0.000933
H	-1.400799	1.770304	-0.000040
C	0.685617	0.941500	0.000727
H	1.400805	1.770302	0.001016

	2Me_Me	RI-BP86/SVP	
21			
E(SCF) =	-383.176603		
C	0.000000	0.000000	1.580145
N	0.000000	1.066817	0.712229
C	0.000000	2.443087	1.176974
N	0.000000	-1.066817	0.712229
C	0.000000	-2.443087	1.176974
C	0.000000	-0.690103	-0.640733
C	0.000000	-1.668207	-1.771321
C	0.000000	0.690103	-0.640733
C	0.000000	1.668207	-1.771321
H	0.900331	2.990737	0.827707
H	-0.900331	2.990737	0.827707
H	0.000000	2.414973	2.281214
H	0.900331	-2.990737	0.827707
H	0.000000	-2.414973	2.281214
H	-0.900331	-2.990737	0.827707
H	0.000000	-1.139334	-2.743887
H	0.893152	-2.329551	-1.754147
H	-0.893152	-2.329551	-1.754147
H	0.000000	1.139334	-2.743887
H	-0.893152	2.329551	-1.754147
H	0.893152	2.329551	-1.754147

Molekuele/3R/BP86_TZ2P			
	3Me	BP86/TZ2P	
31			
E(SCF) =	-6.819121		
C	1.073415	2.378325	1.692789

C	0.726637	1.204017	2.280670
C	1.390723	2.688092	0.408937
N	0.971096	0.843209	3.615694
N	-0.070158	0.141427	1.799216
N	2.127776	1.959920	-0.551361
N	1.174446	3.924236	-0.221440
C	0.315623	-0.336984	3.935180
C	-0.343118	-0.760370	2.827309
C	2.396366	2.760535	-1.661159
C	1.791084	3.958550	-1.463672
C	1.773648	1.655402	4.500180
H	0.388001	-0.789006	4.915122
H	-0.960472	-1.635690	2.675317
C	-0.804122	0.232996	0.554920
C	2.825758	0.736092	-0.218931
H	2.972102	2.400919	-2.503548
H	1.731309	4.821650	-2.112789
C	0.434722	4.992853	0.408586
H	-1.462493	-0.637854	0.463389
H	-1.409489	1.154133	0.534216
H	-0.128807	0.259450	-0.311095
H	1.337208	1.664101	5.507576
H	2.813157	1.295832	4.560039
H	1.780882	2.670653	4.079442
H	3.442994	0.433622	-1.072004
H	3.469131	0.889358	0.663123
H	2.125328	-0.076378	0.017586
H	0.902835	5.960698	0.186021
H	-0.616455	5.015967	0.079917
H	0.456315	4.798974	1.490128

	3H	BP86/TZ2P	
19			
E(SCF) =	-4.444919		
C	1.075920	2.474870	1.770200
C	0.765900	1.262660	2.301690
C	1.354400	2.723120	0.462960
N	0.933660	0.872300	3.633120
N	0.121000	0.131880	1.748720
N	1.935930	1.916780	-0.542990
N	1.213920	3.946400	-0.198160
C	0.326890	-0.348400	3.900870
C	-0.195930	-0.802940	2.735500
C	2.246920	2.668370	-1.677220
C	1.780040	3.923630	-1.466610
H	1.315550	1.517430	4.310120

H	0.338580	-0.802450	4.881720
H	-0.731890	-1.718070	2.523200
H	-0.340720	0.191200	0.851340
H	2.370640	1.034990	-0.307510
H	2.739130	2.244890	-2.542200
H	1.781770	4.784910	-2.119710
H	0.879690	4.759910	0.298690

3H.c2v.Conf_c BP86/TZ2P

19

E(SCF) =	-4.439581		
C	0.000000	3.538430	0.250320
N	0.000000	2.425810	1.068600
C	0.000000	1.221990	0.358660
N	0.000000	1.700180	-0.974160
C	0.000000	3.091630	-1.031890
C	0.000000	0.000000	0.969690
C	0.000000	-1.221990	0.358660
N	0.000000	-2.425810	1.068600
C	0.000000	-3.538430	0.250320
C	0.000000	-3.091630	-1.031890
N	0.000000	-1.700180	-0.974160
H	0.000000	-2.399710	2.079220
H	0.000000	-4.549290	0.632980
H	0.000000	-3.643090	-1.962410
H	0.000000	-1.103910	-1.786020
H	0.000000	1.103910	-1.786020
H	0.000000	3.643090	-1.962410
H	0.000000	4.549290	0.632980
H	0.000000	2.399710	2.079220

Molekuele/3R/RI-BP86_SVP

3Me.d2h.Conf_e RI-BP86/SVP

31

E(SCF) =	-647.274581		
C	1.344057	0.000000	0.000000
N	-2.250671	1.106695	0.000000
C	0.000000	0.000000	0.000000
C	-1.344057	0.000000	0.000000
N	2.250671	1.106695	0.000000
C	3.570539	-0.685973	0.000000
C	3.570539	0.685973	0.000000
N	-2.250671	-1.106695	0.000000
C	-3.570539	-0.685973	0.000000
C	-3.570539	0.685973	0.000000
N	2.250671	-1.106695	0.000000

C	-1.795547	-2.471822	0.000000
H	-4.412916	-1.385227	0.000000
H	-4.412916	1.385227	0.000000
C	-1.795547	2.471822	0.000000
C	1.795547	-2.471822	0.000000
H	4.412916	-1.385227	0.000000
H	4.412916	1.385227	0.000000
C	1.795547	2.471822	0.000000
H	-2.668784	3.151226	0.000000
H	-1.169338	2.680050	0.894308
H	-1.169338	2.680050	-0.894308
H	-2.668784	-3.151226	0.000000
H	-1.169338	-2.680050	-0.894308
H	-1.169338	-2.680050	0.894308
H	2.668784	-3.151226	0.000000
H	1.169338	-2.680050	0.894308
H	1.169338	-2.680050	-0.894308
H	2.668784	3.151226	0.000000
H	1.169338	2.680050	-0.894308
H	1.169338	2.680050	0.894308

3Ad

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115

E(SCF) =

-2047.177599

C	-0.086411	-0.065640	-0.054589
C	0.488409	1.143370	-0.317108
C	0.238821	-1.351164	0.263583
N	-0.075844	2.146608	-1.142918
N	1.638017	1.766583	0.255878
N	1.280442	-2.191804	-0.229507
N	-0.522041	-2.201937	1.109292
C	0.633686	3.338106	-0.989874
C	1.673566	3.110807	-0.135686
C	1.104101	-3.490231	0.269538
C	0.017202	-3.488569	1.094186
H	0.378074	4.253776	-1.525506
H	2.470821	3.793622	0.160722
H	1.790218	-4.308768	0.048861
H	-0.381206	-4.305998	1.697049
C	2.343629	1.125970	1.366751
H	2.179059	0.044780	1.184039
C	1.736888	1.434536	2.767334
C	3.881262	1.342956	1.429366
H	0.633978	1.329467	2.694262
C	2.115971	2.854741	3.240560
C	2.299413	0.392484	3.761306

H	4.312311	1.172251	0.419353
C	4.283447	2.743555	1.952441
C	4.441904	0.293966	2.425434
H	1.652175	3.051992	4.231905
H	1.705705	3.618149	2.545876
C	3.653959	2.986336	3.341973
H	2.009879	-0.631571	3.441321
H	1.858035	0.551991	4.769417
C	3.837701	0.519014	3.832048
H	3.992899	3.548190	1.248123
H	5.392069	2.795181	2.025379
H	4.209938	-0.733740	2.071489
H	5.549728	0.376575	2.469662
H	3.919043	4.006109	3.696442
C	4.202935	1.934532	4.331429
H	4.243795	-0.242218	4.533059
H	5.306413	2.037733	4.424243
H	3.778599	2.101986	5.345632
C	-1.391480	1.933290	-1.748049
H	-1.978776	1.428825	-0.943386
C	-1.370191	0.943681	-2.947624
C	-2.132331	3.223764	-2.180567
H	-0.798983	0.048038	-2.628435
C	-0.732122	1.594726	-4.191346
C	-2.831177	0.547052	-3.253187
H	-2.116435	3.956738	-1.344918
C	-1.529936	3.857823	-3.460449
C	-3.598843	2.826878	-2.487947
H	-0.690737	0.857591	-5.022684
H	0.317504	1.888853	-3.972830
C	-1.551699	2.834632	-4.615689
H	-3.280388	0.055906	-2.363184
H	-2.857873	-0.197515	-4.078463
C	-3.640466	1.802304	-3.646194
H	-0.489379	4.205952	-3.297997
H	-2.122187	4.759134	-3.732351
H	-4.076883	2.399173	-1.580714
H	-4.179911	3.734728	-2.760772
H	-1.100052	3.291549	-5.523013
C	-3.012227	2.427687	-4.911513
H	-4.696385	1.521199	-3.851685
H	-3.597340	3.317178	-5.233779
H	-3.045876	1.700493	-5.752282
C	2.130789	-1.756363	-1.337452
H	1.983289	-0.657248	-1.344416
C	1.688928	-2.273437	-2.739280

C	3.655784	-2.008216	-1.171809
H	0.590431	-2.139282	-2.830149
C	2.067356	-3.757021	-2.946651
C	2.414073	-1.414765	-3.802448
H	3.963622	-1.686816	-0.153916
C	4.050452	-3.486004	-1.404238
C	4.378200	-1.144694	-2.237021
H	1.736174	-4.084116	-3.956643
H	1.531697	-4.404203	-2.221287
C	3.597934	-3.935464	-2.812090
H	2.129603	-0.346831	-3.687987
H	2.094191	-1.725151	-4.821071
C	3.943181	-1.582438	-3.655295
H	3.624175	-4.148290	-0.623600
H	5.154472	-3.585351	-1.312950
H	4.144652	-0.069588	-2.079804
H	5.478879	-1.255724	-2.125494
H	3.863671	-5.004049	-2.964867
C	4.312884	-3.066981	-3.871300
H	4.461539	-0.953589	-4.411362
H	5.414114	-3.203877	-3.797459
H	4.017489	-3.388583	-4.893970
C	-1.726984	-1.697840	1.760644
H	-1.787042	-0.670243	1.330513
C	-1.635137	-1.555381	3.305040
C	-3.047572	-2.434112	1.399293
H	-0.666375	-1.075220	3.558499
C	-1.754526	-2.924086	4.013326
C	-2.804945	-0.650106	3.759478
H	-3.086170	-2.574633	0.298361
C	-3.184915	-3.795414	2.120177
C	-4.215589	-1.523595	1.854446
H	-1.688518	-2.779961	5.114268
H	-0.905539	-3.585273	3.738824
C	-3.102900	-3.589618	3.650153
H	-2.718804	0.349231	3.281327
H	-2.753863	-0.487760	4.858552
C	-4.151670	-1.309349	3.384740
H	-2.410122	-4.511558	1.778053
H	-4.161966	-4.255364	1.853206
H	-4.164348	-0.546682	1.327681
H	-5.186190	-1.989900	1.576363
H	-3.183012	-4.572686	4.163231
C	-4.263855	-2.674438	4.100041
H	-4.989362	-0.650899	3.702121
H	-5.239872	-3.152629	3.864248

H	-4.234551	-2.531653	5.202614
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3Me (135)° RI-BP86/SVP

31			
E(SCF) =	-647.293545		
C	1.072230	2.339440	1.661567
C	0.710123	1.179714	2.284194
C	1.406307	2.685566	0.383934
N	0.959252	0.841679	3.631121
N	-0.114743	0.123417	1.825366
N	2.172223	1.979656	-0.576286
N	1.186609	3.938412	-0.226507
C	0.292937	-0.331971	3.973830
C	-0.385878	-0.767182	2.869808
C	2.439805	2.798864	-1.678559
C	1.814843	3.996401	-1.467814
C	1.783087	1.658005	4.489115
H	0.372049	-0.774533	4.971342
H	-1.020412	-1.648082	2.732067
C	-0.828269	0.203007	0.571549
C	2.849772	0.745198	-0.252677
H	3.032671	2.451383	-2.530259
H	1.749251	4.878989	-2.111224
C	0.425073	4.982875	0.414106
H	-1.495354	-0.673976	0.472017
H	-1.437108	1.134166	0.523825
H	-0.135237	0.220610	-0.294941
H	1.365187	1.688530	5.515657
H	2.834394	1.295532	4.540075
H	1.792621	2.678039	4.049635
H	3.474687	0.433128	-1.110640
H	3.496831	0.874808	0.644301
H	2.131772	-0.069192	-0.023145
H	0.875239	5.974908	0.207886
H	-0.638665	4.996164	0.086210
H	0.445454	4.772801	1.504576

3Me.c2v.Conf_c RI-BP86/SVP

31			
E(SCF) =	-647.274574		
C	0.000000	3.583828	0.656010
N	0.000000	2.274090	1.103939
C	0.000000	1.343118	0.018547
N	0.000000	2.224937	-1.108710
C	0.000000	3.554485	-0.715446
C	0.000000	0.000000	0.091670

C	0.000000	-1.343118	0.018547
N	0.000000	-2.274090	1.103939
C	0.000000	-3.583828	0.656010
C	0.000000	-3.554485	-0.715446
N	0.000000	-2.224937	-1.108710
C	0.000000	-1.842154	2.477510
H	0.000000	-4.441035	1.336941
H	0.000000	-4.381023	-1.433369
C	0.000000	-1.750626	-2.466422
C	0.000000	1.750626	-2.466422
H	0.000000	4.381023	-1.433369
H	0.000000	4.441035	1.336941
C	0.000000	1.842154	2.477510
H	0.000000	-2.613995	-3.158067
H	-0.895079	-1.123073	-2.668476
H	0.895079	-1.123073	-2.668476
H	0.000000	-2.727540	3.141236
H	0.893434	-1.217705	2.693698
H	-0.893434	-1.217705	2.693698
H	-0.893434	1.217705	2.693698
H	0.893434	1.217705	2.693698
H	0.000000	2.727540	3.141236
H	0.000000	2.613995	-3.158067
H	0.895079	1.123073	-2.668476
H	-0.895079	1.123073	-2.668476

3Me.cs.Conf_b RI-BP86/SVP

31

E(SCF) =	-647.291525		
C	-0.443333	-3.593090	0.000000
N	0.535918	-2.600177	0.000000
C	-0.059398	-1.314637	0.000000
N	-1.446467	-1.598841	0.000000
C	-1.664349	-2.980204	0.000000
C	0.585541	-0.124111	0.000000
C	0.420854	1.228159	0.000000
N	0.415367	2.105388	1.107200
C	0.415367	3.433507	0.684051
C	0.415367	3.433507	-0.684051
N	0.415367	2.105388	-1.107200
C	0.470383	1.628590	2.467904
H	0.414028	4.269922	1.389465
H	0.414028	4.269922	-1.389465
C	0.470383	1.628590	-2.467904
C	-2.447164	-0.564952	0.000000
H	-2.671355	-3.408434	0.000000

H	-0.189804	-4.657268	0.000000
C	1.963290	-2.800196	0.000000
H	2.424292	-1.791074	0.000000
H	2.304633	-3.352620	0.902938
H	2.304633	-3.352620	-0.902938
H	-3.453227	-1.025404	0.000000
H	-2.355347	0.089189	0.895306
H	-2.355347	0.089189	-0.895306
H	1.010554	2.355639	3.106133
H	-0.539536	1.455022	2.902177
H	1.009240	0.657300	2.463133
H	1.010554	2.355639	-3.106133
H	1.009240	0.657300	-2.463133
H	-0.539536	1.455022	-2.902177

3Me.d2d.Conf_d RI-BP86/SVP

31

E(SCF) =	-647.290221		
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.342155
C	0.000000	0.000000	1.342155
N	0.785580	0.785580	-2.220098
N	-0.785580	-0.785580	-2.220098
N	0.785580	-0.785580	2.220098
N	-0.785580	0.785580	2.220098
C	0.483270	0.483270	-3.549293
C	-0.483270	-0.483270	-3.549293
C	0.483270	-0.483270	3.549293
C	-0.483270	0.483270	3.549293
H	0.981757	0.981757	-4.386014
H	-0.981757	-0.981757	-4.386014
H	0.981757	-0.981757	4.386014
H	-0.981757	0.981757	4.386014
C	-1.743612	1.743612	1.734107
H	-2.516308	1.251612	1.102233
H	-1.251612	2.516308	1.102233
H	-2.239243	2.239243	2.590340
C	1.743612	-1.743612	1.734107
H	2.516308	-1.251612	1.102233
H	1.251612	-2.516308	1.102233
H	2.239243	-2.239243	2.590340
C	1.743612	1.743612	-1.734107
H	2.516308	1.251612	-1.102233
H	1.251612	2.516308	-1.102233
H	2.239243	2.239243	-2.590340
C	-1.743612	-1.743612	-1.734107

H	-2.516308	-1.251612	-1.102233
H	-1.251612	-2.516308	-1.102233
H	-2.239243	-2.239243	-2.590340

	3Me (180°)	RI-BP86/SVP	
31			
E(SCF) =	-647.289887		
C	1.052552	1.774191	1.206163
C	0.546502	1.005033	2.182651
C	1.558607	2.543205	0.229521
N	0.932037	0.934644	3.546429
N	-0.498474	0.052594	2.091709
N	2.561864	2.209936	-0.713767
N	1.214001	3.874566	-0.119843
C	0.173535	-0.025465	4.219425
C	-0.713639	-0.559600	3.327573
C	2.792249	3.277399	-1.583224
C	1.955413	4.296895	-1.225242
C	2.043419	1.680954	4.077394
H	0.319626	-0.240192	5.282446
H	-1.487105	-1.320226	3.472131
C	-1.197717	-0.197175	0.857971
C	3.212395	0.925332	-0.713663
H	3.539508	3.225702	-2.381067
H	1.834717	5.294510	-1.658380
C	0.151663	4.596661	0.531360
H	-1.895882	-1.044928	0.993945
H	-1.772273	0.696291	0.525617
H	-0.479243	-0.443457	0.045702
H	1.903221	1.852554	5.163150
H	3.019877	1.166685	3.919567
H	2.094251	2.659524	3.557035
H	3.876366	0.847165	-1.595487
H	3.815320	0.771897	0.209300
H	2.459419	0.107893	-0.750665
H	0.330083	5.687618	0.454625
H	-0.850268	4.366771	0.099867
H	0.128147	4.305303	1.601698

	3Me	RI-BP86/SVP	
31			
E(SCF) =	-647.293612		
C	1.073363	2.375525	1.690571
C	0.723591	1.195757	2.288051
C	1.393646	2.693351	0.399221
N	0.968620	0.838524	3.630311

N	-0.085089	0.137206	1.806220
N	2.142705	1.965155	-0.557592
N	1.177105	3.937350	-0.229179
C	0.316059	-0.348959	3.949507
C	-0.350564	-0.774416	2.834337
C	2.403275	2.764082	-1.676757
C	1.790409	3.969943	-1.478440
C	1.776478	1.651495	4.506993
H	0.395769	-0.807459	4.939763
H	-0.972214	-1.661338	2.677763
C	-0.804952	0.234504	0.556567
C	2.827046	0.738094	-0.217866
H	2.982505	2.397413	-2.529797
H	1.723405	4.842043	-2.135877
C	0.432051	4.998818	0.403510
H	-1.472040	-0.641432	0.448157
H	-1.414589	1.165758	0.527254
H	-0.117423	0.265887	-0.313880
H	1.344738	1.670843	5.528117
H	2.828731	1.293726	4.568643
H	1.785407	2.675022	4.075784
H	3.452255	0.417846	-1.072594
H	3.474870	0.885255	0.675692
H	2.114762	-0.077399	0.025043
H	0.896422	5.982466	0.188478
H	-0.631690	5.024691	0.076688
H	0.452101	4.796594	1.495436

	3Mes	RI-BP86/SVP	
95			
E(SCF) =	-1885.196609		
C	1.084791	2.280919	1.436869
C	0.378959	1.362489	2.137732
C	2.287375	2.804193	1.101010
N	0.525538	0.912242	3.486639
N	-0.790618	0.673526	1.702188
N	3.519252	2.159159	0.769182
N	2.589083	4.182183	0.894778
C	-0.487596	-0.002577	3.809684
C	-1.287432	-0.149949	2.718576
C	4.488006	3.108816	0.412341
C	3.919870	4.342769	0.493146
H	-0.574926	-0.424676	4.814594
H	-2.201728	-0.734286	2.583268
H	5.484981	2.808130	0.078715
H	4.328449	5.328559	0.254440

C	3.751313	0.752808	0.694964
C	4.313977	-2.014656	0.476361
C	3.131790	-0.007010	-0.333461
C	4.671696	0.154087	1.592942
C	4.937208	-1.223391	1.459065
C	3.416715	-1.383286	-0.408385
H	5.650802	-1.692832	2.156260
H	2.940373	-1.975282	-1.207453
C	1.675689	5.270311	1.050345
C	-0.075134	7.478024	1.310802
C	1.846605	6.171797	2.131444
C	0.658994	5.471437	0.080955
C	-0.204957	6.570751	0.240900
C	0.963332	7.263962	2.236797
H	-0.996184	6.731505	-0.510135
H	1.089263	7.965866	3.077852
C	1.485717	1.370385	4.438194
C	3.318017	2.233808	6.418391
C	1.396869	2.695924	4.941804
C	2.456499	0.463071	4.934938
C	3.352439	0.916892	5.923348
C	2.330657	3.103322	5.913122
H	4.109219	0.214983	6.310958
H	2.262599	4.130256	6.308944
C	-1.404773	0.798755	0.417742
C	-2.696136	1.008077	-2.091554
C	-2.127139	1.979067	0.101958
C	-1.342124	-0.287654	-0.491175
C	-1.995621	-0.158815	-1.732601
C	-2.750172	2.061249	-1.157039
H	-1.946524	-0.999024	-2.444942
H	-3.312953	2.976148	-1.406380
C	2.232638	0.656107	-1.344033
H	2.743632	1.515601	-1.825612
H	1.322197	1.069998	-0.858146
H	1.924181	-0.053807	-2.134821
C	5.355836	0.966389	2.666888
H	6.137925	1.634606	2.247848
H	5.845613	0.307568	3.409346
H	4.636004	1.617985	3.200298
C	4.585097	-3.498772	0.375801
H	4.674989	-3.826489	-0.679921
H	3.758779	-4.090235	0.826459
H	5.517505	-3.781740	0.902717
C	-0.593905	-1.552966	-0.143443
H	0.410959	-1.330309	0.268116

H	-0.472970	-2.198613	-1.034567
H	-1.123083	-2.148884	0.630341
C	-3.354532	1.139815	-3.446296
H	-3.550867	0.150723	-3.905094
H	-2.709678	1.707369	-4.152038
H	-4.317562	1.685536	-3.381075
C	-2.238808	3.099116	1.102801
H	-1.235565	3.530532	1.312706
H	-2.632750	2.730963	2.072818
H	-2.906791	3.902021	0.736949
C	0.530048	4.542503	-1.097645
H	1.489525	4.460423	-1.649253
H	-0.249041	4.890647	-1.802147
H	0.274726	3.516036	-0.754390
C	2.945749	5.970392	3.147790
H	2.802119	6.633479	4.022604
H	3.948621	6.190566	2.723854
H	2.981918	4.921421	3.504356
C	-1.037605	8.633225	1.469914
H	-1.359027	9.035581	0.488183
H	-0.589898	9.463218	2.051555
H	-1.958469	8.316760	2.006686
C	2.533114	-0.956099	4.423697
H	2.478961	-0.990000	3.317665
H	1.695372	-1.580119	4.801317
H	3.476515	-1.440333	4.740995
C	0.301199	3.621725	4.481506
H	-0.695467	3.150262	4.608282
H	0.399882	3.849818	3.397811
H	0.312257	4.571514	5.049229
C	4.315618	2.710028	7.450020
H	5.135132	3.293848	6.977408
H	4.784201	1.862940	7.988542
H	3.840896	3.373609	8.201091

	3NMe2	RI-BP86/SVP	
51			
E(SCF) =	-1025.520587		
C	-0.000075	0.517276	-0.000187
C	-1.256684	0.030192	0.118080
C	1.256622	0.030319	-0.118213
N	-1.745624	-1.024290	0.941779
N	-2.453253	0.617527	-0.369363
N	1.745772	-1.024315	-0.941558
N	2.453077	0.618001	0.369092
C	-3.141846	-0.918093	1.104227

C	-3.575900	0.087672	0.294412
C	3.141982	-0.918018	-1.103931
C	3.575851	0.088054	-0.294395
H	-3.715023	-1.642682	1.691534
H	-4.595706	0.397142	0.045414
H	3.715276	-1.642708	-1.691000
H	4.595581	0.397782	-0.045426
N	-0.881335	-1.700273	1.800429
N	-2.416182	1.817774	-1.075499
N	0.881596	-1.700794	-1.799957
N	2.415826	1.818389	1.074918
C	1.154094	-3.124911	-1.867151
H	0.323671	-3.625108	-2.405792
H	1.205440	-3.535507	-0.840388
H	2.105074	-3.391402	-2.401931
C	0.724170	-1.032942	-3.088668
H	0.421331	0.017288	-2.905898
H	-0.085671	-1.531932	-3.657660
H	1.653903	-1.044331	-3.714598
C	3.349691	1.854406	2.184801
H	3.215846	0.949428	2.808906
H	3.130638	2.744845	2.808642
H	4.429997	1.918205	1.883761
C	2.433589	2.988029	0.202332
H	1.611892	2.885128	-0.533837
H	3.404831	3.126547	-0.340190
H	2.241428	3.894897	0.810216
C	-1.153122	-3.124524	1.867567
H	-1.203327	-3.535233	0.840787
H	-2.104468	-3.391473	2.401469
H	-0.322909	-3.624267	2.406954
C	-0.724272	-1.032179	3.089036
H	-0.421829	0.018147	2.906135
H	0.085731	-1.530752	3.658160
H	-1.654021	-1.043800	3.714941
C	-3.350794	1.853755	-2.184733
H	-3.217628	0.948594	-2.808727
H	-3.131934	2.743970	-2.808964
H	-4.430880	1.917922	-1.882974
C	-2.433261	2.987603	-0.203109
H	-1.611145	2.884679	0.532590
H	-3.404197	3.126351	0.339893
H	-2.241312	3.894313	-0.811299

3H (135°) RI-BP86/SVP

E(SCF) =	-490.163889		
C	1.071688	2.326369	1.650948
C	0.729494	1.166972	2.274917
C	1.386939	2.674954	0.374352
N	0.969709	0.828348	3.619778
N	-0.034803	0.058860	1.831181
N	2.091734	1.975462	-0.637083
N	1.176160	3.925245	-0.236689
C	0.328787	-0.352676	3.985725
C	-0.309728	-0.828844	2.874068
C	2.363479	2.793518	-1.736274
C	1.780122	4.005445	-1.488992
H	1.460404	1.471930	4.236287
H	0.390313	-0.768756	4.995301
H	-0.914050	-1.730962	2.739805
H	-0.489982	0.060092	0.921532
H	2.517410	1.069599	-0.455824
H	2.926395	2.446301	-2.607840
H	1.733793	4.904794	-2.109620
H	0.731564	4.683662	0.275379

3H.c2v.Conf_c RI-BP86/SVP

19			
E(SCF) =	-490.157802		
C	0.000000	3.559695	0.259507
N	0.000000	2.441261	1.075110
C	0.000000	1.233943	0.355422
N	0.000000	1.718744	-0.980229
C	0.000000	3.112276	-1.035744
C	0.000000	0.000000	0.963268
C	0.000000	-1.233943	0.355422
N	0.000000	-2.441261	1.075110
C	0.000000	-3.559695	0.259507
C	0.000000	-3.112276	-1.035744
N	0.000000	-1.718744	-0.980229
H	0.000000	-2.408093	2.093442
H	0.000000	-4.581309	0.650097
H	0.000000	-3.671487	-1.976434
H	0.000000	-1.115055	-1.796186
H	0.000000	1.115055	-1.796186
H	0.000000	3.671487	-1.976434
H	0.000000	4.581309	0.650097
H	0.000000	2.408093	2.093442

3H.c2v.Conf_e RI-BP86/SVP

19

E(SCF) =	-490.146821		
C	0.000000	1.338825	0.001075
N	1.091637	-2.253761	0.000314
C	0.000000	0.000000	0.002022
C	0.000000	-1.338825	0.001075
N	1.091637	2.253761	0.000314
C	-0.686608	3.579131	-0.001151
C	0.686608	3.579131	-0.001151
N	-1.091637	-2.253761	0.000314
C	-0.686608	-3.579131	-0.001151
C	0.686608	-3.579131	-0.001151
N	-1.091637	2.253761	0.000314
H	-2.049423	-1.909801	0.000503
H	-1.386663	-4.420412	-0.002059
H	1.386663	-4.420412	-0.002059
H	2.049423	-1.909801	0.000503
H	-2.049423	1.909801	0.000503
H	-1.386663	4.420412	-0.002059
H	1.386663	4.420412	-0.002059
H	2.049423	1.909801	0.000503

3H.cs.Conf_b RI-BP86/SVP

19			
E(SCF) =	-490.161216		
C	-0.314567	-3.622515	0.000000
N	0.632909	-2.599159	0.000000
C	0.032557	-1.321624	0.000000
N	-1.345858	-1.651844	0.000000
C	-1.547976	-3.034599	0.000000
C	0.654068	-0.124780	0.000000
C	0.454468	1.216408	0.000000
N	0.405624	2.107725	1.093938
C	0.405624	3.440558	0.683792
C	0.405624	3.440558	-0.683792
N	0.405624	2.107725	-1.093938
H	0.497067	1.771741	2.049620
H	0.394471	4.276448	1.389252
H	0.394471	4.276448	-1.389252
H	0.497067	1.771741	-2.049620
H	-2.070828	-0.940154	0.000000
H	-2.544748	-3.485252	0.000000
H	-0.038183	-4.680570	0.000000
H	1.643806	-2.705579	0.000000

3H.d2d.Conf_d RI-BP86/SVP

19

E(SCF) =	-490.160255		
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.336820
C	0.000000	0.000000	1.336820
N	0.776150	-0.776150	-2.233880
N	-0.776150	0.776150	-2.233880
N	0.776150	0.776150	2.233880
N	-0.776150	-0.776150	2.233880
C	0.483080	-0.483080	-3.566400
C	-0.483080	0.483080	-3.566400
C	0.483080	0.483080	3.566400
C	-0.483080	-0.483080	3.566400
H	1.454740	-1.454740	-1.900260
H	0.981450	-0.981450	-4.402850
H	-0.981450	0.981450	-4.402850
H	-1.454740	1.454740	-1.900260
H	1.454740	1.454740	1.900260
H	0.981450	0.981450	4.402850
H	-0.981450	-0.981450	4.402850
H	-1.454740	-1.454740	1.900260

3H (180°) RI-BP86/SVP

19			
E(SCF) =	-490.160254		
C	1.048776	1.673132	1.124419
C	0.643974	0.883996	2.124696
C	1.454097	2.463905	0.125722
N	1.138349	0.790230	3.450013
N	-0.394155	-0.081207	2.141409
N	2.438033	2.223187	-0.866159
N	1.013735	3.765605	-0.223089
C	0.445269	-0.161200	4.199649
C	-0.508489	-0.703458	3.385270
C	2.584133	3.309066	-1.730588
C	1.697107	4.268468	-1.331107
H	1.909965	1.367235	3.772626
H	0.684268	-0.376003	5.245182
H	-1.253818	-1.477156	3.590809
H	-0.964055	-0.264225	1.320350
H	2.974144	1.360245	-0.885407
H	3.297321	3.310228	-2.559921
H	1.495234	5.259279	-1.748224
H	0.299808	4.247991	0.315576

3H RI-BP86/SVP

E(SCF) =	-490.164355		
C	1.075562	2.471345	1.767275
C	0.755340	1.255548	2.308906
C	1.364631	2.728318	0.454093
N	0.928477	0.865988	3.647620
N	0.085791	0.130598	1.765074
N	1.971419	1.931142	-0.548710
N	1.219405	3.959143	-0.207680
C	0.336580	-0.364048	3.918150
C	-0.204363	-0.819647	2.747127
C	2.255198	2.675710	-1.696148
C	1.770680	3.937564	-1.485247
H	1.349468	1.503772	4.319837
H	0.359965	-0.825059	4.909639
H	-0.747974	-1.745074	2.534196
H	-0.333476	0.163528	0.838304
H	2.360393	1.016085	-0.331657
H	2.754665	2.248915	-2.571155
H	1.761155	4.808217	-2.147081
H	0.846512	4.768266	0.284407

Molekuele/4Me/RI-BP86_SVP

4Me (135°)

RI-BP86/SVP

39

E(SCF) =	-652.073276		
C	-0.924660	-0.116316	0.239228
C	-0.777124	0.115005	-1.094650
C	-0.089603	-0.114822	1.314946
N	0.288599	-0.378760	-1.895035
N	-1.800033	0.742755	-1.867595
N	0.905446	0.866551	1.573487
N	-0.260432	-1.024303	2.401825
C	-0.069292	-1.046065	-3.152419
H	0.754995	-0.947045	-3.889168
H	-0.988962	-0.603770	-3.569850
H	-0.259849	-2.136249	-2.993117
C	1.370613	-1.082481	-1.224512
H	2.174513	-1.284945	-1.960351
H	1.030913	-2.059285	-0.796663
H	1.804409	-0.493558	-0.397645
C	-3.049257	0.994641	-1.169803
H	-3.380390	0.074372	-0.652564
H	-3.820878	1.297356	-1.908194
H	-2.967645	1.800136	-0.398004
C	0.932928	1.457158	2.916981
H	1.959642	1.796463	3.167502

H	0.598474	0.718927	3.664520
H	0.251575	2.341024	2.985418
C	1.138553	1.880159	0.556881
H	0.263636	2.569370	0.446656
H	1.338303	1.439910	-0.435637
H	2.022127	2.482252	0.849267
C	0.926169	-1.777645	2.801175
H	1.818799	-1.126027	2.797015
H	1.131273	-2.638456	2.114049
H	0.792377	-2.187973	3.824251
C	-1.451844	-1.853838	2.345150
H	-1.580155	-2.369059	3.319996
H	-1.409507	-2.630261	1.541114
H	-2.338064	-1.221824	2.147073
C	-1.379729	1.876996	-2.687383
H	-0.409954	1.665716	-3.173278
H	-1.260109	2.813353	-2.083889
H	-2.134456	2.079068	-3.476339

	4Me	RI-BP86/SVP	
39			
E(SCF) =	-652.084895		
C	-0.227019	0.045700	0.055863
C	-0.577232	0.089412	-1.237230
C	0.123738	0.005606	1.348915
N	0.225494	-0.421267	-2.300490
N	-1.798017	0.652423	-1.715725
N	1.040579	0.914652	1.956641
N	-0.375489	-0.950110	2.283228
C	-0.419342	-1.412218	-3.161172
H	0.100625	-1.465302	-4.140646
H	-1.472986	-1.125968	-3.329001
H	-0.406720	-2.436658	-2.708559
C	1.594718	-0.767889	-1.974068
H	2.147106	-0.989840	-2.910088
H	1.676095	-1.659911	-1.302130
H	2.092326	0.080060	-1.467817
C	-2.810511	0.951268	-0.722298
H	-2.999261	0.062989	-0.091160
H	-3.755477	1.222877	-1.235940
H	-2.527926	1.796281	-0.044104
C	0.529818	1.647965	3.114338
H	1.372252	2.019979	3.734416
H	-0.099203	0.978353	3.727756
H	-0.092803	2.529454	2.814681
C	1.818662	1.749656	1.062803

H	1.202923	2.515343	0.525810
H	2.320362	1.126685	0.299144
H	2.597186	2.281495	1.647234
C	0.636807	-1.735960	2.987711
H	1.497938	-1.090577	3.237040
H	1.012723	-2.591236	2.369995
H	0.214056	-2.152249	3.926069
C	-1.507988	-1.747909	1.856107
H	-1.895773	-2.322536	2.722108
H	-1.254599	-2.473921	1.042094
H	-2.316339	-1.092723	1.481620
C	-1.657343	1.709867	-2.716071
H	-0.837209	1.454762	-3.410877
H	-1.421669	2.701571	-2.251906
H	-2.599100	1.818401	-3.293852

Molekuele/5/BP86_TZ2P

	5	BP86/TZ2P	
5			
E(SCF) =	-1.420009		
C	0.000000	0.000000	-1.276800
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.276800
O	0.000000	0.000000	2.448500
O	0.000000	0.000000	-2.448500

Molekuele/5/RI-BP86_SVP

	5 (135°)	RI-BP86/SVP	
5			
E(SCF) =	-264.553567		
C	0.039211	0.000000	0.239957
C	0.550795	0.000000	1.445178
C	0.060320	0.000000	2.659143
O	-0.290204	0.000000	3.778590
O	-0.330802	0.000000	-0.873124

5 **RI-BP86/SVP**

5			
E(SCF) =	-264.559533		
C	-0.005334	0.000000	0.159729
C	0.006353	0.000000	1.449935
C	0.017187	0.000000	2.740152
O	0.027082	0.000000	3.916645
O	-0.015968	0.000000	-1.016716

Molekuele/6Ph/BP86_TZ2P

	6.cs	BP86/TZ2P	
37			
E(SCF) =	-8.875689		
C	-0.096436	2.210983	0.000000
C	0.411811	3.381260	0.000000
O	0.807315	4.501932	0.000000
P	-0.021237	0.566295	0.000000
C	1.645896	-0.193141	0.000000
C	-0.879088	-0.118149	1.468252
C	-0.879088	-0.118149	-1.468252
C	-0.845850	-1.481823	-1.795437
C	-1.547887	-1.951266	-2.905822
C	-2.287820	-1.064645	-3.693790
C	-2.320029	0.293858	-3.372875
C	-1.617347	0.767406	-2.263512
C	-1.617347	0.767406	2.263512
C	-2.320029	0.293858	3.372875
C	-2.287820	-1.064645	3.693790
C	-1.547887	-1.951266	2.905822
C	-0.845850	-1.481823	1.795437
C	2.317148	-0.419961	-1.212064
C	3.631768	-0.887370	-1.209284
C	4.289702	-1.124601	0.000000
C	3.631768	-0.887370	1.209284
C	2.317148	-0.419961	1.212064
H	1.811522	-0.230446	-2.158917
H	1.811522	-0.230446	2.158917
H	4.143293	-1.063976	2.154884
H	5.316637	-1.489882	0.000000
H	4.143293	-1.063976	-2.154884
H	-2.836548	-1.434324	4.559967
H	-0.261962	-2.179384	1.195304
H	-1.515542	-3.010749	3.157825
H	-2.891567	0.989048	3.986893
H	-1.623206	1.825432	1.998124
H	-1.623206	1.825432	-1.998124
H	-0.261962	-2.179384	-1.195304
H	-1.515542	-3.010749	-3.157825
H	-2.836548	-1.434324	-4.559967
H	-2.891567	0.989048	-3.986893

Molekuele/6Ph/RI-BP86_SVP

	6 (135°)	RI-BP86/SVP	
37			
E(SCF) =	-1187.061505		
C	3.194092	1.181797	-0.354579

P	3.338156	2.323235	0.867313
C	3.575213	-0.049962	-0.510218
O	3.880619	-1.173594	-0.756036
C	2.044681	2.162356	2.178519
C	4.947411	2.341329	1.769695
C	3.120771	4.005600	0.152213
C	2.788312	6.535138	-1.032983
C	2.892098	5.389262	-1.839194
C	3.056941	4.124930	-1.249732
C	5.226416	1.298680	2.682104
C	6.484679	1.218469	3.296882
C	7.476747	2.170792	3.002621
C	7.207139	3.203006	2.089368
C	5.948023	3.289877	1.471849
C	0.846979	1.500888	1.838019
C	-0.182971	1.381211	2.784192
C	-0.022014	1.915226	4.074472
C	1.173791	2.567366	4.420074
C	2.207064	2.692658	3.476410
C	3.010429	5.156373	0.961413
C	2.846534	6.417459	0.367240
H	2.656757	7.525213	-1.496053
H	2.841461	5.478187	-2.935209
H	3.130918	3.207667	-1.856809
H	4.457292	0.544370	2.910688
H	6.693219	0.404586	4.007985
H	8.464070	2.104640	3.484695
H	7.982268	3.947764	1.852295
H	5.744281	4.098270	0.753720
H	0.743394	1.073469	0.827875
H	-1.115166	0.862095	2.513658
H	-0.828864	1.816180	4.816793
H	1.307359	2.976135	5.433458
H	3.148341	3.187665	3.761610
H	3.044722	5.073630	2.058469
H	2.758796	7.313018	1.001175

6 RI-BP86/SVP

37			
E(SCF) =	-1186.871967		
C	3.145592	0.944659	-0.067630
P	3.312592	2.225341	0.954425
C	3.015719	-0.050914	-0.860505
O	2.894347	-0.980577	-1.600539
C	2.069000	2.230750	2.322583
C	4.963312	2.282724	1.785424

C	3.126950	3.860022	0.110690
C	2.883015	6.319540	-1.287799
C	3.402389	5.170763	-1.947183
C	3.518997	3.945264	-1.245844
C	5.614821	1.051689	2.032878
C	6.881717	1.029040	2.666658
C	7.505579	2.248789	3.050312
C	6.853069	3.484663	2.790697
C	5.583265	3.497367	2.159597
C	0.802482	1.658716	2.058285
C	-0.193549	1.632692	3.065502
C	0.081826	2.177625	4.350576
C	1.359106	2.742051	4.616276
C	2.348483	2.767443	3.600709
C	2.604114	4.998051	0.767409
C	2.479981	6.227799	0.072264
H	2.784173	7.270028	-1.830521
H	3.704056	5.232436	-3.001783
H	3.895602	3.053713	-1.766073
H	5.148431	0.109263	1.714018
H	7.386796	0.071463	2.853587
H	8.491596	2.235701	3.535450
H	7.338622	4.429482	3.070934
H	5.108703	4.463864	1.946016
H	0.595186	1.212830	1.075662
H	-1.174711	1.184047	2.858057
H	-0.685652	2.152602	5.136764
H	1.581103	3.149373	5.612161
H	3.336143	3.185198	3.835118
H	2.263482	4.943080	1.809434
H	2.063604	7.108392	0.580377

Molekuele/PHCP-R

	PHCDP_C__h	RI-BP86/SVP	
11			
E(SCF) =	-800.259336		
C	0.333693	0.151046	0.681690
P	0.127733	-1.253710	1.572150
P	0.018537	1.338930	1.821074
H	-0.871878	-2.228605	1.184649
H	1.218911	-2.192795	1.722169
H	-1.061147	2.282915	1.618073
H	1.030216	2.321449	2.155965
C	-0.391312	0.530312	3.467789
H	-0.641062	1.063470	4.400255
C	-0.334347	-0.809817	3.339339

H	-0.530796	-1.528807	4.151849
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PHCDP_C__iPr_PhRI-BP86/SVP

101

E(SCF) = -2195.250105

C	0.160912	0.028433	0.560429
P	-0.105861	-1.363047	1.455798
P	0.104714	1.320957	1.637294
N	-1.414910	-2.323368	0.819249
N	1.250468	-2.441743	1.719693
N	-1.046421	2.559549	1.211068
N	1.582495	2.205451	1.890379
C	-0.411649	0.528887	3.338510
C	-0.534408	-0.815241	3.166606
C	-0.735968	1.163769	4.642762
C	-1.399527	2.266612	7.179956
C	-0.073130	0.739738	5.823120
C	-1.741936	2.152520	4.769013
C	-2.072129	2.691683	6.022145
C	-0.397801	1.286664	7.073549
H	0.710961	-0.028543	5.745779
H	-2.287222	2.479475	3.872847
H	-2.868172	3.448966	6.093489
H	0.135038	0.941476	7.973217
H	-1.656956	2.694281	8.160907
C	-1.818751	-3.548270	1.543020
H	-1.016686	-3.716858	2.288287
C	-1.855054	-4.830052	0.688818
H	-0.896659	-4.991437	0.158601
H	-2.666148	-4.808761	-0.065320
H	-2.038277	-5.708878	1.340879
C	-3.120417	-3.393689	2.363790
H	-3.106589	-2.452338	2.947682
H	-3.226528	-4.239872	3.074929
H	-4.024326	-3.384102	1.725714
C	-2.009702	-1.923316	-0.481802
H	-1.764444	-0.844101	-0.548809
C	-3.540441	-2.054097	-0.554441
H	-3.883306	-3.108604	-0.582366
H	-3.899454	-1.575805	-1.488699
H	-4.039550	-1.549776	0.294057
C	-1.339635	-2.570503	-1.711130
H	-0.253878	-2.355362	-1.715889
H	-1.764731	-2.138451	-2.641373
H	-1.483515	-3.667969	-1.758752
C	2.224547	2.200790	3.231172

H	1.392966	2.316682	3.955598
C	3.162150	3.399335	3.465878
H	3.451109	3.424818	4.536114
H	2.683186	4.367408	3.223515
H	4.101370	3.319727	2.881466
C	2.952607	0.893381	3.610946
H	3.103948	0.843246	4.709718
H	3.952401	0.817480	3.139471
H	2.363787	0.012426	3.296682
C	2.458064	2.485179	0.710434
H	3.063435	3.366836	1.013415
C	3.432793	1.347279	0.346235
H	4.135746	1.110878	1.166264
H	4.039712	1.638287	-0.536283
H	2.857350	0.435677	0.094048
C	1.687262	2.908616	-0.548860
H	2.416785	3.221505	-1.323295
H	1.007231	3.755643	-0.353813
H	1.093219	2.067522	-0.955453
C	-2.289915	2.167053	0.465379
H	-2.911801	3.085833	0.479141
C	-3.143122	1.110963	1.187206
H	-2.628041	0.136457	1.263612
H	-4.096581	0.958256	0.640714
H	-3.399266	1.444154	2.213443
C	-2.026650	1.856736	-1.016775
H	-1.310856	1.017817	-1.114682
H	-1.588231	2.739159	-1.524455
H	-2.975061	1.599190	-1.533096
C	-1.192178	3.952539	1.746074
H	-2.189469	3.974451	2.252912
C	-0.180318	4.434215	2.786371
H	-0.079412	3.745255	3.644091
H	-0.537631	5.405676	3.185404
H	0.817522	4.588526	2.341112
C	-1.257374	5.005197	0.616093
H	-0.266293	5.141502	0.139712
H	-1.566099	5.984613	1.036163
H	-1.982181	4.742658	-0.178112
C	1.356835	-3.295747	2.930310
H	0.374760	-3.201667	3.438511
C	2.388751	-2.822998	3.976956
H	2.233531	-1.758408	4.231061
H	3.432436	-2.944179	3.631090
H	2.275801	-3.417450	4.907778
C	1.546754	-4.799533	2.646572

H	2.555462	-5.017934	2.243811
H	0.799434	-5.184701	1.927061
H	1.442807	-5.373342	3.590504
C	2.219846	-2.513986	0.597463
H	1.973129	-1.607388	-0.000060
C	3.690805	-2.367430	1.022690
H	4.323493	-2.237080	0.120909
H	4.068809	-3.265052	1.554353
H	3.839381	-1.484760	1.672479
C	2.050059	-3.725546	-0.346517
H	2.603574	-3.543390	-1.291383
H	0.986601	-3.880604	-0.607334
H	2.442730	-4.666762	0.085429
H	-0.916642	-1.460519	3.975891

PHCDP_C__Me RI-BP86/SVP

23

E(SCF) =	-957.454091		
C	0.310176	0.145495	0.751552
P	0.117293	-1.259824	1.648969
P	-0.008126	1.370979	1.853444
C	-1.191492	-2.456145	1.105753
C	1.585739	-2.379188	1.821089
C	-1.428326	2.507252	1.491313
C	1.348706	2.584605	2.207071
C	-0.412617	0.574130	3.508324
H	-0.667342	1.111053	4.439097
C	-0.348713	-0.769409	3.403891
H	-0.544867	-1.465065	4.238660
H	1.370640	-3.271842	2.443012
H	1.890499	-2.703199	0.805905
H	2.417842	-1.799695	2.264847
H	-1.257679	-3.344194	1.766762
H	-2.163124	-1.926488	1.084232
H	-0.950733	-2.782838	0.074374
H	-1.573416	3.272898	2.280424
H	-1.227223	3.009867	0.524171
H	-2.345528	1.897522	1.381539
H	1.054302	3.345741	2.958021
H	2.235517	2.025286	2.561822
H	1.613610	3.089538	1.256623

PHCDP_C__NH2 RI-BP86/SVP

19

E(SCF) =	-1021.630908		
C	0.288290	0.134917	0.841864

P	0.029508	-1.269325	1.716761
P	0.037862	1.354122	1.962151
N	-1.138361	-2.312541	1.040052
N	1.215245	-2.500438	1.985276
N	-1.184752	2.572744	1.841772
N	1.340711	2.444898	2.115178
C	-0.410769	0.555841	3.602659
H	-0.655462	1.109452	4.526084
C	-0.393522	-0.786767	3.482630
H	-0.594324	-1.501758	4.299642
H	1.481923	-2.919296	1.082509
H	2.063910	-2.097355	2.405327
H	-1.406044	-3.134975	1.590935
H	-1.940780	-1.819389	0.638799
H	1.277616	3.146323	2.860546
H	2.257678	1.992159	2.066900
H	-1.006598	3.152803	1.009066
H	-2.112578	2.141827	1.729210

PHCDP_C__NMe2 RI-BP86/SVP

43

E(SCF) =	-1335.843585		
C	0.282231	0.060647	1.076952
P	-0.103396	-1.281319	2.004291
P	0.228582	1.331701	2.168178
N	-1.490086	-2.142302	1.474786
N	0.987283	-2.622661	2.190835
N	-0.862093	2.672831	1.975199
N	1.696435	2.206565	2.320213
C	-0.261178	0.637148	3.840124
H	-0.412758	1.227956	4.760180
C	-0.360333	-0.707679	3.771265
H	-0.594405	-1.361207	4.629505
C	2.166848	-2.385854	3.016599
C	1.298814	-3.356795	0.964178
C	-1.997443	-3.293649	2.204606
C	-2.429184	-1.505761	0.566428
C	1.837729	3.303508	3.264793
C	2.936995	1.622024	1.839285
C	-2.273741	2.398039	2.221801
C	-0.649481	3.490369	0.780746
H	2.957574	-1.792167	2.495423
H	1.892279	-1.842732	3.942071
H	2.613635	-3.359536	3.312881
H	2.055174	-2.835356	0.329306
H	1.696508	-4.362628	1.221254

H	0.378762	-3.486766	0.363710
H	-2.326435	-4.091820	1.500520
H	-1.196340	-3.713047	2.842263
H	-2.874602	-3.037255	2.847485
H	-2.740551	-2.218193	-0.230867
H	-3.354235	-1.155971	1.086274
H	-1.931240	-0.634815	0.096059
H	3.535885	2.382133	1.288036
H	3.572776	1.229552	2.669977
H	2.692026	0.789073	1.150791
H	2.410145	4.143937	2.809560
H	0.837698	3.686191	3.543426
H	2.379804	2.998174	4.192862
H	-1.067829	3.022422	-0.142842
H	-1.132641	4.482519	0.915708
H	0.434470	3.647132	0.624141
H	-2.769294	1.849826	1.383098
H	-2.398412	1.792514	3.140884
H	-2.817921	3.356016	2.368919

PHCDP_h RI-BP86/SVP

10			
E(SCF) =	-816.302382		
C	0.327544	0.148924	0.682915
P	0.121629	-1.221665	1.608554
P	0.025312	1.370874	1.784050
H	-0.902867	-2.186114	1.293249
H	1.208316	-2.142747	1.827831
H	-1.059214	2.310023	1.586747
H	1.038143	2.352253	2.116335
C	-0.375623	0.441616	3.443455
H	-0.628289	0.940890	4.401614
N	-0.325856	-0.829108	3.347894

PHCDP_iPrCyc_PhRI-BP86/SVP

86			
E(SCF) =	-2052.984421		
C	0.588789	-0.279171	0.842269
P	-0.280797	-1.435316	1.672416
P	0.424363	1.143970	1.726478
N	-1.826287	-2.082145	1.073676
N	0.368075	-3.022141	1.839302
N	-0.579287	2.370036	1.013564
N	1.863413	2.016628	2.202747
C	-0.400528	0.420666	3.453458
N	-0.734508	-0.811762	3.288499

C	-0.704639	1.098784	4.741417
C	-1.304618	2.319465	7.229127
C	-0.233776	2.395899	5.046005
C	-1.479718	0.419513	5.717638
C	-1.778800	1.024920	6.943107
C	-0.528412	3.000445	6.277522
H	0.379816	2.926465	4.305624
H	-1.834647	-0.593472	5.480439
H	-2.385986	0.484668	7.685849
H	-0.147799	4.010182	6.495137
H	-1.539749	2.794625	8.194026
C	-2.874306	-2.433793	2.092119
H	-2.384247	-2.756219	3.040757
C	-3.787565	-3.581197	1.632966
H	-3.261254	-4.550973	1.537363
H	-4.277723	-3.347564	0.664575
H	-4.590192	-3.720972	2.384581
C	-3.737196	-1.201490	2.398163
H	-3.119392	-0.343112	2.718223
H	-4.452298	-1.426007	3.216563
H	-4.313787	-0.898871	1.500629
C	-1.350206	-3.170108	0.200236
H	-0.839953	-2.701925	-0.668806
C	2.625565	1.433495	3.347304
H	1.882391	0.868516	3.948999
C	3.211857	2.527840	4.258503
H	3.667082	2.069130	5.159745
H	2.441367	3.247953	4.592848
H	4.012042	3.101047	3.745762
C	3.726525	0.433344	2.943214
H	4.133643	-0.070652	3.843285
H	4.576248	0.937926	2.439590
H	3.325947	-0.338389	2.260888
C	2.752292	2.677114	1.189410
H	3.715601	2.798047	1.726533
C	3.054067	1.843431	-0.068158
H	3.420928	0.831849	0.182394
H	3.826542	2.358768	-0.676798
H	2.154099	1.712884	-0.695907
C	2.306217	4.094961	0.814667
H	3.114763	4.609780	0.255606
H	2.072071	4.695928	1.715303
H	1.411558	4.067877	0.166735
C	-1.350139	2.130782	-0.250635
H	-1.826170	3.113950	-0.443463
C	-2.491775	1.105893	-0.148682

H	-2.118459	0.075161	0.006529
H	-3.086196	1.118503	-1.086896
H	-3.181103	1.347093	0.682544
C	-0.451522	1.848070	-1.464247
H	0.088490	0.889600	-1.334946
H	0.286086	2.661362	-1.615666
H	-1.074924	1.782908	-2.379809
C	-1.042721	3.517102	1.843009
H	-0.261415	3.633982	2.620421
C	-1.110957	4.862474	1.089908
H	-0.195387	5.074355	0.510100
H	-1.244382	5.682429	1.824859
H	-1.977364	4.912593	0.399536
C	-2.397898	3.274946	2.540427
H	-3.230162	3.288687	1.807411
H	-2.598339	4.073637	3.284093
H	-2.425655	2.306004	3.072730
C	1.703839	-3.390288	2.339097
H	1.649818	-4.489469	2.516011
C	1.987197	-2.742152	3.699891
H	1.186855	-2.988695	4.424371
H	2.039984	-1.640271	3.614086
H	2.956866	-3.095959	4.104991
C	2.812817	-3.131564	1.301815
H	2.837581	-2.057539	1.030401
H	2.626334	-3.703584	0.370050
H	3.806588	-3.436200	1.690290
C	-0.324629	-4.000365	0.996766
H	0.383440	-4.513072	0.306461
H	-2.186127	-3.774056	-0.195908
H	-0.814947	-4.791268	1.615201

PHCDP_iPr_Ph RI-BP86/SVP

100

E(SCF) =	-2211.303549		
C	0.189815	0.065696	0.486712
P	-0.060286	-1.315903	1.397179
P	0.111971	1.350729	1.567559
N	-1.375691	-2.283998	0.823177
N	1.292848	-2.363476	1.720766
N	-1.047260	2.590568	1.153856
N	1.573848	2.244178	1.871082
C	-0.423427	0.386909	3.255219
N	-0.494084	-0.887728	3.071310
C	-0.757293	0.957353	4.585648
C	-1.409825	1.962318	7.153208

C	-0.343455	0.276288	5.757560
C	-1.514732	2.143158	4.726340
C	-1.845395	2.634382	5.999461
C	-0.656211	0.780980	7.026546
H	0.229095	-0.656134	5.648912
H	-1.873979	2.662654	3.828313
H	-2.450791	3.549433	6.088921
H	-0.316387	0.245061	7.926312
H	-1.660858	2.354863	8.150512
C	-1.778561	-3.479072	1.602735
H	-0.943310	-3.654185	2.305640
C	-1.900123	-4.776385	0.781778
H	-0.976010	-4.983004	0.207514
H	-2.748547	-4.752187	0.070196
H	-2.073854	-5.631745	1.466574
C	-3.018069	-3.248149	2.493751
H	-2.884091	-2.326208	3.092008
H	-3.143065	-4.098623	3.196702
H	-3.953748	-3.160498	1.909576
C	-2.011886	-1.912389	-0.469112
H	-1.765782	-0.837386	-0.574429
C	-3.544943	-2.034227	-0.491840
H	-3.896483	-3.085513	-0.473560
H	-3.926627	-1.584165	-1.431107
H	-4.015643	-1.497948	0.352875
C	-1.381893	-2.601194	-1.696616
H	-0.295029	-2.394700	-1.739147
H	-1.830936	-2.195452	-2.627337
H	-1.534035	-3.698401	-1.704459
C	2.155562	2.234080	3.239914
H	1.290563	2.344838	3.926613
C	3.082243	3.430560	3.521883
H	3.330657	3.445022	4.602412
H	2.614320	4.401115	3.269899
H	4.043036	3.354270	2.973218
C	2.865680	0.924587	3.643774
H	2.954608	0.858973	4.748219
H	3.889914	0.857546	3.225892
H	2.301329	0.044676	3.284754
C	2.493722	2.522380	0.726210
H	3.096497	3.396582	1.055715
C	3.470005	1.377874	0.388634
H	4.135379	1.125655	1.234987
H	4.115996	1.671191	-0.464881
H	2.897445	0.474245	0.103305
C	1.763584	2.961346	-0.551906

H	2.516151	3.259303	-1.309813
H	1.098043	3.823872	-0.372170
H	1.160738	2.133312	-0.973274
C	-2.322983	2.165257	0.483346
H	-2.961208	3.072101	0.516662
C	-3.118657	1.108975	1.268217
H	-2.602539	0.133028	1.314003
H	-4.107054	0.951679	0.789336
H	-3.305306	1.447910	2.307504
C	-2.126286	1.834220	-1.004563
H	-1.387860	1.017824	-1.123419
H	-1.741694	2.719294	-1.549843
H	-3.089468	1.535732	-1.468575
C	-1.174403	4.006163	1.630194
H	-2.142382	4.046219	2.192527
C	-0.112198	4.553458	2.585069
H	0.039870	3.920196	3.477411
H	-0.456642	5.547140	2.938563
H	0.861945	4.684685	2.083039
C	-1.317322	4.999467	0.453950
H	-0.365549	5.093064	-0.105568
H	-1.581466	6.004129	0.843344
H	-2.105065	4.706476	-0.265698
C	1.371336	-3.207085	2.947302
H	0.405786	-3.034954	3.463221
C	2.440288	-2.771010	3.971577
H	2.345880	-1.697386	4.213114
H	3.473838	-2.957779	3.623774
H	2.300311	-3.343729	4.912226
C	1.495430	-4.721351	2.684469
H	2.496896	-4.992426	2.294923
H	0.738485	-5.087551	1.965306
H	1.357474	-5.274641	3.636267
C	2.260601	-2.481789	0.598073
H	2.036923	-1.584554	-0.020524
C	3.733578	-2.362061	1.022575
H	4.368650	-2.256898	0.119201
H	4.090740	-3.261029	1.565514
H	3.901061	-1.475184	1.662031
C	2.059711	-3.709156	-0.318772
H	2.617660	-3.562064	-1.267063
H	0.992298	-3.842938	-0.575902
H	2.427979	-4.649659	0.135101

PHCDP_Me RI-BP86/SVP

E(SCF) =	-973.499953		
C	0.319308	0.152828	0.703595
P	0.127082	-1.238271	1.612104
P	0.005813	1.379719	1.799859
C	-1.208057	-2.423146	1.150123
C	1.582095	-2.342163	1.866677
C	-1.424511	2.519634	1.485576
C	1.350880	2.594849	2.198101
C	-0.388237	0.434925	3.440202
H	-0.648882	0.921926	4.405684
N	-0.329222	-0.838732	3.348336
H	1.343021	-3.174256	2.557392
H	1.895770	-2.746951	0.884328
H	2.412198	-1.736381	2.277395
H	-1.286678	-3.250099	1.882661
H	-2.164730	-1.869035	1.100968
H	-0.986963	-2.831394	0.144277
H	1.050061	3.304283	2.995862
H	2.252826	2.034518	2.510241
H	1.595053	3.164167	1.278716
H	-1.580253	3.235036	2.318759
H	-1.225004	3.085362	0.553303
H	-2.335883	1.910220	1.334382

	PHCDP_NH2	RI-BP86/SVP	
18			
E(SCF) =	-1037.676351		
C	0.335699	0.149763	0.712789
P	0.107330	-1.237206	1.625907
P	0.026853	1.375611	1.805655
N	-1.102827	-2.423016	1.343371
H	-1.081308	-2.727118	0.360656
H	-2.040379	-2.054614	1.550038
N	1.430420	-2.286585	1.653730
H	2.342979	-1.823691	1.662872
H	1.364168	-3.088765	2.288200
N	-1.192928	2.486020	1.359907
H	-1.462566	3.189512	2.055943
H	-1.997560	2.049273	0.901648
N	1.151663	2.581320	2.319649
H	1.312674	3.266174	1.567476
H	2.055958	2.160738	2.570376
C	-0.368749	0.450379	3.439493
H	-0.596821	0.960366	4.402190
N	-0.359805	-0.827052	3.354778

PHCDP_NMe2 RI-BP86/SVP

42

E(SCF) =	-1351.890118		
C	0.333102	0.012709	0.697945
P	0.090811	-1.330652	1.671373
P	0.230097	1.286506	1.778047
N	-1.240227	-2.406390	1.466506
N	1.375044	-2.445764	1.684487
N	-1.015486	2.424887	1.464547
N	1.531536	2.392447	2.088072
C	-0.050935	0.433562	3.471591
N	-0.193645	-0.839422	3.410908
H	-0.136569	0.966169	4.444504
C	-2.093071	2.075666	0.553371
H	-1.790651	1.184530	-0.031313
H	-2.294843	2.914841	-0.150434
H	-3.045303	1.849058	1.091157
C	-1.272505	3.556540	2.343082
H	-0.393460	3.734547	2.990606
H	-2.168903	3.393004	2.988606
H	-1.456699	4.482996	1.752058
C	1.902975	3.295108	0.998531
H	2.447928	4.174220	1.406505
H	0.992175	3.655658	0.484526
H	2.557230	2.804030	0.238584
C	2.688453	1.835171	2.780791
H	3.284061	2.657205	3.233379
H	3.364042	1.251466	2.108990
H	2.368273	1.162538	3.601466
C	2.684548	-2.060067	1.181839
H	3.410007	-1.853036	2.004850
H	2.575532	-1.148618	0.562285
H	3.110332	-2.875869	0.555344
C	1.341531	-3.642675	2.514186
H	1.973813	-3.534557	3.426438
H	1.717187	-4.522524	1.943881
H	0.301579	-3.848774	2.826085
C	-1.330290	-3.033318	0.148935
H	-0.317837	-3.311035	-0.202091
H	-1.791936	-2.368368	-0.619894
H	-1.940238	-3.960102	0.218961
C	-2.530804	-2.011570	2.021307
H	-2.397153	-1.645662	3.056935
H	-3.198818	-2.898917	2.052528
H	-3.047990	-1.219856	1.424697

PHCDP_NMe2Me RI-BP86/SVP

45

E(SCF) = -1391.185197

C	0.329171	0.016523	0.719207
P	0.090683	-1.326629	1.697291
P	0.214489	1.283970	1.804287
N	-1.235452	-2.408211	1.476581
N	1.378601	-2.439038	1.700088
N	-1.019544	2.433557	1.470532
N	1.528438	2.383965	2.116887
C	-0.086809	0.426595	3.517472
N	-0.201505	-0.850945	3.419031
C	-0.245187	1.168004	4.814300
H	0.580030	1.894091	4.963791
H	-0.292440	0.466089	5.669291
H	-1.181747	1.765562	4.791047
C	-2.089876	2.081734	0.551589
H	-1.787660	1.181159	-0.018555
H	-2.276738	2.913819	-0.164840
H	-3.050321	1.869467	1.080932
C	-1.273570	3.586561	2.318781
H	-0.394826	3.783657	2.960773
H	-2.170294	3.444264	2.970800
H	-1.460464	4.496846	1.703641
C	1.880046	3.314565	1.043177
H	2.459395	4.167612	1.459039
H	0.961871	3.710432	0.570999
H	2.496825	2.833562	0.246188
C	2.707115	1.777971	2.729670
H	3.329364	2.566232	3.206158
H	3.347288	1.231445	1.995357
H	2.415643	1.055613	3.517666
C	2.682749	-2.053189	1.185081
H	3.415603	-1.840588	2.000436
H	2.566228	-1.144779	0.562264
H	3.105467	-2.870708	0.558470
C	1.353335	-3.631749	2.535230
H	1.987605	-3.517567	3.445673
H	1.731062	-4.512960	1.968154
H	0.315132	-3.841333	2.851037
C	-1.312057	-3.026365	0.154438
H	-0.295708	-3.299152	-0.189075
H	-1.768125	-2.357510	-0.614593
H	-1.920479	-3.955102	0.212236
C	-2.532542	-2.020748	2.020121
H	-2.409779	-1.659723	3.058698

H	-3.198451	-2.910170	2.040087
H	-3.046776	-1.227564	1.422384

PA/Di_Prot/RI-BP86_SVP

(H+)2-5

RI-BP86/SVP

7

E(SCF) = -264.882049

C	0.148378	0.037282	0.147582
C	-0.668015	0.070851	1.377038
C	0.079993	0.054697	2.649587
O	0.576804	0.045000	3.657090
O	0.699795	0.014153	-0.830879
H	-1.316922	1.002927	1.352721
H	-1.375534	-0.817770	1.363891

(H+)2-3Ad

RI-BP86/SVP

117

E(SCF) = -2047.974675

C	-0.497907	-0.062876	-0.005182
C	0.322817	1.178402	-0.276062
C	0.165789	-1.348784	0.416249
N	-0.030438	2.097523	-1.225831
N	1.395184	1.669921	0.413289
N	1.142894	-2.043039	-0.239389
N	-0.193255	-2.061837	1.526753
C	0.848545	3.161439	-1.148651
C	1.736064	2.895503	-0.136938
C	1.423671	-3.185328	0.492813
C	0.595696	-3.194262	1.588194
H	0.777762	4.029879	-1.805344
H	2.580328	3.484377	0.222723
H	2.182761	-3.906919	0.190668
H	0.516139	-3.922328	2.396892
C	1.980680	1.070810	1.652472
H	1.650770	0.013896	1.611305
C	1.402175	1.695898	2.954730
C	3.532727	1.054092	1.733293
H	0.296299	1.778241	2.861275
C	2.016410	3.084459	3.245438
C	1.763327	0.722711	4.104980
H	3.946882	0.670204	0.776026
C	4.157953	2.427929	2.082736
C	3.878652	0.073371	2.887831
H	1.568401	3.482129	4.179597
H	1.750120	3.816495	2.452709
C	3.551057	2.966090	3.396326

H	1.304891	-0.275006	3.924361
H	1.333200	1.103578	5.054276
C	3.298065	0.597617	4.222551
H	4.055963	3.167626	1.262609
H	5.252693	2.287251	2.199118
H	3.485252	-0.943030	2.664513
H	4.981234	-0.024449	2.960254
H	3.977291	3.965826	3.618385
C	3.890521	1.987825	4.542034
H	3.549335	-0.114178	5.035919
H	4.990901	1.917613	4.669660
H	3.483850	2.363602	5.504185
C	-1.268680	2.026417	-2.078468
H	-2.032443	1.608427	-1.390116
C	-1.147076	1.082850	-3.304957
C	-1.814396	3.404933	-2.545529
H	-0.680696	0.120765	-2.994039
C	-0.308014	1.726539	-4.431616
C	-2.590088	0.819180	-3.803796
H	-1.845704	4.101063	-1.679746
C	-1.021520	4.024256	-3.724975
C	-3.262012	3.131407	-3.040839
H	-0.224829	1.007722	-5.273198
H	0.731183	1.925445	-4.086822
C	-0.976614	3.036429	-4.907942
H	-3.192361	0.331325	-3.005795
H	-2.558726	0.109816	-4.656529
C	-3.239850	2.151479	-4.237412
H	0.011108	4.323317	-3.449899
H	-1.528577	4.964510	-4.024927
H	-3.883889	2.725151	-2.213891
H	-3.726489	4.093553	-3.338846
H	-0.378880	3.475214	-5.732938
C	-2.414512	2.754790	-5.394652
H	-4.279762	1.961296	-4.573750
H	-2.883424	3.694365	-5.753886
H	-2.400737	2.057920	-6.259005
C	1.731187	-1.667566	-1.562163
H	1.313980	-0.658015	-1.754902
C	1.274485	-2.595146	-2.725707
C	3.279764	-1.535829	-1.582414
H	0.173363	-2.738391	-2.668030
C	1.998437	-3.961728	-2.700016
C	1.642899	-1.860263	-4.040395
H	3.605468	-0.923870	-0.713572
C	4.005467	-2.903051	-1.583182

C	3.629711	-0.801096	-2.904111
H	1.648309	-4.559992	-3.566645
H	1.719263	-4.556818	-1.805010
C	3.528831	-3.754328	-2.781495
H	1.111462	-0.886137	-4.101784
H	1.294239	-2.465945	-4.902183
C	3.170492	-1.645181	-4.115412
H	3.877452	-3.445832	-0.623868
H	5.096950	-2.716684	-1.660955
H	3.153039	0.203768	-2.927203
H	4.725602	-0.632277	-2.944471
H	4.036222	-4.740537	-2.758957
C	3.879871	-3.016947	-4.092454
H	3.421347	-1.107630	-5.053121
H	4.978974	-2.883540	-4.173522
H	3.568911	-3.622450	-4.969291
C	-1.276271	-1.674351	2.492457
H	-1.102728	-0.590160	2.665280
C	-1.196278	-2.363593	3.881690
C	-2.707927	-1.861076	1.912345
H	-0.159000	-2.286222	4.274549
C	-1.674068	-3.839420	3.876140
C	-2.156796	-1.559215	4.801416
H	-2.754930	-1.444984	0.881990
C	-3.116295	-3.351283	1.884951
C	-3.663870	-1.065708	2.835768
H	-1.639594	-4.215572	4.919491
H	-1.008337	-4.512129	3.297380
C	-3.108968	-3.928674	3.318062
H	-1.828625	-0.499219	4.870641
H	-2.100969	-1.973936	5.828590
C	-3.605266	-1.645719	4.265631
H	-2.435802	-3.936376	1.227393
H	-4.127616	-3.436339	1.436353
H	-3.390738	0.013019	2.839542
H	-4.696543	-1.130214	2.434941
H	-3.427442	-4.990818	3.289046
C	-4.061950	-3.120433	4.224707
H	-4.275453	-1.060807	4.928593
H	-5.103931	-3.187515	3.847291
H	-4.068161	-3.550605	5.247849
H	-1.089372	-0.262186	-0.921509
H	-1.248244	0.180755	0.775267

(H+)2-3Me

RI-BP86/SVP

E(SCF) =	-648.042303		
C	1.008920	2.608246	1.898302
C	0.582707	1.236536	2.357376
C	1.459756	2.774957	0.468826
N	1.031977	0.611048	3.481027
N	-0.387411	0.450246	1.813916
N	2.447057	2.087626	-0.169467
N	1.018236	3.740480	-0.384688
C	0.344430	-0.579921	3.640666
C	-0.543031	-0.682247	2.595688
C	2.620773	2.617390	-1.437096
C	1.727750	3.654172	-1.570365
C	2.035839	1.118964	4.432706
H	0.535601	-1.258642	4.479107
H	-1.267615	-1.467166	2.352371
C	-1.208745	0.764476	0.635615
C	3.252292	0.993505	0.392307
H	3.360547	2.221292	-2.141455
H	1.547210	4.332292	-2.411628
C	0.001618	4.769199	-0.103231
H	-1.809921	-0.125177	0.378929
H	-1.898832	1.600705	0.860794
H	-0.568862	1.014332	-0.230577
H	2.243027	0.327372	5.173431
H	2.980845	1.363214	3.913087
H	1.648856	2.008565	4.965647
H	3.968446	0.655112	-0.376576
H	3.826792	1.350991	1.268177
H	2.609959	0.138009	0.672895
H	-0.203404	5.319113	-1.038002
H	-0.941258	4.304194	0.239391
H	0.374699	5.485337	0.653793
H	1.821261	2.953199	2.573096
H	0.174952	3.320503	2.074225

	(H+)2-4Me	RI-BP86/SVP	
41			
E(SCF) =	-652.807050		
C	0.153519	-0.098415	0.023426
C	-0.419297	0.021003	-1.386961
C	0.239748	1.112443	0.949493
N	0.142099	-0.724325	-2.359935
N	-1.510161	0.778586	-1.619912
N	0.614005	2.315446	0.469016
N	0.022564	0.915741	2.265344
C	-0.631514	-1.270107	-3.497009

H	-0.400604	-0.751632	-4.448173
H	-1.713015	-1.224416	-3.290758
H	-0.347813	-2.335167	-3.607426
C	1.531175	-1.225044	-2.319539
H	1.923770	-1.235508	-3.354212
H	1.572558	-2.260864	-1.924101
H	2.193612	-0.570446	-1.726426
C	-2.472509	1.145415	-0.570273
H	-2.286553	0.594001	0.365331
H	-3.492990	0.879392	-0.913106
H	-2.450859	2.236681	-0.376565
C	0.268345	3.594647	1.120239
H	1.135203	4.052055	1.636550
H	-0.561883	3.457021	1.832449
H	-0.061258	4.294691	0.327266
C	1.382336	2.480501	-0.773939
H	0.776151	2.989742	-1.549912
H	1.750520	1.515598	-1.157969
H	2.269024	3.112433	-0.563946
C	0.708942	1.699871	3.315727
H	1.579462	2.231881	2.899222
H	1.076295	0.982229	4.075345
H	0.027638	2.414383	3.817915
C	-0.776136	-0.199419	2.813193
H	-1.297408	0.162852	3.719787
H	-0.127972	-1.051322	3.105082
H	-1.552000	-0.543394	2.106893
C	-1.839622	1.345058	-2.942931
H	-0.955830	1.334754	-3.601890
H	-2.149886	2.397278	-2.787754
H	-2.679542	0.812967	-3.431452
H	-0.415544	-0.898462	0.538650
H	1.172862	-0.529527	-0.043682

	(H+)2-3H	RI-BP86/SVP	
21			
E(SCF) =	-490.893399		
C	0.843258	2.662179	1.879247
C	0.540162	1.262103	2.352212
C	1.325574	2.820654	0.458769
N	0.999991	0.693411	3.491479
N	-0.312195	0.360412	1.808266
N	2.396046	2.237182	-0.132158
N	0.819565	3.677158	-0.459483
C	0.442793	-0.559685	3.673249
C	-0.391769	-0.773793	2.598576

C	2.567135	2.721128	-1.418154
C	1.563452	3.641454	-1.625298
H	1.648523	1.140818	4.151900
H	0.677892	-1.191920	4.537277
H	-1.025011	-1.630612	2.341000
H	-0.850637	0.500449	0.945258
H	3.017328	1.551415	0.312950
H	3.375592	2.380546	-2.075333
H	1.326768	4.262086	-2.497281
H	0.013543	4.296327	-0.304892
H	1.596471	3.102013	2.568610
H	-0.064411	3.291523	2.005789

(H+)-2-1Cl RI-BP86/SVP

11			
E(SCF) =	-3481.898420		
C	-0.302094	0.053476	0.961100
P	-0.186071	-1.602414	0.121369
P	-0.136309	1.686613	0.085964
H	0.479364	0.048763	1.757508
Cl	-0.279500	3.051590	1.514954
Cl	-1.604964	1.903589	-1.230953
Cl	1.628193	1.803886	-0.815255
Cl	-0.513800	-2.929103	1.556020
Cl	-1.569497	-1.750084	-1.294145
Cl	1.625726	-1.847672	-0.650250
H	-1.297394	0.075432	1.465001

(H+)-2-1Cy RI-BP86/SVP

107			
E(SCF) =	-2132.005146		
C	-0.099508	-0.187071	-0.841663
P	1.711175	-0.092647	-0.323261
P	-1.794848	0.079892	-0.091890
C	-2.965769	-0.417822	-1.485860
C	-3.563662	-0.210547	-3.950147
C	-4.540327	-2.090301	-2.564595
C	-4.082985	-1.654367	-3.962494
C	-3.444035	-1.889353	-1.497001
C	-2.454417	-0.019158	-2.896365
H	-4.398388	0.492422	-3.734484
H	-5.441332	-1.509692	-2.266595
H	-3.278005	-2.334157	-4.320788
H	-2.585606	-2.561451	-1.718843
H	-1.596873	-0.672654	-3.168822
H	-3.849411	0.218825	-1.247603

H	-3.167565	0.075701	-4.945723
H	-4.847732	-3.155775	-2.564819
H	-4.915911	-1.756269	-4.686743
H	-3.843506	-2.185448	-0.508101
H	-2.088577	1.027512	-2.922610
C	-2.293651	1.824383	0.360084
C	-2.168635	3.770246	1.992456
C	-3.043872	4.146851	-0.349017
C	-2.281531	4.764767	0.829847
C	-2.416328	2.818347	-0.819913
C	-1.526479	2.439897	1.550175
H	-3.179601	3.564211	2.408419
H	-4.100568	3.962370	-0.054233
H	-1.263477	5.070215	0.499061
H	-1.410188	3.017463	-1.246473
H	-0.474392	2.625101	1.246286
H	-3.332780	1.606588	0.707713
H	-1.575014	4.198932	2.825354
H	-3.082668	4.847887	-1.207331
H	-2.785335	5.692703	1.167379
H	-3.037255	2.395387	-1.633212
H	-1.497518	1.740231	2.410180
C	-1.968350	-0.959432	1.447469
C	-3.440923	-1.607685	3.420111
C	-1.614523	-3.176177	2.639492
C	-3.012771	-3.072702	3.264706
C	-1.538490	-2.438874	1.287472
C	-3.378246	-0.838288	2.085331
H	-2.783318	-1.101616	4.161560
H	-0.863245	-2.745814	3.339709
H	-3.746379	-3.612096	2.625493
H	-2.202210	-2.951364	0.564335
H	-4.140571	-1.248686	1.388513
H	-1.241982	-0.471500	2.139821
H	-4.471056	-1.538316	3.824264
H	-1.327673	-4.236899	2.488572
H	-3.030349	-3.582731	4.248689
H	-0.509439	-2.508858	0.876912
H	-3.646494	0.222804	2.262509
C	2.456726	-1.477678	-1.359892
C	4.596057	-2.573152	-2.203346
C	2.419465	-3.858355	-2.249360
C	3.943166	-3.956361	-2.095586
C	1.804327	-2.875949	-1.230789
C	3.996359	-1.567980	-1.198376
H	4.466630	-2.175429	-3.234162

H	2.166629	-3.522547	-3.279593
H	4.190032	-4.412274	-1.111197
H	1.955947	-3.273150	-0.205810
H	4.241195	-1.892818	-0.163610
H	2.245719	-1.102753	-2.390626
H	5.689674	-2.637452	-2.031915
H	1.944654	-4.852239	-2.120760
H	4.360801	-4.637953	-2.863536
H	0.705995	-2.835196	-1.394406
H	4.471057	-0.578391	-1.348291
C	2.439572	1.490722	-1.049767
C	2.131729	3.840271	-1.966889
C	4.403513	3.104020	-1.133440
C	3.445169	4.288181	-1.311934
C	3.746281	1.950233	-0.349707
C	1.466292	2.681305	-1.196442
H	2.326336	3.512773	-3.012260
H	4.733350	2.730464	-2.127982
H	3.231042	4.746446	-0.320857
H	3.508635	2.302314	0.677019
H	1.156813	3.036832	-0.189273
H	2.704625	1.150208	-2.078138
H	1.416960	4.685602	-2.036225
H	5.323847	3.418268	-0.600682
H	3.923380	5.081444	-1.920789
H	4.468337	1.116112	-0.243736
H	0.542521	2.378081	-1.730593
C	2.206856	-0.224762	1.467255
C	2.282091	0.875307	3.755420
C	2.757175	-1.601950	3.521160
C	2.187912	-0.501615	4.426991
C	2.090254	-1.615506	2.130094
C	1.610813	0.879612	2.367974
H	3.349584	1.166994	3.642833
H	3.852506	-1.453338	3.395790
H	1.123615	-0.727128	4.663537
H	1.020234	-1.890799	2.237172
H	0.522792	0.692496	2.490202
H	3.295092	-0.010086	1.345257
H	1.814597	1.657167	4.388086
H	2.634979	-2.600265	3.988279
H	2.721486	-0.491262	5.398557
H	2.563146	-2.395168	1.502215
H	1.711799	1.879831	1.899576
H	-0.193818	-1.238759	-1.187819
H	-0.116207	0.423957	-1.768093

-----	(H+)2-1F	RI-BP86/SVP	
11			
E(SCF) =	-1319.826481		
C	-0.079485	0.153890	-0.720978
P	-1.640596	0.089319	0.225876
P	1.559536	0.020045	0.075102
F	-1.708202	-1.180238	1.091754
F	-2.786818	0.080748	-0.792916
F	-1.775284	1.316902	1.140761
F	1.696225	1.030715	1.226809
F	1.779315	-1.395112	0.632839
F	2.612737	0.317908	-0.999086
H	-0.132401	-0.661084	-1.490283
H	-0.087325	1.122030	-1.288001

-----	(H+)2-1H	RI-BP86/SVP	
11			
E(SCF) =	-724.733361		
C	-0.132712	0.000030	1.100518
P	-0.867661	-1.624784	1.610958
P	-0.867795	1.624760	1.610960
H	-0.093268	0.000046	-0.014495
H	0.925984	0.000046	1.452658
H	-0.048156	-2.641321	1.042669
H	-2.196165	-1.773144	1.122329
H	-0.875057	-1.772578	3.026475
H	-0.048136	2.641353	1.042995
H	-0.875547	1.772461	3.026487
H	-2.196168	1.773131	1.121987

-----	(H+)2-1H2Me	RI-BP86/SVP	
17			
E(SCF) =	-803.377256		
C	0.000040	0.473160	0.000113
P	1.612581	-0.445436	0.000245
P	-1.612527	-0.445320	-0.000248
H	1.631361	-1.300947	1.136834
H	1.631014	-1.301759	-1.135736
C	3.028171	0.676938	-0.000306
C	-3.028314	0.676804	0.000219
H	-1.631054	-1.300740	-1.136905
H	-1.631155	-1.301749	1.135650
H	-3.946740	0.050342	-0.000286
H	-3.013562	1.306257	0.913320
H	-3.013329	1.307388	-0.912095

H	3.946777	0.050740	0.000038
H	3.013152	1.306508	-0.913319
H	3.013136	1.307386	0.912105
H	0.000219	1.138290	-0.893507
H	-0.000012	1.138210	0.893794

(H+)2-1HMe2 RI-BP86/SVP

23

E(SCF) =	-882.005335		
C	0.000516	-0.661131	0.356473
P	-1.628595	-0.049492	-0.296711
P	1.632060	-0.062910	-0.301837
C	-2.911284	-1.234921	0.178880
H	-1.510709	-0.056250	-1.715243
C	-2.022876	1.632907	0.243791
C	2.916787	-1.218537	0.237329
H	1.528560	-0.130734	-1.719824
C	2.010072	1.644201	0.168318
H	3.883249	-0.888766	-0.198544
H	2.995643	-1.211474	1.343621
H	2.691116	-2.242461	-0.122226
H	-3.013961	1.902264	-0.178621
H	-2.083919	1.672018	1.350486
H	-1.277601	2.363930	-0.124574
H	-3.876323	-0.890019	-0.248339
H	-2.677738	-2.240052	-0.225817
H	-2.998056	-1.279137	1.283733
H	3.008913	1.897041	-0.246080
H	1.271309	2.354091	-0.251216
H	2.048410	1.736357	1.272829
H	0.002552	-0.514152	1.460085
H	-0.002725	-1.761732	0.189202

(H+)2-1Me RI-BP86/SVP

29

E(SCF) =	-960.625967		
C	-0.164239	0.004461	1.234979
P	-0.850156	-1.661065	1.701515
P	-0.904701	1.661550	1.645036
H	-0.056188	-0.007121	0.127212
H	0.872728	0.022984	1.639056
C	-2.572020	-1.851709	1.161143
H	-2.667264	-1.646029	0.076363
H	-3.251924	-1.193978	1.736773
H	-2.874918	-2.903691	1.344999
C	0.195729	-2.862340	0.831984

H	1.254358	-2.750460	1.140847
H	0.111520	-2.729217	-0.265138
H	-0.146942	-3.884320	1.095796
C	-0.716050	-1.928986	3.491073
H	0.335383	-1.810323	3.821122
H	-1.036977	-2.968760	3.709686
H	-1.369209	-1.237868	4.057458
C	-2.442939	1.921373	0.718589
H	-2.261645	1.809526	-0.369109
H	-2.791466	2.957368	0.911362
H	-3.237351	1.222005	1.042222
C	0.333291	2.876119	1.110991
H	1.275095	2.748101	1.681173
H	-0.065471	3.893822	1.302699
H	0.536946	2.771449	0.026480
C	-1.201779	1.840533	3.426322
H	-0.275245	1.639425	4.000019
H	-2.016967	1.174318	3.769488
H	-1.511172	2.889053	3.618978

	(H+)2-1Mes	RI-BP86/SVP	
125			
E(SCF) =	-2817.413653		
C	-0.000053	-0.000195	0.495353
P	-1.887548	0.047936	0.019922
P	1.887435	-0.047970	0.019884
C	-2.381330	1.734096	-0.557443
C	-2.559887	-0.314993	1.725589
C	2.559765	0.313507	1.725850
C	-2.350590	-1.286619	-1.167591
C	2.350428	1.287622	-1.166510
C	2.381371	-1.733602	-0.558889
C	-1.733486	2.284054	-1.712075
C	-2.031502	3.599673	-2.110283
C	-2.969459	4.399831	-1.435703
C	-3.660204	3.804725	-0.364585
C	-2.040965	0.388652	2.864533
C	-2.386294	-0.053930	4.157095
C	-3.422016	2.491965	0.087917
C	-3.255093	-1.132186	4.388915
C	-3.857918	-1.711123	3.257330
C	-3.563386	-1.326260	1.935611
C	2.040820	-0.391054	2.864201
C	2.386127	0.050486	4.157138
C	3.254979	1.128490	4.389841
C	3.857823	1.708359	3.258727

C	3.563304	1.324579	1.936705
C	-3.264217	-1.052378	-2.255653
C	-3.478755	-2.096033	-3.175980
C	-2.894296	-3.370455	-3.057425
C	-2.105233	-3.604403	-1.918779
C	-1.828385	-2.607334	-0.964862
C	1.828184	2.608158	-0.962702
C	2.104900	3.605991	-1.915863
C	2.893905	3.372994	-3.054734
C	3.478303	2.098651	-3.174420
C	3.263941	1.054275	-2.254872
C	1.733553	-2.282734	-1.713911
C	2.031625	-3.598062	-2.113092
C	2.969653	-4.398646	-1.439162
C	3.660336	-3.804321	-0.367554
C	3.422079	-2.491931	0.085935
H	4.454574	-4.380313	0.132888
H	1.520969	-4.000059	-3.002036
H	1.981725	-0.503989	5.019243
H	4.626993	2.482960	3.406823
H	1.701538	4.616080	-1.742198
H	4.174518	1.912417	-4.007397
H	-4.454479	4.380342	0.136221
H	-1.520915	4.002255	-2.999002
H	-1.982012	0.499922	5.019655
H	-4.627145	-2.485789	3.404766
H	-1.702008	-4.614681	-1.745896
H	-4.175189	-1.909184	-4.008632
C	4.122331	-0.178598	-2.463630
H	4.581710	-0.543709	-1.526782
H	4.946489	0.068727	-3.158212
H	3.576455	-1.034786	-2.904023
C	1.025858	3.046245	0.242731
H	-0.057219	2.850647	0.109891
H	1.125456	4.139401	0.378964
H	1.359873	2.571197	1.183934
C	3.163082	4.448941	-4.072868
H	2.655692	5.398194	-3.819036
H	2.824986	4.133975	-5.081836
H	4.250680	4.652752	-4.156062
C	-1.221630	1.666861	2.824860
H	-1.290306	2.210455	1.865370
H	-0.150958	1.490752	3.062793
H	-1.593921	2.359629	3.605133
C	-4.430255	-1.968484	0.869866
H	-3.961419	-2.853900	0.397667

H	-4.701297	-1.274893	0.054566
H	-5.372542	-2.313577	1.335842
C	-3.584451	-1.609101	5.778339
H	-4.680932	-1.653073	5.937768
H	-3.147228	-0.956038	6.556494
H	-3.200813	-2.638345	5.941227
C	4.430189	1.967629	0.871473
H	4.701166	1.274696	0.055592
H	5.372508	2.312275	1.337716
H	3.961389	2.853450	0.400004
C	1.221431	-1.669195	2.823502
H	1.290063	-2.212010	1.863576
H	0.150766	-1.493240	3.061590
H	1.593702	-2.362593	3.603225
C	3.584804	1.603956	5.779656
H	4.681322	1.641174	5.940779
H	3.142534	0.953704	6.557306
H	3.207349	2.635589	5.941627
C	3.258762	-5.814396	-1.861009
H	2.916777	-6.532112	-1.085592
H	4.347776	-5.981335	-1.985702
H	2.756525	-6.075593	-2.811135
C	0.803990	-1.491329	-2.594005
H	-0.002718	-0.998698	-2.028404
H	0.316678	-2.145175	-3.339766
H	1.348437	-0.699059	-3.148233
C	4.369738	-2.000319	1.161837
H	5.250157	-2.668393	1.200870
H	3.921760	-1.997654	2.173842
H	4.741028	-0.976700	0.975039
C	-4.122575	0.180699	-2.463307
H	-4.581919	0.545004	-1.526127
H	-4.946752	-0.065983	-3.158089
H	-3.576675	1.037253	-2.902965
C	-1.026016	-3.046389	0.240186
H	-1.359991	-2.572111	1.181791
H	0.057052	-2.850651	0.107458
H	-1.125559	-4.139664	0.375515
C	-3.162497	-4.445236	-4.077038
H	-2.809766	-4.134619	-5.082435
H	-4.250835	-4.638913	-4.172631
H	-2.666486	-5.398731	-3.816666
C	-4.369739	1.999556	1.163393
H	-3.921788	1.996024	2.175409
H	-4.741111	0.976122	0.975753
H	-5.250094	2.667681	1.202966

C	-0.804031	1.493203	-2.592775
H	-0.316308	2.147601	-3.337784
H	-1.348671	0.701690	-3.147907
H	0.002354	0.999705	-2.027483
C	-3.257905	5.816127	-1.856160
H	-4.347324	5.986568	-1.971775
H	-2.762562	6.075236	-2.810484
H	-2.906937	6.533204	-1.084108
H	-0.024528	-0.874403	1.164700
H	0.024426	0.873676	1.165115

(H+)2-1NH2 RI-BP86/SVP

23

E(SCF) = -1056.896035

C	-0.033255	0.077179	-1.040514
P	-1.618609	0.004153	-0.092342
P	1.570697	0.079813	-0.121634
N	1.458907	-1.233546	0.894301
H	1.083361	-2.114270	0.520685
H	2.243188	-1.400505	1.541952
N	2.676119	0.244371	-1.338226
H	2.524497	-0.179586	-2.261093
H	3.672870	0.351148	-1.104166
N	1.895356	1.331241	0.887805
H	2.346596	2.187109	0.547576
H	1.591290	1.331820	1.866265
N	-1.924095	-1.320440	0.825593
H	-1.600300	-1.395112	1.794822
H	-2.382989	-2.148240	0.430591
N	-2.747926	-0.068943	-1.295865
H	-3.739963	-0.194057	-1.051109
H	-2.614188	0.423851	-2.186754
N	-1.486121	1.237150	1.017442
H	-2.257658	1.354218	1.690811
H	-1.116888	2.143698	0.704216
H	-0.045620	-0.788623	-1.739201
H	-0.034434	0.992081	-1.673650

(H+)2-1NMe2 RI-BP86/SVP

59

E(SCF) = -1528.225367

C	0.026546	0.699791	-0.459121
P	1.760889	0.135068	-0.024628
P	-1.721440	0.092457	-0.139992
H	0.093522	0.817591	-1.560808
N	-2.264296	0.841379	1.250776

N	-1.812922	-1.571095	-0.023993
N	-2.584643	0.629967	-1.460344
N	1.795082	-0.373249	1.569440
N	2.214907	-1.014485	-1.135696
N	2.786003	1.428852	-0.265039
C	3.629044	-1.233351	-1.507374
H	3.738271	-1.171907	-2.609575
H	3.966112	-2.238725	-1.179603
H	4.279023	-0.471144	-1.044008
C	1.295621	-2.031910	-1.662444
H	0.243523	-1.779996	-1.434302
H	1.514050	-3.032717	-1.233827
H	1.412042	-2.097684	-2.763919
C	3.395510	2.197914	0.833319
H	4.470711	2.357366	0.613243
H	3.324252	1.650682	1.788508
H	2.915224	3.192510	0.949875
C	2.944894	2.037395	-1.599174
H	2.460424	3.036079	-1.643504
H	2.510123	1.390279	-2.383598
H	4.022927	2.167899	-1.825804
C	1.042915	0.293359	2.644782
H	0.712957	-0.470504	3.378008
H	0.139479	0.789264	2.244709
H	1.655840	1.044318	3.187694
C	2.905611	-1.230887	2.033013
H	2.505082	-1.995071	2.729177
H	3.686226	-0.647851	2.566253
H	3.374935	-1.755765	1.182018
C	-2.171220	2.300946	1.446046
H	-1.627003	2.536348	2.384619
H	-3.184900	2.747627	1.520144
H	-1.659774	2.795709	0.598829
C	-3.125781	0.154660	2.232954
H	-4.159442	0.559046	2.204071
H	-2.722262	0.304140	3.255059
H	-3.171233	-0.928743	2.029713
C	-1.008756	-2.341322	0.939619
H	-0.703645	-3.300270	0.474875
H	-1.587295	-2.578026	1.858216
H	-0.095698	-1.786948	1.225540
C	-2.973539	-2.309127	-0.567141
H	-2.612681	-3.206127	-1.109272
H	-3.544701	-1.679856	-1.271028
H	-3.654336	-2.640544	0.244923
C	-3.905440	1.277753	-1.343826

H	-3.890782	2.262732	-1.853459
H	-4.178076	1.430871	-0.285788
H	-4.689150	0.649769	-1.816759
C	-2.168030	0.349444	-2.845478
H	-1.233533	-0.241571	-2.878482
H	-2.017278	1.295399	-3.406495
H	-2.946895	-0.242026	-3.370853
H	0.000527	1.739549	-0.069872

	(H+)2-1Ph	RI-BP86/SVP	
71			
E(SCF) =	-2109.930184		
C	0.000120	-0.000309	1.007506
P	1.542991	0.715621	0.233030
P	-1.542865	-0.715854	0.232906
C	1.145124	2.207965	-0.714897
C	2.538067	1.166718	1.688434
C	2.443918	-0.481800	-0.789876
C	-1.145372	-2.208245	-0.715098
C	-2.538091	-1.166779	1.688260
C	-2.443411	0.481867	-0.789989
H	0.367316	-0.802210	1.681681
H	-0.367027	0.801361	1.681984
C	0.257973	3.173869	-0.167205
C	0.022616	4.385483	-0.860298
C	0.677315	4.636449	-2.101924
C	1.569964	3.667542	-2.641089
C	1.806703	2.454196	-1.945593
C	2.773675	0.215129	2.718649
C	3.563297	0.570992	3.838295
C	4.124331	1.878494	3.930351
C	3.891247	2.823237	2.891769
C	3.097950	2.467361	1.770905
C	3.770756	-0.833979	-0.427913
C	4.518251	-1.714017	-1.251357
C	3.943051	-2.237031	-2.443187
C	2.612943	-1.873987	-2.805412
C	1.866044	-0.999484	-1.980721
C	-0.258226	-3.174269	-0.167610
C	-0.023424	-4.386049	-0.860604
C	-0.678555	-4.636999	-2.102002
C	-1.571333	-3.668049	-2.640878
C	-1.807538	-2.454548	-1.945470
C	-2.773619	-0.215132	2.718443
C	-3.563320	-0.570872	3.838073
C	-4.124496	-1.878312	3.930152

C	-3.891491	-2.823110	2.891603
C	-3.098119	-2.467354	1.770753
C	-3.770011	0.834781	-0.427884
C	-4.517121	1.715198	-1.251273
C	-3.941785	2.237830	-2.443204
C	-2.611886	1.874115	-2.805529
C	-1.865372	0.999233	-1.980895
H	-4.249932	0.430426	0.472485
H	-5.546985	1.986198	-0.974339
H	-4.524956	2.914177	-3.087447
H	-2.171657	2.271877	-3.731690
H	-0.847989	0.741307	-2.295743
H	-2.377406	0.808357	2.676544
H	-3.750312	0.160356	4.638725
H	-4.739111	-2.154715	4.801066
H	-4.329045	-3.830457	2.958723
H	-2.939388	-3.215910	0.983778
H	0.247091	-3.026084	0.795777
H	0.657484	-5.141210	-0.440378
H	-0.502357	-5.583371	-2.636810
H	-2.087699	-3.867489	-3.591934
H	-2.516944	-1.734207	-2.373687
H	2.939152	3.215880	0.983909
H	4.328696	3.830632	2.958867
H	4.738876	2.154996	4.801281
H	3.750356	-0.160198	4.638967
H	2.377582	-0.808407	2.676767
H	-0.658079	5.140675	-0.439785
H	-0.247177	3.025576	0.796255
H	2.515870	1.733806	-2.374127
H	2.086045	3.867028	-3.592289
H	0.500587	5.582641	-2.636875
H	4.250586	-0.429263	0.472342
H	0.848536	-0.742013	-2.295538
H	2.172800	-2.272073	-3.731476
H	4.526526	-2.913060	-3.087487
H	5.548260	-1.984524	-0.974480

	(H+)2-1THP	RI-BP86/SVP	
83			
E(SCF) =	-1992.481253		
H	0.756084	1.528510	-0.948797
C	0.623582	0.885966	-0.054968
P	1.391919	-0.754091	-0.468254
P	-1.120333	1.202876	0.510453
N	-1.778123	-0.055836	1.373428

C	-3.184462	-0.537522	1.181074
C	-3.316519	-1.648982	2.232130
C	-2.425985	-1.159365	3.384630
C	-1.209162	-0.563156	2.659118
H	-3.347746	-0.898933	0.146274
H	-3.915004	0.277208	1.377366
H	-4.370065	-1.809776	2.530213
H	-2.935785	-2.609228	1.826395
H	-2.139641	-1.961955	4.090644
H	-2.947246	-0.373538	3.969183
H	-0.439817	-1.336048	2.445349
H	-0.725135	0.252466	3.234251
N	-1.005382	2.538076	1.495705
C	-0.241365	3.767953	1.120129
C	-0.543734	4.743532	2.269332
C	-1.967570	4.358108	2.697396
C	-1.956380	2.824846	2.620911
H	-0.594985	4.169738	0.144414
H	0.843755	3.555866	1.026637
H	0.169794	4.582493	3.103387
H	-0.450058	5.798935	1.950585
H	-2.714323	4.775472	1.989985
H	-2.233495	4.718760	3.709315
H	-2.960302	2.397769	2.429745
H	-1.569277	2.382098	3.563914
N	-2.001936	1.516587	-0.862390
C	-3.167715	2.453644	-0.879245
C	-3.381952	2.700920	-2.377497
C	-3.039545	1.339484	-3.001957
C	-1.822920	0.858642	-2.188236
H	-2.937048	3.376142	-0.311328
H	-4.064806	1.980813	-0.422614
H	-4.413033	3.034886	-2.600460
H	-2.687525	3.486768	-2.740087
H	-2.817638	1.395537	-4.084673
H	-3.885417	0.633647	-2.871938
H	-0.870881	1.196914	-2.657166
H	-1.786850	-0.245788	-2.100230
N	0.454181	-1.831756	-1.315124
C	0.669552	-2.119625	-2.773830
C	-0.468530	-3.095727	-3.119944
C	-0.764433	-3.806332	-1.790425
C	-0.648578	-2.670134	-0.766370
H	1.663010	-2.589734	-2.927641
H	0.630472	-1.196449	-3.386241
H	-1.363806	-2.538422	-3.465813

H	-0.179824	-3.787706	-3.933707
H	-0.003101	-4.586822	-1.583926
H	-1.757548	-4.294145	-1.765384
H	-0.413153	-3.022033	0.255846
H	-1.592431	-2.084073	-0.713356
N	2.710453	-0.306354	-1.381178
C	3.923856	-1.177241	-1.472830
C	4.941338	-0.281426	-2.191830
C	4.065276	0.528565	-3.158895
C	2.811714	0.849733	-2.326975
H	3.712136	-2.094810	-2.065843
H	4.260184	-1.489673	-0.464416
H	5.445277	0.387205	-1.463757
H	5.725362	-0.872013	-2.702521
H	3.791495	-0.086963	-4.040192
H	4.555938	1.446836	-3.533830
H	1.907052	0.945979	-2.963230
H	2.943703	1.797096	-1.760312
N	1.802546	-1.466761	0.981281
C	2.504625	-0.689267	2.054738
C	3.041028	-1.772935	3.005383
C	3.305982	-2.967667	2.077745
C	2.109336	-2.930444	1.119341
H	1.807023	0.004895	2.566574
H	3.335086	-0.088790	1.621697
H	3.939006	-1.431208	3.554263
H	2.270579	-2.033603	3.759891
H	3.376571	-3.932465	2.615336
H	4.256983	-2.829349	1.521946
H	1.234316	-3.451532	1.564996
H	2.315676	-3.396067	0.136446
H	1.274489	1.318142	0.732618

	(H+)2-2Ad	RI-BP86/SVP	
59			
E(SCF) =	-1005.190207		
C	0.000006	-0.160715	-0.006503
N	1.155556	0.743151	-0.001695
N	-1.155600	0.743167	-0.003403
C	-0.718502	1.994536	-0.000760
C	0.718479	1.994521	0.000661
H	0.000749	-0.803589	-0.913329
C	2.568549	0.274710	-0.000840
C	2.814899	-0.602070	1.275949
C	4.280517	-1.088203	1.255740
C	4.528501	-1.955313	0.002126

C	4.281968	-1.090220	-1.253245
C	2.816301	-0.604180	-1.275491
C	5.236792	0.119256	1.267473
C	4.992038	0.970233	0.000073
C	3.529382	1.477851	-0.000868
C	5.238046	0.117378	-1.265741
C	-2.568530	0.274760	-0.002403
C	-2.812896	-0.617160	-1.268234
C	-4.278642	-1.102956	-1.245339
C	-4.528493	-1.955229	0.018235
C	-4.283809	-1.075389	1.263485
C	-2.818318	-0.589011	1.283053
C	-5.234501	0.104576	-1.272563
C	-4.992033	0.970127	-0.014803
C	-3.529388	1.477775	-0.016361
C	-5.240322	0.131927	1.260510
H	1.383684	2.867525	0.003213
H	-1.383709	2.867538	0.000413
H	2.611713	0.009203	2.180402
H	2.128857	-1.476454	1.281149
H	4.430945	-1.704629	2.169504
H	5.570172	-2.333152	0.003031
H	3.867706	-2.848272	0.002426
H	4.433482	-1.708158	-2.165753
H	2.130619	-1.478853	-1.279892
H	2.613911	0.005349	-2.181336
H	3.355427	2.109283	-0.900569
H	3.354944	2.109864	0.898311
H	5.659785	1.855077	-0.000167
H	6.288318	-0.230551	1.289597
H	5.088489	0.732235	2.181704
H	6.289652	-0.232302	-1.286374
H	5.090579	0.728953	-2.181056
H	-2.607827	-0.017203	-2.179873
H	-2.127557	-1.492081	-1.261631
H	-4.427835	-1.730251	-2.151767
H	-3.867700	-2.848118	0.029322
H	-5.570163	-2.333063	0.020249
H	-4.436561	-1.682413	2.183203
H	-2.131906	-1.462962	1.299103
H	-2.617769	0.031764	2.181574
H	-3.358132	2.118129	0.877510
H	-3.352309	2.100870	-0.921255
H	-5.659787	1.854899	-0.025577
H	-6.291835	-0.217859	1.283144
H	-5.094698	0.754147	2.168917

H	-5.084367	0.706869	-2.193573
H	-6.286104	-0.245154	-1.292676
H	-0.000733	-0.814086	0.892825

(H+)2-2Cl RI-BP86/SVP

11			
E(SCF) =	-1145.455502		
C	-0.000028	-0.826113	0.000691
N	-1.136491	0.113367	-0.000008
Cl	-2.728946	-0.430921	-0.000249
N	1.136631	0.113548	-0.000200
Cl	2.728944	-0.430952	-0.000196
C	-0.725151	1.371967	0.000229
H	-1.403615	2.245358	0.000038
C	0.725085	1.372118	0.000184
H	1.403209	2.245773	-0.000374
H	-0.000047	-1.466844	0.915922
H	0.000079	-1.468684	-0.913193

(H+)2-2F RI-BP86/SVP

11			
E(SCF) =	-424.659959		
C	0.000023	-1.017619	0.000208
N	-1.105211	-0.049632	0.000358
F	-2.342568	-0.473693	-0.000215
N	1.105187	-0.049749	-0.000080
F	2.342493	-0.473705	-0.000201
C	-0.733487	1.208848	-0.000073
H	-1.432101	2.071587	-0.000545
C	0.733596	1.208758	0.000085
H	1.432365	2.071372	0.000588
H	0.000318	-1.660247	0.920393
H	-0.000528	-1.660384	-0.919964

(H+)2-2H RI-BP86/SVP

11			
E(SCF) =	-226.537096		
C	-0.000456	-1.181503	-0.000002
N	-1.120188	-0.259988	-0.000114
H	-2.113827	-0.579534	-0.000169
N	1.120035	-0.260798	0.000009
H	2.113409	-0.581088	0.000093
C	-0.737258	0.990296	0.000022
H	-1.424112	1.858701	0.000058
C	0.738004	0.989737	-0.000026
H	1.425436	1.857688	0.000054

H	-0.001507	-1.850210	0.903309
H	-0.000071	-1.851239	-0.902571

	(H+)2-2Me	RI-BP86/SVP	
17			
E(SCF) =	-305.152463		
C	-0.000042	-0.932003	0.000094
N	1.149243	-0.023722	0.000066
C	2.542860	-0.499528	-0.000073
N	-1.149196	-0.023738	-0.000054
C	-2.542880	-0.499527	-0.000063
C	-0.729639	1.220435	-0.000007
H	-1.401262	2.096687	-0.000009
C	0.729639	1.220440	0.000032
H	1.401222	2.096723	0.000087
H	3.223029	0.370810	0.000750
H	2.713092	-1.122831	0.903318
H	2.713366	-1.121303	-0.904485
H	-3.222994	0.370850	-0.001863
H	-2.712703	-1.123537	-0.903025
H	-2.713738	-1.120520	0.904822
H	0.000191	-1.586895	-0.904246
H	-0.000163	-1.586657	0.904670

	(H+)2-2Mes	RI-BP86/SVP	
49			
E(SCF) =	-924.191618		
C	0.000004	-0.253203	-0.150658
N	-1.163234	0.422739	0.455481
N	1.163225	0.422737	0.455469
C	0.704969	1.440771	1.210220
C	-0.704967	1.440774	1.210222
H	0.000000	-1.342819	0.034253
C	2.514529	0.114863	0.158481
C	2.953713	-1.255557	0.154757
C	4.290855	-1.498368	-0.165356
C	5.205000	-0.464035	-0.502907
C	4.729681	0.866719	-0.491815
C	3.412008	1.200837	-0.153854
C	-2.514538	0.114872	0.158509
C	-2.953723	-1.255551	0.154759
C	-4.290879	-1.498345	-0.165270
C	-5.205037	-0.463993	-0.502763
C	-4.729722	0.866749	-0.491653
C	-3.412022	1.200854	-0.153757
C	2.089100	-2.425395	0.573315

C	6.625645	-0.786533	-0.838223
C	3.003444	2.653144	-0.217633
C	-2.089079	-2.425389	0.573249
C	-6.625588	-0.786575	-0.838380
C	-3.003471	2.653164	-0.217514
H	4.656731	-2.536343	-0.130235
H	5.417531	1.678148	-0.774475
H	1.474221	-2.818895	-0.264760
H	1.426104	-2.187332	1.429450
H	2.728307	-3.267356	0.897418
H	6.682853	-1.589518	-1.603458
H	7.148757	-1.189564	0.057973
H	7.188291	0.093918	-1.197119
H	3.648690	3.195310	-0.933539
H	1.954381	2.807193	-0.544414
H	3.129451	3.162401	0.761831
H	1.365788	2.078350	1.808103
H	-1.365775	2.078350	1.808120
H	-4.656765	-2.536313	-0.130122
H	-5.417600	1.678186	-0.774208
H	-2.728261	-3.267411	0.897236
H	-1.474128	-2.818784	-0.264821
H	-1.426138	-2.187368	1.429440
H	-6.682189	-1.585961	-1.607493
H	-7.147599	-1.194704	0.056089
H	-7.189500	0.094781	-1.193009
H	-3.648696	3.195325	-0.933440
H	-3.129524	3.162412	0.761949
H	-1.954396	2.807229	-0.544247
H	-0.000005	-0.066373	-1.245549

(H+)2-2NH2 RI-BP86/SVP

15

E(SCF) =

-337.175151

C	0.000046	-0.974468	0.000547
N	-1.150350	-0.037945	-0.056387
N	-2.397627	-0.494495	0.068513
N	1.150353	-0.037952	0.056612
N	2.397620	-0.494557	-0.069778
C	-0.713811	1.222552	-0.032296
H	-1.381652	2.098626	-0.037161
C	0.713785	1.222515	0.032544
H	1.381641	2.098591	0.036812
H	3.147786	0.209166	-0.137531
H	2.625062	-1.391489	0.384411
H	-3.147998	0.208932	0.136620

H	-2.624495	-1.392037	-0.384661
H	-0.068113	-1.598269	0.918714
H	0.067677	-1.602475	-0.914703

(H+)2-2NMe2 RI-BP86/SVP

27

E(SCF) =	-494.350294		
C	-0.000010	0.702884	-0.000018
N	-1.151311	-0.225659	-0.005032
N	-2.416586	0.217193	0.049044
N	1.151294	-0.225663	0.005043
N	2.416586	0.217192	-0.049121
C	-0.707917	-1.498909	-0.005658
H	-1.368071	-2.373545	-0.008614
C	0.707895	-1.498910	0.005754
H	1.368048	-2.373550	0.008766
H	0.008548	1.337002	-0.911328
C	-2.671308	1.644788	-0.145190
C	-3.466332	-0.797804	0.092374
C	3.466340	-0.797816	-0.092445
C	2.671334	1.644784	0.145245
H	3.754607	1.812558	0.019042
H	2.149076	2.257228	-0.619423
H	2.385469	1.979808	1.166943
H	4.437416	-0.282744	-0.184500
H	3.474110	-1.411307	0.836227
H	3.331568	-1.456824	-0.976963
H	-3.754576	1.812572	-0.019017
H	-2.149069	2.257155	0.619544
H	-2.385398	1.979908	-1.166838
H	-4.437418	-0.282735	0.184245
H	-3.473988	-1.411392	-0.836226
H	-3.331653	-1.456720	0.976968
H	-0.008559	1.337042	0.911264

(H+)2-2Ph RI-BP86/SVP

31

E(SCF) =	-688.441999		
C	-0.000010	0.360255	0.000024
N	1.164391	-0.551988	-0.021206
C	2.497856	-0.098315	-0.014556
N	-1.164389	-0.551997	0.021019
C	-2.497860	-0.098322	0.014514
C	0.704397	-1.817015	-0.015057
H	1.358163	-2.697484	-0.037965
C	-0.704384	-1.817021	0.014506

H	-1.358149	-2.697499	0.037079
H	0.027530	0.992693	0.910418
C	3.561843	-1.025628	0.183768
C	4.876785	-0.565245	0.176867
C	5.150958	0.807589	-0.021063
C	4.094473	1.726772	-0.210744
C	2.771502	1.285428	-0.207992
H	3.370787	-2.092084	0.367613
H	5.701606	-1.274833	0.337612
H	6.192691	1.162910	-0.024332
H	4.312930	2.792894	-0.369416
H	1.968829	2.017230	-0.377289
C	-3.561900	-1.025660	-0.183422
C	-4.876833	-0.565254	-0.176380
C	-5.150951	0.807623	0.021316
C	-4.094422	1.726826	0.210638
C	-2.771459	1.285461	0.207750
H	-3.370902	-2.092178	-0.366963
H	-5.701694	-1.274870	-0.336796
H	-6.192676	1.162959	0.024695
H	-4.312837	2.792984	0.369127
H	-1.968739	2.017289	0.376716
H	-0.027521	0.992926	-0.910207

(H+)2-2Me_Me RI-BP86/SVP

23

E(SCF) =	-383.783162		
C	0.000107	-1.514729	-0.000310
N	1.142929	-0.612126	-0.008168
C	2.527733	-1.123749	-0.006797
N	-1.142798	-0.612248	0.007655
C	-2.527660	-1.123837	0.007450
C	-0.746143	0.649485	0.004529
C	-1.610044	1.842567	-0.010371
C	0.746131	0.649585	-0.005026
C	1.609763	1.842846	0.010473
H	3.081639	-0.699524	-0.867706
H	3.028762	-0.835757	0.939684
H	2.506073	-2.224616	-0.091435
H	-3.034904	-0.821501	-0.931085
H	-2.505506	-2.225853	0.075192
H	-3.075801	-0.712843	0.878563
H	-1.260181	2.587359	0.736641
H	-1.528760	2.346988	-1.003022
H	-2.674978	1.612095	0.171659
H	1.529288	2.345890	1.003905

H	2.674655	1.612769	-0.172355
H	1.259199	2.588516	-0.735288
H	-0.006367	-2.167785	-0.904942
H	0.006640	-2.168125	0.904093

	(H+)2-6	RI-BP86/SVP	
39			
E(SCF) =	-1187.480261		
C	3.498055	1.632817	-0.583465
P	3.442189	2.977337	0.925947
C	3.900919	0.331784	-0.230270
O	4.250169	-0.693329	0.125236
C	2.063294	2.477262	1.952879
C	5.043637	2.842238	1.720845
C	3.183895	4.494518	0.009852
H	4.214590	2.023783	-1.342840
H	2.479382	1.589177	-1.032789
C	2.774569	6.928295	-1.377321
C	1.847625	5.850461	-1.536582
C	2.049736	4.633836	-0.844819
C	6.236211	2.891284	0.939269
C	7.493727	2.829326	1.584407
C	7.564439	2.725417	3.008305
C	6.367389	2.687813	3.781468
C	5.103599	2.743602	3.140358
C	0.964447	3.365799	2.131440
C	-0.117903	2.977841	2.961467
C	-0.106504	1.705137	3.603531
C	1.004165	0.821877	3.422687
C	2.088681	1.207080	2.601360
C	4.117201	5.559290	0.170580
C	3.904148	6.779240	-0.519205
H	2.614955	7.875161	-1.919400
H	0.976604	5.974521	-2.199304
H	1.307992	3.834661	-0.983122
H	6.226178	3.002386	-0.154305
H	8.423070	2.867409	0.994375
H	8.545960	2.679640	3.508320
H	6.425880	2.619296	4.879148
H	4.199529	2.728291	3.763638
H	0.935288	4.359593	1.665603
H	-0.967260	3.661849	3.115570
H	-0.950935	1.402579	4.244778
H	1.011811	-0.154051	3.933397
H	2.939137	0.515780	2.520723
H	4.989725	5.476595	0.832364

H	4.610089	7.615038	-0.392054
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PA/Mono_Prot/CBS-QB3

(H+)-1Cl

cbs-qb3

10

E(SCF) = -3482.646176

C	-0.000040	-0.000930	0.933310
P	1.521470	0.027740	0.189800
P	-1.521530	-0.028110	0.189640
H	-0.000120	-0.001420	2.017930
Cl	-2.858510	-0.711670	1.503960
Cl	-1.573860	-1.174950	-1.458700
Cl	-2.242080	1.748460	-0.437130
Cl	2.858460	0.706740	1.506430
Cl	2.241170	-1.747310	-0.442330
Cl	1.574890	1.179460	-1.455130

(H+)-1F

cbs-qb3

10

E(SCF) = -1320.549098

C	0.000030	-0.834130	0.007540
P	1.489900	-0.092360	0.005170
P	-1.489870	-0.092490	-0.003430
F	2.346300	-0.315700	-1.238900
F	2.428430	-0.567200	1.109490
F	1.396420	1.422270	0.146570
F	-2.342440	-0.282200	1.248920
F	-1.397360	1.417990	-0.184360
F	-2.431400	-0.597240	-1.091700
H	-0.000020	-1.923620	0.018530

(H+)-1H

cbs-qb3

10

E(SCF) = -724.776183

C	0.000000	0.671230	-0.008910
P	1.513420	-0.113710	0.002500
P	-1.513410	-0.113710	0.002500
H	-0.000010	1.750460	0.099610
H	2.436130	0.443010	-0.895270
H	1.379710	-1.455580	-0.369120
H	2.247340	-0.170790	1.203790
H	-1.379830	-1.455450	-0.369650
H	-2.247160	-0.171250	1.203880
H	-2.436220	0.443430	-0.894910

-----	(H+)-1Me	cbs-qb3	
28			
E(SCF) =	-960.841192		
C	-0.499859	-0.011177	-0.622476
P	0.006676	-1.562901	-0.088783
P	-0.132138	1.565117	-0.051878
H	-1.294546	-0.040427	-1.360396
C	-0.873258	-2.788626	-1.090547
H	-1.949229	-2.679001	-0.946170
H	-0.573820	-3.795281	-0.794157
H	-0.635845	-2.639653	-2.144934
C	-0.338053	-1.972643	1.654721
H	0.191311	-1.282468	2.315711
H	-0.009853	-2.989120	1.884066
H	-1.409363	-1.885873	1.843094
C	1.784195	-1.902690	-0.292408
H	2.376493	-1.223705	0.323597
H	2.059585	-1.759650	-1.338262
H	2.011131	-2.928240	0.007781
C	-0.328570	2.744542	-1.414449
H	-0.150861	3.763033	-1.063945
H	-1.346025	2.680389	-1.805929
H	0.372309	2.502072	-2.213925
C	1.566493	1.722549	0.572120
H	1.740371	2.750014	0.898046
H	2.278540	1.470804	-0.214401
H	1.725008	1.066128	1.430225
C	-1.188825	2.203930	1.291677
H	-0.914022	3.228181	1.555271
H	-1.090704	1.569528	2.174783
H	-2.231300	2.184738	0.967648

-----	(H+)-1NH2	cbs-qb3	
22			
E(SCF) =	=		
C	-0.000010	0.869440	-0.000090
P	-1.519610	0.103030	0.070250
P	1.519610	0.103030	-0.070270
N	1.408970	-1.161700	-1.138020
H	0.942480	-0.974890	-2.014310
H	2.198500	-1.788480	-1.229940
N	2.608380	1.317600	-0.316610
H	2.365300	2.074770	-0.938750
H	3.594350	1.096320	-0.298460

N	2.257220	-0.697730	1.186870
H	2.534820	-0.141880	1.984820
H	1.884690	-1.602190	1.441720
N	-2.257380	-0.697770	-1.186790
H	-1.884820	-1.602210	-1.441680
H	-2.535030	-0.141930	-1.984730
N	-2.608360	1.317600	0.316660
H	-3.594340	1.096340	0.298520
H	-2.365250	2.074760	0.938800
N	-1.408820	-1.161680	1.138010
H	-2.198320	-1.788490	1.229980
H	-0.942340	-0.974800	2.014290
H	-0.000020	1.951040	-0.000250

PA/Mono_Prot/RI-BP86_SVP

(H⁺)-5 RI-BP86/SVP

6			
E(SCF) =	-264.846645		
H	-1.695664	0.103693	1.348650
C	0.102691	0.039195	0.193924
C	-0.584189	0.068327	1.379336
C	0.036769	0.055822	2.600855
O	0.512053	0.046889	3.641205
O	0.634200	0.016074	-0.818629

(H⁺)-3Ad RI-BP86/SVP

116			
E(SCF) =	-2047.661682		
C	-0.178798	-0.002953	0.084998
C	0.517442	1.165984	-0.314984
C	0.325819	-1.256647	0.525695
N	-0.008452	2.127930	-1.167692
N	1.762883	1.634593	0.085260
N	1.462925	-1.943653	0.117777
N	-0.303527	-2.056263	1.467447
C	0.909300	3.164525	-1.301495
C	2.007688	2.851450	-0.553577
C	1.535222	-3.142423	0.830694
C	0.446849	-3.212796	1.652759
H	0.719730	4.042757	-1.918783
H	2.947165	3.392714	-0.445219
H	2.358032	-3.846653	0.711757
H	0.167365	-3.986176	2.368447
C	2.552065	1.060367	1.206406
H	2.669147	-0.015094	0.965240

C	1.825999	1.149496	2.580333
C	3.986001	1.637034	1.362749
H	0.777645	0.808729	2.455904
C	1.849120	2.589444	3.137607
C	2.572047	0.199192	3.546929
H	4.497251	1.630861	0.375330
C	4.024374	3.057181	1.985972
C	4.732981	0.681106	2.331910
H	1.289806	2.617102	4.096922
H	1.321748	3.283967	2.447767
C	3.307043	3.053535	3.351233
H	2.536930	-0.843979	3.163264
H	2.060015	0.194918	4.532645
C	4.034361	0.667037	3.711984
H	3.563347	3.823146	1.331527
H	5.086713	3.357570	2.108124
H	4.769966	-0.346416	1.909022
H	5.785312	1.018364	2.438241
H	3.313148	4.080344	3.773515
C	4.038087	2.090421	4.311242
H	4.574590	-0.028037	4.388976
H	5.080784	2.436580	4.475764
H	3.542922	2.086595	5.305939
C	-1.366262	2.041193	-1.755173
H	-2.019646	1.754624	-0.901987
C	-1.509582	0.945194	-2.848742
C	-1.928520	3.379445	-2.305318
H	-1.043887	0.007646	-2.480829
C	-0.842868	1.386266	-4.170054
C	-3.023872	0.723393	-3.073137
H	-1.781575	4.180159	-1.548445
C	-1.309121	3.794702	-3.664629
C	-3.448091	3.153604	-2.526017
H	-0.930456	0.566584	-4.914229
H	0.245397	1.557944	-4.018101
C	-1.514068	2.672045	-4.702076
H	-3.505615	0.382106	-2.130548
H	-3.175516	-0.085873	-3.818416
C	-3.674345	2.033603	-3.568902
H	-0.228223	4.029771	-3.586166
H	-1.800933	4.730779	-4.004029
H	-3.942468	2.894134	-1.564925
H	-3.910818	4.100535	-2.874847
H	-1.043637	2.967346	-5.663491
C	-3.025466	2.435744	-4.911561
H	-4.764826	1.878220	-3.709401

H	-3.502380	3.356830	-5.309291
H	-3.190016	1.639435	-5.668896
C	2.193396	-1.618955	-1.134882
H	2.069787	-0.525346	-1.243044
C	1.562991	-2.276494	-2.395614
C	3.723574	-1.890657	-1.133075
H	0.461295	-2.138626	-2.353974
C	1.914821	-3.777789	-2.491246
C	2.137967	-1.532414	-3.624975
H	4.170711	-1.478410	-0.202777
C	4.097034	-3.385954	-1.289900
C	4.292866	-1.137117	-2.365934
H	1.433520	-4.206237	-3.395861
H	1.497489	-4.338031	-1.627270
C	3.448802	-3.959850	-2.568130
H	1.865357	-0.455649	-3.581646
H	1.683016	-1.939853	-4.552468
C	3.672469	-1.701451	-3.666525
H	3.817305	-3.990313	-0.403838
H	5.203026	-3.464641	-1.357129
H	4.085989	-0.048081	-2.282124
H	5.397016	-1.251686	-2.387923
H	3.690296	-5.040235	-2.652743
C	4.006373	-3.204057	-3.794237
H	4.083776	-1.149459	-4.537925
H	5.105347	-3.350905	-3.864479
H	3.569647	-3.612781	-4.730410
C	-1.518008	-1.621806	2.188190
H	-1.383704	-0.519982	2.263564
C	-1.678387	-2.167436	3.633175
C	-2.837238	-1.874230	1.403109
H	-0.719092	-2.042256	4.179924
C	-2.149519	-3.642779	3.693820
C	-2.777322	-1.297255	4.300819
H	-2.701884	-1.556391	0.346881
C	-3.237754	-3.365530	1.447842
C	-3.935045	-1.013478	2.071669
H	-2.297228	-3.920792	4.758965
H	-1.390508	-4.351434	3.304902
C	-3.468115	-3.808528	2.910631
H	-2.466405	-0.230453	4.318649
H	-2.899665	-1.610890	5.358777
C	-4.116210	-1.454474	3.540750
H	-2.453596	-3.994636	0.972430
H	-4.161337	-3.514080	0.849354
H	-3.662286	0.063476	2.019840

H	-4.890165	-1.128694	1.516861
H	-3.779265	-4.874096	2.930850
C	-4.559611	-2.933770	3.565006
H	-4.889200	-0.821863	4.025767
H	-5.523749	-3.051878	3.025586
H	-4.736579	-3.266274	4.610089
H	-1.273212	0.069811	0.032578

(H+)-3Me RI-BP86/SVP

32

E(SCF) = -647.771480

C	1.075327	2.498496	1.794623
C	0.698380	1.245054	2.340296
C	1.420187	2.751480	0.442561
N	0.916942	0.839237	3.639122
N	-0.017345	0.227450	1.736783
N	2.075640	1.918672	-0.445568
N	1.227652	3.942886	-0.222943
C	0.342967	-0.412939	3.841672
C	-0.224802	-0.800313	2.660171
C	2.272128	2.595143	-1.652183
C	1.758249	3.853415	-1.507050
C	1.659905	1.610121	4.626038
H	0.397231	-0.927254	4.805510
H	-0.763299	-1.715254	2.397108
C	-0.717463	0.352887	0.463268
C	2.738460	0.673450	-0.074668
H	2.765469	2.123557	-2.506922
H	1.714798	4.688208	-2.212517
C	0.547809	5.099214	0.343649
H	-1.502247	-0.422341	0.409590
H	-1.192745	1.352375	0.403096
H	-0.040606	0.232748	-0.405387
H	1.985627	0.938925	5.440629
H	2.551862	2.060251	4.147785
H	1.037809	2.419993	5.058665
H	3.490704	0.426613	-0.844612
H	3.249489	0.806409	0.899795
H	2.029706	-0.173314	0.012854
H	0.219878	5.764630	-0.474789
H	-0.339065	4.762398	0.915399
H	1.215708	5.669406	1.021012
H	1.103440	3.353754	2.484286

(H+)-4Me RI-BP86/SVP

40

E(SCF) =	-652.555884		
C	0.068097	0.027856	-0.019596
C	-0.418217	0.054987	-1.355760
C	0.180363	1.093497	0.915537
N	0.028625	-0.883992	-2.252287
N	-1.354729	0.954784	-1.805874
N	0.358046	2.407490	0.553421
N	0.152302	0.813431	2.259345
C	-0.856572	-1.508463	-3.239636
H	-0.560428	-1.269325	-4.282494
H	-1.900035	-1.188483	-3.077576
H	-0.815235	-2.611174	-3.117240
C	1.318692	-1.548560	-2.079596
H	1.759766	-1.749863	-3.076876
H	1.220764	-2.521613	-1.548907
H	2.011103	-0.901443	-1.512302
C	-2.355414	1.546780	-0.924679
H	-2.416800	0.975180	0.017967
H	-3.347746	1.514397	-1.420929
H	-2.129358	2.609178	-0.688938
C	-0.152630	3.521403	1.355408
H	0.657227	4.085330	1.865490
H	-0.863474	3.150396	2.114171
H	-0.688635	4.233202	0.693485
C	1.023220	2.792810	-0.686484
H	0.304931	3.166001	-1.448103
H	1.574775	1.932555	-1.104731
H	1.747910	3.607174	-0.477337
C	1.016084	1.503268	3.221883
H	1.720897	2.170583	2.697030
H	1.610998	0.749915	3.779736
H	0.436014	2.095229	3.960493
C	-0.497300	-0.390732	2.773022
H	-0.944879	-0.167734	3.762755
H	0.221326	-1.229661	2.906457
H	-1.300822	-0.715413	2.088213
C	-1.387967	1.430637	-3.190594
H	-0.454497	1.154318	-3.711160
H	-1.475867	2.537142	-3.195036
H	-2.251624	1.025259	-3.759658
H	0.404768	-0.953986	0.340658

	(H+)-3H	RI-BP86/SVP	
20			
E(SCF) =	-490.644721		
C	1.017311	2.552947	1.806545

C	0.700363	1.295610	2.356555
C	1.344224	2.798719	0.458731
N	0.637227	0.985155	3.691867
N	0.368291	0.123598	1.709037
N	1.693906	1.900085	-0.527754
N	1.401018	4.026022	-0.152817
C	0.249507	-0.340907	3.877731
C	0.071592	-0.881912	2.636992
C	1.994823	2.571993	-1.718604
C	1.801950	3.902686	-1.482205
H	0.884221	1.638243	4.436620
H	0.145440	-0.784648	4.871666
H	-0.228688	-1.887868	2.331488
H	0.091657	0.091409	0.726288
H	1.976892	0.939030	-0.328665
H	2.308220	2.044208	-2.623396
H	1.903819	4.767372	-2.143709
H	1.142232	4.899739	0.307436
H	1.009170	3.414637	2.486098

(H+)-1Cl RI-BP86/SVP

10			
E(SCF) =	-3481.707697		
C	-0.209995	0.008685	0.919127
P	0.036752	-1.522365	0.196063
P	-0.187489	1.544577	0.170623
H	-0.503382	-0.006034	1.982620
Cl	0.412559	2.925904	1.500223
Cl	-1.959418	2.240914	-0.527679
Cl	1.036383	1.559356	-1.432278
Cl	-0.482480	-2.913914	1.542800
Cl	-1.025382	-1.837560	-1.499306
Cl	1.939791	-1.932329	-0.360593

(H+)-1Cy RI-BP86/SVP

106			
E(SCF) =	-2131.693313		
C	-0.074337	-0.121479	-0.728439
P	1.619506	-0.153898	-0.303300
P	-1.690775	0.144275	-0.143878
C	-2.873535	-0.365951	-1.530151
C	-3.394012	-0.306963	-4.026105
C	-4.496045	-2.041003	-2.551505
C	-3.976312	-1.725324	-3.960301
C	-3.426375	-1.808302	-1.466019
C	-2.315488	-0.088669	-2.948324

H	-4.207508	0.439955	-3.887907
H	-5.378463	-1.399359	-2.330885
H	-3.186506	-2.459697	-4.236188
H	-2.591492	-2.529560	-1.603844
H	-1.476773	-0.792585	-3.144691
H	-3.731838	0.323881	-1.362241
H	-2.957590	-0.107517	-5.026792
H	-4.854831	-3.089465	-2.491637
H	-4.787266	-1.847201	-4.707568
H	-3.871402	-2.016164	-0.473822
H	-1.897812	0.934249	-3.028828
C	-2.266478	1.909709	0.235575
C	-2.070380	3.958077	1.749259
C	-2.796387	4.242996	-0.654630
C	-2.047396	4.880556	0.523116
C	-2.254116	2.841459	-0.996438
C	-1.520397	2.557289	1.419458
H	-3.115403	3.861118	2.119849
H	-3.877631	4.162783	-0.402976
H	-0.991939	5.077471	0.228306
H	-1.213139	2.928368	-1.375614
H	-0.443633	2.641635	1.156869
H	-3.330198	1.759403	0.532769
H	-1.486027	4.398177	2.584016
H	-2.736328	4.889645	-1.554651
H	-2.488064	5.867573	0.773430
H	-2.858883	2.413058	-1.820108
H	-1.579334	1.916886	2.323986
C	-2.043982	-0.775444	1.461073
C	-3.586401	-1.207354	3.441807
C	-1.830670	-2.920174	2.809985
C	-3.229127	-2.699937	3.405938
C	-1.706153	-2.283247	1.413906
C	-3.451921	-0.539802	2.058434
H	-2.915115	-0.684674	4.159956
H	-1.067277	-2.479648	3.491280
H	-3.979984	-3.245863	2.791777
H	-2.402754	-2.803450	0.727666
H	-4.222237	-0.957742	1.373481
H	-1.306649	-0.299121	2.151216
H	-4.618619	-1.060190	3.821740
H	-1.599368	-4.003777	2.744690
H	-3.289642	-3.133921	4.425207
H	-0.691972	-2.433523	0.993685
H	-3.672768	0.541950	2.155349
C	2.343136	-1.608460	-1.263985

C	4.384499	-2.938933	-2.000527
C	2.081334	-3.987527	-2.114355
C	3.580611	-4.242911	-1.898887
C	1.540184	-2.921924	-1.143427
C	3.852818	-1.852697	-1.043551
H	4.335378	-2.554983	-3.044124
H	1.909957	-3.649803	-3.161449
H	3.736335	-4.696025	-0.893983
H	1.610385	-3.311859	-0.105335
H	4.027585	-2.175784	0.006680
H	2.213333	-1.243404	-2.311795
H	5.458292	-3.121978	-1.788465
H	1.502977	-4.927039	-1.993387
H	3.957234	-4.984172	-2.633518
H	0.466066	-2.725413	-1.332249
H	4.433923	-0.920560	-1.190382
C	2.587861	1.317647	-1.046486
C	2.473859	3.640437	-2.075580
C	4.664597	2.786383	-1.132207
C	3.796890	4.024981	-1.396850
C	3.900780	1.713824	-0.330044
C	1.712130	2.564486	-1.280547
H	2.681547	3.254655	-3.099038
H	4.995308	2.349468	-2.100995
H	3.581270	4.535812	-0.431413
H	3.664300	2.123175	0.676293
H	1.397298	2.985288	-0.299113
H	2.861871	0.919242	-2.051550
H	1.827973	4.533476	-2.207267
H	5.589660	3.065466	-0.586231
H	4.351304	4.758742	-2.017524
H	4.558776	0.836172	-0.166867
H	0.779968	2.277854	-1.807080
C	2.138297	-0.248589	1.487334
C	2.262506	0.926137	3.742095
C	2.557456	-1.587039	3.603571
C	2.060420	-0.415039	4.462163
C	1.909344	-1.596174	2.205419
C	1.614448	0.924535	2.345267
H	3.351216	1.132143	3.637649
H	3.662818	-1.520601	3.491457
H	0.978062	-0.553784	4.684275
H	0.821000	-1.785457	2.305170
H	0.513815	0.825457	2.455967
H	3.239639	-0.119940	1.383307
H	1.846187	1.761155	4.343033

H	2.356538	-2.554710	4.108243
H	2.577817	-0.408394	5.443516
H	2.322005	-2.434540	1.610704
H	1.791210	1.896821	1.842023
H	-0.113510	-0.268275	-1.822680

(H+)-1F			
RI-BP86/SVP			
10			
E(SCF) =	-1319.708192		
C	0.000009	-0.004165	-0.651126
P	-1.503250	-0.120065	0.092497
P	1.502802	0.121683	0.092065
F	-2.164250	-1.532681	0.169239
F	-2.602847	0.705988	-0.636098
F	-1.472911	0.345264	1.580824
F	2.153236	1.538966	0.175475
F	1.480567	-0.348584	1.579026
F	2.605450	-0.693217	-0.643989
H	0.001193	-0.013189	-1.757903

(H+)-1H			
RI-BP86/SVP			
10			
E(SCF) =	-724.536965		
C	-0.000030	0.035627	1.195657
P	-1.535122	-0.010082	1.969227
P	1.535225	-0.010317	1.968895
H	-0.000234	-0.101785	0.101760
H	-2.514362	0.696544	1.216438
H	-1.503577	0.604179	3.253053
H	-2.195172	-1.256909	2.242243
H	1.502877	0.601096	3.254030
H	2.196248	-1.257211	2.239085
H	2.514136	0.698857	1.217993

(H+)-1H2Me			
RI-BP86/SVP			
16			
E(SCF) =	-803.149049		
C	-0.049290	-0.757562	-0.246214
P	1.641127	-0.524366	0.006634
P	-1.354003	0.104616	0.477211
H	2.311211	-1.357313	-0.928084
H	2.228428	-0.943580	1.250775
C	2.267762	1.175911	-0.198280
C	-2.815196	0.236946	-0.598602
H	-1.885533	-0.367119	1.727566
H	-0.933608	1.416795	0.835134

H	-3.620943	0.779558	-0.066316
H	-2.540381	0.765294	-1.530819
H	-3.167744	-0.784356	-0.844454
H	3.367853	1.173267	-0.064292
H	2.008203	1.546356	-1.208060
H	1.825840	1.841017	0.569364
H	-0.319832	-1.705432	-0.739912

(H⁺)-1HMe2 RI-BP86/SVP

22

E(SCF) =	-881.757973		
C	-0.041190	0.557800	-0.359717
P	1.476093	-0.085875	0.157604
P	-1.593959	-0.191287	-0.294704
C	2.492321	-1.005252	-1.062007
H	1.240480	-1.029037	1.198181
C	2.548783	1.215006	0.854260
C	-2.893323	1.070967	-0.471559
H	-1.927622	-1.140053	-1.325008
C	-1.880095	-1.158198	1.225740
H	-3.888307	0.585105	-0.489667
H	-2.830464	1.784396	0.372356
H	-2.743233	1.616883	-1.423464
H	3.512693	0.784724	1.188584
H	2.743968	1.973203	0.069686
H	2.031947	1.700159	1.703270
H	3.420941	-1.386531	-0.591905
H	1.907439	-1.854049	-1.465928
H	2.755414	-0.326194	-1.897359
H	-2.900771	-1.587773	1.194055
H	-1.158261	-1.994794	1.298975
H	-1.777111	-0.500440	2.110140
H	0.021906	1.449889	-1.005710

(H⁺)-1Me RI-BP86/SVP

28

E(SCF) =	-960.359166		
C	-0.501529	-0.010242	1.458298
P	-0.016286	-1.574911	2.016057
P	-0.140776	1.575754	2.046528
H	-1.287204	-0.034241	0.686197
C	-0.883538	-2.806160	0.988457
H	-1.977255	-2.688407	1.112367
H	-0.588633	-3.828147	1.294918
H	-0.617620	-2.650700	-0.074771
C	-0.414360	-1.971192	3.765949

H	0.109991	-1.266510	4.441594
H	-0.097482	-3.002275	4.020629
H	-1.505527	-1.869076	3.923309
C	1.777874	-1.926932	1.859663
H	2.362076	-1.229555	2.490660
H	2.081146	-1.790632	0.803813
H	2.000839	-2.963790	2.181198
C	-0.393753	2.768925	0.689016
H	-0.211065	3.801521	1.044856
H	-1.438345	2.693758	0.328002
H	0.292907	2.530348	-0.145181
C	1.583216	1.752981	2.634349
H	1.760816	2.796293	2.961446
H	2.285604	1.499097	1.817827
H	1.766758	1.086199	3.499790
C	-1.180473	2.185576	3.436275
H	-0.915343	3.225584	3.713820
H	-1.045735	1.529186	4.318198
H	-2.244796	2.147690	3.131848

	(H+)-1Mes	RI-BP86/SVP	
124			
E(SCF) =	-2817.068856		
C	-0.003211	-0.528333	-0.165550
P	-1.673769	0.012015	0.060946
P	1.709733	-0.084564	-0.152784
C	-2.621719	-0.571159	1.606758
C	-2.615889	-1.008630	-1.250616
C	2.571740	-1.252494	-1.368804
C	-1.843500	1.870031	-0.101541
C	2.612392	-0.510431	1.473703
C	1.955079	1.726700	-0.501462
C	-1.980299	-1.050824	2.788820
C	-2.738565	-1.732450	3.763113
C	-4.123870	-1.924675	3.654327
C	-4.754899	-1.344143	2.540846
C	-2.503008	-2.438359	-1.123205
C	-2.972720	-3.264348	-2.162335
C	-4.049734	-0.668839	1.525921
C	-3.589661	-2.763457	-3.321464
C	-3.794860	-1.380211	-3.369244
C	-3.357123	-0.491005	-2.360276
C	1.863619	-1.949546	-2.401588
C	2.476693	-3.057121	-3.025474
C	3.778100	-3.484528	-2.727874
C	4.509992	-2.684213	-1.835007

C	3.957222	-1.575306	-1.167929
C	-2.362848	2.704341	0.948585
C	-2.503996	4.086821	0.702429
C	-2.156484	4.700296	-0.511592
C	-1.611344	3.874089	-1.504482
C	-1.443466	2.487414	-1.332498
C	2.396319	-1.837347	1.983388
C	2.917913	-2.193669	3.241770
C	3.651920	-1.304581	4.043274
C	3.931567	-0.048668	3.488941
C	3.472933	0.364186	2.218018
C	1.482441	2.662804	0.468522
C	1.684714	4.040211	0.253981
C	2.346190	4.538944	-0.877190
C	2.777823	3.601208	-1.832889
C	2.598569	2.210959	-1.689247
H	3.275009	3.963829	-2.746829
H	1.311883	4.745488	1.013931
H	1.906203	-3.585146	-3.806883
H	5.574039	-2.912284	-1.659946
H	2.742352	-3.220120	3.602752
H	4.582589	0.643562	4.048132
H	-5.852721	-1.400742	2.457391
H	-2.213174	-2.107518	4.656423
H	-2.864335	-4.354539	-2.043058
H	-4.349349	-0.952494	-4.220685
H	-1.308011	4.317130	-2.466384
H	-2.906744	4.711914	1.515278
C	4.086874	1.683250	1.769775
H	3.960938	1.921741	0.704541
H	5.174753	1.653625	1.980393
H	3.683348	2.540753	2.345630
C	1.639315	-2.937964	1.269279
H	1.942670	-3.921346	1.675986
H	1.816124	-2.961111	0.178906
H	0.546806	-2.846840	1.429764
C	4.138354	-1.695691	5.416227
H	4.418921	-2.766604	5.460655
H	3.341585	-1.538525	6.174883
H	5.012328	-1.092870	5.730371
C	-2.019356	-3.188672	0.104184
H	-1.234481	-2.681483	0.685373
H	-1.638465	-4.188085	-0.181737
H	-2.867633	-3.343837	0.803645
C	-3.861298	0.927967	-2.555414
H	-3.496345	1.355173	-3.510503

H	-3.602203	1.629737	-1.751380
H	-4.968005	0.901348	-2.627968
C	-4.030425	-3.677803	-4.437088
H	-4.763583	-3.187099	-5.105616
H	-4.486453	-4.608549	-4.044373
H	-3.164310	-3.983371	-5.062385
C	4.943734	-0.761359	-0.357188
H	4.653488	0.297322	-0.258549
H	5.929098	-0.784377	-0.863886
H	5.091545	-1.165478	0.663602
C	0.525624	-1.556594	-2.988759
H	0.253929	-0.516504	-2.766241
H	-0.308466	-2.192661	-2.628246
H	0.568363	-1.684209	-4.089206
C	4.382261	-4.708507	-3.367893
H	5.454710	-4.559654	-3.603171
H	3.855450	-4.988288	-4.300522
H	4.321418	-5.579265	-2.680151
C	2.596461	6.014296	-1.067655
H	2.354605	6.338143	-2.099972
H	3.667731	6.255964	-0.900864
H	2.003697	6.627238	-0.362201
C	0.830995	2.282776	1.777204
H	0.358445	1.287718	1.763021
H	0.056307	3.025146	2.042489
H	1.569638	2.272680	2.604087
C	3.093525	1.357515	-2.839134
H	3.422148	2.009298	-3.670406
H	2.314300	0.679936	-3.234850
H	3.952870	0.718730	-2.561373
C	-2.752375	2.274598	2.349307
H	-3.710051	1.721337	2.379880
H	-2.873079	3.172527	2.984477
H	-1.999312	1.625501	2.828423
C	-0.852359	1.753860	-2.511542
H	-1.208569	0.716538	-2.611667
H	0.249602	1.720450	-2.419039
H	-1.085054	2.289528	-3.451521
C	-2.382293	6.173324	-0.741441
H	-2.278536	6.755898	0.194831
H	-3.410309	6.354971	-1.122646
H	-1.679848	6.584843	-1.491880
C	-4.906962	-0.025029	0.456274
H	-5.160130	-0.732999	-0.357832
H	-4.434596	0.860404	-0.003124
H	-5.863084	0.310373	0.904690

C	-0.538439	-0.791095	3.140655
H	-0.138886	-1.578584	3.807115
H	-0.449232	0.167883	3.696766
H	0.113378	-0.717514	2.256871
C	-4.904136	-2.696729	4.688611
H	-5.910869	-2.262752	4.848893
H	-4.378181	-2.726943	5.662371
H	-5.054585	-3.748557	4.363003
H	-0.046299	-1.589010	-0.447089

(H+)-1NH2 RI-BP86/SVP

22

E(SCF) = -1056.632823

C	-0.001425	0.000681	-0.934155
P	-1.525120	-0.087965	-0.143156
P	1.524654	0.088148	-0.147592
N	1.490368	-1.004119	1.135849
H	1.140172	-1.940132	0.911655
H	2.295890	-1.022446	1.771699
N	2.661572	-0.028548	-1.369773
H	2.499081	-0.700843	-2.124369
H	3.648491	0.071790	-1.113668
N	2.152510	1.415499	0.687221
H	2.335085	2.251950	0.122493
H	1.697908	1.639369	1.578440
N	-2.151145	-1.416988	0.690413
H	-1.693666	-1.643375	1.579530
H	-2.335877	-2.251945	0.124170
N	-2.665745	0.032233	-1.361532
H	-3.651904	-0.068574	-1.102695
H	-2.505388	0.706461	-2.114857
N	-1.486228	1.001209	1.142792
H	-2.289748	1.018382	1.781200
H	-1.136382	1.937610	0.919670
H	-0.003105	0.001603	-2.033326

(H+)-1NMe2 RI-BP86/SVP

58

E(SCF) = -1527.929492

C	-0.024690	0.060956	-0.857460
P	1.568670	0.016170	-0.186266
P	-1.613337	0.002637	-0.180979
H	-0.027749	-0.094175	-1.946795
N	-1.754253	1.020109	1.177609
N	-2.215774	-1.477928	0.425273
N	-2.688923	0.321824	-1.453061

N	1.774574	-0.482172	1.422172
N	2.450372	-1.011502	-1.200719
N	2.293534	1.552250	-0.161485
C	3.901497	-0.886073	-1.345778
H	4.178490	-0.968976	-2.418221
H	4.448638	-1.681410	-0.790608
H	4.253214	0.094814	-0.983868
C	1.896945	-2.220659	-1.814121
H	0.811202	-2.285795	-1.622513
H	2.382591	-3.138936	-1.412290
H	2.061530	-2.205998	-2.913456
C	3.479332	1.892652	0.630177
H	4.360826	2.088351	-0.020900
H	3.735439	1.072961	1.324109
H	3.294361	2.813562	1.224887
C	1.991783	2.519458	-1.218044
H	1.902895	3.537943	-0.784105
H	1.030584	2.262103	-1.700849
H	2.786593	2.546852	-1.996984
C	1.411410	0.343676	2.573628
H	0.491076	-0.028517	3.075505
H	1.239191	1.388588	2.263228
H	2.234026	0.336873	3.321678
C	2.116806	-1.863865	1.754941
H	1.266745	-2.403221	2.229243
H	2.968169	-1.882309	2.469592
H	2.419326	-2.421069	0.850902
C	-1.129366	2.347458	1.134014
H	-0.907657	2.680095	2.169344
H	-1.798513	3.110063	0.672876
H	-0.183543	2.316496	0.565927
C	-2.999813	1.033190	1.961880
H	-3.699611	1.820806	1.601468
H	-2.767861	1.249195	3.025917
H	-3.515669	0.059418	1.907657
C	-1.775345	-1.976997	1.730725
H	-0.857603	-2.604038	1.643951
H	-2.572512	-2.610140	2.173495
H	-1.564136	-1.146839	2.426282
C	-2.406960	-2.569856	-0.538288
H	-1.490330	-3.196166	-0.640816
H	-2.669754	-2.174924	-1.535186
H	-3.230311	-3.228828	-0.192929
C	-4.133593	0.115529	-1.291341
H	-4.665393	1.080561	-1.133575
H	-4.342047	-0.547091	-0.433630

H	-4.553555	-0.355857	-2.205806
C	-2.366106	1.219349	-2.565362
H	-1.285509	1.440158	-2.599357
H	-2.912014	2.185090	-2.473875
H	-2.660177	0.754016	-3.530788

	(H+)-1Ph	RI-BP86/SVP	
70			
E(SCF) =	-2109.621415		
C	-0.000127	-0.000132	0.572304
P	1.582058	0.126519	-0.127843
P	-1.582138	-0.126597	-0.128272
C	2.025117	1.787684	-0.782284
C	2.759536	-0.248194	1.231505
C	1.924262	-1.041079	-1.509130
C	-2.025010	-1.787581	-0.783296
C	-2.759953	0.247709	1.230895
C	-1.924028	1.041392	-1.509309
H	-0.000268	-0.000240	1.671845
C	1.286125	2.904746	-0.328575
C	1.634222	4.212302	-0.750872
C	2.732125	4.402661	-1.634691
C	3.475039	3.277147	-2.090089
C	3.121636	1.973583	-1.662543
C	2.427202	-1.235104	2.194022
C	3.336594	-1.553290	3.232918
C	4.589581	-0.884509	3.311971
C	4.919484	0.105141	2.345373
C	4.004777	0.420380	1.309188
C	2.441301	-2.329188	-1.226441
C	2.667032	-3.253789	-2.276125
C	2.370546	-2.892060	-3.619856
C	1.853037	-1.597778	-3.901275
C	1.633650	-0.676051	-2.846963
C	-1.286148	-2.904768	-0.329683
C	-1.634129	-4.212208	-0.752432
C	-2.731784	-4.402325	-1.636612
C	-3.474568	-3.276685	-2.091913
C	-3.121284	-1.973239	-1.663910
C	-2.427892	1.234381	2.193750
C	-3.337544	1.552251	3.232516
C	-4.590517	0.883389	3.311098
C	-4.920146	-0.106023	2.344162
C	-4.005180	-0.420943	1.308108
C	-2.441168	2.329408	-1.226380
C	-2.666654	3.254307	-2.275855

C	-2.369821	2.892972	-3.619614
C	-1.852212	1.598782	-3.901276
C	-1.633069	0.676757	-2.847174
H	-2.696109	2.626265	-0.200938
H	-3.080743	4.248313	-2.055201
H	-2.548881	3.607264	-4.436365
H	-1.634748	1.312240	-4.939961
H	-1.254293	-0.323331	-3.092904
H	-1.466099	1.760171	2.158145
H	-3.076016	2.313819	3.980900
H	-5.298063	1.126256	4.117275
H	-5.883320	-0.632160	2.405173
H	-4.280043	-1.200871	0.587474
H	-0.435242	-2.764457	0.348528
H	-1.058754	-5.079867	-0.400637
H	-3.005542	-5.414517	-1.968271
H	-4.322266	-3.421879	-2.776656
H	-3.708020	-1.122086	-2.033214
H	4.279846	1.200486	0.588826
H	5.882669	0.631216	2.406749
H	5.296926	-1.127623	4.118250
H	3.074854	-2.315043	3.981041
H	1.465391	-1.760837	2.158050
H	1.058744	5.079864	-0.399005
H	0.435028	2.764249	0.349356
H	3.708473	1.122531	-2.031919
H	4.322928	3.422528	-2.774555
H	3.005976	5.414944	-1.965996
H	2.695975	-2.626345	-0.201020
H	1.254960	0.324117	-3.092500
H	1.635840	-1.310932	-4.939933
H	2.549794	-3.606122	-4.436767
H	3.081044	-4.247868	-2.055654

	(H+)-1THP	RI-BP86/SVP	
82			
E(SCF) =	-1992.167165		
H	1.062694	1.691899	-0.152781
C	0.455872	0.783261	-0.016066
P	1.314194	-0.668703	-0.391489
P	-1.180884	1.107960	0.422364
N	-1.878861	-0.215587	1.207298
C	-3.347344	-0.470524	1.255042
C	-3.491876	-1.528803	2.357868
C	-2.389822	-1.143584	3.355137
C	-1.221969	-0.738968	2.440625

H	-3.724412	-0.830771	0.277648
H	-3.917128	0.449223	1.509082
H	-4.507363	-1.534719	2.799163
H	-3.301370	-2.541669	1.944856
H	-2.116619	-1.960250	4.051236
H	-2.716189	-0.278111	3.969159
H	-0.572763	-1.606097	2.194325
H	-0.574918	0.034879	2.903236
N	-1.175451	2.517697	1.344901
C	0.028831	3.253136	1.808261
C	-0.502712	4.142447	2.945011
C	-1.957165	4.416403	2.531508
C	-2.409343	3.063246	1.963641
H	0.453850	3.874465	0.986537
H	0.824294	2.558770	2.144423
H	-0.476403	3.589057	3.907078
H	0.100314	5.062104	3.072600
H	-1.994407	5.193544	1.739618
H	-2.598272	4.757996	3.367047
H	-3.229981	3.160656	1.224353
H	-2.772284	2.396248	2.779054
N	-2.320518	1.425941	-0.806406
C	-2.473657	2.799190	-1.368395
C	-2.472795	2.602484	-2.891572
C	-3.100824	1.211216	-3.052708
C	-2.481936	0.423076	-1.888355
H	-1.666450	3.473292	-1.020399
H	-3.439406	3.238385	-1.030840
H	-3.026535	3.401976	-3.421080
H	-1.431656	2.601014	-3.277402
H	-2.896139	0.740200	-4.033929
H	-4.202822	1.268355	-2.932888
H	-1.489447	0.004189	-2.178227
H	-3.122245	-0.425119	-1.568546
N	0.537131	-1.956662	-1.159755
C	0.483249	-2.037586	-2.644010
C	-0.628815	-3.067125	-2.924516
C	-0.663421	-3.927216	-1.651141
C	-0.428766	-2.893502	-0.541889
H	1.462010	-2.378184	-3.047463
H	0.257479	-1.055124	-3.112439
H	-1.601934	-2.550591	-3.057755
H	-0.434894	-3.649252	-3.846000
H	0.161337	-4.670044	-1.660441
H	-1.613625	-4.480748	-1.520710
H	-0.014838	-3.345136	0.380927

H	-1.375161	-2.374425	-0.268563
N	2.562816	-0.172275	-1.409727
C	3.800366	-0.964666	-1.596507
C	4.678182	-0.061177	-2.478201
C	3.648317	0.687679	-3.338254
C	2.511176	0.978098	-2.345736
H	3.590453	-1.933597	-2.107732
H	4.280688	-1.197834	-0.624175
H	5.244063	0.653778	-1.845262
H	5.413894	-0.638614	-3.070543
H	3.282947	0.032804	-4.156957
H	4.048052	1.610578	-3.801424
H	1.521122	1.063070	-2.837879
H	2.694267	1.936106	-1.807168
N	1.954509	-1.421456	0.978928
C	2.533263	-0.590455	2.068388
C	3.222323	-1.613200	2.985093
C	3.688805	-2.700589	2.004825
C	2.508108	-2.801991	1.027904
H	1.745004	-0.007577	2.585245
H	3.272142	0.139094	1.664443
H	4.045383	-1.162252	3.572521
H	2.490659	-2.035989	3.705175
H	3.918471	-3.668459	2.491500
H	4.605928	-2.370168	1.472124
H	1.743639	-3.508833	1.424300
H	2.797643	-3.165943	0.022885

	(H+)-2Ad	RI-BP86/SVP	
58			
E(SCF) =	-1005.000640		
C	-0.237088	5.273253	21.100159
N	-0.529355	5.606532	19.823398
N	-1.273326	5.601475	21.899160
C	-2.261718	6.163775	21.105453
C	-1.797181	6.166868	19.809896
H	0.694437	4.810241	21.431521
C	0.395422	5.389988	18.650946
C	1.710006	6.176523	18.884384
C	2.663640	5.945583	17.688926
C	2.974880	4.437578	17.565221
C	1.664436	3.656718	17.322567
C	0.706246	3.877898	18.516289
C	1.990763	6.448519	16.393986
C	0.682638	5.663404	16.159406
C	-0.275474	5.890605	17.353848

C	0.990277	4.156558	16.027106
C	-1.364261	5.404384	23.388722
C	-0.073041	4.746109	23.920261
C	-0.187995	4.553249	25.452209
C	-0.378226	5.927441	26.129144
C	-1.670967	6.583828	25.599836
C	-1.555513	6.782859	24.070493
C	-1.393756	3.641552	25.765340
C	-2.684890	4.301380	25.236373
C	-2.574173	4.489181	23.705209
C	-2.882895	5.677510	25.909421
H	-2.276520	6.524176	18.896318
H	-3.213365	6.517783	21.510493
H	1.481068	7.257126	19.002607
H	2.196661	5.837510	19.824382
H	3.600553	6.511371	17.872526
H	3.680246	4.263860	16.726344
H	3.480405	4.069884	18.484427
H	1.880321	2.571112	17.241908
H	1.175564	3.499387	19.449949
H	-0.240228	3.314825	18.370918
H	-1.226447	5.342925	17.179467
H	-0.514824	6.972195	17.440050
H	0.182110	6.029102	15.239126
H	2.675519	6.311236	15.531560
H	1.782231	7.537666	16.463847
H	1.658158	3.980801	15.158520
H	0.057179	3.585979	15.831345
H	0.083329	3.759816	23.431384
H	0.806235	5.386693	23.690836
H	0.748193	4.079712	25.813647
H	0.497721	6.581962	25.931186
H	-0.437943	5.801857	27.230089
H	-1.811442	7.577791	26.072979
H	-0.696176	7.442076	23.823222
H	-2.471733	7.277140	23.683328
H	-3.508998	4.941401	23.311466
H	-2.442578	3.509939	23.197248
H	-3.557033	3.648348	25.447102
H	-2.990987	5.550790	27.006604
H	-3.822212	6.151877	25.551943
H	-1.253311	2.640346	25.304027
H	-1.470228	3.478346	26.860304

(H+)-2Cl

RI-BP86/SVP

E(SCF) =	-1145.346129		
C	0.062943	-1.221815	0.000333
N	-1.033625	-0.431076	0.000544
Cl	-2.635428	-1.018405	0.000423
N	1.123780	-0.383361	0.000126
Cl	2.749556	-0.900642	-0.000531
C	-0.672907	0.908958	0.000356
H	-1.411906	1.717637	0.000299
C	0.704514	0.939193	0.000205
H	1.406559	1.780181	-0.000060
H	0.087659	-2.317579	-0.000075

(H+)-2F RI-BP86/SVP

10			
E(SCF) =	-424.582125		
C	0.068722	-1.213202	0.000155
N	-1.009317	-0.401263	0.000671
F	-2.259832	-0.866260	0.001021
N	1.102788	-0.345986	0.000134
F	2.376057	-0.744983	-0.000271
C	-0.680136	0.934532	0.000122
H	-1.431969	1.732497	-0.000024
C	0.704189	0.970781	0.000054
H	1.413284	1.806957	-0.000176
H	0.097353	-2.309746	-0.000456

(H+)-2H RI-BP86/SVP

10			
E(SCF) =	-226.449739		
C	0.069789	-1.203752	0.000217
N	-1.031637	-0.432938	0.000538
H	-1.992320	-0.794635	0.000468
N	1.127712	-0.373739	0.000158
H	2.106338	-0.683581	-0.000274
C	-0.676422	0.905813	0.000383
H	-1.416436	1.712344	0.000339
C	0.700083	0.943239	0.000096
H	1.394205	1.789640	-0.000216
H	0.099828	-2.299065	-0.000480

(H+)-2Me RI-BP86/SVP

16			
E(SCF) =	-305.024672		
C	-0.173303	-0.028834	1.644701
N	-0.013251	1.073497	2.404476
C	-0.111672	2.462909	1.937034

N	-0.009842	-1.119084	2.420819
C	-0.104091	-2.515624	1.974093
C	0.262990	-0.700737	3.714557
H	0.435478	-1.407377	4.532791
C	0.260624	0.675366	3.704375
H	0.430786	1.394698	4.511981
H	-0.920717	2.982492	2.483574
H	0.849290	2.982289	2.110184
H	-0.339519	2.467869	0.857100
H	-0.911784	-3.029412	2.528080
H	-0.331476	-2.537410	0.894275
H	0.858271	-3.029612	2.155368
H	-0.398990	-0.037195	0.572602

	(H+)-2Mes	RI-BP86/SVP	
48			
E(SCF) =	-923.992426		
N	-1.098208	-0.002722	0.645273
C	-2.473718	-0.010065	0.172379
N	1.098090	0.003539	0.645452
C	-3.156879	1.223869	0.073482
C	-4.489075	1.181728	-0.380733
H	-5.043038	2.129182	-0.470827
C	-5.130475	-0.025451	-0.720131
C	-4.400943	-1.227104	-0.597655
H	-4.887255	-2.181335	-0.855178
C	-3.067679	-1.253708	-0.153169
C	-2.502775	2.534921	0.442268
H	-1.526484	2.675229	-0.066049
H	-2.313833	2.609811	1.534052
H	-3.148747	3.387485	0.163070
C	-6.560843	-0.045039	-1.199441
H	-6.639246	-0.515078	-2.201282
H	-6.988323	0.972931	-1.264497
H	-7.200205	-0.641061	-0.515821
C	-2.310536	-2.556743	-0.040482
H	-2.993633	-3.418063	-0.157893
H	-1.531786	-2.650978	-0.827378
H	-1.801480	-2.664007	0.939194
C	0.000011	0.000035	-0.138980
C	-0.688287	-0.001195	1.973710
H	-1.410680	-0.006695	2.795643
C	0.687948	0.003297	1.973824
H	1.410197	0.009562	2.795877
C	2.473665	0.010328	0.172717
C	3.068240	1.253736	-0.152498

C	4.402014	1.226723	-0.595517
H	4.889176	2.180878	-0.851680
C	5.131196	0.024836	-0.717523
C	4.489443	-1.182048	-0.377602
H	5.043743	-2.129516	-0.465468
C	3.156782	-1.223764	0.075199
C	2.311636	2.557081	-0.039809
H	2.994947	3.418110	-0.158081
H	1.532352	2.651222	-0.826180
H	1.803297	2.664964	0.940181
C	6.559033	0.042822	-1.204385
H	6.616607	0.413974	-2.248853
H	7.182547	0.722821	-0.588749
H	7.017445	-0.963297	-1.176054
C	2.502454	-2.534392	0.445103
H	3.148582	-3.387284	0.167275
H	2.312764	-2.608057	1.536843
H	1.526510	-2.675243	-0.063729
H	0.000108	-0.000474	-1.234030

(H+)-2NH2 RI-BP86/SVP

14			
E(SCF) =	-337.021615		
C	0.037994	-1.224174	-0.001441
N	-1.053319	-0.441427	-0.116681
N	-2.330337	-0.988243	-0.256175
N	1.111516	-0.417596	0.116707
N	2.400524	-0.936054	0.253912
C	-0.668929	0.899545	-0.070966
H	-1.394218	1.716918	-0.146752
C	0.697087	0.914553	0.076370
H	1.403801	1.747747	0.155287
H	2.988206	-0.613257	-0.527451
H	2.807882	-0.619005	1.144777
H	-2.925627	-0.680335	0.525422
H	-2.743960	-0.678175	-1.146635
H	0.050268	-2.319841	-0.003542

(H+)-2NMe2 RI-BP86/SVP

26			
E(SCF) =	-494.148291		
C	0.010761	-1.247849	-0.001423
N	-1.042414	-0.450404	-0.266494
N	-2.307047	-0.978092	-0.586959
N	1.071254	-0.461419	0.267388
N	2.330999	-1.002237	0.585176

C	-0.645501	0.885873	-0.164638
H	-1.333128	1.719823	-0.337409
C	0.686664	0.878940	0.171926
H	1.381926	1.705697	0.348709
H	0.005701	-2.343012	-0.004007
C	-3.310077	-0.646953	0.434422
C	-2.701957	-0.647885	-1.963186
C	3.336681	-0.676307	-0.435282
C	2.729502	-0.681331	1.962560
H	3.639180	-1.267530	2.191421
H	2.960894	0.398628	2.122140
H	1.935080	-0.995656	2.665460
H	4.246150	-1.262584	-0.205904
H	2.972826	-0.987010	-1.432781
H	3.615176	0.403998	-0.461178
H	-4.224855	-1.223828	0.202330
H	-2.949544	-0.965045	1.430795
H	-3.578575	0.435769	0.464561
H	-3.616982	-1.224616	-2.194777
H	-2.923156	0.434831	-2.118456
H	-1.910217	-0.966770	-2.667052

	(H+)-2Ph	RI-BP86/SVP	
30			
E(SCF) =	-688.255360		
C	0.013348	-1.158694	-0.098920
N	-1.087652	-0.466315	0.271120
C	-2.452021	-0.882291	0.048139
N	1.109424	-0.462029	0.277632
C	2.476728	-0.872643	0.062767
C	-0.680839	0.709483	0.892024
H	-1.399608	1.418748	1.313115
C	0.694351	0.712162	0.896093
H	1.407823	1.424227	1.321444
H	0.016857	-2.091852	-0.670863
C	-3.375257	0.045570	-0.465779
C	-4.700333	-0.364321	-0.677095
C	-5.089561	-1.683456	-0.387656
C	-4.154394	-2.599889	0.122483
C	-2.828017	-2.203183	0.351055
H	-3.059322	1.067932	-0.720770
H	-5.429817	0.351989	-1.082331
H	-6.129339	-1.998486	-0.558427
H	-4.460172	-3.629106	0.360473
H	-2.102646	-2.906172	0.787177
C	3.399304	0.058798	-0.445828

C	4.727218	-0.345876	-0.649247
C	5.119949	-1.663422	-0.357318
C	4.185414	-2.583483	0.147418
C	2.856145	-2.192003	0.368071
H	3.080865	1.079875	-0.702839
H	5.456238	0.373269	-1.050277
H	6.161949	-1.974362	-0.521919
H	4.493834	-3.611465	0.387329
H	2.131001	-2.897825	0.799965

(H+)-2Me_Me RI-BP86/SVP

22

E(SCF) =	-383.618282		
C	1.051382	-1.010095	0.000000
N	-0.272598	-1.254379	0.000000
C	-0.888341	-2.583547	0.000000
N	1.242510	0.322432	0.000000
C	2.546008	0.990865	0.000000
C	0.000000	0.963846	0.000000
C	-0.134933	2.449159	0.000000
C	-0.963167	-0.038455	0.000000
C	-2.452598	0.036943	0.000000
H	-1.515458	-2.710786	0.902526
H	-1.515458	-2.710786	-0.902526
H	-0.095423	-3.351599	0.000000
H	2.648087	1.622623	0.902480
H	3.345164	0.229344	0.000000
H	2.648087	1.622623	-0.902480
H	-1.201195	2.737736	0.000000
H	0.334348	2.905243	0.896009
H	0.334348	2.905243	-0.896009
H	-2.783737	1.090739	0.000000
H	-2.889587	-0.449987	-0.896093
H	-2.889587	-0.449987	0.896093
H	1.840918	-1.769073	0.000000

(H+)-PHCDP_C__hRI-BP86/SVP

12

E(SCF) =	-800.693170		
C	0.308926	0.138684	0.792862
P	0.124326	-1.362750	1.605637
P	0.006014	1.438860	1.873073
H	-0.888153	-2.272143	1.154998
H	1.256738	-2.233944	1.712938
H	-1.081899	2.329600	1.593748
H	1.063382	2.366141	2.152897

C	-0.378833	0.537297	3.414460
H	-0.631024	1.058386	4.352378
C	-0.322065	-0.804059	3.286443
H	-0.522367	-1.512059	4.106846
H	0.579145	0.251012	-0.265037

(H+)-PHCDP_C__iPr_RI-BP86/SVP

102

E(SCF) = -2195.726921

C	0.096717	0.027368	0.644948
P	-0.114537	-1.472272	1.472987
P	0.083023	1.413290	1.701911
N	-1.382801	-2.394347	0.782106
N	1.262985	-2.464812	1.731898
N	-1.046078	2.597944	1.194188
N	1.579712	2.191952	1.951067
C	-0.413069	0.526561	3.292114
C	-0.518765	-0.822006	3.122204
C	-0.729979	1.166959	4.594377
C	-1.393848	2.256204	7.128594
C	-0.199992	0.612962	5.787610
C	-1.604168	2.275445	4.701387
C	-1.934230	2.809848	5.956371
C	-0.525913	1.154548	7.038994
H	0.491037	-0.240897	5.724652
H	-2.058844	2.699488	3.796509
H	-2.627999	3.661704	6.018007
H	-0.096267	0.714282	7.951357
H	-1.650908	2.680272	8.110639
C	-1.727105	-3.682889	1.454038
H	-0.873973	-3.878808	2.132277
C	-1.789419	-4.901471	0.518499
H	-0.858623	-5.018210	-0.068519
H	-2.642150	-4.852951	-0.185534
H	-1.923754	-5.819010	1.125739
C	-2.976966	-3.595189	2.355337
H	-2.951661	-2.689271	2.992724
H	-3.019690	-4.480705	3.021673
H	-3.918195	-3.575874	1.775632
C	-2.069514	-1.927508	-0.460893
H	-1.885648	-0.836338	-0.468369
C	-3.595060	-2.110453	-0.450737
H	-3.903135	-3.171978	-0.516373
H	-4.019891	-1.598693	-1.337437
H	-4.060479	-1.665948	0.448648
C	-1.443129	-2.484063	-1.753646

H	-0.355181	-2.277695	-1.796284
H	-1.908100	-1.996595	-2.634847
H	-1.588265	-3.575323	-1.865736
C	2.183389	2.263747	3.325004
H	1.327466	2.419541	4.011680
C	3.119532	3.467825	3.517207
H	3.375603	3.543840	4.592610
H	2.658028	4.427168	3.217533
H	4.076561	3.350981	2.970462
C	2.890999	0.973738	3.777341
H	3.038186	0.988225	4.876421
H	3.890868	0.858597	3.315390
H	2.293811	0.080570	3.519149
C	2.477918	2.483429	0.783215
H	3.046056	3.384267	1.093833
C	3.497338	1.369441	0.485413
H	4.170091	1.175175	1.340293
H	4.133433	1.662363	-0.374062
H	2.983246	0.423388	0.228202
C	1.740205	2.884541	-0.501505
H	2.490256	3.208017	-1.249701
H	1.041465	3.722114	-0.338570
H	1.173943	2.048904	-0.956480
C	-2.336979	2.183221	0.522473
H	-2.954026	3.101374	0.579253
C	-3.144853	1.125449	1.288084
H	-2.645361	0.141063	1.317486
H	-4.130344	0.992268	0.798386
H	-3.337250	1.445263	2.331299
C	-2.171702	1.889672	-0.975209
H	-1.579288	0.975708	-1.159515
H	-1.667972	2.730609	-1.489765
H	-3.167276	1.752571	-1.444174
C	-1.148495	4.044383	1.635099
H	-2.117322	4.096974	2.187233
C	-0.083712	4.583094	2.587863
H	0.039734	3.968117	3.497778
H	-0.410086	5.589729	2.917064
H	0.897822	4.692668	2.094834
C	-1.271597	5.003306	0.433629
H	-0.318978	5.081367	-0.126180
H	-1.522172	6.017083	0.804360
H	-2.065050	4.713283	-0.280172
C	1.387363	-3.316074	2.961557
H	0.397862	-3.244123	3.460168
C	2.405224	-2.801256	3.995379

H	2.223490	-1.738951	4.241661
H	3.450908	-2.900497	3.651024
H	2.308181	-3.389063	4.930749
C	1.614500	-4.811346	2.676952
H	2.627025	-5.006960	2.274315
H	0.874761	-5.223936	1.964745
H	1.528386	-5.379891	3.624494
C	2.223427	-2.549655	0.589256
H	2.006466	-1.632103	-0.001243
C	3.695127	-2.435994	1.015652
H	4.327043	-2.322112	0.112316
H	4.050380	-3.342679	1.543879
H	3.866788	-1.557866	1.665877
C	2.011288	-3.745598	-0.360472
H	2.590313	-3.584848	-1.292586
H	0.946920	-3.853030	-0.641440
H	2.353907	-4.702491	0.075556
H	0.371443	0.103257	-0.412117
H	-0.888157	-1.465862	3.935631

(H+)-PHCDP_C__MRI-BP86/SVP

24

E(SCF) =	-957.917668		
C	0.282864	0.135867	0.865667
P	0.111669	-1.370539	1.687816
P	-0.024091	1.474825	1.908492
C	-1.207061	-2.492306	1.090040
C	1.611135	-2.414211	1.818877
C	-1.447792	2.544982	1.480987
C	1.370628	2.623268	2.209336
C	-0.400866	0.579236	3.460667
H	-0.656774	1.109606	4.392772
C	-0.336954	-0.764110	3.356468
H	-0.534856	-1.453376	4.193901
H	1.414248	-3.320658	2.425012
H	1.915213	-2.724416	0.798810
H	2.429651	-1.823030	2.270911
H	-1.281921	-3.395171	1.728044
H	-2.171392	-1.950377	1.080546
H	-0.962049	-2.804476	0.054810
H	-1.603458	3.327632	2.249819
H	-1.241253	3.034689	0.508009
H	-2.356261	1.921736	1.381031
H	1.093587	3.402353	2.946985
H	2.245267	2.049785	2.569741
H	1.635406	3.114964	1.251569

H	0.555841	0.230844	-0.193171
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(H+)-PHCDP_C__NERI-BP86/SVP

20

E(SCF) =	-1022.094485		
C	0.263858	0.126013	0.952293
P	0.016760	-1.379473	1.745301
P	0.033662	1.458615	2.014225
N	-1.117511	-2.306188	0.949425
N	1.181576	-2.564326	2.028146
N	-1.176328	2.626642	1.906043
N	1.367569	2.457896	2.032886
C	-0.396626	0.559622	3.558766
H	-0.629400	1.102552	4.489723
C	-0.384574	-0.782307	3.436812
H	-0.601212	-1.488383	4.255514
H	1.955206	-2.306841	2.651646
H	1.518312	-3.064646	1.196024
H	-1.326561	-3.255933	1.272827
H	-1.881861	-1.828993	0.465282
H	1.353591	3.327857	2.574387
H	2.290896	2.039051	1.897603
H	-2.141531	2.299312	2.027670
H	-1.096154	3.278886	1.115929
H	0.535523	0.224520	-0.106897

(H+)-PHCDP_C__NMRI-BP86/SVP

44

E(SCF) =	-1336.309368		
C	0.259710	0.064359	1.159968
P	-0.091293	-1.391200	2.017885
P	0.211357	1.447902	2.190212
N	-1.454646	-2.189651	1.430987
N	1.028374	-2.656245	2.179018
N	-0.899854	2.713255	1.978942
N	1.681829	2.268479	2.261134
C	-0.264298	0.639621	3.770082
H	-0.422005	1.220735	4.693455
C	-0.303235	-0.708463	3.710267
H	-0.521440	-1.358046	4.573728
C	2.160961	-2.497393	3.095739
C	1.338177	-3.470046	0.995198
C	-1.908998	-3.458537	2.013678
C	-2.445635	-1.520067	0.587082
C	1.841730	3.484662	3.068299
C	2.939872	1.648312	1.842193

C	-2.302601	2.502752	2.348176
C	-0.721409	3.615673	0.832981
H	3.028795	-1.987386	2.618549
H	1.868610	-1.917181	3.991567
H	2.495477	-3.499061	3.435410
H	2.195887	-3.057240	0.417163
H	1.599930	-4.499977	1.314066
H	0.458803	-3.527700	0.327822
H	-2.144455	-4.186085	1.208276
H	-1.120301	-3.892977	2.653550
H	-2.828683	-3.311592	2.621896
H	-2.691454	-2.160807	-0.286123
H	-3.387628	-1.324557	1.146092
H	-2.044773	-0.558726	0.219143
H	3.505954	2.347418	1.190848
H	3.579854	1.399483	2.717732
H	2.737253	0.721956	1.275546
H	2.370545	4.265445	2.481692
H	0.854939	3.882724	3.364944
H	2.439950	3.280352	3.983620
H	-1.267052	3.257921	-0.069546
H	-1.106929	4.622848	1.093434
H	0.350942	3.710424	0.581635
H	-2.896082	2.039581	1.526967
H	-2.385306	1.855650	3.242076
H	-2.763149	3.481338	2.594896
H	0.485969	0.105444	0.086866

(H+)-PHCDP RI-BP86/SVP

11			
E(SCF) =	-816.718278		
C	0.303240	0.149369	0.774111
P	0.114750	-1.320029	1.645692
P	0.013160	1.470761	1.827501
H	-0.920861	-2.230912	1.268946
H	1.241004	-2.183158	1.822032
H	-1.086799	2.356877	1.576199
H	1.068933	2.395262	2.126459
C	-0.359229	0.453332	3.373702
H	-0.613167	0.931755	4.341438
N	-0.304765	-0.818227	3.257823
H	0.563603	0.230124	-0.290186

(H+)-PHCDP_iPrCyc RI-BP86/SVP

87	
E(SCF) =	-2053.456567

C	0.534550	-0.277243	0.925706
P	-0.322957	-1.539159	1.701131
P	0.422970	1.228885	1.781274
N	-1.833401	-2.163468	1.116696
N	0.438225	-3.045850	1.740846
N	-0.586746	2.387052	1.037560
N	1.878797	2.011954	2.230282
C	-0.378194	0.413070	3.387515
N	-0.722649	-0.825233	3.219130
C	-0.691781	1.094622	4.660156
C	-1.311985	2.298622	7.143669
C	-0.235313	2.399041	4.966755
C	-1.462977	0.399702	5.631166
C	-1.770578	0.998531	6.855965
C	-0.541421	2.994966	6.197110
H	0.376267	2.943515	4.235794
H	-1.810869	-0.615546	5.395885
H	-2.372742	0.450916	7.596158
H	-0.175559	4.008020	6.420967
H	-1.555294	2.768178	8.108729
C	-2.920310	-2.459626	2.133087
H	-2.446759	-2.738938	3.101769
C	-3.816534	-3.628662	1.704566
H	-3.285700	-4.599149	1.658691
H	-4.301797	-3.438079	0.725311
H	-4.624500	-3.741788	2.453641
C	-3.779055	-1.210627	2.361059
H	-3.169763	-0.343864	2.677007
H	-4.523818	-1.403443	3.159286
H	-4.323862	-0.936906	1.435697
C	-1.388911	-3.263121	0.231640
H	-0.934613	-2.816226	-0.679589
C	2.643921	1.420887	3.383573
H	1.904573	0.843329	3.977495
C	3.215287	2.515476	4.299805
H	3.670480	2.051132	5.197027
H	2.439689	3.225757	4.641542
H	4.013736	3.097677	3.796480
C	3.750708	0.440297	2.957969
H	4.169443	-0.064024	3.851301
H	4.592564	0.957297	2.455517
H	3.362352	-0.337061	2.274473
C	2.762735	2.720444	1.233416
H	3.736086	2.775118	1.759019
C	3.006694	1.935765	-0.063766
H	3.390068	0.916948	0.134264

H	3.758033	2.464040	-0.684373
H	2.085022	1.853811	-0.671397
C	2.349968	4.166899	0.954352
H	3.174895	4.695093	0.435469
H	2.130196	4.715862	1.890371
H	1.462318	4.212380	0.299298
C	-1.379483	2.125953	-0.221316
H	-1.884547	3.097582	-0.381513
C	-2.492503	1.078194	-0.095609
H	-2.104543	0.048743	0.019595
H	-3.120602	1.101750	-1.009705
H	-3.154007	1.294801	0.763707
C	-0.510390	1.906334	-1.466218
H	0.011989	0.931421	-1.449070
H	0.236874	2.714306	-1.589138
H	-1.157749	1.913732	-2.366074
C	-1.024893	3.599340	1.814323
H	-0.232957	3.751189	2.574023
C	-1.090029	4.891922	0.976657
H	-0.210585	5.034561	0.324395
H	-1.140692	5.759325	1.664526
H	-1.999935	4.937946	0.345834
C	-2.375495	3.396641	2.525800
H	-3.207658	3.355842	1.794655
H	-2.578154	4.249850	3.203892
H	-2.402304	2.472688	3.132541
C	1.757534	-3.432293	2.296464
H	1.669458	-4.528239	2.465213
C	2.005041	-2.791510	3.665790
H	1.183354	-3.027727	4.369257
H	2.090007	-1.690402	3.588700
H	2.952882	-3.168250	4.098142
C	2.901162	-3.203476	1.296161
H	3.037785	-2.123489	1.089091
H	2.701405	-3.713806	0.332717
H	3.855750	-3.602188	1.693911
C	-0.323619	-4.065484	0.996812
H	0.346336	-4.609808	0.297712
H	-2.241900	-3.876937	-0.102842
H	-0.773978	-4.812414	1.689933
H	1.126507	-0.419710	0.016239

(H+)-PHCDP_iPr_PIRI-BP86/SVP

101

E(SCF) =	-2211.776368		
C	0.140691	0.094512	0.568269

P	-0.018956	-1.411959	1.395918
P	0.098000	1.447939	1.662229
N	-1.322824	-2.338735	0.811596
N	1.356341	-2.395543	1.620451
N	-1.018999	2.643756	1.146142
N	1.587136	2.201464	2.020303
C	-0.418037	0.376591	3.203999
N	-0.390568	-0.904260	3.001040
C	-0.843926	0.917082	4.511774
C	-1.704057	1.862074	7.034386
C	-0.761076	0.088999	5.660362
C	-1.377399	2.221450	4.650839
C	-1.808149	2.686828	5.901739
C	-1.179131	0.561949	6.908971
H	-0.354530	-0.926258	5.551307
H	-1.488140	2.862285	3.766860
H	-2.233449	3.697387	5.991865
H	-1.097305	-0.086241	7.794259
H	-2.035906	2.230570	8.016655
C	-1.631611	-3.595779	1.562619
H	-0.719526	-3.787561	2.159405
C	-1.818743	-4.841370	0.681925
H	-0.954043	-5.010850	0.012483
H	-2.735373	-4.793860	0.063331
H	-1.917215	-5.731465	1.335064
C	-2.776798	-3.431915	2.581604
H	-2.620870	-2.526638	3.199494
H	-2.795599	-4.309468	3.259582
H	-3.770550	-3.367317	2.100993
C	-2.106884	-1.896345	-0.381599
H	-1.911620	-0.808708	-0.437267
C	-3.628383	-2.058896	-0.241898
H	-3.950961	-3.117770	-0.253354
H	-4.118344	-1.564894	-1.104731
H	-4.014778	-1.587067	0.680279
C	-1.595480	-2.501565	-1.702678
H	-0.514536	-2.304544	-1.845553
H	-2.132875	-2.042219	-2.557345
H	-1.755059	-3.594992	-1.761551
C	2.049468	2.391688	3.440994
H	1.134505	2.625411	4.021755
C	3.001583	3.586837	3.621194
H	3.124728	3.774393	4.706183
H	2.624890	4.520165	3.164090
H	4.013636	3.381741	3.218534
C	2.676576	1.142382	4.080944

H	2.831607	1.314291	5.165178
H	3.662150	0.898412	3.639206
H	2.023758	0.257898	3.973379
C	2.590441	2.419360	0.923373
H	3.196241	3.277388	1.276951
C	3.542650	1.231353	0.711489
H	4.104364	0.981268	1.630543
H	4.284984	1.474171	-0.075586
H	2.979715	0.333600	0.394115
C	1.977433	2.871428	-0.409736
H	2.798177	3.129647	-1.107708
H	1.342833	3.767486	-0.292849
H	1.375411	2.082809	-0.900590
C	-2.350628	2.210022	0.569043
H	-2.968088	3.127090	0.644657
C	-3.098445	1.169892	1.415185
H	-2.602047	0.182957	1.426993
H	-4.116355	1.026116	1.000886
H	-3.215623	1.513932	2.461668
C	-2.282559	1.872627	-0.927167
H	-1.701008	0.954034	-1.120942
H	-1.813970	2.695082	-1.500321
H	-3.306293	1.721304	-1.325759
C	-1.072106	4.126023	1.457056
H	-2.014547	4.251696	2.042458
C	0.038540	4.736667	2.308666
H	0.173021	4.233106	3.281974
H	-0.249762	5.784954	2.522851
H	1.009321	4.758436	1.783409
C	-1.226193	4.962884	0.170872
H	-0.318684	4.900858	-0.461606
H	-1.374951	6.026375	0.443739
H	-2.093139	4.661937	-0.445372
C	1.583615	-3.167123	2.889314
H	0.672294	-2.972339	3.490618
C	2.761291	-2.651603	3.737726
H	2.737709	-1.551942	3.830902
H	3.745462	-2.943613	3.326956
H	2.692164	-3.082422	4.757328
C	1.698397	-4.689988	2.697739
H	2.645770	-4.975798	2.200441
H	0.861393	-5.115387	2.111674
H	1.696720	-5.179936	3.692101
C	2.196713	-2.580744	0.395633
H	1.959730	-1.688035	-0.226637
C	3.707250	-2.519685	0.669116

H	4.247229	-2.461753	-0.296979
H	4.072117	-3.427522	1.188066
H	3.984618	-1.634728	1.270366
C	1.845463	-3.818233	-0.453760
H	2.356875	-3.751183	-1.435481
H	0.758452	-3.881071	-0.644637
H	2.170756	-4.762386	0.021598
H	0.337121	0.206982	-0.502606

(H+)-PHCDP_Me RI-BP86/SVP

23

E(SCF) = -973.950355

C	0.296522	0.124955	0.807289
P	0.117844	-1.361647	1.669061
P	-0.006827	1.464733	1.844210
C	-1.226368	-2.475693	1.154350
C	1.601835	-2.393762	1.883259
C	-1.445740	2.536283	1.469798
C	1.376543	2.614078	2.196855
C	-0.373149	0.442181	3.378845
H	-0.635287	0.920752	4.345947
N	-0.312257	-0.833145	3.281202
H	1.380021	-3.251051	2.548397
H	1.920117	-2.770033	0.890179
H	2.415200	-1.778195	2.311420
H	-1.306360	-3.329451	1.855258
H	-2.177557	-1.911529	1.128719
H	-1.004818	-2.853995	0.136069
H	1.087890	3.357697	2.966278
H	2.259086	2.037783	2.532684
H	1.635988	3.151537	1.262033
H	-1.602697	3.284649	2.272072
H	-1.249350	3.070573	0.517963
H	-2.349752	1.910689	1.346774
H	0.567123	0.203349	-0.253792

(H+)-PHCDP_NH2 RI-BP86/SVP

19

E(SCF) = -1038.129327

C	0.322701	0.190708	0.880118
P	0.124762	-1.303251	1.720433
P	0.074884	1.519745	1.931077
H	0.591566	0.271669	-0.181232
N	-1.094521	-2.422105	1.498604
H	-1.195936	-2.841445	0.568001
H	-1.990978	-2.241161	1.962491

N	1.469744	-2.249916	1.566965
H	2.387112	-1.814573	1.442297
H	1.469228	-3.202489	1.946053
N	-1.135005	2.549459	1.425578
H	-1.341079	3.412229	1.939083
H	-1.913377	2.159557	0.888232
N	1.213411	2.657885	2.419246
H	1.422637	3.410332	1.751158
H	2.063350	2.303216	2.872139
H	-0.465746	0.977540	4.448982
C	-0.252977	0.491245	3.472918
N	-0.261377	-0.784704	3.358357

(H+)-PHCDP_NMe2RI-BP86/SVP

43

E(SCF) =	-1352.348065		
C	0.355612	0.006772	0.786350
P	0.068469	-1.431808	1.703746
P	0.269101	1.398918	1.792630
N	-1.278952	-2.416835	1.489929
N	1.355727	-2.496278	1.644803
N	-0.986672	2.456975	1.411181
N	1.567198	2.447063	2.081874
C	-0.015777	0.462338	3.395466
N	-0.206776	-0.805249	3.323730
H	-0.115947	0.992994	4.366121
C	-2.079651	2.071278	0.516580
H	-1.853306	1.102855	0.035016
H	-2.211997	2.839224	-0.274986
H	-3.038522	1.979616	1.072401
C	-1.221063	3.692909	2.169397
H	-0.374634	3.896096	2.849284
H	-2.154437	3.616259	2.768708
H	-1.329150	4.555150	1.477607
C	1.938833	3.448596	1.072692
H	2.323476	4.359165	1.576790
H	1.057550	3.732137	0.468861
H	2.729458	3.070092	0.386781
C	2.694129	1.960224	2.882882
H	3.158652	2.813503	3.418523
H	3.478277	1.471456	2.261493
H	2.355990	1.231718	3.645999
C	2.699505	-2.092907	1.220991
H	3.401950	-2.079605	2.082635
H	2.671595	-1.086521	0.767178
H	3.088262	-2.813403	0.471077

C	1.290518	-3.818658	2.284061
H	1.958434	-3.856487	3.170889
H	1.615488	-4.602182	1.567783
H	0.257653	-4.038327	2.605019
C	-1.420264	-3.099121	0.197497
H	-0.426354	-3.272148	-0.257656
H	-2.042538	-2.517686	-0.519246
H	-1.901079	-4.087049	0.352507
C	-2.539888	-2.151957	2.190736
H	-2.337510	-1.767570	3.207138
H	-3.096987	-3.106071	2.288434
H	-3.189044	-1.428758	1.646572
H	0.572552	0.025852	-0.289136

(H+)-PHCDP_NMe2MRI-BP86/SVP

46

E(SCF) = -1391.647284

C	0.354389	0.021781	0.820631
P	0.077755	-1.423135	1.731247
P	0.246912	1.400425	1.838936
H	0.592971	0.053979	-0.249937
N	-1.259270	-2.419342	1.490327
N	1.372624	-2.479487	1.655898
N	-1.005858	2.464007	1.451911
N	1.554616	2.447387	2.117383
C	-0.059072	0.454982	3.458914
N	-0.211341	-0.820233	3.341601
C	-0.247491	1.180151	4.754992
H	0.555109	1.924313	4.929911
H	-0.294136	0.462158	5.594675
H	-1.201743	1.749696	4.724841
C	-2.089632	2.078956	0.545948
H	-1.851714	1.117328	0.056305
H	-2.223072	2.853674	-0.238913
H	-3.052466	1.972667	1.092901
C	-1.255728	3.690086	2.217975
H	-0.407785	3.907543	2.891628
H	-2.183945	3.598344	2.824932
H	-1.386134	4.554099	1.531919
C	1.886292	3.493160	1.139016
H	2.308493	4.374096	1.665293
H	0.981193	3.813749	0.592867
H	2.637185	3.139516	0.397117
C	2.726336	1.900677	2.808689
H	3.223949	2.705740	3.387824
H	3.471366	1.472578	2.100466

H	2.435648	1.103060	3.519767
C	2.713258	-2.063363	1.236820
H	3.415533	-2.047377	2.098952
H	2.678284	-1.055422	0.786936
H	3.110020	-2.776846	0.484192
C	1.317877	-3.805598	2.287042
H	1.980427	-3.843072	3.178237
H	1.655097	-4.582141	1.568627
H	0.285203	-4.037912	2.599923
C	-1.379865	-3.084230	0.187361
H	-0.378824	-3.248670	-0.255002
H	-1.992741	-2.494808	-0.531373
H	-1.860697	-4.075309	0.321181
C	-2.531509	-2.169796	2.174450
H	-2.345510	-1.795391	3.197465
H	-3.085275	-3.127727	2.253421
H	-3.177430	-1.444304	1.628801

	(H+)-6	RI-BP86/SVP	
38			
E(SCF) =	-1187.278072		
C	3.203021	0.995478	-0.096154
P	3.396165	2.362740	1.039775
C	2.514862	-0.112501	0.199899
O	1.912001	-1.076009	0.450962
C	2.118232	2.208626	2.320996
C	5.056408	2.324628	1.777983
C	3.214050	3.912969	0.107870
H	3.675773	1.049177	-1.091476
C	2.960086	6.298942	-1.396100
C	3.993496	5.367415	-1.705586
C	4.121665	4.175807	-0.952010
C	5.708716	1.082402	1.978614
C	6.984823	1.049914	2.593714
C	7.606064	2.262535	3.008128
C	6.944575	3.506578	2.801364
C	5.668924	3.537835	2.184785
C	0.763576	2.021039	1.934410
C	-0.239082	1.906618	2.928019
C	0.111489	1.981315	4.307007
C	1.470389	2.171614	4.684601
C	2.474677	2.285442	3.689968
C	2.186547	4.833952	0.424173
C	2.060246	6.030236	-0.327762
H	2.860346	7.224968	-1.981937
H	4.691589	5.577837	-2.528921

H	4.936957	3.483624	-1.203145
H	5.252836	0.137318	1.655683
H	7.499736	0.090362	2.746724
H	8.599070	2.238636	3.481566
H	7.428224	4.442943	3.115317
H	5.182914	4.509492	2.024874
H	0.465149	1.966424	0.878622
H	-1.289357	1.758003	2.637355
H	-0.667526	1.889583	5.078777
H	1.741080	2.225376	5.749024
H	3.517668	2.423733	4.003786
H	1.482193	4.650399	1.245650
H	1.266236	6.751294	-0.085448

LS-Addukte/BH3-CL/RI-BP86_SVP

	BH3-2Me	RI-BP86/SVP	
19			
E(SCF) =	-331.268397		
C	1.151053	0.818039	5.350397
N	1.358770	0.027199	4.249777
N	0.968022	-0.066817	6.381843
B	1.142770	2.409659	5.341409
H	0.271369	2.772004	4.532449
H	2.245392	2.783550	4.906445
H	0.927298	2.872379	6.463969
C	1.060531	-1.380537	5.932099
C	1.307552	-1.319545	4.585101
C	1.601716	0.570239	2.920472
H	1.448920	-2.114849	3.847277
H	0.943802	-2.238954	6.599847
C	0.711236	0.313439	7.765124
H	-0.264884	-0.088974	8.101157
H	1.512817	-0.071117	8.426439
H	0.692772	1.417451	7.806782
H	1.719369	-0.262322	2.203602
H	0.755317	1.216011	2.617434
H	2.515135	1.195805	2.928489

C(NMe2)2-BH3 RI-BP86/SVP

23			
E(SCF) =	-333.642138		
C	0.120696	0.014340	1.265553
N	0.846250	1.015826	1.849309
N	-0.251366	-1.014552	2.086735
C	0.539368	-1.474178	3.229436
C	-1.254358	-1.978045	1.637122

C	0.692280	1.422688	3.246886
C	1.617018	1.967459	1.051037
H	2.601615	2.136790	1.536837
H	1.093819	2.946009	0.972472
H	1.762387	1.568793	0.034810
H	0.050642	-1.288695	4.210775
H	1.579208	1.193953	3.877233
H	0.536499	2.522051	3.275784
H	-0.198346	0.945052	3.691344
H	1.534183	-0.995011	3.228413
H	0.695740	-2.569207	3.133427
H	-0.784773	-2.841291	1.116698
H	-1.815197	-2.352774	2.517910
H	-1.947560	-1.487647	0.932974
B	-0.342301	0.029268	-0.269617
H	0.133010	0.959801	-0.914236
H	-0.129126	-1.073005	-0.789373
H	-1.578578	0.191506	-0.212203

CO_BH3 RI-BP86/SVP

6			
E(SCF) =	-139.868566		
C	0.015108	0.000171	0.066659
O	-0.014134	0.000127	1.215181
B	0.053715	-0.000013	-1.449149
H	-1.123163	-0.000154	-1.802630
H	0.654400	1.026593	-1.757638
H	0.654496	-1.026724	-1.757228

PH3_BH3 RI-BP86/SVP

8			
E(SCF) =	-369.695003		
P	0.220019	0.088974	0.037890
H	-0.220244	-0.627552	1.193546
H	1.258017	-0.795156	-0.390813
H	-0.804165	-0.309907	-0.875790
B	0.621863	1.973157	0.214612
H	-0.439818	2.460100	0.590529
H	1.520451	1.998827	1.049681
H	0.964509	2.302952	-0.916431

PMe3_BH3 RI-BP86/SVP

17			
E(SCF) =	-487.584529		
P	0.097117	-0.171595	0.122740
C	0.081781	-0.092082	1.962273

C	1.345159	-1.467815	-0.267949
C	0.896811	1.403735	-0.396315
H	1.091791	0.084470	2.382727
H	-0.598054	0.723113	2.278578
H	-0.321414	-1.045206	2.356910
H	1.466512	-1.526425	-1.367310
H	2.326950	-1.259612	0.201951
H	0.966019	-2.446348	0.086300
H	1.008397	1.400954	-1.498283
H	1.889632	1.545053	0.075380
H	0.234007	2.247736	-0.122249
B	-1.625652	-0.476065	-0.665097
H	-1.422750	-0.500574	-1.879882
H	-1.999485	-1.557129	-0.207678
H	-2.316991	0.476391	-0.301297

	PPh3_BH3	RI-BP86/SVP	
38			
E(SCF) =	-1062.212354		
P	-1.104777	-0.044710	-0.019142
C	-0.362837	0.201538	-1.689662
C	-0.352279	-1.603780	0.616605
C	-0.389503	1.296223	1.025725
B	-3.038955	-0.068346	-0.028076
H	-3.375209	1.068897	-0.352172
H	-3.348452	-0.922174	-0.856600
H	-3.364102	-0.363762	1.120202
C	0.847432	-0.416370	-2.083674
C	1.371490	-0.202207	-3.383366
C	0.680878	0.637545	-4.299054
C	-0.538966	1.252959	-3.904604
C	-1.057515	1.029749	-2.605122
H	1.386258	-1.083365	-1.398357
H	2.307748	-0.690418	-3.686800
H	1.082341	0.802948	-5.308626
H	-1.084111	1.893678	-4.611110
H	-2.010960	1.494285	-2.319750
C	0.851907	-1.619969	1.359276
C	1.384779	-2.844868	1.833956
C	0.709176	-4.066192	1.564393
C	-0.504594	-4.048447	0.823642
C	-1.032034	-2.819064	0.356838
H	-1.980804	-2.816608	-0.196412
H	-1.038342	-4.987200	0.621869
H	1.117452	-5.017248	1.933945
H	2.316157	-2.851075	2.416607

H	1.378815	-0.686271	1.594577
C	-1.094977	1.669815	2.195756
C	-0.596618	2.696682	3.035154
C	0.613683	3.364110	2.700678
C	1.315199	2.995852	1.520441
C	0.811317	1.964355	0.688792
H	1.357826	1.708336	-0.228069
H	2.244058	3.516636	1.250241
H	0.999378	4.165880	3.345798
H	-1.150242	2.984186	3.939421
H	-2.041381	1.176062	2.454204

LS-Addukte/LS-4Me

(BH3)2-4Me

RI-BP86/SVP

47

E(SCF) =	-705.316749		
C	-0.159263	-0.368310	0.067795
C	-0.497662	0.067935	-1.292222
C	-0.003961	0.716115	1.044581
N	-0.067454	-0.541649	-2.438347
N	-1.402295	1.092109	-1.506787
N	0.636492	1.893834	0.704141
N	-0.351805	0.635165	2.364678
C	-1.020780	-0.898163	-3.490637
H	-0.778614	-0.419044	-4.464368
H	-2.048135	-0.631073	-3.191461
H	-0.989625	-2.000034	-3.627381
C	1.214983	-1.226463	-2.572641
H	1.672982	-0.933452	-3.542695
H	1.075526	-2.327646	-2.561548
H	1.885336	-0.967889	-1.736427
C	-2.374698	1.528880	-0.512639
H	-2.524403	0.723628	0.228239
H	-3.348404	1.709742	-1.015426
H	-2.067551	2.474444	-0.014301
C	0.387458	3.148097	1.407399
H	1.242599	3.465942	2.044385
H	-0.510825	3.058188	2.043137
H	0.211725	3.951792	0.660309
C	1.541287	2.019398	-0.431679
H	1.059426	2.526815	-1.295937
H	1.908091	1.017625	-0.717108
H	2.420395	2.626352	-0.127460
C	0.595819	1.034867	3.406545
H	1.553397	1.351607	2.960373
H	0.802685	0.149646	4.044862

H	0.198699	1.846654	4.054300
C	-1.455977	-0.172125	2.874916
H	-2.021944	0.431280	3.618015
H	-1.075616	-1.087990	3.373514
H	-2.118372	-0.491925	2.053610
C	-1.400355	1.891200	-2.727861
H	-0.470601	1.716910	-3.297419
H	-1.450165	2.967284	-2.454976
H	-2.268014	1.674571	-3.389954
B	1.303703	-1.262352	0.502125
H	2.309869	-0.604069	0.164224
H	1.287624	-1.391272	1.728503
H	1.281200	-2.359055	-0.046027
B	-1.358620	-1.663046	0.185557
H	-1.122601	-2.338812	1.181348
H	-2.504275	-1.167814	0.232025
H	-1.244904	-2.344061	-0.836342

	BH3-4Me	RI-BP86/SVP	
43			
E(SCF) =	-678.724100		
C	0.093867	-0.332439	0.014769
C	-0.341552	0.026557	-1.294335
C	0.196234	0.696489	0.984230
N	0.182844	-0.539194	-2.438301
N	-1.395919	0.905520	-1.520328
N	0.556393	2.014867	0.667434
N	0.054162	0.471497	2.339590
C	-0.661718	-1.016175	-3.527141
H	-0.425056	-0.524325	-4.497362
H	-1.725595	-0.843023	-3.288956
H	-0.515168	-2.111465	-3.654229
C	1.563258	-0.993966	-2.503964
H	2.030992	-0.618164	-3.442115
H	1.629617	-2.101369	-2.477147
H	2.122294	-0.615723	-1.630749
C	-2.468308	1.088398	-0.555722
H	-2.429207	0.281834	0.197006
H	-3.452313	1.050474	-1.075290
H	-2.404889	2.068400	-0.031460
C	-0.016194	3.159878	1.357589
H	0.742116	3.738756	1.935122
H	-0.803846	2.825690	2.056332
H	-0.477375	3.863014	0.626425
C	1.441562	2.349260	-0.431337
H	0.904859	2.780913	-1.307829

H	1.979434	1.444897	-0.765212
H	2.189378	3.105445	-0.098645
C	0.920682	1.097728	3.327480
H	1.729303	1.657520	2.824944
H	1.384887	0.310742	3.961278
H	0.373783	1.794445	4.003930
C	-0.881903	-0.513111	2.863530
H	-1.721800	-0.008919	3.396758
H	-0.370326	-1.189438	3.578721
H	-1.261799	-1.147019	2.040706
C	-1.477698	1.759434	-2.697139
H	-0.533756	1.704259	-3.268344
H	-1.640298	2.816422	-2.388874
H	-2.317069	1.480512	-3.374823
B	0.313255	-1.929932	0.383978
H	1.045913	-2.043961	1.380475
H	-0.806690	-2.440065	0.625293
H	0.787286	-2.559975	-0.571898

	CO2-4Me	RI-BP86/SVP	
42			
E(SCF) =	-840.561133		
C	-0.005998	-0.066759	-0.030335
C	-0.469864	0.076659	-1.361357
C	0.100818	1.025605	0.865812
N	0.027516	-0.683803	-2.392976
N	-1.502760	0.938497	-1.714121
N	0.521304	2.290723	0.470169
N	-0.139804	0.890086	2.212438
C	-0.872599	-1.449525	-3.254122
H	-0.578414	-1.371622	-4.322640
H	-1.912411	-1.098136	-3.139530
H	-0.836616	-2.514088	-2.936504
C	1.385052	-1.217664	-2.360789
H	1.817147	-1.164504	-3.383840
H	1.383369	-2.262750	-1.987592
H	2.007975	-0.618806	-1.672048
C	-2.513414	1.376866	-0.767805
H	-2.501601	0.721740	0.120618
H	-3.519625	1.320833	-1.238451
H	-2.355136	2.427321	-0.433385
C	0.104662	3.501494	1.163436
H	0.941645	3.993997	1.709321
H	-0.689733	3.257442	1.891652
H	-0.293171	4.239810	0.431957
C	1.343762	2.508914	-0.706678

H	0.762960	2.929163	-1.559004
H	1.794996	1.554161	-1.028121
H	2.159556	3.226423	-0.468386
C	0.857069	1.318081	3.192912
H	1.603328	1.982166	2.724033
H	1.390059	0.415862	3.563700
H	0.385599	1.847734	4.048100
C	-1.049408	-0.129056	2.725270
H	-1.620347	0.294999	3.579911
H	-0.485235	-1.032093	3.037966
H	-1.755879	-0.435184	1.932731
C	-1.604815	1.528864	-3.041225
H	-0.680999	1.322617	-3.611094
H	-1.736565	2.630703	-2.957269
H	-2.470349	1.135046	-3.621674
C	0.417848	-1.530887	0.485974
O	1.104348	-1.533473	1.535301
O	0.005282	-2.474194	-0.229642

LS-Addukte/LS-6Ph

(BH3)2-6

RI-BP86/SVP

45

E(SCF) = -1240.094642

C	3.582929	1.380155	-0.569754
P	3.554551	2.656711	0.688732
C	2.405685	1.088710	-1.176307
O	1.441550	0.745765	-1.732243
C	2.269308	2.352854	1.956974
C	5.157751	2.733235	1.554479
C	3.191428	4.312661	-0.015089
B	3.796920	-0.266690	0.136604
H	3.960997	-1.010786	-0.821600
H	2.803308	-0.538237	0.809240
H	4.821041	-0.114592	0.803612
H	4.003248	1.533251	-2.968853
B	4.641234	1.741015	-1.932993
H	5.583046	0.965393	-1.814972
H	4.933741	2.935677	-1.846576
C	2.542766	6.889309	-1.017501
C	2.238046	5.727723	-1.778610
C	2.566277	4.443545	-1.277150
C	6.356757	2.390407	0.883870
C	7.597174	2.516012	1.556474
C	7.642287	2.988940	2.896894
C	6.434065	3.329764	3.564176
C	5.193631	3.199167	2.892616

C	1.070422	3.106263	1.959346
C	0.053980	2.821642	2.905303
C	0.237442	1.777979	3.853009
C	1.442223	1.021454	3.845399
C	2.454148	1.306183	2.896477
C	3.502999	5.467189	0.743364
C	3.181086	6.754381	0.246129
H	2.298048	7.886633	-1.409601
H	1.764347	5.824363	-2.765167
H	2.360931	3.569243	-1.907251
H	6.335354	2.014955	-0.148226
H	8.525487	2.239232	1.038480
H	8.605988	3.082946	3.417421
H	6.461963	3.684852	4.603485
H	4.273074	3.443665	3.437332
H	0.908559	3.917309	1.238011
H	-0.876414	3.405846	2.904776
H	-0.550583	1.552894	4.585689
H	1.584160	0.206121	4.567898
H	3.367265	0.697670	2.890406
H	4.011070	5.391285	1.712811
H	3.432836	7.648839	0.832360

BH3-6

RI-BP86/SVP

41

E(SCF) =	-1213.496118		
C	3.355357	0.850674	-0.047778
P	3.415921	2.268892	0.952345
C	2.530183	-0.146616	0.232159
O	1.826987	-1.076557	0.396641
C	2.095283	2.273759	2.228840
C	4.994405	2.420728	1.874746
C	3.190150	3.775745	-0.064165
B	4.410850	0.748613	-1.393147
H	4.963443	1.856498	-1.448883
H	3.731519	0.545905	-2.402498
H	5.230502	-0.150054	-1.176450
C	2.718634	6.082496	-1.642253
C	2.276604	4.807518	-2.091565
C	2.515309	3.655482	-1.301674
C	6.146150	1.752578	1.394077
C	7.370501	1.864007	2.099759
C	7.443901	2.642809	3.287196
C	6.281058	3.304877	3.769207
C	5.058459	3.191127	3.062861
C	0.981572	3.140123	2.131351

C	-0.060243	3.071468	3.090969
C	0.010487	2.128080	4.151937
C	1.130605	1.255423	4.245812
C	2.169075	1.330574	3.285563
C	3.641525	5.039160	0.384322
C	3.405781	6.194465	-0.401985
H	2.543027	6.975880	-2.257973
H	1.766887	4.711259	-3.059938
H	2.209349	2.667894	-1.672960
H	6.097076	1.148707	0.475769
H	8.263329	1.344167	1.726276
H	8.393636	2.727868	3.834072
H	6.331062	3.897724	4.692892
H	4.167432	3.688370	3.467542
H	0.906253	3.870251	1.315293
H	-0.925070	3.744469	3.012208
H	-0.797734	2.069957	4.894570
H	1.187493	0.520980	5.061114
H	3.025231	0.648952	3.377244
H	4.195275	5.145477	1.325361
H	3.763798	7.175289	-0.060443

LS-Addukte/LS-C3O2/BP86_TZ2P

(BH3)2-5.c2v BP86/TZ2P

13

E(SCF) =	-2.592871		
C	1.187667	0.000000	-0.464724
C	0.000000	0.000000	0.143210
C	-1.187667	0.000000	-0.464724
O	-2.259625	0.000000	-0.885864
O	2.259625	0.000000	-0.885864
B	0.000000	1.713615	1.142452
B	0.000000	-1.713615	1.142452
H	0.000000	1.255675	2.249576
H	1.015184	2.207936	0.712103
H	-1.015184	2.207936	0.712103
H	1.015184	-2.207936	0.712103
H	0.000000	-1.255675	2.249576
H	-1.015184	-2.207936	0.712103

BH3-5.cs BP86/TZ2P

9

E(SCF) =	-2.012708		
C	1.185334	-0.362444	0.000000
C	-0.024701	0.166467	0.000000
C	-1.192555	-0.448925	0.000000

O	-2.271729	-0.868531	0.000000
O	2.284912	-0.726929	0.000000
B	0.000053	1.985942	0.000000
H	1.192610	2.205332	0.000000
H	-0.562113	2.247836	-1.036095
H	-0.562113	2.247836	1.036095

LS-Addukte/LS-C3O2/RI-BP86_SVP

(BH3)2-5.c2v BP86/TZ2P

13			
E(SCF) =	-2.592871		
C	1.187667	0.000000	-0.464724
C	0.000000	0.000000	0.143210
C	-1.187667	0.000000	-0.464724
O	-2.259625	0.000000	-0.885864
O	2.259625	0.000000	-0.885864
B	0.000000	1.713615	1.142452
B	0.000000	-1.713615	1.142452
H	0.000000	1.255675	2.249576
H	1.015184	2.207936	0.712103
H	-1.015184	2.207936	0.712103
H	1.015184	-2.207936	0.712103
H	0.000000	-1.255675	2.249576
H	-1.015184	-2.207936	0.712103

(BH3)2-5 RI-BP86/SVP

13			
E(SCF) =	-317.729243		
C	1.211688	0.000177	-0.481750
C	0.000206	0.001902	0.111533
C	-1.210672	-0.004489	-0.482960
O	-2.299077	-0.029817	-0.870840
O	2.300530	0.021363	-0.868640
B	-0.011834	1.616184	1.140392
B	0.009905	-1.605986	1.154371
H	0.704809	1.264189	2.060780
H	0.399962	2.448967	0.346944
H	-1.207483	1.682356	1.402627
H	1.205225	-1.670504	1.418175
H	-0.707878	-1.245696	2.070566
H	-0.401671	-2.444188	0.366557

BH3-5.cs BP86/TZ2P

9			
E(SCF) =	-2.012708		
C	1.185334	-0.362444	0.000000

C	-0.024701	0.166467	0.000000
C	-1.192555	-0.448925	0.000000
O	-2.271729	-0.868531	0.000000
O	2.284912	-0.726929	0.000000
B	0.000053	1.985942	0.000000
H	1.192610	2.205332	0.000000
H	-0.562113	2.247836	-1.036095
H	-0.562113	2.247836	1.036095

	BH3-5	RI-BP86/SVP	
9			
E(SCF) =	-291.149278		
C	0.287417	-0.000037	0.258991
C	-0.220312	0.000005	1.490460
C	0.383005	0.000050	2.677207
O	0.792863	0.000101	3.765721
O	0.643565	-0.000072	-0.848872
B	-2.031839	-0.000006	1.455617
H	-2.260424	0.000098	0.246705
H	-2.313349	-1.051029	2.015697
H	-2.313372	1.050890	2.015919

LS-Addukte/LS-CDC-R/BP86_TZ2P
(BH3)2-3.c2v BP86/TZ2P

27			
E(SCF) =	-5.739498		
B	1.475345	0.000000	-1.760010
B	-1.475345	0.000000	-1.760010
H	-2.402192	0.000000	-0.893712
H	-1.581445	1.016029	-2.422614
H	-1.581445	-1.016029	-2.422614
H	1.581445	1.016029	-2.422614
H	2.402192	0.000000	-0.893712
H	1.581445	-1.016029	-2.422614
C	0.000000	0.000000	-0.929083
C	0.000000	1.219569	-0.100722
N	-1.073542	1.935263	0.296059
C	-0.682605	3.099916	0.927794
C	0.682605	3.099916	0.927794
N	1.073542	1.935262	0.296059
C	0.000000	-1.219569	-0.100722
N	1.073542	-1.935263	0.296059
C	0.682605	-3.099917	0.927794
C	-0.682605	-3.099917	0.927794
N	-1.073542	-1.935263	0.296059
H	1.999933	1.620450	-0.007851

H	1.387416	3.824978	1.308856
H	-1.387416	3.824978	1.308856
H	-1.999933	1.620451	-0.007851
H	1.999933	-1.620451	-0.007851
H	1.387416	-3.824979	1.308855
H	-1.387417	-3.824979	1.308854
H	-1.999933	-1.620451	-0.007851

BH3-3.cs

BP86/TZ2P

23

E(SCF) =

-5.121127

C	0.763971	-0.008573	0.000000
C	0.110780	1.219281	0.000000
C	0.115250	-1.237863	0.000000
N	0.809089	2.404243	0.000000
N	-1.217992	1.630723	0.000000
N	-1.218966	-1.633288	0.000000
N	0.797170	-2.432393	0.000000
C	-0.034683	3.497078	0.000000
C	-1.306465	3.024433	0.000000
C	-1.325411	-3.026903	0.000000
C	-0.059271	-3.514116	0.000000
H	1.827653	2.365112	0.000000
H	0.329605	4.514301	0.000000
H	-2.254466	3.542617	0.000000
H	-2.018878	1.021807	0.000000
H	-2.012209	-1.014528	0.000000
H	-2.279840	-3.533315	0.000000
H	0.292954	-4.535682	0.000000
H	1.819935	-2.380581	0.000000
B	2.404855	0.066029	0.000000
H	2.926522	-1.051980	0.000000
H	2.790015	0.668479	-1.002873
H	2.790015	0.668479	1.002873

LS-Addukte/LS-CDC-R/RI-BP86_SVP

(BH3)2-3Me

RI-BP86/SVP

39

E(SCF) =

-700.562734

C	1.111525	2.587305	1.915797
C	0.726644	1.230404	2.333154
C	1.434613	2.657789	0.482626
N	1.016712	0.578964	3.506147
N	-0.125817	0.385652	1.648031
N	2.201286	1.746819	-0.218800
N	1.163067	3.665524	-0.409193

C	0.347804	-0.638835	3.553999
C	-0.359653	-0.766125	2.392465
C	2.401904	2.191843	-1.521576
C	1.760073	3.392326	-1.634594
C	1.725937	1.124997	4.662001
H	0.430620	-1.302923	4.418651
H	-1.010590	-1.567247	2.031480
C	-0.814041	0.704614	0.401525
C	2.846876	0.567469	0.348228
H	2.986026	1.618028	-2.246368
H	1.679846	4.085173	-2.476597
C	0.545316	4.957038	-0.113341
B	-0.276297	3.430666	2.518922
H	-0.024406	4.628440	2.667869
H	-1.242223	3.263616	1.743879
H	-0.548086	2.940041	3.623732
B	2.573996	3.284699	2.529135
H	2.401753	3.719039	3.670206
H	3.491365	2.436501	2.500381
H	2.867058	4.229855	1.783163
H	2.412635	0.355734	5.064408
H	2.286375	2.024198	4.343930
H	0.990156	1.419285	5.436564
H	-1.727346	0.085262	0.338174
H	-1.108120	1.771928	0.433286
H	-0.180052	0.503958	-0.485366
H	3.717097	0.308265	-0.282171
H	3.206079	0.825354	1.363615
H	2.160171	-0.301732	0.389871
H	1.334887	5.730909	-0.037553
H	-0.162501	5.216005	-0.923930
H	0.021750	4.887219	0.858640

	BH3-3Me	RI-BP86/SVP	
35			
E(SCF) =	-673.945528		
C	1.168465	2.611987	1.878597
C	0.649757	1.371511	2.311838
C	1.534558	2.736795	0.513996
N	0.674512	0.830789	3.597575
N	-0.134624	0.468932	1.567802
N	2.243560	1.814014	-0.263205
N	1.367801	3.839274	-0.318670
C	-0.066989	-0.345750	3.637832
C	-0.569216	-0.574299	2.390394
C	2.505207	2.349053	-1.524766

C	1.967450	3.605734	-1.550252
C	1.543847	1.249194	4.689827
H	-0.160534	-0.929850	4.557989
H	-1.208358	-1.378437	2.014520
C	-0.713358	0.764456	0.272027
C	2.830245	0.595392	0.259776
H	3.060127	1.796213	-2.288034
H	1.951461	4.351744	-2.350000
C	0.512080	4.980330	-0.031785
B	1.470737	3.870135	2.926122
H	1.595035	4.933212	2.307073
H	0.559200	3.963515	3.766388
H	2.565344	3.684994	3.501779
H	0.982115	1.211528	5.643822
H	2.426780	0.577441	4.763818
H	1.880799	2.287055	4.497515
H	-1.601124	0.122735	0.117477
H	-1.024057	1.829748	0.242796
H	-0.003161	0.596294	-0.564362
H	0.049114	5.324798	-0.977656
H	-0.271955	4.665619	0.682308
H	1.075792	5.803337	0.447130
H	3.691110	0.304702	-0.371247
H	3.176035	0.781383	1.296731
H	2.103958	-0.244476	0.289959

	CO2-3Me	RI-BP86/SVP	
34			
E(SCF) =	-835.782377		
C	1.082408	2.618336	1.872257
C	0.682065	1.342957	2.348533
C	1.447175	2.791339	0.511834
N	0.961579	0.767238	3.575544
N	-0.144775	0.426458	1.698773
N	2.217017	1.927098	-0.266754
N	1.183408	3.874475	-0.308138
C	0.308886	-0.452121	3.687019
C	-0.370363	-0.675699	2.519913
C	2.424590	2.480792	-1.527799
C	1.790975	3.693983	-1.542459
C	1.876571	1.312789	4.571027
H	0.387462	-1.065773	4.588775
H	-0.997323	-1.516026	2.208961
C	-0.833365	0.694614	0.450749
C	2.876518	0.740984	0.244887
H	3.008271	1.971305	-2.299598

H	1.716369	4.443847	-2.334958
C	0.321649	4.999062	0.036164
C	1.122278	3.857066	2.865445
O	1.750037	4.855574	2.433728
O	0.520849	3.676974	3.953251
H	2.053321	0.543340	5.344941
H	2.836269	1.574431	4.080035
H	1.442021	2.252336	4.975129
H	-1.708655	0.023903	0.368296
H	-1.176783	1.748774	0.447229
H	-0.180083	0.542608	-0.433589
H	0.138377	5.593927	-0.877485
H	-0.641549	4.613793	0.429114
H	0.805179	5.580223	0.850615
H	3.722580	0.482040	-0.418349
H	3.259658	0.952149	1.263626
H	2.190908	-0.129531	0.308738

LS-Addukte/LS-CDP-R/BP86_TZ2P

	B2H5+-1H	BP86/TZ2P	
16			
E(SCF) =	-2.295605		
C	0.122475	5.991006	12.637916
P	-0.691678	7.010282	11.466011
P	0.935499	6.605214	14.065080
H	0.124769	7.962521	10.804059
H	-1.225224	6.180959	10.462311
H	-1.773215	7.780969	11.963745
H	2.016879	7.491250	13.826306
H	0.118432	7.310317	14.985284
H	1.469288	5.509819	14.768696
B	0.933233	4.740754	11.935966
B	-0.684819	4.584005	12.923648
H	-0.640719	4.218173	14.066836
H	-1.725680	4.488551	12.331896
H	1.974753	4.471808	12.470419
H	0.889486	4.742060	10.735645
H	0.125544	3.730657	12.283935

(BH3)2-1H.c2v **BP86/TZ2P**

17			
E(SCF) =	-2.623459		
C	0.000000	0.000000	0.337363
P	0.000000	-1.498378	-0.549431
P	0.000000	1.498378	-0.549431
H	1.118698	-1.784815	-1.379114

H	-1.118698	-1.784815	-1.379114
H	0.000000	-2.536154	0.401240
H	1.118698	1.784815	-1.379114
H	0.000000	2.536154	0.401240
H	-1.118698	1.784815	-1.379114
B	1.510687	0.000000	1.119614
B	-1.510687	0.000000	1.119614
H	-1.550810	-1.011966	1.802469
H	-2.396077	0.000000	0.264803
H	-1.550810	1.011966	1.802469
H	1.550810	1.011966	1.802469
H	2.396077	0.000000	0.264803
H	1.550810	-1.011966	1.802469

	BH3-1H.cs	BP86/TZ2P	
13			
E(SCF) =	-1.980524		
C	0.001556	0.301040	0.000000
P	1.513602	-0.432368	0.000000
P	-1.461714	-0.534224	0.000000
B	-0.120518	2.005774	0.000000
H	1.035308	2.414526	0.000000
H	-0.710418	2.344875	1.016907
H	-0.710418	2.344875	-1.016907
H	1.924677	-1.291672	1.076491
H	2.513245	0.562257	0.000000
H	1.924677	-1.291672	-1.076491
H	-1.821690	-1.408363	1.079796
H	-1.821690	-1.408363	-1.079796
H	-2.525914	0.391253	0.000000

LS-Addukte/LS-CDP-R/RI-BP86_SVP
(AlCl3)2-1H **RI-BP86/SVP**

17			
E(SCF) =	-3970.062519		
C	-0.115910	0.092183	0.967586
P	-1.052773	-1.242689	1.663646
P	-0.552051	1.699448	1.576161
Al	1.866168	-0.226276	1.653623
Cl	2.961197	1.492107	0.994249
Cl	1.547766	-0.139922	3.815787
Cl	2.346816	-2.223601	1.049980
Al	-0.329172	0.063874	-1.129052
Cl	-1.245344	2.007558	-1.488163
Cl	1.496887	-0.216770	-2.176725
Cl	-1.752066	-1.562489	-1.395736

H	-0.504324	-2.470377	1.218669
H	-2.448376	-1.286062	1.386667
H	-0.951082	-1.284613	3.088711
H	0.342089	2.657657	1.039735
H	-0.392617	1.795004	2.993531
H	-1.869769	2.170956	1.316303

(AlCl₃)₂-1Me RI-BP86/SVP

35

E(SCF) =	-4205.863586		
C	0.215929	0.026071	0.738651
P	-0.478459	-1.562427	1.277799
P	-0.636872	1.470142	1.434005
Al	2.277048	0.094373	1.271244
Cl	3.285563	1.532553	0.046969
Cl	2.329282	0.754945	3.370430
Cl	3.149976	-1.890689	1.241663
Al	0.149157	0.144273	-1.386821
Cl	0.139494	2.210477	-2.046141
Cl	1.716767	-1.052895	-2.219692
Cl	-1.801241	-0.693740	-1.969869
C	0.385996	2.973944	1.343681
H	1.225893	2.884933	2.058322
H	-0.259603	3.832484	1.615200
H	0.769634	3.094644	0.313250
C	-1.087187	1.331515	3.209103
H	-0.161039	1.140088	3.786096
H	-1.829971	0.531776	3.387295
H	-1.527935	2.297518	3.525667
C	-2.203990	1.888299	0.580028
H	-1.961957	2.226560	-0.446660
H	-2.698980	2.707907	1.137658
H	-2.878148	1.016007	0.517811
C	-0.001194	-2.925994	0.169298
H	1.094522	-2.908911	0.018577
H	-0.524025	-2.807059	-0.798382
H	-0.306122	-3.873269	0.656498
C	0.060682	-2.077137	2.952393
H	1.147305	-2.289836	2.918950
H	-0.492483	-2.995572	3.232145
H	-0.124413	-1.285425	3.699568
C	-2.312831	-1.636256	1.327763
H	-2.605417	-2.670216	1.597816
H	-2.695806	-1.395097	0.316509
H	-2.735247	-0.944264	2.079891

	(AlCl ₃) ₂ -1Ph	RI-BP86/SVP	
77			
E(SCF) =	-5355.038989		
C	0.004180	-0.729400	-0.054389
P	-1.573855	0.267341	-0.002365
P	1.565080	0.299030	0.044069
C	1.878693	1.397051	-1.428501
C	1.729777	1.452814	1.496878
C	3.178107	-0.621066	0.068945
C	-1.538808	1.948950	-0.810993
C	-2.227194	0.632144	1.691203
C	-3.023889	-0.538597	-0.831081
Al	-0.064481	-2.018054	-1.835722
Cl	-0.650239	-0.895310	-3.619726
Cl	1.889633	-2.790126	-2.327139
Cl	-1.549277	-3.531926	-1.519173
Al	-0.012878	-2.273028	1.538945
Cl	-1.922169	-2.614443	2.491180
Cl	1.333384	-1.534397	3.087934
Cl	0.767220	-4.174951	0.899779
C	-1.086297	2.106943	-2.143052
C	-2.103595	3.065533	-0.140044
C	-2.217829	4.318186	-0.790191
C	-1.774053	4.469949	-2.131913
C	-1.207921	3.354652	-2.804231
C	-1.398312	0.667309	2.833582
C	-1.936073	1.002219	4.101804
C	-3.315751	1.308016	4.235174
C	-4.151489	1.275127	3.084685
C	-3.607171	0.940414	1.821737
C	2.155423	0.762634	-2.665780
C	2.519525	1.527054	-3.800529
C	2.632960	2.940523	-3.703859
C	2.387587	3.573063	-2.455800
C	2.016008	2.802167	-1.326388
C	0.878368	2.573267	1.651223
C	1.059984	3.484206	2.720750
C	2.104292	3.278667	3.660951
C	2.957401	2.151857	3.514067
C	2.768289	1.248810	2.439280
C	3.357530	-1.983922	0.377501
C	4.660677	-2.543722	0.421797
C	5.798865	-1.739739	0.159076
C	5.618903	-0.363399	-0.151780
C	4.317536	0.187786	-0.196774
C	-3.739498	-1.554596	-0.150803

C	-4.906139	-2.115470	-0.722968
C	-5.369707	-1.664807	-1.988540
C	-4.654887	-0.642211	-2.667014
C	-3.490152	-0.081293	-2.087665
H	-2.470501	2.984528	0.889469
H	-2.660618	5.171179	-0.257695
H	-1.872332	5.437852	-2.643782
H	-0.860153	3.452142	-3.841668
H	-0.659155	1.262270	-2.699899
H	-0.337698	0.397200	2.789370
H	-1.282297	0.995554	4.984345
H	-3.737907	1.551584	5.220376
H	-5.223651	1.496626	3.176854
H	-4.279189	0.912798	0.955729
H	-3.395066	-1.939184	0.817127
H	-5.438315	-2.915630	-0.191014
H	-6.267611	-2.108545	-2.441399
H	-4.996652	-0.289155	-3.649147
H	-2.973732	0.704784	-2.644235
H	4.219698	1.250650	-0.446092
H	6.488803	0.272891	-0.363829
H	6.807360	-2.175902	0.187962
H	4.774797	-3.611843	0.651061
H	2.522067	-2.663884	0.567972
H	0.388680	4.347573	2.824183
H	0.061891	2.768698	0.948930
H	3.433192	0.381911	2.367790
H	3.761953	1.970895	4.239855
H	2.248860	3.980097	4.494843
H	2.131908	-0.330799	-2.767557
H	1.856103	3.327784	-0.379994
H	2.491696	4.662475	-2.361626
H	2.924699	3.535231	-4.581141
H	2.724037	1.017060	-4.751980

	AlCl3-1H	RI-BP86/SVP	
13			
E(SCF) =	-2347.105119		
C	0.705189	-0.151149	-0.506099
P	2.091082	-0.123236	0.481744
P	0.708091	0.407784	-2.113657
Al	-1.050424	0.044107	0.466525
Cl	-0.401706	0.768486	2.419438
Cl	-2.092286	1.509153	-0.768929
Cl	-2.129571	-1.808596	0.602353
H	2.503593	1.061898	1.186272

H	3.315827	-0.472428	-0.181372
H	2.020495	-1.060634	1.547888
H	0.581512	1.804181	-2.437877
H	1.875943	0.066563	-2.876060
H	-0.352695	-0.145398	-2.881455

	AlCl3-1Me	RI-BP86/SVP	
31			
E(SCF) =	-2582.902992		
C	0.646329	0.104291	-0.403817
P	2.051057	-0.126506	0.560513
P	0.605161	0.301581	-2.112109
Al	-1.064048	0.582081	0.549222
Cl	-0.654836	1.036903	2.655262
Cl	-1.898967	2.383191	-0.391770
Cl	-2.481884	-1.056511	0.413872
C	2.663167	1.370903	1.441289
H	3.533226	1.136448	2.087024
H	1.826613	1.753307	2.059340
H	2.944097	2.139893	0.695428
C	1.775397	-1.368611	1.880360
H	2.689576	-1.500265	2.492382
H	1.483095	-2.327834	1.411947
H	0.945950	-1.006436	2.519667
C	3.558746	-0.741658	-0.306624
H	4.358303	-0.895301	0.444725
H	3.916837	-0.002201	-1.048477
H	3.352075	-1.704038	-0.810968
C	0.975100	1.997862	-2.736246
H	2.011296	2.278435	-2.462376
H	0.268151	2.681417	-2.224347
H	0.848647	2.074307	-3.835123
C	-1.055728	-0.071650	-2.784019
H	-1.388551	-1.059685	-2.413786
H	-1.019391	-0.055114	-3.890786
H	-1.764606	0.697880	-2.419510
C	1.719744	-0.788827	-3.101775
H	2.783830	-0.538010	-2.941170
H	1.488140	-0.657470	-4.177345
H	1.544328	-1.844695	-2.819224

	AlCl3-1Ph	RI-BP86/SVP	
73			
E(SCF) =	-3732.133630		
C	6.282892	3.449427	6.393615
P	5.973132	2.282216	7.628212

P	7.290832	4.832088	6.669362
C	5.406765	3.023298	9.230788
C	4.644044	1.079931	7.178093
C	7.363125	1.122323	8.040883
C	7.806568	5.117822	8.428766
C	8.930591	4.816640	5.796513
C	6.446532	6.413072	6.210054
Al	5.538099	3.190986	4.525272
Cl	6.404783	1.402013	3.618813
Cl	3.369536	3.117713	4.601383
Cl	6.176391	4.881037	3.311416
C	5.957743	2.694196	10.489654
H	6.802206	2.000788	10.573611
C	5.442950	3.279707	11.674373
H	5.883284	3.023908	12.647580
C	4.363807	4.200886	11.605587
H	3.959728	4.651052	12.523091
C	3.817483	4.543445	10.338020
H	2.989168	5.262553	10.272532
C	4.345113	3.960500	9.160938
H	3.925563	4.253412	8.189883
C	3.320926	1.202200	7.661642
H	3.024546	2.032460	8.310774
C	2.338599	0.244279	7.309491
H	1.310604	0.352856	7.680319
C	2.677519	-0.847549	6.465463
H	1.914130	-1.584460	6.179444
C	4.009227	-0.973702	5.986411
H	4.280748	-1.805486	5.322499
C	4.987487	-0.015154	6.348014
H	6.003482	-0.131970	5.954591
C	8.589236	1.251283	7.354128
H	8.716833	2.036963	6.597472
C	9.650253	0.340156	7.593442
H	10.596005	0.440762	7.043303
C	9.479846	-0.714825	8.528888
H	10.295471	-1.427789	8.714314
C	8.236491	-0.858208	9.207127
H	8.090753	-1.687680	9.912832
C	7.182959	0.053456	8.955386
H	6.218719	-0.105123	9.455363
C	7.139151	6.074962	9.228730
H	6.305866	6.661444	8.822524
C	7.542014	6.300026	10.568846
H	7.018307	7.047191	11.180219
C	8.623878	5.562152	11.120971

H	8.941733	5.737726	12.158203
C	9.294577	4.598972	10.318896
H	10.135308	4.026814	10.734679
C	8.885344	4.383284	8.980263
H	9.431678	3.646196	8.379978
C	9.972978	5.685785	6.209454
H	9.843427	6.359318	7.065504
C	11.221889	5.680041	5.541767
H	12.023116	6.357732	5.867085
C	11.440967	4.793836	4.451626
H	12.406572	4.789388	3.926677
C	10.402364	3.912402	4.048596
H	10.557358	3.222587	3.207673
C	9.154967	3.925497	4.722523
H	8.372212	3.233266	4.384384
C	7.171054	7.595525	5.933962
H	8.266007	7.596812	5.894537
C	6.485870	8.804282	5.656520
H	7.053347	9.715582	5.423851
C	5.064373	8.835142	5.657189
H	4.531073	9.768449	5.428901
C	4.339287	7.643464	5.928247
H	3.241298	7.647218	5.896485
C	5.033869	6.439365	6.201865
H	4.464399	5.514105	6.354516

	B2H5+-1H	RI-BP86/SVP	
16			
E(SCF) =	-776.616043		
C	0.122539	5.984553	12.637017
P	-0.696025	7.014992	11.459465
P	0.939916	6.607905	14.072876
H	0.127850	7.973756	10.797448
H	-1.237808	6.191729	10.443628
H	-1.782152	7.790453	11.964737
H	2.025765	7.500924	13.828495
H	0.115146	7.319097	14.995021
H	1.481766	5.514617	14.790174
B	0.935710	4.735778	11.933187
B	-0.687475	4.578472	12.924470
H	-0.650030	4.197742	14.078971
H	-1.743478	4.470764	12.330676
H	1.992471	4.454098	12.465290
H	0.898293	4.726851	10.717539
H	0.125504	3.711204	12.280819

	B2H5+-1Ph	RI-BP86/SVP	
76			
E(SCF) =	-2161.687876		
C	0.142154	5.961625	12.650764
P	-0.629358	6.996397	11.365012
P	0.884213	6.612518	14.190524
C	0.606859	7.762795	10.250667
C	-1.724340	6.030937	10.240380
C	-1.703730	8.328257	12.045466
C	1.966652	8.092347	13.984386
C	-0.374810	7.124367	15.434404
C	1.914214	5.329066	15.003006
B	0.892745	4.718789	11.879658
B	-0.635603	4.540660	12.954827
H	-0.429076	4.081373	14.061688
H	-1.760566	4.415821	12.513894
H	1.954479	4.328190	12.303958
H	0.800865	4.752709	10.669835
H	0.063296	3.697087	12.171345
C	3.303432	8.105246	14.455781
C	4.099755	9.271674	14.327116
C	3.559170	10.445394	13.736309
C	2.209081	10.442039	13.287526
C	1.422675	9.272343	13.415308
C	-1.510072	6.311798	15.688343
C	-2.426807	6.661749	16.708383
C	-2.215616	7.833395	17.487755
C	-1.075062	8.643796	17.237381
C	-0.157458	8.285244	16.217614
C	3.139903	4.908194	14.422521
C	3.945737	3.945336	15.076687
C	3.530437	3.391382	16.319383
C	2.306469	3.818512	16.902077
C	1.504688	4.785139	16.244535
C	-2.651504	7.986806	13.043341
C	-3.554770	8.958564	13.539220
C	-3.515272	10.288579	13.037499
C	-2.560997	10.632971	12.040750
C	-1.661440	9.655282	11.548337
C	1.992589	7.643992	10.503796
C	2.934081	8.214209	9.610888
C	2.487703	8.906950	8.452878
C	1.092684	9.012345	8.189995
C	0.157640	8.436387	9.083742
C	-3.110186	5.907121	10.504572
C	-3.946358	5.189864	9.613671

C	-3.398060	4.590621	8.446550
C	-2.007944	4.723705	8.178246
C	-1.177208	5.441853	9.072612
H	3.745855	7.231803	14.947433
H	5.134933	9.270381	14.697166
H	4.174416	11.351996	13.639275
H	1.776265	11.351583	12.847830
H	0.376610	9.318194	13.089829
H	0.719350	8.924637	16.059918
H	-0.900143	9.546616	17.839556
H	-2.924173	8.105386	18.284049
H	-3.298907	6.022198	16.906004
H	-1.687185	5.392679	15.114090
H	0.568666	5.094457	16.723612
H	1.979193	3.397319	17.863017
H	4.152392	2.638599	16.825627
H	4.890609	3.618775	14.619640
H	3.489063	5.307377	13.464603
H	-0.935345	9.955895	10.783639
H	-2.524503	11.659839	11.649963
H	-4.217161	11.045477	13.417241
H	-4.285921	8.685994	14.313222
H	-2.699640	6.971612	13.454600
H	-0.909645	8.499102	8.834371
H	0.743099	9.528687	7.284490
H	3.215723	9.346732	7.755438
H	4.010408	8.113065	9.807296
H	2.361393	7.094526	11.377230
H	-0.110637	5.529089	8.835210
H	-1.576463	4.267283	7.276348
H	-4.045151	4.032030	7.754457
H	-5.020947	5.097034	9.824651
H	-3.572439	6.364211	11.385565

	(BCl3)2-1H	RI-BP86/SVP	
17			
E(SCF) =	-3534.759883		
C	-0.024349	0.001204	0.929122
P	-0.771591	-1.528171	1.576283
P	-0.836334	1.514958	1.533953
B	-0.338756	-0.009514	-0.740661
Cl	-2.226744	-0.394821	-0.879452
Cl	-0.045040	1.710893	-1.393642
Cl	0.610466	-1.305774	-1.615075
B	1.537958	0.024468	1.597022
Cl	2.580695	1.340660	0.871668

Cl	2.259882	-1.685734	1.434388
Cl	1.261365	0.388142	3.474016
H	-0.547137	-2.564514	0.637776
H	-2.177995	-1.462813	1.776411
H	-0.236916	-1.915402	2.832342
H	0.115792	2.563104	1.528021
H	-1.334448	1.430186	2.863217
H	-1.951875	1.896437	0.744503

	(BCI3)2-1Me	RI-BP86/SVP	
35			
E(SCF) =	-3770.539656		
C	-0.022832	0.001207	0.933195
P	-0.856921	-1.550869	1.586328
P	-0.865550	1.536566	1.613926
B	-0.175096	0.022576	-0.796460
B	1.628455	-0.004889	1.470121
Cl	-1.955864	-0.511232	-1.334105
Cl	0.040164	1.754909	-1.505924
Cl	1.006098	-1.119931	-1.618820
Cl	2.680992	1.159560	0.514705
Cl	2.389531	-1.727528	1.403713
Cl	1.745896	0.513124	3.330988
C	-2.407795	2.010829	0.744143
H	-2.167663	2.261788	-0.304778
H	-2.818438	2.894299	1.272801
H	-3.144426	1.189446	0.753634
C	0.200626	3.017423	1.586926
H	1.030129	2.873390	2.302268
H	-0.438218	3.872190	1.887070
H	0.599970	3.159314	0.568470
C	-1.408469	1.441782	3.372146
H	-0.532360	1.218119	4.006664
H	-2.203439	0.690872	3.527681
H	-1.816809	2.438363	3.633278
C	-2.693121	-1.480410	1.720637
H	-3.033102	-0.739114	2.465512
H	-3.026714	-2.483695	2.052566
H	-3.117164	-1.254684	0.725882
C	-0.572843	-3.018006	0.538964
H	0.511019	-3.145759	0.378907
H	-1.083625	-2.869882	-0.429369
H	-1.000262	-3.883379	1.084269
C	-0.350928	-2.035383	3.280316
H	0.729406	-2.267202	3.282610
H	-0.942895	-2.932948	3.549849

H	-0.543392	-1.225846	4.004990
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(BCl3)2-1Ph	RI-BP86/SVP
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77

E(SCF) =	-4919.703957
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C	-0.000158	-0.961077	-0.024614
P	-1.652841	0.148207	0.029560
P	1.646701	0.157093	-0.003177
C	1.931826	1.229055	-1.512952
C	1.808674	1.388185	1.396591
C	3.307230	-0.706923	0.071980
C	-1.584266	1.895524	-0.676640
C	-2.349313	0.506885	1.719642
C	-3.118357	-0.556645	-0.886297
B	-0.071996	-1.875915	-1.503428
Cl	-0.604498	-0.830581	-3.005017
Cl	1.616651	-2.572389	-1.924356
Cl	-1.290177	-3.259089	-1.391034
B	0.032956	-2.053247	1.363732
Cl	-1.683108	-2.395294	2.034702
Cl	1.052136	-1.295484	2.778854
Cl	0.778807	-3.723237	1.040133
C	-1.048202	2.195164	-1.952151
C	-2.243696	2.935075	0.036697
C	-2.364914	4.234586	-0.510955
C	-1.832067	4.523572	-1.796095
C	-1.172362	3.491789	-2.512210
C	-1.521934	0.803765	2.826606
C	-2.088056	1.183163	4.068005
C	-3.497602	1.278928	4.214991
C	-4.329271	0.993500	3.099344
C	-3.756444	0.616644	1.859714
C	2.202064	0.604760	-2.757845
C	2.574140	1.373162	-3.887664
C	2.699520	2.784775	-3.785621
C	2.457023	3.409983	-2.534210
C	2.079960	2.634427	-1.409614
C	0.930497	2.487144	1.536029
C	1.131128	3.460783	2.547153
C	2.227154	3.344931	3.440121
C	3.113613	2.241294	3.304975
C	2.902983	1.276237	2.292079
C	3.548056	-1.970385	0.652065
C	4.868433	-2.477983	0.745917
C	5.969263	-1.719336	0.268098
C	5.728423	-0.442135	-0.304342

C	4.407145	0.058732	-0.398934
C	-3.802331	-1.695342	-0.396006
C	-4.985447	-2.151724	-1.026282
C	-5.497393	-1.474471	-2.165331
C	-4.810846	-0.333424	-2.658038
C	-3.630636	0.120187	-2.019051
H	-2.679097	2.759951	1.025573
H	-2.883022	5.017591	0.059629
H	-1.934218	5.528664	-2.229490
H	-0.752541	3.689987	-3.507643
H	-0.554932	1.415364	-2.542018
H	-0.436435	0.685291	2.773881
H	-1.428878	1.380140	4.924268
H	-3.939440	1.559126	5.181413
H	-5.421706	1.057903	3.195815
H	-4.430493	0.407640	1.022208
H	-3.417035	-2.247109	0.467522
H	-5.493488	-3.045155	-0.638927
H	-6.407942	-1.834795	-2.664391
H	-5.186940	0.196738	-3.543171
H	-3.131323	0.997984	-2.438162
H	4.271496	1.049873	-0.843793
H	6.565487	0.161601	-0.680273
H	6.991949	-2.116225	0.335431
H	5.029250	-3.472148	1.184408
H	2.727897	-2.602607	1.007614
H	0.432926	4.304142	2.636901
H	0.077694	2.622233	0.864230
H	3.593236	0.427912	2.235393
H	3.962172	2.128873	3.993503
H	2.388066	4.094788	4.227389
H	2.152288	-0.485751	-2.858132
H	1.926256	3.160820	-0.463529
H	2.568360	4.497769	-2.430644
H	2.996245	3.382061	-4.659492
H	2.774326	0.866558	-4.841691

	BCI3-1H	RI-BP86/SVP	
13			
E(SCF) =	-2129.453106		
C	-0.002523	-0.030585	0.008845
P	1.427819	0.208156	0.906090
P	-0.085506	0.047388	-1.692623
B	-1.408379	0.086324	0.819600
Cl	-1.065868	1.116960	2.380112
Cl	-2.643391	0.960418	-0.331572

Cl	-2.064157	-1.588475	1.297348
H	1.780878	1.493153	1.442147
H	2.601625	-0.122048	0.155965
H	1.535849	-0.615361	2.064336
H	-0.442996	1.257239	-2.379437
H	1.162549	-0.277559	-2.314122
H	-0.994889	-0.882350	-2.275770

	BCl3-1Me	RI-BP86/SVP	
31			
E(SCF) =	-2365.244185		
C	0.062777	0.174821	-0.042071
P	1.503788	0.219434	0.910385
P	-0.052789	0.054160	-1.761982
B	-1.354638	0.176996	0.782975
Cl	-1.246306	1.151638	2.423016
Cl	-2.772800	0.998133	-0.199996
Cl	-1.887822	-1.593847	1.197592
C	1.963755	1.878407	1.571853
H	2.832525	1.814612	2.257866
H	1.079206	2.273547	2.106167
H	2.203809	2.547128	0.721900
C	1.422743	-0.886319	2.373359
H	2.392285	-0.877871	2.909593
H	1.169329	-1.906330	2.028633
H	0.610799	-0.529936	3.034048
C	3.065837	-0.314323	0.089619
H	3.867343	-0.282704	0.853625
H	3.348613	0.365366	-0.734463
H	2.979369	-1.348425	-0.291643
C	-0.480238	1.620312	-2.637047
H	0.342773	2.347196	-2.490127
H	-1.401258	2.014925	-2.167853
H	-0.641936	1.448667	-3.720480
C	1.457637	-0.493763	-2.665797
H	2.280051	0.238129	-2.572030
H	1.189187	-0.576090	-3.737390
H	1.795263	-1.483573	-2.307256
C	-1.308951	-1.168821	-2.305253
H	-1.087770	-2.138123	-1.820529
H	-1.293058	-1.263641	-3.409023
H	-2.301314	-0.824969	-1.959291

	BCl3-1Ph	RI-BP86/SVP	
73			
E(SCF) =	-3514.474846		

C	-0.103544	0.909131	-0.502006
P	1.492063	0.213372	-0.439785
P	-1.498721	0.052234	0.090710
C	2.323891	0.193906	-2.095567
C	2.687403	0.939876	0.790440
C	1.530576	-1.570843	0.072244
C	-1.687483	-0.049535	1.935978
C	-3.133342	0.793425	-0.375901
C	-1.607375	-1.680792	-0.555306
B	-0.249268	2.476240	-0.974681
Cl	-0.836832	3.584215	0.465743
Cl	-1.440568	2.655185	-2.421170
Cl	1.430579	3.157611	-1.533454
C	1.506859	0.290312	-3.245299
C	2.076798	0.205705	-4.538994
C	3.479184	0.026690	-4.688211
C	4.299863	-0.055880	-3.530875
C	3.720092	0.026900	-2.239893
C	2.414396	2.181366	1.410145
C	3.315500	2.719970	2.363205
C	4.500488	2.015384	2.706741
C	4.766086	0.758621	2.098296
C	3.858039	0.224665	1.151301
C	1.453541	-1.915074	1.444538
C	1.526031	-3.268611	1.854724
C	1.685464	-4.297051	0.886459
C	1.766632	-3.953579	-0.490053
C	1.688966	-2.595960	-0.889660
C	-0.706162	0.544053	2.758148
C	-0.844738	0.533214	4.170159
C	-1.980361	-0.077349	4.765848
C	-2.980436	-0.659196	3.936843
C	-2.834848	-0.635637	2.528695
C	-3.894580	0.298507	-1.459532
C	-5.165367	0.850135	-1.755230
C	-5.687095	1.905996	-0.960497
C	-4.926850	2.393886	0.136155
C	-3.659299	1.833328	0.427936
C	-1.463817	-1.849088	-1.955552
C	-1.611336	-3.125975	-2.548414
C	-1.892982	-4.257676	-1.734789
C	-2.013974	-4.093165	-0.329013
C	-1.873529	-2.807916	0.253717
H	-1.224474	-0.990245	-2.595384
H	-1.504351	-3.243407	-3.635704
H	-2.007771	-5.251952	-2.188557

H	-2.212182	-4.964794	0.309253
H	-1.955030	-2.715888	1.342685
H	-3.523410	-0.511199	-2.095651
H	-5.743883	0.465391	-2.605765
H	-6.667558	2.343774	-1.194099
H	-5.314254	3.215412	0.753633
H	-3.085450	2.240681	1.266893
H	0.154104	1.054661	2.306421
H	-0.082124	1.010871	4.800530
H	-2.095985	-0.084485	5.858760
H	-3.873096	-1.110909	4.391044
H	-3.641634	-1.048103	1.909334
H	4.071019	-0.765164	0.730038
H	5.672449	0.199133	2.367383
H	5.203436	2.435941	3.439457
H	3.096066	3.690420	2.828950
H	1.511362	2.752108	1.153928
H	1.437631	0.307608	-5.426478
H	0.434278	0.495963	-3.138447
H	4.383379	-0.011138	-1.368991
H	5.387126	-0.170612	-3.637144
H	3.927776	-0.026867	-5.689882
H	1.352645	-1.141691	2.214897
H	1.760290	-2.355569	-1.957345
H	1.891381	-4.740648	-1.245789
H	1.750054	-5.348402	1.199752
H	1.468239	-3.522131	2.922115

	(BeCl₂)₂-1H	RI-BP86/SVP	
15			
E(SCF) =	-2594.394347		
C	-0.129765	-0.000017	1.013680
P	-0.813692	-1.533497	1.523743
P	-0.793064	1.520448	1.586205
Be	-0.187876	0.054238	-0.812291
Cl	-0.534474	1.805210	-1.542149
Cl	-0.212333	-1.640454	-1.718193
Be	1.640865	-0.038121	1.465021
Cl	2.298843	-1.786671	1.942864
Cl	2.498229	1.664761	1.704733
H	-0.216825	-2.584424	0.790107
H	-2.218903	-1.665762	1.287440
H	-0.703637	-1.861725	2.908206
H	0.036554	2.585986	1.167965
H	-0.863525	1.640016	3.010472
H	-2.126392	1.834782	1.186125

-----	BeCl2-1H	RI-BP86/SVP	
12			
E(SCF) =	-1659.269473		
C	0.174117	-0.109739	-0.006075
P	1.512699	0.438096	0.890808
P	-0.011745	-0.022405	-1.695516
Be	-1.149561	-0.842683	0.904443
Cl	-0.932950	-0.944326	2.832617
Cl	-2.676480	-1.467197	-0.122153
H	2.817450	-0.125661	0.649491
H	1.236547	0.158744	2.262674
H	1.875331	1.833035	0.859118
H	0.926636	-0.698165	-2.556433
H	-0.015066	1.261271	-2.351677
H	-1.279683	-0.599393	-2.004898

-----	BeCl2-1Me	RI-BP86/SVP	
33			
E(SCF) =	-2830.196719		
C	-0.269191	0.029140	0.952527
P	-0.968357	-1.541259	1.367603
P	-0.745232	1.498219	1.814143
Be	-0.163384	0.298786	-0.932178
Cl	-0.566475	2.124287	-1.608008
Cl	-0.800911	-1.183926	-2.092969
Be	1.515450	-0.111527	1.023453
Cl	2.510399	-0.425912	2.647043
Cl	2.241125	0.105651	-0.781203
C	0.077508	-2.871120	0.683499
C	-2.670290	-1.804599	0.749685
C	-1.024990	-1.936347	3.163843
C	0.492097	2.805626	1.513773
C	-0.778578	1.368000	3.649271
C	-2.380075	2.166110	1.335954
H	-3.021353	-2.823086	1.008104
H	-3.355036	-1.056986	1.195113
H	-2.633254	-1.674842	-0.351718
H	-0.394420	-3.849436	0.899939
H	0.161977	-2.719160	-0.411533
H	1.073304	-2.826536	1.168364
H	-1.272248	-3.009690	3.285198
H	-0.025968	-1.736741	3.599238
H	-1.791280	-1.339080	3.691204
H	-0.873334	2.385657	4.077339
H	-1.631384	0.759308	4.001854

H	0.173719	0.913159	3.986358
H	0.160844	3.737665	2.011999
H	1.462594	2.483568	1.941704
H	0.573714	2.963027	0.419272
H	-2.586680	3.107961	1.881471
H	-2.341147	2.351586	0.242623
H	-3.172769	1.428014	1.566141

	BeCl2-1Ph	RI-BP86/SVP	
75			
E(SCF) =	-3979.407594		
C	-0.014745	0.369535	1.188691
P	-1.571147	0.171284	0.330131
P	1.564711	0.173526	0.354806
C	1.700134	-1.309913	-0.746633
C	2.174607	1.544452	-0.726851
C	2.899117	-0.113156	1.609957
C	-1.701151	-1.278868	-0.832771
C	-2.071390	1.574006	-0.767777
C	-2.974636	-0.123945	1.495807
Be	0.214541	-0.493558	2.767336
Cl	0.406474	-2.373831	3.164646
Cl	0.334027	0.862966	4.209735
Be	-0.173086	1.992996	2.314099
Cl	-2.010186	2.649569	2.592015
Cl	1.138794	3.425905	1.885470
C	-2.262593	-2.503359	-0.399726
C	-1.257370	-1.162413	-2.173954
C	-1.376488	-2.248394	-3.073624
C	-1.945648	-3.475694	-2.636178
C	-2.387203	-3.597919	-1.291848
C	-1.492596	2.858031	-0.639286
C	-1.938247	3.926815	-1.457503
C	-2.971832	3.719214	-2.408967
C	-3.553146	2.427755	-2.539959
C	-3.101995	1.363755	-1.722429
C	1.185316	-2.553248	-0.304543
C	1.375131	-3.722483	-1.078900
C	2.080988	-3.655998	-2.311665
C	2.598529	-2.409280	-2.754139
C	2.411115	-1.243747	-1.969387
C	1.381677	1.978788	-1.815112
C	1.858423	2.971487	-2.705153
C	3.149208	3.535378	-2.515549
C	3.952653	3.087571	-1.432562
C	3.465850	2.093298	-0.547790

C	3.244317	0.894569	2.546496
C	4.284323	0.676064	3.483195
C	4.991713	-0.555667	3.494773
C	4.650597	-1.562913	2.552089
C	3.612128	-1.339378	1.615889
C	-2.848963	-1.054076	2.552398
C	-3.949159	-1.329731	3.402632
C	-5.193989	-0.681846	3.190700
C	-5.321053	0.245278	2.120018
C	-4.215365	0.521821	1.280837
H	-0.826827	-0.227888	-2.549688
H	-1.030305	-2.142721	-4.110673
H	-2.046120	-4.319667	-3.332843
H	-2.834518	-4.538727	-0.942815
H	-2.628578	-2.626414	0.626197
H	-0.701693	3.064893	0.094607
H	-1.486011	4.920671	-1.337644
H	-3.324837	4.551112	-3.034809
H	-4.355860	2.257241	-3.270367
H	-3.569619	0.378943	-1.843717
H	-1.909028	-1.587140	2.752752
H	-3.828110	-2.038159	4.233569
H	-6.046076	-0.883046	3.854776
H	-6.272027	0.770591	1.958585
H	-4.332481	1.282612	0.502003
H	3.375833	-2.141538	0.909165
H	5.185613	-2.522090	2.554032
H	5.791452	-0.730448	4.228399
H	4.529724	1.462507	4.209877
H	2.714742	1.858819	2.556758
H	1.225856	3.312198	-3.536187
H	0.379439	1.573551	-1.986115
H	4.106119	1.773893	0.282143
H	4.950007	3.519333	-1.272719
H	3.520481	4.313622	-3.196899
H	0.657633	-2.632808	0.656840
H	2.836447	-0.298625	-2.327002
H	3.152361	-2.348733	-3.700977
H	2.229411	-4.562861	-2.914727
H	0.976838	-4.682437	-0.723899

	(BeH2)2-1H	RI-BP86/SVP	
15			
E(SCF) =	-755.988429		
C	-0.107868	0.000144	0.996666
P	-0.730155	-1.557278	1.429295

P	-0.683398	1.545922	1.525180
Be	-0.306942	0.058868	-0.832500
H	-0.453494	1.355487	-1.310209
H	-0.492847	-1.201664	-1.387090
Be	1.635764	-0.043694	1.585148
H	2.086035	-1.337359	1.818594
H	2.121971	1.219735	1.898885
H	0.014652	-2.572003	0.788738
H	-2.094308	-1.851272	1.094918
H	-0.712794	-1.924501	2.816453
H	0.090639	2.575427	0.945781
H	-0.654821	1.827266	2.932025
H	-2.038428	1.899691	1.212046

(BeH2)2-1Me RI-BP86/SVP

33			
E(SCF) =	-991.794384		
C	-0.204460	-0.007245	1.160285
P	-0.937304	-1.551740	1.432585
P	-0.710496	1.482811	1.881176
Be	-0.059273	0.275064	-0.782954
H	-0.421347	1.601964	-1.103130
H	-0.534158	-0.869251	-1.461678
Be	1.538836	-0.062336	0.670622
H	2.673162	-0.285939	1.413438
H	1.495498	0.196358	-0.738370
C	0.121306	-2.851179	0.710076
C	-2.603184	-1.777799	0.692969
C	-1.150051	-2.061294	3.197386
C	0.525545	2.773589	1.509817
C	-0.846784	1.497458	3.725328
C	-2.326132	2.138100	1.303548
H	-2.955665	-2.821214	0.815105
H	-3.327009	-1.089828	1.172258
H	-2.503119	-1.522486	-0.381138
H	-0.330283	-3.849202	0.872310
H	0.207938	-2.628073	-0.372922
H	1.123542	-2.808254	1.182679
H	-1.504046	-3.110025	3.256905
H	-0.177127	-1.972660	3.718525
H	-1.890132	-1.412553	3.704656
H	-1.046365	2.524840	4.090585
H	-1.671136	0.839340	4.061474
H	0.104039	1.132104	4.159592
H	0.221683	3.737560	1.962278
H	1.510413	2.462361	1.913599

H	0.582034	2.855390	0.405195
H	-2.523181	3.142669	1.727675
H	-2.264280	2.186265	0.197820
H	-3.142092	1.450720	1.601414

	(BeH2)2-1Ph	RI-BP86/SVP	
75			
E(SCF) =	-2141.032698		
C	0.041319	0.425162	1.069380
P	-1.544221	0.448331	0.308598
P	1.541317	-0.061054	0.324600
C	1.619238	-1.802772	-0.289657
C	2.204921	1.015452	-1.021935
C	2.859568	0.054334	1.608910
C	-1.497821	-0.686862	-1.203675
C	-2.251924	1.957835	-0.536271
C	-2.861816	-0.341292	1.333289
Be	0.131383	-0.086486	2.819548
H	0.502505	-1.267219	3.409881
H	-0.172931	1.116332	3.542919
Be	-0.339585	1.897879	2.243788
H	-1.746612	1.801057	1.994071
H	0.358273	3.104638	2.218725
C	-1.945795	-2.027987	-1.146338
C	-0.984968	-0.195599	-2.431597
C	-0.928874	-1.018248	-3.582809
C	-1.389200	-2.361311	-3.519324
C	-1.895365	-2.863726	-2.291052
C	-1.811994	3.268569	-0.241100
C	-2.370367	4.383590	-0.913757
C	-3.398805	4.197138	-1.877090
C	-3.851445	2.881935	-2.165933
C	-3.269773	1.770792	-1.505468
C	1.371433	-2.828568	0.658931
C	1.403076	-4.188034	0.267617
C	1.676435	-4.533571	-1.085002
C	1.907520	-3.504926	-2.036599
C	1.877421	-2.144647	-1.636655
C	1.526103	2.205976	-1.359212
C	2.064164	3.090645	-2.328575
C	3.298961	2.784960	-2.960186
C	3.994451	1.595594	-2.603290
C	3.449451	0.720031	-1.633462
C	2.904501	1.212011	2.425476
C	3.932904	1.358720	3.390886
C	4.926404	0.353308	3.535847

C	4.884402	-0.798767	2.703341
C	3.854041	-0.944175	1.742501
C	-2.520010	-1.431998	2.165206
C	-3.505052	-2.061587	2.967179
C	-4.849110	-1.603381	2.933438
C	-5.189830	-0.506909	2.094754
C	-4.198088	0.119451	1.300219
H	-0.642280	0.842700	-2.520994
H	-0.540224	-0.614829	-4.527999
H	-1.357997	-3.002836	-4.410798
H	-2.253835	-3.900085	-2.228408
H	-2.354795	-2.443115	-0.217503
H	-1.059860	3.434241	0.547422
H	-2.019035	5.395969	-0.672309
H	-3.844573	5.061849	-2.388382
H	-4.649546	2.724652	-2.904262
H	-3.622781	0.765920	-1.767890
H	-1.482837	-1.795488	2.227564
H	-3.222620	-2.895037	3.624723
H	-5.615044	-2.081942	3.559030
H	-6.222638	-0.133398	2.074273
H	-4.481420	0.986068	0.691387
H	3.838342	-1.848209	1.122265
H	5.648262	-1.580750	2.811483
H	5.720934	0.464064	4.287002
H	3.952069	2.252205	4.029816
H	2.146194	2.008349	2.328497
H	1.531579	4.018235	-2.579142
H	0.593019	2.476236	-0.848761
H	4.021940	-0.172397	-1.351028
H	4.961107	1.365131	-3.071915
H	3.723583	3.469873	-3.707486
H	1.151079	-2.571916	1.707309
H	2.038707	-1.371302	-2.396081
H	2.102154	-3.762753	-3.086236
H	1.701209	-5.588277	-1.392945
H	1.215354	-4.976449	1.009287

	BeH2-1H	RI-BP86/SVP	
12			
E(SCF) =	-740.061668		
C	0.137760	-0.131012	0.019128
P	1.467541	0.412871	0.919212
P	-0.054767	-0.046533	-1.663167
Be	-1.204530	-0.872933	0.942212
H	-0.952702	-0.897446	2.318608

H	-2.252406	-1.288956	0.113535
H	2.783459	-0.144220	0.701867
H	1.224825	0.149429	2.294995
H	1.843742	1.808428	0.910413
H	0.868061	-0.722824	-2.546448
H	-0.072112	1.229981	-2.341025
H	-1.311577	-0.615210	-2.006931

	BeH2-1Me	RI-BP86/SVP	
30			
E(SCF) =	-975.853041		
C	-0.980057	0.053919	0.834545
P	-1.067634	-1.570694	1.322155
P	-0.874400	1.525277	1.676349
Be	-1.029345	0.258906	-0.929598
H	-0.971167	1.578703	-1.407580
H	-1.124856	-0.916751	-1.692910
C	0.295492	-2.599040	0.637890
C	-2.592173	-2.418567	0.736961
C	-1.029652	-1.946765	3.133906
C	0.610586	2.508601	1.216986
C	-0.809229	1.476426	3.525390
C	-2.278168	2.661363	1.323433
H	-2.585564	-3.499944	0.981000
H	-3.474036	-1.930948	1.196299
H	-2.631308	-2.271139	-0.360761
H	0.169762	-3.672387	0.884893
H	0.278589	-2.451013	-0.460308
H	1.260251	-2.227973	1.035305
H	-1.091262	-3.041872	3.291594
H	-0.088136	-1.575343	3.582214
H	-1.886803	-1.465569	3.642885
H	-0.737365	2.507114	3.926023
H	-1.724062	1.001449	3.928873
H	0.074999	0.901705	3.861907
H	0.613701	3.505916	1.700935
H	1.518854	1.943803	1.504126
H	0.586894	2.614333	0.114091
H	-2.142249	3.651225	1.803714
H	-2.323819	2.770492	0.221521
H	-3.217639	2.193694	1.677252

	BeH2-1Ph	RI-BP86/SVP	
72			
E(SCF) =	-2125.092089		
C	0.088357	0.635912	0.416340

P	1.520441	-0.120390	-0.113618
P	-1.489241	-0.016724	0.391763
C	1.751115	-0.280681	-1.941499
C	2.992591	0.820637	0.480035
C	1.878793	-1.793182	0.611855
C	-2.238090	-0.241611	2.073201
C	-2.662139	1.099558	-0.505228
C	-1.735352	-1.651919	-0.450891
Be	0.114482	2.453809	0.438525
H	-0.775042	3.067742	1.323476
H	1.009259	3.091338	-0.427493
C	1.340748	-1.439745	-2.645457
C	1.385215	-1.472277	-4.061601
C	1.829560	-0.333707	-4.787474
C	2.217044	0.838832	-4.082285
C	2.173550	0.863141	-2.666463
C	2.869685	1.680986	1.592965
C	4.008914	2.338969	2.119791
C	5.285098	2.131746	1.529126
C	5.408025	1.259593	0.413250
C	4.262658	0.604500	-0.103332
C	1.375216	-2.051162	1.908895
C	1.712365	-3.246220	2.591039
C	2.564656	-4.200169	1.970839
C	3.080208	-3.937340	0.672387
C	2.743106	-2.734068	0.003297
C	-1.743783	0.572291	3.119449
C	-2.279038	0.460597	4.426774
C	-3.314004	-0.477188	4.694329
C	-3.811080	-1.293143	3.641921
C	-3.275748	-1.169320	2.335156
C	-2.141342	1.985651	-1.475851
C	-3.007265	2.840151	-2.203785
C	-4.406636	2.809277	-1.958210
C	-4.927799	1.919295	-0.978983
C	-4.054396	1.068024	-0.257962
C	-2.149261	-1.686187	-1.805019
C	-2.292843	-2.920663	-2.486346
C	-2.017026	-4.141537	-1.812757
C	-1.598818	-4.110302	-0.454463
C	-1.461387	-2.870690	0.217851
H	-2.370105	-0.756838	-2.345143
H	-2.621090	-2.932812	-3.534583
H	-2.130752	-5.101465	-2.335557
H	-1.383865	-5.048156	0.075658
H	-1.139859	-2.877577	1.265600

H	-1.056802	2.037657	-1.662562
H	-2.591524	3.538677	-2.942450
H	-5.080312	3.478470	-2.511257
H	-6.006687	1.902428	-0.773323
H	-4.477991	0.407111	0.508017
H	-0.960747	1.314616	2.902602
H	-1.898924	1.104497	5.231448
H	-3.730129	-0.567769	5.707481
H	-4.611679	-2.018171	3.842828
H	-3.674077	-1.813144	1.541043
H	4.382287	-0.061431	-0.966702
H	6.390670	1.097602	-0.050095
H	6.169940	2.645275	1.930062
H	3.901646	3.018455	2.975875
H	1.887749	1.854787	2.056803
H	1.070020	-2.376436	-4.599831
H	0.966751	-2.322506	-2.111776
H	2.443521	1.787459	-2.136514
H	2.544435	1.729956	-4.635056
H	1.864308	-0.355875	-5.885547
H	0.729246	-1.311954	2.403730
H	3.173450	-2.548549	-0.987912
H	3.748444	-4.664850	0.191564
H	2.832032	-5.128185	2.495215
H	1.323012	-3.432375	3.601553

	(BeO)2-1H	RI-BP86/SVP	
13			
E(SCF) =	-903.999419		
C	-0.140166	-0.001385	1.020068
P	-0.820499	-1.536449	1.519395
P	-0.792300	1.521256	1.591713
Be	-0.271881	0.053981	-0.713303
O	-0.680689	0.119275	-2.013459
Be	1.525458	-0.030012	1.519227
O	2.710724	-0.060246	2.194393
H	-0.087324	-2.577604	0.896684
H	-2.185814	-1.790211	1.162952
H	-0.773094	-1.845553	2.918400
H	-0.036667	2.576167	1.021314
H	-0.742609	1.760343	3.004507
H	-2.151257	1.817567	1.245028

	(BeO)2-1Me	RI-BP86/SVP	
31			
E(SCF) =	-1139.823364		

C	-0.167555	-0.002000	1.042066
P	-0.796972	-1.572748	1.584544
P	-0.849851	1.556971	1.553315
Be	-0.424927	0.078474	-0.674118
O	-1.068780	0.355919	-1.850240
Be	1.448133	-0.066764	1.679019
O	2.440796	-0.334569	2.583784
C	0.146708	-2.843230	0.678591
C	-2.564746	-1.851471	1.189897
C	-0.522330	-1.899822	3.362001
C	0.218691	2.846084	0.830966
C	-0.840879	1.821020	3.366592
C	-2.532897	1.868946	0.911333
H	-0.205246	-3.853735	0.964028
H	0.010559	-2.686102	-0.410421
H	1.217409	-2.724043	0.942554
H	-0.696895	-2.969151	3.591234
H	0.541371	-1.616353	3.553694
H	-1.195377	-1.278441	3.983760
H	-2.834019	-2.912399	1.358677
H	-3.207856	-1.214445	1.827678
H	-2.721686	-1.582938	0.124282
H	-2.810554	2.931958	1.050807
H	-2.490746	1.605442	-0.172872
H	-3.274318	1.227783	1.425966
H	-1.071171	2.878055	3.603579
H	-1.594512	1.173051	3.854853
H	0.170159	1.556504	3.741622
H	-0.149345	3.850130	1.118980
H	1.255648	2.702107	1.195786
H	0.190447	2.730913	-0.272010

	(BeO)2-1Ph	RI-BP86/SVP	
73			
E(SCF) =	-2289.451925		
C	0.000271	0.000233	1.033737
P	-1.555984	0.231862	0.175800
P	1.556117	-0.231728	0.175084
C	1.821965	-1.828147	-0.705511
C	1.867979	1.163910	-0.972839
C	2.868395	-0.246107	1.464879
C	-1.868417	-1.164036	-0.971646
C	-1.822440	1.828062	-0.705017
C	-2.867538	0.246423	1.466337
Be	-0.342463	-1.344391	2.069641
O	-0.548078	-2.632006	2.506739

Be	0.343466	1.345029	2.069241
O	0.549930	2.632592	2.506094
C	-2.140595	-2.438708	-0.415016
C	-1.718693	-1.025265	-2.370024
C	-1.889400	-2.138457	-3.208684
C	-2.204120	-3.392826	-2.660164
C	-2.316824	-3.540360	-1.267878
C	-1.184315	2.997807	-0.232978
C	-1.515826	4.238838	-0.803844
C	-2.478150	4.329217	-1.821482
C	-3.137654	3.169651	-2.264156
C	-2.821428	1.923244	-1.703530
C	1.184109	-2.997772	-0.232825
C	1.515232	-4.238925	-0.803653
C	2.476916	-4.329537	-1.821876
C	3.136170	-3.170077	-2.265204
C	2.820320	-1.923546	-1.704642
C	1.717575	1.024870	-2.371116
C	1.887869	2.137902	-3.210071
C	2.202833	3.392382	-2.661944
C	2.316214	3.540183	-1.269742
C	2.140429	2.438691	-0.416581
C	2.705964	-1.087712	2.590911
C	3.724145	-1.162339	3.553125
C	4.910467	-0.426913	3.393431
C	5.085409	0.379792	2.257775
C	4.072035	0.469682	1.290576
C	-2.704455	1.088111	2.592208
C	-3.722044	1.162789	3.555042
C	-4.908442	0.427317	3.396130
C	-5.084067	-0.379454	2.260624
C	-4.071274	-0.469412	1.292826
H	-1.464813	-0.049956	-2.809531
H	-1.774754	-2.021877	-4.297024
H	-2.345908	-4.261925	-3.320790
H	-2.530409	-4.526904	-0.829699
H	-2.140231	-2.586579	0.681822
H	-0.472975	2.964304	0.622556
H	-1.018815	5.145765	-0.427602
H	-2.731723	5.307242	-2.259014
H	-3.912563	3.233897	-3.043192
H	-3.370845	1.030897	-2.036489
H	-1.793231	1.705238	2.725329
H	-3.580532	1.809554	4.433713
H	-5.701830	0.488488	4.156578
H	-6.014371	-0.951426	2.125059

H	-4.221306	-1.107075	0.410524
H	4.221520	1.107317	0.408158
H	6.015662	0.951697	2.121577
H	5.704303	-0.488025	4.153416
H	3.583180	-1.809077	4.431904
H	1.794827	-1.704833	2.724605
H	1.772671	2.021116	-4.298330
H	1.463527	0.049466	-2.810316
H	2.140573	2.586773	0.680231
H	2.530001	4.526814	-0.831855
H	2.344289	4.261355	-3.322807
H	0.473268	-2.964014	0.623128
H	3.369542	-1.031282	-2.038138
H	3.910584	-3.234501	-3.044718
H	2.730193	-5.307659	-2.259364
H	1.018456	-5.145767	-0.426897

BeO-1H RI-BP86/SVP

11			
E(SCF) =	-814.068171		
C	-0.002849	0.014600	0.066017
P	1.363647	0.507021	0.940519
P	-0.132057	0.053228	-1.623700
Be	-0.971257	-1.169357	0.852934
O	-1.711204	-2.134722	1.479765
H	2.472438	-0.387331	1.179119
H	1.033395	0.860690	2.280270
H	2.078857	1.658718	0.457352
H	0.361271	-1.026416	-2.447121
H	0.462808	1.171281	-2.307237
H	-1.491159	0.091243	-2.048709

BeO-1Me RI-BP86/SVP

29			
E(SCF) =	-1049.868899		
C	0.067899	0.200727	-0.011870
P	1.425928	0.587343	0.943043
P	-0.118065	0.129965	-1.702636
Be	-0.878157	-0.995256	0.781354
O	-1.537224	-2.010310	1.426803
C	2.692165	-0.743946	1.145145
C	0.864548	0.931665	2.650887
C	2.407751	2.065303	0.436361
C	0.601407	-1.343952	-2.557947
C	0.529033	1.561905	-2.670140
C	-1.904180	0.043954	-2.093966

H	-2.075226	-0.105325	-3.178083
H	-2.333303	-0.801107	-1.515904
H	-2.389710	0.977995	-1.752049
H	0.255375	1.462367	-3.739161
H	0.097358	2.497596	-2.265831
H	1.632475	1.611960	-2.592244
H	0.333492	-1.378992	-3.633324
H	1.704471	-1.328564	-2.454717
H	0.214000	-2.246957	-2.045059
H	3.186417	2.288330	1.192293
H	2.904067	1.882689	-0.536588
H	1.731586	2.936272	0.338564
H	1.720792	1.073825	3.339057
H	0.222839	1.833491	2.641845
H	0.246313	0.067391	2.974238
H	3.481286	-0.466577	1.872968
H	2.160881	-1.652323	1.494039
H	3.156797	-0.963949	0.163712

	BeO-1Ph	RI-BP86/SVP	
71			
E(SCF) =	-2199.121781		
C	0.135656	0.445783	0.726959
P	1.568923	-0.251066	0.114971
P	-1.481189	-0.001037	0.386764
C	1.484146	-0.801671	-1.646575
C	3.001429	0.921105	0.143338
C	2.189380	-1.700407	1.095205
C	-2.498148	-0.435641	1.879540
C	-2.419785	1.400493	-0.374453
C	-1.708674	-1.444829	-0.740641
Be	0.287024	1.548377	2.014477
O	0.396228	2.372871	3.105289
C	1.625607	-2.148048	-2.049609
C	1.543995	-2.497587	-3.422246
C	1.319511	-1.493294	-4.401193
C	1.167399	-0.138021	-3.994234
C	1.247089	0.200084	-2.622149
C	3.132753	1.884993	1.172430
C	4.267669	2.734917	1.206904
C	5.282623	2.622056	0.219388
C	5.150842	1.648683	-0.808354
C	4.015172	0.803403	-0.841336
C	1.457099	-2.074049	2.243906
C	1.906915	-3.135937	3.069425
C	3.102896	-3.829255	2.741996

C	3.847958	-3.442948	1.592445
C	3.392806	-2.377492	0.778118
C	-2.234694	0.198174	3.119031
C	-3.039620	-0.092795	4.249491
C	-4.116561	-1.014236	4.148816
C	-4.383279	-1.642704	2.901980
C	-3.577377	-1.349732	1.774677
C	-1.733347	2.606076	-0.636505
C	-2.420712	3.714907	-1.193128
C	-3.806187	3.612977	-1.490842
C	-4.497851	2.399111	-1.218808
C	-3.804301	1.300194	-0.656259
C	-2.123459	-1.282864	-2.082308
C	-2.273490	-2.411660	-2.927704
C	-2.007121	-3.715236	-2.429050
C	-1.580130	-3.877444	-1.081856
C	-1.430324	-2.744209	-0.246518
H	-2.332881	-0.285304	-2.487841
H	-2.595024	-2.277969	-3.969404
H	-2.128615	-4.592105	-3.080224
H	-1.370080	-4.881879	-0.689163
H	-1.103680	-2.893223	0.790951
H	-0.667371	2.691636	-0.378066
H	-1.885791	4.656595	-1.376421
H	-4.345163	4.471622	-1.915159
H	-5.572522	2.321907	-1.433206
H	-4.364532	0.384356	-0.430060
H	-1.412336	0.934875	3.237822
H	-2.823986	0.406698	5.204287
H	-4.740257	-1.236288	5.026078
H	-5.214629	-2.355324	2.813428
H	-3.803259	-1.855629	0.828289
H	3.933935	0.072335	-1.654853
H	5.927896	1.555602	-1.579199
H	6.161154	3.281685	0.249136
H	4.350826	3.483976	2.006643
H	2.364303	2.017772	1.962316
H	1.651051	-3.546944	-3.728313
H	1.789186	-2.942104	-1.311228
H	1.128161	1.250593	-2.325087
H	0.990452	0.644560	-4.744862
H	1.260209	-1.760749	-5.465435
H	0.553122	-1.511647	2.520554
H	4.002691	-2.077387	-0.083125
H	4.783874	-3.963592	1.347380
H	3.460670	-4.648080	3.381807

H	1.341022	-3.409638	3.970416
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(BH3)2-1H	RI-BP86/SVP
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17

E(SCF) =	-777.399488		
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C	-0.091552	0.000474	0.982621
P	-0.770183	-1.525635	1.516479
P	-0.778439	1.512337	1.545591
B	-0.431418	0.041754	-0.680661
H	-0.426411	1.239640	-1.020496
H	-1.575129	-0.418962	-0.869298
H	0.440447	-0.599860	-1.263643
B	1.458674	-0.027896	1.675449
H	1.805333	-1.222254	1.736383
H	1.388993	0.424093	2.836045
H	2.209800	0.627531	0.955838
H	-0.153156	-2.541177	0.747227
H	-2.170868	-1.754951	1.319615
H	-0.555775	-1.914703	2.875456
H	0.094286	2.543182	1.121768
H	-0.894016	1.724990	2.957867
H	-2.062716	1.891337	1.044431

(BH3)2-1Me	RI-BP86/SVP
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35

E(SCF) =	-1013.192837		
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C	-0.043794	-0.000758	0.950086
P	-0.738967	-1.534795	1.549605
P	-0.799579	1.522467	1.501921
B	-0.260436	-0.022241	-0.742094
H	-0.166912	1.139498	-1.169573
H	-1.399832	-0.450366	-1.033219
H	0.619392	-0.722533	-1.242210
B	1.554708	0.031211	1.545583
H	2.002687	-1.126469	1.543338
H	1.575890	0.450784	2.724644
H	2.235041	0.743498	0.807686
C	0.296523	2.917079	1.083795
H	1.236308	2.810246	1.655331
H	-0.214328	3.868121	1.330540
H	0.524056	2.862432	0.003467
C	-2.424716	1.911154	0.742852
H	-2.311874	1.843784	-0.355374
H	-2.744904	2.929605	1.038124
H	-3.189349	1.181266	1.069396
C	-1.083997	1.675448	3.314704

H	-0.145484	1.401062	3.833500
H	-1.904061	1.005960	3.640285
H	-1.358592	2.718242	3.568785
C	-2.567475	-1.702539	1.413769
H	-2.861288	-1.423354	0.383780
H	-3.076484	-1.042319	2.142992
H	-2.868545	-2.749346	1.616222
C	-0.070954	-2.916382	0.566770
H	1.032227	-2.852338	0.591216
H	-0.414869	-2.804300	-0.477439
H	-0.419380	-3.873746	1.000752
C	-0.365366	-1.932669	3.301912
H	0.728653	-1.850975	3.442923
H	-0.711321	-2.958052	3.538072
H	-0.868091	-1.215234	3.977605

(BH3)2-1Ph RI-BP86/SVP

77

E(SCF) =	-2162.412604		
C	0.000014	0.000019	1.311360
P	-1.559370	0.073697	0.394643
P	1.559386	-0.073682	0.394623
C	1.838433	-1.502315	-0.767664
C	1.956034	1.392575	-0.674030
C	2.973480	-0.130575	1.582348
C	-1.955988	-1.392531	-0.674061
C	-1.838490	1.502365	-0.767587
C	-2.973450	0.130492	1.582391
B	0.029625	-1.479885	2.207758
H	-0.862779	-2.249353	1.828691
H	1.117442	-2.037773	2.026912
H	-0.080400	-1.217949	3.404199
B	-0.029583	1.479917	2.207763
H	-1.117419	2.037785	2.026974
H	0.862790	2.249404	1.828657
H	0.080506	1.217981	3.404198
C	-2.730259	-2.457356	-0.152581
C	-1.477871	-1.475633	-2.004423
C	-1.776642	-2.598897	-2.813422
C	-2.557831	-3.663935	-2.288568
C	-3.031960	-3.588827	-0.950982
C	-1.191783	2.748590	-0.579946
C	-1.483908	3.847151	-1.425687
C	-2.430571	3.714056	-2.475886
C	-3.077041	2.464336	-2.672306
C	-2.780395	1.370874	-1.822803

C	1.191733	-2.748545	-0.580024
C	1.483792	-3.847075	-1.425826
C	2.430382	-3.713945	-2.476087
C	3.076851	-2.464223	-2.672501
C	2.780272	-1.370792	-1.822934
C	1.477824	1.475789	-2.004350
C	1.776613	2.599079	-2.813305
C	2.557918	3.664031	-2.288448
C	3.032144	3.588809	-0.950902
C	2.730420	2.457314	-0.152545
C	2.804893	0.131786	2.961289
C	3.923367	0.105465	3.829936
C	5.219051	-0.186720	3.325967
C	5.383813	-0.453002	1.939987
C	4.262375	-0.423426	1.074778
C	-2.804802	-0.131709	2.961355
C	-3.923266	-0.105466	3.830018
C	-5.219001	0.186480	3.326041
C	-5.383825	0.452602	1.940037
C	-4.262397	0.423104	1.074814
H	-0.874977	-0.670794	-2.438445
H	-1.399054	-2.650698	-3.843490
H	-2.792557	-4.538193	-2.911734
H	-3.632704	-4.408140	-0.533274
H	-3.106841	-2.420589	0.876574
H	-0.472093	2.881896	0.236856
H	-0.973864	4.805706	-1.261721
H	-2.663070	4.568227	-3.127389
H	-3.811766	2.346274	-3.480538
H	-3.295076	0.421754	-2.010105
H	-1.810846	-0.355023	3.368368
H	-3.780513	-0.305067	4.900398
H	-6.085084	0.213479	4.001983
H	-6.378797	0.688784	1.539366
H	-4.423067	0.649042	0.014996
H	4.422992	-0.649500	0.014980
H	6.378743	-0.689373	1.539323
H	6.085141	-0.213783	4.001898
H	3.780660	0.305188	4.900300
H	1.810973	0.355279	3.368296
H	1.398949	2.650969	-3.843341
H	0.874839	0.671017	-2.438374
H	3.107074	2.420461	0.876581
H	3.632977	4.408054	-0.533191
H	2.792658	4.538310	-2.911580
H	0.472098	-2.881876	0.236824

H	3.294955	-0.421670	-2.010224
H	3.811524	-2.346136	-3.480776
H	2.662827	-4.568091	-3.127642
H	0.973753	-4.805633	-1.261863

BH3-1H RI-BP86/SVP

13			
E(SCF) =	-750.760546		
C	0.099857	-0.449569	-0.057058
P	1.410142	-0.032175	0.928679
P	-0.099607	0.057016	-1.659020
B	-1.330599	-0.166840	0.787808
H	-1.056393	0.477215	1.822703
H	-1.867168	-1.247394	1.057017
H	-2.072469	0.547582	0.080520
H	2.735772	-0.206582	0.399864
H	1.441004	-0.837817	2.104575
H	1.525635	1.278667	1.532094
H	1.007044	-0.106300	-2.562293
H	-0.526924	1.400443	-1.988168
H	-1.132944	-0.684699	-2.303201

BH3-1Me RI-BP86/SVP

31			
E(SCF) =	-986.550492		
C	0.281628	0.529214	-0.190625
P	1.539145	0.166930	0.888809
P	0.012845	0.039453	-1.792416
B	-1.124132	1.049528	0.585215
H	-1.135118	0.633114	1.762402
H	-2.123816	0.563267	0.016559
H	-1.193148	2.291255	0.574144
C	1.840035	1.589340	2.010369
H	2.566536	1.336015	2.807409
H	0.863762	1.868042	2.451581
H	2.209130	2.443212	1.410193
C	1.241840	-1.244163	2.050577
H	2.020376	-1.313816	2.836984
H	1.209042	-2.188616	1.472592
H	0.250142	-1.075992	2.513558
C	3.198598	-0.214902	0.175175
H	3.937877	-0.326523	0.992884
H	3.519177	0.608144	-0.491533
H	3.168951	-1.159302	-0.401158
C	-0.847829	1.366521	-2.725006
H	-0.174120	2.241678	-2.800898

H	-1.735224	1.658360	-2.131064
H	-1.152654	1.026605	-3.734351
C	1.489234	-0.364499	-2.824943
H	2.196566	0.486520	-2.818722
H	1.170406	-0.562212	-3.867484
H	2.001771	-1.266250	-2.438846
C	-1.083643	-1.434448	-2.025903
H	-0.569922	-2.333876	-1.633108
H	-1.355465	-1.593321	-3.089061
H	-1.995885	-1.255126	-1.424565

	BH3-1Ph	RI-BP86/SVP	
73			
E(SCF) =	-2135.790472		
C	-0.125610	0.700303	-0.372664
P	1.462636	0.064121	-0.412848
P	-1.548961	-0.041077	0.222900
C	2.233002	0.309318	-2.083193
C	2.696214	0.782016	0.790995
C	1.643902	-1.754259	-0.106199
C	-1.844821	0.072075	2.058553
C	-3.021008	0.776145	-0.539162
C	-1.805028	-1.844601	-0.145462
B	-0.136204	2.364662	-0.657843
H	-0.495436	2.998579	0.352955
H	-0.869362	2.646910	-1.615961
H	1.025116	2.692903	-0.955358
C	1.387840	0.669139	-3.156443
C	1.911756	0.820616	-4.464287
C	3.296982	0.609678	-4.702698
C	4.148142	0.255802	-3.620355
C	3.613712	0.109787	-2.315792
C	2.439731	2.035612	1.396297
C	3.366062	2.595925	2.311101
C	4.565233	1.904024	2.630273
C	4.823539	0.643839	2.026689
C	3.891414	0.090188	1.114767
C	1.755388	-2.246407	1.217771
C	1.911844	-3.632784	1.460970
C	1.945478	-4.545512	0.371409
C	1.814625	-4.055847	-0.956334
C	1.667208	-2.664945	-1.188327
C	-1.005601	0.938164	2.794643
C	-1.169069	1.082130	4.196264
C	-2.180623	0.346843	4.871199
C	-3.026625	-0.525417	4.131534

C	-2.858672	-0.656332	2.731003
C	-2.990867	1.041380	-1.930099
C	-4.112676	1.612290	-2.578336
C	-5.277461	1.936248	-1.830041
C	-5.300214	1.688906	-0.431809
C	-4.172862	1.111513	0.206513
C	-2.272382	-2.230437	-1.425924
C	-2.473753	-3.595695	-1.743173
C	-2.204192	-4.598752	-0.772272
C	-1.727431	-4.215983	0.509477
C	-1.530436	-2.845982	0.815560
H	-2.503645	-1.478228	-2.189021
H	-2.845296	-3.879125	-2.737333
H	-2.362900	-5.659297	-1.011801
H	-1.508173	-4.982661	1.264474
H	-1.158332	-2.581430	1.811466
H	-2.080384	0.849349	-2.507814
H	-4.074035	1.828399	-3.654524
H	-6.146248	2.389952	-2.326835
H	-6.187325	1.955528	0.158230
H	-4.210120	0.956363	1.290680
H	-0.230865	1.514746	2.271758
H	-0.516240	1.763747	4.758225
H	-2.310536	0.452989	5.957298
H	-3.810653	-1.095502	4.648667
H	-3.522848	-1.336589	2.182776
H	4.110698	-0.894401	0.685072
H	5.745826	0.098431	2.269274
H	5.286952	2.339246	3.335589
H	3.157677	3.573595	2.766470
H	1.532046	2.595378	1.130637
H	1.251556	1.118704	-5.289765
H	0.327781	0.871394	-2.959014
H	4.297417	-0.143181	-1.497549
H	5.222147	0.105419	-3.794698
H	3.710224	0.732164	-5.713497
H	1.737889	-1.559188	2.073416
H	1.580890	-2.305865	-2.221699
H	1.832216	-4.754925	-1.803282
H	2.071373	-5.621749	0.553826
H	2.010573	-4.003514	2.490469

	(CO2)2-1H	RI-BP86/SVP	
15			
E(SCF) =	-1101.051113		
C	-0.070822	-0.002914	0.953410

P	-0.443745	-1.580515	1.727561
P	-0.906336	1.578802	1.199342
C	-0.187133	0.151607	-0.628153
O	0.180726	-0.627930	-1.467618
O	-0.747729	1.350313	-0.720041
C	1.434036	-0.144948	1.443738
O	1.429117	-1.345642	1.996611
O	2.332461	0.631226	1.240798
H	-0.192096	-2.872945	1.166248
H	-1.905988	-1.670107	1.474961
H	-0.631811	-1.642431	3.149303
H	-0.271798	2.850166	1.035907
H	-0.934390	1.653119	2.674683
H	-2.330722	1.672109	1.065070

(CO₂)₂-1Me RI-BP86/SVP

33

E(SCF) =	-1336.850029		
C	-0.152375	-0.000075	1.033450
P	-0.636785	-1.630249	1.792990
P	-0.994683	1.630802	1.348708
C	-0.311805	0.024309	-0.558128
O	-0.054220	-0.941180	-1.275074
O	-0.745551	1.193647	-0.858687
C	1.371055	-0.024626	1.520449
O	1.573875	-1.192858	2.010235
O	2.126609	0.939970	1.415149
C	-2.476677	-1.731425	1.515836
H	-2.693550	-1.616785	0.435203
H	-3.016020	-0.946872	2.082624
H	-2.856579	-2.718376	1.847531
C	-0.510755	-1.864035	3.609979
H	0.440527	-2.380708	3.824738
H	-1.378492	-2.445983	3.978362
H	-0.486430	-0.883608	4.119367
C	-0.052479	-3.079354	0.854368
H	0.910293	-3.415175	1.274308
H	0.099938	-2.705856	-0.182447
H	-0.819068	-3.878086	0.871326
C	-2.745160	1.864425	0.845369
H	-3.289524	2.439594	1.620049
H	-3.235701	0.883863	0.706455
H	-2.756174	2.388023	-0.126142
C	-1.108109	1.731998	3.206003
H	-0.097005	1.615512	3.644313
H	-1.776743	0.948721	3.614682

H	-1.509912	2.719719	3.508451
C	0.045737	3.079536	0.973426
H	1.091221	2.705243	1.040252
H	-0.130149	3.878281	1.719754
H	-0.163994	3.415555	-0.055725

	(CO2)2-1Ph	RI-BP86/SVP	
75			
E(SCF) =	-2486.062422		
C	0.039027	-0.729940	-0.476681
P	1.665304	0.006052	0.079121
P	-1.647753	0.075018	-0.139961
C	1.636273	0.870348	1.705007
C	2.282088	1.256883	-1.133542
C	3.011145	-1.245509	0.110689
C	-1.865094	0.128929	1.723694
C	-1.846120	1.817457	-0.695728
C	-3.200306	-0.858902	-0.533389
C	0.012172	-2.213545	0.260183
C	-0.070388	-0.769176	-2.036295
O	0.722021	-2.232586	1.295299
O	-0.722338	-3.051339	-0.269965
O	-1.218708	-0.294983	-2.371558
O	0.849805	-1.182752	-2.746722
C	1.327512	0.161616	2.889708
C	1.977115	2.241348	1.778804
C	2.001981	2.894660	3.021958
C	1.699115	2.188199	4.197048
C	1.364702	0.825461	4.125401
C	1.457702	1.890914	-2.085795
C	2.003626	2.835946	-2.970363
C	3.367990	3.158857	-2.914741
C	4.196523	2.525203	-1.972818
C	3.660694	1.574599	-1.091872
C	-1.961490	-1.120767	2.385434
C	-2.205372	-1.179392	3.765192
C	-2.379025	0.000998	4.507880
C	-2.316219	1.242326	3.857198
C	-2.063904	1.306745	2.475560
C	-1.080903	2.867166	-0.144695
C	-1.261406	4.186291	-0.595729
C	-2.203642	4.467049	-1.597044
C	-2.954673	3.420378	-2.160840
C	-2.773822	2.101063	-1.721930
C	-3.269976	-1.981930	-1.380941
C	-4.514922	-2.581365	-1.631411

C	-5.691075	-2.059945	-1.068481
C	-5.621959	-0.936837	-0.228330
C	-4.380064	-0.345938	0.052659
C	3.197191	-2.083594	-1.009515
C	4.269695	-2.988752	-1.016291
C	5.161075	-3.052522	0.067906
C	4.976763	-2.206322	1.173618
C	3.902206	-1.303027	1.202484
H	2.235434	2.800039	0.868141
H	2.270260	3.961131	3.068233
H	1.726590	2.700981	5.170848
H	1.125263	0.265869	5.041923
H	1.060558	-0.902709	2.809460
H	0.391996	1.642403	-2.166185
H	1.350019	3.311302	-3.716711
H	3.790749	3.896178	-3.614318
H	5.270720	2.760724	-1.930034
H	4.323651	1.067870	-0.374761
H	2.491706	-2.017813	-1.855915
H	4.405673	-3.651835	-1.884188
H	6.000346	-3.764750	0.053207
H	5.668515	-2.251422	2.028636
H	3.758123	-0.657528	2.080313
H	-4.338147	0.519837	0.730289
H	-6.535471	-0.519505	0.222002
H	-6.662810	-2.532416	-1.279708
H	-4.558801	-3.469351	-2.279970
H	-2.354306	-2.403251	-1.807180
H	-0.656294	4.995650	-0.160017
H	-0.330350	2.664276	0.631951
H	-3.335000	1.280276	-2.188663
H	-3.682180	3.629716	-2.959642
H	-2.346973	5.500907	-1.946683
H	-1.875965	-2.059016	1.818293
H	-2.046348	2.290461	1.988491
H	-2.473308	2.173877	4.422351
H	-2.580623	-0.048842	5.589148
H	-2.272187	-2.161061	4.258246

	CO2-1H	RI-BP86/SVP	
12			
E(SCF) =	-912.604053		
C	0.193590	-0.036812	1.201289
P	-1.503106	0.039660	1.656206
P	1.649974	0.112190	2.064674
C	-0.071247	-0.282361	-0.252122

O	0.706297	-0.437594	-1.179644
O	-1.413300	-0.286983	-0.265347
H	-2.344123	1.163626	1.390281
H	-1.413985	0.285312	3.104932
H	-2.344466	-1.108888	1.776053
H	1.400683	0.319910	3.450093
H	2.576841	-0.987185	2.062122
H	2.558612	1.180126	1.740853

	CO2-1Me	RI-BP86/SVP	
30			
E(SCF) =	-1148.394927		
C	0.066692	0.028564	1.438864
P	-1.558307	0.106948	2.026290
P	1.645071	0.131336	2.138892
C	0.122169	-0.196931	-0.082297
O	1.285108	-0.267813	-0.575163
O	-1.001576	-0.284881	-0.656463
C	2.643462	1.513420	1.460730
H	3.689621	1.473629	1.824318
H	2.175806	2.474602	1.749910
H	2.599461	1.384295	0.361936
C	1.670517	0.400292	3.961715
H	2.724188	0.451490	4.301120
H	1.171123	-0.434824	4.488322
H	1.169192	1.350940	4.224556
C	2.644240	-1.387367	1.888530
H	3.690427	-1.244048	2.224996
H	2.600381	-1.581052	0.799236
H	2.177053	-2.224385	2.442922
C	-1.716101	0.374033	3.842711
H	-1.249238	1.332060	4.139976
H	-1.242243	-0.453761	4.403376
H	-2.791720	0.408746	4.107093
C	-2.527335	1.474072	1.278724
H	-2.096170	2.442140	1.599880
H	-3.595885	1.417945	1.567279
H	-2.403598	1.346337	0.185841
C	-2.514176	-1.426463	1.706329
H	-2.074593	-2.256860	2.292363
H	-2.390544	-1.618413	0.622854
H	-3.583535	-1.299333	1.968100

	CO2-1Ph	RI-BP86/SVP	
72			
E(SCF) =	-2297.629154		

C	-0.142829	0.765782	-0.238465
P	1.557043	0.314507	-0.425935
P	-1.621017	-0.020101	0.202452
C	2.167836	0.100551	-2.153916
C	2.906058	0.951444	0.697534
C	1.645317	-1.476593	0.221611
C	-1.929733	-0.172991	2.021024
C	-3.024141	0.976873	-0.455418
C	-1.890918	-1.719159	-0.483025
C	0.009833	2.217256	-0.632188
O	1.284090	2.305333	-0.967272
O	-0.830696	3.113581	-0.630455
C	1.319238	-0.510508	-3.105617
C	1.730955	-0.643573	-4.455321
C	3.007528	-0.167047	-4.858807
C	3.857996	0.448383	-3.900414
C	3.434595	0.581337	-2.554361
C	2.766511	2.158140	1.421555
C	3.798052	2.602190	2.287085
C	4.995568	1.847827	2.417351
C	5.141885	0.640701	1.682315
C	4.093461	0.193257	0.840304
C	1.455820	-1.671864	1.614812
C	1.569974	-2.954354	2.202721
C	1.882190	-4.080096	1.391360
C	2.074609	-3.896388	-0.003061
C	1.959033	-2.601956	-0.574526
C	-1.220917	0.713180	2.864682
C	-1.434895	0.696511	4.265828
C	-2.364986	-0.219594	4.829314
C	-3.080020	-1.108524	3.979664
C	-2.864001	-1.079430	2.579385
C	-2.938174	1.505249	-1.766828
C	-4.033618	2.206859	-2.325301
C	-5.224384	2.388526	-1.568770
C	-5.303910	1.864487	-0.251119
C	-4.203450	1.160057	0.300397
C	-2.478276	-1.865201	-1.764342
C	-2.674380	-3.150784	-2.325336
C	-2.283800	-4.310678	-1.601749
C	-1.693599	-4.164859	-0.317720
C	-1.498211	-2.874121	0.234110
H	-2.809448	-0.989407	-2.335652
H	-3.136435	-3.251614	-3.316933
H	-2.437111	-5.310189	-2.032033
H	-1.379180	-5.052437	0.247391

H	-1.019510	-2.794028	1.216962
H	-2.013635	1.416989	-2.348688
H	-3.951757	2.634292	-3.333780
H	-6.070974	2.943963	-1.995824
H	-6.213739	2.014506	0.345516
H	-4.283812	0.783637	1.326976
H	-0.502238	1.422866	2.430760
H	-0.883788	1.390403	4.915394
H	-2.532122	-0.239341	5.915422
H	-3.801331	-1.816068	4.411282
H	-3.430398	-1.771223	1.943086
H	4.219540	-0.757845	0.307802
H	6.063937	0.050625	1.772774
H	5.801927	2.196802	3.077115
H	3.676882	3.540883	2.844405
H	1.874183	2.780727	1.293178
H	1.062774	-1.110619	-5.191500
H	0.324806	-0.872765	-2.813179
H	4.090131	1.093224	-1.839349
H	4.839189	0.835333	-4.206963
H	3.330135	-0.263285	-5.904497
H	1.245199	-0.816258	2.270164
H	2.131076	-2.493300	-1.652135
H	2.323822	-4.756145	-0.639786
H	1.986716	-5.077281	1.840936
H	1.435362	-3.078688	3.286180

(CS2)2-1Ph RI-BP86/SVP

75

E(SCF) =	-3777.773170		
C	0.083750	-0.895834	-0.613270
P	1.792860	-0.100386	0.040904
P	-1.754808	0.036075	-0.171834
C	1.761052	1.103293	1.471051
C	2.387367	1.001099	-1.341174
C	3.250142	-1.205892	0.358891
C	-2.047469	-0.227156	1.674546
C	-1.960510	1.873444	-0.342254
C	-3.356527	-0.757234	-0.723793
C	0.010754	-2.264408	0.071862
C	0.090177	-0.836894	-2.144347
S	0.719259	-2.281034	1.623603
S	-0.828813	-3.505244	-0.681212
S	-1.132908	0.149978	-2.802009
S	1.318418	-1.649483	-2.929402
C	1.164992	0.788341	2.715430

C	2.456201	2.336353	1.338568
C	2.548524	3.237326	2.427434
C	1.942802	2.917970	3.672941
C	1.249329	1.685829	3.809326
C	1.561850	2.034474	-1.849829
C	2.031433	2.896892	-2.871561
C	3.341623	2.735841	-3.395655
C	4.173468	1.703095	-2.883541
C	3.695091	0.844462	-1.864144
C	-2.300492	-1.556509	2.112329
C	-2.654656	-1.825754	3.456746
C	-2.768210	-0.762639	4.392608
C	-2.529789	0.568151	3.959678
C	-2.173085	0.827126	2.611650
C	-1.114015	2.789915	0.323898
C	-1.297862	4.188677	0.168147
C	-2.342943	4.683971	-0.653216
C	-3.193654	3.762008	-1.325815
C	-2.995114	2.369844	-1.175014
C	-3.455623	-1.701024	-1.770057
C	-4.719114	-2.233872	-2.133241
C	-5.896881	-1.809410	-1.461842
C	-5.795596	-0.856990	-0.411996
C	-4.527885	-0.346430	-0.037577
C	3.454285	-2.412642	-0.352103
C	4.602633	-3.201093	-0.099447
C	5.560987	-2.787691	0.866950
C	5.354028	-1.573585	1.573574
C	4.203840	-0.784914	1.318360
H	2.943589	2.612112	0.396779
H	3.098258	4.181114	2.308309
H	2.016725	3.612587	4.521762
H	0.777719	1.419211	4.764891
H	0.643318	-0.168749	2.840526
H	0.543110	2.188360	-1.478581
H	1.372261	3.681572	-3.266960
H	3.704979	3.396381	-4.195113
H	5.185183	1.561288	-3.286962
H	4.352603	0.045104	-1.503474
H	2.722037	-2.742924	-1.100939
H	4.743688	-4.141859	-0.648647
H	6.447769	-3.404213	1.068750
H	6.083615	-1.243312	2.325375
H	4.071075	0.140133	1.890424
H	-4.479068	0.368627	0.792383
H	-6.697474	-0.522106	0.118146

H	-6.876154	-2.218355	-1.747282
H	-4.779986	-2.980265	-2.936617
H	-2.561874	-2.053266	-2.295260
H	-0.626627	4.886790	0.686807
H	-0.295076	2.446338	0.966420
H	-3.645307	1.682469	-1.729840
H	-4.001071	4.130821	-1.973101
H	-2.491006	5.765976	-0.774881
H	-2.256627	-2.399388	1.409526
H	-2.027577	1.871163	2.319029
H	-2.635490	1.402871	4.665754
H	-3.048897	-0.968278	5.435095
H	-2.839200	-2.861871	3.771287

(CS2)2-1H RI-BP86/SVP

15			
E(SCF) =	-2392.794585		
C	-0.025600	-0.145739	0.934395
P	-0.762583	-1.734860	1.535787
P	-0.609691	1.728242	1.395644
C	-0.229033	-0.092623	-0.580473
S	-0.409653	-1.531274	-1.415822
S	-0.277736	1.534992	-1.107485
C	1.410684	-0.083470	1.455734
S	2.192083	-1.517995	1.819781
S	1.909725	1.546527	1.604977
H	-0.308016	-3.019935	1.171161
H	-2.156194	-1.707909	1.228576
H	-0.758547	-1.702554	2.962547
H	-0.557188	3.164386	1.347073
H	-0.656645	1.581997	2.830088
H	-2.020837	1.574156	1.138840

(CS2)2-1Me RI-BP86/SVP

33			
E(SCF) =	-2628.561504		
C	-0.063081	-0.001907	1.003133
P	-0.914209	-1.637025	1.621153
P	-0.891324	1.605697	1.697189
C	-0.244274	0.038337	-0.532698
S	0.659296	-1.007104	-1.477798
S	-1.475725	1.115004	-1.041572
C	1.372299	-0.031967	1.578112
S	1.548210	-1.155446	2.860581
S	2.504051	1.056899	1.001680
C	-2.709702	1.691393	1.991700

H	-2.902443	2.601452	2.595307
H	-3.051881	0.814453	2.573476
H	-3.243463	1.740191	1.028381
C	-0.272755	3.179905	0.991952
H	0.688320	2.941054	0.490376
H	-0.089923	3.893202	1.821685
H	-0.996305	3.573310	0.258636
C	-2.474935	-1.721691	0.615103
H	-2.217511	-1.756081	-0.460158
H	-3.130056	-0.848289	0.784217
H	-3.015117	-2.647769	0.896416
C	-0.081190	-3.189002	1.115151
H	0.444991	-3.627140	1.980172
H	0.648532	-2.910078	0.325922
H	-0.835475	-3.883157	0.692503
C	-1.607598	-1.797287	3.325174
H	-0.836121	-2.219949	3.990512
H	-2.506040	-2.446174	3.286597
H	-1.905779	-0.808743	3.720946
C	-0.264725	1.725713	3.440797
H	0.830337	1.882137	3.415160
H	-0.460540	0.807711	4.023055
H	-0.751847	2.593307	3.928975

	CS2-1H	RI-BP86/SVP	
12			
E(SCF) =	-1558.490528		
C	-0.000408	-0.035470	1.211740
P	-1.617676	0.073831	1.880786
P	1.617531	0.074677	1.878939
C	-0.001242	-0.261551	-0.208466
S	1.583273	-0.363560	-0.851639
S	-1.586609	-0.363680	-0.849533
H	-2.476390	1.176736	1.597119
H	-1.392934	0.300566	3.293604
H	-2.478539	-1.060728	1.956841
H	1.394358	0.301724	3.291939
H	2.479014	-1.059448	1.954128
H	2.475402	1.177902	1.593933

	CS2-1Me	RI-BP86/SVP	
30			
E(SCF) =	-1794.260582		
C	0.048323	-0.048250	1.260410
P	-1.632218	0.069362	1.851476
P	1.628877	0.096482	2.042970

C	0.048536	-0.323140	-0.172623
S	1.464844	-0.502108	-1.101718
S	-1.568740	-0.441026	-0.791415
C	-2.630494	-1.491824	1.929278
H	-2.100542	-2.265865	1.346221
H	-3.611669	-1.319984	1.448190
H	-2.778581	-1.820957	2.978932
C	-1.575631	0.426188	3.696010
H	-1.077126	1.388514	3.917209
H	-1.083149	-0.386912	4.261457
H	-2.625032	0.497680	4.047106
C	-2.622824	1.551698	1.340911
H	-2.764495	2.250924	2.191203
H	-3.607101	1.217864	0.962149
H	-2.092190	2.047532	0.508771
C	2.634884	-1.437435	1.957185
H	3.657774	-1.250602	2.340974
H	2.666799	-1.739400	0.892128
H	2.138120	-2.218705	2.565374
C	2.643905	1.485960	1.401795
H	3.664809	1.449122	1.831781
H	2.150229	2.438689	1.676839
H	2.679496	1.374042	0.300558
C	1.589130	0.439770	3.849387
H	2.642615	0.500284	4.187142
H	1.086810	-0.371387	4.406508
H	1.092842	1.401956	4.069848

	CS2-1Ph	RI-BP86/SVP	
72			
E(SCF) =	-2943.499521		
C	0.000074	-0.000008	-0.911121
P	1.648703	0.026756	-0.237061
P	-1.648661	-0.026753	-0.237320
C	2.648820	-1.512267	-0.484084
C	2.594102	1.547738	-0.666073
C	1.664303	0.059552	1.631054
C	-2.648653	1.512343	-0.484397
C	-2.594055	-1.547638	-0.666682
C	-1.664605	-0.059755	1.630780
C	0.000194	0.000068	-2.373231
S	1.529514	0.057080	-3.137369
S	-1.528968	-0.056860	-3.137676
C	-2.170256	2.561220	-1.303662
C	-2.906605	3.764549	-1.426513
C	-4.140665	3.921287	-0.735089

C	-4.615439	2.870699	0.093837
C	-3.860911	1.676885	0.228347
C	-1.895193	-2.778878	-0.661151
C	-2.574921	-3.989819	-0.940958
C	-3.969708	-3.977681	-1.212811
C	-4.669966	-2.739352	-1.206200
C	-3.984102	-1.532172	-0.930137
C	-2.118673	-1.190416	2.348987
C	-2.258774	-1.144750	3.759671
C	-1.942710	0.044059	4.467709
C	-1.483960	1.182982	3.749257
C	-1.352616	1.126317	2.341556
C	2.170607	-2.561122	-1.303485
C	2.907045	-3.764401	-1.426297
C	4.141010	-3.921108	-0.734698
C	4.615600	-2.870541	0.094360
C	3.860979	-1.676781	0.228832
C	1.895196	2.778951	-0.660445
C	2.574911	3.989956	-0.940011
C	3.969726	3.977906	-1.211718
C	4.670028	2.739601	-1.205204
C	3.984177	1.532357	-0.929386
C	2.118258	1.190117	2.349481
C	2.258112	1.144275	3.760184
C	1.941913	-0.044618	4.468020
C	1.483279	-1.183448	3.749345
C	1.352181	-1.126605	2.341628
H	2.387411	2.116648	1.828739
H	2.619958	2.027574	4.303819
H	2.054047	-0.087855	5.560214
H	1.237431	-2.108847	4.287331
H	1.022336	-2.027858	1.810543
H	0.813155	2.804038	-0.479083
H	2.021063	4.938535	-0.956491
H	4.499694	4.913345	-1.436910
H	5.744938	2.718017	-1.430339
H	4.539166	0.588266	-0.976365
H	1.245470	-2.435737	-1.879180
H	2.532648	-4.570478	-2.071694
H	4.720794	-4.848430	-0.840931
H	5.561715	-2.986140	0.640493
H	4.226750	-0.901079	0.912970
H	-4.539055	-0.588055	-0.977040
H	-5.744851	-2.717699	-1.431444
H	-4.499684	-4.913070	-1.438192
H	-2.021105	-4.938414	-0.957510

H	-0.813171	-2.804024	-0.479681
H	-2.532066	4.570641	-2.071809
H	-1.245037	2.435819	-1.879222
H	-4.226830	0.901164	0.912383
H	-5.561630	2.986321	0.639834
H	-4.720376	4.848651	-0.841350
H	-2.387722	-2.116885	1.828082
H	-1.022679	2.027636	1.810641
H	-1.238213	2.108316	4.287401
H	-2.055034	0.087158	5.559889
H	-2.620707	-2.028119	4.303133

(H+)-1H RI-BP86/SVP

10			
E(SCF) =	-724.536965		
C	-0.000030	0.035627	1.195657
P	-1.535122	-0.010082	1.969227
P	1.535225	-0.010317	1.968895
H	-0.000234	-0.101785	0.101760
H	-2.514362	0.696544	1.216438
H	-1.503577	0.604179	3.253053
H	-2.195172	-1.256909	2.242243
H	1.502877	0.601096	3.254030
H	2.196248	-1.257211	2.239085
H	2.514136	0.698857	1.217993

(H+)-1Me RI-BP86/SVP

28			
E(SCF) =	-960.359166		
C	-0.501529	-0.010242	1.458298
P	-0.016286	-1.574911	2.016057
P	-0.140776	1.575754	2.046528
H	-1.287204	-0.034241	0.686197
C	-0.883538	-2.806160	0.988457
H	-1.977255	-2.688407	1.112367
H	-0.588633	-3.828147	1.294918
H	-0.617620	-2.650700	-0.074771
C	-0.414360	-1.971192	3.765949
H	0.109991	-1.266510	4.441594
H	-0.097482	-3.002275	4.020629
H	-1.505527	-1.869076	3.923309
C	1.777874	-1.926932	1.859663
H	2.362076	-1.229555	2.490660
H	2.081146	-1.790632	0.803813
H	2.000839	-2.963790	2.181198
C	-0.393753	2.768925	0.689016

H	-0.211065	3.801521	1.044856
H	-1.438345	2.693758	0.328002
H	0.292907	2.530348	-0.145181
C	1.583216	1.752981	2.634349
H	1.760816	2.796293	2.961446
H	2.285604	1.499097	1.817827
H	1.766758	1.086199	3.499790
C	-1.180473	2.185576	3.436275
H	-0.915343	3.225584	3.713820
H	-1.045735	1.529186	4.318198
H	-2.244796	2.147690	3.131848

	(H+)-1Ph	RI-BP86/SVP	
70			
E(SCF) =	-2109.621415		
C	-0.000127	-0.000132	0.572304
P	1.582058	0.126519	-0.127843
P	-1.582138	-0.126597	-0.128272
C	2.025117	1.787684	-0.782284
C	2.759536	-0.248194	1.231505
C	1.924262	-1.041079	-1.509130
C	-2.025010	-1.787581	-0.783296
C	-2.759953	0.247709	1.230895
C	-1.924028	1.041392	-1.509309
H	-0.000268	-0.000240	1.671845
C	1.286125	2.904746	-0.328575
C	1.634222	4.212302	-0.750872
C	2.732125	4.402661	-1.634691
C	3.475039	3.277147	-2.090089
C	3.121636	1.973583	-1.662543
C	2.427202	-1.235104	2.194022
C	3.336594	-1.553290	3.232918
C	4.589581	-0.884509	3.311971
C	4.919484	0.105141	2.345373
C	4.004777	0.420380	1.309188
C	2.441301	-2.329188	-1.226441
C	2.667032	-3.253789	-2.276125
C	2.370546	-2.892060	-3.619856
C	1.853037	-1.597778	-3.901275
C	1.633650	-0.676051	-2.846963
C	-1.286148	-2.904768	-0.329683
C	-1.634129	-4.212208	-0.752432
C	-2.731784	-4.402325	-1.636612
C	-3.474568	-3.276685	-2.091913
C	-3.121284	-1.973239	-1.663910
C	-2.427892	1.234381	2.193750

C	-3.337544	1.552251	3.232516
C	-4.590517	0.883389	3.311098
C	-4.920146	-0.106023	2.344162
C	-4.005180	-0.420943	1.308108
C	-2.441168	2.329408	-1.226380
C	-2.666654	3.254307	-2.275855
C	-2.369821	2.892972	-3.619614
C	-1.852212	1.598782	-3.901276
C	-1.633069	0.676757	-2.847174
H	-2.696109	2.626265	-0.200938
H	-3.080743	4.248313	-2.055201
H	-2.548881	3.607264	-4.436365
H	-1.634748	1.312240	-4.939961
H	-1.254293	-0.323331	-3.092904
H	-1.466099	1.760171	2.158145
H	-3.076016	2.313819	3.980900
H	-5.298063	1.126256	4.117275
H	-5.883320	-0.632160	2.405173
H	-4.280043	-1.200871	0.587474
H	-0.435242	-2.764457	0.348528
H	-1.058754	-5.079867	-0.400637
H	-3.005542	-5.414517	-1.968271
H	-4.322266	-3.421879	-2.776656
H	-3.708020	-1.122086	-2.033214
H	4.279846	1.200486	0.588826
H	5.882669	0.631216	2.406749
H	5.296926	-1.127623	4.118250
H	3.074854	-2.315043	3.981041
H	1.465391	-1.760837	2.158050
H	1.058744	5.079864	-0.399005
H	0.435028	2.764249	0.349356
H	3.708473	1.122531	-2.031919
H	4.322928	3.422528	-2.774555
H	3.005976	5.414944	-1.965996
H	2.695975	-2.626345	-0.201020
H	1.254960	0.324117	-3.092500
H	1.635840	-1.310932	-4.939933
H	2.549794	-3.606122	-4.436767
H	3.081044	-4.247868	-2.055654

	(H+)2-1H	RI-BP86/SVP	
11			
E(SCF) =	-724.733361		
C	-0.132712	0.000030	1.100518
P	-0.867661	-1.624784	1.610958
P	-0.867795	1.624760	1.610960

H	-0.093268	0.000046	-0.014495
H	0.925984	0.000046	1.452658
H	-0.048156	-2.641321	1.042669
H	-2.196165	-1.773144	1.122329
H	-0.875057	-1.772578	3.026475
H	-0.048136	2.641353	1.042995
H	-0.875547	1.772461	3.026487
H	-2.196168	1.773131	1.121987

	(H+)2-1Me	RI-BP86/SVP	
29			
E(SCF) =	-960.625967		
C	-0.164239	0.004461	1.234979
P	-0.850156	-1.661065	1.701515
P	-0.904701	1.661550	1.645036
H	-0.056188	-0.007121	0.127212
H	0.872728	0.022984	1.639056
C	-2.572020	-1.851709	1.161143
H	-2.667264	-1.646029	0.076363
H	-3.251924	-1.193978	1.736773
H	-2.874918	-2.903691	1.344999
C	0.195729	-2.862340	0.831984
H	1.254358	-2.750460	1.140847
H	0.111520	-2.729217	-0.265138
H	-0.146942	-3.884320	1.095796
C	-0.716050	-1.928986	3.491073
H	0.335383	-1.810323	3.821122
H	-1.036977	-2.968760	3.709686
H	-1.369209	-1.237868	4.057458
C	-2.442939	1.921373	0.718589
H	-2.261645	1.809526	-0.369109
H	-2.791466	2.957368	0.911362
H	-3.237351	1.222005	1.042222
C	0.333291	2.876119	1.110991
H	1.275095	2.748101	1.681173
H	-0.065471	3.893822	1.302699
H	0.536946	2.771449	0.026480
C	-1.201779	1.840533	3.426322
H	-0.275245	1.639425	4.000019
H	-2.016967	1.174318	3.769488
H	-1.511172	2.889053	3.618978

	(H+)2-1Ph	RI-BP86/SVP	
71			
E(SCF) =	-2109.930184		
C	0.000120	-0.000309	1.007506

P	1.542991	0.715621	0.233030
P	-1.542865	-0.715854	0.232906
C	1.145124	2.207965	-0.714897
C	2.538067	1.166718	1.688434
C	2.443918	-0.481800	-0.789876
C	-1.145372	-2.208245	-0.715098
C	-2.538091	-1.166779	1.688260
C	-2.443411	0.481867	-0.789989
H	0.367316	-0.802210	1.681681
H	-0.367027	0.801361	1.681984
C	0.257973	3.173869	-0.167205
C	0.022616	4.385483	-0.860298
C	0.677315	4.636449	-2.101924
C	1.569964	3.667542	-2.641089
C	1.806703	2.454196	-1.945593
C	2.773675	0.215129	2.718649
C	3.563297	0.570992	3.838295
C	4.124331	1.878494	3.930351
C	3.891247	2.823237	2.891769
C	3.097950	2.467361	1.770905
C	3.770756	-0.833979	-0.427913
C	4.518251	-1.714017	-1.251357
C	3.943051	-2.237031	-2.443187
C	2.612943	-1.873987	-2.805412
C	1.866044	-0.999484	-1.980721
C	-0.258226	-3.174269	-0.167610
C	-0.023424	-4.386049	-0.860604
C	-0.678555	-4.636999	-2.102002
C	-1.571333	-3.668049	-2.640878
C	-1.807538	-2.454548	-1.945470
C	-2.773619	-0.215132	2.718443
C	-3.563320	-0.570872	3.838073
C	-4.124496	-1.878312	3.930152
C	-3.891491	-2.823110	2.891603
C	-3.098119	-2.467354	1.770753
C	-3.770011	0.834781	-0.427884
C	-4.517121	1.715198	-1.251273
C	-3.941785	2.237830	-2.443204
C	-2.611886	1.874115	-2.805529
C	-1.865372	0.999233	-1.980895
H	-4.249932	0.430426	0.472485
H	-5.546985	1.986198	-0.974339
H	-4.524956	2.914177	-3.087447
H	-2.171657	2.271877	-3.731690
H	-0.847989	0.741307	-2.295743
H	-2.377406	0.808357	2.676544

H	-3.750312	0.160356	4.638725
H	-4.739111	-2.154715	4.801066
H	-4.329045	-3.830457	2.958723
H	-2.939388	-3.215910	0.983778
H	0.247091	-3.026084	0.795777
H	0.657484	-5.141210	-0.440378
H	-0.502357	-5.583371	-2.636810
H	-2.087699	-3.867489	-3.591934
H	-2.516944	-1.734207	-2.373687
H	2.939152	3.215880	0.983909
H	4.328696	3.830632	2.958867
H	4.738876	2.154996	4.801281
H	3.750356	-0.160198	4.638967
H	2.377582	-0.808407	2.676767
H	-0.658079	5.140675	-0.439785
H	-0.247177	3.025576	0.796255
H	2.515870	1.733806	-2.374127
H	2.086045	3.867028	-3.592289
H	0.500587	5.582641	-2.636875
H	4.250586	-0.429263	0.472342
H	0.848536	-0.742013	-2.295538
H	2.172800	-2.272073	-3.731476
H	4.526526	-2.913060	-3.087487
H	5.548260	-1.984524	-0.974480

LS-Addukte/LS-CDP-R/RI-BP86_TZVP

(AlCl3)2-1H RI-BP86/TZVP

17

E(SCF) =	-3971.398275		
C	-0.054361	0.084886	0.989801
P	-1.210255	-1.046338	1.734154
P	-0.303005	1.784026	1.459338
Al	1.861047	-0.447384	1.682147
Cl	2.989182	1.389275	1.553825
Cl	1.405367	-0.905592	3.776652
Cl	2.531724	-2.169793	0.623568
Al	-0.370013	-0.031119	-1.088342
Cl	-2.106870	1.289995	-1.293526
Cl	1.337091	0.749010	-2.096070
Cl	-0.959819	-2.082953	-1.409838
H	-0.733836	-2.369818	1.604168
H	-2.505554	-1.040387	1.146666
H	-1.445370	-0.860668	3.123851
H	0.398111	2.630812	0.572139
H	0.163964	2.114120	2.761594
H	-1.649963	2.237915	1.434848

	(AlCl₃)₂-1Me	RI-BP86/TZVP	
35			
E(SCF) =	-4207.448828		
C	0.233024	0.027802	0.725085
P	-0.470709	-1.563229	1.272199
P	-0.630060	1.472376	1.428047
Al	2.291438	0.099376	1.274363
Cl	3.310830	1.558904	0.078915
Cl	2.344806	0.716387	3.390191
Cl	3.183264	-1.877356	1.200250
Al	0.150865	0.141048	-1.401927
Cl	0.192291	2.204858	-2.070843
Cl	1.694615	-1.080434	-2.252520
Cl	-1.821094	-0.652730	-1.986718
C	0.382391	2.990836	1.340083
H	1.231835	2.909841	2.028365
H	-0.263859	3.828521	1.638002
H	0.741029	3.140128	0.315523
C	-1.086799	1.337102	3.207723
H	-0.181788	1.136997	3.794555
H	-1.836152	0.554845	3.376998
H	-1.516000	2.300700	3.515050
C	-2.211417	1.886556	0.587335
H	-2.006882	2.179748	-0.449722
H	-2.672852	2.726782	1.124842
H	-2.895065	1.030991	0.586266
C	0.002586	-2.942393	0.171046
H	1.090292	-2.957039	0.039387
H	-0.492826	-2.827597	-0.800066
H	-0.329962	-3.871601	0.654938
C	0.052501	-2.077565	2.957605
H	1.135796	-2.249955	2.966259
H	-0.472098	-3.010413	3.207509
H	-0.191012	-1.309028	3.698861
C	-2.310513	-1.641597	1.327737
H	-2.591668	-2.671124	1.588843
H	-2.708855	-1.395036	0.335684
H	-2.723625	-0.966981	2.086851

	(AlCl₃)₂-1Ph	RI-BP86/TZVP	
77			
E(SCF) =	-5358.161597		
C	0.008850	-0.745685	-0.054389
P	-1.583975	0.261464	-0.003654
P	1.569690	0.317306	0.024877

C	1.876883	1.413112	-1.453134
C	1.726141	1.469885	1.481856
C	3.189072	-0.598103	0.060753
C	-1.538919	1.945539	-0.809735
C	-2.236084	0.621060	1.692936
C	-3.035105	-0.542706	-0.843621
Al	-0.069989	-2.023798	-1.828363
Cl	-0.658369	-0.940309	-3.651200
Cl	1.888252	-2.812406	-2.321331
Cl	-1.534846	-3.568550	-1.526325
Al	0.005503	-2.269605	1.562639
Cl	-1.920990	-2.658127	2.482866
Cl	1.302384	-1.552479	3.176985
Cl	0.808044	-4.184186	0.958564
C	-1.101916	2.106129	-2.134540
C	-2.083675	3.052185	-0.131594
C	-2.186608	4.290788	-0.769617
C	-1.760409	4.440615	-2.092190
C	-1.221410	3.345317	-2.769956
C	-1.405279	0.668079	2.817976
C	-1.934459	0.992143	4.070165
C	-3.292953	1.280192	4.207353
C	-4.127659	1.240789	3.085512
C	-3.606703	0.912045	1.833232
C	2.110329	0.790809	-2.691430
C	2.474776	1.553474	-3.802402
C	2.633825	2.937485	-3.688524
C	2.434187	3.556007	-2.451909
C	2.059237	2.800609	-1.337401
C	0.896722	2.594447	1.625959
C	1.083471	3.484702	2.686353
C	2.096210	3.259799	3.621538
C	2.919980	2.139284	3.489695
C	2.740147	1.249180	2.428714
C	3.361781	-1.934523	0.426446
C	4.646323	-2.483392	0.492634
C	5.766141	-1.705935	0.200719
C	5.599503	-0.366329	-0.165845
C	4.321512	0.186529	-0.240543
C	-3.743019	-1.561391	-0.183024
C	-4.898824	-2.093026	-0.754539
C	-5.355736	-1.627865	-1.989858
C	-4.654569	-0.616990	-2.649776
C	-3.501499	-0.071381	-2.081533
H	-2.436022	2.951940	0.893888
H	-2.611909	5.137449	-0.228187

H	-1.852766	5.406298	-2.592190
H	-0.886418	3.444842	-3.803157
H	-0.692573	1.261149	-2.688425
H	-0.349315	0.414632	2.748689
H	-1.276615	0.995020	4.939802
H	-3.705916	1.522881	5.187887
H	-5.193107	1.454569	3.183576
H	-4.270336	0.872478	0.970040
H	-3.394611	-1.945725	0.774222
H	-5.430451	-2.889380	-0.232122
H	-6.255879	-2.052436	-2.437685
H	-4.998513	-0.246006	-3.616146
H	-2.981185	0.721014	-2.611966
H	4.215087	1.230552	-0.532601
H	6.464880	0.254130	-0.403811
H	6.766015	-2.140257	0.251443
H	4.753862	-3.533219	0.767337
H	2.520110	-2.588308	0.635656
H	0.430267	4.353862	2.777664
H	0.101763	2.793048	0.910174
H	3.384272	0.376869	2.347980
H	3.707826	1.946305	4.219130
H	2.242363	3.954280	4.450570
H	2.045296	-0.292618	-2.794857
H	1.929151	3.301872	-0.380835
H	2.574750	4.632846	-2.345091
H	2.929099	3.529177	-4.556855
H	2.643535	1.052646	-4.756526

AlCl3-1H RI-BP86/TZVP

13			
E(SCF) =	-2347.906520		
C	0.698916	-0.087785	-0.485754
P	2.107821	-0.107955	0.477557
P	0.720797	0.396415	-2.122055
Al	-1.062854	0.075117	0.479497
Cl	-0.470320	0.741869	2.474294
Cl	-2.149768	1.559914	-0.697749
Cl	-2.101546	-1.813987	0.528277
H	2.540908	1.056732	1.195472
H	3.307011	-0.461484	-0.217762
H	2.034823	-1.064608	1.522332
H	0.597926	1.776170	-2.498162
H	1.890166	0.017192	-2.853759
H	-0.338828	-0.186859	-2.863418

	AlCl3-1Me	RI-BP86/TZVP	
31			
E(SCF) =	-2583.957582		
C	0.626789	0.119502	-0.388475
P	2.046058	-0.107127	0.566955
P	0.600549	0.294804	-2.105430
Al	-1.087165	0.592007	0.559958
Cl	-0.707796	0.977491	2.687994
Cl	-1.906629	2.427381	-0.333373
Cl	-2.527544	-1.033602	0.371321
C	2.645144	1.382702	1.479297
H	3.511561	1.136957	2.109576
H	1.824271	1.754412	2.105734
H	2.922402	2.158146	0.753069
C	1.808977	-1.391405	1.860968
H	2.720317	-1.498763	2.465429
H	1.564828	-2.342946	1.372096
H	0.973272	-1.091862	2.505844
C	3.564010	-0.672680	-0.323643
H	4.364581	-0.813059	0.415145
H	3.893649	0.079937	-1.050942
H	3.380380	-1.625704	-0.832861
C	1.026364	1.970619	-2.765321
H	2.062920	2.218353	-2.499560
H	0.352367	2.693226	-2.286136
H	0.908601	2.017274	-3.857312
C	-1.068553	-0.045918	-2.784548
H	-1.401455	-1.037536	-2.455459
H	-1.022654	0.000271	-3.881193
H	-1.777599	0.705321	-2.414521
C	1.684458	-0.845271	-3.081456
H	2.745895	-0.620930	-2.931430
H	1.450259	-0.726584	-4.148244
H	1.482600	-1.881326	-2.781925

	AlCl3-1Ph	RI-BP86/TZVP	
73			
E(SCF) =	-3734.722976		
C	6.291782	3.450180	6.389889
P	5.972228	2.280862	7.634886
P	7.307557	4.835316	6.691115
C	5.389328	3.027826	9.233328
C	4.646012	1.073855	7.175747
C	7.366183	1.121884	8.057152
C	7.825310	5.111524	8.453489
C	8.942304	4.823174	5.803555

C	6.458953	6.417205	6.228264
Al	5.530760	3.208161	4.526808
Cl	6.387036	1.416386	3.581581
Cl	3.351611	3.133578	4.600688
Cl	6.129459	4.882076	3.256001
C	5.927814	2.707842	10.486850
H	6.772284	2.023707	10.564144
C	5.398108	3.282699	11.646794
H	5.831586	3.033049	12.616750
C	4.323871	4.172130	11.566975
H	3.908560	4.612498	12.475112
C	3.790339	4.505144	10.317665
H	2.957314	5.206372	10.244341
C	4.325104	3.943874	9.156447
H	3.919274	4.218910	8.181532
C	3.343081	1.166143	7.687153
H	3.068893	1.972066	8.365773
C	2.382741	0.216314	7.333178
H	1.371208	0.300357	7.733539
C	2.712422	-0.828435	6.466280
H	1.957312	-1.564056	6.183904
C	4.011012	-0.928387	5.961282
H	4.276706	-1.736240	5.278171
C	4.979137	0.011325	6.319492
H	5.985255	-0.075652	5.912077
C	8.578801	1.234456	7.367594
H	8.692029	2.011532	6.609566
C	9.619898	0.333376	7.617153
H	10.557216	0.424849	7.065981
C	9.451092	-0.688444	8.554225
H	10.260784	-1.394580	8.746367
C	8.231267	-0.822101	9.228510
H	8.086690	-1.634243	9.943178
C	7.188553	0.071209	8.975347
H	6.227928	-0.066955	9.474606
C	7.176281	6.070434	9.245825
H	6.354505	6.654056	8.830512
C	7.589297	6.291123	10.562735
H	7.079648	7.042693	11.167664
C	8.653123	5.560416	11.098805
H	8.978917	5.740196	12.124828
C	9.303126	4.602735	10.314355
H	10.138317	4.031692	10.723491
C	8.894395	4.379848	8.997487
H	9.421525	3.643804	8.390540
C	9.981713	5.683127	6.202850

H	9.853116	6.342884	7.062158
C	11.201195	5.678562	5.520993
H	12.000820	6.349642	5.839682
C	11.396973	4.812073	4.440740
H	12.349574	4.809360	3.907955
C	10.373344	3.944086	4.052330
H	10.516655	3.261738	3.213238
C	9.150325	3.946592	4.729619
H	8.365374	3.257018	4.415790
C	7.176893	7.586839	5.938662
H	8.266044	7.574629	5.905849
C	6.495671	8.772600	5.654773
H	7.061068	9.675450	5.417631
C	5.097406	8.799145	5.655323
H	4.568376	9.724954	5.422734
C	4.380491	7.632268	5.931606
H	3.289836	7.636267	5.903746
C	5.058049	6.444145	6.216143
H	4.501626	5.520900	6.383495

(BCl3)2-1H RI-BP86/TZVP

17			
E(SCF) =	-3535.983881		
C	-0.018263	0.001138	0.924165
P	-0.789273	-1.524137	1.584919
P	-0.848384	1.510431	1.549236
B	-0.321471	-0.001996	-0.743029
Cl	-2.209711	-0.431289	-0.916737
Cl	-0.067155	1.730524	-1.399340
Cl	0.663010	-1.261399	-1.635333
B	1.544002	0.017272	1.580483
Cl	2.611896	1.297648	0.824434
Cl	2.261266	-1.705317	1.456923
Cl	1.300655	0.425158	3.465692
H	-0.586853	-2.573567	0.662943
H	-2.189621	-1.434362	1.789879
H	-0.250286	-1.905655	2.836377
H	0.083088	2.570867	1.561486
H	-1.349681	1.401222	2.871269
H	-1.958250	1.886771	0.756525

(BCl3)2-1Me RI-BP86/TZVP

35			
E(SCF) =	-3772.012033		
C	-0.001710	0.001339	0.916298
P	-0.850612	-1.554462	1.579568

P	-0.857541	1.540283	1.609022
B	-0.164559	0.024560	-0.809293
B	1.642926	-0.006597	1.463349
Cl	-1.958437	-0.491923	-1.341338
Cl	0.069068	1.755488	-1.521612
Cl	1.000490	-1.134484	-1.646309
Cl	2.706193	1.174882	0.528061
Cl	2.411218	-1.727394	1.379358
Cl	1.750801	0.493548	3.335763
C	-2.412278	2.012396	0.749933
H	-2.208878	2.227053	-0.303363
H	-2.789978	2.911233	1.258447
H	-3.156386	1.212626	0.815891
C	0.199719	3.035295	1.587793
H	1.034311	2.899491	2.283097
H	-0.441140	3.869142	1.909627
H	0.577976	3.206289	0.576757
C	-1.408996	1.447405	3.370362
H	-0.554403	1.221460	4.014720
H	-2.206855	0.712004	3.516169
H	-1.808902	2.440095	3.620786
C	-2.691752	-1.485925	1.721550
H	-3.022593	-0.760995	2.472282
H	-3.013207	-2.485517	2.046340
H	-3.130248	-1.257054	0.745841
C	-0.573811	-3.036058	0.539701
H	0.498397	-3.193047	0.397872
H	-1.064345	-2.896421	-0.428947
H	-1.022476	-3.880704	1.082787
C	-0.357720	-2.037120	3.283205
H	0.717235	-2.236981	3.321093
H	-0.925401	-2.946785	3.527017
H	-0.601749	-1.248122	4.001281

(BCl3)2-1Ph **RI-BP86/TZVP**

77

E(SCF) =	-4922.713861		
C	0.012245	-0.937601	-0.028832
P	-1.689616	0.142445	0.044361
P	1.703054	0.200123	-0.032709
C	2.015994	1.295265	-1.529209
C	1.862776	1.449181	1.356105
C	3.311350	-0.755466	0.093275
C	-1.608429	1.902327	-0.601991
C	-2.425259	0.427338	1.735497
C	-3.129059	-0.548420	-0.931554

B	-0.036888	-1.866043	-1.496442
Cl	-0.732140	-0.866923	-2.981732
Cl	1.689267	-2.424399	-2.001551
Cl	-1.096979	-3.382519	-1.374654
B	0.074786	-1.963393	1.372124
Cl	-1.639021	-2.552717	1.885183
Cl	0.769974	-1.056219	2.912441
Cl	1.126223	-3.473905	1.124890
C	-1.018274	2.228986	-1.833270
C	-2.297094	2.908518	0.106206
C	-2.368077	4.208703	-0.399057
C	-1.763334	4.528278	-1.617880
C	-1.094368	3.532934	-2.332228
C	-1.669754	0.979746	2.779220
C	-2.273941	1.299204	3.997486
C	-3.639882	1.082438	4.188095
C	-4.401897	0.550352	3.144824
C	-3.804299	0.227792	1.924768
C	2.019978	0.783690	-2.839759
C	2.375174	1.598301	-3.917913
C	2.752259	2.927586	-3.713308
C	2.783761	3.434220	-2.412907
C	2.422346	2.628298	-1.329876
C	0.970624	2.527285	1.462067
C	1.160325	3.523393	2.424761
C	2.251837	3.464359	3.292708
C	3.157699	2.406515	3.179292
C	2.971214	1.410571	2.218816
C	3.622225	-1.564891	1.197660
C	4.879626	-2.167083	1.295735
C	5.842385	-1.972139	0.304945
C	5.543393	-1.153708	-0.786556
C	4.290455	-0.548230	-0.894349
C	-3.690772	-1.800380	-0.636422
C	-4.845672	-2.223326	-1.299614
C	-5.450795	-1.413529	-2.261724
C	-4.896670	-0.165290	-2.555107
C	-3.744697	0.267362	-1.896421
H	-2.783854	2.682689	1.052371
H	-2.908675	4.970548	0.165075
H	-1.823136	5.544378	-2.011764
H	-0.627817	3.760269	-3.291607
H	-0.530703	1.456348	-2.422074
H	-0.604391	1.148665	2.663174
H	-1.662306	1.709750	4.802247
H	-4.108479	1.326043	5.143069

H	-5.471441	0.378032	3.275504
H	-4.417670	-0.186526	1.127993
H	-3.231034	-2.442722	0.108976
H	-5.261704	-3.203444	-1.061865
H	-6.348577	-1.752525	-2.781568
H	-5.354700	0.480042	-3.306336
H	-3.330652	1.239401	-2.151969
H	4.086355	0.073919	-1.761335
H	6.283158	-0.985623	-1.570838
H	6.819760	-2.451413	0.382871
H	5.092582	-2.801816	2.157164
H	2.897637	-1.725342	1.990109
H	0.448103	4.347878	2.485140
H	0.130831	2.619097	0.778226
H	3.694617	0.601978	2.150750
H	4.022105	2.349067	3.842666
H	2.402248	4.240973	4.044403
H	1.769874	-0.256615	-3.025560
H	2.471864	3.053136	-0.331422
H	3.094957	4.463654	-2.227925
H	3.034659	3.558182	-4.558355
H	2.362961	1.175047	-4.923567

BCl3-1H Σ -BP86/TZVP

13

E(SCF) =	-2130.199571		
C	0.924518	-0.001629	0.076390
P	1.730210	1.506596	0.048790
P	1.722720	-1.513916	0.048993
B	-0.686574	0.001352	0.000364
Cl	-1.218267	1.578927	-0.920370
Cl	-1.224872	-1.564409	-0.936301
Cl	-1.445658	-0.006266	1.718385
H	1.771671	2.277453	-1.155166
H	3.110804	1.387782	0.382979
H	1.234936	2.459471	0.983428
H	1.763200	-2.283601	-1.155808
H	3.102936	-1.404173	0.387686
H	1.217814	-2.464400	0.980842

BCl3-1Me Σ -BP86/TZVP

31

E(SCF) =	-2366.242457		
C	0.039260	0.189101	-0.028866
P	1.494588	0.224393	0.917479
P	-0.063046	0.055837	-1.757256

B	-1.369669	0.208584	0.789035
Cl	-1.257620	1.180334	2.433408
Cl	-2.784312	1.039690	-0.196023
Cl	-1.930058	-1.567163	1.210974
C	1.975192	1.879679	1.587371
H	2.846375	1.794405	2.252679
H	1.119472	2.290186	2.134638
H	2.216321	2.541613	0.744729
C	1.431026	-0.901676	2.371610
H	2.366377	-0.817351	2.942610
H	1.293436	-1.928851	2.012003
H	0.577507	-0.631755	3.002534
C	3.055848	-0.304611	0.084650
H	3.846410	-0.289023	0.847046
H	3.341461	0.383419	-0.718222
H	2.967703	-1.323130	-0.308968
C	-0.477737	1.617329	-2.656970
H	0.344108	2.332211	-2.515730
H	-1.393743	2.030646	-2.220401
H	-0.621217	1.425226	-3.729989
C	1.453345	-0.499388	-2.653620
H	2.263989	0.232666	-2.575480
H	1.180817	-0.597839	-3.713144
H	1.792733	-1.474140	-2.286236
C	-1.309965	-1.180180	-2.307567
H	-1.025933	-2.163046	-1.912037
H	-1.342303	-1.203133	-3.405925
H	-2.292153	-0.909293	-1.905934

	BCl3-1Ph	RI-BP86/TZVP	
73			
E(SCF) =	-3517.007279		
C	-0.101226	0.921028	-0.507671
P	1.496249	0.200753	-0.429122
P	-1.503729	0.047486	0.085032
C	2.341771	0.163943	-2.081909
C	2.686975	0.948516	0.795907
C	1.518223	-1.579942	0.101832
C	-1.669266	-0.077172	1.934710
C	-3.144743	0.802200	-0.349523
C	-1.621482	-1.674333	-0.599232
B	-0.253769	2.453824	-1.038923
Cl	-0.878777	3.633010	0.349356
Cl	-1.442059	2.577296	-2.514092
Cl	1.413215	3.166074	-1.610723
C	1.545851	0.230862	-3.233835

C	2.132498	0.130847	-4.497445
C	3.515645	-0.030984	-4.620293
C	4.313004	-0.080692	-3.473049
C	3.730641	0.017466	-2.206225
C	2.416422	2.195944	1.376874
C	3.304471	2.740709	2.309433
C	4.466312	2.051974	2.668324
C	4.732910	0.800782	2.104294
C	3.844829	0.246918	1.178109
C	1.442710	-1.911112	1.465339
C	1.517877	-3.244855	1.873184
C	1.679604	-4.260614	0.926202
C	1.759786	-3.937235	-0.431030
C	1.681168	-2.604153	-0.843400
C	-0.717485	0.551190	2.745793
C	-0.849539	0.525494	4.138510
C	-1.935357	-0.126825	4.727211
C	-2.904841	-0.734241	3.920206
C	-2.780982	-0.700715	2.529739
C	-3.921601	0.318146	-1.412063
C	-5.176552	0.871684	-1.673830
C	-5.667902	1.909556	-0.878200
C	-4.902472	2.385449	0.189105
C	-3.650093	1.831840	0.460346
C	-1.503075	-1.807909	-1.993881
C	-1.667597	-3.054903	-2.600135
C	-1.935912	-4.183997	-1.819593
C	-2.029361	-4.059998	-0.431235
C	-1.877822	-2.810676	0.179087
H	-1.276679	-0.929675	-2.600616
H	-1.582139	-3.143285	-3.684568
H	-2.062273	-5.159627	-2.292180
H	-2.218831	-4.940040	0.185759
H	-1.940770	-2.732228	1.263913
H	-3.558059	-0.491224	-2.042452
H	-5.768613	0.488994	-2.506775
H	-6.646403	2.345042	-1.088310
H	-5.275497	3.197302	0.815297
H	-3.058284	2.220108	1.286765
H	0.108793	1.089290	2.278702
H	-0.106996	1.028270	4.760299
H	-2.040065	-0.145393	5.813463
H	-3.768655	-1.222562	4.374795
H	-3.566129	-1.135594	1.909130
H	4.047219	-0.747146	0.777007
H	5.629404	0.247634	2.390211

H	5.159072	2.484128	3.392753
H	3.084164	3.714856	2.749107
H	1.516736	2.747969	1.101485
H	1.506448	0.204475	-5.388194
H	0.475792	0.419069	-3.134779
H	4.368517	0.002783	-1.322984
H	5.395834	-0.185317	-3.561396
H	3.973941	-0.100773	-5.608370
H	1.340848	-1.127480	2.215528
H	1.757559	-2.360103	-1.902814
H	1.890329	-4.723745	-1.175932
H	1.749151	-5.301796	1.246237
H	1.461045	-3.487213	2.935714

(BH3)2-1H Σ -BP86/TZVP

17

E(SCF) =	-777.721885		
C	-0.085780	0.000466	0.977904
P	-0.780693	-1.523004	1.534832
P	-0.798651	1.509224	1.551917
B	-0.415736	0.033785	-0.679984
H	-0.274970	1.198896	-1.048937
H	-1.585156	-0.312984	-0.866009
H	0.382881	-0.708449	-1.222336
B	1.461193	-0.019636	1.659993
H	1.865272	-1.179631	1.595610
H	1.384650	0.318965	2.844182
H	2.155410	0.735069	1.003344
H	-0.166913	-2.536936	0.766893
H	-2.179095	-1.748978	1.347229
H	-0.548233	-1.896055	2.891157
H	0.072553	2.538233	1.131494
H	-0.922865	1.717921	2.959984
H	-2.075997	1.873013	1.033402

(BH3)2-1Me Σ -BP86/TZVP

35

E(SCF) =	-1013.771169		
C	-0.035232	-0.000667	0.942900
P	-0.742444	-1.534201	1.553321
P	-0.804158	1.521924	1.504516
B	-0.252204	-0.023354	-0.744409
H	-0.155728	1.125435	-1.166882
H	-1.378374	-0.448526	-1.033486
H	0.620712	-0.718441	-1.230967
B	1.558506	0.032377	1.537206

H	2.001851	-1.112481	1.531748
H	1.580785	0.449952	2.702606
H	2.224119	0.738684	0.802375
C	0.300418	2.917595	1.089016
H	1.230324	2.805649	1.657426
H	-0.202862	3.861322	1.339125
H	0.527027	2.870847	0.018137
C	-2.429224	1.912573	0.734877
H	-2.321318	1.805972	-0.351037
H	-2.725308	2.938461	0.992424
H	-3.199248	1.216212	1.089326
C	-1.091175	1.674153	3.321563
H	-0.164472	1.397109	3.839299
H	-1.909366	1.014795	3.640044
H	-1.358147	2.709827	3.571721
C	-2.575654	-1.701815	1.418970
H	-2.871500	-1.421365	0.400469
H	-3.077385	-1.050950	2.147188
H	-2.870974	-2.741241	1.616266
C	-0.074240	-2.916878	0.562243
H	1.019602	-2.861083	0.586555
H	-0.416252	-2.799999	-0.472011
H	-0.424809	-3.866775	0.987937
C	-0.358586	-1.933514	3.308082
H	0.721893	-1.813789	3.451298
H	-0.663222	-2.965218	3.529773
H	-0.888467	-1.249149	3.982127

	(BH3)2-1Ph	RI-BP86/TZVP	
77			
E(SCF) =	-2164.517968		
C	0.000017	-0.000087	1.327621
P	-1.559181	0.071478	0.383184
P	1.559206	-0.071553	0.383160
C	1.829879	-1.514266	-0.767351
C	1.940358	1.403411	-0.681727
C	2.987009	-0.140879	1.561498
C	-1.940404	-1.403436	-0.681744
C	-1.829828	1.514263	-0.767245
C	-2.986949	0.140840	1.561565
B	0.019494	-1.470255	2.233143
H	-0.847121	-2.245298	1.844907
H	1.106164	-2.012759	2.091239
H	-0.126749	-1.194598	3.409540
B	-0.019452	1.469907	2.233417
H	-1.105998	2.012613	2.091325

H	0.847395	2.244883	1.845568
H	0.126425	1.194001	3.409802
C	-2.710658	-2.457149	-0.163390
C	-1.448605	-1.500903	-1.993737
C	-1.734068	-2.619978	-2.779070
C	-2.504978	-3.662587	-2.257028
C	-2.987875	-3.580063	-0.947869
C	-1.240341	2.766118	-0.520245
C	-1.534212	3.855462	-1.344198
C	-2.414680	3.718740	-2.420254
C	-3.001470	2.476920	-2.676125
C	-2.712275	1.381667	-1.857164
C	1.240274	-2.766098	-0.520520
C	1.534064	-3.855363	-1.344607
C	2.414593	-3.718590	-2.420608
C	3.001419	-2.476765	-2.676371
C	2.712302	-1.381588	-1.857278
C	1.448554	1.500893	-1.993716
C	1.734010	2.619980	-2.779036
C	2.504922	3.662583	-2.256984
C	2.987833	3.580038	-0.947832
C	2.710626	2.457112	-0.163368
C	2.844771	0.130215	2.929803
C	3.967268	0.095043	3.761412
C	5.228949	-0.211686	3.244437
C	5.369848	-0.486383	1.881471
C	4.253717	-0.453484	1.041793
C	-2.844628	-0.129956	2.929920
C	-3.967092	-0.094713	3.761570
C	-5.228824	0.211786	3.244584
C	-5.369801	0.486223	1.881574
C	-4.253702	0.453257	1.041857
H	-0.849744	-0.694741	-2.417945
H	-1.347475	-2.677439	-3.797712
H	-2.729453	-4.537343	-2.869989
H	-3.587794	-4.391040	-0.531702
H	-3.094661	-2.397933	0.854075
H	-0.565928	2.887040	0.326270
H	-1.067016	4.819308	-1.136259
H	-2.644498	4.575660	-3.056291
H	-3.690675	2.354081	-3.513540
H	-3.178416	0.421607	-2.076731
H	-1.863044	-0.366990	3.338502
H	-3.845697	-0.303225	4.825819
H	-6.099585	0.241911	3.902208
H	-6.348028	0.735685	1.466981

H	-4.379517	0.686074	-0.015609
H	4.379473	-0.686479	-0.015641
H	6.348033	-0.736025	1.466889
H	6.099737	-0.241745	3.902028
H	3.845932	0.303752	4.825629
H	1.863233	0.367474	3.338367
H	1.347412	2.677452	-3.797676
H	0.849733	0.694715	-2.417949
H	3.094681	2.397859	0.854075
H	3.587760	4.391007	-0.531659
H	2.729371	4.537359	-2.869927
H	0.565695	-2.887022	0.325862
H	3.178378	-0.421493	-2.076831
H	3.690695	-2.353893	-3.513723
H	2.644301	-4.575435	-3.056785
H	1.066867	-4.819222	-1.136731

BH3-1H Σ I-BP86/TZVP

13			
E(SCF) =	-751.053222		
C	0.067938	-0.401015	-0.036773
P	1.419942	-0.027167	0.921229
P	-0.088610	0.064462	-1.662861
B	-1.359074	-0.152896	0.804712
H	-1.103399	0.479023	1.834529
H	-1.861982	-1.237525	1.063366
H	-2.111756	0.534495	0.107430
H	2.718713	-0.208113	0.344739
H	1.464712	-0.862178	2.071921
H	1.562060	1.263405	1.553290
H	1.046740	-0.106268	-2.519471
H	-0.528828	1.390331	-2.028272
H	-1.093104	-0.707005	-2.310318

BH3-1Me Σ I-BP86/TZVP

31			
E(SCF) =	-987.099627		
C	0.272017	0.528442	-0.185174
P	1.540804	0.163749	0.889600
P	0.013528	0.036554	-1.794320
B	-1.128725	1.052710	0.587376
H	-1.137317	0.645501	1.752540
H	-2.117057	0.572693	0.025046
H	-1.190855	2.280226	0.570523
C	1.836950	1.593417	2.010555
H	2.547692	1.336647	2.807905

H	0.867723	1.876606	2.439980
H	2.217566	2.435317	1.418459
C	1.246094	-1.245728	2.062144
H	2.010642	-1.292590	2.850807
H	1.239720	-2.187676	1.497633
H	0.255990	-1.091715	2.509784
C	3.202822	-0.219207	0.173619
H	3.933481	-0.324142	0.987188
H	3.519887	0.594558	-0.489855
H	3.173835	-1.159188	-0.391246
C	-0.851343	1.370564	-2.721855
H	-0.179293	2.233523	-2.810689
H	-1.725147	1.666138	-2.127675
H	-1.164505	1.028082	-3.717571
C	1.493566	-0.365921	-2.828415
H	2.195850	0.476441	-2.819280
H	1.173652	-0.555303	-3.862132
H	1.997318	-1.264074	-2.450259
C	-1.089025	-1.438009	-2.035931
H	-0.571807	-2.336523	-1.673753
H	-1.371351	-1.573531	-3.089826
H	-1.986607	-1.273409	-1.426406

BH3-1Ph

RI-BP86/TZVP

73

E(SCF) =	-2137.870433		
C	-0.112890	0.696163	-0.344869
P	1.474933	0.039084	-0.399444
P	-1.550990	-0.049738	0.235313
C	2.220317	0.295066	-2.084202
C	2.715320	0.766202	0.792751
C	1.657047	-1.780309	-0.086821
C	-1.859614	0.061922	2.072052
C	-3.005667	0.799531	-0.533549
C	-1.817850	-1.849324	-0.154420
B	-0.103661	2.347509	-0.657903
H	-0.472437	2.990344	0.327780
H	-0.807059	2.618270	-1.623395
H	1.053834	2.656795	-0.934619
C	1.341981	0.437290	-3.166579
C	1.840275	0.578112	-4.464132
C	3.220429	0.583105	-4.688458
C	4.100380	0.455077	-3.609278
C	3.604144	0.314753	-2.309908
C	2.448064	1.994593	1.417753
C	3.371227	2.539956	2.315051

C	4.566869	1.872326	2.597070
C	4.837237	0.647258	1.980903
C	3.916278	0.095024	1.085060
C	1.763335	-2.261262	1.229456
C	1.933383	-3.626726	1.470263
C	1.988054	-4.526078	0.400578
C	1.864675	-4.056019	-0.909822
C	1.703990	-2.688743	-1.154457
C	-1.039502	0.928455	2.807064
C	-1.222968	1.071873	4.185887
C	-2.222185	0.345602	4.840431
C	-3.045198	-0.520696	4.112387
C	-2.869569	-0.660223	2.732441
C	-2.954953	1.097710	-1.905338
C	-4.053748	1.680201	-2.539843
C	-5.205080	1.989423	-1.808987
C	-5.250788	1.718930	-0.439313
C	-4.154887	1.127993	0.198038
C	-2.287821	-2.213532	-1.427315
C	-2.493831	-3.556267	-1.749390
C	-2.231132	-4.554069	-0.804990
C	-1.755545	-4.200446	0.459596
C	-1.551692	-2.855933	0.785826
H	-2.512499	-1.444179	-2.166345
H	-2.870271	-3.821938	-2.738846
H	-2.397185	-5.603447	-1.055065
H	-1.541457	-4.972026	1.201033
H	-1.186364	-2.594834	1.778309
H	-2.038407	0.903827	-2.460712
H	-4.000116	1.914726	-3.604298
H	-6.059821	2.453601	-2.304419
H	-6.138439	1.974739	0.141895
H	-4.197052	0.939360	1.270357
H	-0.266730	1.491900	2.281673
H	-0.582874	1.753505	4.748629
H	-2.361530	0.453855	5.917678
H	-3.825348	-1.091528	4.619677
H	-3.515461	-1.340073	2.174076
H	4.131502	-0.873614	0.631384
H	5.764525	0.114218	2.199499
H	5.285539	2.303921	3.296296
H	3.154304	3.498626	2.789835
H	1.529076	2.529692	1.172114
H	1.148905	0.700423	-5.299900
H	0.270063	0.465309	-2.965540
H	4.301187	0.239577	-1.474976

H	5.178923	0.473668	-3.776526
H	3.610693	0.698767	-5.701305
H	1.733400	-1.564296	2.068483
H	1.630379	-2.325434	-2.180309
H	1.903946	-4.753302	-1.748361
H	2.128446	-5.592103	0.588525
H	2.028156	-3.987308	2.496259

(CO2)2-1H RI-BP86/TZVP

15

E(SCF) = -1101.741990

C	-0.092106	-0.000257	0.987063
P	-0.524083	-1.626065	1.714554
P	-0.894314	1.625846	1.254795
C	-0.267052	0.067857	-0.589806
O	-0.060984	-0.874116	-1.334082
O	-0.661481	1.287063	-0.808842
C	1.412127	-0.067797	1.492475
O	1.542658	-1.285967	1.926627
O	2.182982	0.874252	1.446881
H	-0.152373	-2.725300	0.910420
H	-1.959126	-1.711677	1.548354
H	-0.462739	-1.859908	3.108288
H	-0.028908	2.724953	1.064217
H	-1.037862	1.710396	2.692469
H	-2.242970	1.860632	0.898407

(CO2)2-1Me RI-BP86/TZVP

33

E(SCF) = -1337.788469

C	-0.153333	-0.000964	1.029619
P	-0.854679	-1.600777	1.632489
P	-0.882735	1.601262	1.591621
C	-0.397740	-0.002904	-0.582236
O	0.086679	-0.955568	-1.208416
O	-1.126297	0.962308	-0.942984
C	1.378281	0.002772	1.599808
O	1.574177	-0.942915	2.411440
O	2.095986	0.940480	1.227692
C	-2.508580	-1.851858	0.858085
H	-2.393441	-1.816874	-0.232744
H	-3.218159	-1.076568	1.169745
H	-2.900676	-2.834891	1.152954
C	-1.141312	-1.753334	3.438288
H	-0.203398	-1.520747	3.952890
H	-1.438793	-2.790093	3.649758

H	-1.950254	-1.086174	3.763211
C	0.139886	-3.015683	1.045835
H	1.007194	-3.138171	1.699293
H	0.460397	-2.761000	0.025411
H	-0.503103	-3.907221	1.037004
C	-2.707932	1.760167	1.492758
H	-2.974461	2.795827	1.746709
H	-3.197549	1.089180	2.210542
H	-3.014747	1.535631	0.466106
C	-0.474018	1.843068	3.373272
H	0.616170	1.800635	3.492380
H	-0.933021	1.068344	3.998375
H	-0.838936	2.827150	3.697746
C	-0.092825	3.018303	0.752634
H	0.968098	2.752937	0.638357
H	-0.201964	3.903001	1.395867
H	-0.557600	3.158629	-0.226335

	(CO2)2-1Ph	RI-BP86/TZVP	
75			
E(SCF) =	-2488.542288		
C	0.021862	-0.615647	-0.578108
P	1.669814	0.049134	-0.016401
P	-1.628583	0.137570	-0.068472
C	1.648866	0.842183	1.647809
C	2.373501	1.321654	-1.154345
C	2.938315	-1.288699	0.041678
C	-1.849187	0.275339	1.787845
C	-1.922169	1.846585	-0.699393
C	-3.111530	-0.905787	-0.456221
C	0.041526	-2.300759	-0.025124
C	-0.060046	-0.534815	-2.132044
O	0.317335	-2.370761	1.183766
O	-0.214653	-3.090512	-0.922558
O	-1.222889	-0.189384	-2.514644
O	0.965537	-0.789287	-2.788139
C	1.332817	0.079991	2.787332
C	1.993109	2.197753	1.786170
C	2.016794	2.786861	3.053806
C	1.709520	2.027665	4.185810
C	1.370326	0.677759	4.048680
C	1.587875	2.096127	-2.019151
C	2.188571	3.072435	-2.817844
C	3.569103	3.281280	-2.763502
C	4.355807	2.505284	-1.907249
C	3.763685	1.525376	-1.107586

C	-1.914088	-0.915683	2.537087
C	-2.209808	-0.877890	3.900165
C	-2.456981	0.341449	4.539145
C	-2.410322	1.525174	3.801208
C	-2.114452	1.493728	2.433950
C	-1.151277	2.927657	-0.242951
C	-1.399712	4.218873	-0.720467
C	-2.418222	4.438022	-1.650726
C	-3.178855	3.359357	-2.115382
C	-2.930525	2.067684	-1.649654
C	-3.096659	-2.007344	-1.322922
C	-4.277314	-2.722645	-1.544429
C	-5.474010	-2.334131	-0.937487
C	-5.490737	-1.228235	-0.082486
C	-4.311797	-0.524753	0.172118
C	3.085375	-2.141242	-1.065441
C	4.079933	-3.121545	-1.043253
C	4.930075	-3.249550	0.058914
C	4.787737	-2.390192	1.151928
C	3.791759	-1.410461	1.149663
H	2.259191	2.789156	0.909930
H	2.287581	3.839340	3.153296
H	1.736603	2.487291	5.175407
H	1.126394	0.081644	4.929065
H	1.053943	-0.967626	2.663080
H	0.515763	1.929372	-2.101346
H	1.569941	3.657448	-3.499675
H	4.033608	4.039072	-3.396783
H	5.436602	2.650366	-1.868860
H	4.387847	0.910464	-0.458019
H	2.422020	-2.021775	-1.925475
H	4.184179	-3.791313	-1.898195
H	5.703550	-4.019678	0.067634
H	5.447217	-2.484043	2.016336
H	3.682946	-0.752512	2.011222
H	-4.333519	0.320845	0.860543
H	-6.418642	-0.914951	0.398883
H	-6.392313	-2.892919	-1.127085
H	-4.253193	-3.588635	-2.207515
H	-2.175228	-2.313186	-1.810612
H	-0.791524	5.051229	-0.362709
H	-0.349000	2.771770	0.479636
H	-3.496766	1.223956	-2.040950
H	-3.962661	3.520519	-2.857134
H	-2.613648	5.445797	-2.021128
H	-1.716335	-1.875304	2.063240

H	-2.118832	2.427948	1.875974
H	-2.616348	2.482904	4.282397
H	-2.697220	0.366172	5.603703
H	-2.254172	-1.812587	4.461815

CO2-1H RI-BP86/TZVP

12

E(SCF) = -913.079767

C	0.175173	-0.035792	1.214119
P	-1.518112	0.042586	1.683034
P	1.653606	0.110571	2.058698
C	-0.064920	-0.276570	-0.233903
O	0.750001	-0.425650	-1.136048
O	-1.402600	-0.287546	-0.289614
H	-2.346721	1.160011	1.384363
H	-1.439809	0.283480	3.124117
H	-2.346157	-1.111584	1.764239
H	1.426329	0.328673	3.441363
H	2.560773	-0.998066	2.040146
H	2.548207	1.170886	1.698877

CO2-1Me RI-BP86/TZVP

30

E(SCF) = -1149.124996

C	0.067916	0.021649	1.411758
P	-1.560846	0.103887	2.011651
P	1.648659	0.128699	2.125212
C	0.123111	-0.201482	-0.097858
O	1.286951	-0.273348	-0.591303
O	-1.001739	-0.288013	-0.672673
C	2.659345	1.517076	1.464241
H	3.682657	1.478579	1.863747
H	2.185527	2.467588	1.742481
H	2.663820	1.405607	0.373410
C	1.659109	0.400101	3.951941
H	2.702910	0.452817	4.290583
H	1.164795	-0.429020	4.472050
H	1.160798	1.342584	4.208312
C	2.663940	-1.388783	1.895252
H	3.687197	-1.232649	2.265128
H	2.668015	-1.599022	0.819056
H	2.193540	-2.219052	2.438188
C	-1.704102	0.370035	3.833607
H	-1.239870	1.319249	4.126531
H	-1.235024	-0.453035	4.385721
H	-2.769908	0.405790	4.097735

C	-2.543256	1.479071	1.283468
H	-2.105223	2.435781	1.596906
H	-3.591775	1.423742	1.608691
H	-2.468209	1.370979	0.194848
C	-2.534574	-1.428004	1.709284
H	-2.090127	-2.252621	2.281894
H	-2.461035	-1.635236	0.635068
H	-3.583112	-1.288250	2.008014

CO2-1Ph Σ I-BP86/TZVP

72

E(SCF) = -2299.892026

C	0.013030	0.683884	0.192121
P	1.577364	0.073351	-0.314881
P	-1.579172	0.015170	0.459404
C	1.953743	0.265131	-2.113002
C	3.032264	0.631315	0.691799
C	1.732588	-1.762012	0.022244
C	-2.214985	0.165054	2.192179
C	-2.812379	0.903476	-0.592756
C	-1.762291	-1.761108	-0.004896
C	0.128958	2.184157	0.054999
O	1.250747	2.484832	-0.497581
O	-0.775891	2.942468	0.471095
C	1.059345	-0.281803	-3.046122
C	1.285374	-0.122592	-4.416924
C	2.404192	0.585953	-4.863701
C	3.287151	1.146125	-3.934534
C	3.063430	0.991833	-2.564731
C	2.886120	1.547649	1.741127
C	3.991546	1.893285	2.522368
C	5.249472	1.343860	2.253120
C	5.397542	0.429267	1.206918
C	4.289803	0.063079	0.436116
C	1.819632	-2.159559	1.370060
C	2.049568	-3.493784	1.707314
C	2.195972	-4.456413	0.701726
C	2.110584	-4.072781	-0.637901
C	1.885752	-2.732851	-0.977236
C	-1.802275	1.279723	2.941881
C	-2.274554	1.449469	4.245433
C	-3.153126	0.517686	4.808815
C	-3.574659	-0.584095	4.059259
C	-3.111191	-0.761201	2.751286
C	-2.403510	1.456074	-1.814750
C	-3.341940	2.062417	-2.652638

C	-4.687172	2.124059	-2.275284
C	-5.093552	1.579915	-1.053374
C	-4.159356	0.971823	-0.210345
C	-2.269450	-2.096163	-1.271453
C	-2.410183	-3.436176	-1.641563
C	-2.055697	-4.452084	-0.749635
C	-1.553300	-4.123908	0.512966
C	-1.405525	-2.786171	0.886179
H	-2.573247	-1.308170	-1.961680
H	-2.810588	-3.684106	-2.626050
H	-2.173211	-5.498474	-1.036474
H	-1.271463	-4.911393	1.213237
H	-1.013664	-2.543245	1.873230
H	-1.349150	1.434895	-2.093694
H	-3.014845	2.505427	-3.594645
H	-5.416712	2.606398	-2.928246
H	-6.139568	1.637880	-0.747366
H	-4.480205	0.567986	0.750762
H	-1.155359	2.025364	2.472126
H	-1.956957	2.320238	4.821652
H	-3.515983	0.654480	5.829220
H	-4.266221	-1.310373	4.490231
H	-3.449083	-1.622599	2.173808
H	4.409914	-0.674332	-0.359990
H	6.373871	-0.009306	0.992867
H	6.111895	1.626209	2.859645
H	3.869790	2.608892	3.337300
H	1.915081	1.999313	1.936650
H	0.582387	-0.549427	-5.134712
H	0.172160	-0.818823	-2.703112
H	3.729094	1.467915	-1.845482
H	4.147962	1.722981	-4.277181
H	2.579930	0.714682	-5.933128
H	1.732524	-1.411738	2.160991
H	1.853116	-2.446781	-2.028313
H	2.232041	-4.814683	-1.429292
H	2.387186	-5.498773	0.963340
H	2.127168	-3.780826	2.757785

(CS2)2-1H RI-BP86/TZVP

15

E(SCF) = -2393.651936

C	-0.026092	-0.165590	0.934838
P	-0.775514	-1.739516	1.545797
P	-0.593635	1.739191	1.383152
C	-0.237750	-0.103618	-0.571072

S	-0.436820	-1.519596	-1.445359
S	-0.290816	1.533051	-1.088236
C	1.399594	-0.094402	1.462144
S	2.216144	-1.505260	1.851903
S	1.886927	1.545194	1.613995
H	-0.284294	-2.999698	1.151504
H	-2.161415	-1.726278	1.229380
H	-0.758642	-1.721220	2.967091
H	-0.547607	3.172884	1.339525
H	-0.647105	1.593271	2.813679
H	-2.002206	1.585529	1.132483

(CS2)2-1Me RI-BP86/TZVP

33

E(SCF) = -2629.673600

C	-0.045119	-0.002577	0.981427
P	-0.910297	-1.633209	1.597520
P	-0.868369	1.606158	1.701730
C	-0.243211	0.034593	-0.546885
S	0.603284	-1.074674	-1.480875
S	-1.413159	1.172207	-1.068148
C	1.396310	-0.024469	1.527856
S	1.647943	-1.174870	2.772243
S	2.485028	1.108194	0.935750
C	-2.696230	1.699862	1.969386
H	-2.886954	2.629546	2.525112
H	-3.045812	0.860663	2.582898
H	-3.215080	1.714554	1.008299
C	-0.266219	3.211525	1.035216
H	0.621242	3.008137	0.423231
H	0.007361	3.860325	1.880085
H	-1.052541	3.656606	0.417994
C	-2.484605	-1.713613	0.614845
H	-2.246329	-1.780786	-0.453270
H	-3.112228	-0.830416	0.774585
H	-3.034773	-2.612767	0.926255
C	-0.100301	-3.221458	1.144485
H	0.324272	-3.672701	2.046481
H	0.697570	-2.996965	0.425817
H	-0.849505	-3.874666	0.673926
C	-1.592245	-1.760457	3.312406
H	-0.776526	-1.791562	4.038133
H	-2.180416	-2.689016	3.351438
H	-2.266415	-0.923009	3.529029
C	-0.276516	1.676948	3.460625
H	0.816139	1.766450	3.475232

H	-0.557840	0.780877	4.023883
H	-0.724439	2.561527	3.935125

	(CS2)2-1Ph	RI-BP86/TZVP	
75			
E(SCF) =	-3780.417553		
C	0.105849	-0.913731	-0.617961
P	1.816799	-0.080584	0.010970
P	-1.774328	0.012362	-0.176965
C	1.759707	1.106147	1.455006
C	2.416254	1.023041	-1.361553
C	3.262208	-1.194626	0.364574
C	-2.051429	-0.249842	1.671878
C	-1.963033	1.854304	-0.357563
C	-3.405509	-0.755884	-0.704745
C	0.021547	-2.278081	0.051504
C	0.105750	-0.851262	-2.144358
S	0.708828	-2.364840	1.609304
S	-0.830023	-3.496322	-0.747819
S	-1.158920	0.082097	-2.805017
S	1.362522	-1.612072	-2.948285
C	1.197969	0.757346	2.693120
C	2.406367	2.352610	1.326842
C	2.483430	3.224410	2.416032
C	1.916165	2.871685	3.643925
C	1.274857	1.637746	3.775849
C	1.594703	2.036548	-1.883065
C	2.074869	2.888399	-2.881159
C	3.377849	2.745206	-3.363781
C	4.202262	1.743225	-2.842962
C	3.727218	0.885484	-1.849022
C	-2.298466	-1.566882	2.113230
C	-2.642015	-1.818566	3.442997
C	-2.750408	-0.767005	4.356814
C	-2.519430	0.542354	3.929015
C	-2.169938	0.799322	2.598563
C	-1.113830	2.758037	0.297933
C	-1.285681	4.138327	0.132706
C	-2.311063	4.628387	-0.676269
C	-3.160208	3.729594	-1.333115
C	-2.984131	2.354301	-1.184450
C	-3.535852	-1.690987	-1.738175
C	-4.799426	-2.189580	-2.070759
C	-5.939018	-1.743682	-1.396963
C	-5.811578	-0.807283	-0.367222
C	-4.549276	-0.327961	-0.006601

C	3.481001	-2.390504	-0.337300
C	4.617922	-3.153210	-0.066959
C	5.544415	-2.737379	0.895088
C	5.327984	-1.544850	1.588862
C	4.192636	-0.771215	1.329001
H	2.859333	2.642799	0.380857
H	2.996094	4.180782	2.299464
H	1.979829	3.553185	4.494207
H	0.827307	1.348042	4.727725
H	0.714865	-0.213735	2.799320
H	0.576210	2.169093	-1.521707
H	1.419635	3.661736	-3.284889
H	3.749145	3.409548	-4.145920
H	5.220501	1.620158	-3.215537
H	4.374698	0.100208	-1.461502
H	2.763289	-2.710912	-1.093291
H	4.772513	-4.085920	-0.611809
H	6.428693	-3.341588	1.104466
H	6.041933	-1.207662	2.342366
H	4.038457	0.152016	1.885597
H	-4.463260	0.383597	0.814624
H	-6.692847	-0.451830	0.169487
H	-6.923391	-2.129738	-1.667681
H	-4.884989	-2.932369	-2.865298
H	-2.651977	-2.056030	-2.257391
H	-0.610065	4.824885	0.645358
H	-0.307151	2.399785	0.935373
H	-3.636941	1.665313	-1.719924
H	-3.961473	4.100233	-1.974560
H	-2.447708	5.703796	-0.800905
H	-2.256907	-2.399281	1.409023
H	-2.023708	1.831947	2.288938
H	-2.622260	1.376083	4.626227
H	-3.028365	-0.965957	5.393532
H	-2.823600	-2.846388	3.760475

CS2-1H **RI-BP86/TZVP**

12			
E(SCF) =	-1559.052400		
C	-0.000111	-0.034998	1.206925
P	-1.618099	0.075181	1.888552
P	1.617955	0.076445	1.887954
C	-0.000979	-0.260430	-0.201495
S	1.584936	-0.364568	-0.855304
S	-1.589078	-0.364686	-0.850873
H	-2.467582	1.175853	1.593163

H	-1.387745	0.300649	3.294506
H	-2.468728	-1.061739	1.952102
H	1.389081	0.302296	3.293864
H	2.469387	-1.059946	1.949950
H	2.466744	1.176942	1.590049

	CS2-1Me	RI-BP86/TZVP	
30			
E(SCF) =	-1795.077997		
C	0.042110	-0.052451	1.240636
P	-1.641972	0.068354	1.847488
P	1.634887	0.091957	2.019087
C	0.035849	-0.324716	-0.177615
S	1.460309	-0.504890	-1.104913
S	-1.587616	-0.441120	-0.794578
C	-2.649035	-1.490612	1.938522
H	-2.092888	-2.284324	1.428394
H	-3.591892	-1.341110	1.399875
H	-2.847351	-1.766345	2.984811
C	-1.569248	0.424506	3.693289
H	-1.075180	1.378847	3.910622
H	-1.080417	-0.382800	4.251229
H	-2.608289	0.495628	4.045466
C	-2.640956	1.554288	1.351047
H	-2.836366	2.200646	2.219420
H	-3.585360	1.220130	0.906160
H	-2.081395	2.098095	0.582493
C	2.648935	-1.445120	1.958004
H	3.654513	-1.243870	2.353937
H	2.706468	-1.772289	0.913957
H	2.154523	-2.210313	2.571647
C	2.657157	1.493163	1.397924
H	3.660304	1.449188	1.845339
H	2.164693	2.433027	1.681912
H	2.719442	1.410436	0.307242
C	1.590391	0.437453	3.830148
H	2.634696	0.498492	4.165863
H	1.093456	-0.367221	4.381977
H	1.098433	1.391441	4.046675

	CS2-1Ph	RI-BP86/TZVP	
72			
E(SCF) =	-2945.847717		
C	0.000054	-0.000106	-0.918552
P	1.653462	0.026826	-0.228334
P	-1.653434	-0.026835	-0.228506

C	2.655161	-1.509857	-0.503569
C	2.590808	1.560979	-0.644457
C	1.672516	0.031307	1.640036
C	-2.654888	1.509968	-0.503868
C	-2.590836	-1.560838	-0.645044
C	-1.672874	-0.031520	1.639832
C	0.000166	0.000094	-2.368033
S	1.529316	0.084863	-3.144938
S	-1.528717	-0.084737	-3.145405
C	-2.166233	2.548906	-1.309519
C	-2.895963	3.732087	-1.438949
C	-4.125488	3.881083	-0.785990
C	-4.610717	2.851202	0.022860
C	-3.870039	1.674147	0.180049
C	-1.901523	-2.782509	-0.594048
C	-2.575748	-3.979867	-0.848941
C	-3.942127	-3.969582	-1.141644
C	-4.630722	-2.751451	-1.184659
C	-3.963406	-1.551520	-0.935854
C	-2.165059	-1.127099	2.365335
C	-2.315499	-1.047508	3.754318
C	-1.976882	0.124761	4.431937
C	-1.484916	1.221796	3.715894
C	-1.340827	1.146895	2.330522
C	2.166689	-2.548908	-1.309187
C	2.896547	-3.732027	-1.438460
C	4.126043	-3.880836	-0.785403
C	4.611073	-2.850860	0.023444
C	3.870254	-1.673875	0.180489
C	1.901477	2.782621	-0.593097
C	2.575661	3.980061	-0.847730
C	3.942013	3.969875	-1.140550
C	4.630624	2.751766	-1.183955
C	3.963350	1.551760	-0.935408
C	2.164615	1.126756	2.365791
C	2.314813	1.046954	3.754791
C	1.976039	-0.125402	4.432178
C	1.484149	-1.222310	3.715886
C	1.340303	-1.147196	2.330502
H	2.449805	2.041861	1.847628
H	2.707104	1.905100	4.303537
H	2.100540	-0.189977	5.514565
H	1.220769	-2.144121	4.236883
H	0.986179	-2.020565	1.780721
H	0.830062	2.792644	-0.383815
H	2.026573	4.923049	-0.822452

H	4.467386	4.904534	-1.342742
H	5.694947	2.733737	-1.425171
H	4.501860	0.607173	-1.011799
H	1.231827	-2.416888	-1.852704
H	2.510665	-4.533871	-2.070014
H	4.700156	-4.801608	-0.902384
H	5.562151	-2.963087	0.546929
H	4.235750	-0.896616	0.853243
H	-4.501913	-0.606907	-1.011949
H	-5.695061	-2.733339	-1.425797
H	-4.467538	-4.904182	-1.344012
H	-2.026673	-4.922871	-0.823965
H	-0.830085	-2.792584	-0.384891
H	-2.509913	4.533866	-2.070483
H	-1.231388	2.416714	-1.853024
H	-4.235721	0.896936	0.852758
H	-5.561810	2.963582	0.546286
H	-4.699506	4.801897	-0.903108
H	-2.450097	-2.042146	1.846987
H	-0.986613	2.020350	1.780936
H	-1.221667	2.143542	4.237071
H	-2.101573	0.189170	5.514312
H	-2.707859	-1.905748	4.302868

	(H+)-1H	RI-BP86/TZVP	
10			
E(SCF) =	-724.799616		
C	-0.000045	0.057421	1.190284
P	-1.536176	-0.013197	1.970780
P	1.536136	-0.012834	1.970713
H	0.000002	-0.078236	0.108268
H	-2.515339	0.681955	1.215328
H	-1.505729	0.607084	3.247442
H	-2.174503	-1.266367	2.246712
H	1.506150	0.608639	3.246817
H	2.174292	-1.265860	2.247726
H	2.515202	0.681393	1.214313

	(H+)-1Me	RI-BP86/TZVP	
28			
E(SCF) =	-960.877574		
C	-0.483489	-0.009328	1.442457
P	-0.014784	-1.578167	2.015468
P	-0.135913	1.578898	2.044707
H	-1.231971	-0.033235	0.649500
C	-0.883209	-2.807160	0.977234

H	-1.967520	-2.687471	1.093557
H	-0.595453	-3.821044	1.283068
H	-0.610297	-2.654785	-0.074429
C	-0.435508	-1.965752	3.766778
H	0.089159	-1.274481	4.440237
H	-0.135566	-2.991995	4.019526
H	-1.516995	-1.851375	3.912394
C	1.782365	-1.949562	1.881655
H	2.360079	-1.260230	2.510738
H	2.096353	-1.824818	0.837870
H	1.986496	-2.978120	2.209511
C	-0.420505	2.775109	0.689909
H	-0.252004	3.798812	1.048565
H	-1.457393	2.686729	0.339999
H	0.259561	2.555122	-0.141692
C	1.596619	1.777228	2.616537
H	1.763347	2.813703	2.938660
H	2.285993	1.532949	1.799361
H	1.794827	1.118251	3.472391
C	-1.166973	2.173593	3.454076
H	-0.904282	3.204840	3.728378
H	-1.016438	1.521117	4.324111
H	-2.224989	2.131311	3.164547

(H+)-1Ph Σ -BP86/TZVP

70

E(SCF) = -2111.668978

C	-0.000131	-0.000138	0.553178
P	1.591330	0.109052	-0.143475
P	-1.591416	-0.109139	-0.143905
C	2.035212	1.754287	-0.847638
C	2.754459	-0.214684	1.245597
C	1.949090	-1.107930	-1.484503
C	-2.035106	-1.754179	-0.848646
C	-2.754893	0.214193	1.244969
C	-1.948853	1.108226	-1.484673
H	-0.000269	-0.000272	1.641894
C	1.314133	2.879649	-0.424924
C	1.674607	4.151634	-0.876644
C	2.755849	4.304282	-1.749619
C	3.478348	3.183745	-2.173808
C	3.122226	1.909014	-1.726716
C	2.439712	-1.190318	2.208241
C	3.333625	-1.460259	3.247034
C	4.542603	-0.762840	3.332695
C	4.856612	0.208171	2.377997

C	3.967532	0.485335	1.336170
C	2.500629	-2.359181	-1.164568
C	2.723647	-3.302603	-2.170255
C	2.396043	-3.007299	-3.497219
C	1.850389	-1.761457	-3.820183
C	1.630157	-0.810361	-2.819908
C	-1.314066	-2.879640	-0.426131
C	-1.674419	-4.151506	-0.878283
C	-2.755506	-4.303937	-1.751488
C	-3.477983	-3.183303	-2.175459
C	-3.121978	-1.908689	-1.727939
C	-2.440393	1.189555	2.207969
C	-3.334568	1.459196	3.246614
C	-4.543563	0.761746	3.331772
C	-4.857329	-0.208993	2.376718
C	-3.967985	-0.485857	1.335036
C	-2.500537	2.359358	-1.164522
C	-2.723297	3.303076	-2.169988
C	-2.395285	3.008190	-3.496945
C	-1.849469	1.762475	-3.820124
C	-1.629496	0.811083	-2.820072
H	-2.775105	2.592599	-0.134855
H	-3.165182	4.267701	-1.916368
H	-2.575051	3.745317	-4.280724
H	-1.605395	1.524288	-4.856511
H	-1.228268	-0.168034	-3.084902
H	-1.496832	1.733752	2.150622
H	-3.083060	2.214315	3.992684
H	-5.239193	0.972594	4.145161
H	-5.795250	-0.761694	2.444502
H	-4.216285	-1.256259	0.604903
H	-0.469220	-2.748820	0.252252
H	-1.109713	-5.024707	-0.548860
H	-3.035707	-5.297436	-2.104558
H	-4.320488	-3.300735	-2.858488
H	-3.688077	-1.039688	-2.066927
H	4.216015	1.255949	0.606325
H	5.794520	0.760846	2.446173
H	5.238026	-0.973922	4.146200
H	3.081926	-2.215589	3.992826
H	1.496162	-1.734494	2.150500
H	1.109880	5.024760	-0.547056
H	0.469157	2.748659	0.253263
H	3.688323	1.040087	-2.065898
H	4.320974	3.301347	-2.856659
H	3.036142	5.297874	-2.102355

H	2.774892	-2.592742	-0.134892
H	1.229079	0.168866	-3.084562
H	1.606634	-1.522944	-4.856571
H	2.576014	-3.744193	-4.281170
H	3.165409	-4.267327	-1.916796

(H+)2-1H RI-BP86/TZVP

11			
E(SCF) =	-724.999415		
C	-0.119089	0.000021	1.091612
P	-0.868491	-1.622237	1.611365
P	-0.868597	1.622214	1.611413
H	-0.084530	0.000037	-0.012117
H	0.926958	0.000053	1.445465
H	-0.059405	-2.645407	1.049459
H	-2.194614	-1.759173	1.124389
H	-0.876265	-1.759654	3.023973
H	-0.059579	2.645441	1.049515
H	-0.876340	1.759602	3.024024
H	-2.194728	1.759103	1.124444

(H+)2-1Me RI-BP86/TZVP

29			
E(SCF) =	-961.145376		
C	-0.152492	0.004550	1.228843
P	-0.839949	-1.661024	1.714229
P	-0.911384	1.661479	1.630420
H	-0.047197	-0.015290	0.131154
H	0.873440	0.031338	1.632733
C	-2.592397	-1.833472	1.248148
H	-2.731991	-1.614283	0.181045
H	-3.231906	-1.181161	1.856794
H	-2.893652	-2.875391	1.431683
C	0.158324	-2.872225	0.789912
H	1.222358	-2.760711	1.039487
H	0.016290	-2.740081	-0.291331
H	-0.168998	-3.883591	1.071705
C	-0.629147	-1.940858	3.501358
H	0.428924	-1.839981	3.779040
H	-0.955221	-2.966128	3.729948
H	-1.237469	-1.243760	4.090941
C	-2.412923	1.932587	0.636335
H	-2.182274	1.836841	-0.433428
H	-2.771905	2.954571	0.827243
H	-3.208175	1.228539	0.910865
C	0.353250	2.886177	1.162787

H	1.254869	2.759461	1.777380
H	-0.055096	3.893184	1.331979
H	0.612237	2.781730	0.100300
C	-1.288344	1.822599	3.405224
H	-0.397114	1.608965	4.010396
H	-2.113962	1.161255	3.698106
H	-1.597673	2.860900	3.595826

(H+)2-1Ph Σ -BP86/TZVP

71

E(SCF) = -2111.982354

C	-0.000192	-0.000141	0.585987
P	1.700663	-0.049267	-0.199019
P	-1.700782	0.049192	-0.199587
C	2.022623	1.482264	-1.124648
C	2.800561	-0.120047	1.256619
C	1.969140	-1.512555	-1.249084
C	-2.022453	-1.482085	-1.125730
C	-2.801175	0.119600	1.255694
C	-1.968869	1.512767	-1.249352
H	-0.031695	-0.875305	1.252765
H	0.031079	0.874845	1.253008
C	1.662292	2.725743	-0.570305
C	2.003998	3.902332	-1.236674
C	2.705547	3.846024	-2.447291
C	3.069226	2.612000	-2.994041
C	2.734298	1.425202	-2.336188
C	2.589918	-1.082728	2.264294
C	3.457474	-1.140932	3.355094
C	4.532977	-0.249172	3.446043
C	4.745828	0.700666	2.443563
C	3.883594	0.771794	1.346231
C	2.985788	-2.422431	-0.904610
C	3.250972	-3.511204	-1.739407
C	2.517437	-3.691774	-2.914670
C	1.510765	-2.782717	-3.262481
C	1.232789	-1.694805	-2.435691
C	-1.662310	-2.725715	-0.571605
C	-2.003824	-3.902123	-1.238392
C	-2.704998	-3.845483	-2.449210
C	-3.068489	-2.611310	-2.995747
C	-2.733749	-1.424690	-2.337477
C	-2.590862	1.082008	2.263698
C	-3.458789	1.139931	3.354220
C	-4.534334	0.248160	3.444564
C	-4.746857	-0.701408	2.441758

C	-3.884250	-0.772253	1.344700
C	-2.985622	2.422569	-0.904991
C	-3.250488	3.511575	-1.739586
C	-2.516531	3.692452	-2.914538
C	-1.509754	2.783471	-3.262240
C	-1.232094	1.695327	-2.435649
H	-3.575792	2.279555	-0.000345
H	-4.040938	4.213369	-1.471853
H	-2.733249	4.539210	-3.566988
H	-0.943050	2.919695	-4.183754
H	-0.448988	0.995021	-2.726685
H	-1.771157	1.800667	2.202822
H	-3.297186	1.884927	4.133993
H	-5.209674	0.297517	4.299541
H	-5.587403	-1.392724	2.509875
H	-4.057632	-1.516132	0.567124
H	-1.133519	-2.789673	0.380830
H	-1.729519	-4.866001	-0.808504
H	-2.975533	-4.768720	-2.963216
H	-3.624116	-2.568219	-3.933135
H	-3.032407	-0.465880	-2.761856
H	4.057231	1.515885	0.568914
H	5.586343	1.391975	2.512151
H	5.208027	-0.298749	4.301236
H	3.295616	-1.886140	4.134613
H	1.770244	-1.801383	2.202947
H	1.729544	4.866092	-0.806616
H	1.133206	2.789445	0.381983
H	3.033102	0.466509	-2.760729
H	3.625142	2.569165	-3.931269
H	2.976227	4.769401	-2.960968
H	3.575636	-2.279652	0.000285
H	0.449777	-0.994432	-2.726818
H	0.944394	-2.918698	-4.184237
H	2.734402	-4.538351	-3.567273
H	4.041343	-4.213053	-1.471587

LS-Addukte/LS-CDP-R/RI-MP2-SVP

	BCI3-1H	RI-MP2/SVP	
13			
E(SCF) =	-2125.362844		
C	0.014041	0.151166	-0.009036
P	1.424435	0.210137	0.908286
P	-0.088999	0.034115	-1.685635
B	-1.393192	0.170110	0.802595
Cl	-1.099726	1.114163	2.389964

Cl	-2.652502	1.012010	-0.293482
Cl	-1.931167	-1.566003	1.177012
H	1.789364	1.411646	1.543789
H	2.579133	-0.087701	0.159607
H	1.487059	-0.699177	1.977451
H	-0.516590	1.146727	-2.434124
H	1.140897	-0.275093	-2.297258
H	-0.951743	-0.968840	-2.158249

	BCl3-1Me	RI-MP2/SVP	
31			
E(SCF) =	-2359.473584		
C	0.069085	0.264210	-0.051131
P	1.485500	0.238294	0.902605
P	-0.056475	0.076258	-1.743882
B	-1.345979	0.252743	0.773776
Cl	-1.224325	1.203835	2.391854
Cl	-2.739031	1.046487	-0.209567
Cl	-1.823792	-1.523008	1.159514
C	1.985161	1.844355	1.604302
H	2.864940	1.732040	2.255074
H	1.140531	2.252260	2.169952
H	2.221398	2.522239	0.771892
C	1.382785	-0.910930	2.305883
H	2.330858	-0.899515	2.862975
H	1.174145	-1.914698	1.914236
H	0.554348	-0.612867	2.957253
C	3.027802	-0.293805	0.084295
H	3.815958	-0.289327	0.850290
H	3.321827	0.396657	-0.714341
H	2.932066	-1.310025	-0.315766
C	-0.502363	1.583187	-2.666815
H	0.301109	2.320083	-2.526612
H	-1.432117	1.982666	-2.247585
H	-0.626274	1.365663	-3.738008
C	1.443924	-0.461690	-2.633213
H	2.246299	0.281239	-2.560877
H	1.168828	-0.568851	-3.691891
H	1.796578	-1.430995	-2.261693
C	-1.264604	-1.188047	-2.236230
H	-0.975428	-2.139725	-1.772393
H	-1.279470	-1.277618	-3.332171
H	-2.255070	-0.906380	-1.863330

	BCl3-1Ph	RI-MP2/SVP	
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E(SCF) =	-3500.927206		
C	-0.109136	0.899384	-0.470003
P	1.462245	0.201133	-0.415771
P	-1.467256	0.019581	0.111311
C	2.236008	0.178415	-2.060831
C	2.646155	0.906768	0.782054
C	1.477390	-1.547518	0.099316
C	-1.648481	-0.066652	1.920569
C	-3.076747	0.719705	-0.363994
C	-1.512475	-1.686662	-0.522752
B	-0.269539	2.455490	-0.925897
Cl	-0.871433	3.525850	0.508282
Cl	-1.465597	2.618355	-2.356167
Cl	1.374199	3.158437	-1.489298
C	1.390636	0.380825	-3.167897
C	1.919913	0.337380	-4.484078
C	3.308875	0.091826	-4.680525
C	4.158234	-0.098677	-3.551425
C	3.613701	-0.052797	-2.241521
C	2.383862	2.146339	1.395538
C	3.307747	2.686549	2.330635
C	4.496634	1.972742	2.651066
C	4.743751	0.707127	2.042333
C	3.811343	0.178200	1.114810
C	1.384756	-1.859623	1.472054
C	1.396427	-3.211745	1.899775
C	1.511495	-4.256370	0.937332
C	1.615853	-3.932715	-0.446342
C	1.596308	-2.573933	-0.857522
C	-0.679214	0.551368	2.727606
C	-0.825942	0.559616	4.142124
C	-1.961231	-0.059952	4.735576
C	-2.952662	-0.668039	3.906600
C	-2.793661	-0.659640	2.498411
C	-3.771117	0.279649	-1.507810
C	-5.010716	0.872734	-1.859287
C	-5.550131	1.920059	-1.058124
C	-4.845107	2.352394	0.100929
C	-3.610458	1.743893	0.444580
C	-1.341262	-1.832870	-1.916858
C	-1.438776	-3.112184	-2.519697
C	-1.694713	-4.256472	-1.708977
C	-1.839418	-4.103458	-0.300601
C	-1.748760	-2.812405	0.286417
H	-1.119013	-0.953040	-2.527016
H	-1.312497	-3.218235	-3.602400

H	-1.771767	-5.249230	-2.165306
H	-2.016556	-4.978072	0.333285
H	-1.840988	-2.703688	1.368552
H	-3.364673	-0.511616	-2.137114
H	-5.542028	0.532481	-2.753528
H	-6.498637	2.392594	-1.334659
H	-5.242075	3.161238	0.722396
H	-3.065576	2.087427	1.324826
H	0.162164	1.060770	2.251237
H	-0.076351	1.056759	4.766496
H	-2.085869	-0.052782	5.823805
H	-3.841344	-1.122704	4.356453
H	-3.574295	-1.080027	1.857459
H	3.984165	-0.811079	0.685068
H	5.646902	0.141591	2.293624
H	5.214247	2.389562	3.365991
H	3.098342	3.655819	2.794715
H	1.475869	2.702189	1.152226
H	1.261683	0.519594	-5.339671
H	0.339643	0.630469	-2.999513
H	4.276756	-0.169980	-1.383204
H	5.231029	-0.265001	-3.691445
H	3.726862	0.070684	-5.692642
H	1.329798	-1.059289	2.212304
H	1.681238	-2.321764	-1.917514
H	1.712984	-4.726958	-1.193172
H	1.529439	-5.303030	1.259867
H	1.328823	-3.447432	2.966919

	BH3-1Ph	RI-MP2/SVP	
73			
E(SCF) =	-2124.433804		
C	-0.160639	0.737768	-0.421096
P	1.405056	0.087696	-0.413735
P	-1.516189	-0.061632	0.203435
C	2.151425	0.234746	-2.067272
C	2.616132	0.828258	0.742569
C	1.519885	-1.676055	0.010996
C	-1.738508	-0.024400	2.015520
C	-3.004872	0.727175	-0.477508
C	-1.658833	-1.828896	-0.249924
B	-0.218243	2.394919	-0.692957
H	-0.586653	2.996114	0.325395
H	-0.977106	2.644208	-1.628396
H	0.918008	2.757504	-0.997925
C	1.343075	0.755803	-3.094087

C	1.866534	0.897670	-4.407601
C	3.207569	0.506420	-4.680296
C	4.018973	-0.019927	-3.631374
C	3.484163	-0.148727	-2.324368
C	2.365591	2.096191	1.304484
C	3.313869	2.683963	2.185175
C	4.516876	1.993415	2.502117
C	4.759158	0.707114	1.936815
C	3.804261	0.131776	1.061338
C	1.527524	-2.043968	1.373180
C	1.600984	-3.411538	1.741094
C	1.651820	-4.412839	0.727510
C	1.621091	-4.033591	-0.645577
C	1.553864	-2.658535	-0.996233
C	-0.820184	0.753695	2.742776
C	-0.930183	0.858437	4.156945
C	-1.974413	0.168625	4.834333
C	-2.905953	-0.616069	4.089509
C	-2.784072	-0.705270	2.680276
C	-3.005743	0.992140	-1.863118
C	-4.134471	1.590976	-2.476617
C	-5.267343	1.940765	-1.685755
C	-5.247289	1.697761	-0.283518
C	-4.109288	1.092717	0.314369
C	-1.792521	-2.129529	-1.623113
C	-1.930273	-3.472108	-2.057007
C	-1.920594	-4.528630	-1.100010
C	-1.756689	-4.222390	0.279705
C	-1.622979	-2.870406	0.695734
H	-1.788046	-1.325184	-2.360885
H	-2.044021	-3.693124	-3.123226
H	-2.031533	-5.568595	-1.425052
H	-1.727661	-5.024954	1.023250
H	-1.476297	-2.647201	1.753013
H	-2.107057	0.792552	-2.448362
H	-4.121025	1.808745	-3.549200
H	-6.138060	2.415481	-2.150253
H	-6.098254	1.990301	0.339381
H	-4.087720	0.947688	1.395159
H	-0.040306	1.292435	2.196045
H	-0.217837	1.473462	4.716274
H	-2.068088	0.244206	5.923000
H	-3.715198	-1.143166	4.605437
H	-3.501616	-1.301330	2.109881
H	3.982674	-0.866470	0.656203
H	5.677663	0.162960	2.179335

H	5.251651	2.445927	3.176710
H	3.112936	3.672755	2.609972
H	1.452849	2.636693	1.040108
H	1.239998	1.318952	-5.200061
H	0.325322	1.076462	-2.850679
H	4.113661	-0.539322	-1.522726
H	5.053864	-0.314640	-3.832087
H	3.619455	0.618715	-5.688887
H	1.491640	-1.269306	2.145230
H	1.534756	-2.357295	-2.047600
H	1.650048	-4.797187	-1.429208
H	1.712719	-5.471183	1.002728
H	1.618853	-3.694890	2.798499

CO2-1H RI-MP2/SVP

12			
E(SCF) =	-909.937970		
C	0.180686	-0.030809	1.239060
P	-1.509834	0.036542	1.647842
P	1.646430	0.110168	2.057510
C	-0.061118	-0.271210	-0.205262
O	0.732318	-0.421253	-1.112776
O	-1.392936	-0.278160	-0.237305
H	-2.329230	1.145775	1.382007
H	-1.445397	0.274577	3.072839
H	-2.327791	-1.099916	1.756967
H	1.442620	0.327836	3.427069
H	2.535519	-0.984025	2.030031
H	2.524503	1.151475	1.691408

CO2-1Me RI-MP2/SVP

30			
E(SCF) =	-1144.059764		
C	0.066848	0.028584	1.437901
P	-1.540583	0.105062	2.013775
P	1.628334	0.129302	2.125603
C	0.122082	-0.196861	-0.080731
O	1.279962	-0.265778	-0.561659
O	-0.997935	-0.283146	-0.641856
C	2.619819	1.500135	1.472235
H	3.639248	1.481244	1.884066
H	2.126041	2.446067	1.733898
H	2.632326	1.375677	0.382419
C	1.638766	0.395387	3.928362
H	2.683419	0.446628	4.266740
H	1.142461	-0.434341	4.447238

H	1.140250	1.338539	4.185203
C	2.620717	-1.371330	1.895840
H	3.640087	-1.233982	2.284704
H	2.633443	-1.566736	0.816469
H	2.127424	-2.201840	2.419304
C	-1.682030	0.369198	3.811309
H	-1.217264	1.319540	4.102624
H	-1.210926	-0.453443	4.363875
H	-2.748577	0.404198	4.075260
C	-2.504259	1.461343	1.292001
H	-2.044528	2.414384	1.587682
H	-3.549771	1.426671	1.630964
H	-2.438054	1.337733	0.204026
C	-2.491415	-1.410250	1.714998
H	-2.023711	-2.233573	2.272210
H	-2.425065	-1.605081	0.637489
H	-3.537620	-1.288614	2.030989

	CO2-1Ph	RI-MP2/SVP	
72			
E(SCF) =	-2285.511366		
C	0.099142	0.667512	0.456676
P	1.523861	0.012384	-0.240998
P	-1.499839	0.059584	0.547861
C	1.728574	0.273394	-2.021649
C	3.034499	0.558622	0.596022
C	1.667289	-1.783946	0.053537
C	-2.256762	0.189100	2.189830
C	-2.596176	0.883201	-0.639282
C	-1.634284	-1.703892	0.138382
C	0.150777	2.192764	0.294917
O	1.178216	2.573442	-0.332103
O	-0.805514	2.840354	0.764437
C	0.789655	-0.319646	-2.890331
C	0.855235	-0.074382	-4.286037
C	1.868058	0.784229	-4.803545
C	2.796232	1.399532	-3.914112
C	2.715595	1.143630	-2.519656
C	2.971449	1.440697	1.687649
C	4.163528	1.798504	2.373360
C	5.413868	1.263516	1.949660
C	5.461914	0.361948	0.845917
C	4.262320	0.007691	0.177112
C	1.798056	-2.154433	1.411453
C	2.017745	-3.506926	1.769740
C	2.095560	-4.502605	0.750828

C	1.960246	-4.124278	-0.613703
C	1.754468	-2.758449	-0.955672
C	-1.746217	1.144767	3.088974
C	-2.326654	1.279616	4.379539
C	-3.419073	0.447379	4.757603
C	-3.924737	-0.519013	3.839150
C	-3.337641	-0.643364	2.554277
C	-2.012271	1.533619	-1.742971
C	-2.839311	2.161394	-2.711330
C	-4.255326	2.132406	-2.560549
C	-4.833672	1.477638	-1.433780
C	-3.994578	0.854907	-0.473488
C	-2.033931	-2.104709	-1.151756
C	-2.096384	-3.484820	-1.481612
C	-1.755655	-4.461166	-0.502485
C	-1.359769	-4.046596	0.803172
C	-1.299366	-2.664391	1.115077
H	-2.324165	-1.350620	-1.889001
H	-2.416146	-3.794532	-2.481894
H	-1.805835	-5.527330	-0.748261
H	-1.103689	-4.790917	1.563403
H	-1.005480	-2.339591	2.116375
H	-0.923646	1.593318	-1.831307
H	-2.380946	2.686171	-3.555634
H	-4.896964	2.628332	-3.296554
H	-5.919877	1.468868	-1.299357
H	-4.437791	0.381207	0.405437
H	-0.930805	1.796883	2.762456
H	-1.934985	2.028747	5.074766
H	-3.870361	0.549842	5.750257
H	-4.762302	-1.163805	4.123986
H	-3.712990	-1.396857	1.856786
H	4.289077	-0.699815	-0.657450
H	6.418111	-0.057795	0.518020
H	6.335609	1.543302	2.470448
H	4.116535	2.492658	3.218091
H	2.007271	1.856999	1.989940
H	0.123553	-0.532063	-4.959551
H	-0.005405	-0.951694	-2.486170
H	3.379839	1.660599	-1.823111
H	3.555445	2.087915	-4.298211
H	1.920736	0.986616	-5.878555
H	1.747384	-1.381493	2.185851
H	1.689587	-2.473561	-2.007294
H	2.028631	-4.877998	-1.404497
H	2.269697	-5.550745	1.016643

H	2.132624	-3.783888	2.822857
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CS2-1H	RI-MP2/SVP
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12

E(SCF) =	-1555.127145		
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C	-0.000189	-0.029227	1.234429
P	-1.588545	0.077781	1.904831
P	1.588603	0.078915	1.903616
C	-0.001184	-0.258127	-0.192294
S	1.555657	-0.362666	-0.846233
S	-1.559676	-0.363048	-0.842591
H	-2.423382	1.152648	1.575685
H	-1.388281	0.300598	3.292387
H	-2.422746	-1.046585	1.928694
H	1.389586	0.301885	3.291249
H	2.423255	-1.045117	1.926587
H	2.422681	1.153944	1.573033

CS2-1Me	RI-MP2/SVP
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30

E(SCF) =	-1789.219950		
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C	0.047109	-0.045926	1.277949
P	-1.614429	0.069520	1.852911
P	1.607478	0.096011	2.041591
C	0.030854	-0.321099	-0.156793
S	1.414075	-0.503482	-1.095424
S	-1.581280	-0.429806	-0.738532
C	-2.605918	-1.468983	1.935415
H	-2.031737	-2.263410	1.444261
H	-3.535789	-1.331636	1.369773
H	-2.831860	-1.744300	2.976925
C	-1.544605	0.420500	3.674321
H	-1.049638	1.375177	3.890461
H	-1.055158	-0.388205	4.230656
H	-2.584109	0.491796	4.027124
C	-2.596873	1.534217	1.356638
H	-2.819514	2.178433	2.220936
H	-3.528466	1.201887	0.882119
H	-2.018981	2.085591	0.605607
C	2.601673	-1.420555	1.953153
H	3.598366	-1.245083	2.383784
H	2.679655	-1.710027	0.898770
H	2.079874	-2.203195	2.521445
C	2.609459	1.467997	1.401366
H	3.605681	1.458573	1.867286
H	2.092256	2.407734	1.640432

H	2.687829	1.347787	0.314611
C	1.584507	0.437379	3.829943
H	2.635269	0.495124	4.148242
H	1.093770	-0.367300	4.388466
H	1.098702	1.393753	4.052623

	CS2-1Ph	RI-MP2/SVP	
72			
E(SCF) =	-2930.675655		
C	-0.000048	-0.000835	-0.897308
P	1.604741	0.041806	-0.213704
P	-1.604893	-0.041949	-0.213723
C	2.595967	-1.446977	-0.527328
C	2.498998	1.571333	-0.575200
C	1.608513	-0.015468	1.613979
C	-2.592748	1.450238	-0.521834
C	-2.502065	-1.568218	-0.581620
C	-1.608945	0.007482	1.614206
C	-0.000137	0.002852	-2.368609
S	1.501556	0.186462	-3.129667
S	-1.501733	-0.176915	-3.130764
C	-2.104835	2.462919	-1.369314
C	-2.848211	3.660610	-1.537158
C	-4.088100	3.829964	-0.854216
C	-4.564926	2.803089	0.010722
C	-3.802613	1.617782	0.182581
C	-1.759261	-2.761497	-0.505594
C	-2.388445	-4.007008	-0.766191
C	-3.773947	-4.041814	-1.096019
C	-4.514002	-2.825032	-1.169106
C	-3.869476	-1.587778	-0.910109
C	-2.122697	-1.050296	2.387039
C	-2.220987	-0.923964	3.799675
C	-1.793793	0.275142	4.433988
C	-1.275293	1.345199	3.644580
C	-1.193245	1.204242	2.237469
C	2.109781	-2.458118	-1.377600
C	2.855725	-3.653616	-1.549605
C	4.096428	-3.822267	-0.867956
C	4.571533	-2.796958	-0.000222
C	3.806646	-1.613915	0.175786
C	1.754674	2.763122	-0.491128
C	2.381378	4.010913	-0.746836
C	3.765994	4.049458	-1.079889
C	4.507640	2.834147	-1.161152
C	3.865537	1.594629	-0.907096

C	2.122816	1.038437	2.391690
C	2.221345	0.905349	3.803698
C	1.793918	-0.296634	4.432375
C	1.274931	-1.362778	3.637993
C	1.192607	-1.215090	2.231590
H	2.461304	1.959612	1.912062
H	2.631095	1.726187	4.400928
H	1.869369	-0.408013	5.519344
H	0.950290	-2.294919	4.111255
H	0.824211	-2.042242	1.618099
H	0.683442	2.716842	-0.273155
H	1.798027	4.936186	-0.703627
H	4.254715	5.006244	-1.291377
H	5.565360	2.852530	-1.441898
H	4.416166	0.659038	-1.029555
H	1.175805	-2.301595	-1.924588
H	2.481371	-4.434693	-2.218983
H	4.680694	-4.737788	-1.008862
H	5.517530	-2.922402	0.536199
H	4.147307	-0.845896	0.876090
H	-4.419154	-0.650824	-1.026183
H	-5.572450	-2.840421	-1.447275
H	-4.264583	-4.996774	-1.311286
H	-1.806338	-4.933335	-0.729294
H	-0.687360	-2.717691	-0.290323
H	-2.472529	4.442855	-2.204432
H	-1.171521	2.306127	-1.917342
H	-4.144534	0.848444	0.880812
H	-5.510310	2.928999	0.548118
H	-4.670385	4.747234	-0.991924
H	-2.460954	-1.969302	1.903107
H	-0.825258	2.034460	1.627920
H	-0.950781	2.275161	4.122199
H	-1.869024	0.381313	5.521494
H	-2.630328	-1.747785	4.393066

	(H+)-1H	RI-MP2/SVP	
10			
E(SCF) =	-722.879559		
C	-0.000040	0.004023	1.190178
P	-1.520245	-0.005841	1.966349
P	1.520228	-0.005566	1.966228
H	-0.000030	-0.159348	0.109640
H	-2.480385	0.722290	1.252843
H	-1.449065	0.583307	3.236121
H	-2.181541	-1.222807	2.224358

H	1.449305	0.584247	3.235705
H	2.181490	-1.222427	2.224820
H	2.480272	0.722122	1.252141

	(H+)-1Me	RI-MP2/SVP	
28			
E(SCF) =	-957.024143		
C	-0.520244	-0.010253	1.424660
P	-0.007425	-1.545337	1.993752
P	-0.164871	1.549081	2.041655
H	-1.304538	-0.040662	0.663260
C	-0.901444	-2.801558	1.055392
H	-1.980153	-2.684848	1.224320
H	-0.586508	-3.803724	1.376033
H	-0.685207	-2.675173	-0.013900
C	-0.321950	-1.872457	3.753593
H	0.221877	-1.144090	4.372400
H	0.013338	-2.882768	4.028847
H	-1.397875	-1.773302	3.951901
C	1.761009	-1.891097	1.772716
H	2.361844	-1.181208	2.356705
H	2.014424	-1.779898	0.709805
H	1.997402	-2.911706	2.106335
C	-0.320808	2.766031	0.716064
H	-0.127871	3.777353	1.099726
H	-1.341596	2.725535	0.310600
H	0.390950	2.524213	-0.083810
C	1.517783	1.661409	2.703789
H	1.704300	2.682569	3.064605
H	2.242972	1.414048	1.917469
H	1.642733	0.971617	3.550335
C	-1.240295	2.142741	3.381886
H	-0.963449	3.160150	3.694230
H	-1.161294	1.463740	4.242382
H	-2.281595	2.139732	3.030365

	(H+)-1Ph	RI-MP2/SVP	
70			
E(SCF) =	-2098.514520		
C	-0.000142	-0.000172	0.670328
P	1.535726	0.143102	-0.083887
P	-1.535823	-0.143222	-0.084310
C	1.910689	1.780370	-0.752290
C	2.755697	-0.222186	1.197806
C	1.782192	-1.013217	-1.455904
C	-1.910638	-1.780299	-0.753267

C	-2.756109	0.221705	1.197186
C	-1.781936	1.013503	-1.456050
H	-0.000280	-0.000314	1.759822
C	1.144324	2.869206	-0.293698
C	1.435881	4.183819	-0.746919
C	2.507453	4.391577	-1.662992
C	3.282399	3.281555	-2.117052
C	2.980034	1.974736	-1.656402
C	2.441882	-1.191039	2.177655
C	3.389681	-1.514390	3.183118
C	4.657854	-0.862276	3.197490
C	4.963289	0.114685	2.205158
C	4.005118	0.431738	1.205774
C	2.160766	-2.339926	-1.156752
C	2.288531	-3.293657	-2.199269
C	2.026083	-2.907585	-3.547779
C	1.643709	-1.566140	-3.838881
C	1.522060	-0.621145	-2.785436
C	-1.144407	-2.869271	-0.294771
C	-1.435881	-4.183761	-0.748402
C	-2.507229	-4.391259	-1.664796
C	-3.282064	-3.281108	-2.118729
C	-2.979788	-1.974415	-1.657664
C	-2.442535	1.190280	2.177388
C	-3.390580	1.513342	3.182711
C	-4.658756	0.861224	3.196586
C	-4.963946	-0.115456	2.203902
C	-4.005531	-0.432222	1.204661
C	-2.160578	2.340124	-1.156596
C	-2.288056	3.294176	-2.198856
C	-2.025256	2.908512	-3.547414
C	-1.642784	1.567161	-3.838819
C	-1.521423	0.621843	-2.785629
H	-2.381144	2.630504	-0.125361
H	-2.597258	4.319755	-1.970019
H	-2.127772	3.639615	-4.357534
H	-1.453130	1.262364	-4.873807
H	-1.243363	-0.409932	-3.010847
H	-1.466377	1.682633	2.170369
H	-3.146813	2.259708	3.946552
H	-5.394160	1.105116	3.971778
H	-5.931712	-0.628234	2.214592
H	-4.236758	-1.197933	0.460367
H	-0.331419	-2.687110	0.413312
H	-0.843264	-5.033318	-0.393035
H	-2.738869	-5.402107	-2.019396

H	-4.108486	-3.438583	-2.820406
H	-3.571854	-1.123672	-2.007634
H	4.236530	1.197659	0.461753
H	5.931051	0.627460	2.216232
H	5.393069	-1.106393	3.972790
H	3.145725	-2.260971	3.946688
H	1.465726	-1.683389	2.170257
H	0.843177	5.033276	-0.391456
H	0.331143	2.686840	0.414111
H	3.572158	1.124085	-2.006501
H	4.108993	3.439230	-2.818480
H	2.739150	5.402520	-2.017284
H	2.381080	-2.630612	-0.125549
H	1.244118	0.410714	-3.010418
H	1.454328	-1.261030	-4.873827
H	2.128834	-3.638437	-4.358097
H	2.597663	-4.319309	-1.970662

	(H+)2-1Ph	RI-MP2/SVP	
71			
E(SCF) =	-2098.826485		
C	-0.001017	-0.005768	0.671452
P	1.629043	-0.039180	-0.169959
P	-1.629500	0.034616	-0.172503
C	1.811983	1.440577	-1.148735
C	2.797977	-0.011929	1.183772
C	1.814283	-1.524940	-1.145517
C	-1.818070	-1.443165	-1.153154
C	-2.800737	0.012105	1.179437
C	-1.805636	1.521628	-1.147938
H	-0.026576	-0.887626	1.328846
H	0.023318	0.873084	1.332909
C	1.371448	2.664430	-0.588717
C	1.581216	3.873309	-1.298230
C	2.241905	3.845664	-2.566040
C	2.698590	2.607045	-3.107788
C	2.486597	1.398775	-2.389590
C	2.565156	-0.768776	2.358450
C	3.527155	-0.754930	3.400749
C	4.722913	0.014023	3.254827
C	4.946972	0.767269	2.063359
C	3.977411	0.752349	1.024854
C	2.564019	-2.598527	-0.611722
C	2.696311	-3.801329	-1.357777
C	2.078097	-3.914396	-2.638321
C	1.329480	-2.818403	-3.168822

C	1.196847	-1.625527	-2.416295
C	-1.374584	-2.668824	-0.599653
C	-1.591240	-3.875821	-1.310443
C	-2.261599	-3.844454	-2.572994
C	-2.721170	-2.603975	-3.108192
C	-2.502480	-1.397742	-2.388684
C	-2.567232	0.768012	2.354604
C	-3.531121	0.757802	3.395181
C	-4.729518	-0.006614	3.247164
C	-4.954236	-0.759025	2.055312
C	-3.982765	-0.747758	1.018552
C	-2.540145	2.603484	-0.609823
C	-2.663094	3.807811	-1.354998
C	-2.050829	3.914091	-2.638973
C	-1.317733	2.809758	-3.173840
C	-1.194263	1.615358	-2.422155
H	-3.040859	2.515264	0.358827
H	-3.243401	4.644898	-0.948991
H	-2.158053	4.836977	-3.222897
H	-0.864289	2.882236	-4.169143
H	-0.643334	0.774355	-2.843483
H	-1.659996	1.367162	2.481486
H	-3.357976	1.336346	4.310194
H	-5.476021	-0.016328	4.051369
H	-5.871881	-1.347749	1.939509
H	-4.153048	-1.332494	0.109204
H	-0.880509	-2.705512	0.376486
H	-1.258288	-4.830832	-0.887511
H	-2.438824	-4.777671	-3.122500
H	-3.256839	-2.581227	-4.064794
H	-2.882663	-0.452262	-2.786759
H	4.147088	1.337503	0.115640
H	5.862683	1.359310	1.949167
H	5.467931	0.026571	4.060367
H	3.354666	-1.334241	4.315402
H	1.660020	-1.371502	2.483381
H	1.250999	4.827022	-0.870258
H	0.885707	2.698061	0.391752
H	2.864648	0.454641	-2.792827
H	3.227097	2.587207	-4.068424
H	2.414004	4.780411	-3.114564
H	3.068602	-2.504937	0.354410
H	0.633254	-0.791132	-2.833962
H	0.870916	-2.896068	-4.161388
H	2.192123	-4.836114	-3.222808
H	3.287990	-4.631981	-0.954988

LS-Addukte/LS-CDP-R/RI-MP2-TZVP

	BCI3-1H	RI-MP2/TZVP	
13			
E(SCF) =	-2126.097559		
C	0.017473	0.441084	-0.032070
P	1.416435	0.179989	0.894742
P	-0.080849	0.023295	-1.675189
B	-1.369423	0.313866	0.783855
Cl	-1.173884	1.202332	2.409145
Cl	-2.729474	1.041297	-0.260049
Cl	-1.729997	-1.503580	1.103537
H	1.795484	1.247027	1.717641
H	2.560778	-0.054218	0.116002
H	1.401330	-0.898132	1.799011
H	-0.664903	0.989337	-2.502845
H	1.173087	-0.198419	-2.266162
H	-0.815048	-1.130616	-2.006698

BCI3-1Me **RI-MP2/TZVP**

31			
E(SCF) =	-2360.453072		
C	0.056271	0.301431	-0.045941
P	1.482166	0.248403	0.907173
P	-0.062847	0.086092	-1.744146
B	-1.345030	0.271365	0.772385
Cl	-1.233425	1.212874	2.397213
Cl	-2.749068	1.054703	-0.204378
Cl	-1.818891	-1.514524	1.157109
C	2.000219	1.843640	1.633803
H	2.838592	1.693257	2.316313
H	1.160274	2.283931	2.162072
H	2.302545	2.504963	0.821268
C	1.378912	-0.924077	2.298841
H	2.329786	-0.927722	2.834116
H	1.165290	-1.912097	1.894349
H	0.571508	-0.642581	2.967652
C	3.023335	-0.283429	0.078844
H	3.805480	-0.282438	0.838657
H	3.313535	0.405957	-0.709491
H	2.926193	-1.289160	-0.321895
C	-0.520733	1.579001	-2.694271
H	0.299151	2.293986	-2.619721
H	-1.417394	2.013986	-2.263905
H	-0.690522	1.322876	-3.741598
C	1.445636	-0.450517	-2.627736

H	2.237095	0.290798	-2.557255
H	1.172971	-0.560510	-3.677793
H	1.797886	-1.409127	-2.255540
C	-1.259909	-1.200367	-2.228048
H	-0.962530	-2.135003	-1.755342
H	-1.254161	-1.302885	-3.314398
H	-2.254123	-0.938084	-1.879941

	BCl3-1Ph	RI-MP2/TZVP	
73			
E(SCF) =	-3503.738706		
C	0.056714	-0.852835	-0.210914
P	-1.507541	-0.168455	-0.000882
P	1.419951	0.181336	-0.027089
C	-2.583998	-0.423628	-1.442853
C	-2.413893	-0.662761	1.505026
C	-1.467461	1.645610	0.193870
C	1.844676	0.648148	1.682299
C	2.992753	-0.538789	-0.589224
C	1.241726	1.710381	-1.000930
B	0.233568	-2.434986	-0.460747
Cl	1.126879	-3.259294	0.988613
Cl	1.196103	-2.746434	-2.039937
Cl	-1.453032	-3.246741	-0.621835
C	-1.966439	-0.731679	-2.658375
C	-2.734989	-0.834825	-3.814614
C	-4.100997	-0.556770	-3.775726
C	-4.718119	-0.278985	-2.556434
C	-3.957261	-0.172075	-1.394248
C	-1.979496	-1.768487	2.242575
C	-2.626867	-2.102831	3.429973
C	-3.744179	-1.383005	3.851699
C	-4.152714	-0.256926	3.137944
C	-3.511525	0.086566	1.949637
C	-1.152370	2.197416	1.442090
C	-1.148356	3.580252	1.609429
C	-1.436971	4.416475	0.531553
C	-1.787614	3.865499	-0.701654
C	-1.773597	2.484685	-0.883494
C	1.073406	0.128582	2.722812
C	1.413472	0.410132	4.044902
C	2.475292	1.269479	4.323547
C	3.273018	1.752780	3.283840
C	2.946827	1.466157	1.960719
C	3.509167	-0.271923	-1.860041
C	4.735950	-0.811872	-2.233265

C	5.412750	-1.676917	-1.375961
C	4.916197	-1.909049	-0.094712
C	3.693076	-1.370432	0.291086
C	0.855768	1.532525	-2.337829
C	0.771697	2.630748	-3.188413
C	1.004622	3.914736	-2.694418
C	1.386449	4.089299	-1.364619
C	1.486773	2.993531	-0.508329
H	0.649940	0.532579	-2.702614
H	0.478434	2.488407	-4.222132
H	0.940865	4.770518	-3.356120
H	1.561544	5.086921	-0.978436
H	1.751535	3.142090	0.530534
H	2.991556	0.389431	-2.540415
H	5.129809	-0.609051	-3.221760
H	6.360999	-2.106096	-1.675960
H	5.444855	-2.568363	0.582704
H	3.304816	-1.563431	1.281221
H	0.266633	-0.555063	2.486788
H	0.820476	-0.003663	4.851985
H	2.737499	1.490748	5.351139
H	4.121731	2.389303	3.503938
H	3.588308	1.808498	1.155801
H	-3.815640	0.981301	1.418786
H	-5.003847	0.322433	3.475518
H	-4.245076	-1.649073	4.774638
H	-2.289042	-2.964401	3.993326
H	-1.119069	-2.334522	1.912731
H	-2.258998	-1.095531	-4.752285
H	-0.915183	-0.993204	-2.665698
H	-4.446797	0.038297	-0.452594
H	-5.784775	-0.092786	-2.518578
H	-4.696339	-0.636504	-4.677257
H	-0.965890	1.553861	2.291734
H	-2.047548	2.060013	-1.841695
H	-2.031562	4.512791	-1.535878
H	-1.450543	5.491414	0.668828
H	-0.906525	4.001931	2.578387

BH3-1Ph

RI-MP2/TZVP

73

E(SCF) = -2126.796296

C	-0.055224	-0.369574	-1.234769
P	1.449271	-0.133775	-0.479563
P	-1.478660	-0.049454	-0.365870
C	2.528556	-1.582965	-0.700913

C	2.425841	1.312601	-1.036047
C	1.366656	0.141416	1.319940
C	-1.926516	1.703229	-0.069396
C	-2.879808	-0.744294	-1.294285
C	-1.541163	-0.849716	1.285327
B	0.014585	-0.566773	-2.903559
H	-0.521552	0.378162	-3.466631
H	-0.504784	-1.622303	-3.221281
H	1.205142	-0.604269	-3.187102
C	1.926761	-2.769724	-1.128266
C	2.696098	-3.923183	-1.265750
C	4.040684	-3.915755	-0.896849
C	4.645251	-2.724105	-0.495969
C	3.885158	-1.564666	-0.363225
C	2.107274	1.933663	-2.250107
C	2.810395	3.068699	-2.650647
C	3.872366	3.549530	-1.885282
C	4.169751	2.951271	-0.661549
C	3.475471	1.813902	-0.254063
C	1.067887	1.423206	1.800667
C	0.993800	1.649939	3.172903
C	1.161899	0.591408	4.065472
C	1.465190	-0.683796	3.587011
C	1.539637	-0.918562	2.215592
C	-1.092076	2.665004	-0.645139
C	-1.371980	4.020679	-0.483196
C	-2.449215	4.421309	0.306119
C	-3.306730	3.464053	0.851150
C	-3.033140	2.107044	0.690657
C	-2.766869	-2.064182	-1.747379
C	-3.800270	-2.637636	-2.480374
C	-4.976276	-1.925328	-2.712184
C	-5.069128	-0.596562	-2.305632
C	-4.041922	-0.015276	-1.564235
C	-1.322801	-2.234746	1.316425
C	-1.404712	-2.932752	2.516866
C	-1.620966	-2.246469	3.712130
C	-1.823703	-0.868640	3.687296
C	-1.746710	-0.164499	2.485787
H	-1.118386	-2.767716	0.396696
H	-1.240849	-4.004042	2.526252
H	-1.687688	-2.789734	4.647327
H	-1.977701	-0.326594	4.613331
H	-1.872486	0.909536	2.489778
H	-1.836352	-2.597717	-1.613791
H	-3.704392	-3.657149	-2.833461

H	-5.777837	-2.374115	-3.286156
H	-5.966496	-0.026360	-2.513692
H	-4.120561	1.021034	-1.265292
H	-0.254200	2.335367	-1.249014
H	-0.719179	4.761153	-0.930392
H	-2.665688	5.475151	0.434046
H	-4.156214	3.774481	1.448105
H	-3.703149	1.367917	1.115759
H	3.700331	1.369045	0.708606
H	4.980539	3.332833	-0.052181
H	4.415155	4.431870	-2.202339
H	2.565839	3.539610	-3.595401
H	1.301708	1.537904	-2.856595
H	2.234342	-4.839483	-1.613691
H	0.886200	-2.742742	-1.432158
H	4.361998	-0.643015	-0.054534
H	5.696061	-2.711505	-0.232215
H	4.635847	-4.815171	-0.999752
H	0.950260	2.249441	1.109249
H	1.780985	-1.907649	1.842852
H	1.604313	-1.504654	4.280791
H	1.114569	0.771533	5.133138
H	0.775923	2.645594	3.542533

	CO2-1H	RI-MP2/TZVP	
12			
E(SCF) =	-910.409794		
C	0.178411	-0.035091	1.236697
P	-1.514096	0.037127	1.658542
P	1.651245	0.109712	2.059192
C	-0.060898	-0.268843	-0.197688
O	0.738743	-0.416157	-1.104834
O	-1.396050	-0.277716	-0.242180
H	-2.318757	1.147396	1.376710
H	-1.443215	0.273463	3.080258
H	-2.320782	-1.103179	1.750759
H	1.435611	0.331919	3.423628
H	2.528741	-0.989409	2.029093
H	2.516818	1.151778	1.679213

	CO2-1Me	RI-MP2/TZVP	
30			
E(SCF) =	-1144.777103		
C	0.067750	0.023209	1.414065
P	-1.541927	0.103536	2.005431
P	1.630244	0.127773	2.117472

C	0.122917	-0.200729	-0.097353
O	1.282116	-0.269826	-0.580743
O	-0.998050	-0.287028	-0.661442
C	2.635849	1.502648	1.475520
H	3.633575	1.479646	1.916637
H	2.141038	2.440857	1.725500
H	2.687391	1.388566	0.395247
C	1.626775	0.394269	3.925223
H	2.662163	0.446204	4.263134
H	1.134744	-0.430561	4.436295
H	1.131138	1.329568	4.176620
C	2.638964	-1.371769	1.899099
H	3.636286	-1.220784	2.315177
H	2.691224	-1.573575	0.831752
H	2.145679	-2.199281	2.408479
C	-1.669835	0.368859	3.808829
H	-1.207268	1.311332	4.094166
H	-1.202662	-0.448831	4.353596
H	-2.727113	0.404982	4.072961
C	-2.520663	1.463411	1.293771
H	-2.059096	2.408879	1.577707
H	-3.546515	1.424875	1.663526
H	-2.494218	1.349366	0.212597
C	-2.509868	-1.411061	1.717424
H	-2.040939	-2.231298	2.260471
H	-2.484162	-1.612945	0.649135
H	-3.536047	-1.275572	2.062646

CO2-1Ph

RI-MP2/TZVP

72

E(SCF) =

-2288.063164

C	0.110032	0.744672	0.534755
P	1.514968	0.069268	-0.197656
P	-1.485122	0.107415	0.591670
C	1.693899	0.307777	-1.988165
C	3.060878	0.579155	0.603882
C	1.621999	-1.735389	0.086327
C	-2.308958	0.214406	2.206961
C	-2.577050	0.932757	-0.600298
C	-1.560361	-1.653353	0.151027
C	0.177455	2.255587	0.341131
O	1.209162	2.604476	-0.311036
O	-0.760233	2.935885	0.809095
C	0.690994	-0.205141	-2.817516
C	0.774694	-0.039151	-4.198351
C	1.811388	0.716088	-4.744002

C	2.805620	1.235538	-3.913522
C	2.731854	1.066124	-2.533641
C	3.054317	1.445443	1.697482
C	4.256513	1.754630	2.328832
C	5.445350	1.149080	1.921869
C	5.448037	0.289722	0.823908
C	4.248484	-0.036842	0.196213
C	1.859916	-2.137557	1.410169
C	2.102721	-3.474604	1.704378
C	2.032008	-4.435416	0.694224
C	1.798857	-4.039652	-0.620786
C	1.566876	-2.697392	-0.924901
C	-1.891476	1.196698	3.111313
C	-2.532227	1.303899	4.342924
C	-3.524812	0.393324	4.705871
C	-3.948523	-0.573649	3.795602
C	-3.313882	-0.694701	2.560770
C	-2.007315	1.532115	-1.727802
C	-2.835479	2.087002	-2.700373
C	-4.221318	1.978213	-2.588528
C	-4.784711	1.405393	-1.448493
C	-3.966000	0.845923	-0.470425
C	-1.959908	-2.042379	-1.131926
C	-1.997783	-3.396187	-1.464428
C	-1.609129	-4.356465	-0.532847
C	-1.238573	-3.968503	0.755791
C	-1.189028	-2.619727	1.093796
H	-2.282432	-1.296275	-1.849689
H	-2.310787	-3.696588	-2.457502
H	-1.652737	-5.408339	-0.789535
H	-0.953752	-4.715423	1.486793
H	-0.907718	-2.317690	2.095832
H	-0.931512	1.628996	-1.806206
H	-2.393835	2.565958	-3.565973
H	-4.861080	2.414049	-3.346412
H	-5.861697	1.345631	-1.346951
H	-4.407015	0.405285	0.415615
H	-1.137342	1.909693	2.799886
H	-2.215350	2.066830	5.043590
H	-4.014373	0.480475	5.668339
H	-4.722630	-1.279043	4.073152
H	-3.624887	-1.467229	1.866615
H	4.244164	-0.734821	-0.634817
H	6.369567	-0.181394	0.503641
H	6.376043	1.396667	2.417790
H	4.256309	2.430196	3.175532

H	2.129988	1.914114	2.008164
H	-0.007830	-0.433063	-4.836300
H	-0.134536	-0.755771	-2.382747
H	3.464388	1.524753	-1.882003
H	3.599996	1.839019	-4.335669
H	1.874837	0.855983	-5.816389
H	1.926390	-1.388451	2.192595
H	1.430456	-2.401382	-1.956634
H	1.767626	-4.779849	-1.411974
H	2.231518	-5.476452	0.920003
H	2.305938	-3.772403	2.726538

CS2-1H RI-MP2/TZVP

12

E(SCF) =	-1555.684860		
C	-0.000267	-0.029346	1.228916
P	-1.589863	0.079058	1.911551
P	1.589727	0.080207	1.910279
C	-0.001078	-0.257344	-0.184103
S	1.559068	-0.363863	-0.845308
S	-1.562569	-0.362544	-0.842740
H	-2.413338	1.154391	1.570789
H	-1.383245	0.300249	3.295305
H	-2.412164	-1.049773	1.922785
H	1.384635	0.302499	3.293958
H	2.412786	-1.048105	1.920989
H	2.412088	1.155571	1.566973

CS2-1Me RI-MP2/TZVP

30

E(SCF) =	-1790.025861		
C	0.013021	-0.094166	1.287974
P	-1.619413	0.081962	1.917047
P	1.606923	0.070928	1.989544
C	-0.013898	-0.420781	-0.118269
S	1.419134	-0.439805	-1.021868
S	-1.592496	-0.759089	-0.700266
C	-2.610215	-1.439876	2.178746
H	-2.021238	-2.283357	1.826240
H	-3.514120	-1.392856	1.576204
H	-2.857414	-1.560288	3.235309
C	-1.521601	0.686293	3.662323
H	-1.002330	1.641301	3.722138
H	-1.052336	-0.036783	4.324163
H	-2.547000	0.838928	4.003057
C	-2.610164	1.449234	1.199468

H	-2.844148	2.189519	1.966668
H	-3.522072	1.049221	0.763327
H	-2.029134	1.900976	0.398788
C	2.670319	-1.397089	1.736375
H	3.064544	-1.728718	2.698844
H	3.478857	-1.160897	1.051044
H	2.069805	-2.181292	1.281751
C	2.542432	1.567273	1.526477
H	3.541683	1.519915	1.963409
H	2.012793	2.435932	1.918874
H	2.603576	1.620104	0.443881
C	1.583075	0.201108	3.814108
H	2.623357	0.229717	4.140595
H	1.107847	-0.673614	4.253537
H	1.088412	1.104671	4.156576

	CS2-1Ph	RI-MP2/TZVP	
72			
E(SCF) =	-2933.312408		
C	-0.000095	0.001977	-0.966542
P	1.599881	0.058958	-0.276340
P	-1.600005	-0.057356	-0.276382
C	2.593458	-1.437834	-0.549255
C	2.478822	1.593665	-0.650496
C	1.565072	0.036926	1.552947
C	-2.593179	1.440848	-0.542918
C	-2.479317	-1.590240	-0.657067
C	-1.565059	-0.043189	1.552970
C	-0.000176	0.005137	-2.418856
S	1.520775	0.161589	-3.167355
S	-1.521137	-0.148006	-3.167990
C	-2.075877	2.482451	-1.318426
C	-2.785471	3.675131	-1.421052
C	-3.976385	3.851908	-0.714250
C	-4.495867	2.805570	0.045459
C	-3.777193	1.618311	0.179958
C	-1.734804	-2.770518	-0.574354
C	-2.360107	-3.996722	-0.786681
C	-3.737410	-4.050624	-0.995283
C	-4.472586	-2.867552	-1.089374
C	-3.856481	-1.637088	-0.881959
C	-2.112546	-1.087447	2.304477
C	-2.179600	-0.985168	3.694347
C	-1.758323	0.177748	4.332994
C	-1.205147	1.220059	3.585531
C	-1.156593	1.131655	2.199044

C	2.076355	-2.476356	-1.329014
C	2.786306	-3.668372	-1.436728
C	3.977378	-3.847728	-0.730841
C	4.496699	-2.804374	0.033071
C	3.777664	-1.617920	0.172652
C	1.734162	2.773447	-0.562269
C	2.359181	4.000688	-0.769408
C	3.736389	4.055731	-0.978324
C	4.471723	2.873202	-1.077893
C	3.855889	1.641731	-0.875729
C	2.112631	1.077911	2.308929
C	2.179916	0.969560	3.698330
C	1.758806	-0.196160	4.331951
C	1.205595	-1.235235	3.580022
C	1.156812	-1.140769	2.193943
H	2.459837	1.981602	1.824250
H	2.617788	1.774200	4.277601
H	1.825305	-0.283054	5.410129
H	0.888755	-2.149789	4.066999
H	0.776225	-1.970982	1.607791
H	0.660885	2.718193	-0.412549
H	1.779657	4.914799	-0.716934
H	4.222387	5.009939	-1.140668
H	5.537501	2.914182	-1.268063
H	4.422605	0.724889	-0.981829
H	1.158940	-2.325311	-1.884351
H	2.386721	-4.475503	-2.038863
H	4.530328	-4.774053	-0.828524
H	5.418347	-2.941710	0.585747
H	4.146473	-0.835088	0.826702
H	-4.423091	-0.719703	-0.983850
H	-5.538453	-2.907522	-1.279258
H	-4.223617	-5.004026	-1.161687
H	-1.780725	-4.911155	-0.738415
H	-0.661449	-2.716060	-0.424908
H	-2.385760	4.484613	-2.019938
H	-1.158581	2.333463	-1.874511
H	-4.146089	0.832918	0.830879
H	-5.417406	2.940873	0.598819
H	-4.529026	4.778832	-0.807924
H	-2.459887	-1.988986	1.815900
H	-0.776026	1.964392	1.616473
H	-0.888192	2.132463	4.076449
H	-1.824640	0.259929	5.411551
H	-2.617465	-1.792291	4.270159

	(H+)-1Ph	RI-MP2/TZVP	
70			
E(SCF) =	-2100.844502		
C	0.001233	-0.020662	1.217024
P	1.515828	-0.081574	0.396114
P	-1.516366	0.083874	0.404488
C	1.910907	1.392262	-0.584530
C	2.807609	-0.274757	1.642966
C	1.610690	-1.493740	-0.745960
C	-1.880471	-1.385128	-0.589145
C	-2.806326	0.264763	1.655937
C	-1.639802	1.500844	-0.733348
H	0.015336	0.144943	2.285143
C	1.339530	2.606474	-0.189147
C	1.657043	3.773173	-0.877634
C	2.473155	3.717102	-2.008176
C	3.058340	2.509382	-2.388459
C	2.755507	1.335796	-1.700035
C	2.571649	-1.066397	2.774567
C	3.577242	-1.221024	3.725296
C	4.834022	-0.655581	3.512750
C	5.058238	0.149877	2.397269
C	4.059043	0.317863	1.442074
C	1.996708	-2.739194	-0.236123
C	1.961848	-3.864678	-1.054823
C	1.458407	-3.772851	-2.352509
C	1.100848	-2.529776	-2.871749
C	1.142788	-1.396997	-2.061625
C	-1.358937	-2.609782	-0.158291
C	-1.625939	-3.765403	-0.885807
C	-2.474710	-3.713528	-1.992298
C	-3.001441	-2.493591	-2.415654
C	-2.744489	-1.331826	-1.689867
C	-2.592811	1.082839	2.773211
C	-3.598811	1.222435	3.725583
C	-4.837245	0.612305	3.529478
C	-5.039397	-0.219119	2.429307
C	-4.039253	-0.370418	1.472030
C	-2.050138	2.741349	-0.230705
C	-2.005838	3.869531	-1.046103
C	-1.473130	3.785849	-2.332483
C	-1.089732	2.547730	-2.845359
C	-1.134300	1.414579	-2.036518
H	-2.458389	2.817325	0.770224
H	-2.343612	4.823621	-0.659867
H	-1.438919	4.666582	-2.961924

H	-0.709911	2.471541	-3.857183
H	-0.860678	0.452490	-2.446929
H	-1.638210	1.573814	2.921849
H	-3.436391	1.855887	4.588652
H	-5.618715	0.726952	4.269911
H	-5.994123	-0.709696	2.287445
H	-4.199669	-1.013881	0.615408
H	-0.707538	-2.635785	0.707276
H	-1.229209	-4.715614	-0.550056
H	-2.686629	-4.615330	-2.553427
H	-3.667334	-2.457771	-3.269169
H	-3.175034	-0.389237	-2.006746
H	4.235715	0.942272	0.574628
H	6.027979	0.606300	2.243652
H	5.614891	-0.782496	4.251863
H	3.398451	-1.833041	4.600548
H	1.599846	-1.519827	2.930570
H	1.222085	4.715587	-0.568306
H	0.694814	2.635151	0.681927
H	3.217189	0.399619	-1.992153
H	3.710845	2.472023	-3.252154
H	2.709902	4.624372	-2.550411
H	2.378229	-2.820558	0.774931
H	0.896285	-0.430694	-2.479104
H	0.742799	-2.448434	-3.891014
H	1.428181	-4.651963	-2.984455
H	2.281497	-4.822808	-0.663253

	(H+)2-1Ph	RI-MP2/TZVP	
71			
E(SCF) =	-2101.168353		
C	0.000670	-0.000357	1.236757
P	-1.593673	0.054325	0.321835
P	1.593826	-0.054516	0.319747
C	-1.738120	-1.436213	-0.661601
C	-2.859096	0.060423	1.594795
C	-1.680904	1.538496	-0.686871
C	1.736975	1.436524	-0.663115
C	2.860924	-0.061238	1.591035
C	1.679772	-1.538189	-0.689804
H	0.040446	0.877594	1.887904
H	-0.038279	-0.878705	1.887419
C	-1.333236	-2.652410	-0.091348
C	-1.499733	-3.831114	-0.809576
C	-2.148043	-3.809747	-2.046561
C	-2.571767	-2.601735	-2.598494

C	-2.407958	-1.411515	-1.891393
C	-2.707023	0.819001	2.764967
C	-3.721770	0.810391	3.717899
C	-4.905494	0.114166	3.473014
C	-5.042339	-0.656430	2.318789
C	-4.034230	-0.666396	1.358976
C	-2.258175	2.687061	-0.129126
C	-2.294059	3.863552	-0.875316
C	-1.708430	3.912130	-2.139324
C	-1.156004	2.759299	-2.700239
C	-1.093479	1.583445	-1.959813
C	1.332825	2.652420	-0.091696
C	1.498371	3.831500	-0.809524
C	2.145056	3.810784	-2.047372
C	2.568076	2.603066	-2.600486
C	2.405193	1.412473	-1.893798
C	2.710338	-0.820236	2.761125
C	3.726375	-0.812112	3.712687
C	4.909857	-0.115949	3.466464
C	5.045246	0.655050	2.312335
C	4.035837	0.665511	1.353896
C	2.257716	-2.687026	-0.133316
C	2.292655	-3.863166	-0.880102
C	1.705462	-3.911138	-2.143408
C	1.152352	-2.758037	-2.703090
C	1.090767	-1.582528	-1.962037
H	2.740737	-2.649121	0.835606
H	2.753701	-4.748823	-0.461146
H	1.750363	-4.824606	-2.723559
H	0.727395	-2.786342	-3.698894
H	0.678000	-0.691466	-2.412467
H	1.805398	-1.382935	2.959184
H	3.617740	-1.396304	4.617577
H	5.699662	-0.119805	4.206723
H	5.957452	1.209761	2.133741
H	4.145681	1.259695	0.454367
H	0.864548	2.689160	0.885179
H	1.194505	4.773779	-0.370790
H	2.293337	4.734220	-2.593490
H	3.088360	2.594076	-3.550208
H	2.771242	0.481765	-2.309505
H	-4.145207	-1.260267	0.459380
H	-5.954716	-1.211189	2.141221
H	-5.694303	0.117653	4.214336
H	-3.611991	1.394262	4.622857
H	-1.801884	1.381737	2.962010

H	-1.195299	-4.773624	-0.371732
H	-0.863669	-2.689668	0.884888
H	-2.774531	-0.480585	-2.306139
H	-3.093300	-2.592244	-3.547526
H	-2.297056	-4.732897	-2.592963
H	-2.739989	2.648698	0.840377
H	-0.681261	0.692599	-2.411172
H	-0.732275	2.788082	-3.696551
H	-1.754073	4.825869	-2.718992
H	-2.754601	4.749003	-0.455372

LS-Addukte/LS-NHC-R

(BH3)2-2Ad

RI-BP86/SVP

65

E(SCF) = -1057.817685

N	1.076946	-0.751202	-0.051358
N	-1.121212	-0.737501	-0.099212
C	-0.022848	0.061256	0.153013
C	0.658490	-2.019545	-0.428364
C	-0.705629	-2.012666	-0.454234
C	2.542505	-0.381595	0.015252
C	2.914696	0.490593	-1.210214
C	4.413579	0.863400	-1.150516
C	4.698891	1.636568	0.156278
C	4.366328	0.740274	1.370045
C	2.869315	0.361597	1.332742
C	3.412727	-1.666647	-0.031224
C	4.915746	-1.301936	0.023912
C	5.271484	-0.417976	-1.190804
C	5.224031	-0.539538	1.327997
C	-2.581565	-0.355833	-0.021931
C	-2.941414	0.101161	1.416007
C	-4.431612	0.503080	1.480790
C	-4.705299	1.635708	0.465073
C	-4.393841	1.139878	-0.965250
C	-2.903228	0.746619	-1.064819
C	-3.468255	-1.585912	-0.354651
C	-4.967106	-1.205979	-0.277792
C	-5.272296	-0.084672	-1.292718
C	-5.308743	-0.720136	1.145913
H	1.345624	-2.835009	-0.650797
H	-1.393072	-2.822289	-0.696294
H	2.693584	-0.079430	-2.138682
H	2.295552	1.408057	-1.234379
H	4.650862	1.506347	-2.024304
H	5.766253	1.944354	0.191829

H	4.091630	2.565713	0.187522
H	4.563412	1.296384	2.311104
H	2.248303	1.269607	1.423354
H	2.608745	-0.291070	2.194120
H	3.151712	-2.336820	0.816401
H	3.228242	-2.224405	-0.973245
H	5.501947	-2.245360	-0.010697
H	6.352850	-0.162419	-1.170040
H	5.090729	-0.972997	-2.137164
H	6.305154	-0.286480	1.374399
H	5.004821	-1.179246	2.210599
H	-2.732795	-0.732818	2.121223
H	-2.300450	0.952755	1.708492
H	-4.657181	0.859435	2.508513
H	-4.083269	2.523717	0.704964
H	-5.767121	1.957104	0.532964
H	-4.592774	1.953788	-1.694135
H	-2.255158	1.627012	-0.902632
H	-2.673099	0.355774	-2.079531
H	-3.241418	-1.957470	-1.376875
H	-3.264065	-2.412092	0.360031
H	-5.565288	-2.110021	-0.521865
H	-6.349632	0.184341	-1.247513
H	-5.071473	-0.435651	-2.328357
H	-5.133800	-1.532795	1.884381
H	-6.386268	-0.455542	1.208112
B	-0.078608	1.592693	0.673579
H	-1.180774	2.075063	0.601094
H	0.322074	1.669374	1.834752
H	0.869383	2.301719	0.132382
B	0.464284	3.078164	-0.927408
H	-0.183872	4.025756	-0.513287
H	1.651551	3.338602	-1.140666
H	-0.045177	2.397458	-1.809685

	(BH3)2-2H.c2v	BP86/TZ2P	
17			
E(SCF) =	-3.278377		
B	0.000000	-1.335712	-1.816157
B	0.000000	1.335712	-1.816157
H	1.029938	1.853605	-1.442746
H	-1.029938	1.853605	-1.442746
H	0.000000	1.031553	-2.969812
H	1.029938	-1.853605	-1.442746
H	-1.029938	-1.853605	-1.442746
H	0.000000	-1.031553	-2.969812

C	0.000000	0.000000	-0.470202
N	-1.062888	0.000000	0.394005
C	-0.686288	0.000000	1.708135
C	0.686288	0.000000	1.708135
N	1.062888	0.000000	0.394005
H	2.015806	0.000000	0.049400
H	1.391096	0.000000	2.528118
H	-1.391096	0.000000	2.528118
H	-2.015806	0.000000	0.049400

(BH3)2-2H RI-BP86/SVP

17

E(SCF) =	-279.320691		
C	-0.103502	0.453710	-0.042262
N	0.160186	-0.871277	-0.079336
N	1.120956	1.042626	0.041978
B	-2.778527	-0.714981	0.117218
H	-2.382093	-0.809565	1.267038
H	-2.300095	-1.540500	-0.674686
H	-3.987932	-0.590192	-0.001384
C	2.138341	0.096774	0.060169
C	1.519486	-1.127859	-0.020291
H	-0.648420	-1.521118	-0.146571
H	1.934836	-2.139075	-0.038019
H	3.196215	0.364883	0.127038
H	1.243127	2.055825	0.083999
B	-1.523444	1.176560	-0.073623
H	-2.497857	0.439758	-0.531468
H	-1.786613	1.724907	0.986997
H	-1.555263	1.971995	-1.015109

BH3-2Ad RI-BP86/SVP

61

E(SCF) =	-1031.211191		
N	1.096916	0.659304	-0.021730
N	-1.096911	0.659396	-0.021677
C	-0.000057	-0.184025	-0.012886
C	0.682123	1.986115	-0.033537
C	-0.681980	1.986175	-0.033532
C	2.549279	0.261603	-0.007388
C	2.908093	-0.391525	1.353202
C	4.395208	-0.809443	1.359720
C	4.656703	-1.802802	0.205090
C	4.339558	-1.123070	-1.146120
C	2.852665	-0.707852	-1.177410
C	3.448199	1.513976	-0.182066

C	4.942009	1.109263	-0.168949
C	5.283393	0.439082	1.179043
C	5.228223	0.124928	-1.321684
C	-2.549284	0.261696	-0.007378
C	-2.852736	-0.707353	-1.177752
C	-4.339579	-1.122752	-1.146381
C	-4.656554	-1.802897	0.204669
C	-4.395090	-0.809847	1.359560
C	-2.907986	-0.391839	1.353049
C	-3.448330	1.514054	-0.181602
C	-4.942125	1.109251	-0.168534
C	-5.283374	0.438671	1.179282
C	-5.228376	0.125209	-1.321515
H	1.370607	2.830725	-0.042725
H	-1.370374	2.830850	-0.042770
H	2.705255	0.337704	2.167721
H	2.254924	-1.269604	1.516253
H	4.623941	-1.297062	2.331575
H	5.716837	-2.137030	0.224153
H	4.028106	-2.709300	0.331904
H	4.525001	-1.838144	-1.975897
H	2.196236	-1.594094	-1.099068
H	2.610998	-0.200704	-2.136955
H	3.208481	2.026081	-1.138864
H	3.267868	2.236836	0.642257
H	5.552361	2.029000	-0.297414
H	6.358529	0.158060	1.201469
H	5.119710	1.152128	2.016534
H	6.303327	-0.157395	-1.321405
H	5.022318	0.608230	-2.301545
H	-2.611323	-0.199760	-2.137114
H	-2.196191	-1.593536	-1.099758
H	-4.525057	-1.837621	-1.976323
H	-4.027863	-2.709370	0.331209
H	-5.716653	-2.137237	0.223691
H	-4.623746	-1.297749	2.331291
H	-2.254755	-1.269908	1.515870
H	-2.705157	0.337203	2.167744
H	-3.268034	2.236660	0.642948
H	-3.208689	2.026492	-1.138239
H	-5.552563	2.028968	-0.296733
H	-6.358487	0.157556	1.201703
H	-5.119695	1.151500	2.016960
H	-5.022614	0.608795	-2.301266
H	-6.303460	-0.157189	-1.321182
B	0.000006	-1.801886	-0.057273

H	-1.000175	-2.267758	0.483044
H	0.000990	-2.136677	-1.254796
H	0.999380	-2.267818	0.484649

	BH3-2H.cs1	BP86/TZ2P	
13			
E(SCF) =	-2.725099		
C	-0.001336	0.707465	0.000000
N	1.059176	-0.138313	0.000000
N	-1.067795	-0.135339	0.000000
B	0.023791	2.288791	0.000000
H	1.190078	2.649143	0.000000
H	-0.573618	2.673066	0.996523
H	-0.573618	2.673066	-0.996523
C	-0.685381	-1.467741	0.000000
C	0.674492	-1.471069	0.000000
H	2.007581	0.218208	0.000000
H	1.379641	-2.289845	0.000000
H	-1.393573	-2.284228	0.000000
H	-2.019008	0.211817	0.000000

	BH3-2H	RI-BP86/SVP	
13			
E(SCF) =	-252.704911		
C	1.162688	0.811839	5.326949
N	1.306774	0.006638	4.235704
N	0.948399	-0.072785	6.342561
B	1.274493	2.393071	5.405575
H	0.931213	2.871330	4.317872
H	2.473210	2.646226	5.615917
H	0.589948	2.794280	6.354241
C	0.969900	-1.392467	5.907560
C	1.199850	-1.341495	4.555594
H	1.473841	0.398923	3.307730
H	1.285487	-2.140198	3.813825
H	0.815790	-2.244319	6.575454
H	0.794828	0.248432	7.299728

	CO2-2Ad	RI-BP86/SVP	
60			
E(SCF) =	-1193.030901		
N	1.101518	0.896980	-0.000421
N	-1.101510	0.896999	-0.000280
C	-0.000010	0.087511	-0.000281
C	0.683936	2.225450	-0.000615
C	-0.683915	2.225456	-0.000489

C	2.536679	0.440573	-0.000188
C	2.822091	-0.391120	1.277790
C	4.288688	-0.873969	1.263162
C	4.537611	-1.729783	0.000972
C	4.289007	-0.875014	-1.261989
C	2.822394	-0.392211	-1.277380
C	3.482192	1.666489	-0.000620
C	4.957021	1.194634	-0.000209
C	5.231596	0.347116	1.260260
C	5.231940	0.346048	-1.259880
C	-2.536650	0.440592	-0.000049
C	-2.822549	-0.391307	-1.277793
C	-4.289155	-0.874129	-1.262531
C	-4.537591	-1.729767	-0.000126
C	-4.288478	-0.874834	1.262622
C	-2.821870	-0.391997	1.277370
C	-3.482184	1.666508	0.000546
C	-4.957008	1.194641	0.000823
C	-5.231413	0.346233	1.260721
C	-5.232078	0.346949	-1.259423
H	1.378092	3.066396	-0.000757
H	-1.378045	3.066427	-0.000548
H	2.634952	0.248055	2.168189
H	2.121246	-1.245432	1.349002
H	4.467836	-1.486879	2.171912
H	5.580340	-2.114715	0.001254
H	3.865145	-2.613531	0.001246
H	4.468369	-1.488698	-2.170176
H	2.121652	-1.246638	-1.348009
H	2.635416	0.246156	-2.168390
H	3.296563	2.294473	-0.898771
H	3.296353	2.295283	0.896923
H	5.609950	2.093823	-0.000492
H	6.293480	0.019411	1.271348
H	5.073794	0.956287	2.176928
H	6.293819	0.018309	-1.270397
H	5.074398	0.954445	-2.177106
H	-2.635705	0.247698	-2.168372
H	-2.121778	-1.245661	-1.349072
H	-4.468664	-1.487167	-2.171123
H	-3.865141	-2.613529	-0.000551
H	-5.580325	-2.114685	0.000045
H	-4.467478	-1.488388	2.170967
H	-2.121040	-1.246380	1.347879
H	-2.634577	0.246522	2.168206
H	-3.296173	2.294666	0.898497

H	-3.296736	2.295133	-0.897193
H	-5.609939	2.093828	0.001251
H	-6.293290	0.018501	1.271715
H	-5.073495	0.954749	2.177803
H	-5.074650	0.956001	-2.176235
H	-6.293959	0.019221	-1.270045
C	-0.000068	-1.479845	-0.000614
O	0.000428	-1.981541	1.143749
O	-0.000624	-1.980570	-1.145436

	CO2-2H	RI-BP86/SVP	
12			
E(SCF) =	-414.514226		
C	0.010439	0.007045	0.000008
N	1.353594	-0.064250	0.000006
C	1.909299	1.205251	0.000003
C	0.849322	2.089699	-0.000016
N	-0.300117	1.315685	0.000014
H	1.793341	-0.994040	0.000016
H	2.987793	1.388877	-0.000005
H	0.836816	3.183631	-0.000023
H	-1.293708	1.581578	0.000024
C	-0.986822	-1.187472	-0.000001
O	-2.172572	-0.796698	-0.000002
O	-0.390708	-2.284393	-0.000026

M-Komplexe/M-CDP_vs_M-NHC/BP86_TZ2P

	Ag6-1H	BP86/TZ2P	
11			
E(SCF) =	-1.553129		
C	-0.272228	0.116935	0.879016
P	-0.815529	-1.229540	1.725371
P	0.095036	0.039165	-0.759246
H	-0.282704	-2.501630	1.345378
H	-2.206865	-1.565044	1.808461
H	-0.511083	-1.177799	3.107482
H	0.665910	-1.179149	-1.245485
H	1.054047	1.000960	-1.160217
H	-0.894730	0.263998	-1.771486
Ag	-0.978518	1.971157	1.560496
Cl	-1.722871	4.012100	2.307794

	Ag6-1H.c2v	BP86/TZ2P	
11			
E(SCF) =	-1.553131		
C	0.000000	0.000000	1.354240

P	0.000000	1.482370	2.123780
P	0.000000	-1.482370	2.123780
H	0.000000	1.478620	3.553370
H	-1.083210	2.366260	1.849630
H	1.083210	2.366260	1.849630
H	0.000000	-1.478620	3.553370
H	1.083210	-2.366260	1.849630
H	-1.083210	-2.366260	1.849630
Ag	0.000000	0.000000	-0.738170
Cl	0.000000	0.000000	-3.036570

	Ag6-2H.cs	BP86/TZ2P	
11			
E(SCF) =	-2.273423		
C	-0.049404	-0.059904	0.000000
N	1.311297	-0.086005	0.000000
C	1.875725	1.180708	0.000000
C	0.833429	2.053343	0.000000
N	-0.314266	1.274972	0.000000
H	1.832395	-0.953627	0.000000
H	2.943089	1.351627	0.000000
H	0.813991	3.134149	0.000000
H	-1.259986	1.635448	0.000000
Ag	-1.366128	-1.630741	0.000000
Cl	-2.836755	-3.383432	0.000000

	Au6-1H	BP86/TZ2P	
11			
E(SCF) =	-1.575822		
C	-0.267030	0.134536	0.890157
P	-0.846851	-1.201766	1.743883
P	0.075052	0.078732	-0.762222
H	-0.353899	-2.475423	1.327390
H	-2.245497	-1.490322	1.862525
H	-0.498764	-1.164427	3.115839
H	0.595236	-1.156042	-1.255831
H	1.068660	1.012326	-1.143982
H	-0.912964	0.362524	-1.760472
Au	-0.990006	1.935678	1.539125
Cl	-1.751335	3.958722	2.287819

	Au6-1H.c2v	BP86/TZ2P	
11			
E(SCF) =	-1.575709		
C	0.000000	0.000000	1.488710
P	0.000000	1.492350	2.251480

P	0.000000	-1.492350	2.251480
H	0.000000	1.470310	3.678520
H	-1.085390	2.372500	1.973650
H	1.085390	2.372500	1.973650
H	0.000000	-1.470310	3.678520
H	1.085390	-2.372500	1.973650
H	-1.085390	-2.372500	1.973650
Au	0.000000	0.000000	-0.551140
Cl	0.000000	0.000000	-2.839000

Au6-2H.cs

BP86/TZ2P

11			
E(SCF) =	-2.303097		
C	-0.108795	-0.131076	0.000000
N	1.253134	-0.162557	0.000000
C	1.813290	1.105593	0.000000
C	0.771156	1.978292	0.000000
N	-0.378857	1.204113	0.000000
H	1.768051	-1.033939	0.000000
H	2.880314	1.277465	0.000000
H	0.752915	3.058933	0.000000
H	-1.327126	1.558029	0.000000
Au	-1.379839	-1.646851	0.000000
Cl	-2.843363	-3.390427	0.000000

Cr2-1H.c2v

BP86/TZ2P

16			
E(SCF) =	-3.057136		
Cr	0.000000	0.000000	0.545926
C	0.000000	0.000000	-1.426570
P	0.000000	1.513791	-2.200735
P	0.000000	-1.513791	-2.200735
H	0.000000	1.542128	-3.632986
H	1.100457	2.355301	-1.903461
H	-1.100457	2.355301	-1.903461
H	0.000000	-1.542128	-3.632986
H	-1.100457	-2.355301	-1.903461
H	1.100457	-2.355301	-1.903461
Cl	2.034073	0.000000	1.521016
C	0.000000	-1.869294	0.743984
O	0.000000	-3.007271	0.980678
Cl	-2.034073	0.000000	1.521016
C	0.000000	1.869294	0.743984
O	0.000000	3.007271	0.980678

Cr2-2H

BP86/TZ2P

16			
E(SCF) =	-3.781612		
C	0.079913	-0.037168	-1.454739
N	0.817118	0.777906	-2.249645
H	1.629907	1.262805	-1.877940
N	-0.849450	-0.539012	-2.305760
H	-1.523223	-1.229446	-1.984686
C	-0.696515	-0.063073	-3.595479
H	-1.339993	-0.355608	-4.413583
C	0.372689	0.781758	-3.559508
H	0.839466	1.366082	-4.340333
Cr	0.321572	-0.429135	0.585395
Cl	2.374513	0.430561	0.503833
Cl	-0.963854	-2.236762	0.385673
C	-0.690804	0.800702	1.416136
O	-1.344871	1.592606	1.971823
C	0.602476	-0.862924	2.415814
O	0.730657	-1.075282	3.542609

	Cr2-2H.c2v	BP86/TZ2P	
16			
E(SCF) =	-3.757150		
C	0.000000	0.000000	-1.529936
N	0.000000	1.059643	-2.376615
H	0.000000	2.018450	-2.052350
N	0.000000	-1.059643	-2.376615
H	0.000000	-2.018450	-2.052350
C	0.000000	-0.678986	-3.712756
H	0.000000	-1.389342	-4.527423
C	0.000000	0.678986	-3.712756
H	0.000000	1.389342	-4.527423
Cr	0.000000	0.000000	0.621587
Cl	2.226124	0.000000	0.414250
Cl	-2.226124	0.000000	0.414250
C	0.000000	1.175967	2.031342
O	0.000000	1.947022	2.899774
C	0.000000	-1.175967	2.031342
O	0.000000	-1.947022	2.899774

	Cr3-1H	BP86/TZ2P	
18			
E(SCF) =	-4.016570		
Cr	-1.588653	-0.129547	2.853788
C	0.456700	-0.047490	2.556006
P	1.210948	-1.467708	2.037063
P	1.144624	1.489194	2.412511

H	2.636841	-1.463057	1.876342
H	0.826762	-2.035131	0.789681
H	1.028570	-2.572993	2.898862
H	2.568436	1.587878	2.263277
H	0.919462	2.334917	3.522252
H	0.728233	2.332900	1.344663
C	-2.937164	-0.011302	1.626663
O	-3.758768	0.070186	0.800630
C	-1.857784	1.713910	3.108935
O	-2.169868	2.826014	3.280266
C	-2.722175	-0.328410	4.283167
O	-3.400500	-0.457428	5.223378
C	-1.773282	-1.990828	2.659722
O	-2.033677	-3.124663	2.559577

	Cr3-1H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.016625		
Cr	0.000000	0.000000	-0.483359
C	0.000000	0.000000	1.577161
P	0.000000	-1.503779	2.339702
P	0.000000	1.503779	2.339702
H	0.000000	-1.546011	3.774112
H	1.092459	-2.360416	2.052024
H	-1.092459	-2.360416	2.052024
H	0.000000	1.546011	3.774112
H	-1.092459	2.360416	2.052024
H	1.092459	2.360416	2.052024
C	1.352355	0.000000	-1.718516
O	2.257572	0.000000	-2.455495
C	0.000000	1.865357	-0.720566
O	0.000000	2.994567	-1.018985
C	-1.352355	0.000000	-1.718516
O	-2.257572	0.000000	-2.455495
C	0.000000	-1.865357	-0.720566
O	0.000000	-2.994567	-1.018985

	Cr3-2H	BP86/TZ2P	
18			
E(SCF) =	-4.729120		
Cr	-0.408028	1.010263	2.996084
C	-1.545641	2.081471	3.916404
O	-2.275088	2.791030	4.489581
C	1.000339	1.718014	4.022699
O	1.826424	2.185819	4.699099
C	-0.579886	-0.361203	4.244879

O	-0.686969	-1.219634	5.024333
C	-1.895184	0.313076	2.079890
O	-2.857049	-0.086328	1.556263
C	0.029583	2.285758	1.419687
N	1.024629	3.218782	1.312779
H	1.681334	3.384061	2.066041
N	-0.607950	2.421714	0.216649
H	-1.423260	1.868385	-0.018046
C	1.000835	3.905872	0.113794
H	1.710213	4.682057	-0.137944
C	-0.047572	3.393811	-0.590229
H	-0.426751	3.638328	-1.572833

	Cr3-2H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.724594		
C	0.000000	0.000000	-1.540264
N	0.000000	1.059045	-2.397144
H	0.000000	2.014150	-2.057051
N	0.000000	-1.059045	-2.397144
H	0.000000	-2.014150	-2.057051
C	0.000000	0.682745	-3.723773
H	0.000000	1.389755	-4.541885
C	0.000000	-0.682745	-3.723773
H	0.000000	-1.389755	-4.541885
Cr	0.000000	0.000000	0.588478
C	1.300314	0.000000	1.868983
O	2.170787	0.000000	2.647721
C	0.000000	-1.874779	0.696503
O	0.000000	-3.032196	0.839097
C	-1.300314	0.000000	1.868983
O	-2.170787	0.000000	2.647721
C	0.000000	1.874779	0.696503
O	0.000000	3.032196	0.839097

	Cr4-1H	BP86/TZ2P	
20			
E(SCF) =	-4.608777		
Cr	-1.811476	-0.088191	2.113746
C	0.432485	-0.161221	2.104035
P	1.162404	-1.084849	3.297149
P	1.233403	1.130952	1.397623
H	2.588861	-1.162814	3.291037
H	0.787146	-2.452429	3.265442
H	0.926268	-0.819257	4.685149
H	2.661262	1.096906	1.382971

H	1.013946	2.470635	1.857193
H	0.921734	1.312932	0.026150
C	-3.660281	-0.062874	2.075170
O	-4.823548	-0.045812	2.051453
C	-1.712132	1.375872	3.308590
O	-1.637209	2.271375	4.042105
C	-2.018200	-1.271961	3.572058
O	-2.245947	-1.991516	4.456044
C	-1.681049	-1.562896	0.927146
O	-1.584826	-2.462924	0.205938
C	-1.926310	1.085979	0.635103
O	-2.100027	1.794308	-0.269313

Cr4-1H.c2v BP86/TZ2P

20			
E(SCF) =	-4.608559		
Cr	0.000000	0.000000	0.457249
C	0.000000	0.000000	-1.781345
P	0.000000	1.462286	-2.589510
P	0.000000	-1.462286	-2.589510
H	0.000000	1.430465	-4.016819
H	1.081975	2.353887	-2.327730
H	-1.081975	2.353887	-2.327730
H	0.000000	-1.430465	-4.016819
H	-1.081975	-2.353887	-2.327730
H	1.081975	-2.353887	-2.327730
C	0.000000	0.000000	2.306378
O	0.000000	0.000000	3.470287
C	-1.352558	-1.325934	0.489179
O	-2.188697	-2.127364	0.560218
C	-1.352558	1.325934	0.489179
O	-2.188697	2.127364	0.560218
C	1.352558	1.325934	0.489179
O	2.188697	2.127364	0.560218
C	1.352558	-1.325934	0.489179
O	2.188697	-2.127364	0.560218

Cr4-2H.c2v BP86/TZ2P

20			
E(SCF) =	-5.339375		
C	0.000000	0.000000	-1.421831
N	0.000000	1.060438	-2.280671
N	0.000000	-1.060438	-2.280671
C	0.000000	0.679233	-3.615028
C	0.000000	-0.679233	-3.615028
H	0.000000	2.017876	-1.952215

H	0.000000	-2.017876	-1.952215
H	0.000000	1.389186	-4.430329
H	0.000000	-1.389186	-4.430329
Cr	0.000000	0.000000	0.667666
C	-1.895480	0.000000	0.623387
C	0.000000	0.000000	2.540732
C	1.895480	0.000000	0.623387
C	0.000000	-1.884431	0.671821
C	0.000000	1.884431	0.671821
O	0.000000	-3.046607	0.664109
O	3.052704	0.000000	0.597196
O	-3.052704	0.000000	0.597196
O	0.000000	3.046607	0.664109
O	0.000000	0.000000	3.701225

Cu6-1H BP86/TZ2P

11			
E(SCF) =	-1.596629		
C	-0.178180	0.156325	0.929184
P	-0.819425	-1.177836	1.747819
P	0.094452	0.106511	-0.739354
H	-0.300760	-2.465742	1.400697
H	-2.220601	-1.485018	1.774216
H	-0.566935	-1.121495	3.138694
H	0.681916	-1.086658	-1.267673
H	1.010437	1.099523	-1.159503
H	-0.939820	0.313035	-1.712148
Cu	-0.908232	1.796571	1.516323
Cl	-1.676660	3.617732	2.192001

Cu6-1H.c2v BP86/TZ2P

11			
E(SCF) =	-1.596534		
C	0.000000	0.000000	1.054626
P	0.000000	1.486363	1.827253
P	0.000000	-1.486363	1.827253
H	0.000000	1.479104	3.257407
H	-1.083793	2.371719	1.557435
H	1.083793	2.371719	1.557435
H	0.000000	-1.479104	3.257407
H	1.083793	-2.371719	1.557435
H	-1.083793	-2.371719	1.557435
Cu	0.000000	0.000000	-0.829535
Cl	0.000000	0.000000	-2.920549

Cu6-2H.c2v BP86/TZ2P

11			
E(SCF) =	-2.319286		
C	0.000000	-0.679940	3.103363
C	0.000000	0.679940	3.103363
N	0.000000	1.062934	1.771405
C	0.000000	0.000000	0.913294
N	0.000000	-1.062934	1.771405
Cu	0.000000	0.000000	-0.932413
Cl	0.000000	0.000000	-3.015786
H	0.000000	2.018887	1.439576
H	0.000000	-2.018887	1.439576
H	0.000000	-1.387510	3.920490
H	0.000000	1.387510	3.920490

Hf1-1H BP86/TZ2P

14			
E(SCF) =	-2.243839		
Hf	0.000000	0.000000	-0.539173
Cl	0.000000	-2.427546	-0.200008
Cl	2.012637	0.000000	-1.763722
Cl	-2.012637	0.000000	-1.763722
Cl	0.000000	2.427546	-0.200008
C	0.000000	0.000000	1.723861
P	0.000000	-1.456257	2.611625
H	1.098194	-2.336297	2.463092
H	-1.098194	-2.336297	2.463092
H	0.000000	-1.237731	4.021620
P	0.000000	1.456257	2.611625
H	0.000000	1.237731	4.021620
H	-1.098194	2.336297	2.463092
H	1.098194	2.336297	2.463092

Hf1-2H BP86/TZ2P

14			
E(SCF) =	-2.954233		
C	0.000000	0.000000	1.557387
N	0.000000	1.061934	2.397770
H	0.000000	2.007803	2.011740
N	0.000000	-1.061934	2.397770
H	0.000000	-2.007803	2.011740
C	0.000000	-0.683726	3.721262
H	0.000000	-1.391715	4.538660
C	0.000000	0.683726	3.721262
H	0.000000	1.391715	4.538660
Hf	0.000000	0.000000	-0.788695
Cl	-1.971078	0.000000	-2.050292

Cl	0.000000	2.393028	-0.347834
Cl	1.971078	0.000000	-2.050292
Cl	0.000000	-2.393028	-0.347834

	Mo2-1H.c2v	BP86/TZ2P	
16			
E(SCF) =	-3.114757		
C	0.000000	0.000000	-1.569091
P	0.000000	-1.518587	-2.342582
P	0.000000	1.518587	-2.342582
H	1.100742	2.357161	-2.043370
H	-1.100742	2.357161	-2.043370
H	0.000000	1.549568	-3.775948
H	1.100742	-2.357161	-2.043370
H	-1.100742	-2.357161	-2.043370
H	0.000000	-1.549568	-3.775948
Mo	0.000000	0.000000	0.516502
Cl	2.132047	0.000000	1.538666
Cl	-2.132047	0.000000	1.538666
C	0.000000	-2.006190	0.666155
C	0.000000	2.006190	0.666155
O	0.000000	-3.159834	0.838576
O	0.000000	3.159834	0.838576

	Mo2-2H	BP86/TZ2P	
16			
E(SCF) =	-3.842388		
C	0.128122	0.001521	-1.262985
N	0.012272	1.241489	-1.822582
H	0.156166	2.092918	-1.289081
N	-0.173437	-0.827841	-2.303010
H	-0.163824	-1.839060	-2.157514
C	-0.473226	-0.138285	-3.458598
H	-0.741949	-0.629387	-4.383779
C	-0.350953	1.184942	-3.153815
H	-0.487933	2.068868	-3.761144
Mo	0.777566	-0.670085	0.670328
Cl	2.863592	-0.515003	1.643190
Cl	0.319319	-2.887495	-0.122079
C	0.586711	1.261085	0.959797
O	0.375287	2.408067	1.061771
C	-0.728758	-0.507280	1.863910
O	-1.604524	-0.400883	2.630988

	Mo2-2H.c2v	BP86/TZ2P	
16			

E(SCF) =	-3.806633		
C	0.000000	0.000000	-1.671670
N	0.000000	1.059211	-2.521902
H	0.000000	2.019681	-2.201458
N	0.000000	-1.059211	-2.521902
H	0.000000	-2.019681	-2.201458
C	0.000000	-0.679083	-3.857181
H	0.000000	-1.389061	-4.672311
C	0.000000	0.679083	-3.857181
H	0.000000	1.389061	-4.672311
Mo	0.000000	0.000000	0.637035
Cl	2.331976	0.000000	0.347787
Cl	-2.331976	0.000000	0.347787
C	0.000000	1.115965	2.221224
O	0.000000	1.807613	3.162630
C	0.000000	-1.115965	2.221224
O	0.000000	-1.807613	3.162630

-----	Mo3-1H	BP86/TZ2P	
18			
E(SCF) =	-4.059784		
Mo	-1.644513	-0.136320	2.897946
C	0.561188	-0.044173	2.543430
P	1.321918	-1.450141	1.996006
P	1.253383	1.486973	2.365925
H	2.753354	-1.455869	1.894616
H	0.988088	-1.975689	0.713884
H	1.087298	-2.581470	2.809177
H	2.682450	1.583152	2.275314
H	0.974675	2.368979	3.433935
H	0.886798	2.299108	1.253476
C	-3.127604	-0.015353	1.638727
O	-3.971391	0.064565	0.832889
C	-1.903948	1.862250	3.167525
O	-2.191550	2.979386	3.333762
C	-2.928682	-0.344399	4.370368
O	-3.633896	-0.471702	5.292195
C	-1.812972	-2.150495	2.677625
O	-2.049413	-3.286527	2.569068

-----	Mo3-1H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.059731		
Mo	0.000139	-0.000012	0.540000
C	0.000076	-0.000028	-1.690105
P	0.000168	1.491485	-2.473602

P	-0.000217	-1.491482	-2.473722
H	-0.000041	1.507691	-3.908615
H	1.090530	2.357224	-2.199639
H	-1.089826	2.357590	-2.199291
H	-0.000483	-1.507627	-3.908730
H	-1.090427	-2.357323	-2.199467
H	1.089927	-2.357539	-2.199848
C	1.382255	0.000036	1.925685
O	2.259668	0.000165	2.697478
C	-0.000023	-2.021864	0.755153
O	-0.000302	-3.157301	1.018397
C	-1.382004	-0.000035	1.925650
O	-2.259461	-0.000044	2.697404
C	-0.000109	2.021831	0.755137
O	-0.000354	3.157274	1.018362

	Mo3-2H	BP86/TZ2P	
18			
E(SCF) =	-4.773271		
Mo	-0.394697	0.941256	3.026979
C	-1.603384	2.090663	3.995394
O	-2.333515	2.802723	4.567267
C	1.134392	1.713087	4.124749
O	1.972885	2.179178	4.783983
C	-0.637300	-0.486032	4.420847
O	-0.768772	-1.321702	5.220133
C	-1.996392	0.190919	2.021878
O	-2.944524	-0.212136	1.480063
C	0.056391	2.328808	1.347819
N	1.049323	3.265330	1.241989
H	1.706734	3.430483	1.994141
N	-0.584804	2.470851	0.146643
H	-1.400878	1.919738	-0.088877
C	1.018271	3.961773	0.047185
H	1.723568	4.742762	-0.201576
C	-0.030546	3.451900	-0.655777
H	-0.414817	3.703204	-1.634788

	Mo3-2H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.767334		
C	0.000000	0.000000	-1.780287
N	0.000000	1.058859	-2.636853
H	0.000000	2.014255	-2.298441
N	0.000000	-1.058859	-2.636853
H	0.000000	-2.014255	-2.298441

C	0.000000	0.682220	-3.964728
H	0.000000	1.389065	-4.783313
C	0.000000	-0.682220	-3.964728
H	0.000000	-1.389065	-4.783313
Mo	0.000000	0.000000	0.520302
C	1.339929	0.000000	1.934078
O	2.191995	0.000000	2.734647
C	0.000000	-2.028916	0.643840
O	0.000000	-3.182325	0.802671
C	-1.339929	0.000000	1.934078
O	-2.191995	0.000000	2.734647
C	0.000000	2.028916	0.643840
O	0.000000	3.182325	0.802671

	Mo4-1H	BP86/TZ2P	
20			
E(SCF) =	-4.652962		
Mo	-1.814825	0.078424	2.160353
C	-1.780047	0.324704	0.122745
O	-1.804365	0.460368	-1.027126
C	0.543328	0.116270	2.197786
P	1.307851	1.519055	1.700113
C	-3.806711	0.007275	2.094488
O	-4.968776	-0.035974	2.059811
C	-2.002230	2.103286	2.404675
O	-2.196052	3.239124	2.540651
C	-1.932860	-0.154308	4.193636
O	-2.061548	-0.273194	5.339868
C	-1.833037	-1.954113	1.887795
O	-1.919334	-3.097283	1.716231
P	1.325217	-1.034733	3.127634
H	2.754341	-1.041115	3.129502
H	1.022417	-2.376011	2.771553
H	1.063773	-1.116397	4.532562
H	2.736894	1.533009	1.671663
H	1.050538	2.754021	2.375895
H	0.982568	1.922258	0.377311

	Mo4-1H.c2v	BP86/TZ2P	
20			
E(SCF) =	-4.653130		
Mo	0.000000	0.000000	0.455183
C	0.000000	0.000000	-1.898685
P	0.000000	1.467833	-2.694213
P	0.000000	-1.467833	-2.694213
H	0.000000	1.460135	-4.123042

H	1.082024	2.355292	-2.419918
H	-1.082024	2.355292	-2.419918
H	0.000000	-1.460135	-4.123042
H	-1.082024	-2.355292	-2.419918
H	1.082024	-2.355292	-2.419918
C	0.000000	0.000000	2.450020
O	0.000000	0.000000	3.613499
C	-1.459331	-1.439540	0.521266
O	-2.292306	-2.239743	0.620528
C	-1.459331	1.439540	0.521266
O	-2.292306	2.239743	0.620528
C	1.459331	1.439540	0.521266
O	2.292306	2.239743	0.620528
C	1.459331	-1.439540	0.521266
O	2.292306	-2.239743	0.620528

	Mo4-2H.c2v	BP86/TZ2P	
20			
E(SCF) =	-5.379775		
C	0.000000	0.000000	-1.637792
N	0.000000	1.059909	-2.497930
N	0.000000	-1.059909	-2.497930
C	0.000000	0.679453	-3.831969
C	0.000000	-0.679453	-3.831969
H	0.000000	2.017069	-2.168867
H	0.000000	-2.017069	-2.168867
H	0.000000	1.388812	-4.647955
H	0.000000	-1.388812	-4.647955
Mo	0.000000	0.000000	0.600175
C	0.000000	-2.043289	0.610279
C	0.000000	0.000000	2.625308
C	0.000000	2.043289	0.610279
C	2.053762	0.000000	0.578774
C	-2.053762	0.000000	0.578774
O	3.210515	0.000000	0.569312
O	0.000000	3.204215	0.612945
O	0.000000	-3.204215	0.612945
O	-3.210515	0.000000	0.569312
O	0.000000	0.000000	3.785270

	Ti1-1H	BP86/TZ2P	
14			
E(SCF) =	-2.176465		
Ti	0.000000	0.000000	-0.716231
Cl	0.000000	2.330078	-0.412671
Cl	-1.897300	0.000000	-1.877641

Cl	1.897300	0.000000	-1.877641
Cl	0.000000	-2.330078	-0.412671
C	0.000000	0.000000	1.409159
P	0.000000	1.460101	2.301068
H	-1.103002	2.337539	2.183600
H	1.103002	2.337539	2.183600
H	0.000000	1.202745	3.705886
P	0.000000	-1.460101	2.301068
H	0.000000	-1.202745	3.705886
H	1.103002	-2.337539	2.183600
H	-1.103002	-2.337539	2.183600

Ti1-2H.c2v BP86/TZ2P

14			
E(SCF) =	-2.885359		
Ti	0.000000	0.000000	-0.765447
Cl	-1.853858	0.000000	-1.966787
Cl	0.000000	2.293800	-0.399457
Cl	1.853858	0.000000	-1.966787
Cl	0.000000	-2.293800	-0.399457
C	0.000000	0.000000	1.464521
N	0.000000	1.061714	2.304960
H	0.000000	2.006920	1.916708
N	0.000000	-1.061714	2.304960
H	0.000000	-2.006920	1.916708
C	0.000000	-0.683507	3.628348
H	0.000000	-1.392051	4.445461
C	0.000000	0.683507	3.628348
H	0.000000	1.392051	4.445461

W2-1H.c2v BP86/TZ2P

16			
E(SCF) =	-3.118939		
W	0.000000	0.000000	0.519909
Cl	2.125764	0.000000	1.557318
Cl	-2.125764	0.000000	1.557318
C	0.000000	-2.002935	0.650558
C	0.000000	2.002935	0.650558
O	0.000000	-3.165389	0.785256
O	0.000000	3.165389	0.785256
C	0.000000	0.000000	-1.561404
P	0.000000	-1.520996	-2.341674
P	0.000000	1.520996	-2.341674
H	1.102408	2.356862	-2.043595
H	-1.102408	2.356862	-2.043595
H	0.000000	1.549232	-3.775383

H	1.102408	-2.356862	-2.043595
H	-1.102408	-2.356862	-2.043595
H	0.000000	-1.549232	-3.775383

	W2-2H	BP86/TZ2P	
16			
E(SCF) =	-3.834076		
C	0.000810	-0.106348	-1.529852
N	1.000322	0.174818	-2.406842
H	1.834314	0.670584	-2.104177
N	-0.935457	-0.698988	-2.316938
H	-1.832656	-0.984450	-1.934461
C	-0.539714	-0.783610	-3.638894
H	-1.154889	-1.221659	-4.412679
C	0.701329	-0.223352	-3.696524
H	1.374776	-0.079837	-4.530151
W	-0.092615	0.327644	0.657466
Cl	1.674582	1.823965	0.327755
Cl	-2.403711	0.001074	0.517462
C	-0.227978	0.837744	2.598370
O	-0.282781	1.086980	3.731808
C	0.616027	-1.159302	1.635651
O	1.043000	-2.067738	2.249765

	W2-2H.c2v	BP86/TZ2P	
16			
E(SCF) =	-3.814100		
C	0.000000	0.000000	-1.642918
N	0.000000	1.060402	-2.489492
H	0.000000	2.020042	-2.166894
N	0.000000	-1.060402	-2.489492
H	0.000000	-2.020042	-2.166894
C	0.000000	-0.679009	-3.824124
H	0.000000	-1.389442	-4.638783
C	0.000000	0.679009	-3.824124
H	0.000000	1.389442	-4.638783
W	0.000000	0.000000	0.629298
Cl	2.327546	0.000000	0.315421
Cl	-2.327546	0.000000	0.315421
C	0.000000	1.108128	2.227648
O	0.000000	1.812507	3.163351
C	0.000000	-1.108128	2.227648
O	0.000000	-1.812507	3.163351

	W3-1H	BP86/TZ2P	
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E(SCF) =	-4.065740		
W	-1.650806	-0.131585	2.859968
C	0.523189	-0.043371	2.532286
P	1.286482	-1.462887	2.010250
P	1.218266	1.494336	2.382688
H	2.718311	-1.463032	1.913767
H	0.955299	-1.996914	0.732499
H	1.048367	-2.580778	2.840328
H	2.648036	1.582999	2.295711
H	0.937127	2.359085	3.463675
H	0.854614	2.313801	1.276490
C	-3.169020	-0.014219	1.625390
O	-4.015799	0.064641	0.821364
C	-1.912166	1.862621	3.141320
O	-2.179587	2.985315	3.319950
C	-2.875589	-0.345959	4.388376
O	-3.529793	-0.477754	5.347944
C	-1.822337	-2.144305	2.650326
O	-2.038707	-3.287606	2.551309

	W3-1H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.065813		
W	0.000000	0.000000	0.359660
C	1.405755	0.000000	1.733698
O	2.307202	0.000000	2.478951
C	0.000000	-2.019318	0.576957
O	0.000000	-3.161887	0.818906
C	-1.405755	0.000000	1.733698
O	-2.307202	0.000000	2.478951
C	0.000000	2.019318	0.576957
O	0.000000	3.161887	0.818906
C	0.000000	0.000000	-1.834964
P	0.000000	-1.500914	-2.612424
P	0.000000	1.500914	-2.612424
H	0.000000	1.518567	-4.047119
H	1.093210	2.359231	-2.332183
H	-1.093210	2.359231	-2.332183
H	0.000000	-1.518567	-4.047119
H	-1.093210	-2.359231	-2.332183
H	1.093210	-2.359231	-2.332183

	W3-2H	BP86/TZ2P	
18			
E(SCF) =	-4.775761		
W	-0.427223	0.982036	3.043921

C	-1.646102	2.070389	4.075812
O	-2.381506	2.750926	4.681314
C	1.105343	1.749132	4.133611
O	1.953420	2.215726	4.783654
C	-0.607755	-0.499278	4.388083
O	-0.688275	-1.377951	5.148840
C	-2.023698	0.232009	2.037104
O	-2.968418	-0.168710	1.483420
C	0.048378	2.332714	1.357151
N	1.056685	3.251924	1.244130
H	1.704023	3.425615	2.003655
N	-0.574229	2.452836	0.143665
H	-1.395323	1.906728	-0.087974
C	1.050898	3.918812	0.034438
H	1.769855	4.684467	-0.222601
C	0.004456	3.405882	-0.671859
H	-0.362285	3.639220	-1.661961

	W3-2H.c2v	BP86/TZ2P	
18			
E(SCF) =	-4.772022		
W	0.000000	0.000000	0.419273
C	-1.355889	0.000000	1.829116
O	-2.228495	0.000000	2.608858
C	0.000000	2.025738	0.535420
O	0.000000	3.184506	0.670370
C	1.355889	0.000000	1.829116
O	2.228495	0.000000	2.608858
C	0.000000	-2.025738	0.535420
O	0.000000	-3.184506	0.670370
C	0.000000	0.000000	-1.844767
N	0.000000	-1.059966	-2.699645
H	0.000000	-2.015037	-2.357859
N	0.000000	1.059966	-2.699645
H	0.000000	2.015037	-2.357859
C	0.000000	-0.682868	-4.025189
H	0.000000	-1.389542	-4.843758
C	0.000000	0.682868	-4.025189
H	0.000000	1.389542	-4.843758

	W4-1H	BP86/TZ2P	
20			
E(SCF) =	-4.662818		
W	-1.812140	0.079960	2.155037
C	-1.778548	0.334055	0.119258
O	-1.804058	0.473738	-1.031496

C	0.524405	0.124889	2.204121
P	1.295312	1.515138	1.680402
C	-3.809910	0.007803	2.086494
O	-4.972949	-0.034435	2.052801
C	-1.997861	2.103685	2.407292
O	-2.182187	3.241639	2.549384
C	-1.931460	-0.160396	4.184801
O	-2.057053	-0.284990	5.332327
C	-1.827518	-1.951914	1.887779
O	-1.906939	-3.098570	1.726279
P	1.301242	-1.029387	3.135546
H	2.729398	-1.022879	3.149651
H	1.009718	-2.370894	2.769787
H	1.019607	-1.112648	4.535393
H	2.723559	1.523552	1.676652
H	1.021968	2.761164	2.326631
H	0.989904	1.886555	0.343217

	W4-1H.c2v	BP86/TZ2P	
22			
E(SCF) =	-4.663005		
C	0.000000	0.000000	-1.881739
P	0.000000	1.471140	-2.673419
P	0.000000	-1.471140	-2.673419
H	0.000000	1.460233	-4.101404
H	1.083548	2.354855	-2.395008
H	-1.083548	2.354855	-2.395008
H	0.000000	-1.460233	-4.101404
H	-1.083548	-2.354855	-2.395008
H	1.083548	-2.354855	-2.395008
W	0.000000	0.000000	0.453210
C	0.000000	0.000000	2.452947
O	0.000000	0.000000	3.617349
C	-1.457068	-1.439499	0.522365
O	-2.290382	-2.241282	0.622426
C	-1.457068	1.439499	0.522365
O	-2.290382	2.241282	0.622426
C	1.457068	1.439499	0.522365
O	2.290382	2.241282	0.622426
C	1.457068	-1.439499	0.522365
O	2.290382	-2.241282	0.622426
XX	0.000000	1.000000	0.453210
XX	0.000000	1.000000	2.452947

	W4-2H.c2v	BP86/TZ2P	
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E(SCF) =	-5.390807		
C	0.000000	0.000000	-1.735553
N	0.000000	1.060310	-2.595326
N	0.000000	-1.060310	-2.595326
C	0.000000	0.679649	-3.928388
C	0.000000	-0.679649	-3.928388
H	0.000000	2.017234	-2.265269
H	0.000000	-2.017234	-2.265269
H	0.000000	1.389060	-4.744153
H	0.000000	-1.389060	-4.744153
W	0.000000	0.000000	0.492152
C	-2.052260	0.000000	0.485659
C	0.000000	0.000000	2.520635
C	2.052260	0.000000	0.485659
C	0.000000	-2.041675	0.486313
C	0.000000	2.041675	0.486313
O	0.000000	-3.203897	0.469450
O	3.210171	0.000000	0.493765
O	-3.210171	0.000000	0.493765
O	0.000000	3.203897	0.469450
O	0.000000	0.000000	3.681255

	Zr1-1H.c2v	BP86/TZ2P	
14			
E(SCF) =	-2.237559		
Zr	0.000000	0.000000	-0.665470
Cl	0.000000	-2.438714	-0.292925
Cl	2.025698	0.000000	-1.897170
Cl	-2.025698	0.000000	-1.897170
Cl	0.000000	2.438714	-0.292925
C	0.000000	0.000000	1.622415
P	0.000000	-1.455600	2.509194
H	1.097655	-2.336057	2.361147
H	-1.097655	-2.336057	2.361147
H	0.000000	-1.238143	3.920050
P	0.000000	1.455600	2.509194
H	0.000000	1.238143	3.920050
H	-1.097655	2.336057	2.361147
H	1.097655	2.336057	2.361147

	Zr1-2H.c2v	BP86/TZ2P	
14			
E(SCF) =	-2.947828		
C	0.000000	0.000000	1.569964
N	0.000000	1.061795	2.411244
H	0.000000	2.007866	2.026325

N	0.000000	-1.061795	2.411244
H	0.000000	-2.007866	2.026325
C	0.000000	-0.683574	3.735173
H	0.000000	-1.391734	4.552361
C	0.000000	0.683574	3.735173
H	0.000000	1.391734	4.552361
Zr	0.000000	0.000000	-0.807898
Cl	-1.975499	0.000000	-2.088347
Cl	0.000000	2.401851	-0.327867
Cl	1.975499	0.000000	-2.088347
Cl	0.000000	-2.401851	-0.327867

M-Komplexe/M-CDP_vs_M-NHC/RI-BP86_SVP

	Ag6-2H	RI-BP86/SVP	
11			
E(SCF) =	-833.331923		
C	-0.043374	-0.062213	0.000000
N	1.322520	-0.087855	0.000000
C	1.884689	1.182393	0.000000
C	0.829902	2.060027	0.000000
N	-0.316717	1.276311	0.000000
H	1.847185	-0.963624	0.000000
H	2.963763	1.359521	0.000000
H	0.807432	3.153300	0.000000
H	-1.273504	1.632459	0.000000
Ag	-1.365574	-1.634669	0.000000
Cl	-2.858484	-3.384426	0.000000

	Au6-1H	RI-BP86/SVP	
11			
E(SCF) =	-1320.217744		
C	-0.311692	0.124843	0.868759
P	-0.824948	-1.238836	1.740826
P	0.100113	0.050863	-0.777134
H	-0.266546	-2.497878	1.323382
H	-2.219265	-1.604677	1.858100
H	-0.482508	-1.179804	3.125162
H	0.669957	-1.191852	-1.226993
H	1.088662	1.010257	-1.150515
H	-0.864908	0.284477	-1.828603
Au	-0.999108	1.940193	1.539415
Cl	-1.734196	4.001867	2.310744

	Au6-2H	RI-BP86/SVP	
11			
E(SCF) =	-822.151435		

C	-0.102910	-0.125986	0.000000
N	1.263759	-0.160407	0.000000
C	1.825375	1.110025	0.000000
C	0.773035	1.990291	0.000000
N	-0.378079	1.213101	0.000000
H	1.780570	-1.041061	0.000000
H	2.904852	1.284168	0.000000
H	0.753489	3.083544	0.000000
H	-1.336269	1.566024	0.000000
Au	-1.383088	-1.651976	0.000000
Cl	-2.872829	-3.420299	0.000000

Cr2-1H

RI-BP86/SVP

16

E(SCF) = -2915.500596

Cr	-1.550970	-0.116615	2.754468
C	0.379655	-0.036879	2.457357
P	1.162897	-1.503926	2.053643
P	1.099997	1.515563	2.456130
H	2.589115	-1.477451	1.820727
H	0.708233	-2.167015	0.871556
H	1.054247	-2.538724	3.029100
H	2.525839	1.609578	2.238698
H	0.951058	2.252959	3.667882
H	0.614941	2.446456	1.485490
Cl	-2.787944	0.069004	0.864334
C	-1.814878	1.719601	3.009801
O	-2.108869	2.835376	3.191166
Cl	-2.232524	-0.374307	4.903414
C	-1.725530	-1.973319	2.589373
O	-1.963482	-3.114525	2.515362

Cr2-2H

RI-BP86/SVP

16

E(SCF) = -2417.444065

C	0.118415	0.014180	-1.225312
N	-0.017925	1.251035	-1.798025
H	0.109549	2.117740	-1.268747
N	-0.143853	-0.834931	-2.261950
H	-0.114983	-1.851395	-2.076092
C	-0.434765	-0.166826	-3.434279
H	-0.671625	-0.680758	-4.370303
C	-0.352716	1.174484	-3.139213
H	-0.501075	2.058483	-3.765820
Cr	0.715414	-0.614307	0.621891
Cl	2.710663	-0.510442	1.522885

Cl	0.247928	-2.739127	-0.037846
C	0.583696	1.179630	0.919363
O	0.444195	2.333894	1.074869
C	-0.660291	-0.517429	1.783368
O	-1.530627	-0.459232	2.561435

	Cr3-1H	RI-BP86/SVP	
18			
E(SCF) =	-2221.783016		
Cr	-1.596851	-0.130101	2.857542
C	0.438280	-0.048563	2.567927
P	1.199529	-1.471355	2.030817
P	1.135402	1.494380	2.407229
H	2.639715	-1.464983	1.881064
H	0.832918	-2.031560	0.759751
H	1.010711	-2.601316	2.877402
H	2.573672	1.586682	2.268156
H	0.904581	2.367415	3.508862
H	0.737687	2.338902	1.315246
C	-2.927302	-0.011103	1.616913
O	-3.734246	0.072364	0.770026
C	-1.851050	1.709424	3.114516
O	-2.151894	2.829142	3.290663
C	-2.723845	-0.328811	4.287289
O	-3.395997	-0.458880	5.237689
C	-1.766589	-1.987135	2.665754
O	-2.015960	-3.128821	2.567523

	Cr3-2H	RI-BP86/SVP	
18			
E(SCF) =	-1723.704826		
Cr	-0.412563	1.008655	3.004115
C	-1.544935	2.092023	3.908012
O	-2.275084	2.815212	4.472636
C	1.004141	1.713198	4.013193
O	1.847182	2.178337	4.678918
C	-0.583981	-0.361121	4.250481
O	-0.687766	-1.225274	5.030799
C	-1.885680	0.311873	2.073959
O	-2.840380	-0.094992	1.532329
C	0.022747	2.283436	1.430978
N	1.021098	3.220662	1.326572
H	1.682233	3.384265	2.088047
N	-0.618952	2.418691	0.224314
H	-1.440064	1.857850	-0.010062
C	0.998636	3.909585	0.125732

H	1.715885	4.694938	-0.129425
C	-0.058657	3.392545	-0.584894
H	-0.441180	3.639978	-1.579275

Cr4-1H RI-BP86/SVP

20			
E(SCF) =	-2335.067478		
Cr	-1.817161	-0.090596	2.110694
C	0.410089	-0.179315	2.080133
P	1.136303	-1.082065	3.308705
P	1.207428	1.147234	1.403393
H	2.573720	-1.179943	3.292800
H	0.738782	-2.454661	3.311893
H	0.920901	-0.782219	4.708155
H	2.646316	1.101877	1.360253
H	1.014890	2.489081	1.911852
H	0.865270	1.376227	0.035656
C	-3.665730	-0.058643	2.080416
O	-4.833686	-0.037171	2.061981
C	-1.676406	1.365510	3.300807
O	-1.559266	2.261246	4.037776
C	-2.022524	-1.272653	3.565313
O	-2.249396	-1.996003	4.453612
C	-1.661014	-1.559344	0.928270
O	-1.532343	-2.461858	0.206453
C	-1.932766	1.077010	0.632957
O	-2.101670	1.786276	-0.278690

Cr4-2H RI-BP86/SVP

20			
E(SCF) =	-1837.006700		
C	2.069359	0.068924	0.000483
N	2.921695	0.933002	-0.634133
N	2.937013	-0.780217	0.634517
C	4.261008	0.638811	-0.408206
C	4.270849	-0.462889	0.407612
H	2.579808	1.704952	-1.208225
H	2.608989	-1.558059	1.208765
H	5.080808	1.222714	-0.835664
H	5.100924	-1.032550	0.834460
Cr	-0.013656	0.049760	0.000469
C	0.051165	-1.093611	-1.504157
C	-1.884872	0.031586	0.000114
C	0.028272	1.194590	1.504900
C	-0.003922	-1.447427	1.139104
C	-0.033306	1.546967	-1.138158

O	0.006849	-2.376755	1.845691
O	0.055680	1.899033	2.430125
O	0.093208	-1.796899	-2.429713
O	-0.041813	2.476277	-1.844767
O	-3.050124	0.020237	-0.000217

Cu6-1H			
RI-BP86/SVP			
11			
E(SCF) =	-2824.889783		
C	-0.170693	0.147797	0.926501
P	-0.821202	-1.187701	1.750095
P	0.097683	0.101084	-0.749842
H	-0.298213	-2.494865	1.424992
H	-2.234588	-1.506089	1.767264
H	-0.586447	-1.117394	3.154684
H	0.705365	-1.089875	-1.297322
H	1.003047	1.116815	-1.176110
H	-0.947854	0.295886	-1.734071
Cu	-0.903919	1.794567	1.517035
Cl	-1.687618	3.639225	2.199920

Cu6-2H			
RI-BP86/SVP			
11			
E(SCF) =	-2326.819668		
C	-0.195383	-1.075937	-1.174950
C	-0.588274	-1.648953	0.008031
N	-0.705344	-0.605422	0.917157
C	-0.404350	0.617087	0.371170
N	-0.093639	0.286370	-0.923929
Cu	-0.414903	2.293791	1.182620
Cl	-0.432785	4.193589	2.103795
H	-0.983332	-0.706022	1.893780
H	0.180521	0.990672	-1.609492
H	0.014450	-1.521978	-2.151105
H	-0.788482	-2.692632	0.265922

Hf1-1H			
RI-BP86/SVP			
14			
E(SCF) =	-2613.024820		
Hf	0.922804	0.031455	2.008903
Cl	2.653188	1.389970	3.145958
Cl	2.507158	-1.301715	0.806765
Cl	-0.042105	-0.752472	4.056601
Cl	-1.005955	-0.688428	0.633242
C	0.342061	2.061802	1.172986
P	1.220292	3.486081	1.579621

H	2.599337	3.564477	1.224493
H	1.242496	3.913634	2.940095
H	0.688048	4.649257	0.921852
P	-0.986245	2.243891	0.092239
H	-1.163565	3.613056	-0.311398
H	-2.294470	1.911989	0.553234
H	-0.941703	1.579083	-1.168811

Hf1-2H

RI-BP86/SVP

14

E(SCF) = -2114.942193

Hf	0.000278	-0.000084	1.263416
Cl	1.693098	1.129928	2.493883
Cl	-1.339649	2.013262	0.794014
Cl	-1.692788	-1.130078	2.493531
Cl	1.340521	-2.013361	0.794383
C	0.000141	0.000021	-1.097333
N	0.589359	-0.891381	-1.937922
H	1.114901	-1.684692	-1.538342
N	-0.589253	0.891568	-1.937667
H	-1.114746	1.684781	-1.537849
C	-0.380977	0.575629	-3.264046
H	-0.775771	1.173443	-4.090771
C	0.380170	-0.575633	-3.264205
H	0.774715	-1.173404	-4.091081

Mo2-1H

RI-BP86/SVP

16

E(SCF) = -1939.331289

Mo	-1.644201	-0.117386	2.749312
C	0.397717	-0.028763	2.398347
P	1.206298	-1.510497	2.075301
P	1.135566	1.522900	2.439753
H	2.630051	-1.468594	1.833480
H	0.746746	-2.231949	0.933272
H	1.122448	-2.494631	3.104639
H	2.558543	1.605314	2.203326
H	1.010159	2.231271	3.671486
H	0.638301	2.471554	1.496730
Cl	-3.008747	0.106008	0.797160
C	-1.856191	1.867388	3.032775
O	-2.068888	3.005457	3.209400
Cl	-2.262712	-0.425408	5.040094
C	-1.770290	-2.116522	2.520609
O	-1.933013	-3.270366	2.402817

	Mo2-2H	RI-BP86/SVP	
16			
E(SCF) =	-1441.264257		
C	0.127162	0.000179	-1.264443
N	0.004111	1.242694	-1.827543
H	0.148406	2.102416	-1.291021
N	-0.167287	-0.841816	-2.300927
H	-0.142900	-1.860892	-2.132401
C	-0.468270	-0.160211	-3.463389
H	-0.733209	-0.664002	-4.397324
C	-0.355415	1.177637	-3.162779
H	-0.498299	2.067162	-3.782735
Mo	0.777583	-0.665263	0.672089
Cl	2.892618	-0.499283	1.650396
Cl	0.292025	-2.895797	-0.139369
C	0.595374	1.273867	0.971137
O	0.397423	2.426669	1.081322
C	-0.740349	-0.521125	1.865590
O	-1.626973	-0.427235	2.627623

	Mo3-1H	RI-BP86/SVP	
18			
E(SCF) =	-1245.595292		
Mo	-1.653632	-0.136338	2.899548
C	0.538472	-0.044803	2.551813
P	1.310816	-1.456207	1.992201
P	1.245397	1.493756	2.364409
H	2.756584	-1.460675	1.923930
H	1.010409	-1.966038	0.681385
H	1.055264	-2.609752	2.785777
H	2.689133	1.577655	2.305340
H	0.946711	2.401102	3.419473
H	0.913983	2.300427	1.220858
C	-3.130116	-0.014270	1.618193
O	-3.961976	0.065772	0.793886
C	-1.889580	1.870124	3.170629
O	-2.150610	2.998536	3.338921
C	-2.933951	-0.346738	4.388878
O	-3.631050	-0.475868	5.321987
C	-1.798672	-2.157437	2.678615
O	-2.008422	-3.303565	2.568526

	Mo3-2H	RI-BP86/SVP	
18			
E(SCF) =	-747.515781		
Mo	-0.392453	0.935642	3.028189

C	-1.601918	2.107796	3.979590
O	-2.332391	2.837025	4.538369
C	1.145723	1.708168	4.123497
O	1.988935	2.175802	4.784325
C	-0.638289	-0.497844	4.430614
O	-0.776174	-1.330812	5.237632
C	-1.994228	0.182588	2.013967
O	-2.945798	-0.221984	1.468699
C	0.054182	2.329024	1.351743
N	1.046874	3.272841	1.251055
H	1.711007	3.433360	2.010013
N	-0.595960	2.473259	0.150516
H	-1.415809	1.911610	-0.084501
C	1.011736	3.975871	0.057272
H	1.722004	4.769046	-0.192890
C	-0.046539	3.460804	-0.651663
H	-0.438221	3.717663	-1.639997

	Mo4-1H	RI-BP86/SVP	
20			
E(SCF) =	-1358.878140		
Mo	-1.842673	-0.065421	2.118052
C	0.505693	-0.087720	2.093218
P	1.272335	-1.343788	2.916501
P	1.289262	1.374660	1.791935
H	2.709457	-1.416595	2.839132
H	0.878670	-2.645068	2.471128
H	1.086279	-1.530295	4.338223
H	2.726935	1.357909	1.697268
H	1.107387	2.513595	2.664395
H	0.909600	1.983811	0.554692
C	-3.847901	-0.079713	2.056219
O	-5.014891	-0.089723	2.016317
C	-1.914306	1.765641	3.039210
O	-2.005117	2.798697	3.570871
C	-1.954863	-0.954837	3.962818
O	-2.083690	-1.448614	5.010766
C	-1.814692	-1.903519	1.202150
O	-1.825920	-2.942559	0.678083
C	-1.838723	0.831104	0.270719
O	-1.881103	1.332425	-0.779268

	Mo4-2H	RI-BP86/SVP	
20			
E(SCF) =	-860.812935		
C	2.212127	0.063550	-0.000641

N	3.064129	0.945220	0.609708
N	3.081055	-0.801898	-0.610361
C	4.403466	0.646404	0.392808
C	4.414352	-0.477961	-0.392394
H	2.719921	1.731804	1.161639
H	2.752163	-1.594894	-1.162473
H	5.223156	1.242210	0.803775
H	5.245409	-1.058272	-0.802705
Mo	-0.025070	0.041117	-0.000561
C	-0.022696	-1.559399	-1.276364
C	-2.058113	0.019459	-0.000082
C	-0.056959	1.641662	1.274878
C	0.025805	-1.238845	1.607013
C	-0.002428	1.322573	-1.607655
O	0.059358	-1.962875	2.515874
O	-0.080109	2.553897	2.000756
O	-0.025463	-2.471641	-2.002632
O	0.014641	2.047975	-2.515880
O	-3.222667	0.006990	0.000297

Ti1-1H

RI-BP86/SVP

14

E(SCF) =

-3414.359072

Ti	0.898301	0.123533	1.968076
Cl	2.567060	1.376490	3.058613
Cl	2.363444	-1.181279	0.908461
Cl	0.027093	-0.642619	3.872633
Cl	-0.925655	-0.603022	0.668084
C	0.359246	2.011268	1.190154
P	1.237378	3.435464	1.606125
H	2.609719	3.540020	1.235027
H	1.248958	3.876628	2.961604
H	0.679771	4.585647	0.942484
P	-0.973804	2.188224	0.111013
H	-1.133682	3.567124	-0.272964
H	-2.286764	1.874883	0.569171
H	-0.929722	1.549719	-1.162703

Ti1-2H

RI-BP86/SVP

14

E(SCF) =

-2916.275803

Ti	-0.001239	0.000541	1.165661
Cl	1.505234	-1.100393	2.354271
Cl	1.349109	1.854981	0.788394
Cl	-1.498249	1.094939	2.373439
Cl	-1.359281	-1.848026	0.788048

C	-0.001012	0.000676	-1.058844
N	0.629470	0.862575	-1.898621
H	1.188023	1.628522	-1.489708
N	-0.629779	-0.862258	-1.898861
H	-1.189285	-1.627648	-1.490271
C	-0.405615	-0.558042	-3.225282
H	-0.827604	-1.137504	-4.051709
C	0.408243	0.556613	-3.225121
H	0.831987	1.135024	-4.051386

	W2-1H	RI-BP86/SVP	
16			
E(SCF) =	-1938.238244		
W	-1.664405	-0.118275	2.752626
C	0.386596	-0.029132	2.400703
P	1.206951	-1.511284	2.078212
P	1.135391	1.523902	2.435870
H	2.630530	-1.463286	1.834523
H	0.747105	-2.235230	0.938594
H	1.127743	-2.491964	3.110571
H	2.559559	1.599723	2.202430
H	1.007469	2.236150	3.664423
H	0.643053	2.468401	1.486714
Cl	-3.040846	0.111434	0.793725
C	-1.853242	1.881829	3.039974
O	-2.027966	3.029757	3.216041
Cl	-2.295443	-0.433561	5.052327
C	-1.767954	-2.130898	2.514371
O	-1.892755	-3.291791	2.387397

	W2-2H	RI-BP86/SVP	
16			
E(SCF) =	-1440.170620		
C	0.122727	-0.011314	-1.264758
N	-0.001671	1.235378	-1.821383
H	0.137036	2.090721	-1.275034
N	-0.174010	-0.847633	-2.307958
H	-0.140334	-1.867397	-2.154403
C	-0.477245	-0.157899	-3.464944
H	-0.745597	-0.655313	-4.401320
C	-0.362714	1.177998	-3.155657
H	-0.506721	2.071224	-3.770070
W	0.778197	-0.660440	0.683350
Cl	2.903381	-0.570186	1.673413
Cl	0.384044	-2.911403	-0.149897
C	0.599366	1.297493	0.974400

O	0.410352	2.457484	1.052942
C	-0.765903	-0.491821	1.863855
O	-1.658910	-0.401892	2.623688

	W3-1H	RI-BP86/SVP	
18			
E(SCF) =	-1244.498821		
W	-1.666052	-0.132552	2.865676
C	0.521001	-0.042293	2.528968
P	1.309682	-1.460972	1.996432
P	1.243308	1.497420	2.367682
H	2.756525	-1.464909	1.972821
H	1.047607	-1.967940	0.677334
H	1.022949	-2.608741	2.786218
H	2.688390	1.570522	2.351584
H	0.913002	2.400065	3.416220
H	0.949786	2.303313	1.214408
C	-3.192261	-0.013045	1.604932
O	-4.023951	0.067994	0.779237
C	-1.892762	1.889583	3.147626
O	-2.122808	3.024883	3.326130
C	-2.909790	-0.349645	4.410996
O	-3.553403	-0.482682	5.382764
C	-1.801748	-2.170818	2.649243
O	-1.980713	-3.324504	2.546100

	W3-2H	RI-BP86/SVP	
18			
E(SCF) =	-746.416930		
W	-0.425790	0.971251	3.050979
C	-1.650793	2.111312	4.053160
O	-2.384290	2.826759	4.628917
C	1.145800	1.738907	4.130555
O	2.020444	2.197615	4.758618
C	-0.630813	-0.514348	4.431415
O	-0.721437	-1.388352	5.202564
C	-2.020817	0.206453	2.004753
O	-2.947648	-0.206158	1.421062
C	0.040914	2.347691	1.356891
N	1.045550	3.279267	1.248901
H	1.702325	3.447060	2.013303
N	-0.594943	2.475090	0.145132
H	-1.418954	1.917322	-0.086649
C	1.028666	3.960208	0.043110
H	1.748855	4.742174	-0.214033
C	-0.027731	3.442318	-0.667716

H	-0.406658	3.685292	-1.664532
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W4-1H	RI-BP86/SVP
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20

E(SCF) =	-1357.783630		
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W	-1.852708	-0.062405	2.124692
C	0.497763	-0.073070	2.124478
P	1.274810	-1.354604	2.899176
P	1.289525	1.382005	1.804813
H	2.712124	-1.407979	2.823000
H	0.894310	-2.644381	2.408518
H	1.081631	-1.588037	4.312009
H	2.727109	1.355954	1.721809
H	1.101141	2.527476	2.665522
H	0.920514	1.980235	0.558069
C	-3.879533	-0.082672	2.051568
O	-5.047148	-0.096213	2.006243
C	-1.925809	1.792368	3.037784
O	-2.005168	2.832116	3.560393
C	-1.956958	-0.946196	3.992226
O	-2.064537	-1.433918	5.046461
C	-1.814222	-1.922812	1.216429
O	-1.811519	-2.966656	0.698925
C	-1.830158	0.830390	0.256917
O	-1.849427	1.328389	-0.796602

W4-2H	RI-BP86/SVP
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20

E(SCF) =	-859.718479		
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C	2.209907	0.072726	0.000298
N	3.061874	0.964484	-0.596342
N	3.079506	-0.802032	0.596680
C	4.400837	0.662691	-0.383888
C	4.412176	-0.473877	0.383798
H	2.716303	1.759318	-1.136093
H	2.749891	-1.603560	1.136530
H	5.220220	1.265270	-0.785522
H	5.243409	-1.060182	0.785174
W	-0.039047	0.049703	0.000319
C	0.000447	-1.252341	-1.613390
C	-2.092967	0.027891	0.000500
C	-0.027419	1.352730	1.613720
C	-0.013597	-1.556958	1.296064
C	-0.048520	1.656483	-1.295623
O	0.014982	-2.466310	2.027096
O	-0.018828	2.084498	2.517996

O	0.025023	-1.983282	-2.518042
O	-0.040486	2.566014	-2.026919
O	-3.258182	0.015488	0.000646

	Zr1-1H	RI-BP86/SVP	
14			
E(SCF) =	-2612.043345		
Zr	0.924068	0.027544	2.010261
Cl	2.652128	1.401946	3.140628
Cl	2.506418	-1.314085	0.817449
Cl	-0.037147	-0.760548	4.056267
Cl	-1.009472	-0.678293	0.626793
C	0.341772	2.063626	1.171877
P	1.219730	3.485940	1.579831
H	2.598949	3.565182	1.225171
H	1.242615	3.912509	2.940686
H	0.688101	4.650744	0.923509
P	-0.985674	2.244050	0.092128
H	-1.164826	3.613180	-0.312348
H	-2.293959	1.911133	0.552507
H	-0.941365	1.579153	-1.168978

	Zr1-2H	RI-BP86/SVP	
14			
E(SCF) =	-2113.961152		
Zr	-0.000282	-0.001074	1.270473
Cl	1.684679	-1.130830	2.508018
Cl	1.341540	2.008762	0.782005
Cl	-1.682507	1.125532	2.514912
Cl	-1.344646	-2.008686	0.779798
C	-0.000185	0.000154	-1.099187
N	0.592269	0.889634	-1.939117
H	1.119677	1.681044	-1.538223
N	-0.592229	-0.888708	-1.940060
H	-1.119965	-1.680322	-1.539997
C	-0.382189	-0.573336	-3.266545
H	-0.779048	-1.169226	-4.093687
C	0.382833	0.575264	-3.265936
H	0.780053	1.171791	-4.092445

M-Komplexe/M-NHC_Isomere/nNHC-Komplexe

Fe5(n)

18		BP86/TZ2P	
-4.74161257			
C	-0.001578	-0.004684	0.000000
N	1.360796	-0.004571	0.000000

C	1.896123	1.275007	0.000000
C	0.835621	2.124193	0.000000
N	-0.297556	1.324469	0.000000
H	1.891954	-0.866569	0.000000
H	2.959545	1.467861	0.000000
H	0.790759	3.204107	0.000000
H	-1.252349	1.664266	0.000000
Fe	-1.187293	-1.575271	0.000000
C	-2.247537	-3.008075	0.000000
C	-2.583649	-0.475006	0.000000
C	-0.441221	-2.069531	1.548604
C	-0.441221	-2.069531	-1.548604
O	-2.934009	-3.939250	0.000000
O	-3.458323	0.296588	0.000000
O	0.040469	-2.389726	-2.556759
O	0.040469	-2.389726	2.556759

Ru5(n)

18

BP86/TZ2P

-4.7282674

C	0.061070	0.089350	0.000000
N	1.422920	0.100198	0.000000
C	1.948203	1.383960	0.000000
C	0.880688	2.224841	0.000000
N	-0.245727	1.416084	0.000000
H	1.961224	-0.757298	0.000000
H	3.010077	1.585809	0.000000
H	0.828157	3.304706	0.000000
H	-1.203021	1.749194	0.000000
Ru	-1.201820	-1.598042	0.000000
C	-2.362645	-3.140293	0.000000
C	-2.699077	-0.380618	0.000000
C	-0.379643	-2.138184	1.672923
C	-0.379643	-2.138184	-1.672923
O	-3.057502	-4.063310	0.000000
O	-3.545605	0.421641	0.000000
O	0.112027	-2.462784	-2.674414
O	0.112027	-2.462784	2.674414

Os5(n)

18

BP86/TZ2P

-4.78910565

C	0.072085	0.101702	0.000000
N	1.432754	0.111299	0.000000
C	1.957525	1.394514	0.000000
C	0.889930	2.235190	0.000000

N	-0.235989	1.427208	0.000000
H	1.969443	-0.747587	0.000000
H	3.019326	1.595939	0.000000
H	0.837195	3.314860	0.000000
H	-1.193944	1.758822	0.000000
Os	-1.200807	-1.592646	0.000000
C	-2.369386	-3.144595	0.000000
C	-2.694372	-0.371510	0.000000
C	-0.376236	-2.132668	1.668940
C	-0.376236	-2.132668	-1.668940
O	-3.062472	-4.069469	0.000000
O	-3.549457	0.425768	0.000000
O	0.120730	-2.455390	-2.671451
O	0.120730	-2.455390	2.671451

M-Komplexe/M-NHC_Isomere/aNHC-Komplexe

Ti1(a)

14		BP86/TZ2P	
-2.86635955			
Ti	-0.755296	0.047825	0.000000
Cl	-1.939852	-0.030620	1.871999
Cl	-0.492954	2.318496	0.000000
Cl	-1.939852	-0.030620	-1.871999
Cl	-0.367951	-2.287618	0.000000
C	1.457780	0.088283	0.000000
C	2.382729	1.113561	0.000000
H	2.225921	2.183134	0.000000
N	2.253441	-1.056042	0.000000
H	1.790723	-1.977850	0.000000
C	3.554372	-0.777046	0.000000
H	4.378001	-1.477983	0.000000
N	3.653988	0.564198	0.000000
H	4.529223	1.075962	0.000000

Hf1(a)

14		BP86/TZ2P	
-2.93566464			
C	1.546303	0.071774	0.000000
C	2.474947	1.092551	0.000000
H	2.319456	2.162896	0.000000
N	2.339206	-1.076183	0.000000
H	1.880655	-1.998726	0.000000
C	3.641153	-0.801002	0.000000
H	4.462530	-1.504426	0.000000
N	3.744694	0.539983	0.000000
H	4.621883	1.049023	0.000000

Hf	-0.780474	0.032600	0.000000
Cl	-2.017475	-0.056401	1.993956
Cl	-0.481864	2.417424	0.000000
Cl	-2.017475	-0.056401	-1.993956
Cl	-0.315389	-2.395581	0.000000

Zr1(a)

14		BP86/TZ2P	
-2.9291665			
C	1.561042	0.079778	0.000000
C	2.490913	1.099702	0.000000
H	2.338173	2.170177	0.000000
N	2.353362	-1.069002	0.000000
H	1.895717	-1.991640	0.000000
C	3.656095	-0.795014	0.000000
H	4.477149	-1.498884	0.000000
N	3.760980	0.545718	0.000000
H	4.638882	1.053360	0.000000
Zr	-0.796897	0.042502	0.000000
Cl	-2.050232	-0.043814	2.001257
Cl	-0.453740	2.437155	0.000000
Cl	-2.050232	-0.043814	-2.001257
Cl	-0.297400	-2.395130	0.000000

Cr4(a)

20		BP86/TZ2P	
-5.31751126			
C	-0.078103	1.407850	0.000000
C	-1.118521	2.323167	0.000000
N	1.048160	2.245860	0.000000
N	-0.599841	3.611622	0.000000
C	0.737199	3.551999	0.000000
H	-2.187497	2.161217	0.000000
H	1.999122	1.891304	0.000000
H	-1.132969	4.473417	0.000000
H	1.418255	4.391243	0.000000
Cr	-0.009300	-0.699136	0.000000
C	1.866393	-0.644897	0.000000
C	0.024310	-2.567357	0.000000
C	-1.898680	-0.721566	0.000000
C	-0.012684	-0.634041	1.892013
C	-0.012684	-0.634041	-1.892013
O	-0.012199	-0.584487	3.049903
O	-3.059080	-0.732742	0.000000
O	3.029893	-0.573055	0.000000
O	-0.012199	-0.584487	-3.049903

O	0.047044	-3.729347	0.000000
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Mo4(a)

20		BP86/TZ2P	
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-5.35805946

C	-0.066597	1.625058	0.000000
C	-1.096167	2.552553	0.000000
N	1.068310	2.452994	0.000000
N	-0.564772	3.836260	0.000000
C	0.771856	3.762277	0.000000
H	-2.167118	2.402553	0.000000
H	2.014835	2.088103	0.000000
H	-1.088377	4.703994	0.000000
H	1.461113	4.594965	0.000000
Mo	-0.014518	-0.626078	0.000000
C	2.021771	-0.598560	0.000000
C	0.007396	-2.647308	0.000000
C	-2.062918	-0.635725	0.000000
C	-0.016203	-0.584407	2.050963
C	-0.016203	-0.584407	-2.050963
O	-0.016273	-0.552245	3.208561
O	-3.222371	-0.634717	0.000000
O	3.185146	-0.561500	0.000000
O	-0.016273	-0.552245	-3.208561
O	0.022240	-3.808866	0.000000

W4(a)

20		BP86/TZ2P	
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-5.36937039

C	0.052709	1.735481	0.000000
C	1.076457	2.669550	0.000000
N	-1.087845	2.554881	0.000000
N	0.536091	3.948292	0.000000
C	-0.800026	3.865583	0.000000
H	2.148101	2.525687	0.000000
H	-2.031542	2.182178	0.000000
H	1.054349	4.819061	0.000000
H	-1.495140	4.693072	0.000000
W	0.015849	-0.509399	0.000000
C	0.017861	-0.495799	2.050529
C	0.000734	-2.531784	0.000000
C	0.017861	-0.495799	-2.050529
C	-2.019518	-0.477590	0.000000
C	2.062916	-0.502316	0.000000
O	-3.184060	-0.431153	0.000000
O	0.018349	-0.496392	-3.209713

O	0.018349	-0.496392	3.209713
O	3.223571	-0.491588	0.000000
O	-0.011443	-3.694262	0.000000

Fe5(a)

18

BP86/TZ2P

-4.71977056

C	0.054993	-0.051285	0.000000
C	1.438911	0.011541	0.000000
N	1.831126	1.341956	0.000000
C	0.747227	2.127243	0.000000
N	-0.309834	1.301456	0.000000
H	2.168952	-0.785417	0.000000
H	2.784610	1.684270	0.000000
H	0.735579	3.207724	0.000000
H	-1.278337	1.611159	0.000000
Fe	-1.197019	-1.601767	0.000000
C	-2.276722	-3.015686	0.000000
C	-2.546504	-0.455941	0.000000
C	-0.444411	-2.089435	1.546241
C	-0.444411	-2.089435	-1.546241
O	-2.978337	-3.937310	0.000000
O	-3.367966	0.378439	0.000000
O	0.049689	-2.391312	-2.554919
O	0.049689	-2.391312	2.554919

Ru5(a)

18

BP86/TZ2P

-4.7069536

C	0.118071	0.037210	0.000000
C	1.500449	0.115489	0.000000
N	1.877786	1.451015	0.000000
C	0.784494	2.223339	0.000000
N	-0.262771	1.385756	0.000000
H	2.239476	-0.673387	0.000000
H	2.827182	1.804975	0.000000
H	0.760824	3.303801	0.000000
H	-1.234365	1.685696	0.000000
Ru	-1.211233	-1.625719	0.000000
C	-2.393244	-3.146771	0.000000
C	-2.651283	-0.355908	0.000000
C	-0.381119	-2.149780	1.673549
C	-0.381119	-2.149780	-1.673549
O	-3.103902	-4.059539	0.000000
O	-3.430213	0.518586	0.000000
O	0.126180	-2.432214	-2.680706

O	0.126180	-2.432214	2.680706
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Os5(a)

18

BP86/TZ2P

-4.76810386

C	0.128512	0.060506	0.000000
C	1.509257	0.144094	0.000000
N	1.879969	1.481048	0.000000
C	0.783099	2.247914	0.000000
N	-0.259747	1.406313	0.000000
H	2.251594	-0.641543	0.000000
H	2.827928	1.838274	0.000000
H	0.753240	3.328046	0.000000
H	-1.233737	1.699441	0.000000
Os	-1.206094	-1.613472	0.000000
C	-2.404897	-3.136964	0.000000
C	-2.639508	-0.334447	0.000000
C	-0.369649	-2.147415	1.664175
C	-0.369649	-2.147415	-1.664175
O	-3.123230	-4.044401	0.000000
O	-3.421835	0.541038	0.000000
O	0.142475	-2.446075	-2.667331
O	0.142475	-2.446075	2.667331

Cu6(a)

11

BP86/TZ2P

-2.29791186

C	-0.712241	3.052895	0.000000
N	0.626336	3.095070	0.000000
C	1.130439	1.801688	0.000000
C	0.077588	0.898113	0.000000
N	-1.042347	1.751744	0.000000
H	2.197000	1.622883	0.000000
H	-1.996835	1.411161	0.000000
H	-1.379811	3.902786	0.000000
H	1.168630	3.951068	0.000000
Cu	0.018449	-0.951322	0.000000
Cl	-0.036225	-3.040359	0.000000

Ag6(a)

11

BP86/TZ2P

-2.25294715

C	0.005508	-0.103793	0.000000
C	1.388380	-0.089257	0.000000
N	1.834907	1.226731	0.000000
C	0.781195	2.052102	0.000000

N	-0.305761	1.264209	0.000000
H	2.090925	-0.911503	0.000000
H	2.800414	1.535545	0.000000
H	0.813824	3.132554	0.000000
H	-1.255519	1.617939	0.000000
Ag	-1.359481	-1.638368	0.000000
Cl	-2.874932	-3.363495	0.000000

Au6(a)

11		BP86/TZ2P	
-2.28212898			
C	-0.043559	-0.179415	0.000000
C	1.341397	-0.155873	0.000000
N	1.768996	1.164159	0.000000
C	0.708344	1.980928	0.000000
N	-0.372950	1.186126	0.000000
H	2.048834	-0.973232	0.000000
H	2.731429	1.480551	0.000000
H	0.730809	3.061204	0.000000
H	-1.329581	1.521333	0.000000
Au	-1.373773	-1.653943	0.000000
Cl	-2.896333	-3.359855	0.000000

M-Komplexe/M-NHC_Isomere/NHI-Komplexe

Ti1(I)

14		BP86/TZ2P	
-2.90456337			
Ti	0.329239	0.734022	0.000000
Cl	1.264712	0.023605	1.889512
Cl	1.264712	0.023605	-1.889512
Cl	1.254238	2.762410	0.000000
Cl	-1.787805	1.484505	0.000000
N	-0.661277	-1.353561	0.000000
C	0.037698	-2.547677	0.000000
H	1.118947	-2.570202	0.000000
C	-1.948940	-1.670135	0.000000
H	-2.767263	-0.962614	0.000000
N	-2.100360	-3.016405	0.000000
H	-2.985444	-3.507890	0.000000
C	-0.844260	-3.593210	0.000000
H	-0.697805	-4.664886	0.000000

Hf1(I)

14		BP86/TZ2P	
-2.97402925			
N	-0.807896	-1.606755	0.000000

C	-0.136662	-2.819019	0.000000
H	0.943839	-2.868670	0.000000
C	-2.105347	-1.894631	0.000000
H	-2.905865	-1.166577	0.000000
N	-2.285514	-3.235170	0.000000
H	-3.182269	-3.705667	0.000000
C	-1.043670	-3.842364	0.000000
H	-0.922733	-4.917084	0.000000
Hf	0.251314	0.531043	0.000000
Cl	1.243631	-0.243118	1.989265
Cl	1.243631	-0.243118	-1.989265
Cl	1.229773	2.675011	0.000000
Cl	-1.988563	1.325372	0.000000

Zr1(I)

14		BP86/TZ2P	
-2.96794357			
N	-0.760907	-1.509645	0.000000
C	-0.092376	-2.723438	0.000000
H	0.988212	-2.775740	0.000000
C	-2.058466	-1.795417	0.000000
H	-2.858228	-1.066494	0.000000
N	-2.242219	-3.136144	0.000000
H	-3.139708	-3.605112	0.000000
C	-1.001301	-3.745582	0.000000
H	-0.883097	-4.820717	0.000000
Zr	0.312421	0.658838	0.000000
Cl	1.309301	-0.128219	1.999379
Cl	1.309301	-0.128219	-1.999379
Cl	1.290206	2.819133	0.000000
Cl	-1.948824	1.439935	0.000000

Cr4(I)

20		BP86/TZ2P	
-5.34813551			
N	-0.179100	1.508164	0.000000
C	-1.366451	2.218752	0.000000
C	0.793853	2.411453	0.000000
C	-1.100515	3.562801	0.000000
N	0.274436	3.666192	0.000000
H	-2.326291	1.720685	0.000000
H	1.854965	2.202585	0.000000
H	-1.748263	4.428704	0.000000
H	0.810732	4.524555	0.000000
Cr	0.068957	-0.639094	0.000000
C	1.954296	-0.506874	0.000000

C	0.275020	-2.476868	0.000000
C	-1.801866	-0.932127	0.000000
C	0.065409	-0.608259	1.899675
C	0.065409	-0.608259	-1.899675
O	0.068317	-0.611740	3.056509
O	-2.935271	-1.175280	0.000000
O	3.114742	-0.485015	0.000000
O	0.068317	-0.611740	-3.056509
O	0.405469	-3.632718	0.000000

Mo4(I)

20

BP86/TZ2P

-5.39259897

N	0.051649	1.724523	0.000000
C	-1.019024	2.602443	0.000000
C	1.146447	2.476777	0.000000
C	-0.559246	3.893175	0.000000
N	0.816591	3.793728	0.000000
H	-2.041111	2.248661	0.000000
H	2.165284	2.113316	0.000000
H	-1.072397	4.845259	0.000000
H	1.472510	4.564792	0.000000
Mo	-0.022779	-0.573256	0.000000
C	2.016159	-0.724198	0.000000
C	-0.092920	-2.559235	0.000000
C	-2.071429	-0.583063	0.000000
C	-0.022603	-0.586364	2.053444
C	-0.022603	-0.586364	-2.053444
O	-0.022218	-0.631752	3.209316
O	-3.227997	-0.650250	0.000000
O	3.167146	-0.867916	0.000000
O	-0.022218	-0.631752	-3.209316
O	-0.133376	-3.721532	0.000000

W4(I)

20

BP86/TZ2P

-5.40062171

N	0.118661	1.802713	0.000000
C	-0.921675	2.716396	0.000000
C	1.240035	2.515900	0.000000
C	-0.416672	3.989239	0.000000
N	0.954709	3.842011	0.000000
H	-1.954767	2.397033	0.000000
H	2.244832	2.115884	0.000000
H	-0.897125	4.957976	0.000000
H	1.637455	4.589360	0.000000

W	-0.035391	-0.474437	0.000000
C	1.996600	-0.674908	0.000000
C	-0.176069	-2.462304	0.000000
C	-2.079972	-0.393934	0.000000
C	-0.036453	-0.484427	2.050736
C	-0.036453	-0.484427	-2.050736
O	-0.036723	-0.524023	3.208194
O	-3.239917	-0.394679	0.000000
O	3.147618	-0.830153	0.000000
O	-0.036723	-0.524023	-3.208194
O	-0.257757	-3.623022	0.000000

Fe5(I)

18

BP86/TZ2P

-4.7409346

N	0.071609	0.057122	0.000000
C	1.453331	-0.008867	0.000000
C	1.968246	1.260011	0.000000
N	0.876718	2.102830	0.000000
C	-0.248741	1.345305	0.000000
H	1.969775	-0.958727	0.000000
H	2.985681	1.626479	0.000000
H	0.901054	3.114662	0.000000
H	-1.250537	1.752338	0.000000
Fe	-1.183853	-1.553881	0.000000
C	-2.203259	-2.983646	0.000000
C	-2.633431	-0.503830	0.000000
C	-0.477042	-2.056283	1.576773
C	-0.477042	-2.056283	-1.576773
O	-2.872617	-3.929316	0.000000
O	-3.589659	0.159641	0.000000
O	-0.038544	-2.392175	-2.597824
O	-0.038544	-2.392175	2.597824

Ru5(I)

18

BP86/TZ2P

-4.73071009

N	0.133288	0.149407	0.000000
C	1.516483	0.100131	0.000000
C	2.016257	1.375717	0.000000
N	0.914155	2.205390	0.000000
C	-0.201910	1.435024	0.000000
H	2.044503	-0.843340	0.000000
H	3.028611	1.755923	0.000000
H	0.926802	3.217680	0.000000
H	-1.209013	1.829840	0.000000

Ru	-1.199295	-1.579171	0.000000
C	-2.316477	-3.095486	0.000000
C	-2.746985	-0.411856	0.000000
C	-0.408458	-2.133655	1.692925
C	-0.408458	-2.133655	-1.692925
O	-3.000280	-4.029915	0.000000
O	-3.689367	0.271622	0.000000
O	0.040047	-2.497231	-2.700119
O	0.040047	-2.497231	2.700119

Os5(I)

18		BP86/TZ2P	
-4.78784913			
N	0.133496	0.147836	0.000000
C	1.516313	0.098769	0.000000
C	2.012601	1.374685	0.000000
N	0.908787	2.202288	0.000000
C	-0.205583	1.432383	0.000000
H	2.043697	-0.844925	0.000000
H	3.024364	1.755954	0.000000
H	0.918724	3.214590	0.000000
H	-1.214022	1.822998	0.000000
Os	-1.202326	-1.585834	0.000000
C	-2.326359	-3.118040	0.000000
C	-2.728931	-0.398526	0.000000
C	-0.402246	-2.117623	1.690103
C	-0.402246	-2.117623	-1.690103
O	-3.007612	-4.054708	0.000000
O	-3.648642	0.320753	0.000000
O	0.065380	-2.458596	-2.700106
O	0.065380	-2.458596	2.700106

Cu6(I)

11		BP86/TZ2P	
-2.32977123			
N	-0.675999	3.031799	0.000000
C	0.702982	3.072849	0.000000
C	1.112730	1.766774	0.000000
N	0.000899	0.935148	0.000000
C	-1.066936	1.732258	0.000000
H	2.117783	1.367475	0.000000
H	-2.099781	1.411415	0.000000
H	-1.296467	3.831314	0.000000
H	1.254664	4.003024	0.000000
Cu	0.004009	-0.930033	0.000000
Cl	0.007274	-2.998999	0.000000

Ag6(I)

11		BP86/TZ2P		
-2.28497804				
N	-0.015294	-0.019144	0.000000	
C	1.366591	-0.088013	0.000000	
C	1.885445	1.180019	0.000000	
N	0.795925	2.026085	0.000000	
C	-0.331050	1.270480	0.000000	
H	1.887393	-1.036123	0.000000	
H	2.903124	1.545898	0.000000	
H	0.826699	3.038095	0.000000	
H	-1.332273	1.680476	0.000000	
Ag	-1.369380	-1.635955	0.000000	
Cl	-2.840741	-3.372139	0.000000	

Au6(I)

11		BP86/TZ2P		
-2.30029506				
N	-0.070874	-0.087150	0.000000	
C	1.311521	-0.162580	0.000000	
C	1.827543	1.105671	0.000000	
N	0.739003	1.953166	0.000000	
C	-0.390886	1.203752	0.000000	
H	1.824285	-1.114431	0.000000	
H	2.845954	1.469062	0.000000	
H	0.770149	2.964861	0.000000	
H	-1.393929	1.607477	0.000000	
Au	-1.385473	-1.651703	0.000000	
Cl	-2.833943	-3.372377	0.000000	

M-Komplexe/NiCO2-Komplexe/BP86_TZ2P

	Ni(CO)2-5.cs	BP86/TZ2P		
10				
E(SCF) =	-2.743292			
Ni	0.375367	0.341700	0.000000	
C	2.003234	-0.443964	0.000000	
C	0.487190	2.108235	0.000000	
O	0.569663	3.254694	0.000000	
O	3.051348	-0.913167	0.000000	
C	-1.009776	-0.985746	0.000000	
C	-1.198667	-2.271992	0.000000	
O	-1.327409	-3.432862	0.000000	
C	-1.647256	0.205694	0.000000	
O	-2.585513	0.937665	0.000000	

	Ni(CO)2-3.c2v	BP86/TZ2P	
24			
E(SCF) =	-5.813191		
C	0.000000	0.000000	0.494913
C	0.000000	1.220740	1.180137
C	0.000000	-1.220740	1.180137
N	0.000000	2.446141	0.553080
N	0.000000	1.578732	2.527947
N	0.000000	-1.578732	2.527947
N	0.000000	-2.446141	0.553080
C	0.000000	3.497745	1.443996
C	0.000000	2.964994	2.690835
C	0.000000	-2.964994	2.690835
C	0.000000	-3.497745	1.443996
H	0.000000	2.460900	-0.468464
H	0.000000	4.529670	1.123877
H	0.000000	3.435104	3.663953
H	0.000000	0.937880	3.302617
H	0.000000	-0.937880	3.302617
H	0.000000	-3.435104	3.663953
H	0.000000	-4.529670	1.123877
H	0.000000	-2.460900	-0.468464
Ni	0.000000	0.000000	-1.505989
C	0.000000	-1.433269	-2.505216
O	0.000000	-2.287102	-3.304045
C	0.000000	1.433269	-2.505216
O	0.000000	2.287102	-3.304045

	Ni(CO)2-1H.c2v	BP86/TZ2P	
14			
E(SCF) =	-2.697776		
Ni	0.000000	0.000000	0.806434
C	0.000000	1.513842	1.689170
O	0.000000	2.460827	2.367279
C	0.000000	-1.513842	1.689170
O	0.000000	-2.460827	2.367279
C	0.000000	0.000000	-1.146990
P	0.000000	-1.463428	-1.999694
H	0.000000	-2.581787	-1.141719
H	1.081557	-1.792400	-2.887991
H	-1.081557	-1.792400	-2.887991
P	0.000000	1.463428	-1.999694
H	0.000000	2.581787	-1.141719
H	-1.081557	1.792400	-2.887991
H	1.081557	1.792400	-2.887991

Ni(CO)2-2H.c2v2 BP86/TZ2P

14

E(SCF) =	-3.418076		
Ni	0.000000	0.000000	-0.871031
C	0.000000	-1.527203	-1.747008
C	0.000000	1.527203	-1.747008
O	0.000000	2.497948	-2.387301
O	0.000000	-2.497948	-2.387301
C	0.000000	0.000000	1.055630
N	0.000000	-1.059977	1.919962
C	0.000000	-0.681146	3.251167
C	0.000000	0.681146	3.251167
N	0.000000	1.059977	1.919962
H	0.000000	2.013464	1.579898
H	0.000000	-2.013464	1.579898
H	0.000000	1.386933	4.070244
H	0.000000	-1.386933	4.070244

M-Komplexe/NiCO2-Komplexe/RI-BP86_SVP**Ni(CO)2-1H RI-BP86/SVP**

14

E(SCF) =	-2459.127632		
Ni	-0.116641	0.053899	1.067041
C	-0.078901	0.270679	-0.674787
O	0.070800	0.448101	-1.820594
C	1.410813	0.278048	1.903027
O	2.477701	0.459935	2.345116
C	-1.751056	-0.445020	2.010843
P	-1.648550	-0.186870	3.679709
H	-0.580607	-0.912476	4.281573
H	-2.766977	-0.564444	4.526799
H	-1.401027	1.123284	4.238062
P	-3.145932	-0.184060	1.089748
H	-3.134624	-0.906479	-0.137912
H	-3.506031	1.127448	0.599776
H	-4.438198	-0.562046	1.635649

Ni(CO)2-1Ph RI-BP86/SVP

74

E(SCF) =	-3844.161477		
Ni	-1.231617	-0.022018	2.659211
C	0.736813	0.018715	2.540517
C	-2.239710	1.405125	2.490558
O	-3.037718	2.258999	2.429196
C	-2.147087	-1.491247	2.952465
O	-2.892792	-2.376821	3.123112

P	1.463316	-1.374921	3.175433
P	1.323223	1.489185	1.933349
C	3.315094	-1.542061	3.106382
C	0.861667	-2.907888	2.328517
C	1.145893	-1.650020	4.991733
C	3.161180	1.744537	1.794630
C	0.759905	2.948878	2.926422
C	0.790058	1.831439	0.182404
C	6.156685	-1.730414	3.016320
C	4.113940	-0.748257	3.967051
C	3.944786	-2.424078	2.197380
C	5.358572	-2.523208	2.149118
C	5.526202	-0.837609	3.926903
H	3.650064	-0.059267	4.684025
H	3.348273	-3.053981	1.525512
H	5.836946	-3.218069	1.445463
H	6.136144	-0.218130	4.598050
H	7.252392	-1.805921	2.985348
C	0.016370	-5.214058	0.892644
C	0.575175	-2.821892	0.945545
C	0.725377	-4.147491	2.992973
C	0.299410	-5.298724	2.282286
C	0.156423	-3.966013	0.224172
H	0.646645	-1.853602	0.432992
H	0.916637	-4.235968	4.069112
H	0.174805	-6.254366	2.809275
H	-0.074696	-3.888754	-0.846950
H	-0.322066	-6.102349	0.341528
C	0.631772	-2.038382	7.767465
C	1.967350	-2.514098	5.758216
C	0.074615	-0.979224	5.621202
C	-0.189851	-1.168194	7.000802
C	1.715242	-2.710907	7.138691
H	2.820298	-3.032134	5.301674
H	-0.571360	-0.308568	5.032040
H	-1.031640	-0.645399	7.475223
H	2.357409	-3.382177	7.725226
H	0.431793	-2.189612	8.837453
C	5.979258	2.071103	1.535612
C	3.884080	0.995406	0.832544
C	3.854890	2.652101	2.628382
C	5.257603	2.819773	2.503068
C	5.284485	1.153300	0.699401
H	3.367285	0.289242	0.170276
H	3.316561	3.249077	3.375300
H	5.785681	3.533648	3.149844

H	5.835712	0.568375	-0.049095
H	7.065516	2.199804	1.432077
C	-0.020640	5.132401	4.576716
C	0.692738	2.793856	4.331658
C	0.434848	4.196465	2.347663
C	0.040448	5.285979	3.165700
C	0.308170	3.876683	5.158913
H	0.908980	1.818506	4.787059
H	0.451971	4.336258	1.260243
H	-0.231609	6.246279	2.707083
H	0.249360	3.744911	6.247927
H	-0.333587	5.972463	5.212079
C	-0.028593	2.319082	-2.502406
C	1.461307	2.799066	-0.606156
C	-0.282203	1.105809	-0.380336
C	-0.697504	1.343444	-1.714564
C	1.056801	3.046314	-1.941437
H	2.315096	3.359315	-0.204092
H	-0.808553	0.352093	0.226152
H	-1.538088	0.776374	-2.137363
H	1.582886	3.798022	-2.545710
H	-0.346378	2.508546	-3.537211

M-Komplexe/NiCO3_Komplexe/BP86_TZ2P

	Ni(CO)3-5.cs	BP86/TZ2P	
12			
E(SCF) =	-3.325233		
Ni	0.308471	-0.549274	0.000000
C	1.277120	-0.508021	1.518006
C	1.277120	-0.508021	-1.518006
C	-0.928071	-1.851455	0.000000
O	1.924668	-0.560930	2.469479
O	1.924668	-0.560930	-2.469479
O	-1.647402	-2.751986	0.000000
C	-0.763454	1.299498	0.000000
C	-2.074530	1.239995	0.000000
O	-3.229663	1.098511	0.000000
C	0.043397	2.335212	0.000000
O	0.822841	3.199219	0.000000

Ni(CO)3-1Ph **BP86/TZ2P**

76			
E(SCF) =	-18.220689		
Ni	-1.003495	2.130822	1.796366
C	-0.771396	2.038355	0.020083
O	-0.494124	2.156746	-1.096963

C	0.611226	2.016714	2.544980
O	1.706315	2.116622	2.920265
C	-1.677218	3.752371	2.141774
O	-1.986660	4.857802	2.299061
C	-2.403770	0.656490	2.555296
P	-1.937143	-0.184641	3.957316
C	-0.522415	-1.364191	3.788831
C	-3.236000	-1.150455	4.850601
C	-1.437552	0.956158	5.309640
P	-3.372972	0.062836	1.290692
C	-2.557132	-0.995862	0.009816
C	-4.124400	1.477240	0.385815
C	-4.847745	-0.981692	1.705918
C	-4.493130	-0.543852	5.007300
C	-5.487933	-1.160635	5.764383
C	-5.239244	-2.389047	6.382358
C	-3.987406	-2.990175	6.247609
C	-2.987683	-2.373008	5.491859
H	-4.683659	0.419562	4.533831
H	-6.459141	-0.678995	5.874642
H	-6.017625	-2.871794	6.973427
H	-3.780654	-3.941919	6.736693
H	-2.011147	-2.847663	5.411580
C	-0.827152	0.455403	6.470409
C	-0.559164	1.302314	7.545713
C	-0.910614	2.653181	7.478461
C	-1.538303	3.151253	6.335300
C	-1.805478	2.305077	5.257119
H	-0.565096	-0.600053	6.540577
H	-0.081036	0.903735	8.440044
H	-0.700049	3.313896	8.319457
H	-1.819143	4.202366	6.278105
H	-2.291243	2.680019	4.358587
C	0.794809	-0.992706	4.099585
C	1.859360	-1.856118	3.830675
C	1.625336	-3.104019	3.251378
C	0.318572	-3.482640	2.929287
C	-0.742439	-2.615817	3.186835
H	0.996017	-0.023581	4.551189
H	2.874868	-1.545789	4.074900
H	2.457569	-3.777347	3.045704
H	0.124166	-4.451483	2.468513
H	-1.754667	-2.917945	2.918711
C	-4.257847	1.511848	-1.007986
C	-4.877703	2.598450	-1.629650
C	-5.377175	3.654514	-0.867310

C	-5.244697	3.628680	0.523906
C	-4.616470	2.550573	1.145765
H	-3.856904	0.705018	-1.618972
H	-4.958680	2.620318	-2.715936
H	-5.855583	4.503256	-1.356001
H	-5.615475	4.458668	1.124416
H	-4.477697	2.538353	2.226648
C	-6.122903	-0.416024	1.858343
C	-7.216772	-1.211404	2.206359
C	-7.052729	-2.582105	2.410612
C	-5.788841	-3.157182	2.258366
C	-4.696927	-2.364409	1.905124
H	-6.270645	0.650001	1.689246
H	-8.201406	-0.755751	2.309844
H	-7.907335	-3.202466	2.680959
H	-5.652270	-4.227535	2.409477
H	-3.722528	-2.831631	1.760037
C	-3.304102	-1.677111	-0.966733
C	-2.667311	-2.503763	-1.893192
C	-1.279304	-2.664887	-1.850871
C	-0.532492	-1.999796	-0.877491
C	-1.167956	-1.170809	0.050122
H	-4.389199	-1.576971	-0.994116
H	-3.257072	-3.027730	-2.644917
H	-0.782916	-3.312682	-2.573880
H	0.548917	-2.123822	-0.835040
H	-0.590782	-0.649139	0.814044

M-Komplexe/NiCO3_Komplexe/RI-BP86_SVP

Ni(CO)3-3Me RI-BP86/SVP

38

E(SCF) = -2495.578740

C	0.794459	2.720574	1.752811
C	0.657600	1.464196	2.389076
C	1.576236	2.789619	0.598389
N	1.682735	0.637198	2.849521
N	-0.508960	0.823299	2.797744
N	1.835152	1.736457	-0.317427
N	2.207040	3.898088	0.009364
C	1.155239	-0.460207	3.529036
C	-0.207647	-0.338580	3.496238
C	2.590880	2.207712	-1.396225
C	2.822112	3.533085	-1.186661
H	1.790896	-1.218866	3.994662
H	-0.986801	-0.981183	3.916533
H	2.890058	1.554505	-2.220944

H	3.383037	4.257835	-1.783690
Ni	0.019927	4.254007	2.973583
C	1.435643	5.068110	3.713128
O	2.335864	5.584399	4.245057
C	-0.921214	3.569897	4.339367
O	-1.535370	3.250794	5.277932
C	-1.031947	5.275815	1.937713
O	-1.738609	5.944470	1.296103
C	3.087289	0.986810	2.758837
H	3.513832	0.737757	1.764474
H	3.651786	0.447022	3.541940
H	3.187768	2.080587	2.909546
C	-1.835944	1.224836	2.367791
H	-1.808513	2.309495	2.152769
H	-2.568487	1.028861	3.173147
H	-2.141753	0.677078	1.450027
C	2.374285	5.207850	0.607485
H	3.227813	5.234208	1.319337
H	1.460091	5.479245	1.163825
H	2.553983	5.948771	-0.194992
C	1.122459	0.476355	-0.340100
H	1.499461	-0.250845	0.408725
H	1.223687	0.024594	-1.345255
H	0.044363	0.648802	-0.135355

Ni(CO)₃-3Ad RI-BP86/SVP

122

E(SCF) =	-3895.451660		
C	-0.197791	0.465399	0.655487
C	0.662619	1.349899	-0.060671
C	0.153514	-0.857656	0.872769
N	0.303639	2.144209	-1.153305
N	1.982994	1.702566	0.226170
N	1.271054	-1.590082	0.319690
N	-0.469680	-1.772418	1.771423
C	1.378172	2.939805	-1.526890
C	2.418529	2.660389	-0.683803
C	1.355517	-2.825772	0.990598
C	0.315384	-2.927002	1.855256
H	1.332115	3.646197	-2.355788
H	3.431017	3.064696	-0.680092
H	2.199765	-3.503425	0.859506
H	0.108408	-3.714174	2.580746
C	2.740384	1.157838	1.377148
H	2.615623	0.057991	1.295703
C	2.168638	1.585262	2.755822

C	4.263795	1.455154	1.356951
H	1.070862	1.442649	2.732656
C	2.505317	3.055982	3.078916
C	2.802252	0.656794	3.815973
H	4.681394	1.208511	0.355636
C	4.615550	2.916517	1.738682
C	4.903049	0.522367	2.419923
H	2.047376	3.329354	4.053550
H	2.054169	3.732943	2.322122
C	4.036320	3.252032	3.128597
H	2.539627	-0.401117	3.600457
H	2.381455	0.892794	4.816544
C	4.335118	0.845522	3.822469
H	4.233620	3.647912	0.998156
H	5.721989	3.026514	1.742573
H	4.707734	-0.540902	2.162980
H	6.006175	0.658251	2.412830
H	4.273273	4.307980	3.381177
C	4.658852	2.312018	4.183995
H	4.795660	0.163760	4.569880
H	5.759560	2.464831	4.228627
H	4.260409	2.551526	5.193770
C	-1.061097	2.125491	-1.709172
H	-1.664524	1.828180	-0.824817
C	-1.296226	1.053213	-2.804246
C	-1.603004	3.491146	-2.212917
H	-0.851641	0.097015	-2.459054
C	-0.685654	1.484610	-4.155652
C	-2.826444	0.884383	-2.952337
H	-1.383851	4.272328	-1.454927
C	-1.052276	3.909716	-3.599626
C	-3.139048	3.320287	-2.357707
H	-0.843757	0.682599	-4.908887
H	0.415103	1.615396	-4.062814
C	-1.337191	2.802630	-4.636378
H	-3.263045	0.554250	-1.986518
H	-3.047394	0.089564	-3.697472
C	-3.456052	2.221751	-3.400497
H	0.033035	4.135922	-3.576645
H	-1.546606	4.856713	-3.907309
H	-3.591108	3.059529	-1.378838
H	-3.588936	4.286224	-2.673468
H	-0.906981	3.093508	-5.619037
C	-2.864513	2.617002	-4.771178
H	-4.557688	2.104114	-3.485909
H	-3.329726	3.558536	-5.136205

H	-3.091896	1.833118	-5.526560
C	1.737194	-1.409029	-1.072413
H	1.390858	-0.393484	-1.340744
C	1.101987	-2.380781	-2.116632
C	3.279822	-1.417108	-1.278340
H	0.005981	-2.422140	-1.938215
C	1.705757	-3.802482	-2.049654
C	1.385527	-1.799065	-3.523763
H	3.750952	-0.774041	-0.506716
C	3.891730	-2.837755	-1.221930
C	3.559493	-0.831619	-2.685765
H	1.228495	-4.435554	-2.829472
H	1.476361	-4.283904	-1.078290
C	3.232099	-3.740417	-2.289089
H	0.935792	-0.789423	-3.621915
H	0.906544	-2.438872	-4.296655
C	2.909375	-1.724981	-3.767132
H	3.796375	-3.283668	-0.211254
H	4.984452	-2.765210	-1.414874
H	3.165513	0.205723	-2.752888
H	4.656962	-0.770173	-2.852973
H	3.660823	-4.763972	-2.226897
C	3.507799	-3.146573	-3.688120
H	3.104151	-1.291331	-4.771995
H	4.602224	-3.114400	-3.882487
H	3.060868	-3.793623	-4.474133
C	-1.906483	-1.725617	2.094550
H	-2.166509	-0.664534	1.915816
C	-2.292719	-2.039966	3.567306
C	-2.800084	-2.588826	1.152744
H	-1.624962	-1.470600	4.245724
C	-2.246655	-3.548856	3.912225
C	-3.757217	-1.563412	3.754294
H	-2.482343	-2.409205	0.103077
C	-2.713613	-4.095511	1.487779
C	-4.262942	-2.120287	1.342346
H	-2.596960	-3.686765	4.958751
H	-1.212807	-3.949577	3.893585
C	-3.160362	-4.339627	2.948685
H	-3.833042	-0.474203	3.554694
H	-4.065820	-1.718205	4.811021
C	-4.696860	-2.347113	2.807787
H	-1.685420	-4.479537	1.323131
H	-3.371179	-4.663740	0.793447
H	-4.362343	-1.048648	1.075175
H	-4.930477	-2.686735	0.656392

H	-3.096369	-5.425071	3.181012
C	-4.615833	-3.855092	3.130524
H	-5.740186	-1.989077	2.945086
H	-5.297150	-4.426639	2.462553
H	-4.953573	-4.045460	4.172926
Ni	-1.528340	1.718046	1.757281
C	-1.024075	3.433476	1.545991
C	-3.244469	1.604727	1.251259
C	-1.335503	1.338629	3.502948
O	-4.383296	1.651614	0.998099
O	-1.263192	1.218787	4.659560
O	-0.828772	4.581928	1.510665

Ni(CO)3-3Mes RI-BP86/SVP

102

E(SCF) =	-3733.433910		
C	0.766433	2.715943	1.886450
C	0.213718	1.557678	2.503245
C	1.976350	2.938503	1.254534
N	0.139882	1.358456	3.903271
N	-0.583768	0.507100	1.993125
N	2.959618	1.999816	0.764465
N	2.593370	4.204398	1.011887
C	-0.735659	0.321909	4.212456
C	-1.191283	-0.193366	3.040301
C	4.127315	2.703667	0.373528
C	3.889236	4.027146	0.513791
H	-0.949019	0.043124	5.247489
H	-1.889941	-1.010191	2.842390
H	4.998965	2.172432	-0.017799
H	4.537343	4.890074	0.335393
Ni	-0.772926	4.160087	2.278875
C	-0.369372	5.223955	3.674159
O	-0.323249	5.980715	4.558903
C	-2.375380	3.437263	2.660743
O	-3.501942	3.214069	2.870872
C	-1.113921	5.163817	0.833256
O	-1.518841	5.856850	-0.011560
C	2.741657	0.794530	-0.007378
C	2.747918	-1.402656	-1.814972
C	2.019117	0.878120	-1.232962
C	3.495810	-0.367744	0.297795
C	3.473092	-1.445448	-0.614348
C	2.023244	-0.228043	-2.097640
H	4.075009	-2.339976	-0.382469
H	1.473469	-0.147815	-3.049455

C	2.194929	5.548446	1.345120
C	1.707709	8.277081	1.913283
C	2.473765	6.052755	2.639141
C	1.752250	6.407617	0.309213
C	1.500242	7.757283	0.622488
C	2.211391	7.409020	2.901055
H	1.131117	8.422990	-0.174607
H	2.407345	7.797258	3.913728
C	0.797155	2.092099	4.955849
C	2.102816	3.347362	7.140394
C	0.030173	2.808287	5.910146
C	2.199793	1.938160	5.123578
C	2.824296	2.575344	6.208783
C	0.712185	3.435682	6.974319
H	3.911922	2.449833	6.335913
H	0.118544	4.009237	7.704589
C	-0.694655	-0.085020	0.673283
C	-1.197184	-1.540738	-1.707775
C	-1.504501	0.490472	-0.337194
C	-0.135779	-1.381876	0.509085
C	-0.409304	-2.085212	-0.678776
C	-1.716084	-0.247365	-1.518468
H	0.014680	-3.095247	-0.798896
H	-2.345967	0.202285	-2.303569
C	1.346332	2.159033	-1.651746
H	2.086384	2.983205	-1.716274
H	0.580157	2.477625	-0.917702
H	0.865394	2.048588	-2.641927
C	4.364670	-0.490360	1.529715
H	5.242229	-1.134088	1.323180
H	3.810379	-0.963215	2.367537
H	4.728959	0.486218	1.894760
C	2.756937	-2.560537	-2.785553
H	2.989987	-2.223535	-3.816864
H	1.764302	-3.057425	-2.829639
H	3.502715	-3.328695	-2.501786
C	0.709866	-2.036733	1.577240
H	1.310175	-1.294922	2.136392
H	1.404083	-2.769369	1.123995
H	0.089570	-2.578861	2.322072
C	-1.461886	-2.303961	-2.985106
H	-1.295440	-3.391364	-2.854853
H	-0.791467	-1.962597	-3.803428
H	-2.501469	-2.155601	-3.340742
C	-2.195864	1.812546	-0.154621
H	-1.546559	2.554892	0.349830

H	-3.097579	1.701925	0.483992
H	-2.526314	2.226480	-1.126527
C	1.574469	5.908713	-1.104063
H	2.549421	5.649768	-1.569809
H	1.090082	6.676218	-1.736633
H	0.952369	4.994213	-1.136432
C	3.049973	5.153118	3.699199
H	3.203757	5.698776	4.649014
H	4.024817	4.726076	3.381436
H	2.376350	4.295336	3.895944
C	1.387074	9.717753	2.238244
H	1.369948	10.350173	1.328793
H	2.121611	10.150634	2.947047
H	0.387662	9.802006	2.717226
C	3.002521	1.070089	4.194680
H	3.072045	1.508867	3.180240
H	2.533202	0.071459	4.077013
H	4.030006	0.922980	4.578433
C	-1.478124	2.897818	5.888802
H	-1.910227	2.331718	6.741976
H	-1.925635	2.507188	4.961341
H	-1.803605	3.950615	6.002910
C	2.806852	4.057183	8.273084
H	3.237477	5.022465	7.929516
H	3.646084	3.454175	8.674532
H	2.114838	4.285973	9.107000

Ni(CO)3-3NMe2 RI-BP86/SVP

58

E(SCF) =	-2873.807189		
C	-0.090034	0.123409	-0.087702
C	1.265243	-0.276500	0.007759
C	-0.509174	1.373588	0.262941
N	1.905488	-0.789881	1.135092
N	2.202821	-0.447230	-1.002681
N	0.289836	2.511096	0.645369
N	-1.841945	1.867731	0.350601
C	3.172606	-1.283699	0.815943
C	3.348379	-1.092229	-0.526080
C	-0.549058	3.642807	0.813594
C	-1.833300	3.242118	0.653315
H	3.835179	-1.729362	1.562415
H	4.195682	-1.337737	-1.170555
H	-0.152224	4.602564	1.160063
H	-2.766553	3.789845	0.821907
Ni	-1.174146	-1.658656	-0.186829

C	-1.885721	-1.694170	1.457572
O	-2.337773	-1.711167	2.532818
C	-0.171508	-3.122935	-0.454888
O	0.329692	-4.169315	-0.593792
C	-2.410742	-1.497659	-1.474384
O	-3.252333	-1.436493	-2.279783
N	1.254864	-0.916102	2.358135
N	1.962840	-0.055157	-2.325773
N	1.597137	2.632574	0.127847
N	-2.910326	1.243948	-0.292244
C	2.490039	3.311821	1.055562
H	3.526367	3.247317	0.667652
H	2.455873	2.811913	2.041774
H	2.256139	4.398310	1.203635
C	1.607026	3.204526	-1.220715
H	0.998257	2.560716	-1.884547
H	2.647066	3.207911	-1.602304
H	1.218330	4.252904	-1.255776
C	-4.063798	1.050887	0.571929
H	-3.743760	0.555850	1.507367
H	-4.785965	0.386199	0.057157
H	-4.600984	2.001049	0.832053
C	-3.210335	1.809740	-1.602589
H	-2.278443	1.855692	-2.198962
H	-3.659485	2.835474	-1.559145
H	-3.916485	1.138190	-2.128841
C	1.485988	0.198537	3.266676
H	1.226647	1.145580	2.756194
H	2.537630	0.256065	3.650312
H	0.806570	0.085136	4.133819
C	1.371182	-2.241929	2.948190
H	1.145935	-3.005315	2.180419
H	0.612284	-2.330859	3.750025
H	2.374406	-2.457338	3.398573
C	3.159930	0.422691	-2.998718
H	3.673022	1.175444	-2.370274
H	2.852692	0.908519	-3.945807
H	3.892165	-0.383923	-3.262426
C	1.215893	-1.066479	-3.077659
H	0.309006	-1.337213	-2.501630
H	1.815473	-1.988316	-3.281792
H	0.903849	-0.622464	-4.042953

Ni(CO)₃-3H RI-BP86/SVP

26

E(SCF) = -2338.474817

C	1.028154	2.599651	1.905119
C	0.657979	1.321574	2.332557
C	1.401524	2.753651	0.566427
N	0.448815	0.919939	3.639283
N	0.381166	0.160467	1.585388
N	1.699055	1.806338	-0.430147
N	1.597872	3.965425	-0.069145
C	0.005368	-0.393190	3.708259
C	-0.062574	-0.868097	2.428401
C	2.143760	2.450022	-1.593949
C	2.055440	3.795725	-1.367601
H	0.564894	1.579158	4.411862
H	-0.204808	-0.889075	4.659944
H	-0.353012	-1.852192	2.049781
H	0.108278	0.236214	0.602686
H	1.975861	0.856104	-0.173019
H	2.449213	1.898564	-2.487730
H	2.260420	4.639876	-2.031772
H	1.467508	4.832849	0.459979
Ni	0.997929	4.272659	3.093491
C	2.624549	5.018291	2.962306
O	3.680804	5.509972	2.944038
C	0.695411	3.862260	4.799152
O	0.500599	3.655010	5.934217
C	-0.364646	5.266913	2.480727
O	-1.274158	5.909644	2.137587

Ni(CO)₃-1Cy RI-BP86/SVP

112

E(SCF) =	-3979.493073		
C	0.085414	-0.386934	-0.089883
P	-1.546603	0.151637	-0.185034
P	1.570336	0.406819	0.228276
C	3.114342	-0.312552	-0.644277
C	5.402591	-1.409112	-0.657855
C	4.061780	-1.274767	-2.802217
C	5.094984	-2.082960	-2.003095
C	2.789792	-1.010851	-1.978245
C	4.123940	-1.154903	0.166010
H	5.918723	-0.438784	-0.842187
H	4.513584	-0.303878	-3.112257
H	4.693014	-3.103777	-1.815974
H	2.283219	-1.968204	-1.748742
H	3.675838	-2.130614	0.439945
H	3.654325	0.629934	-0.889865
H	6.108732	-2.028130	-0.064472

H	3.794053	-1.806007	-3.740134
H	6.027272	-2.217362	-2.592044
H	2.060146	-0.421941	-2.568201
H	4.399036	-0.647477	1.112419
C	2.105956	0.566944	2.053855
C	1.734464	1.769766	4.281187
C	2.560312	-0.619745	4.269595
C	1.745065	0.432148	5.034356
C	2.078518	-0.775468	2.815587
C	1.261136	1.603557	2.824912
H	2.761304	2.201488	4.283364
H	3.634700	-0.324825	4.271507
H	0.698727	0.070187	5.150181
H	1.037718	-1.161315	2.806599
H	0.203976	1.262704	2.818815
H	3.159121	0.928732	2.011863
H	1.087707	2.507387	4.803237
H	2.509235	-1.602424	4.784606
H	2.143970	0.567621	6.062269
H	2.689802	-1.539630	2.304822
H	1.273468	2.592163	2.322795
C	1.725604	2.213039	-0.397251
C	2.980207	4.444136	-0.375713
C	1.719801	3.749022	-2.451539
C	2.934402	4.514312	-1.908005
C	1.686636	2.296007	-1.941447
C	2.953671	2.989965	0.135447
H	2.107282	4.993900	0.044069
H	0.790207	4.276942	-2.140583
H	3.866489	4.068550	-2.323479
H	2.570969	1.768651	-2.359252
H	3.888491	2.483270	-0.194734
H	0.812376	2.711428	-0.005361
H	3.885117	4.958100	0.012922
H	1.719370	3.753043	-3.562332
H	2.915484	5.570855	-2.249899
H	0.796010	1.762225	-2.330049
H	2.979657	2.994522	1.242362
C	-2.317755	-0.553666	-1.774182
C	-4.302369	-0.989300	-3.307468
C	-1.948715	-1.094148	-4.235106
C	-3.416490	-0.757618	-4.540218
C	-1.430332	-0.314921	-3.013882
C	-3.792969	-0.216245	-2.073359
H	-4.318600	-2.076386	-3.068659
H	-1.850854	-2.184344	-4.039855

H	-3.493847	0.309278	-4.852468
H	-1.409760	0.767890	-3.265900
H	-3.908133	0.874881	-2.261769
H	-2.256486	-1.642462	-1.549356
H	-5.354063	-0.701272	-3.520897
H	-1.308391	-0.880443	-5.117374
H	-3.784970	-1.359260	-5.398199
H	-0.388118	-0.602776	-2.769143
H	-4.439561	-0.457597	-1.206518
C	-2.680206	-0.599992	1.185626
C	-2.735486	-1.688261	3.489705
C	-4.865085	-0.762477	2.478805
C	-4.101527	-1.048331	3.780285
C	-4.029533	0.088558	1.500115
C	-1.910888	-0.851134	2.496510
H	-2.886143	-2.704687	3.064705
H	-5.131023	-1.725548	1.987993
H	-3.951472	-0.091976	4.331879
H	-3.852110	1.082607	1.965104
H	-1.654466	0.124728	2.967992
H	-2.921172	-1.594069	0.751462
H	-2.162875	-1.826691	4.431658
H	-5.825218	-0.246510	2.694949
H	-4.704578	-1.700341	4.447474
H	-4.622224	0.273845	0.582077
H	-0.950296	-1.350701	2.259449
C	-2.136285	1.966870	-0.147860
C	-2.552503	4.065349	1.239228
C	-2.630521	4.185499	-1.289591
C	-2.306998	4.945756	0.005099
C	-1.867407	2.849289	-1.382427
C	-1.787496	2.732219	1.146020
H	-3.642369	3.855480	1.331028
H	-3.725014	3.983625	-1.331850
H	-1.238748	5.260618	-0.012105
H	-0.783305	3.057505	-1.470242
H	-0.697849	2.941582	1.169314
H	-3.234971	1.790500	-0.131074
H	-2.261187	4.602982	2.166649
H	-2.397393	4.811539	-2.177284
H	-2.904191	5.880160	0.067366
H	-2.159023	2.324928	-2.312729
H	-1.994491	2.113394	2.041389
Ni	0.078376	-2.571516	-0.181777
C	-1.365193	-3.413144	0.471891
O	-2.165745	-4.190558	0.815297

C	0.172476	-3.132323	-1.891161
O	0.208547	-3.693940	-2.911829
C	1.412865	-3.335111	0.737345
O	2.157953	-4.048381	1.283166

Ni(CO)3-1F RI-BP86/SVP

16			
E(SCF) =	-3167.636070		
Ni	-0.291625	0.847207	1.285959
C	-0.210226	0.464214	-0.469411
O	-0.048461	0.293723	-1.605075
C	1.259376	0.357739	2.054050
O	2.319244	0.123075	2.462004
C	-0.652499	2.594359	1.572324
O	-0.795774	3.736840	1.706500
C	-1.840739	-0.244625	2.140884
P	-1.686163	-0.461965	3.742091
F	-0.434703	-1.302380	4.222630
F	-2.845093	-1.211813	4.534685
F	-1.503850	0.810316	4.671119
P	-3.154874	-0.339349	1.192313
F	-3.000075	-1.157219	-0.153989
F	-3.765216	0.999320	0.601752
F	-4.478511	-1.006547	1.773320

Ni(CO)3-1H RI-BP86/SVP

16			
E(SCF) =	-2572.403707		
Ni	-0.253846	0.766516	1.261505
C	-0.184132	0.401666	-0.494280
O	-0.088577	0.203399	-1.636553
C	1.286908	0.306420	2.058434
O	2.317252	0.050984	2.534264
C	-1.723371	-0.426045	2.058807
P	-1.695552	-0.425392	3.745823
H	-0.475103	-0.953596	4.265973
H	-2.682595	-1.206618	4.457868
H	-1.761406	0.797612	4.522916
P	-3.171931	-0.300556	1.202691
H	-3.039200	-0.737271	-0.150317
H	-3.825688	0.972417	0.965954
H	-4.313017	-1.068330	1.650019
C	-0.657521	2.493861	1.562661
O	-0.861405	3.627827	1.725387

Ni(CO)3-1Me RI-BP86/SVP

34

E(SCF) =	-2808.188347		
Ni	-0.495206	1.357094	1.431559
C	-0.340377	1.051603	-0.321876
O	-0.145130	0.913383	-1.464715
C	1.085532	0.980779	2.173286
O	2.167309	0.805601	2.576362
C	-2.036031	0.199574	2.270331
P	-1.707279	-0.403398	3.815249
C	-0.357305	-1.667458	3.961305
C	-3.084336	-1.217772	4.755621
C	-1.171254	0.923408	4.973960
P	-3.243399	-0.268798	1.183417
C	-2.770644	-1.478118	-0.142182
C	-3.905922	1.160969	0.231758
C	-4.787282	-1.043055	1.862214
C	-1.025895	3.037885	1.792916
O	-1.354585	4.130853	2.021966
H	-0.187062	-1.965933	5.015647
H	-0.640047	-2.557868	3.365932
H	0.578205	-1.250491	3.544288
H	-2.742599	-1.454339	5.782752
H	-3.954673	-0.537077	4.814570
H	-3.392043	-2.159582	4.263228
H	-0.917203	0.511091	5.970739
H	-0.291659	1.436831	4.543804
H	-1.992754	1.660083	5.066547
H	-5.520699	-1.187001	1.044205
H	-4.566878	-2.029466	2.312247
H	-5.231688	-0.383544	2.631611
H	-4.672611	0.837135	-0.499784
H	-4.344459	1.884349	0.946175
H	-3.069332	1.656799	-0.294246
H	-3.615291	-1.683510	-0.830827
H	-1.919834	-1.070973	-0.719570
H	-2.448043	-2.422580	0.338605

Ni(CO)₃-1Mes RI-BP86/SVP

130

E(SCF) =	-4664.799952		
C	0.060416	-0.717242	-1.007786
P	1.597530	-0.034800	-0.403711
P	-1.614842	-0.559932	-0.399117
C	2.207387	1.864556	-0.603726
C	3.086112	-0.747451	-1.417687
C	-2.666310	-2.144430	-0.689966

C	1.796219	-0.459869	1.461852
C	-2.771871	0.778978	-1.188281
C	-1.819560	-0.049467	1.481949
C	1.474839	2.873108	-1.299547
C	1.964277	4.198205	-1.379077
C	3.189140	4.592395	-0.837604
C	3.940717	3.581823	-0.217604
C	3.076596	-0.422562	-2.819794
C	3.990050	-1.028042	-3.701623
C	3.496487	2.251231	-0.095007
C	4.971454	-1.932188	-3.273834
C	5.072283	-2.118565	-1.892682
C	4.199913	-1.528078	-0.947009
C	-2.200553	-3.357436	-0.092072
C	-2.966867	-4.533733	-0.115776
C	-4.230824	-4.586888	-0.714987
C	-4.662525	-3.416786	-1.349558
C	-3.922392	-2.210518	-1.396789
C	1.737263	0.492960	2.533760
C	1.703381	0.032467	3.870260
C	1.735827	-1.320055	4.225193
C	1.819989	-2.240012	3.170492
C	1.850660	-1.854643	1.816298
C	-2.541523	1.284088	-2.503889
C	-3.241895	2.423641	-2.955124
C	-4.222085	3.064178	-2.185548
C	-4.557233	2.453154	-0.965404
C	-3.887893	1.318189	-0.462294
C	-1.470413	1.303305	1.806990
C	-1.528829	1.770347	3.135621
C	-1.914191	0.958002	4.206895
C	-2.323833	-0.338846	3.875221
C	-2.332890	-0.855802	2.558966
H	-2.712697	-0.988303	4.676517
H	-1.267471	2.824658	3.323082
H	-2.550846	-5.434549	0.364204
H	-5.625650	-3.437887	-1.884073
H	-3.020729	2.798350	-3.968443
H	-5.403852	2.853518	-0.382531
H	4.929711	3.831706	0.201416
H	1.346809	4.938792	-1.914724
H	3.917081	-0.775131	-4.771419
H	5.890464	-2.746568	-1.502493
H	1.870382	-3.317583	3.399196
H	1.651388	0.790925	4.668507
C	-4.528625	0.708322	0.772768

H	-4.385026	-0.383957	0.832050
H	-5.620593	0.897016	0.735617
H	-4.153333	1.146116	1.718560
C	-1.697308	0.580868	-3.538524
H	-1.237601	1.296049	-4.247168
H	-2.344184	-0.090011	-4.146492
H	-0.914970	-0.061127	-3.096524
C	-4.915027	4.319088	-2.658880
H	-4.900517	4.403197	-3.763516
H	-4.414266	5.225887	-2.255260
H	-5.970297	4.356571	-2.321601
C	2.198231	0.632226	-3.442191
H	1.171631	0.611702	-3.046041
H	2.143596	0.494568	-4.537335
H	2.627872	1.636654	-3.249610
C	4.720803	-1.734325	0.471599
H	4.973009	-2.799834	0.639736
H	4.060482	-1.402408	1.283256
H	5.675209	-1.178244	0.577353
C	5.872762	-2.649752	-4.247077
H	6.832705	-2.944971	-3.779018
H	6.094253	-2.026546	-5.136424
H	5.385703	-3.579090	-4.613349
C	-4.561706	-1.184067	-2.314613
H	-5.014334	-0.322417	-1.791993
H	-5.365421	-1.679540	-2.891672
H	-3.843206	-0.777755	-3.044519
C	-0.846299	-3.468187	0.523085
H	-0.554884	-2.594738	1.132649
H	-0.114923	-3.523976	-0.304593
H	-0.758831	-4.384324	1.139997
C	-5.048813	-5.854188	-0.738449
H	-6.119684	-5.648662	-0.933039
H	-4.968718	-6.409562	0.217649
H	-4.691682	-6.535934	-1.540173
C	-1.911895	1.454742	5.631874
H	-0.932398	1.257484	6.119028
H	-2.685599	0.949635	6.243787
H	-2.086741	2.547881	5.684773
C	-1.126933	2.356232	0.787751
H	-0.557328	1.945270	-0.055313
H	-0.537541	3.173361	1.242217
H	-2.043242	2.808947	0.359708
C	-3.037283	-2.196818	2.471858
H	-3.651534	-2.339201	3.381442
H	-2.336668	-3.049933	2.423675

H	-3.709076	-2.279703	1.600902
C	1.774066	2.001907	2.420530
H	2.820003	2.371808	2.443591
H	1.255687	2.450553	3.289021
H	1.325431	2.399063	1.501266
C	2.034518	-2.999505	0.847623
H	1.722299	-2.756208	-0.180460
H	1.470856	-3.883896	1.189069
H	3.090285	-3.318704	0.816025
C	1.656992	-1.770528	5.663614
H	1.983539	-0.974275	6.361319
H	2.281855	-2.667954	5.845711
H	0.614154	-2.041310	5.936751
C	4.486136	1.330280	0.571082
H	5.073223	0.786680	-0.194460
H	4.013523	0.579070	1.223147
H	5.201342	1.911964	1.184627
C	0.198327	2.656005	-2.067416
H	0.384607	2.811542	-3.150082
H	-0.581049	3.383756	-1.771838
H	-0.198759	1.640058	-1.940686
C	3.690200	6.014160	-0.916366
H	3.739980	6.478770	0.091453
H	3.032870	6.645739	-1.545016
H	4.715222	6.059276	-1.339229
Ni	0.253319	-2.268377	-2.655901
C	-1.236962	-3.231314	-2.974086
O	-2.006764	-3.964778	-3.450527
C	1.570688	-3.465213	-2.382943
O	2.334354	-4.340945	-2.478548
C	0.561000	-1.688005	-4.332664
O	0.708267	-1.631385	-5.488402

Ni(CO)₃-1Ph RI-BP86/SVP

76

E(SCF) =

Ni	-3957.428137		
Ni	-1.029749	2.119506	1.793701
C	-0.807390	2.016074	0.013976
O	-0.554647	2.128964	-1.117267
C	0.588333	2.003229	2.553669
O	1.683311	2.097766	2.942976
C	-1.696208	3.755306	2.120486
O	-2.004394	4.870778	2.256605
C	-2.396008	0.687400	2.563094
P	-1.922979	-0.178772	3.954435
C	-0.500125	-1.367123	3.781589

C	-3.236394	-1.153604	4.844872
C	-1.425470	0.955356	5.328832
P	-3.362095	0.082605	1.292793
C	-2.544342	-0.995126	0.009591
C	-4.114493	1.501386	0.374746
C	-4.846809	-0.969506	1.713511
C	-4.507841	-0.545338	4.980688
C	-5.527407	-1.164110	5.743401
C	-5.277992	-2.407695	6.386695
C	-3.999444	-3.013537	6.261778
C	-2.984693	-2.382649	5.498280
H	-4.712106	0.418889	4.499369
H	-6.510363	-0.683998	5.839897
H	-6.065591	-2.891645	6.980639
H	-3.794683	-3.968873	6.764032
H	-2.002325	-2.865274	5.435706
C	-0.818227	0.441729	6.500468
C	-0.547871	1.293503	7.599286
C	-0.898649	2.670399	7.535661
C	-1.528080	3.179178	6.367669
C	-1.791496	2.316643	5.273547
H	-0.556894	-0.620410	6.582957
H	-0.070791	0.891241	8.503289
H	-0.688121	3.334529	8.385412
H	-1.806497	4.240195	6.309873
H	-2.272255	2.709664	4.369299
C	0.826959	-0.991773	4.101496
C	1.911636	-1.865057	3.833173
C	1.676288	-3.133332	3.238588
C	0.345754	-3.511548	2.907045
C	-0.727047	-2.627190	3.171943
H	1.041422	-0.017358	4.555049
H	2.936172	-1.555454	4.081042
H	2.514334	-3.812880	3.030456
H	0.153607	-4.486057	2.437781
H	-1.740281	-2.936895	2.889674
C	-4.246794	1.530531	-1.031343
C	-4.877338	2.628967	-1.670470
C	-5.386825	3.707029	-0.898890
C	-5.248412	3.680222	0.516758
C	-4.611302	2.582178	1.143038
H	-3.840262	0.726217	-1.655143
H	-4.959521	2.651876	-2.765561
H	-5.869279	4.562317	-1.391943
H	-5.617044	4.520969	1.120055
H	-4.469754	2.588160	2.231418

C	-6.132444	-0.398523	1.865177
C	-7.244360	-1.201353	2.223703
C	-7.076036	-2.595533	2.439560
C	-5.786540	-3.174111	2.285811
C	-4.685516	-2.361396	1.922261
H	-6.294059	0.672438	1.691679
H	-8.238912	-0.746557	2.328132
H	-7.934755	-3.222055	2.717729
H	-5.646927	-4.251701	2.446653
H	-3.707168	-2.836339	1.785267
C	-3.301219	-1.684565	-0.971224
C	-2.661210	-2.528451	-1.911971
C	-1.249123	-2.694547	-1.872649
C	-0.491811	-2.016048	-0.880402
C	-1.143778	-1.172923	0.055182
H	-4.394265	-1.592070	-1.006900
H	-3.253947	-3.057430	-2.670841
H	-0.748228	-3.344953	-2.603223
H	0.598537	-2.141394	-0.837935
H	-0.551406	-0.652430	0.819570

Ni(CO)3-1THP RI-BP86/SVP

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E(SCF) =	-3839.967557		
C	0.038845	-0.265922	-0.044836
P	-1.571242	0.251153	-0.116192
P	1.486792	0.591355	0.106177
N	1.395392	2.319011	0.137463
C	1.001771	3.008106	-1.113305
C	1.397049	4.475792	-0.881332
C	2.635681	4.359396	0.019710
C	2.268040	3.195196	0.953812
H	-0.080026	2.880684	-1.312612
H	1.553967	2.595551	-1.990433
H	1.583518	5.018342	-1.829527
H	0.584761	5.011401	-0.345146
H	2.870709	5.290768	0.572959
H	3.526728	4.096912	-0.589303
H	1.716065	3.579269	1.845564
H	3.150959	2.641471	1.328888
N	2.433413	0.301639	1.512078
C	1.790963	0.548057	2.825136
C	2.344279	-0.548053	3.755793
C	3.691962	-0.907123	3.110827
C	3.382988	-0.832256	1.608915
H	0.682187	0.502184	2.736358

H	2.049312	1.563186	3.204779
H	2.435065	-0.203249	4.805104
H	1.678317	-1.433425	3.748035
H	4.069466	-1.905050	3.409913
H	4.465380	-0.156478	3.381338
H	2.928686	-1.781181	1.249227
H	4.295211	-0.650210	1.005091
N	2.607114	0.199123	-1.128998
C	3.913524	0.854865	-1.245388
C	4.679363	-0.062564	-2.221157
C	3.571178	-0.699297	-3.107734
C	2.232514	-0.232282	-2.482201
H	4.403957	0.957839	-0.257733
H	3.819618	1.884529	-1.675813
H	5.435770	0.499149	-2.804997
H	5.216104	-0.848244	-1.653359
H	3.642883	-1.803089	-3.089235
H	3.643862	-0.379324	-4.166274
H	1.461395	-1.023251	-2.426571
H	1.806756	0.611564	-3.078348
N	-2.577096	-0.386159	1.115836
C	-3.938088	0.130949	1.372420
C	-4.377212	-0.579470	2.667359
C	-3.047703	-0.827853	3.394955
C	-2.113187	-1.219461	2.242206
H	-4.638952	-0.077820	0.537214
H	-3.927505	1.236428	1.511533
H	-5.104374	0.021301	3.249430
H	-4.862103	-1.548713	2.425375
H	-3.109669	-1.611365	4.176092
H	-2.693035	0.107253	3.880145
H	-2.210562	-2.304412	2.012487
H	-1.044839	-1.027453	2.454593
N	-1.907040	1.938020	-0.029265
C	-2.760470	2.693747	-0.964194
C	-3.394254	3.784299	-0.084869
C	-2.287827	4.082654	0.940551
C	-1.661543	2.699876	1.211999
H	-3.509893	2.039909	-1.451229
H	-2.161023	3.163616	-1.784301
H	-3.706773	4.673860	-0.667930
H	-4.296374	3.385669	0.426154
H	-2.659624	4.568083	1.864800
H	-1.532021	4.762483	0.493101
H	-2.147200	2.201961	2.085162
H	-0.575583	2.764741	1.427413

N	-2.328369	-0.193416	-1.578816
C	-1.567889	-0.162788	-2.843197
C	-2.621189	-0.503274	-3.909770
C	-3.570860	-1.452300	-3.162193
C	-3.643619	-0.835266	-1.754094
H	-0.749617	-0.917900	-2.821589
H	-1.097731	0.828263	-3.020859
H	-3.162147	0.415285	-4.223859
H	-2.171016	-0.953340	-4.816869
H	-3.130642	-2.467671	-3.100102
H	-4.569317	-1.543182	-3.634563
H	-3.826108	-1.600597	-0.973271
H	-4.477306	-0.090759	-1.700795
Ni	0.253922	-2.388207	-0.053786
C	0.512239	-3.023191	1.600286
O	0.674691	-3.586229	2.609951
C	-1.249726	-3.125849	-0.684459
O	-2.157295	-3.767427	-1.041040
C	1.634595	-2.987410	-1.030272
O	2.488509	-3.571566	-1.569877

Ni(CO)₃-2Ad RI-BP86/SVP

64

E(SCF) =

	-2852.831762		
C	0.047131	5.234115	21.232628
N	-1.142901	5.199886	21.955760
N	-0.382062	5.221655	19.907759
Ni	1.968047	5.445988	21.948692
C	2.228591	7.221518	22.078548
C	2.366593	4.670856	23.527352
C	3.318016	4.726662	20.992846
O	4.337751	4.332966	20.589164
C	-2.243236	5.159286	21.106238
C	-1.769779	5.172840	19.831825
C	0.452168	5.219597	18.650275
C	1.412929	6.432357	18.626004
C	2.271599	6.411808	17.341696
C	3.074283	5.093104	17.272721
C	2.101149	3.892292	17.249835
C	1.237975	3.889762	18.532720
C	1.353682	6.521353	16.108007
C	0.384129	5.322171	16.102444
C	-0.461663	5.327118	17.397492
C	1.182346	4.004130	16.015757
C	-1.332768	5.166119	23.452618
C	-0.813545	3.824036	24.026376

C	-0.998045	3.793559	25.561307
C	-0.246920	4.981256	26.204934
C	-0.810907	6.311655	25.657156
C	-0.622366	6.364984	24.124714
C	-2.499943	3.897269	25.898146
C	-3.048597	5.227139	25.339287
C	-2.843187	5.264702	23.806574
C	-2.311777	6.412939	25.994003
O	2.445684	8.358756	22.180076
O	2.871162	4.243209	24.486683
H	-2.327675	5.155518	18.896765
H	-3.276106	5.128214	21.449762
H	0.814994	7.367926	18.681145
H	2.054124	6.405596	19.525778
H	2.971428	7.274043	17.369591
H	3.706390	5.082549	16.358465
H	3.762213	5.013751	18.138222
H	2.678446	2.944089	17.206681
H	1.866951	3.751315	19.431461
H	0.514021	3.046224	18.511215
H	-1.166067	4.469528	17.360919
H	-1.064872	6.259120	17.443813
H	-0.308320	5.400282	15.236807
H	1.955963	6.529970	15.173893
H	0.784944	7.476441	16.133447
H	1.784027	3.983384	15.081541
H	0.488522	3.136341	15.970808
H	-1.374728	2.989828	23.551580
H	0.250013	3.691841	23.754425
H	-0.588513	2.837068	25.950556
H	0.839334	4.906955	25.996527
H	-0.364766	4.946857	27.309688
H	-0.263197	7.164767	26.111384
H	0.450785	6.344197	23.862211
H	-1.039227	7.309411	23.712457
H	-3.270377	6.205034	23.396857
H	-3.400089	4.415890	23.356555
H	-4.138413	5.300266	25.543933
H	-2.466189	6.397728	27.094558
H	-2.726164	7.375856	25.623591
H	-3.054226	3.038236	25.460826
H	-2.654147	3.853262	26.997875

Ni(CO)3-2F RI-BP86/SVP

16

E(SCF) = -2272.500369

Ni	1.000059	0.002049	-0.003307
N	-1.839210	1.032656	-0.007584
C	1.557662	-0.142091	1.702348
O	1.940331	-0.234945	2.793866
C	1.578134	1.550895	-0.727006
O	2.007068	2.528264	-1.181644
C	1.552667	-1.419412	-0.966807
O	1.953611	-2.322004	-1.575565
N	-1.830845	-1.022444	-0.004922
C	-0.940859	0.008759	-0.012848
C	-3.178421	0.688574	0.000510
C	-3.172749	-0.689827	0.002209
F	-1.451034	2.334635	-0.008771
F	-1.430005	-2.320498	-0.003986
H	-3.990192	1.421079	0.003797
H	-3.978396	-1.429067	0.007484

Ni(CO)3-2H RI-BP86/SVP

16			
E(SCF) =	-2074.337580		
Ni	2.639567	4.870043	7.469446
N	3.138665	2.023512	8.320255
C	3.348932	5.382028	5.898580
O	3.806009	5.723740	4.885897
N	1.859792	2.099949	6.619582
C	0.965470	5.496785	7.659606
O	-0.113393	5.911583	7.783252
C	2.546071	2.922207	7.473773
C	2.838408	0.701057	8.011707
C	2.014815	0.750406	6.916514
H	3.735121	2.326688	9.090508
H	1.300562	2.474526	5.853015
H	3.224010	-0.149680	8.580506
H	1.539609	-0.048835	6.340838
C	3.676372	5.383036	8.843447
O	4.341872	5.745301	9.726630

Ni(CO)3-2Me RI-BP86/SVP

22			
E(SCF) =	-2152.898848		
Ni	2.668625	4.874694	7.455755
N	3.254088	2.013837	8.226846
C	3.902877	5.292191	6.217793
O	4.700281	5.562634	5.416302
N	1.694924	2.105072	6.736934
C	1.075732	5.606293	7.056763

O	0.069693	6.143000	6.825487
C	2.528132	2.910837	7.477868
C	2.873102	0.700061	7.973689
C	1.883877	0.757938	7.028315
C	4.296820	2.393952	9.171178
C	0.731834	2.602150	5.762731
H	3.336780	-0.156877	8.471421
H	1.315194	-0.038642	6.539294
C	3.144401	5.477812	9.081352
O	3.426473	5.934795	10.113448
H	0.428434	1.774350	5.095388
H	-0.166397	3.014226	6.263900
H	1.197354	3.406156	5.164461
H	4.934033	1.515621	9.383956
H	4.912722	3.198882	8.731144
H	3.860414	2.766026	10.119372

Ni(CO)3-2Me_ges RI-BP86/SVP

24

E(SCF) = -2154.096799

Ni	2.716340	4.856388	7.413583
N	3.361835	2.033783	8.047755
C	4.280105	5.213699	6.604355
O	5.273738	5.470191	6.057927
N	1.526569	2.122392	6.868550
C	1.427504	5.734729	6.517298
O	0.658608	6.417456	5.971544
C	2.501613	2.888339	7.429038
C	2.924855	0.630241	8.015236
C	1.763353	0.676157	7.011052
C	4.489752	2.403473	8.873517
C	0.457350	2.563726	6.002270
H	3.751498	-0.039577	7.698069
H	0.851137	0.156674	7.372082
C	2.658218	5.414925	9.121734
O	2.593783	5.809258	10.213524
H	0.624472	2.232765	4.952019
H	-0.515845	2.149097	6.342409
H	0.402821	3.664638	6.021173
H	5.398659	1.841579	8.568363
H	4.674882	3.485402	8.755674
H	4.294281	2.187686	9.948500
H	2.601021	0.303577	9.030442
H	2.031873	0.232638	6.024519

Ni(CO)3-2Mes RI-BP86/SVP

54

E(SCF) = -2771.851928

Ni	5.309226	6.072785	14.390234
N	2.645710	7.092664	15.377352
C	2.778686	6.486048	16.679640
O	6.996630	7.044816	16.617914
N	3.006317	7.740494	13.347680
O	4.904358	3.169849	14.792094
C	2.267394	5.183231	16.884162
O	6.860014	6.417923	11.888911
C	2.398293	4.621019	18.167981
H	2.012048	3.603106	18.339091
C	3.005291	5.316935	19.231338
C	3.472335	6.623474	18.990150
H	3.937103	7.191351	19.812394
C	3.366908	7.233958	17.726245
C	1.586129	4.426247	15.769492
H	2.226935	4.369649	14.867453
H	0.640436	4.920429	15.461108
H	1.342139	3.393734	16.082680
C	3.175021	4.669775	20.586443
H	4.143448	4.127547	20.646645
H	2.375158	3.930874	20.790969
H	3.170878	5.419553	21.402160
C	3.849023	8.647162	17.502681
H	4.371221	9.034166	18.397727
H	4.547174	8.705906	16.644300
H	3.005207	9.333578	17.277806
C	3.582990	7.011571	14.367201
C	1.531597	7.843533	14.997318
H	0.687472	8.014247	15.671879
C	1.759427	8.253756	13.712637
H	1.156772	8.857934	13.028184
C	3.593195	7.968210	12.050174
C	3.318699	7.056354	11.005145
C	3.875151	7.321914	9.740239
H	3.673572	6.617556	8.916866
C	4.684487	8.449481	9.501338
C	4.932361	9.330361	10.572082
H	5.568358	10.215231	10.407280
C	4.401073	9.112387	11.856549
C	2.490151	5.819577	11.253290
H	2.353412	5.237331	10.322601
H	2.987130	5.167256	12.001725
H	1.486209	6.064275	11.657821
C	5.306340	8.684626	8.144485

H	6.306631	8.204122	8.083059
H	4.688276	8.257465	7.330281
H	5.450158	9.764168	7.940640
C	4.714526	10.042592	13.002915
H	5.338596	10.892616	12.668216
H	3.795561	10.452936	13.470495
H	5.264938	9.499855	13.799868
C	6.308384	6.687958	15.750627
C	5.028986	4.315567	14.632545
C	6.196480	6.325877	12.838952

Ni(CO)3-2-tBu RI-BP86/SVP

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E(SCF) = -2388.592648

C	2.289052	2.788295	7.249443
N	1.526157	1.847609	6.565624
N	3.054091	2.010291	8.111758
Ni	2.127922	4.843819	7.193373
C	1.678872	5.593231	5.613129
C	3.605093	5.801277	7.595553
C	0.853179	5.231836	8.399250
O	0.036487	5.534088	9.169334
C	1.811691	0.557332	6.996066
C	2.766057	0.658960	7.961973
C	4.144596	2.478761	9.051534
C	3.563017	3.481299	10.064364
O	4.424070	6.598028	7.816642
C	0.563820	2.096065	5.423750
C	1.368595	2.634682	4.224030
O	1.407362	6.270791	4.706690
C	4.703639	1.284390	9.852530
C	5.293303	3.061956	8.204496
C	-0.555206	3.047741	5.882971
C	-0.102608	0.772391	4.994259
H	3.244096	-0.131514	8.540042
H	1.328247	-0.335586	6.600525
H	5.482298	1.670901	10.537985
H	5.186351	0.523853	9.207272
H	3.929215	0.794718	10.476132
H	6.075690	3.491682	8.860992
H	4.929434	3.853575	7.527203
H	5.755772	2.265380	7.587015
H	2.787493	2.993287	10.688755
H	3.102358	4.344404	9.555524
H	4.366914	3.848725	10.732436
H	-1.139559	2.588646	6.705934

H	-0.144704	4.005251	6.244818
H	-1.243704	3.251939	5.039200
H	0.624095	0.034004	4.601270
H	-0.686229	0.308122	5.814213
H	-0.810613	1.000070	4.174227
H	2.074215	1.861332	3.858385
H	1.952976	3.528501	4.502484
H	0.686780	2.904275	3.393249

M-Komplexe/XRay_Komplexe/BP86_TZ2P

Au2Cl2-1H.c2v BP86/TZ2P

13			
E(SCF) =	-1.788283		
C	0.000000	0.000000	0.884300
P	-1.507170	0.000000	1.772340
P	1.507170	0.000000	1.772340
H	-1.775280	1.110470	2.624750
H	-1.775280	-1.110470	2.624750
H	-2.596140	0.000000	0.881520
H	1.775280	1.110470	2.624750
H	2.596140	0.000000	0.881520
H	1.775280	-1.110470	2.624750
Au	0.000000	-1.794070	-0.162660
Cl	0.000000	-3.742760	-1.335950
Au	0.000000	1.794070	-0.162660
Cl	0.000000	3.742760	-1.335950

Au2Cl2-2H.c2v BP86/TZ2P

13			
E(SCF) =	-2.487890		
C	0.681373	0.000000	3.520840
C	-0.681373	0.000000	3.520840
N	-1.074304	0.000000	2.200316
C	0.000000	0.000000	1.334505
N	1.074304	0.000000	2.200316
Au	0.000000	-1.337778	-0.287232
Au	0.000000	1.337778	-0.287232
Cl	0.000000	3.306204	-1.410447
Cl	0.000000	-3.306204	-1.410447
H	-2.031108	0.000000	1.868734
H	2.031108	0.000000	1.868734
H	1.385372	0.000000	4.341073
H	-1.385372	0.000000	4.341073

(ReO3)+-1H.cs BP86/TZ2P

E(SCF) =	-2.318936		
Re	-0.148819	0.732692	0.000000
O	-1.062105	1.108847	1.404384
O	1.432259	1.418394	0.000000
O	-1.062105	1.108847	-1.404384
C	0.233251	-1.280508	0.000000
P	1.899743	-1.735795	0.000000
P	-1.070175	-2.408256	0.000000
H	-1.941874	-2.306176	1.113337
H	-0.629177	-3.753369	0.000000
H	-1.941874	-2.306176	-1.113337
H	2.648308	-1.284492	1.113642
H	2.648308	-1.284492	-1.113642
H	2.065387	-3.142372	0.000000

(ReO3)+-2H.cs BP86/TZ2P

13			
E(SCF) =	-3.007312		
Re	0.042663	-0.800793	0.000000
O	-0.707909	-1.407580	-1.413186
O	1.742365	-1.023178	0.000000
O	-0.707909	-1.407580	1.413186
C	-0.180041	1.288612	0.000000
N	0.835006	2.185324	0.000000
H	1.818847	1.923538	0.000000
N	-1.305437	2.039135	0.000000
H	-2.248915	1.657997	0.000000
C	-1.006792	3.379539	0.000000
H	-1.769814	4.147816	0.000000
C	0.360461	3.472365	0.000000
H	1.013304	4.336134	0.000000

W_(CO)2tpMod_1H.c BP86/TZ2P

40			
E(SCF) =	-9.063308		
C	0.176429	-2.272320	0.000000
P	1.880992	-2.581252	0.000000
P	-1.009309	-3.521572	0.000000
H	-0.552454	-4.878695	0.000000
H	-1.885450	-3.505260	1.110913
H	-1.885450	-3.505260	-1.110913
H	2.571026	-2.025862	1.107155
H	2.571026	-2.025862	-1.107155
H	2.309370	-3.936961	0.000000
W	-0.576399	-0.317535	0.000000
C	-2.058052	-0.719714	1.255685

O	-2.962692	-0.980117	1.948942
N	0.971776	0.306646	1.483783
C	1.288457	-0.152908	2.713934
C	2.300878	0.627469	3.279917
C	2.567177	1.606309	2.327958
N	1.767044	1.395410	1.258897
B	1.540056	2.260611	0.000000
N	1.767044	1.395410	-1.258897
N	0.971776	0.306646	-1.483783
C	1.288457	-0.152908	-2.713934
C	2.300878	0.627469	-3.279917
C	2.567177	1.606309	-2.327958
N	-0.963399	1.805068	0.000000
N	0.060508	2.724914	0.000000
C	-0.457720	3.966411	0.000001
C	-1.851872	3.877647	0.000001
C	-2.120657	2.514734	0.000001
C	-2.058052	-0.719714	-1.255685
O	-2.962692	-0.980117	-1.948942
H	2.276492	3.203986	0.000000
H	-2.562512	4.694363	0.000001
H	2.759835	0.514052	-4.253956
H	2.759835	0.514052	4.253956
H	0.192322	4.834261	0.000001
H	-3.069966	1.992975	0.000001
H	3.257823	2.441359	-2.343425
H	0.756813	-1.001827	-3.127945
H	3.257823	2.441359	2.343425
H	0.756812	-1.001827	3.127945

W_(CO)2tpMod_2H.a BP86/TZ2P

40

E(SCF) =	-9.758692		
C	-0.343418	2.293888	0.000000
N	0.261712	3.517617	0.000000
N	-1.667521	2.625026	0.000000
C	-1.877609	3.980395	0.000000
C	-0.632591	4.556301	0.000000
H	1.272828	3.613423	0.000000
H	-2.397302	1.918751	0.000000
H	-2.861616	4.430186	0.000000
H	-0.336300	5.596963	0.000000
W	0.577607	0.311669	0.000000
C	2.018428	0.898714	-1.233183
O	2.901906	1.267199	-1.900643
C	2.018428	0.898714	1.233183

O	2.901906	1.267199	1.900643
N	-0.929747	-0.369020	1.472806
C	-1.305239	0.088424	2.687033
C	-2.264480	-0.756527	3.249923
C	-2.435974	-1.772704	2.314591
N	-1.635534	-1.522059	1.255221
N	-0.929747	-0.369020	-1.472806
N	-1.635534	-1.522059	-1.255221
C	-2.435974	-1.772704	-2.314591
C	-2.264480	-0.756526	-3.249923
C	-1.305239	0.088424	-2.687033
N	1.132131	-1.728303	0.000000
N	0.174041	-2.723894	0.000000
C	0.782269	-3.918635	0.000000
C	2.171932	-3.729711	0.000000
C	2.342598	-2.356416	0.000000
B	-1.342943	-2.368316	0.000000
H	-1.999151	-3.368912	0.000000
H	2.937276	-4.495564	0.000000
H	-2.751594	-0.658686	-4.211874
H	-2.751594	-0.658687	4.211874
H	0.200002	-4.833777	0.000000
H	3.249701	-1.764747	0.000000
H	-3.057817	-2.660183	-2.337922
H	-0.857042	0.988680	-3.090603
H	-3.057817	-2.660184	2.337922
H	-0.857042	0.988680	3.090603

	WO3_1H.cs	BP86/TZ2P	
13			
E(SCF) =	-2.598092		
W	-0.524111	-0.554100	0.000000
O	-1.814812	0.674559	0.000000
O	-0.435214	-1.533710	1.451503
O	-0.435214	-1.533710	-1.451503
C	1.034809	0.901500	0.000000
P	0.277964	2.425421	0.000000
H	-0.538395	2.745753	1.108120
H	-0.538395	2.745753	-1.108120
H	1.229173	3.491379	0.000000
P	2.681548	0.571665	0.000000
H	3.539953	1.704504	0.000000
H	3.174166	-0.192388	-1.092863
H	3.174166	-0.192388	1.092863

M-Komplexe/XRay_Komplexe/RI-BP86_SVP

	Ag-1H_2	RI-BP86/SVP	
19			
E(SCF) =	-1595.236931		
C	-0.126477	2.097135	-0.018550
P	-1.061252	2.898294	1.154522
H	-1.317000	4.291979	0.916206
H	-0.651494	2.948984	2.537049
H	-2.371176	2.355352	1.311215
P	1.015101	2.963776	-0.934667
H	0.730897	4.356370	-1.145405
H	1.180198	2.466397	-2.261401
H	2.397516	3.045444	-0.530227
Ag	-0.000015	-0.000068	0.028752
C	0.126362	-2.097212	-0.021411
P	-1.016212	-2.962612	-0.937430
H	-2.398252	-3.044440	-0.531763
H	-0.732457	-4.355025	-1.149945
H	-1.182494	-2.463768	-2.263473
P	1.062541	-2.899804	1.149534
H	0.654564	-2.951882	2.532530
H	2.372786	-2.357306	1.305134
H	1.317689	-4.293280	0.909364

	Ag-1Ph_2	RI-BP86/SVP	
139			
E(SCF) =	-4365.333380		
Ag	6.188986	10.961201	0.107218
C	7.347175	9.256765	-0.474775
P	8.035664	8.263697	0.742449
P	7.261481	8.840029	-2.138662
C	4.977209	12.611123	0.722155
P	5.646095	14.033437	1.403143
P	3.301679	12.434620	0.388454
C	7.444916	8.725942	2.432871
C	9.876459	8.396023	0.949929
C	7.690180	6.446832	0.617979
C	8.529495	7.670964	-2.821994
C	7.470096	10.350538	-3.192818
C	5.648575	8.104270	-2.704674
C	2.834580	12.472938	-1.414168
C	2.663416	10.796820	0.983179
C	4.835873	14.596755	2.970104
C	5.768826	15.538155	0.317162
C	2.147491	13.667814	1.143630
C	7.425338	13.802356	1.854324
C	8.331330	13.440495	0.827350

C	9.714398	13.306643	1.101192
C	10.204865	13.544531	2.415944
C	9.298785	13.923544	3.441239
C	7.914364	14.054968	3.155471
C	8.693901	5.457211	0.735420
C	10.646576	9.005390	-0.063520
C	8.363784	4.082783	0.617839
C	7.018194	3.689881	0.382868
C	6.008191	4.685003	0.261783
C	6.348639	6.054681	0.376830
C	7.746319	10.021413	2.922140
C	7.366344	10.397675	4.234096
C	6.678721	9.474700	5.070829
C	6.380049	8.176191	4.579917
C	6.768212	7.806406	3.265883
C	12.051916	9.134954	0.077660
C	12.692245	8.656723	1.252480
C	11.914686	8.054792	2.281449
C	10.512491	7.928023	2.127235
C	6.980776	10.399950	-4.519371
C	7.231920	11.532922	-5.333980
C	7.980710	12.627713	-4.821305
C	8.471091	12.578037	-3.487491
C	8.213189	11.439717	-2.682721
C	5.551431	7.323660	-3.883977
C	4.301770	6.795738	-4.293915
C	3.133654	7.050465	-3.523978
C	3.231412	7.834834	-2.342469
C	4.486525	8.354317	-1.940315
C	9.680319	8.174921	-3.477791
C	10.672083	7.293684	-3.974870
C	10.518116	5.888981	-3.819273
C	9.362518	5.381002	-3.165518
C	8.375914	6.269941	-2.671304
C	4.357498	15.910452	3.177331
C	3.749702	16.266159	4.408949
C	3.621352	15.303431	5.445670
C	4.093511	13.977833	5.233681
C	4.690789	13.630958	3.998381
C	5.222941	15.491928	-0.984232
C	5.345577	16.602831	-1.858156
C	6.027030	17.771920	-1.425752
C	6.593059	17.813078	-0.120090
C	6.466503	16.697084	0.742420
C	3.815946	12.172952	-2.385959
C	3.493110	12.180335	-3.765550

C	2.171669	12.492740	-4.184991
C	1.182730	12.797961	-3.209914
C	1.516439	12.786628	-1.832940
C	3.395421	10.090731	1.963686
C	2.900892	8.871632	2.493520
C	1.659493	8.351306	2.037410
C	0.924895	9.059657	1.046218
C	1.428957	10.276845	0.524137
C	1.972362	14.939581	0.542636
C	1.111971	15.899478	1.129568
C	0.417581	15.591677	2.331759
C	0.597984	14.318759	2.938437
C	1.460751	13.364379	2.343485
H	5.558700	6.809686	0.264104
H	4.966221	4.389327	0.076033
H	6.759715	2.624957	0.293718
H	9.149565	3.319773	0.707087
H	9.742366	5.732618	0.901626
H	6.542422	6.790518	2.919756
H	5.864452	7.451142	5.225057
H	6.395139	9.758449	6.094284
H	7.622724	11.397920	4.608772
H	8.294765	10.746496	2.304824
H	9.931862	7.478758	2.943639
H	12.404110	7.694456	3.197118
H	13.780846	8.755653	1.369716
H	12.647417	9.604535	-0.717206
H	10.156056	9.390696	-0.965404
H	8.583936	11.401410	-1.648761
H	9.048375	13.422782	-3.087125
H	8.179080	13.506057	-5.452035
H	6.853671	11.564676	-6.365395
H	6.397564	9.571095	-4.939051
H	4.552138	8.954885	-1.019796
H	2.335568	8.039075	-1.740059
H	2.163415	6.641651	-3.840229
H	4.234028	6.185680	-5.205624
H	6.437928	7.098680	-4.490190
H	7.491264	5.847221	-2.179700
H	9.232046	4.296562	-3.046949
H	11.283038	5.201365	-4.207396
H	11.557055	7.693926	-4.488742
H	9.814967	9.253029	-3.631098
H	5.033775	12.598712	3.841978
H	3.988242	13.226144	6.028152
H	3.153937	15.578727	6.401841

H	3.373614	17.287267	4.560619
H	4.431313	16.670666	2.390828
H	6.937493	16.743161	1.733001
H	7.135514	18.709222	0.212532
H	6.127253	18.636040	-2.097961
H	4.922160	16.557662	-2.871184
H	4.724245	14.580812	-1.342267
H	7.239537	14.364881	3.962764
H	9.672459	14.124420	4.455004
H	11.277924	13.445580	2.632796
H	10.413757	13.029887	0.300924
H	7.971256	13.275805	-0.197146
H	0.737110	13.047565	-1.106170
H	0.160370	13.047835	-3.526700
H	1.915685	12.502556	-5.254010
H	4.267531	11.946633	-4.508844
H	4.846302	11.938697	-2.075911
H	2.487833	15.202120	-0.389137
H	0.975594	16.880468	0.653446
H	-0.256027	16.331377	2.787262
H	0.065117	14.074304	3.867589
H	1.579019	12.387100	2.827664
H	0.842991	10.798570	-0.241987
H	-0.036649	8.663819	0.690372
H	1.267762	7.409420	2.447256
H	3.478750	8.332734	3.256765
H	4.360848	10.484139	2.312954

Ag-(H+)-1H_2 RI-BP86/SVP

21			
E(SCF) =	-1595.679155		
C	-0.386064	2.194013	-0.257222
P	-1.030032	2.942498	1.269051
H	-1.422738	4.314417	1.175801
H	-0.097310	2.878177	2.340035
H	-2.189796	2.231264	1.676073
P	0.966225	3.091934	-1.079194
H	0.724599	4.475805	-1.346612
H	1.219482	2.488098	-2.339408
H	2.177840	3.044555	-0.336934
Ag	-0.000358	0.000044	-0.113297
H	-1.237138	2.207839	-0.978874
C	0.385846	-2.193566	-0.260784
H	1.236312	-2.206175	-0.983161
P	-0.966998	-3.090608	-1.082878
H	-2.177960	-3.044522	-0.339474

H	-0.725346	-4.474052	-1.352476
H	-1.221478	-2.485007	-2.342001
P	1.031024	-2.944117	1.263967
H	0.099063	-2.881416	2.335713
H	2.190992	-2.233329	1.671178
H	1.423834	-4.315854	1.168497

Ag-(H+)-1Ph_2 RI-BP86/SVP

141

E(SCF) =	-4365.970273		
Ag	-0.001283	0.003596	-0.000340
C	-1.174006	-1.492650	1.173302
H	-1.293885	-2.267414	0.385115
P	-2.879187	-1.003445	1.618180
P	-0.070545	-2.288106	2.398822
C	-3.944384	-2.397331	2.141884
C	-3.720425	-0.367241	0.121600
C	-2.924143	0.300360	2.889535
C	-0.790027	-3.598671	3.465633
C	1.227130	-3.113398	1.401072
C	0.665171	-1.098692	3.571994
P	2.877714	1.005738	-1.618174
C	1.173085	1.498071	-1.174737
H	1.294449	2.274736	-0.388573
P	0.072468	2.291058	-2.403148
C	-1.230316	3.113524	-1.410848
C	-1.366568	1.609819	-4.697272
C	0.794277	3.604327	-3.464434
C	3.945491	2.397390	-2.143195
C	2.921098	-0.299350	-2.888048
C	3.717598	0.370939	-0.120228
C	4.889770	-0.407300	-0.300417
C	5.710889	-0.722059	0.810734
C	5.365736	-0.251065	2.109143
C	4.185916	0.523588	2.284336
C	3.366781	0.835331	1.169692
C	-1.429000	-3.225220	4.677753
C	-1.987243	-4.213358	5.524220
C	-1.904277	-5.589115	5.165654
C	-1.250728	-5.961866	3.957629
C	-0.696400	-4.968700	3.111617
C	0.853680	-3.956730	0.320387
C	1.828133	-4.743427	-0.340905
C	3.189457	-4.688529	0.073398
C	3.563201	-3.826259	1.140743
C	2.582670	-3.042923	1.803175

C	1.382403	-1.623310	4.681842
C	1.953797	-0.747312	5.637475
C	1.796075	0.661360	5.497738
C	1.073804	1.181334	4.388143
C	0.518002	0.300776	3.426912
C	-5.161193	-2.129838	2.823873
C	-6.077038	-3.180431	3.078007
C	-5.789347	-4.502910	2.635515
C	-4.578042	-4.761994	1.935072
C	-3.662245	-3.709505	1.688500
C	-4.890171	0.414275	0.303132
C	-5.712944	0.729395	-0.806716
C	-5.371815	0.255636	-2.105148
C	-4.194166	-0.522030	-2.281798
C	-3.373419	-0.834256	-1.168459
C	-3.169410	-0.015743	4.249464
C	-3.192833	1.012137	5.225627
C	-2.972375	2.363965	4.840970
C	-2.728151	2.676416	3.473126
C	-2.703644	1.647218	2.501024
C	1.426497	3.235791	-4.681835
C	1.986599	4.226672	-5.523934
C	1.912426	5.600322	-5.155959
C	1.265877	5.968451	-3.942619
C	0.709637	4.972717	-3.101015
C	-0.865341	3.952069	-0.323540
C	-1.844614	4.736397	0.333396
C	-3.202745	4.683620	-0.091444
C	-3.568442	3.826142	-1.165422
C	-2.582920	3.045539	-1.823635
C	-1.932967	0.733212	-5.639844
C	-1.786083	-0.672677	-5.486932
C	-1.075119	-1.191818	-4.369907
C	-0.518228	-0.304750	-3.411813
C	-0.657350	1.100104	-3.574710
C	5.157987	2.128399	-2.832156
C	6.076246	3.176842	-3.086624
C	5.795339	4.498537	-2.637577
C	4.588342	4.759053	-1.930215
C	3.670104	3.708787	-1.683291
C	3.159304	0.016516	-4.249334
C	3.181577	-1.011989	-5.224833
C	2.966828	-2.364182	-4.838215
C	2.729231	-2.676279	-3.469160
C	2.705771	-1.646445	-2.497658
H	-0.171707	-5.300347	2.207963

H	-1.160528	-7.025680	3.692005
H	-2.326070	-6.360767	5.828246
H	-2.469273	-3.926443	6.470535
H	-1.468038	-2.178936	5.003281
H	2.903642	-2.395108	2.628148
H	4.612109	-3.783586	1.467627
H	3.945210	-5.321038	-0.417355
H	1.530648	-5.423835	-1.152546
H	-0.187929	-4.046984	-0.015663
H	-0.049823	0.726284	2.588683
H	0.934160	2.267272	4.293049
H	2.219642	1.340358	6.254217
H	2.504490	-1.155004	6.498796
H	1.492061	-2.704871	4.838669
H	-2.745725	-3.945774	1.136755
H	-4.360886	-5.780789	1.583084
H	-6.504937	-5.317501	2.826334
H	-7.018123	-2.974813	3.609852
H	-5.432228	-1.121265	3.158214
H	-2.488461	-1.459484	-1.340123
H	-3.932979	-0.898724	-3.280835
H	-6.027102	0.473977	-2.962286
H	-6.629936	1.320049	-0.661565
H	-5.194336	0.777893	1.292740
H	-2.539990	1.920468	1.448905
H	-2.580672	3.723313	3.173757
H	-3.007698	3.164665	5.595945
H	-3.397746	0.770733	6.279362
H	-3.371750	-1.044275	4.570740
H	0.190447	5.301073	-2.192959
H	1.182787	7.030942	-3.669469
H	2.335619	6.374200	-5.815076
H	2.463442	3.943450	-6.473999
H	1.458984	2.191557	-5.014656
H	-2.897344	2.401472	-2.654522
H	-4.614828	3.785156	-1.500512
H	-3.962125	5.314051	0.396395
H	-1.553204	5.413634	1.149856
H	0.173641	4.040283	0.021223
H	0.045483	-0.719149	-2.564343
H	-0.942908	-2.277885	-4.263472
H	-2.208496	-1.357952	-6.238301
H	-2.476738	1.126831	-6.509344
H	-1.462973	2.690547	-4.855826
H	2.757394	3.945968	-1.125544
H	4.376563	5.777155	-1.572970

H	6.512881	5.311370	-2.828562
H	7.014013	2.970041	-3.623846
H	5.423827	1.120241	-3.171842
H	2.479904	1.458181	1.340090
H	3.921939	0.898282	3.283397
H	6.019650	-0.469155	2.967403
H	6.629710	-1.310162	0.666735
H	5.197138	-0.768409	-1.289967
H	2.546847	-1.919394	-1.444773
H	2.585699	-3.723310	-3.168335
H	3.001230	-3.165352	-5.592721
H	3.381099	-0.770778	-6.279635
H	3.356760	1.045481	-4.572278

(AuCl)₂-1H RI-BP86/SVP

13			
E(SCF) =	-1916.303040		
C	0.007137	0.015247	1.079707
P	-0.793568	-1.397276	1.781227
P	0.075678	0.121461	-0.684374
H	-0.235018	-2.687883	1.494655
H	-2.184779	-1.587407	1.484561
H	-0.757356	-1.320233	3.194794
H	0.780315	-0.913964	-1.385246
H	0.746362	1.307215	-1.071008
H	-1.169719	0.185908	-1.394779
Au	-1.100782	1.668846	1.711356
Cl	-2.305924	3.502317	2.424496
Au	1.990858	-0.073089	1.726357
Cl	4.178866	-0.148993	2.454824

(AuCl)₂-2H RI-BP86/SVP

13			
E(SCF) =	-1418.203903		
C	-0.428409	-0.961700	-1.199773
C	-0.823737	-1.537598	-0.014528
N	-0.371967	-0.710082	0.993828
C	0.307381	0.390810	0.501586
N	0.248534	0.195146	-0.867585
Au	-0.172526	2.307056	1.270871
Au	2.172586	0.898196	1.372102
Cl	4.368698	0.736928	2.033015
Cl	-1.378325	4.196677	1.782773
H	-0.503516	-0.859585	1.996022
H	0.670248	0.853375	-1.525854
H	-0.577519	-1.285627	-2.233692

H	-1.381686	-2.457907	0.179351
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(AuCl) 2-1Ph	RI-BP86/SVP
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73

E(SCF) =	-3301.350151
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C	3.421696	5.420471	6.301712
P	5.213711	5.461722	6.474650
P	2.648191	4.106997	5.342886
C	5.771626	6.871710	7.530192
C	5.887088	3.959273	7.309360
C	6.228076	5.684378	4.934664
C	2.831161	2.363033	5.955726
C	0.814545	4.312020	5.248884
C	3.206491	4.082783	3.583528
Au	2.705701	5.427192	8.282477
Au	2.714808	7.195305	5.414764
Cl	1.872876	9.156335	4.478726
Cl	1.914455	5.508008	10.473352
C	2.708112	1.271064	5.057514
H	2.595281	1.427590	3.979091
C	2.716998	-0.060664	5.538600
H	2.618020	-0.898438	4.834635
C	2.839797	-0.315187	6.931774
H	2.837799	-1.347502	7.309234
C	2.949920	0.778176	7.832085
H	3.030136	0.598989	8.912853
C	2.942739	2.107117	7.342449
H	3.003573	2.938147	8.063293
C	0.084460	5.165430	6.105274
H	0.591859	5.791675	6.852775
C	-1.329370	5.227516	6.015719
H	-1.884300	5.898521	6.685344
C	-2.020964	4.432580	5.063455
H	-3.116477	4.482744	4.991000
C	-1.283945	3.572832	4.203118
H	-1.809466	2.956274	3.461219
C	0.127319	3.513577	4.300360
H	0.665523	2.844116	3.619534
C	4.285896	3.270903	3.159823
H	4.782876	2.583799	3.853651
C	4.742830	3.325007	1.819582
H	5.581900	2.693297	1.497880
C	4.120735	4.203548	0.891808
H	4.472861	4.249727	-0.148328
C	3.043481	5.027581	1.319932
H	2.562323	5.718738	0.614164

C	2.593509	4.966999	2.661563
H	1.771714	5.626700	2.973774
C	7.564230	5.209771	4.876655
H	7.999572	4.625382	5.694613
C	8.379791	5.491969	3.753836
H	9.413746	5.121729	3.720657
C	7.867904	6.264488	2.676077
H	8.501213	6.492521	1.807130
C	6.534688	6.751269	2.740332
H	6.128999	7.362639	1.922860
C	5.724891	6.462616	3.865672
H	4.702959	6.872690	3.903082
C	6.318398	2.831230	6.570789
H	6.321304	2.840046	5.475279
C	6.763554	1.662998	7.237886
H	7.095817	0.790857	6.658599
C	6.771492	1.615212	8.658214
H	7.114262	0.710433	9.179648
C	6.326225	2.743685	9.400550
H	6.316479	2.713647	10.498858
C	5.883996	3.907667	8.725261
H	5.527940	4.760515	9.319952
C	4.934037	7.946843	7.900113
H	3.876462	7.973584	7.602036
C	5.449645	9.022378	8.667343
H	4.786302	9.850915	8.950323
C	6.811495	9.024927	9.069936
H	7.211221	9.856799	9.666700
C	7.653544	7.941657	8.695242
H	8.707944	7.933517	9.003341
C	7.132755	6.872970	7.926394
H	7.807612	6.052711	7.655707

	(ReO3)+-1H	RI-BP86/SVP	
13			
E(SCF) =	-1027.978830		
C	0.354482	2.071805	1.164235
P	1.713532	3.147752	0.962285
H	2.701615	2.802141	-0.013297
H	2.454332	3.281348	2.170192
H	1.314071	4.463043	0.580614
P	-1.180616	2.334359	0.376691
H	-1.390413	3.702838	0.032621
H	-2.265156	1.953629	1.216240
H	-1.430489	1.638525	-0.848393
Re	0.610123	0.355379	2.263470

O	1.827308	0.770237	3.436568
O	1.153439	-0.931614	1.229636
O	-0.972098	0.013638	2.903869

	(ReO3)+-1Ph	RI-BP86/SVP	
73			
E(SCF) =	-2413.071648		
C	3.557294	8.945825	2.620813
P	4.912822	8.399210	1.605669
P	2.209043	9.963066	2.037564
C	0.675550	9.013911	1.673347
C	1.804339	11.230507	3.302142
C	2.567441	10.896024	0.491968
C	6.172597	9.686073	1.261605
C	5.861318	7.088399	2.468799
C	4.328459	7.683727	0.021221
Re	3.469827	8.266345	4.549684
O	4.798082	8.926974	5.473922
O	3.550384	6.522976	4.554753
O	1.936624	8.806245	5.169897
C	6.791232	7.475915	3.467887
C	7.533676	6.490228	4.163850
C	7.351290	5.113035	3.856519
C	6.425006	4.732389	2.845925
C	5.680788	5.720220	2.154182
C	7.399045	9.295233	0.661597
C	8.409406	10.257691	0.422594
C	8.203141	11.616328	0.796704
C	6.982274	11.998088	1.415923
C	5.972223	11.029683	1.646204
C	4.959694	7.973312	-1.211989
C	4.507047	7.352744	-2.403696
C	3.417043	6.439613	-2.364362
C	2.780125	6.156669	-1.123438
C	3.236615	6.779297	0.064153
C	-0.314021	9.585890	0.831475
C	-1.529587	8.898767	0.592103
C	-1.764017	7.632325	1.196777
C	-0.770059	7.061396	2.038478
C	0.444141	7.753336	2.272163
C	2.836142	11.783703	4.100531
C	2.540633	12.801112	5.040734
C	1.204525	13.267591	5.187900
C	0.171371	12.703260	4.389786
C	0.473022	11.686516	3.448597
C	2.916777	12.268227	0.563689

C	3.145424	13.010419	-0.621201
C	3.020247	12.381272	-1.890724
C	2.657761	11.007496	-1.961126
C	2.430789	10.269873	-0.773341
H	6.954560	8.530162	3.725564
H	8.245921	6.790247	4.945430
H	7.923643	4.345880	4.398462
H	6.284288	3.669341	2.604757
H	4.977970	5.394817	1.378688
H	5.045863	11.337423	2.140855
H	6.828518	13.041933	1.723182
H	8.991304	12.362805	0.619563
H	9.360589	9.955110	-0.038482
H	7.601870	8.247819	0.401445
H	2.725741	6.551983	1.009113
H	1.936672	5.452377	-1.087857
H	3.068865	5.953710	-3.287790
H	4.999723	7.576486	-3.360625
H	5.789868	8.686803	-1.276426
H	1.185883	7.285903	2.932878
H	-0.946850	6.086287	2.514204
H	-2.709013	7.099157	1.015862
H	-2.294071	9.344164	-0.060567
H	-0.160218	10.557511	0.345069
H	-0.349843	11.254294	2.866657
H	-0.865797	13.045619	4.514128
H	0.969123	14.048110	5.926195
H	3.339311	13.215936	5.672026
H	3.869654	11.418866	4.037352
H	2.129944	9.218878	-0.860762
H	2.542819	10.520905	-2.939830
H	3.189380	12.957392	-2.812382
H	3.406288	14.076552	-0.561117
H	2.987481	12.788672	1.527129

W_(CO)2-tp_1Me RI-BP86/SVP

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E(SCF) = -2191.305157

C	-3.447147	1.495656	7.206871
P	-2.544551	-0.000345	7.616838
P	-4.766858	1.892777	8.354642
C	-1.361476	0.186542	9.014923
C	-1.512820	-0.680429	6.278027
C	-3.601479	-1.445273	8.068594
C	-4.480174	1.448328	10.129756
C	-5.194987	3.660359	8.497675

C	-6.355816	1.077527	7.923769
W	-3.148774	2.629516	5.439947
C	-5.075225	3.024494	5.231462
O	-6.217099	3.330777	5.155643
C	-3.237108	4.433036	6.283637
O	-3.318311	5.531143	6.701318
N	-0.878067	2.489093	5.568171
N	-0.159992	1.975238	4.518823
N	-1.570589	3.063876	2.737192
N	-2.569743	3.611194	3.513826
N	-3.070245	0.852232	4.043757
N	-1.960645	0.639676	3.267168
B	-0.873331	1.742683	3.159099
H	-0.054365	1.420750	2.325415
C	1.178296	1.998774	4.803126
C	1.318358	2.547703	6.084500
C	0.013652	2.865731	6.522741
C	-3.009806	4.735318	2.865523
C	-2.276821	4.892196	1.676763
C	-1.373856	3.819908	1.621315
C	-2.111885	-0.496027	2.523652
C	-3.369331	-1.032052	2.838152
C	-3.949149	-0.150743	3.774834
C	-0.380173	3.578158	7.781189
C	2.240531	1.530404	3.857384
C	-4.096895	5.632472	3.366607
C	-0.363265	3.505943	0.563014
C	-1.093055	-1.001147	1.549453
C	-5.311509	-0.234120	4.388101
H	-3.626565	2.034283	10.522914
H	-4.281005	0.371070	10.275876
H	-5.383191	1.713223	10.714151
H	-4.302732	4.255572	8.761540
H	-5.949250	3.747516	9.304867
H	-5.625194	4.041407	7.555568
H	-6.669560	1.430507	6.923089
H	-6.242116	-0.022279	7.905803
H	-7.133085	1.351244	8.664585
H	-0.568318	0.894199	8.707490
H	-0.900264	-0.793488	9.249150
H	-1.859747	0.577551	9.919833
H	-0.820599	0.087722	5.892621
H	-2.149336	-1.046928	5.451608
H	-0.937166	-1.524481	6.705998
H	-2.954830	-2.322341	8.269498
H	-4.267239	-1.683434	7.216675

H	-4.217536	-1.254112	8.966303
H	3.225358	1.555395	4.359056
H	2.304553	2.175833	2.957794
H	2.060310	0.495305	3.505292
H	0.442926	3.545375	8.519903
H	-1.295216	3.149699	8.232642
H	-0.599438	4.646095	7.573066
H	-0.095458	-1.127138	2.014885
H	-0.968803	-0.311589	0.689919
H	-1.411695	-1.981684	1.150407
H	-5.265700	-0.202508	5.494344
H	-5.816013	-1.168088	4.078333
H	-5.944547	0.619942	4.072838
H	0.667109	3.475808	0.970772
H	-0.394973	4.281136	-0.224174
H	-0.556918	2.525266	0.083677
H	-3.798780	6.167232	4.290235
H	-5.026209	5.075383	3.592035
H	-4.330293	6.392377	2.598217
H	-2.389133	5.691236	0.936775
H	-3.820179	-1.935592	2.414475
H	2.256361	2.722776	6.621910

W_(CO)2tpMod_1HRI-BP86/SVP

40

E(SCF) =	-1719.762354		
C	-0.009863	2.690370	6.557380
N	-0.900315	2.416539	5.571401
N	-0.180458	1.983612	4.497739
C	1.143896	1.977268	4.799872
W	-3.139735	2.659576	5.444432
C	-3.417816	1.527401	7.181279
P	-4.610402	2.097261	8.314277
N	-1.622161	3.031740	2.722889
N	-2.583923	3.584584	3.528495
C	-3.032072	4.705129	2.898390
C	-1.472234	3.790295	1.612796
N	-2.995909	0.796059	4.180562
N	-1.954788	0.611095	3.320215
C	-2.122080	-0.548487	2.632786
C	-3.829195	-0.262641	4.023007
C	-5.095424	3.028802	5.203335
O	-6.237149	3.278100	5.102434
C	-3.301493	4.417480	6.394805
O	-3.448477	5.437766	6.954527
P	-2.463755	0.082753	7.426535

B	-0.887307	1.723563	3.140336
H	-0.076928	1.402512	2.293417
C	-2.358810	4.876970	1.683090
H	-2.490331	5.677323	0.948641
C	-3.311139	-1.149777	3.060864
H	-3.749508	-2.087468	2.705640
C	1.299344	2.415188	6.119974
H	2.233974	2.538877	6.675651
H	-0.745121	3.511540	0.841402
H	-3.813347	5.316739	3.363608
H	-1.391715	-0.859476	1.877568
H	-4.766265	-0.313343	4.590664
H	1.885194	1.674934	4.051791
H	-0.358365	3.094329	7.515688
H	-5.925334	2.196484	7.774785
H	-4.358522	3.407059	8.815074
H	-4.828315	1.341116	9.522191
H	-2.623554	-0.885512	6.390376
H	-1.057444	0.325645	7.429947
H	-2.668974	-0.678646	8.622849

W3-2H

RI-BP86/SVP

18

E(SCF) =	-746.416930		
W	-0.425790	0.971251	3.050979
C	-1.650793	2.111312	4.053160
O	-2.384290	2.826759	4.628917
C	1.145800	1.738907	4.130555
O	2.020444	2.197615	4.758618
C	-0.630813	-0.514348	4.431415
O	-0.721437	-1.388352	5.202564
C	-2.020817	0.206453	2.004753
O	-2.947648	-0.206158	1.421062
C	0.040914	2.347691	1.356891
N	1.045550	3.279267	1.248901
H	1.702325	3.447060	2.013303
N	-0.594943	2.475090	0.145132
H	-1.418954	1.917322	-0.086649
C	1.028666	3.960208	0.043110
H	1.748855	4.742174	-0.214033
C	-0.027731	3.442318	-0.667716
H	-0.406658	3.685292	-1.664532

W4-2H

RI-BP86/SVP

20

E(SCF) =	-859.718495
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W	-0.297692	0.830389	3.017770
C	-1.606456	2.181442	3.890481
O	-2.341406	2.939358	4.378997
C	1.264378	1.647688	4.091312
O	2.151269	2.120072	4.685027
C	-0.647534	-0.517928	4.527186
O	-0.846644	-1.283276	5.383042
C	-1.855406	0.029435	1.926180
O	-2.734245	-0.411566	1.297279
C	0.081705	2.306371	1.363400
N	1.058632	3.262358	1.269229
H	1.754624	3.393983	2.004627
N	-0.606840	2.481430	0.191853
H	-1.416249	1.906716	-0.047063
C	0.985381	4.000804	0.095215
H	1.683973	4.805888	-0.148917
C	-0.086237	3.498355	-0.597986
H	-0.508522	3.777872	-1.567193
C	1.018722	-0.492415	2.113358
O	1.757410	-1.234869	1.607104

Zr1-2H

RI-BP86/SVP

14

E(SCF) =	-2113.961152		
Zr	-0.000282	-0.001074	1.270473
Cl	1.684679	-1.130830	2.508018
Cl	1.341540	2.008762	0.782005
Cl	-1.682507	1.125532	2.514912
Cl	-1.344646	-2.008686	0.779798
C	-0.000185	0.000154	-1.099187
N	0.592269	0.889634	-1.939117
H	1.119677	1.681044	-1.538223
N	-0.592229	-0.888708	-1.940060
H	-1.119965	-1.680322	-1.539997
C	-0.382189	-0.573336	-3.266545
H	-0.779048	-1.169226	-4.093687
C	0.382833	0.575264	-3.265936
H	0.780053	1.171791	-4.092445

M-Komplexe/XRay_Komplexe/RI-BP86_TZVP (AuCl)2-1Ph RI-BP86/TZVP

73

E(SCF) =	-3301.726839		
C	3.426039	5.406459	6.303559
P	5.219575	5.444368	6.483646
P	2.655544	4.100486	5.328126

C	5.771640	6.875747	7.512472
C	5.874470	3.952805	7.350804
C	6.226856	5.642285	4.937164
C	2.853843	2.355050	5.928424
C	0.820963	4.301222	5.252444
C	3.211298	4.115211	3.568442
Au	2.697314	5.387215	8.280724
Au	2.738689	7.192561	5.420660
Cl	1.911522	9.168966	4.499202
Cl	1.887826	5.449052	10.467919
C	2.801492	1.267019	5.025292
H	2.736372	1.439695	3.941624
C	2.825783	-0.053173	5.503021
H	2.784985	-0.888786	4.787685
C	2.891971	-0.305249	6.883167
H	2.904913	-1.341201	7.255295
C	2.929991	0.770523	7.784810
H	2.969415	0.587720	8.868931
C	2.908690	2.092236	7.314090
H	2.920129	2.931896	8.031990
C	0.096996	5.178143	6.083864
H	0.622469	5.818490	6.809352
C	-1.303741	5.233658	5.994443
H	-1.854265	5.925114	6.649078
C	-1.990522	4.420895	5.079683
H	-3.087932	4.470901	5.011292
C	-1.272608	3.542370	4.250419
H	-1.801896	2.901741	3.528967
C	0.125878	3.478085	4.337300
H	0.671719	2.786317	3.678640
C	4.321539	3.358227	3.135484
H	4.836831	2.679938	3.830644
C	4.772715	3.455279	1.809234
H	5.637413	2.857751	1.483903
C	4.125568	4.314423	0.906590
H	4.479260	4.389386	-0.133035
C	3.029068	5.082058	1.334813
H	2.522648	5.765442	0.636874
C	2.572462	4.987282	2.658382
H	1.722397	5.603177	2.987921
C	7.526048	5.091881	4.834279
H	7.931881	4.458167	5.635376
C	8.320693	5.355462	3.706571
H	9.329377	4.919624	3.641291
C	7.835915	6.175967	2.675206
H	8.462877	6.385187	1.794887

C	6.552630	6.737142	2.778955
H	6.165464	7.392362	1.984501
C	5.752722	6.476817	3.901768
H	4.751653	6.936685	3.983249
C	6.237093	2.785124	6.644719
H	6.201807	2.766659	5.546086
C	6.654533	1.637636	7.338133
H	6.937865	0.735417	6.775735
C	6.702145	1.641546	8.741548
H	7.029189	0.741659	9.284486
C	6.325545	2.794546	9.451297
H	6.348799	2.802285	10.551253
C	5.912709	3.945878	8.763221
H	5.608250	4.839396	9.328163
C	4.916913	7.908758	7.943988
H	3.845032	7.885815	7.694343
C	5.433203	8.979779	8.692483
H	4.752685	9.778488	9.022112
C	6.797448	9.028197	9.016625
H	7.196237	9.868555	9.605053
C	7.654323	8.000608	8.586289
H	8.725959	8.029738	8.834935
C	7.147122	6.930993	7.834156
H	7.832625	6.136614	7.503163

M-Komplexe/XRay_Komplexe/RI-MP2-SVP

Au2Cl2-1H.c2v RI-MP2/SVP

13			
E(SCF) =	-1910.897126		
C	0.000000	0.000000	1.027783
P	-1.488108	0.000000	1.927342
P	1.488108	0.000000	1.927342
H	-1.714711	1.097110	2.780290
H	-1.714711	-1.097110	2.780290
H	-2.588424	0.000000	1.073150
H	1.714711	1.097110	2.780290
H	2.588424	0.000000	1.073150
H	1.714711	-1.097110	2.780290
Au	0.000000	-1.711336	-0.167889
Cl	0.000000	-3.586985	-1.491998
Au	0.000000	1.711336	-0.167889
Cl	0.000000	3.586985	-1.491998

Au2Cl2-2H RI-MP2/SVP

13	
E(SCF) =	-1413.026456

Au	-1.375010	0.000000	-0.270714
Au	1.375010	0.000000	-0.270714
C	0.000000	0.000000	1.318216
N	0.000000	1.070570	2.177916
N	0.000000	-1.070570	2.177916
C	0.000000	-0.688260	3.490586
C	0.000000	0.688260	3.490586
Cl	3.328530	0.000000	-1.465334
Cl	-3.328530	0.000000	-1.465334
H	0.000000	2.029070	1.839136
H	0.000000	-2.029070	1.839136
H	0.000000	-1.396070	4.314356
H	0.000000	1.396070	4.314356

(AuCl)₂-1Ph RI-MP2/SVP

73

E(SCF) = -3287.152503

C	3.395815	5.463211	6.317192
P	5.153890	5.457151	6.446595
P	2.688475	4.145942	5.383366
C	5.781440	6.824462	7.457660
C	5.735498	3.951840	7.284404
C	6.088493	5.601676	4.884665
C	2.982408	2.454311	6.004648
C	0.882851	4.262217	5.274434
C	3.264160	4.193695	3.659267
Au	2.680074	5.502398	8.280193
Au	2.681679	7.224996	5.449350
Cl	1.849396	9.174786	4.514015
Cl	1.891671	5.594275	10.457167
C	3.090723	1.361788	5.120936
H	3.070746	1.514599	4.040465
C	3.238331	0.064001	5.625513
H	3.329869	-0.775711	4.931645
C	3.242437	-0.161170	7.007045
H	3.351475	-1.176519	7.396726
C	3.098969	0.919873	7.886045
H	3.082836	0.756001	8.966223
C	2.953922	2.218956	7.392533
H	2.834911	3.054619	8.087939
C	0.111494	5.155444	6.034666
H	0.589314	5.855355	6.721436
C	-1.282019	5.150936	5.899869
H	-1.875621	5.853201	6.489263
C	-1.907655	4.257191	5.023579
H	-2.995512	4.261470	4.922055

C	-1.136807	3.359899	4.272340
H	-1.619686	2.659706	3.586424
C	0.254762	3.353155	4.401575
H	0.849285	2.650299	3.811662
C	4.432180	3.528018	3.242676
H	4.936385	2.832135	3.912549
C	4.936952	3.731316	1.953777
H	5.842577	3.206731	1.639340
C	4.296410	4.620151	1.082409
H	4.695539	4.784598	0.078269
C	3.137301	5.290572	1.494872
H	2.633531	5.987073	0.820219
C	2.623717	5.087828	2.780111
H	1.724734	5.622582	3.097208
C	7.342560	4.978626	4.725239
H	7.750257	4.337635	5.508874
C	8.074804	5.168334	3.546910
H	9.042722	4.674037	3.429636
C	7.585036	6.004881	2.537123
H	8.162764	6.155321	1.621550
C	6.355323	6.652932	2.709483
H	5.969857	7.322360	1.936706
C	5.615776	6.467956	3.880412
H	4.660478	6.985003	4.007512
C	6.033481	2.771374	6.578245
H	6.076325	2.778582	5.489522
C	6.307840	1.586898	7.270432
H	6.541497	0.676840	6.712388
C	6.259511	1.565423	8.669294
H	6.466215	0.637963	9.209418
C	5.956339	2.736279	9.376622
H	5.915183	2.725854	10.468525
C	5.686650	3.925550	8.691335
H	5.441074	4.831926	9.250671
C	4.990267	7.898897	7.894044
H	3.926396	7.936884	7.656180
C	5.573900	8.923334	8.649011
H	4.951135	9.752819	8.991125
C	6.937811	8.887562	8.959757
H	7.385463	9.689567	9.551494
C	7.728090	7.819097	8.515305
H	8.793647	7.785651	8.754874
C	7.156765	6.792764	7.758045
H	7.779975	5.962388	7.415185

M-Komplexe/XRay_Komplexe/RI-MP2-TZVP

	(AuCl) ₂ -1Ph	RI-MP2/TZVP	
73			
E(SCF) =	-3289.109321		
C	3.370681	5.495093	6.336624
P	5.134644	5.472791	6.443532
P	2.684880	4.159614	5.404051
C	5.766265	6.815556	7.481416
C	5.718039	3.953625	7.253502
C	6.061715	5.629177	4.878947
C	2.973645	2.472238	6.037542
C	0.884227	4.288623	5.261775
C	3.283960	4.189209	3.688093
Au	2.711949	5.515513	8.302524
Au	2.648496	7.213274	5.428051
Cl	1.832522	9.095967	4.348596
Cl	2.039972	5.506346	10.521515
C	3.007579	1.381927	5.157082
H	2.946530	1.532665	4.087022
C	3.160626	0.089478	5.655602
H	3.184914	-0.748244	4.968583
C	3.186743	-0.132778	7.031175
H	3.287991	-1.140619	7.415729
C	3.124198	0.949401	7.908219
H	3.121105	0.786610	8.979344
C	2.987195	2.244276	7.419346
H	2.917237	3.077583	8.108683
C	0.107090	5.119485	6.071084
H	0.572806	5.796742	6.774205
C	-1.276641	5.126415	5.910140
H	-1.878269	5.777918	6.531390
C	-1.887924	4.251243	5.014889
H	-2.964762	4.260135	4.900092
C	-1.108044	3.420915	4.210046
H	-1.578659	2.744622	3.506900
C	0.274270	3.402468	4.365309
H	0.876084	2.753986	3.738816
C	4.425450	3.485106	3.287603
H	4.887266	2.770528	3.953803
C	4.915897	3.626325	1.991323
H	5.794933	3.070626	1.686817
C	4.324027	4.538168	1.119231
H	4.707025	4.651805	0.112037
C	3.184304	5.239585	1.513791
H	2.710226	5.937814	0.834574
C	2.681283	5.093481	2.803673
H	1.804137	5.653195	3.107568

C	7.340019	5.067346	4.754738
H	7.759654	4.465532	5.550485
C	8.068849	5.248967	3.580776
H	9.056788	4.812375	3.492874
C	7.571340	6.064224	2.565824
H	8.148382	6.217683	1.661750
C	6.311711	6.646702	2.701044
H	5.924826	7.300137	1.928283
C	5.570386	6.458211	3.862668
H	4.601689	6.932461	3.968458
C	6.048655	2.804150	6.526492
H	6.124036	2.842973	5.449211
C	6.380897	1.626413	7.192361
H	6.644384	0.743612	6.621866
C	6.296383	1.565575	8.582131
H	6.550703	0.648947	9.100933
C	5.970110	2.710046	9.310389
H	5.918685	2.673098	10.391871
C	5.649526	3.893886	8.651671
H	5.382568	4.774844	9.224090
C	5.003153	7.924702	7.851184
H	3.954019	7.982525	7.594425
C	5.586553	8.925351	8.625131
H	4.991746	9.780758	8.919828
C	6.939343	8.866229	8.953059
H	7.385533	9.651293	9.550910
C	7.698880	7.757665	8.579413
H	8.749063	7.703691	8.839160
C	7.127876	6.754645	7.802783
H	7.722724	5.895869	7.513195

Metathese/Modell

	ethen	RI-BP86/SVP	
6			
E(SCF) =	-78.528698		
H	-0.027313	0.000000	0.074153
C	-0.000533	0.000000	1.176327
C	1.156704	0.000000	1.854241
H	-0.974872	0.000000	1.692071
H	1.183446	0.000000	2.956282
H	2.130999	0.000000	1.338426

	PMe3	RI-BP86/SVP	
13			
E(SCF) =	-460.943192		
P	-0.015904	-0.000291	-0.008167

C	0.021067	0.006074	1.861848
C	1.211527	-1.374618	-0.329030
C	1.088906	1.472851	-0.336239
H	1.051789	0.052789	2.274282
H	-0.553440	0.876626	2.238456
H	-0.474226	-0.909975	2.243006
H	1.431993	-1.425389	-1.414645
H	2.166179	-1.240120	0.223454
H	0.762928	-2.345092	-0.034562
H	1.305067	1.536399	-1.422044
H	2.051183	1.423974	0.217250
H	0.558201	2.402705	-0.047308

	Ru1a-2	RI-BP86/SVP	
36			
E(SCF) =	-1821.409214		
C	-0.366094	0.518562	-2.403622
N	-0.850244	0.761524	-1.035404
C	-0.140576	0.068408	-0.111947
N	0.860344	-0.589540	-0.756772
C	0.983315	-0.179258	-2.160030
Ru	-0.255790	0.009736	1.927002
P	0.453088	-0.445255	4.158038
C	-0.728592	-1.392914	5.205057
C	1.902905	-1.337188	-0.085297
C	-2.063679	1.516827	-0.830047
C	-1.845718	0.709936	2.446341
Cl	0.880415	2.144005	1.963580
Cl	-1.062744	-2.286189	1.882032
C	1.936887	-1.544069	4.086750
C	0.973732	0.983472	5.196517
H	1.845482	0.515259	-2.291426
H	1.146250	-1.055791	-2.820505
H	-1.086321	-0.127983	-2.956862
H	-0.266415	1.471209	-2.963278
H	2.264910	-2.150300	-0.746903
H	2.769063	-0.698797	0.201132
H	1.464119	-1.814323	0.815585
H	-1.940896	2.564881	-1.177491
H	-2.914245	1.058645	-1.382619
H	-2.300892	1.524146	0.247845
H	-2.740972	0.062294	2.603123
H	-1.964166	1.800722	2.651588
H	-0.253678	-1.756254	6.138461
H	-1.586722	-0.738236	5.453231
H	-1.096699	-2.238405	4.590293

H	2.313690	-1.782622	5.102035
H	1.633968	-2.476483	3.570732
H	2.740724	-1.050175	3.506279
H	1.512589	0.655839	6.108171
H	1.602668	1.646950	4.570915
H	0.070648	1.556550	5.484583

	Ru1b-2	RI-BP86/SVP	
36			
E(SCF) =	-1821.413101		
C	-0.001433	0.123514	-0.159963
Ru	-0.013523	0.173135	1.923834
N	0.978681	-0.352501	-0.983739
N	-1.037362	0.510717	-0.964893
C	0.573076	-0.402720	-2.395516
C	2.147970	-1.118856	-0.600665
C	-0.723473	0.415342	-2.397183
C	-2.365218	0.951999	-0.586291
H	1.361404	0.024076	-3.049767
H	0.412878	-1.460911	-2.709608
H	-1.550793	-0.078235	-2.949089
H	-0.587902	1.431069	-2.835445
H	1.980964	-2.207584	-0.771886
H	3.022055	-0.804752	-1.208955
H	2.385323	-0.931795	0.461036
H	-2.517260	2.037527	-0.780801
H	-3.118404	0.391975	-1.181724
H	-2.539559	0.734670	0.480817
C	-0.756301	1.844140	1.939463
H	-1.118977	2.359321	2.859417
H	-0.839935	2.462954	1.018119
Cl	2.304808	0.635443	2.217012
Cl	-1.691506	-1.499904	1.873144
P	-0.102781	0.029661	4.319294
C	0.680503	-1.526839	4.936436
C	0.761146	1.349659	5.283197
C	-1.790755	-0.018302	5.072384
H	-1.756892	-0.189785	6.167310
H	-2.308103	0.940513	4.869952
H	-2.359405	-0.826869	4.573263
H	0.638538	-1.610343	6.041501
H	0.153710	-2.386125	4.476862
H	1.735914	-1.538598	4.600359
H	0.741540	1.150229	6.373671
H	1.805420	1.404357	4.919311
H	0.277042	2.326187	5.083159

-----	Ru2-2	RI-BP86/SVP	
23			
E(SCF) =	-1360.429372		
C	0.813482	0.282777	-1.973819
C	-0.651585	-0.162823	-2.044280
N	-1.092320	-0.008207	-0.654821
C	-0.032915	0.087495	0.214902
N	1.111103	0.167412	-0.542914
C	-2.513710	-0.005685	-0.368477
Ru	-0.142302	0.146396	2.143824
C	-1.342015	-1.206352	2.278739
C	2.435458	0.552800	-0.094078
Cl	-1.266522	2.176040	2.146804
Cl	1.825528	-0.809110	2.940049
H	0.953057	1.336943	-2.312854
H	1.493392	-0.357033	-2.572730
H	-0.756886	-1.222812	-2.374515
H	-1.264764	0.464191	-2.723609
H	3.199649	-0.023132	-0.655472
H	2.619279	1.638070	-0.269201
H	2.550644	0.322663	0.980145
H	-3.024789	0.676220	-1.081128
H	-2.966905	-1.016068	-0.479687
H	-2.687633	0.371142	0.653804
H	-1.653571	-1.896915	1.465907
H	-1.777710	-1.409118	3.287228

-----	Ru3a-2	RI-BP86/SVP	
29			
E(SCF) =	-1438.972528		
C	-0.579451	-0.178936	2.268562
N	-1.006166	-0.123252	0.863938
C	0.025946	0.156736	0.014843
N	1.125081	0.423542	0.781471
C	0.814966	0.456897	2.217496
Ru	-0.053061	0.042055	-2.009511
Cl	-2.130955	1.200988	-2.146581
C	2.506732	0.579974	0.367721
C	-2.274072	-0.743262	0.524539
C	1.031770	1.516440	-2.135953
Cl	1.266795	-1.911028	-1.800281
H	0.819209	1.505544	2.593534
H	1.573734	-0.110564	2.795081
H	-0.554323	-1.237511	2.618693
H	-1.288497	0.374194	2.917995

H	2.856978	1.632451	0.454500
H	2.627446	0.226459	-0.670664
H	3.150797	-0.048134	1.019620
H	-2.231822	-1.845950	0.678485
H	-2.535771	-0.509578	-0.522293
H	-3.074547	-0.331032	1.172504
H	1.523205	1.836282	-3.078797
H	1.198298	2.194755	-1.271945
C	0.428640	-0.133874	-4.352325
C	-0.744400	-0.803035	-4.092676
H	0.406273	0.888988	-4.759591
H	-1.721578	-0.333294	-4.276968
H	-0.733072	-1.883581	-3.871976
H	1.397876	-0.654774	-4.343871

	Ru3c-2	RI-BP86/SVP	
29			
E(SCF) =	-1438.969823		
N	0.812309	-0.037021	-0.881201
C	0.288342	0.220103	-2.236131
C	-1.230761	0.135274	-2.020601
N	-1.334880	0.349363	-0.569790
C	-0.149741	0.136957	0.047058
C	-2.616568	0.338805	0.114359
Ru	-0.090120	0.180647	2.103896
Cl	0.835231	2.384072	1.606357
C	2.242449	0.003422	-0.641162
C	1.569154	-0.420237	2.506583
Cl	-0.896464	-2.104741	1.836141
C	-1.215989	-0.041605	3.993800
C	-0.688129	1.258981	3.942542
H	0.606576	1.232517	-2.575663
H	0.670069	-0.526658	-2.960363
H	-1.637079	-0.866892	-2.290223
H	-1.795987	0.904791	-2.583638
H	2.594418	1.046536	-0.489878
H	2.476990	-0.578576	0.268692
H	2.767003	-0.455395	-1.501249
H	-3.376534	0.825093	-0.527702
H	-2.931531	-0.693352	0.377332
H	-2.547571	0.934444	1.048141
H	1.742590	-1.502623	2.698108
H	2.422779	0.286738	2.604572
H	-1.308506	2.110931	3.620188
H	-0.741114	-0.837357	4.586860
H	0.222336	1.534895	4.495017

H	-2.263126	-0.239043	3.711900
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	Ru4-2	RI-BP86/SVP	
29			
E(SCF) =	-1438.987570		
C	0.000193	-0.000094	-1.301516
N	0.542185	0.963223	-2.080131
C	0.522410	0.565660	-3.496254
C	-0.522491	-0.565578	-3.496207
N	-0.541923	-0.963349	-2.080133
C	1.418939	2.011652	-1.592417
C	-1.418803	-2.011652	-1.592348
Ru	0.000292	-0.000183	0.685945
C	0.642308	1.182687	2.132296
C	0.000057	-0.000079	2.963756
C	-0.642628	-1.182590	2.132277
Cl	2.124124	-1.117490	0.657266
Cl	-2.123663	1.117137	0.656565
H	0.241622	1.417984	-4.147235
H	1.529553	0.204573	-3.808946
H	-0.241867	-1.417804	-4.147384
H	-1.529711	-0.204437	-3.808591
H	1.118076	2.286114	-0.563616
H	2.482637	1.688088	-1.576338
H	1.317253	2.910175	-2.233226
H	-1.317621	-2.910028	-2.233439
H	-1.117646	-2.286474	-0.563730
H	-2.482393	-1.687761	-1.575778
H	1.740502	1.249706	2.244521
H	0.091531	2.136309	2.236251
H	-0.814635	0.441650	3.568172
H	-1.740872	-1.249089	2.244292
H	-0.092310	-2.136462	2.236398
H	0.814882	-0.441887	3.567925

	Ru_1a-1	RI-BP86/SVP	
46			
E(SCF) =	-2475.505812		
C	0.106603	0.243130	-0.275484
Ru	-0.242504	0.018303	1.835319
P	0.434347	-0.263613	4.063512
C	0.100749	-1.890717	4.867219
C	-1.993770	0.126941	2.324159
Cl	0.277987	2.363511	2.220582
Cl	-0.539322	-2.401662	1.556228
C	2.272386	-0.080877	4.177356

C	-0.185172	0.961929	5.294342
H	-2.679916	-0.753143	2.317985
H	-2.441555	1.107904	2.616933
H	0.613534	-1.971940	5.847050
H	-0.992622	-1.996384	5.008381
H	0.422878	-2.696303	4.180161
H	2.630553	-0.208231	5.219374
H	2.761491	-0.836147	3.531189
H	2.531903	0.930828	3.808660
H	0.321947	0.848457	6.273786
H	-0.010922	1.970521	4.871716
H	-1.275612	0.814345	5.420143
P	1.153729	-0.906892	-1.015696
P	-1.058091	1.142968	-1.159622
C	2.194020	-0.214196	-2.383081
H	2.977465	-0.948084	-2.660110
H	2.671203	0.721052	-2.032394
H	1.588411	0.003203	-3.281661
C	2.414760	-1.485876	0.182514
H	3.153813	-2.135794	-0.326589
H	1.878818	-2.054579	0.968993
H	2.923089	-0.604255	0.618593
C	0.486532	-2.471752	-1.752817
H	1.293411	-3.109062	-2.169843
H	-0.236017	-2.224225	-2.555725
H	-0.043057	-2.993667	-0.930679
C	-0.807500	1.264580	-2.992653
H	0.148017	1.776433	-3.213363
H	-1.636033	1.857369	-3.428205
H	-0.809759	0.262458	-3.463855
C	-1.235467	2.894619	-0.655205
H	-0.329969	3.448052	-0.969705
H	-1.275525	2.943053	0.452014
H	-2.137280	3.338813	-1.121991
C	-2.780875	0.475532	-1.074276
H	-2.783078	-0.559534	-1.467696
H	-3.492920	1.101889	-1.648254
H	-3.084307	0.438094	-0.010915

	Ru_1b-1	RI-BP86/SVP	
46			
E(SCF) =	-2475.507766		
C	0.051718	0.214074	-0.320135
Ru	-0.015488	0.071208	1.913226
C	-0.043171	1.890657	2.061212
H	-0.155505	2.489819	2.996007

H	0.098255	2.498235	1.138849
Cl	2.258062	-0.618997	2.245614
Cl	-2.225755	-0.828516	1.839824
P	-0.186982	-0.141828	4.233770
C	-0.151029	-1.897664	4.815905
C	1.133777	0.655979	5.257859
C	-1.739478	0.516237	4.998457
H	-1.774735	0.328318	6.090721
H	-1.802198	1.607133	4.814542
H	-2.599864	0.032069	4.497887
H	-0.234919	-1.977424	5.919094
H	-0.990172	-2.438658	4.336505
H	0.801354	-2.351861	4.479170
H	0.989315	0.464393	6.340508
H	2.111804	0.258798	4.925141
H	1.126659	1.749131	5.077178
P	1.429388	-0.391075	-1.150101
P	-1.383602	0.637832	-1.166557
C	1.410976	-0.441583	-3.007598
H	2.344322	-0.930769	-3.350694
H	1.372971	0.578033	-3.433253
H	0.550645	-1.031031	-3.379897
C	2.979917	0.549293	-0.827718
H	3.836510	0.106287	-1.374647
H	3.172040	0.520042	0.262066
H	2.823840	1.596711	-1.151136
C	1.851561	-2.146431	-0.765354
H	2.767441	-2.467699	-1.301444
H	0.996241	-2.783994	-1.062916
H	2.011336	-2.225435	0.326776
C	-1.193478	1.543361	-2.781105
H	-0.477885	2.378383	-2.651932
H	-2.178378	1.953740	-3.081384
H	-0.836980	0.877859	-3.587245
C	-2.550146	-0.727037	-1.637541
H	-2.010855	-1.461499	-2.267992
H	-3.437470	-0.349322	-2.186190
H	-2.860131	-1.220557	-0.696054
C	-2.459648	1.818257	-0.256175
H	-1.928405	2.780387	-0.133860
H	-2.704388	1.393539	0.734183
H	-3.388196	1.978093	-0.839469

Ru_1diss-1 RI-BP86/SVP

19

E(SCF) = -1515.560939

Ru	-0.374126	0.013147	2.051893
P	0.407184	-0.219125	4.099846
C	-0.023801	-1.807825	4.927253
C	-2.133391	-0.071837	2.493732
Cl	0.255110	2.242322	1.888174
Cl	0.329322	-2.088429	1.360785
C	2.249272	-0.170488	4.118633
C	-0.103527	1.095902	5.284887
H	-2.841928	0.019685	1.632946
H	-2.611064	-0.201620	3.489785
H	0.453373	-1.879635	5.925687
H	-1.123002	-1.880725	5.036757
H	0.315724	-2.634490	4.274329
H	2.643342	-0.286426	5.148759
H	2.627906	-0.988277	3.475413
H	2.577478	0.798431	3.695187
H	0.374770	0.948730	6.274482
H	0.188092	2.073140	4.854781
H	-1.204355	1.081240	5.400767

	Ru_2-1	RI-BP86/SVP	
33			
E(SCF) =	-2014.518990		
C	-0.109448	-0.203256	-0.044077
Ru	0.044038	-0.778309	1.926825
C	-1.151683	0.422156	2.555233
Cl	2.167883	-0.060259	2.637275
Cl	-1.018008	-2.863528	1.782486
H	-1.606778	1.216563	1.919066
H	-1.463013	0.418600	3.629664
P	1.211227	0.736075	-0.661623
P	-1.398157	-0.861436	-1.007077
C	1.508576	2.292749	0.270138
H	2.345143	2.858951	-0.185762
H	1.761388	2.026125	1.314452
H	0.582792	2.899054	0.250775
C	2.844456	-0.118658	-0.689175
H	3.636272	0.551311	-1.080987
H	2.762237	-1.019861	-1.327584
H	3.087480	-0.417870	0.349216
C	1.086657	1.341390	-2.407971
H	2.001084	1.928826	-2.621553
H	0.206346	1.994836	-2.546643
H	1.042731	0.497353	-3.121531
C	-1.184029	-2.586483	-1.636122
H	-0.275156	-2.627582	-2.268076

H	-2.064149	-2.919792	-2.223021
H	-1.044930	-3.238284	-0.751434
C	-1.848279	0.064708	-2.547434
H	-1.070743	-0.021464	-3.326732
H	-2.025295	1.131631	-2.314091
H	-2.784872	-0.375145	-2.943014
C	-3.007307	-0.896086	-0.123680
H	-2.899081	-1.521487	0.781953
H	-3.781000	-1.325618	-0.790816
H	-3.283700	0.136062	0.162281

	Ru_3a-1	RI-BP86/SVP	
39			
E(SCF) =	-2093.068927		
C	0.008897	0.181937	0.133690
Ru	0.009024	-0.200946	-1.993470
Cl	-2.350521	0.139210	-2.284959
C	0.622945	1.501256	-2.309182
Cl	1.960187	-1.553365	-1.743751
H	0.953963	1.917727	-3.282740
H	0.635941	2.213812	-1.457865
C	0.142065	-0.243634	-4.284493
C	-0.242018	-1.502844	-3.833924
H	-0.607412	0.471668	-4.657094
H	-1.306541	-1.787159	-3.828711
H	0.493191	-2.316918	-3.746794
H	1.191805	-0.048935	-4.556488
P	1.508939	0.339751	0.990700
P	-1.481200	0.042205	1.006817
C	2.282823	-1.200902	1.669783
H	3.221868	-0.981877	2.217981
H	2.482504	-1.864657	0.806953
H	1.565944	-1.699515	2.351307
C	2.854312	1.119185	0.012309
H	3.788290	1.070800	0.606645
H	2.602886	2.177237	-0.188101
H	2.982703	0.564163	-0.934716
C	1.506914	1.455457	2.478206
H	2.555976	1.677125	2.759156
H	1.011459	0.987825	3.347134
H	0.993336	2.404038	2.228121
C	-1.385518	-0.063304	2.857584
H	-0.674024	-0.849021	3.177109
H	-2.392423	-0.329611	3.235491
H	-1.094518	0.905759	3.301910
C	-2.424719	-1.495304	0.632948

H	-1.796351	-2.363604	0.911617
H	-2.635085	-1.514918	-0.452878
H	-3.377367	-1.519525	1.199247
C	-2.674342	1.427248	0.779788
H	-2.189699	2.364278	1.117005
H	-3.602974	1.251692	1.359602
H	-2.904659	1.492949	-0.300957

	Ru_3b-1	RI-BP86/SVP	
39			
E(SCF) =	-2093.062655		
C	0.005072	-0.115372	-0.073719
Ru	-0.045617	0.398328	2.063692
Cl	1.063616	2.394194	1.318403
C	1.184055	-0.861364	2.483490
Cl	-2.040081	-0.961411	2.240977
C	-0.592692	0.557394	4.275819
C	0.424778	1.468037	4.018580
H	1.718702	-0.893753	3.464223
H	1.401826	-1.706276	1.793961
H	1.474743	1.240753	4.266970
H	-0.395137	-0.420135	4.741840
H	0.207946	2.533823	3.856664
H	-1.645201	0.878778	4.302594
P	1.478991	-0.063364	-0.967342
P	-1.486307	-0.131651	-0.945692
C	-1.423697	0.350128	-2.738792
H	-1.126255	1.411461	-2.835146
H	-2.435163	0.223613	-3.173594
H	-0.720883	-0.279984	-3.315383
C	-2.732112	1.069717	-0.319767
H	-2.276460	2.078866	-0.335584
H	-2.995328	0.793099	0.718082
H	-3.637959	1.051162	-0.957994
C	-2.367458	-1.753813	-1.030368
H	-1.716842	-2.480422	-1.555946
H	-3.337750	-1.666266	-1.560702
H	-2.522673	-2.090160	0.012062
C	1.842993	1.427178	-2.018711
H	2.839705	1.349347	-2.498812
H	1.809988	2.298898	-1.336905
H	1.074691	1.550869	-2.803790
C	1.724408	-1.474069	-2.150753
H	2.701420	-1.393008	-2.669827
H	0.922857	-1.499469	-2.913357
H	1.686480	-2.420207	-1.576760

C	3.003188	-0.164714	0.049478
H	3.872407	-0.019331	-0.621563
H	3.081712	-1.150697	0.540329
H	2.971832	0.638600	0.808925

	Ru_3c-1	RI-BP86/SVP	
39			
E(SCF) =	-2093.072770		
C	-0.124109	0.118454	-0.055335
Ru	0.076128	0.447342	2.012210
Cl	1.788872	2.104962	1.393459
C	1.356494	-0.633693	2.716827
Cl	-1.450882	-1.478287	2.275988
C	-1.060237	0.997166	3.829364
C	-0.132794	2.016855	3.560098
H	1.146171	-1.686283	3.005676
H	2.393798	-0.248189	2.833210
H	-0.441871	2.938421	3.040328
H	-0.881382	0.243110	4.609082
H	0.813083	2.097862	4.115125
H	-2.114099	1.103963	3.524734
P	1.236498	0.008927	-1.125003
P	-1.734833	-0.025547	-0.670187
C	1.753251	1.540406	-2.019421
H	2.649314	1.361026	-2.647752
H	1.968506	2.290546	-1.233548
H	0.921792	1.901872	-2.654719
C	2.755919	-0.593178	-0.308687
H	3.545790	-0.743750	-1.070772
H	2.529863	-1.545077	0.207458
H	3.061912	0.172013	0.430086
C	1.018281	-1.233688	-2.483116
H	1.927122	-1.263533	-3.116951
H	0.154288	-0.989031	-3.129396
H	0.856043	-2.231884	-2.032535
C	-1.976284	0.884150	-2.265947
H	-1.740413	1.954219	-2.108854
H	-3.029416	0.785516	-2.597848
H	-1.322991	0.488724	-3.066342
C	-2.994657	0.763684	0.403808
H	-2.682752	1.801968	0.629206
H	-3.057132	0.169472	1.336083
H	-3.971573	0.771772	-0.119541
C	-2.426107	-1.704715	-1.023982
H	-1.802330	-2.212023	-1.784860
H	-3.473918	-1.646446	-1.382788

H	-2.369274	-2.262765	-0.069149
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	Ru_4-1	RI-BP86/SVP	
39			
E(SCF) =	-2093.098956		
C	0.064700	0.034229	-1.417556
Ru	-0.188159	0.216108	0.581620
C	-0.664749	1.660029	1.849972
C	-0.470917	0.420386	2.820945
C	-0.071915	-0.967811	2.164372
Cl	2.180457	0.641196	0.956875
Cl	-2.585328	-0.189483	0.430132
H	0.107070	2.440283	1.998498
H	-1.704922	2.038005	1.840009
H	-1.443154	0.265108	3.326549
H	-0.874089	-1.726093	2.254133
H	0.929608	-1.318244	2.479159
H	0.350251	0.684987	3.514337
P	-0.872617	-1.169160	-2.264018
P	1.210715	1.086474	-2.206804
C	0.006709	-1.898220	-3.721154
H	0.116100	-1.171358	-4.546384
H	-0.578198	-2.760611	-4.097835
H	1.007831	-2.252828	-3.408736
C	-1.184981	-2.657832	-1.244343
H	-0.217017	-3.038311	-0.866377
H	-1.689004	-3.430044	-1.859451
H	-1.828645	-2.349167	-0.396886
C	-2.515206	-0.680218	-2.942717
H	-2.383266	0.149583	-3.663931
H	-3.111493	-0.330312	-2.076598
H	-3.015212	-1.534542	-3.442673
C	0.735856	1.525995	-3.941647
H	1.415779	2.320361	-4.308352
H	-0.302815	1.908993	-3.954729
H	0.816977	0.662202	-4.626082
C	1.298063	2.739404	-1.423545
H	1.957189	3.399358	-2.022455
H	1.704625	2.600472	-0.402158
H	0.276382	3.161316	-1.370933
C	2.957574	0.518629	-2.361583
H	3.585466	1.279936	-2.867464
H	2.987102	-0.429503	-2.932796
H	3.314042	0.341962	-1.327305

Ru_ts34-1.ts	RI-BP86/SVP	
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39

E(SCF) =	-2093.060953		
C	0.059699	-0.478788	-0.010678
Ru	-0.015280	-0.085780	-2.097982
Cl	1.937318	-1.464659	-2.395970
Cl	-2.088024	1.191531	-1.734651
C	0.712779	1.524125	-2.576601
C	-1.043702	-0.706591	-3.915292
C	0.081940	-0.087830	-4.474297
H	1.786902	1.583126	-2.874016
H	0.128253	2.471952	-2.593261
H	-0.021838	0.898267	-4.953988
H	-2.043096	-0.247507	-3.974964
H	-1.003597	-1.799897	-3.748289
H	1.011034	-0.647283	-4.658660
P	-1.402247	-1.059357	0.698068
P	1.305438	0.276155	0.900911
C	-2.604782	0.101893	1.498377
H	-2.110912	0.629721	2.338204
H	-3.498804	-0.433497	1.878901
H	-2.886852	0.836021	0.717734
C	-1.124531	-2.340370	2.004817
H	-0.442759	-3.115757	1.606044
H	-2.093145	-2.803869	2.280784
H	-0.679032	-1.899834	2.915288
C	-2.408534	-1.960322	-0.539664
H	-1.777289	-2.724862	-1.032474
H	-2.763970	-1.217138	-1.280587
H	-3.268161	-2.448322	-0.039078
C	1.268752	-0.006240	2.728725
H	2.098170	0.563560	3.191796
H	1.410177	-1.080381	2.951615
H	0.315095	0.343826	3.168799
C	1.309759	2.122123	0.802777
H	2.130851	2.562723	1.402726
H	0.331282	2.501292	1.155597
H	1.424982	2.415115	-0.258091
C	3.014848	-0.195380	0.441511
H	3.189049	-1.244295	0.748333
H	3.743497	0.477061	0.936997
H	3.107521	-0.163693	-0.662421

Ruts34-2.ts

RI-BP86/SVP

29

E(SCF) =	-1438.963899		
C	0.610673	-0.194522	2.099284

C	-0.842714	-0.668888	1.945229
N	-0.940412	-0.856284	0.490788
C	0.042338	-0.189107	-0.163188
N	0.928329	0.285580	0.742786
C	-2.176785	-1.286674	-0.141343
Ru	-0.007169	-0.037137	-2.181328
Cl	1.522917	-1.898639	-2.253129
C	2.244426	0.816653	0.455830
Cl	-1.648368	1.724368	-1.824573
C	1.226186	1.199968	-2.701361
C	-1.184724	-0.393041	-4.013786
C	0.085366	-0.211912	-4.562801
H	0.729355	0.615412	2.846827
H	1.296542	-1.027851	2.378015
H	-1.054360	-1.611533	2.488947
H	-1.572178	0.102555	2.284647
H	2.214934	1.355031	-0.508583
H	3.008703	0.011736	0.386025
H	2.536264	1.529784	1.252279
H	-2.681395	-2.025347	0.511369
H	-1.947104	-1.796452	-1.099468
H	-2.850547	-0.429190	-0.352799
H	2.266693	0.898074	-2.965008
H	0.953052	2.272933	-2.826625
H	0.327106	0.723757	-5.091789
H	-1.974069	0.369349	-4.100580
H	-1.508016	-1.423272	-3.770532
H	0.791869	-1.049907	-4.664744

Metathese/Real

	1Ph.noBenz	RI-BP86/SVP	
69			
E(SCF) =	-2109.539519		
C	0.169718	0.337843	-0.588703
P	1.693353	-0.110724	-1.078788
P	-1.373676	0.235516	-1.201838
C	2.853017	0.001498	0.365398
C	4.528789	0.207770	2.621777
C	4.243768	-0.195976	0.236916
C	2.308754	0.309045	1.626585
C	3.144245	0.411124	2.751369
C	5.077173	-0.095331	1.362965
H	4.685142	-0.426689	-0.744709
H	1.218937	0.469142	1.687565
H	2.711854	0.652874	3.734896
H	6.161957	-0.250722	1.256090

H	5.184454	0.289042	3.502704
C	2.504664	0.981645	-2.360282
C	3.667701	2.784417	-4.195963
C	2.028386	2.304512	-2.461369
C	3.567220	0.566899	-3.191179
C	4.143043	1.465234	-4.106489
C	2.609044	3.202883	-3.370856
H	1.188166	2.609801	-1.815899
H	3.940592	-0.467616	-3.138950
H	4.966400	1.130089	-4.756465
H	2.231584	4.235216	-3.438299
H	4.120535	3.486343	-4.913331
C	1.949132	-1.827267	-1.746385
C	2.049821	-4.484796	-2.708991
C	1.588229	-2.121497	-3.081107
C	2.348468	-2.883326	-0.897945
C	2.399143	-4.202617	-1.377560
C	1.642737	-3.440869	-3.557946
H	1.258933	-1.314480	-3.754052
H	2.626391	-2.670919	0.145817
H	2.717763	-5.015127	-0.706074
H	1.362578	-3.653706	-4.601094
H	2.092769	-5.518683	-3.084971
C	-1.634419	-0.275379	-2.970593
C	-1.730371	-1.079033	-5.679826
C	-1.239175	0.612821	-3.997841
C	-2.067922	-1.572618	-3.317140
C	-2.115936	-1.969932	-4.664888
C	-1.290574	0.214415	-5.342148
H	-0.885558	1.623665	-3.741351
H	-2.369887	-2.278509	-2.528981
H	-2.459082	-2.984282	-4.921336
H	-0.986148	0.918290	-6.132209
H	-1.771774	-1.390427	-6.735023
C	-2.262772	1.862950	-1.077376
C	-3.546098	4.354708	-0.756754
C	-1.781199	2.795455	-0.136448
C	-3.386384	2.191139	-1.865047
C	-4.023238	3.434256	-1.704947
C	-2.423195	4.033266	0.026326
H	-0.885178	2.528085	0.447748
H	-3.757050	1.484715	-2.624127
H	-4.894195	3.686420	-2.329732
H	-2.041692	4.754865	0.765518
H	-4.046141	5.327844	-0.632992
C	-2.456432	-0.932149	-0.232157

C	-3.971477	-2.744607	1.307716
C	-3.858773	-0.989843	-0.378066
C	-1.822259	-1.781151	0.693616
C	-2.575887	-2.686936	1.458894
C	-4.611751	-1.893758	0.389050
H	-4.373165	-0.324501	-1.087951
H	-0.727655	-1.700784	0.800375
H	-2.070726	-3.348342	2.180013
H	-5.706010	-1.931270	0.271974
H	-4.564410	-3.450482	1.909920

	PCy3	RI-BP86/SVP	
52			
E(SCF) =	-1046.610406		
C	0.142111	2.717770	7.097257
C	-0.044597	2.453524	5.589810
C	-1.446079	2.916558	5.127791
C	-1.694142	4.395780	5.475490
C	-1.483657	4.672857	6.973184
C	-0.097780	4.200819	7.442323
P	0.402190	0.759912	4.849858
C	-0.315056	-0.602444	5.969893
C	0.176120	-0.762571	7.424092
C	-0.392987	-2.043329	8.065978
C	-1.928603	-2.077584	8.001475
C	-2.434194	-1.892582	6.561529
C	-1.859269	-0.618075	5.917091
C	2.258833	0.643491	5.239001
C	3.042984	1.744233	4.488169
C	4.564410	1.619505	4.687718
C	5.079275	0.228877	4.288027
C	4.316499	-0.874144	5.036278
C	2.794709	-0.750721	4.838699
H	0.020157	-1.511107	5.413589
H	-2.255297	0.268948	6.460534
H	-2.207204	-0.522190	4.866343
H	-3.544774	-1.863390	6.540932
H	-2.134594	-2.774413	5.950793
H	-2.337934	-1.261094	8.639294
H	-2.314262	-3.027464	8.429579
H	-0.047029	-2.128146	9.118664
H	0.015963	-2.931536	7.532416
H	-0.143811	0.113922	8.026053
H	1.285107	-0.781260	7.469019
H	2.424924	0.782545	6.332625
H	2.805412	1.675531	3.401782

H	2.711720	2.752253	4.814347
H	5.086370	2.410285	4.107380
H	4.809386	1.806707	5.757933
H	4.943047	0.089205	3.191572
H	6.170532	0.147169	4.479617
H	4.659012	-1.878200	4.705948
H	4.550463	-0.808283	6.123232
H	2.545121	-0.934066	3.768360
H	2.282279	-1.548173	5.416156
H	0.683306	3.106054	5.050678
H	-0.582409	2.098339	7.670053
H	1.154138	2.406706	7.432122
H	0.017668	4.362316	8.535793
H	0.686940	4.820834	6.951990
H	-2.266795	4.137028	7.556746
H	-1.620270	5.753610	7.191409
H	-2.718733	4.694353	5.166164
H	-0.994158	5.029399	4.884326
H	-2.225477	2.293607	5.619912
H	-1.558866	2.748136	4.035975

	real1-1Ph	RI-BP86/SVP	
127			
E(SCF) =	-4210.783341		
C	0.113033	0.206490	0.084909
Ru	0.189750	0.481588	2.337572
C	-1.624135	0.589579	2.452421
P	0.445163	0.708853	4.707975
C	2.233110	0.881892	5.324809
C	2.942175	2.201135	4.955245
C	4.309874	2.292992	5.659617
C	5.206470	1.084708	5.348933
C	4.487154	-0.244322	5.628017
C	3.118484	-0.318158	4.925250
C	-0.120447	-0.816378	5.707413
C	0.363659	-0.960885	7.168579
C	-0.014952	-2.336331	7.752033
C	-1.525669	-2.595113	7.665890
C	-2.020817	-2.442864	6.221353
C	-1.639860	-1.077793	5.617751
C	-0.322632	2.294769	5.428340
C	-1.748737	2.622831	4.938596
C	-2.178186	4.035390	5.377096
C	-2.063725	4.231643	6.896191
C	-0.649751	3.890959	7.389371
C	-0.226528	2.473101	6.959003

Cl	0.801067	2.782804	2.070013
Cl	0.699391	-1.850993	2.530701
H	-2.245106	0.943783	1.598863
H	-2.237238	0.329266	3.341695
H	0.365403	-1.617296	5.103002
H	-2.196686	-0.274420	6.151013
H	-1.963449	-1.053142	4.559901
H	-3.122021	-2.581699	6.168211
H	-1.573457	-3.245648	5.593529
H	-2.060079	-1.867200	8.318427
H	-1.771880	-3.604707	8.059373
H	0.334728	-2.405233	8.804693
H	0.525545	-3.131312	7.190273
H	-0.089257	-0.168772	7.802110
H	1.461875	-0.830953	7.242182
H	2.135262	0.870529	6.434012
H	3.064447	2.257935	3.853175
H	2.328483	3.079896	5.238200
H	4.820079	3.236989	5.370409
H	4.146302	2.355602	6.760125
H	5.492914	1.116506	4.275987
H	6.152665	1.144213	5.929010
H	5.120675	-1.100106	5.310743
H	4.338603	-0.359278	6.726537
H	3.257181	-0.316792	3.822890
H	2.624420	-1.281953	5.162372
H	0.335531	3.053061	4.945636
H	-0.895321	1.736932	7.456822
H	0.799305	2.263237	7.325991
H	-0.587970	3.983968	8.495101
H	0.072902	4.628682	6.972803
H	-2.798439	3.569688	7.409266
H	-2.333995	5.272090	7.177230
H	-3.216722	4.234764	5.036055
H	-1.532013	4.780405	4.860677
H	-2.473822	1.879066	5.338074
H	-1.782651	2.553314	3.833102
P	1.584994	-0.081614	-0.755823
P	-1.362982	0.140736	-0.811529
C	3.084684	-0.129409	0.335269
C	5.572881	-0.026394	1.665379
C	3.826365	-1.308628	0.553212
C	3.589402	1.101814	0.811648
C	4.827471	1.148847	1.470635
C	5.062011	-1.255327	1.219310
H	3.454615	-2.274597	0.187411

H	3.013909	2.027073	0.663759
H	5.216143	2.117087	1.820962
H	5.633463	-2.183018	1.375581
H	6.553336	0.015384	2.164332
C	2.173708	1.238580	-1.944519
C	3.084100	3.347027	-3.587141
C	1.435991	2.432277	-2.045832
C	3.396128	1.122371	-2.645110
C	3.841170	2.167009	-3.470073
C	1.887507	3.481851	-2.865821
H	0.517761	2.542770	-1.449278
H	4.017954	0.221120	-2.530782
H	4.792419	2.065078	-4.015197
H	1.303308	4.412701	-2.929702
H	3.439198	4.168117	-4.228983
C	1.665246	-1.685014	-1.699429
C	1.712418	-4.213182	-2.960605
C	1.990346	-1.793698	-3.066531
C	1.339697	-2.854517	-0.972400
C	1.376163	-4.109830	-1.599151
C	2.008975	-3.052553	-3.692246
H	2.211778	-0.894912	-3.658603
H	1.063032	-2.770407	0.093516
H	1.135446	-5.013638	-1.018077
H	2.254087	-3.121592	-4.763303
H	1.734065	-5.197918	-3.452721
C	-1.283672	-0.501609	-2.553524
C	-1.168691	-1.471898	-5.206396
C	-0.903887	0.351260	-3.614142
C	-1.602967	-1.846812	-2.838738
C	-1.543958	-2.326636	-4.156677
C	-0.846360	-0.132743	-4.931038
H	-0.663421	1.405513	-3.417196
H	-1.906804	-2.523575	-2.027397
H	-1.798794	-3.377256	-4.362713
H	-0.553650	0.546419	-5.746492
H	-1.130442	-1.848814	-6.240118
C	-2.235585	1.774274	-1.047935
C	-3.515955	4.274288	-1.358597
C	-1.870346	2.867083	-0.234264
C	-3.236760	1.950328	-2.031778
C	-3.872604	3.193749	-2.183794
C	-2.513848	4.107647	-0.388972
H	-1.061264	2.756942	0.509116
H	-3.512364	1.119899	-2.699382
H	-4.646625	3.319259	-2.956892

H	-2.217281	4.949881	0.254950
H	-4.013979	5.248789	-1.480171
C	-2.656385	-0.962833	-0.048415
C	-4.522243	-2.812527	0.988020
C	-4.041559	-0.756692	-0.228513
C	-2.214452	-2.094332	0.668216
C	-3.145794	-3.013317	1.181189
C	-4.967220	-1.678472	0.286877
H	-4.408647	0.133628	-0.758120
H	-1.139491	-2.229191	0.864251
H	-2.785303	-3.885635	1.747788
H	-6.044818	-1.504382	0.142729
H	-5.250404	-3.532880	1.392112

	real1-2Mes	RI-BP86/SVP	
107			
E(SCF) =	-3026.032522		
C	3.322234	1.042837	0.066023
C	2.545714	-0.145834	0.127357
C	3.134933	-1.395178	0.461887
C	4.508711	-1.418001	0.774571
C	5.307117	-0.258884	0.736067
C	4.691378	0.958598	0.388700
N	1.188119	-0.116496	-0.351349
C	0.033190	0.089208	0.347074
N	-0.999038	0.034729	-0.548679
C	-0.555848	-0.205044	-1.938425
C	0.967824	-0.340324	-1.796845
Ru	-0.111786	0.406170	2.371182
C	-1.911994	0.577297	2.497695
C	-2.406017	0.201133	-0.314478
C	-2.980994	1.493600	-0.440169
C	-4.376496	1.614829	-0.294475
C	-5.203622	0.502409	-0.046779
C	-4.600750	-0.767506	0.041404
C	-3.211278	-0.948478	-0.096291
C	-2.125310	2.707582	-0.699188
C	-6.694580	0.667861	0.138695
C	-2.598664	-2.322544	0.003856
C	2.332620	-2.671657	0.459782
C	6.794275	-0.331302	0.999691
C	2.717850	2.357813	-0.356364
P	0.354151	0.730371	4.779911
C	2.208619	0.617289	5.106907
C	3.017204	1.792981	4.517670
C	4.502625	1.681343	4.908097

C	5.107134	0.332305	4.490989
C	4.281113	-0.847150	5.026239
C	2.798907	-0.728059	4.629797
C	-0.364367	-0.635041	5.869960
C	0.269133	-0.870599	7.258604
C	-0.293170	-2.155536	7.899661
C	-1.827027	-2.133008	7.988587
C	-2.461490	-1.853516	6.617284
C	-1.901297	-0.564361	5.990481
C	-0.090193	2.433648	5.463008
C	-1.551356	2.864125	5.215149
C	-1.752754	4.345641	5.582320
C	-1.333341	4.641604	7.030570
C	0.108789	4.183578	7.296413
C	0.313346	2.700766	6.929267
Cl	0.206530	2.797438	2.083776
Cl	-0.259030	-1.988206	2.763524
H	1.526876	0.411349	-2.392592
H	1.341892	-1.343647	-2.091481
H	-1.034875	-1.120386	-2.344726
H	-0.854957	0.643381	-2.589973
H	-2.570321	-0.299309	2.695090
H	-2.422648	1.561805	2.397702
H	-5.231849	-1.654079	0.217265
H	-4.829954	2.615495	-0.384876
H	5.299131	1.877038	0.342114
H	4.971896	-2.384179	1.033586
H	2.975881	-3.540695	0.696161
H	1.504211	-2.630847	1.201035
H	1.865433	-2.861096	-0.529836
H	3.490781	3.148409	-0.405779
H	2.243633	2.289218	-1.358232
H	1.923833	2.681351	0.352546
H	7.044360	-1.129129	1.726721
H	7.350505	-0.557938	0.064104
H	7.189932	0.627381	1.389046
H	-2.751040	3.610170	-0.836395
H	-1.421613	2.890938	0.143649
H	-1.502341	2.588779	-1.610526
H	-3.380294	-3.094788	0.137232
H	-2.020900	-2.585010	-0.907621
H	-1.890335	-2.384955	0.859993
H	-7.078018	1.557995	-0.398143
H	-7.252752	-0.219877	-0.219724
H	-6.949413	0.799681	1.212732
H	-0.144303	-1.522190	5.231176

H	-2.188534	0.300415	6.629029
H	-2.358600	-0.394087	4.994850
H	-3.566438	-1.781301	6.708308
H	-2.256522	-2.703212	5.928988
H	-2.139742	-1.339055	8.704948
H	-2.203796	-3.091785	8.404599
H	0.152828	-2.298162	8.907422
H	0.025328	-3.030714	7.289952
H	0.058744	-0.007787	7.927294
H	1.372805	-0.952642	7.189649
H	2.311642	0.661389	6.215206
H	2.910362	1.795828	3.411155
H	2.615924	2.766442	4.864825
H	5.073219	2.518870	4.452971
H	4.598324	1.804683	6.011384
H	5.128223	0.277107	3.381072
H	6.161279	0.256962	4.834183
H	4.692884	-1.809334	4.654085
H	4.360693	-0.883938	6.137150
H	2.700950	-0.796971	3.523988
H	2.223658	-1.585801	5.033391
H	0.527209	3.080344	4.798746
H	-0.309432	2.074210	7.605124
H	1.368282	2.412238	7.117928
H	0.381461	4.349060	8.360873
H	0.808777	4.805278	6.693899
H	-2.019324	4.108395	7.727948
H	-1.442796	5.724157	7.255231
H	-2.813721	4.632218	5.419370
H	-1.150383	4.969602	4.884986
H	-2.244240	2.240501	5.819869
H	-1.806091	2.706497	4.149881

	real2-1Ph	RI-BP86/SVP	
75			
E(SCF) =	-3164.135908		
C	-0.049894	0.013485	-0.027378
Ru	-0.077188	0.427933	2.000410
Cl	0.160973	2.767435	1.776158
Cl	0.848085	-1.668773	2.532680
C	-1.817378	0.279208	2.444551
H	-2.701851	0.039070	1.816262
H	-2.036958	0.459763	3.530634
P	1.509549	-0.037109	-0.799742
P	-1.507185	-0.297221	-0.916195
C	2.898476	0.083242	0.420205

C	5.042052	0.396116	2.228881
C	3.765480	-0.995962	0.690088
C	3.127658	1.328418	1.046439
C	4.187736	1.475591	1.955921
C	4.832065	-0.835676	1.587804
H	3.617003	-1.968025	0.202342
H	2.464854	2.182801	0.847070
H	4.341571	2.446994	2.449629
H	5.499459	-1.686924	1.791103
H	5.874789	0.514498	2.939130
C	1.937158	1.392097	-1.915324
C	2.584844	3.657380	-3.463118
C	1.027999	2.460910	-2.022939
C	3.193231	1.479801	-2.557761
C	3.508448	2.603642	-3.336929
C	1.351040	3.589397	-2.796929
H	0.080994	2.414544	-1.462922
H	3.938641	0.679030	-2.433869
H	4.486960	2.663912	-3.838002
H	0.636616	4.423845	-2.866837
H	2.838007	4.541226	-4.068776
C	-2.667406	1.137187	-1.178903
C	-4.426008	3.312279	-1.583322
C	-2.571601	2.288597	-0.369994
C	-3.642103	1.092387	-2.204690
C	-4.515816	2.174253	-2.402769
C	-3.451192	3.366292	-0.573852
H	-1.791859	2.361448	0.405735
H	-3.713413	0.216409	-2.867077
H	-5.266215	2.127930	-3.207202
H	-3.361915	4.257829	0.065629
H	-5.110498	4.160368	-1.739807
C	-2.564930	-1.613911	-0.141020
C	-4.058115	-3.744665	0.947891
C	-3.961332	-1.679716	-0.340712
C	-1.925078	-2.610848	0.623480
C	-2.672467	-3.670583	1.164333
C	-4.701380	-2.744917	0.198253
H	-4.482131	-0.893612	-0.905202
H	-0.848879	-2.526421	0.840899
H	-2.163555	-4.432100	1.774813
H	-5.789576	-2.787248	0.037051
H	-4.641748	-4.574731	1.375302
C	-1.243280	-0.905409	-2.644082
C	-0.876839	-1.809792	-5.292519
C	-0.951129	0.011479	-3.678662

C	-1.349106	-2.278998	-2.949196
C	-1.166041	-2.726153	-4.267325
C	-0.766619	-0.441437	-4.995026
H	-0.882900	1.087183	-3.462295
H	-1.582657	-3.001985	-2.154375
H	-1.254830	-3.799443	-4.493287
H	-0.543784	0.283544	-5.792785
H	-0.740915	-2.162756	-6.326420
C	1.841771	-1.588158	-1.757099
C	2.323579	-4.052986	-3.043297
C	2.229771	-1.618376	-3.111295
C	1.675834	-2.805299	-1.053825
C	1.927189	-4.028207	-1.694080
C	2.465269	-2.848453	-3.749953
H	2.334739	-0.683898	-3.680127
H	1.357680	-2.781060	0.002403
H	1.809831	-4.968704	-1.133988
H	2.759220	-2.860941	-4.810661
H	2.514943	-5.013799	-3.545660

	real2-2Mes	RI-BP86/SVP	
55			
E(SCF) =	-1979.380876		
C	3.319272	-0.543126	0.376364
C	2.415772	0.455671	-0.074178
C	2.839733	1.801021	-0.250936
C	4.146704	2.143940	0.138375
C	5.042429	1.197057	0.670983
C	4.613565	-0.139503	0.760811
N	1.087066	0.094616	-0.497721
C	0.870351	-0.431756	-1.857067
C	-0.655321	-0.361752	-2.001837
N	-1.105754	-0.192668	-0.606607
C	-0.075796	0.131212	0.244039
C	-2.515287	-0.209771	-0.343107
C	-3.140444	-1.440961	-0.022759
C	-4.534115	-1.442647	0.177911
C	-5.309557	-0.271965	0.061167
C	-4.651354	0.932290	-0.256863
C	-3.259440	0.990802	-0.465200
Ru	-0.083352	0.432481	2.152981
Cl	0.609574	2.649110	2.307408
C	-2.330835	-2.705166	0.134008
C	-6.808701	-0.314864	0.249087
C	-2.574821	2.307701	-0.745802
C	1.930465	2.845466	-0.850168

C	6.420368	1.608231	1.134653
C	2.958348	-2.009035	0.383737
Cl	0.399090	-1.780019	2.725127
C	-1.833493	0.567969	2.585510
H	1.408329	0.184103	-2.605264
H	1.252705	-1.473651	-1.934228
H	-1.092144	-1.279810	-2.443095
H	-0.987046	0.500791	-2.623061
H	-2.732761	0.566376	1.940988
H	-2.011717	0.687865	3.685455
H	-5.028142	-2.392976	0.438455
H	-5.237483	1.862121	-0.339620
H	4.475818	3.188663	0.015302
H	5.313192	-0.906502	1.131141
H	3.667110	-2.584146	1.009848
H	1.940418	-2.186798	0.780322
H	3.013430	-2.434481	-0.642529
H	2.511329	3.726012	-1.185772
H	1.361805	2.455765	-1.718461
H	1.191233	3.186657	-0.095894
H	7.129377	0.757184	1.121856
H	6.839317	2.418741	0.505241
H	6.386754	1.992225	2.177181
H	-3.312981	3.126838	-0.837672
H	-1.867080	2.571250	0.068387
H	-1.984233	2.281685	-1.685139
H	-2.982577	-3.564396	0.381971
H	-1.779291	-2.959658	-0.795685
H	-1.570210	-2.599331	0.936286
H	-7.218133	0.681366	0.507011
H	-7.316852	-0.648841	-0.681432
H	-7.099620	-1.025338	1.048413

	real3a-1Ph	RI-BP86/SVP	
81			
E(SCF) =	-3242.687096		
C	-0.067230	0.257932	-0.120249
Ru	0.020966	0.757648	2.045653
Cl	0.619162	-1.502981	2.562225
C	-1.796943	0.687926	2.266315
C	-0.122988	1.125110	4.306681
C	1.181474	1.348717	3.887550
Cl	0.293895	3.074740	1.489087
H	-2.362533	1.007741	3.166281
H	-2.439273	0.287560	1.454189
H	1.546164	2.371468	3.707561

H	-0.805012	1.975706	4.463571
H	-0.416907	0.161393	4.750345
H	1.940905	0.554539	3.977285
P	1.501298	-0.022211	-0.783786
P	-1.481770	-0.052344	-1.061394
C	2.836331	0.083190	0.499250
C	4.947469	0.358515	2.352550
C	3.555051	-1.050481	0.933903
C	3.193291	1.359216	0.990813
C	4.240102	1.490421	1.919238
C	4.604333	-0.910168	1.854556
H	3.300744	-2.048985	0.555165
H	2.643424	2.253457	0.663284
H	4.501559	2.489523	2.299651
H	5.155473	-1.802920	2.187060
H	5.770947	0.463466	3.075725
C	1.766707	-1.673822	-1.594775
C	2.017902	-4.262569	-2.695234
C	2.313389	-1.850314	-2.883160
C	1.334740	-2.805993	-0.864340
C	1.468033	-4.091898	-1.412188
C	2.437035	-3.139956	-3.428162
H	2.626504	-0.980795	-3.477733
H	0.898781	-2.668826	0.140086
H	1.134167	-4.965705	-0.832024
H	2.860634	-3.264942	-4.436722
H	2.115070	-5.271289	-3.125615
C	2.132611	1.251028	-1.988014
C	3.114049	3.291688	-3.669461
C	1.321723	2.350353	-2.317847
C	3.457825	1.196004	-2.478416
C	3.940632	2.207394	-3.322736
C	1.808914	3.365730	-3.158860
H	0.315720	2.413580	-1.879079
H	4.126955	0.373739	-2.181130
H	4.973300	2.156517	-3.701057
H	1.166462	4.224844	-3.405309
H	3.497421	4.088384	-4.325510
C	-1.285454	-0.069904	-2.908064
C	-0.986146	-0.087655	-5.718743
C	-1.554574	1.091361	-3.665742
C	-0.872880	-1.243641	-3.576944
C	-0.723663	-1.248745	-4.973592
C	-1.403313	1.081739	-5.061077
H	-1.902177	2.006079	-3.163580
H	-0.679165	-2.164537	-3.008656

H	-0.402762	-2.171784	-5.479868
H	-1.621247	1.993533	-5.637793
H	-0.872639	-0.095652	-6.813706
C	-2.803527	1.230241	-0.806165
C	-4.731565	3.280902	-0.589748
C	-2.408631	2.546963	-0.489680
C	-4.173328	0.944939	-0.999165
C	-5.129653	1.967554	-0.893783
C	-3.372205	3.564463	-0.381650
H	-1.350940	2.766988	-0.268497
H	-4.504151	-0.080005	-1.217606
H	-6.194692	1.732374	-1.043583
H	-3.049878	4.582909	-0.116049
H	-5.484508	4.079620	-0.503276
C	-2.351787	-1.671936	-0.740583
C	-3.665983	-4.106632	-0.169123
C	-3.278620	-2.219644	-1.658882
C	-2.077664	-2.364130	0.456993
C	-2.738435	-3.572533	0.739640
C	-3.930766	-3.430163	-1.372553
H	-3.484826	-1.710099	-2.612343
H	-1.325362	-1.974248	1.163750
H	-2.513532	-4.100207	1.679238
H	-4.646118	-3.848847	-2.097409
H	-4.177653	-5.055791	0.053794

	real3b-2Mes	RI-BP86/SVP	
61			
E(SCF) =	-2057.916960		
C	-2.938852	-1.639968	-0.671603
C	-2.427938	-0.337117	-0.903210
C	-3.278706	0.794799	-0.971563
C	-4.659053	0.595198	-0.774968
C	-5.204561	-0.679221	-0.526049
C	-4.327321	-1.780603	-0.482956
N	-1.023087	-0.174920	-1.162588
C	-0.580185	-0.280591	-2.573315
C	0.940189	-0.088232	-2.470842
N	1.155417	0.053770	-1.015190
C	-0.000109	0.011819	-0.286467
C	2.506401	0.205630	-0.531474
C	3.091038	1.500065	-0.462790
C	4.400065	1.612382	0.046065
C	5.157407	0.490785	0.428737
C	4.591526	-0.781991	0.227991
C	3.287027	-0.955235	-0.271245

C	2.419613	2.728391	-1.029593
C	2.814784	-2.346426	-0.622159
C	6.536000	0.645454	1.027305
Ru	0.031314	0.277099	1.800991
Cl	0.746847	-2.014096	1.842680
C	-2.723592	2.176997	-1.213693
C	-6.685849	-0.856381	-0.282931
C	-2.021836	-2.835743	-0.586061
C	-1.734584	0.052290	2.163631
C	0.254136	1.293937	3.870758
C	0.484807	-0.057480	4.046868
Cl	0.071352	2.608414	1.227254
H	1.297795	0.820580	-2.998515
H	1.514598	-0.953686	-2.860726
H	-0.868137	-1.269373	-2.988038
H	-1.077692	0.496903	-3.188907
H	-2.120495	0.164138	3.206207
H	-2.502798	-0.205926	1.409756
H	-4.733603	-2.787735	-0.294283
H	-5.328417	1.469921	-0.817415
H	4.845766	2.617475	0.126197
H	5.188854	-1.680074	0.455641
H	3.213650	-3.092146	0.091749
H	1.715411	-2.435987	-0.606379
H	3.188551	-2.626400	-1.632574
H	2.670896	3.628726	-0.436590
H	2.783193	2.907091	-2.066170
H	1.319760	2.643862	-1.040503
H	7.194013	-0.207467	0.767215
H	7.027821	1.579088	0.689476
H	6.482285	0.687768	2.136786
H	-3.529024	2.935515	-1.189137
H	-1.960763	2.446608	-0.451910
H	-2.225917	2.254266	-2.204101
H	-2.598529	-3.763026	-0.406737
H	-1.441303	-2.980385	-1.521957
H	-1.278079	-2.721208	0.232410
H	-7.282634	-0.089149	-0.814665
H	-7.037441	-1.855372	-0.608471
H	-6.924847	-0.763360	0.798644
H	1.505848	-0.467802	4.054371
H	1.083894	2.003388	3.733956
H	-0.719557	1.751398	4.105920
H	-0.294934	-0.734298	4.429153

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81

E(SCF) = -3242.691976

C	-0.147495	0.113794	-0.137721
Ru	0.041548	0.314401	2.029552
Cl	0.556206	-2.101063	2.019861
C	-1.669556	-0.048852	2.499150
C	1.102875	-0.035411	3.949575
C	0.654454	1.291907	3.957516
Cl	-0.481068	2.697819	1.703972
H	-2.413227	0.768783	2.642923
H	-2.012205	-1.093664	2.669741
H	-0.254273	1.584727	4.504202
H	0.580346	-0.829354	4.501832
H	2.143165	-0.270998	3.670816
H	1.330645	2.120642	3.704443
P	1.419258	0.223369	-0.844557
P	-1.578999	-0.202586	-1.051828
C	2.662140	0.405092	0.518028
C	4.613212	0.868290	2.502817
C	3.572474	-0.615045	0.872591
C	2.740200	1.663433	1.162157
C	3.714008	1.886493	2.152413
C	4.539242	-0.381374	1.861157
H	3.532082	-1.593488	0.376657
H	2.038056	2.468722	0.897387
H	3.767694	2.869278	2.644853
H	5.241724	-1.184237	2.131456
H	5.377382	1.046994	3.274865
C	1.975208	-1.229101	-1.856437
C	2.796607	-3.541609	-3.249945
C	2.464188	-1.128526	-3.175141
C	1.871893	-2.502347	-1.248258
C	2.293964	-3.647661	-1.941365
C	2.869783	-2.282851	-3.867140
H	2.518947	-0.151922	-3.675944
H	1.459189	-2.583717	-0.224769
H	2.223589	-4.632130	-1.453288
H	3.242965	-2.193336	-4.898921
H	3.122341	-4.442374	-3.792957
C	1.802831	1.740989	-1.848841
C	2.367974	4.132561	-3.230889
C	0.810274	2.728393	-1.993014
C	3.096586	1.974535	-2.368905
C	3.372744	3.161920	-3.063892
C	1.091857	3.918588	-2.686826
H	-0.171882	2.574618	-1.521148

H	3.899441	1.236839	-2.215697
H	4.381856	3.336203	-3.468163
H	0.309810	4.686390	-2.788043
H	2.588887	5.065573	-3.771955
C	-1.216524	-0.855169	-2.752569
C	-0.645265	-1.778794	-5.361689
C	-0.885382	0.056287	-3.781000
C	-1.257431	-2.233691	-3.047226
C	-0.972548	-2.690341	-4.344575
C	-0.600280	-0.404371	-5.075942
H	-0.865492	1.136791	-3.577371
H	-1.526641	-2.957225	-2.264805
H	-1.013726	-3.768701	-4.560386
H	-0.349069	0.318936	-5.866843
H	-0.429485	-2.139785	-6.379023
C	-2.769651	1.178345	-1.463677
C	-4.637161	3.210976	-2.058432
C	-2.795348	2.361030	-0.700714
C	-3.691779	1.015940	-2.525390
C	-4.617635	2.028775	-2.820214
C	-3.727734	3.371085	-1.001582
H	-2.076230	2.499516	0.128644
H	-3.691192	0.094783	-3.127628
H	-5.327183	1.893319	-3.651309
H	-3.735388	4.291184	-0.396754
H	-5.362852	4.005486	-2.292440
C	-2.685276	-1.453110	-0.253398
C	-4.310283	-3.456654	0.894140
C	-4.076306	-1.251432	-0.114058
C	-2.112993	-2.660029	0.205944
C	-2.925309	-3.655986	0.771099
C	-4.881742	-2.249391	0.458796
H	-4.536086	-0.309957	-0.444478
H	-1.021386	-2.788801	0.188067
H	-2.462786	-4.585073	1.137370
H	-5.963433	-2.077067	0.568577
H	-4.944084	-4.237182	1.342937

	real3c-2Mes	RI-BP86/SVP	
61			
E(SCF) =	-2057.926421		
C	-3.107764	-1.559332	-0.184108
C	-2.550115	-0.268454	-0.382575
C	-3.371441	0.887365	-0.461140
C	-4.755342	0.730065	-0.252298
C	-5.338718	-0.525315	0.003364

C	-4.498355	-1.654535	0.017683
N	-1.138152	-0.145691	-0.644255
C	-0.664209	-0.252049	-2.045541
C	0.860123	-0.069098	-1.919874
N	1.047918	0.106620	-0.463710
C	-0.120702	0.058295	0.228413
C	2.362177	0.307098	0.100347
C	2.894989	1.624352	0.174259
C	4.181086	1.786629	0.726099
C	4.956450	0.695314	1.161120
C	4.431559	-0.599157	0.986784
C	3.152183	-0.825813	0.442352
C	2.140876	2.820073	-0.348525
C	2.670188	-2.234131	0.205903
C	6.314585	0.906245	1.788690
Ru	-0.088808	0.290624	2.280197
Cl	0.037132	-2.152011	2.407402
C	-2.796039	2.247090	-0.767263
C	-6.821275	-0.655430	0.265295
C	-2.252141	-2.800804	-0.195739
C	-1.862612	0.138021	2.624131
C	0.856408	1.299003	4.064316
C	1.004464	-0.077200	4.220216
Cl	-0.483807	2.671042	1.861505
H	1.234582	0.821283	-2.466276
H	1.432110	-0.949810	-2.278199
H	-0.947593	-1.238144	-2.467744
H	-1.143396	0.530759	-2.668604
H	-2.516899	1.035699	2.638163
H	-2.312907	-0.851587	2.852249
H	-4.936669	-2.652278	0.182833
H	-5.397603	1.624501	-0.301153
H	4.594431	2.805760	0.798204
H	5.043516	-1.472364	1.265504
H	3.468299	-2.964377	0.438885
H	1.786532	-2.463736	0.840587
H	2.369020	-2.393078	-0.850830
H	2.762137	3.733369	-0.281569
H	1.852254	2.689671	-1.412752
H	1.206846	2.986871	0.231126
H	6.993254	0.052462	1.593448
H	6.800302	1.829061	1.414410
H	6.228634	1.007904	2.892255
H	-3.594435	3.012587	-0.802722
H	-2.050618	2.549259	0.000269
H	-2.277768	2.262818	-1.749952

H	-2.871093	-3.705748	-0.045229
H	-1.716414	-2.922382	-1.161490
H	-1.480190	-2.763739	0.603500
H	-7.400457	0.131043	-0.257887
H	-7.208917	-1.642753	-0.055047
H	-7.042068	-0.555119	1.350150
H	1.935542	-0.586437	3.925272
H	1.666594	1.914163	3.641997
H	0.059892	1.857788	4.577082
H	0.331054	-0.663294	4.862574

	real4-1Ph	RI-BP86/SVP	
81			
E(SCF) =	-3242.710001		
C	-0.062443	-0.131318	0.003586
Ru	-0.429923	-0.583388	1.941794
Cl	1.672324	-1.743964	2.099732
C	-1.239029	-2.090217	2.943064
C	-0.828987	-1.108000	4.117407
C	-0.102714	0.241855	3.720435
Cl	-2.559045	0.566615	2.002451
H	-2.334838	-2.197403	2.834948
H	-0.678764	-3.044285	2.964227
H	-0.695443	1.139246	3.981443
H	-1.765406	-0.822066	4.633268
H	-0.122173	-1.667956	4.759456
H	0.950922	0.270528	4.058720
P	1.591946	-0.193763	-0.602564
P	-1.488189	0.147083	-0.998625
C	2.815883	0.764283	0.407480
C	4.676928	2.398030	1.761829
C	4.144983	0.871649	-0.058773
C	2.420594	1.507614	1.533663
C	3.346820	2.320229	2.206421
C	5.072725	1.673262	0.625446
H	4.460754	0.343821	-0.971206
H	1.383117	1.436389	1.892444
H	3.023836	2.892513	3.089460
H	6.108282	1.739815	0.258085
H	5.402982	3.031492	2.294210
C	2.323496	-1.849008	-1.007170
C	3.324172	-4.389253	-1.731449
C	1.608698	-2.671528	-1.901698
C	3.535876	-2.319090	-0.460438
C	4.033664	-3.577413	-0.828460
C	2.107455	-3.935183	-2.262867

H	0.652848	-2.325923	-2.321888
H	4.072336	-1.717526	0.285764
H	4.977633	-3.934758	-0.389315
H	1.536345	-4.566297	-2.961059
H	3.714987	-5.379997	-2.009741
C	1.809484	0.776558	-2.178488
C	2.347757	2.435952	-4.402547
C	1.557028	2.166887	-2.116725
C	2.342639	0.230532	-3.362948
C	2.605411	1.057972	-4.469197
C	1.821658	2.989086	-3.221283
H	1.163927	2.611991	-1.190318
H	2.562593	-0.844296	-3.426471
H	3.022233	0.617075	-5.387641
H	1.624884	4.070126	-3.154789
H	2.565220	3.082332	-5.266817
C	-1.304077	-0.149162	-2.837163
C	-1.115322	-0.613648	-5.627295
C	-1.054612	0.914988	-3.731454
C	-1.470169	-1.449295	-3.367510
C	-1.369299	-1.679487	-4.749482
C	-0.962715	0.684063	-5.112820
H	-0.934435	1.937574	-3.350755
H	-1.714391	-2.289058	-2.701395
H	-1.509112	-2.698920	-5.140547
H	-0.770192	1.529842	-5.789880
H	-1.046837	-0.792532	-6.711339
C	-2.184393	1.862757	-0.966196
C	-3.143604	4.514476	-0.924569
C	-1.631596	2.804312	-0.075762
C	-3.216576	2.261216	-1.843991
C	-3.699461	3.580910	-1.814465
C	-2.104752	4.125378	-0.061732
H	-0.839130	2.481288	0.614456
H	-3.638396	1.550810	-2.570442
H	-4.508861	3.879982	-2.497967
H	-1.667590	4.852011	0.639835
H	-3.519554	5.549052	-0.905254
C	-2.804385	-1.089612	-0.598040
C	-4.730904	-3.103066	-0.164038
C	-4.177270	-0.787593	-0.686846
C	-2.400784	-2.402686	-0.278587
C	-3.363344	-3.404828	-0.066166
C	-5.133372	-1.791382	-0.469005
H	-4.507872	0.240545	-0.887062
H	-1.330437	-2.635520	-0.166550

H	-3.036352	-4.424339	0.189432
H	-6.203736	-1.540247	-0.522466
H	-5.484666	-3.886252	0.009907

	real4-2Mes	RI-BP86/SVP	
6l			
E(SCF) =	-2057.946781		
C	1.030348	3.235021	-1.051277
C	1.562382	1.924385	-1.175631
C	2.941836	1.660438	-0.967362
C	3.762471	2.729674	-0.557905
C	3.262714	4.032762	-0.375042
C	1.899683	4.263920	-0.641373
N	0.697502	0.860045	-1.623657
C	-0.000055	0.000024	-0.842417
N	-0.697679	-0.860030	-1.623552
C	-0.528380	-0.562021	-3.063843
C	0.528065	0.561981	-3.063918
C	-1.562433	-1.924425	-1.175420
C	-2.941928	-1.660650	-0.967204
C	-3.762426	-2.729961	-0.557674
C	-3.262497	-4.032967	-0.374687
C	-1.899426	-4.263959	-0.640957
C	-1.030226	-3.234977	-1.050941
Ru	0.000014	0.000093	1.166860
Cl	1.800570	-1.597077	1.258962
C	-3.528558	-0.287136	-1.174374
C	-4.160183	-5.150860	0.103338
C	0.419660	-3.530304	-1.339451
C	3.528289	0.286833	-1.174441
C	4.160542	5.150574	0.102906
C	-0.419485	3.530522	-1.339876
Cl	-1.800552	1.597318	1.258439
C	0.894065	1.008287	2.610737
C	-0.000005	0.000219	3.443109
C	-0.894287	-1.007748	2.610819
H	0.194892	1.468827	-3.608372
H	1.496227	0.240858	-3.503695
H	-0.195255	-1.468890	-3.608286
H	-1.496580	-0.240915	-3.503543
H	1.978415	0.821071	2.711806
H	0.579943	2.062836	2.712538
H	-0.694059	0.616292	4.045156
H	-1.978602	-0.820321	2.711857
H	-0.580355	-2.062343	2.712752
H	0.694135	-0.615891	4.045010

H	-4.833489	-2.533470	-0.387272
H	-1.493108	-5.283084	-0.535267
H	4.833503	2.533053	-0.387457
H	1.493495	5.283103	-0.535759
H	0.608762	-4.620633	-1.328451
H	0.735825	-3.142261	-2.330041
H	1.073869	-3.051937	-0.577151
H	-4.631758	-0.315731	-1.091916
H	-3.139791	0.431818	-0.419214
H	-3.277484	0.126156	-2.173555
H	-3.842661	-6.132585	-0.300823
H	-4.135010	-5.232325	1.211701
H	-5.216036	-4.981476	-0.186511
H	3.843139	6.132312	-0.301313
H	4.135386	5.232108	1.211263
H	5.216373	4.981042	-0.186938
H	4.631514	0.315343	-1.092271
H	3.139650	-0.431963	-0.419060
H	3.276911	-0.126621	-2.173475
H	-0.608484	4.620868	-1.328735
H	-0.735587	3.142668	-2.330564
H	-1.073798	3.052112	-0.577696

	RuCl2PCy3	RI-BP86/SVP	
58			
E(SCF) =	-2101.224795		
Ru	0.303745	0.529727	2.596141
C	-1.493212	0.443576	2.383669
P	0.454758	0.738395	4.826031
C	2.259263	0.893915	5.398870
C	2.950032	2.207821	4.973100
C	4.380444	2.296624	5.537454
C	5.230010	1.079100	5.145823
C	4.542232	-0.226831	5.568519
C	3.116105	-0.327963	4.998793
C	-0.155026	-0.805267	5.745409
C	0.302767	-0.978165	7.212747
C	-0.105618	-2.362010	7.755698
C	-1.616493	-2.604672	7.628308
C	-2.084290	-2.409280	6.179099
C	-1.677719	-1.030880	5.625741
C	-0.328565	2.325231	5.497582
C	-1.762820	2.613459	5.004831
C	-2.220194	4.020509	5.432470
C	-2.104809	4.232284	6.949257
C	-0.682548	3.927764	7.442089

C	-0.228507	2.514552	7.027765
Cl	0.898356	2.726775	2.116305
Cl	1.058941	-1.666315	2.469818
H	-1.812796	0.335422	1.315720
H	-2.315840	0.483725	3.126355
H	0.337450	-1.594515	5.131896
H	-2.219578	-0.238811	6.189541
H	-1.991293	-0.951091	4.566586
H	-3.185600	-2.531840	6.103836
H	-1.637621	-3.199939	5.535900
H	-2.159691	-1.892395	8.290435
H	-1.877012	-3.622707	7.987547
H	0.218029	-2.455216	8.814241
H	0.442574	-3.148888	7.190699
H	-0.155786	-0.191600	7.849071
H	1.400923	-0.860559	7.306802
H	2.175108	0.903280	6.510275
H	2.973378	2.271370	3.864832
H	2.368128	3.088480	5.313511
H	4.857326	3.235763	5.185439
H	4.334846	2.368745	6.648375
H	5.377246	1.074336	4.042508
H	6.242555	1.150289	5.596663
H	5.134953	-1.106292	5.239287
H	4.501089	-0.277788	6.680759
H	3.160771	-0.398059	3.891365
H	2.642714	-1.273709	5.332523
H	0.322633	3.081305	5.002294
H	-0.878701	1.767936	7.533906
H	0.803995	2.332108	7.390767
H	-0.619261	4.031263	8.546273
H	0.024022	4.675549	7.016817
H	-2.824368	3.561180	7.471484
H	-2.394813	5.269322	7.220754
H	-3.263579	4.192127	5.092875
H	-1.594258	4.775082	4.905669
H	-2.467020	1.857603	5.417629
H	-1.800305	2.530995	3.901499

Fragmente/HG-Fragmente/RI-BP86_SVP

	Ag+_1H	RI-BP86/SVP	
10			
E(SCF) =	-871.019910		
C	-0.429953	0.150518	0.837539
P	-0.838480	-1.243463	1.737993
P	0.089250	0.049210	-0.787600

H	-0.226019	-2.443847	1.252865
H	-2.210736	-1.652811	1.869419
H	-0.441320	-1.188778	3.106856
H	0.651660	-1.221220	-1.135566
H	1.114740	0.979777	-1.129630
H	-0.838565	0.258857	-1.866093
Ag	-0.980819	2.009343	1.586618

	Ag+_1Ph	RI-BP86/SVP	
70			
E(SCF) =	-2256.093497		
C	-1.411854	-1.640957	1.406654
P	-3.064792	-1.298703	1.760401
P	-0.117940	-2.159177	2.422028
C	1.051895	-3.187851	1.431076
C	-0.600268	-3.193143	3.871224
C	0.927544	-0.807456	3.136561
C	-3.372402	-0.421628	3.353320
C	-3.743936	-0.213534	0.428472
C	-4.204916	-2.750785	1.742678
Ag	-0.854828	-1.158777	-0.556017
C	1.652742	-0.989902	4.339957
C	2.479265	0.048114	4.840027
C	2.589314	1.275908	4.130712
C	1.863602	1.455970	2.920316
C	1.035790	0.415049	2.432656
C	-2.519658	0.658738	3.696146
C	-2.720678	1.375257	4.901267
C	-3.779708	1.007494	5.778137
C	-4.628369	-0.081369	5.436915
C	-4.423053	-0.791512	4.226601
C	-3.682477	-4.052061	1.914945
C	-4.544325	-5.178133	1.898893
C	-5.940933	-4.999329	1.701899
C	-6.465215	-3.688304	1.521560
C	-5.597123	-2.569067	1.542475
C	-3.914462	-0.769881	-0.867994
C	-4.371133	0.038309	-1.939289
C	-4.664425	1.414271	-1.715958
C	-4.509528	1.962061	-0.414333
C	-4.051863	1.145602	0.654429
C	-0.407918	-4.596746	3.845073
C	-0.812371	-5.395145	4.944075
C	-1.415067	-4.789582	6.080786
C	-1.602788	-3.379763	6.108123
C	-1.194419	-2.586800	5.007321

C	2.441049	-3.176824	1.698792
C	3.319663	-3.998180	0.946681
C	2.807153	-4.841858	-0.076712
C	1.408952	-4.856092	-0.341331
C	0.538779	-4.029215	0.412148
H	0.071943	-5.087475	2.988657
H	-0.651449	-6.482273	4.923468
H	-1.726232	-5.406132	6.936527
H	-2.059224	-2.905104	6.987971
H	-1.340524	-1.500680	5.061948
H	2.865820	-2.528494	2.475367
H	4.399510	-3.979433	1.151126
H	3.487689	-5.478198	-0.661026
H	1.007591	-5.510380	-1.128198
H	-0.538837	-4.048743	0.197250
H	0.473996	0.567736	1.499371
H	1.948491	2.402316	2.367813
H	3.232087	2.080929	4.515671
H	3.037037	-0.094670	5.776482
H	1.585112	-1.926666	4.908022
H	-2.605748	-4.203515	2.060611
H	-4.136337	-6.189250	2.035489
H	-6.613050	-5.869480	1.683492
H	-7.543470	-3.547729	1.360290
H	-6.023997	-1.569401	1.386099
H	-3.746281	-1.841287	-1.050707
H	-4.519889	-0.398074	-2.937393
H	-5.022868	2.044373	-2.542944
H	-4.749653	3.019401	-0.233326
H	-3.950711	1.593735	1.650658
H	-1.686020	0.946151	3.041886
H	-2.059472	2.213713	5.162197
H	-3.939815	1.561178	6.714779
H	-5.444798	-0.372120	6.112992
H	-5.085475	-1.634084	3.992910

	Ag-(H+)-1H	RI-BP86/SVP	
11			
E(SCF) =	-871.247211		
C	0.798001	0.000063	-0.441860
P	1.584451	1.558943	0.064229
H	2.964108	1.693172	-0.286132
H	1.511554	1.770285	1.468410
H	0.906261	2.635547	-0.568280
P	1.584913	-1.558752	0.064235
H	2.964595	-1.692177	-0.286200

H	0.906765	-2.635288	-0.568393
H	1.512077	-1.770283	1.468394
Ag	-1.359083	-0.000093	0.022412
H	0.783091	-0.000128	-1.556980

	Ag-(H+)-1Ph	RI-BP86/SVP	
71			
E(SCF) =	-2256.413620		
C	-1.527782	-2.005360	1.365703
P	-3.176710	-1.328081	1.812133
P	-0.119380	-2.389337	2.461195
C	1.075683	-3.238730	1.367934
C	-0.530942	-3.517134	3.838577
C	0.687410	-0.899412	3.141786
C	-3.233193	-0.365020	3.354084
C	-3.688276	-0.216819	0.436553
C	-4.390287	-2.683437	1.865190
H	-1.749840	-2.966345	0.853950
Ag	-0.858470	-0.855737	-0.384858
C	1.072582	-0.867596	4.505840
C	1.781837	0.249611	5.019069
C	2.117919	1.336856	4.166155
C	1.744526	1.295705	2.790806
C	1.036422	0.179552	2.287988
C	-2.357688	0.736489	3.550338
C	-2.464485	1.520755	4.724629
C	-3.450634	1.209420	5.705013
C	-4.328884	0.108059	5.500031
C	-4.220825	-0.677248	4.324374
C	-4.023776	-3.960106	2.365073
C	-4.987148	-4.997707	2.422489
C	-6.320199	-4.759335	1.981253
C	-6.682551	-3.474898	1.483556
C	-5.717935	-2.438205	1.424775
C	-3.617996	-0.708813	-0.902356
C	-3.987565	0.128681	-1.987526
C	-4.427089	1.463546	-1.739681
C	-4.512815	1.939262	-0.402768
C	-4.144005	1.097121	0.683913
C	0.037224	-4.816983	3.878325
C	-0.275082	-5.695195	4.947545
C	-1.153935	-5.273945	5.984032
C	-1.717429	-3.965554	5.943339
C	-1.407437	-3.091546	4.873806
C	2.452547	-2.914032	1.463013
C	3.398158	-3.589717	0.649053

C	2.967972	-4.595495	-0.260585
C	1.584128	-4.925592	-0.345661
C	0.642286	-4.250774	0.468733
H	0.735210	-5.164320	3.106060
H	0.172284	-6.699721	4.982599
H	-1.389240	-5.952024	6.818892
H	-2.385842	-3.635376	6.752075
H	-1.845655	-2.085113	4.881371
H	2.817076	-2.148792	2.160404
H	4.466931	-3.339248	0.723596
H	3.701327	-5.121720	-0.891079
H	1.253020	-5.712911	-1.039152
H	-0.410414	-4.555416	0.391204
H	0.788644	0.162746	1.213648
H	2.023328	2.126256	2.125532
H	2.676211	2.199573	4.561840
H	2.082546	0.269960	6.077247
H	0.849133	-1.698149	5.186840
H	-3.008864	-4.171479	2.726405
H	-4.709828	-5.989880	2.807809
H	-7.068602	-5.565832	2.022587
H	-7.711682	-3.290855	1.140535
H	-6.024488	-1.460403	1.030170
H	-3.391259	-1.764131	-1.121128
H	-3.968883	-0.257298	-3.018280
H	-4.718644	2.114004	-2.579056
H	-4.870710	2.961634	-0.207758
H	-4.229075	1.494806	1.703513
H	-1.596190	1.011053	2.809078
H	-1.793580	2.378302	4.879704
H	-3.539279	1.824334	6.614092
H	-5.098334	-0.126434	6.250728
H	-4.916587	-1.515465	4.185842

	Ag6	RI-BP86/SVP	
2			
E(SCF) =	-607.210402		
Ag	0.000000	0.000000	0.308427
Cl	0.000000	0.000000	2.611973

	AlCl3	RI-BP86/SVP	
4			
E(SCF) =	-1622.904760		
Al	0.176817	-0.306023	0.125136
Cl	-0.172453	0.298304	2.100795
Cl	1.922717	0.298637	-0.863093

Cl	-1.219974	-1.515663	-0.862838
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Au2Cl2	RI-BP86/SVP
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4

E(SCF) =	-1192.030365		
Au	0.000000	1.391582	0.000000
Cl	-2.148331	0.009516	0.000000
Au	-0.000011	-1.392074	0.000000
Cl	2.148382	-0.007233	0.000000

AuCl	RI-BP86/SVP
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2

E(SCF) =	-595.997757		
Au	0.000000	0.000000	0.322703
Cl	0.000000	0.000000	2.597697

B2H5+	RI-BP86/SVP
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7

E(SCF) =	-52.307701		
B	-1.287866	4.280748	19.574013
B	-2.807361	4.398192	19.581826
H	-2.089889	3.733011	20.524158
H	-1.960967	5.458942	19.632027
H	-0.097974	4.194802	19.569980
H	-2.091761	3.827231	18.579643
H	-3.996864	4.490229	19.587564

BCl3	RI-BP86/SVP
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4

E(SCF) =	-1405.274703		
B	0.176366	-0.305464	0.124269
Cl	-0.115454	0.199962	1.780070
Cl	1.640147	0.200764	-0.702171
Cl	-0.993952	-1.320007	-0.702168

BeCl2	RI-BP86/SVP
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3

E(SCF) =	-935.076830		
Be	0.534486	0.000000	0.379669
Cl	-0.513298	0.000000	1.863239
Cl	1.581587	0.000000	-1.104375

BeH2	RI-BP86/SVP
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3

E(SCF) =	-15.885380		
Be	0.534245	0.000000	0.379507

H	-0.241153	0.000000	1.477970
H	1.309683	0.000000	-0.718944

BeO RI-BP86/SVP

2			
E(SCF) =	-89.823494		
Be	-0.179437	0.000000	0.000000
O	1.179437	0.000000	0.000000

BH3 RI-BP86/SVP

4			
E(SCF) =	-26.574851		
B	0.176511	-0.305728	0.225127
H	-0.129389	0.224113	1.273113
H	1.240236	-0.046036	-0.299120
H	-0.580250	-1.097095	-0.299121

C(NMe2)2 RI-BP86/SVP

19			
E(SCF) =	-306.970166		
C	0.114000	0.005705	1.305902
N	0.816684	1.032975	1.846436
N	-0.238125	-1.058836	2.070023
C	0.232495	-1.498863	3.396681
C	-1.143798	-2.021475	1.445405
C	1.080525	1.394884	3.251626
C	1.301684	2.040149	0.904404
H	2.411615	2.123537	0.938403
H	0.879666	3.045644	1.134696
H	0.991951	1.729763	-0.108709
H	-0.479203	-1.261758	4.219915
H	2.105293	1.124049	3.593506
H	0.980519	2.495535	3.360302
H	0.342209	0.929495	3.926046
H	1.215796	-1.059248	3.634324
H	0.358157	-2.602129	3.381599
H	-0.677284	-3.031483	1.379210
H	-2.088410	-2.122834	2.026314
H	-1.378924	-1.653142	0.431631

CO RI-BP86/SVP

2			
E(SCF) =	-113.230067		
C	0.000000	0.000000	-0.652573
O	0.000000	0.000000	0.489430

	CO2	RI-BP86/SVP	
3			
E(SCF) =	-188.464208		
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.174890
O	0.000000	0.000000	-1.174890

	Cr4	RI-BP86/SVP	
11			
E(SCF) =	-1610.886051		
Cr	-1.938243	-0.061369	2.126061
C	-3.757679	-0.082775	2.051507
O	-4.922444	-0.096639	2.003157
C	-1.968947	1.647667	2.951647
O	-2.024449	2.691310	3.454314
C	-1.975325	-0.886593	3.835175
O	-2.034769	-1.390546	4.877979
C	-1.862554	-1.769993	1.302531
O	-1.853156	-2.814202	0.798092
C	-1.856357	0.765342	0.419274
O	-1.843265	1.270190	-0.624702

	Cr2 (T)	RI-BP86/SVP	
7			
E(SCF) =	-2191.350433		
Cr	0.000035	0.000023	0.871871
Cl	2.048754	0.000028	0.170965
Cl	-2.048729	0.000033	0.171094
C	0.000072	1.309399	2.158688
O	0.000094	2.146208	2.961016
C	0.000072	-1.309371	2.158670
O	0.000093	-2.146193	2.960984

	Cr3	RI-BP86/SVP	
9			
E(SCF) =	-1497.586341		
Cr	-1.793245	-0.139158	2.893977
C	-3.181873	-0.029038	1.747882
O	-4.076209	0.043972	0.997681
C	-1.866492	1.739911	3.127350
O	-1.994187	2.885449	3.277416
C	-2.930921	-0.335166	4.279962
O	-3.661683	-0.463113	5.184165
C	-1.781644	-2.020525	2.667089
O	-1.857235	-3.173118	2.537182

	CS2	RI-BP86/SVP	
3			
E(SCF) =	-834.320655		
C	0.009955	0.000000	0.000095
S	-0.003769	0.000000	1.571485
S	0.023658	0.000000	-1.571320

	Cu6	RI-BP86/SVP	
2			
E(SCF) =	-2100.677360		
Cu	0.000000	0.000000	0.423035
Cl	0.000000	0.000000	2.497365

	DAD	RI-BP86/SVP	
8			
E(SCF) =	-187.941251		
N	-1.437368	-0.000006	-0.348250
H	-2.446413	-0.000013	-0.584268
N	1.437379	0.000016	-0.348273
H	2.446421	0.000020	-0.584306
C	-0.748473	-0.000008	-1.430083
H	-1.195230	-0.000015	-2.455330
C	0.748466	0.000005	-1.430095
H	1.195206	0.000000	-2.455350

	Mo4	RI-BP86/SVP	
11			
E(SCF) =	-634.697125		
Mo	-1.894667	-0.060948	2.127968
C	-3.838617	-0.084024	2.048031
O	-5.004538	-0.098100	1.999402
C	-1.951821	1.793499	3.022671
O	-2.020286	2.836435	3.524144
C	-1.958882	-0.956738	3.981727
O	-2.031425	-1.460269	5.023396
C	-1.836643	-1.915161	1.233128
O	-1.840545	-2.958682	0.728239
C	-1.829810	0.836050	0.275078
O	-1.829953	1.340328	-0.768747

	Mo2	RI-BP86/SVP	
7			
E(SCF) =	-1215.098031		
Mo	-2.119795	-0.136656	2.826382
Cl	-3.718307	0.036870	1.168616
C	-1.655785	1.851676	2.995990

O	-1.273988	2.946084	3.070892
Cl	-3.060675	-0.425910	4.915542
C	-1.571076	-2.081115	2.489859
O	-1.144416	-3.141778	2.284887

	Mo3	RI-BP86/SVP	
9			
E(SCF) =	-521.399653		
Mo	-1.745016	-0.137734	2.889936
C	-3.249656	-0.020630	1.684883
O	-4.163386	0.050675	0.956879
C	-1.820366	1.898698	3.143185
O	-1.928480	3.046559	3.285456
C	-2.985352	-0.347736	4.355329
O	-3.739652	-0.474626	5.241275
C	-1.728419	-2.176316	2.641649
O	-1.783164	-3.329677	2.514112

	Ni(CO)2	RI-BP86/SVP	
5			
E(SCF) =	-1734.936228		
Ni	-0.274233	-0.052156	0.167154
C	0.377793	-0.103809	1.779185
O	0.778578	-0.388667	2.833772
C	-0.830161	-1.310574	-0.897661
O	-1.134321	-2.305661	-1.418449

	Ni(CO)3	RI-BP86/SVP	
7			
E(SCF) =	-1848.235676		
Ni	-0.514411	-0.033113	0.820839
C	0.689863	-0.512358	2.057343
O	1.463518	-0.823782	2.859432
C	-0.875061	-1.127746	-0.550923
O	-1.108085	-1.834715	-1.436768
C	-1.365457	1.537041	0.960481
O	-1.915782	2.550815	1.051375

	PH3	RI-BP86/SVP	
4			
E(SCF) =	-343.075525		
P	0.079489	0.181519	-0.029589
H	-0.140041	-0.614672	1.151565
H	1.209796	-0.619410	-0.427209
H	-0.832460	-0.619438	-0.806766

	PMe3	RI-BP86/SVP	
13			
E(SCF) =	-460.943192		
P	-0.015904	-0.000291	-0.008167
C	0.021067	0.006074	1.861848
C	1.211527	-1.374618	-0.329030
C	1.088906	1.472851	-0.336239
H	1.051789	0.052789	2.274282
H	-0.553440	0.876626	2.238456
H	-0.474226	-0.909975	2.243006
H	1.431993	-1.425389	-1.414645
H	2.166179	-1.240120	0.223454
H	0.762928	-2.345092	-0.034562
H	1.305067	1.536399	-1.422044
H	2.051183	1.423974	0.217250
H	0.558201	2.402705	-0.047308

	PMes3	RI-BP86/SVP	
61			
E(SCF) =	-1389.338040		
P	0.007075	0.006750	-1.459623
C	0.984315	-1.502225	-1.915416
C	2.544899	-3.894150	-2.177479
C	2.000910	-1.595818	-2.914322
C	0.752074	-2.627733	-1.058183
C	1.524172	-3.793436	-1.214958
C	2.756260	-2.783808	-3.011837
H	1.321334	-4.650764	-0.551648
H	3.533504	-2.843509	-3.791917
C	0.793638	1.529358	-2.168512
C	2.064332	4.011737	-2.837982
C	1.935466	1.990990	-1.434462
C	0.304220	2.322767	-3.250521
C	0.947398	3.542889	-3.549186
C	2.547112	3.206927	-1.790265
H	0.562162	4.141715	-4.391394
H	3.430327	3.537473	-1.218603
C	-1.745665	-0.152589	-2.044737
C	-4.567171	-0.361327	-2.514985
C	-2.669736	0.699678	-1.355393
C	-2.253533	-1.102704	-2.982463
C	-3.647639	-1.185317	-3.185154
C	-4.048213	0.584409	-1.612393
H	-4.024325	-1.919202	-3.917092
H	-4.739865	1.256988	-1.078186
C	2.298759	-0.503993	-3.917231

H	2.834376	0.354900	-3.464527
H	1.374767	-0.086575	-4.362074
H	2.928619	-0.897799	-4.738727
C	-0.320003	-2.613774	0.008938
H	-0.267816	-3.525172	0.635722
H	-1.339820	-2.560413	-0.427446
H	-0.222280	-1.722367	0.663747
C	3.391224	-5.140362	-2.293329
H	3.872661	-5.217492	-3.288159
H	2.792264	-6.058628	-2.127855
H	4.203589	-5.144516	-1.534216
C	2.525608	1.197703	-0.289642
H	3.325332	1.770478	0.218818
H	2.962891	0.236090	-0.632416
H	1.747387	0.929457	0.455577
C	-0.850874	1.916041	-4.137686
H	-0.777514	0.857587	-4.454154
H	-0.877089	2.546399	-5.047902
H	-1.832049	2.015678	-3.630900
C	2.712186	5.335694	-3.169715
H	2.376971	6.131990	-2.469991
H	2.457158	5.671061	-4.194325
H	3.816847	5.282133	-3.089520
C	-2.208417	1.744892	-0.364013
H	-1.540570	1.301439	0.404289
H	-3.071268	2.219008	0.142823
H	-1.618506	2.549015	-0.852599
C	-1.379474	-2.012664	-3.816083
H	-0.521795	-1.471043	-4.259981
H	-1.967311	-2.460991	-4.640709
H	-0.942846	-2.842554	-3.224234
C	-6.055465	-0.496499	-2.737328
H	-6.282120	-0.991201	-3.702385
H	-6.561868	0.489816	-2.727911
H	-6.525886	-1.107857	-1.936607

	PPh3	RI-BP86/SVP	
34			
E(SCF) =	-1035.576021		
P	-1.201722	0.001510	0.001378
C	-0.387080	0.220294	-1.656781
C	-0.386475	-1.544294	0.639086
C	-0.381757	1.325902	1.018600
C	0.731382	-0.525547	-2.099494
C	1.263415	-0.331086	-3.399414
C	0.679454	0.625533	-4.272996

C	-0.444946	1.377348	-3.833487
C	-0.974493	1.165083	-2.537134
H	1.197678	-1.269804	-1.441089
H	2.129272	-0.919566	-3.732543
H	1.088465	0.778694	-5.281182
H	-0.908071	2.113773	-4.504590
H	-1.856764	1.739167	-2.223402
C	0.743846	-1.555109	1.491013
C	1.277022	-2.777879	1.971800
C	0.682166	-4.012204	1.594789
C	-0.454061	-4.007154	0.739469
C	-0.984499	-2.778376	0.275709
H	-1.875787	-2.793058	-0.365999
H	-0.925496	-4.956091	0.448873
H	1.092057	-4.961709	1.965770
H	2.152080	-2.772544	2.636044
H	1.218365	-0.613132	1.794842
C	-0.975042	1.628193	2.271242
C	-0.440984	2.643475	3.101999
C	0.694222	3.386078	2.674969
C	1.284439	3.095388	1.415374
C	0.747642	2.068326	0.598356
H	1.218690	1.860420	-0.371069
H	2.158778	3.667417	1.075791
H	1.106898	4.181616	3.310596
H	-0.908862	2.866241	4.070840
H	-1.865490	1.080258	2.607813

	ReO3+	RI-BP86/SVP	
4			
E(SCF) =	-303.610935		
Re	0.669942	0.444670	1.859055
O	1.820335	0.513402	3.130283
O	1.218746	-0.839460	0.862553
O	-0.746183	-0.176102	2.602799

	Ti1	RI-BP86/SVP	
5			
E(SCF) =	-2690.193488		
Ti	0.769528	0.049502	2.163459
Cl	0.728320	1.711273	3.581496
Cl	2.296845	0.428074	0.647499
Cl	1.234669	-1.802463	3.223262
Cl	-1.183271	-0.133237	1.200214

W_(CO)2-tp_real RI-BP86/SVP

49

E(SCF) =	-1231.278831		
W	-3.067179	2.895478	5.055609
C	-5.053124	3.210613	4.975398
O	-6.197193	3.453764	4.998931
C	-3.308366	4.551882	6.172721
O	-3.539279	5.497162	6.822104
N	-0.948652	2.517624	5.463433
N	-0.186389	2.080557	4.406463
N	-1.589441	3.191764	2.578732
N	-2.595805	3.812048	3.345145
N	-2.991518	0.947599	4.056888
N	-1.937211	0.735229	3.200763
B	-0.876419	1.849017	3.042251
H	-0.062401	1.545295	2.199271
C	1.119837	1.969814	4.789056
C	1.189653	2.331198	6.144468
C	-0.116405	2.675351	6.536407
C	-3.005144	4.956983	2.659885
C	-2.263233	5.041438	1.490423
C	-1.384708	3.924135	1.464779
C	-2.069237	-0.480085	2.592232
C	-3.240241	-1.072308	3.092857
C	-3.798633	-0.154379	4.000308
C	-0.606854	3.104996	7.881837
C	2.221307	1.547773	3.869820
C	-4.061966	5.879521	3.160834
C	-0.389942	3.581739	0.405984
C	-1.107325	-1.008927	1.576716
C	-5.031004	-0.295880	4.834885
H	3.178632	1.518848	4.420811
H	2.341047	2.248850	3.019248
H	2.040341	0.539588	3.445898
H	0.228907	3.497089	8.490213
H	-1.053640	2.257062	8.442510
H	-1.376327	3.898558	7.802182
H	-0.080573	-1.092014	1.986325
H	-1.054981	-0.359566	0.679506
H	-1.425246	-2.014653	1.247638
H	-4.787632	-0.618827	5.869018
H	-5.704445	-1.058680	4.402509
H	-5.590543	0.658310	4.902987
H	0.639089	3.542654	0.815503
H	-0.416665	4.340328	-0.396446
H	-0.602423	2.591037	-0.042842
H	-3.793039	6.312858	4.144645

H	-5.031765	5.358586	3.287870
H	-4.202873	6.707225	2.442709
H	-2.334872	5.820606	0.724450
H	-3.639979	-2.054941	2.822320
H	2.088713	2.346170	6.768977

	W_(CO)2tp	RI-BP86/SVP	
31			
E(SCF) =	-995.508996		
W	-3.062673	2.746220	5.224812
C	-3.272916	4.397004	6.374294
O	-3.457374	5.330136	7.047355
N	-0.914896	2.445065	5.521410
C	-0.048367	2.661343	6.547609
C	1.254759	2.323182	6.153061
C	1.131465	1.918610	4.816676
N	-0.176544	1.990167	4.462906
B	-0.883650	1.743726	3.110183
N	-1.937827	0.627744	3.294090
N	-2.987188	0.843155	4.145734
C	-3.802133	-0.242424	4.055845
C	-3.262404	-1.172851	3.155152
C	-2.087661	-0.573218	2.680629
N	-2.627301	3.668001	3.496185
N	-1.642558	3.080316	2.696405
C	-1.494146	3.832368	1.597221
C	-2.380555	4.937973	1.645523
C	-3.066668	4.798691	2.841654
C	-5.067323	3.013019	5.183951
O	-6.216455	3.203094	5.217818
H	-0.087854	1.462529	2.238708
H	-2.492613	5.727232	0.895226
H	-3.676803	-2.143852	2.867202
H	2.171088	2.382772	6.748280
H	-0.765467	3.551691	0.826215
H	-3.847664	5.417453	3.298071
H	-1.361884	-0.914949	1.933667
H	-4.730200	-0.290640	4.638450
H	1.891350	1.604302	4.091894
H	-0.409252	3.051356	7.507171

	W3	RI-BP86/SVP	
9			
E(SCF) =	-520.293816		
W	-1.782638	-0.138735	2.893588
C	-3.290850	-0.022556	1.673098

O	-4.195057	0.048031	0.930127
C	-1.806944	1.912700	3.142560
O	-1.854098	3.066146	3.284993
C	-3.023705	-0.348454	4.374634
O	-3.765763	-0.475708	5.273369
C	-1.714638	-2.188734	2.639982
O	-1.709795	-3.343477	2.500353

W4 RI-BP86/SVP

11			
E(SCF) =	-633.596766		
W	-1.924924	-0.061021	2.126558
C	-3.883552	-0.084026	2.046229
O	-5.050938	-0.097753	1.997849
C	-1.954588	1.807457	3.029661
O	-1.988365	2.852050	3.533830
C	-1.961608	-0.963382	3.995274
O	-1.999716	-1.467976	5.039511
C	-1.837768	-1.929194	1.226472
O	-1.806901	-2.974177	0.722948
C	-1.831411	0.842569	0.260373
O	-1.797416	1.347843	-0.783669

W2 RI-BP86/SVP

7			
E(SCF) =	-1213.997322		
W	-2.197079	-0.140891	2.841484
Cl	-3.753781	0.037073	1.122610
C	-1.669890	1.827466	2.986363
O	-1.209743	2.898016	3.036545
Cl	-3.057353	-0.427777	4.983082
C	-1.581655	-2.058475	2.499203
O	-1.074542	-3.086241	2.282881

WO3 RI-BP86/SVP

4			
E(SCF) =	-292.791746		
W	0.599571	0.468683	2.156524
O	1.759986	0.701194	3.448981
O	1.148117	-0.947859	1.282784
O	-0.888901	-0.014379	2.945256

Fragmente/HG-Fragmente/RI-BP86_TZVP

AlCl3 RI-BP86/TZVP

4			
E(SCF) =	-1623.445136		

Al	0.000113	0.000020	0.000062
Cl	2.094023	-0.116037	-0.000016
Cl	-0.946553	1.871250	-0.000016
Cl	-1.147556	-1.755228	-0.000016

BCl3 Σ I-BP86/TZVP

4			
E(SCF) =	-1405.756346		
B	0.176453	-0.305614	0.124592
Cl	-0.115804	0.200565	1.781772
Cl	1.641173	0.201053	-0.703185
Cl	-0.994715	-1.320750	-0.703180

BH3 Σ I-BP86/TZVP

4			
E(SCF) =	-26.606769		
B	0.176619	-0.305915	0.224997
H	-0.125936	0.218133	1.261216
H	1.228089	-0.048936	-0.293105
H	-0.571665	-1.088026	-0.293107

CO2 Σ I-BP86/TZVP

3			
E(SCF) =	-188.677277		
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.172138
O	0.000000	0.000000	-1.172138

CS2 Σ I-BP86/TZVP

3			
E(SCF) =	-834.618987		
C	0.009955	0.000000	0.000095
S	-0.003769	0.000000	1.571485
S	0.023658	0.000000	-1.571320

PH3 Σ I-BP86/TZVP

4			
E(SCF) =	-343.189795		
P	0.079481	0.175166	-0.029548
H	-0.140218	-0.612540	1.152554
H	1.210683	-0.617299	-0.427571
H	-0.833161	-0.617327	-0.807435

PMe3 Σ I-BP86/TZVP

13	
E(SCF) =	-461.187053

P	-0.019437	-0.000560	-0.009993
C	0.020886	0.006053	1.864041
C	1.212911	-1.376354	-0.329530
C	1.089874	1.474644	-0.336835
H	1.045343	0.051738	2.265051
H	-0.546260	0.869938	2.237950
H	-0.469037	-0.901921	2.242595
H	1.433471	-1.426004	-1.404998
H	2.155837	-1.236101	0.221500
H	0.769609	-2.338385	-0.036691
H	1.305705	1.537457	-1.412570
H	2.041212	1.419051	0.214803
H	0.565156	2.396378	-0.049021

	PPh3	RI-BP86/TZVP	
34			
E(SCF) =	-1036.585588		
P	-1.210510	0.002025	0.001964
C	-0.391812	0.215381	-1.658911
C	-0.390508	-1.543428	0.644789
C	-0.385149	1.330831	1.015551
C	0.735475	-0.504502	-2.085959
C	1.265140	-0.300049	-3.364807
C	0.680615	0.629335	-4.230017
C	-0.444573	1.349953	-3.814801
C	-0.982493	1.136233	-2.543535
H	1.199297	-1.231879	-1.417803
H	2.140326	-0.869544	-3.684085
H	1.095264	0.786972	-5.227253
H	-0.912278	2.071529	-4.487370
H	-1.874111	1.686297	-2.232433
C	0.744701	-1.553865	1.471076
C	1.275385	-2.763631	1.932162
C	0.683887	-3.977176	1.569326
C	-0.449218	-3.977369	0.748441
C	-0.988017	-2.769403	0.299120
H	-1.885675	-2.774424	-0.324190
H	-0.922353	-4.920212	0.467473
H	1.099356	-4.919632	1.930468
H	2.156750	-2.755859	2.576618
H	1.213898	-0.611888	1.759341
C	-0.979451	1.647474	2.250785
C	-0.436297	2.639778	3.070276
C	0.698208	3.346617	2.656967
C	1.286891	3.050848	1.424030
C	0.751677	2.047515	0.608840

H	1.218683	1.823592	-0.351605
H	2.169461	3.601990	1.093075
H	1.117096	4.130099	3.290981
H	-0.907211	2.870446	4.027777
H	-1.878112	1.113105	2.568885

Fragmente/HG-Fragmente/RI-MP2-SVP

	AlCl3	RI-MP2/SVP	
4			
E(SCF) =	-1620.134958		
Al	-0.000044	-0.000056	0.000045
Cl	-1.981321	-0.615959	-0.000011
Cl	1.524165	-1.407757	-0.000011
Cl	0.457190	2.023759	-0.000011

	BCl3	RI-MP2/SVP	
4			
E(SCF) =	-1402.858420		
B	0.176463	-0.305639	0.124622
Cl	-0.113307	0.196253	1.767634
Cl	1.628655	0.196721	-0.696127
Cl	-0.984705	-1.312079	-0.696129

	BH3	RI-MP2/SVP	
4			
E(SCF) =	-26.370466		
B	0.176633	-0.305937	0.224978
H	-0.125880	0.218032	1.261011
H	1.227877	-0.048978	-0.292994
H	-0.571522	-1.087862	-0.292994

	CO2	RI-MP2/SVP	
3			
E(SCF) =	-187.482102		
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.170368
O	0.000000	0.000000	-1.170368

	CS2	RI-MP2/SVP	
3			
E(SCF) =	-832.635889		
C	0.009951	0.000000	0.000087
S	-0.003697	0.000000	1.563486
S	0.023590	0.000000	-1.563313

	PH3	RI-MP2/SVP	
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4			
E(SCF) =	-342.363706		
P	0.079467	0.154532	-0.029493
H	-0.138811	-0.605682	1.144994
H	1.203479	-0.610413	-0.425028
H	-0.827350	-0.610437	-0.802473

	PMe3	RI-MP2/SVP	
13			
E(SCF) =	-459.392654		
P	0.000010	-0.000015	-0.607052
C	-0.309432	1.592147	0.280159
C	-1.224157	-1.064029	0.280171
C	1.533578	-0.528099	0.280176
H	-0.285544	1.469940	1.373233
H	0.450047	2.330741	-0.009612
H	-1.290393	1.992357	-0.009403
H	-1.079988	-2.113748	-0.008968
H	-1.130632	-0.981815	1.373244
H	-2.243504	-0.775902	-0.010032
H	1.793472	-1.555141	-0.009545
H	1.415797	-0.487633	1.373247
H	2.370659	0.121311	-0.009419

	PPh3	RI-MP2/SVP	
34			
E(SCF) =	-1030.141057		
P	0.000056	-0.000137	-1.248410
C	-0.369844	1.603380	-0.426840
C	1.573687	-0.481504	-0.426836
C	-1.203647	-1.122081	-0.426590
C	0.305019	2.070082	0.717786
C	-0.024144	3.331678	1.282278
C	-1.046993	4.127316	0.691282
C	-1.727102	3.653475	-0.468221
C	-1.375081	2.395341	-1.023094
H	1.091707	1.458163	1.168259
H	0.508121	3.689427	2.169398
H	-1.304226	5.101196	1.120827
H	-2.508127	4.261518	-0.935998
H	-1.877916	2.032812	-1.925879
C	1.640324	-1.298089	0.718684
C	2.897443	-1.643838	1.283212
C	4.098010	-1.157110	0.691339
C	4.027817	-0.332422	-0.469026
C	2.762233	-0.008171	-1.023914

H	2.699752	0.607587	-1.927368
H	4.944972	0.038946	-0.937476
H	5.070007	-1.421277	1.120942
H	2.941063	-2.282744	2.171001
H	0.716969	-1.672488	1.169783
C	-1.388515	-2.387945	-1.023738
C	-2.302248	-3.321637	-0.468703
C	-3.051134	-2.969982	0.691893
C	-2.871978	-1.686937	1.283742
C	-1.943874	-0.771332	0.719064
H	-1.806242	0.215551	1.170035
H	-3.446778	-1.405191	2.171716
H	-3.766053	-3.679481	1.121572
H	-2.439511	-4.301569	-0.937130
H	-0.824417	-2.641738	-1.927437

Fragmente/HG-Fragmente/RI-MP2-TZVP

	AlCl3	RI-MP2/TZVP	
4			
E(SCF) =	-1620.669815		
Al	-0.000030	-0.000037	0.000037
Cl	-1.984011	-0.616816	-0.000009
Cl	1.526225	-1.409707	-0.000009
Cl	0.457805	2.026547	-0.000009

BCl3 **RI-MP2/TZVP**

4			
E(SCF) =	-1403.335321		
B	0.176548	-0.305789	0.124777
Cl	-0.113204	0.196077	1.766844
Cl	1.627863	0.196480	-0.695808
Cl	-0.984100	-1.311514	-0.695812

BH3 **RI-MP2/TZVP**

4			
E(SCF) =	-26.399281		
B	0.176688	-0.306032	0.224965
H	-0.122660	0.212455	1.249933
H	1.216760	-0.051616	-0.287449
H	-0.563680	-1.079553	-0.287449

CO2 **RI-MP2/TZVP**

3			
E(SCF) =	-187.696918		
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169249

O	0.000000	0.000000	-1.169249
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CS2	RI-MP2/TZVP
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3			
E(SCF) =	-832.933585		
C	0.009950	0.000000	0.000087
S	-0.003706	0.000000	1.564547
S	0.023600	0.000000	-1.564373

PH3	RI-MP2/TZVP
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4			
E(SCF) =	-342.475305		
P	0.079464	0.148973	-0.029479
H	-0.139179	-0.603824	1.146970
H	1.205380	-0.608562	-0.425704
H	-0.828881	-0.608587	-0.803787

PMe3	RI-MP2/TZVP
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13			
E(SCF) =	-459.629455		
P	0.000049	-0.000070	-0.616797
C	-0.309796	1.594364	0.280824
C	-1.225909	-1.065463	0.280924
C	1.535708	-0.528908	0.280984
H	-0.282887	1.458545	1.363711
H	0.444278	2.327938	-0.004015
H	-1.284232	1.991451	-0.003246
H	-1.082692	-2.107951	-0.002985
H	-1.121801	-0.974089	1.363803
H	-2.238193	-0.779139	-0.004025
H	1.794038	-1.548733	-0.003825
H	1.404527	-0.484284	1.363857
H	2.366824	0.116455	-0.003012

PPh3	RI-MP2/TZVP
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34			
E(SCF) =	-1031.298573		
P	-0.000402	-0.000723	-1.338947
C	-0.370820	1.589284	-0.474353
C	1.561867	-0.474093	-0.474062
C	-1.191681	-1.116323	-0.473460
C	0.261694	2.004492	0.702861
C	-0.111148	3.198731	1.318235
C	-1.052914	4.033145	0.718981
C	-1.683722	3.630062	-0.457312
C	-1.301887	2.443827	-1.078832

H	0.997604	1.364475	1.175251
H	0.383267	3.507402	2.231877
H	-1.336184	4.963627	1.195670
H	-2.413335	4.276612	-0.930154
H	-1.775304	2.145744	-2.008567
C	1.605660	-1.230534	0.702429
C	2.826432	-1.503799	1.318045
C	4.019671	-1.103284	0.719706
C	3.985530	-0.354409	-0.455926
C	2.767240	-0.093001	-1.077731
H	2.745491	0.466895	-2.006944
H	4.910068	-0.044184	-0.928083
H	4.967203	-1.322414	1.196610
H	2.846902	-2.087147	2.231145
H	0.683656	-1.549387	1.174195
C	-1.467027	-2.349762	-1.077895
C	-2.303046	-3.273486	-0.455759
C	-2.966397	-2.928767	0.721176
C	-2.713818	-1.696131	1.320417
C	-1.866328	-0.776221	0.704454
H	-1.679308	0.180942	1.176878
H	-3.227408	-1.422360	2.234604
H	-3.630338	-3.639243	1.198334
H	-2.498836	-4.228489	-0.928597
H	-0.973029	-2.610681	-2.008094

Fragmente/M-Fragmente/Systematisch/RI-BP86_SVP

	Ag6	RI-BP86/SVP	
2			
E(SCF) =	-607.210397		
Ag	-1.362079	-1.625916	0.000000
Cl	-2.842235	-3.389963	0.000000

	AuCl	RI-BP86/SVP	
2			
E(SCF) =	-595.997757		
Au	0.000000	0.000000	0.322703
Cl	0.000000	0.000000	2.597697

	Cr4	RI-BP86/SVP	
11			
E(SCF) =	-1610.886055		
Cr	-0.000005	0.000018	0.663994
C	-1.898715	-0.000364	0.641258
C	-0.000033	-0.000024	2.485496
C	1.898731	0.000436	0.641234

C	0.000058	-1.898753	0.641993
C	-0.000100	1.898800	0.641922
O	-0.000988	-3.058180	0.666382
O	3.058205	0.000375	0.664011
O	-3.058193	-0.000265	0.664046
O	0.000878	3.058227	0.666281
O	-0.000070	-0.000137	3.651342

Cr2 (T) RI-BP86/SVP

7			
E(SCF) =	-2191.350433		
Cr	0.000035	0.000023	0.871871
Cl	2.048754	0.000028	0.170965
Cl	-2.048729	0.000033	0.171094
C	0.000072	1.309399	2.158688
O	0.000094	2.146208	2.961016
C	0.000072	-1.309371	2.158670
O	0.000093	-2.146193	2.960984

Cr3 RI-BP86/SVP

9			
E(SCF) =	-1497.586341		
Cr	-1.793245	-0.139158	2.893977
C	-3.181873	-0.029038	1.747882
O	-4.076209	0.043972	0.997681
C	-1.866492	1.739911	3.127350
O	-1.994187	2.885449	3.277416
C	-2.930921	-0.335166	4.279962
O	-3.661683	-0.463113	5.184165
C	-1.781644	-2.020525	2.667089
O	-1.857235	-3.173118	2.537182

Cu6 RI-BP86/SVP

2			
E(SCF) =	-2100.677359		
Cu	0.018460	-0.950912	0.000000
Cl	-0.035798	-3.024028	0.000000

Fe5 RI-BP86/SVP

9			
E(SCF) =	-1716.861833		
Fe	-1.190101	-1.587307	0.000171
C	-2.227071	-2.962807	0.000822
C	-2.595431	-0.445890	-0.000590
C	-0.430506	-2.081678	1.566989
C	-0.430005	-2.080074	-1.567298

O	-2.927694	-3.891785	0.000665
O	-3.508329	0.272993	-0.000759
O	0.048129	-2.410336	-2.573529
O	0.047998	-2.411665	2.573175

Hf1 RI-BP86/SVP

5			
E(SCF) =	-1888.844736		
Hf	0.000001	0.000003	-0.969169
Cl	-1.922621	-0.000020	-2.326522
Cl	0.000008	1.922587	0.388221
Cl	1.922582	0.000009	-2.326581
Cl	0.000036	-1.922562	0.388247

Mo4 RI-BP86/SVP

11			
E(SCF) =	-634.697131		
Mo	-0.000090	0.000022	0.597740
C	-0.000028	-2.060278	0.598397
C	0.000044	0.000018	2.543709
C	-0.000056	2.060316	0.598409
C	2.060188	-0.000013	0.596306
C	-2.060378	-0.000053	0.596342
O	3.218920	-0.000096	0.631407
O	0.000091	3.218938	0.637004
O	0.000009	-3.218897	0.636996
O	-3.219115	-0.000161	0.631120
O	0.000175	0.000018	3.710727

Mo2 RI-BP86/SVP

7			
E(SCF) =	-1215.098031		
Mo	-2.119795	-0.136656	2.826382
Cl	-3.718307	0.036870	1.168616
C	-1.655785	1.851676	2.995990
O	-1.273988	2.946084	3.070892
Cl	-3.060675	-0.425910	4.915542
C	-1.571076	-2.081115	2.489859
O	-1.144416	-3.141778	2.284887

Mo3 RI-BP86/SVP

9			
E(SCF) =	-521.399653		
Mo	-1.745016	-0.137734	2.889936
C	-3.249656	-0.020630	1.684883
O	-4.163386	0.050675	0.956879

C	-1.820366	1.898698	3.143185
O	-1.928480	3.046559	3.285456
C	-2.985352	-0.347736	4.355329
O	-3.739652	-0.474626	5.241275
C	-1.728419	-2.176316	2.641649
O	-1.783164	-3.329677	2.514112

Ni(CO)₂ RI-BP86/SVP

5			
E(SCF) =	-1734.936228		
Ni	-0.274233	-0.052156	0.167154
C	0.377793	-0.103809	1.779185
O	0.778578	-0.388667	2.833772
C	-0.830161	-1.310574	-0.897661
O	-1.134321	-2.305661	-1.418449

Ni(CO)₃ RI-BP86/SVP

7			
E(SCF) =	-1848.235676		
Ni	-0.514411	-0.033113	0.820839
C	0.689863	-0.512358	2.057343
O	1.463518	-0.823782	2.859432
C	-0.875061	-1.127746	-0.550923
O	-1.108085	-1.834715	-1.436768
C	-1.365457	1.537041	0.960481
O	-1.915782	2.550815	1.051375

Os₅ RI-BP86/SVP

9			
E(SCF) =	-543.964166		
Os	-1.483344	-1.977901	-0.005939
C	-2.872133	-3.195833	0.611921
C	-2.720259	-0.572712	-0.543387
C	-0.163549	-2.547569	1.308334
C	-0.178063	-1.594365	-1.399894
O	-3.648288	-4.043469	0.779236
O	-3.377128	0.377186	-0.666376
O	0.515416	-1.567960	-2.331195
O	0.574537	-2.675208	2.195948

Ru₅ RI-BP86/SVP

9			
E(SCF) =	-548.142949		
Ru	-1.500598	-2.000342	-0.038772
C	-2.878519	-3.176346	0.622374
C	-2.727102	-0.620711	-0.594896

C	-0.184019	-2.559102	1.254122
C	-0.213139	-1.635418	-1.427444
O	-3.666989	-3.996853	0.845503
O	-3.394115	0.314018	-0.757115
O	0.487842	-1.594796	-2.350334
O	0.568698	-2.706543	2.123967

Ti1 RI-BP86/SVP

5			
E(SCF) =	-2690.193466		
Ti	0.000003	-0.000013	-1.075545
Cl	-1.783322	-0.000004	-2.338886
Cl	0.000033	1.785326	0.185077
Cl	1.783290	0.000000	-2.338942
Cl	-0.000007	-1.785298	0.185157

W1 RI-BP86/SVP

11			
E(SCF) =	-633.596772		
W	-0.000090	-0.000066	0.513876
C	-2.075585	0.000031	0.485227
C	-0.000068	-0.000055	2.474472
C	2.075404	0.000032	0.485189
C	-0.000002	-2.075559	0.485192
C	-0.000002	2.075427	0.485150
O	0.000169	-3.235961	0.487144
O	3.235802	0.000217	0.487184
O	-3.235985	0.000215	0.487239
O	0.000169	3.235826	0.487082
O	-0.000058	-0.000056	3.642921

W3 RI-BP86/SVP

9			
E(SCF) =	-520.293816		
W	-1.782638	-0.138735	2.893588
C	-3.290850	-0.022556	1.673098
O	-4.195057	0.048031	0.930127
C	-1.806944	1.912700	3.142560
O	-1.854098	3.066146	3.284993
C	-3.023705	-0.348454	4.374634
O	-3.765763	-0.475708	5.273369
C	-1.714638	-2.188734	2.639982
O	-1.709795	-3.343477	2.500353

W4 RI-BP86/SVP

11

E(SCF) =	-633.596766		
W	-1.924924	-0.061021	2.126558
C	-3.883552	-0.084026	2.046229
O	-5.050938	-0.097753	1.997849
C	-1.954588	1.807457	3.029661
O	-1.988365	2.852050	3.533830
C	-1.961608	-0.963382	3.995274
O	-1.999716	-1.467976	5.039511
C	-1.837768	-1.929194	1.226472
O	-1.806901	-2.974177	0.722948
C	-1.831411	0.842569	0.260373
O	-1.797416	1.347843	-0.783669

W2 RI-BP86/SVP

7			
E(SCF) =	-1213.997322		
W	-2.197079	-0.140891	2.841484
Cl	-3.753781	0.037073	1.122610
C	-1.669890	1.827466	2.986363
O	-1.209743	2.898016	3.036545
Cl	-3.057353	-0.427777	4.983082
C	-1.581655	-2.058475	2.499203
O	-1.074542	-3.086241	2.282881

Zr1 RI-BP86/SVP

5			
E(SCF) =	-1887.866540		
Zr	0.000000	0.000004	-1.051982
Cl	-1.921769	0.000000	-2.408735
Cl	-0.000004	1.921694	0.304875
Cl	1.921779	0.000016	-2.408721
Cl	-0.000006	-1.921693	0.304865

Fragmente/M-Fragmente/X-Ray

Ag+_1H RI-BP86/SVP

10			
E(SCF) =	-871.019910		
C	-0.429953	0.150518	0.837539
P	-0.838480	-1.243463	1.737993
P	0.089250	0.049210	-0.787600
H	-0.226019	-2.443847	1.252865
H	-2.210736	-1.652811	1.869419
H	-0.441320	-1.188778	3.106856
H	0.651660	-1.221220	-1.135566
H	1.114740	0.979777	-1.129630
H	-0.838565	0.258857	-1.866093

Ag	-0.980819	2.009343	1.586618

	Ag+_1Ph	RI-BP86/SVP	
70			
E(SCF) =	-2256.093497		
C	-1.411854	-1.640957	1.406654
P	-3.064792	-1.298703	1.760401
P	-0.117940	-2.159177	2.422028
C	1.051895	-3.187851	1.431076
C	-0.600268	-3.193143	3.871224
C	0.927544	-0.807456	3.136561
C	-3.372402	-0.421628	3.353320
C	-3.743936	-0.213534	0.428472
C	-4.204916	-2.750785	1.742678
Ag	-0.854828	-1.158777	-0.556017
C	1.652742	-0.989902	4.339957
C	2.479265	0.048114	4.840027
C	2.589314	1.275908	4.130712
C	1.863602	1.455970	2.920316
C	1.035790	0.415049	2.432656
C	-2.519658	0.658738	3.696146
C	-2.720678	1.375257	4.901267
C	-3.779708	1.007494	5.778137
C	-4.628369	-0.081369	5.436915
C	-4.423053	-0.791512	4.226601
C	-3.682477	-4.052061	1.914945
C	-4.544325	-5.178133	1.898893
C	-5.940933	-4.999329	1.701899
C	-6.465215	-3.688304	1.521560
C	-5.597123	-2.569067	1.542475
C	-3.914462	-0.769881	-0.867994
C	-4.371133	0.038309	-1.939289
C	-4.664425	1.414271	-1.715958
C	-4.509528	1.962061	-0.414333
C	-4.051863	1.145602	0.654429
C	-0.407918	-4.596746	3.845073
C	-0.812371	-5.395145	4.944075
C	-1.415067	-4.789582	6.080786
C	-1.602788	-3.379763	6.108123
C	-1.194419	-2.586800	5.007321
C	2.441049	-3.176824	1.698792
C	3.319663	-3.998180	0.946681
C	2.807153	-4.841858	-0.076712
C	1.408952	-4.856092	-0.341331
C	0.538779	-4.029215	0.412148
H	0.071943	-5.087475	2.988657

H	-0.651449	-6.482273	4.923468
H	-1.726232	-5.406132	6.936527
H	-2.059224	-2.905104	6.987971
H	-1.340524	-1.500680	5.061948
H	2.865820	-2.528494	2.475367
H	4.399510	-3.979433	1.151126
H	3.487689	-5.478198	-0.661026
H	1.007591	-5.510380	-1.128198
H	-0.538837	-4.048743	0.197250
H	0.473996	0.567736	1.499371
H	1.948491	2.402316	2.367813
H	3.232087	2.080929	4.515671
H	3.037037	-0.094670	5.776482
H	1.585112	-1.926666	4.908022
H	-2.605748	-4.203515	2.060611
H	-4.136337	-6.189250	2.035489
H	-6.613050	-5.869480	1.683492
H	-7.543470	-3.547729	1.360290
H	-6.023997	-1.569401	1.386099
H	-3.746281	-1.841287	-1.050707
H	-4.519889	-0.398074	-2.937393
H	-5.022868	2.044373	-2.542944
H	-4.749653	3.019401	-0.233326
H	-3.950711	1.593735	1.650658
H	-1.686020	0.946151	3.041886
H	-2.059472	2.213713	5.162197
H	-3.939815	1.561178	6.714779
H	-5.444798	-0.372120	6.112992
H	-5.085475	-1.634084	3.992910

	Ag-(H+)-1H	RI-BP86/SVP	
11			
E(SCF) =	-871.247211		
C	0.798001	0.000063	-0.441860
P	1.584451	1.558943	0.064229
H	2.964108	1.693172	-0.286132
H	1.511554	1.770285	1.468410
H	0.906261	2.635547	-0.568280
P	1.584913	-1.558752	0.064235
H	2.964595	-1.692177	-0.286200
H	0.906765	-2.635288	-0.568393
H	1.512077	-1.770283	1.468394
Ag	-1.359083	-0.000093	0.022412
H	0.783091	-0.000128	-1.556980

Ag-(H+)-1Ph RI-BP86/SVP

71

E(SCF) =	-2256.413620		
C	-1.527782	-2.005360	1.365703
P	-3.176710	-1.328081	1.812133
P	-0.119380	-2.389337	2.461195
C	1.075683	-3.238730	1.367934
C	-0.530942	-3.517134	3.838577
C	0.687410	-0.899412	3.141786
C	-3.233193	-0.365020	3.354084
C	-3.688276	-0.216819	0.436553
C	-4.390287	-2.683437	1.865190
H	-1.749840	-2.966345	0.853950
Ag	-0.858470	-0.855737	-0.384858
C	1.072582	-0.867596	4.505840
C	1.781837	0.249611	5.019069
C	2.117919	1.336856	4.166155
C	1.744526	1.295705	2.790806
C	1.036422	0.179552	2.287988
C	-2.357688	0.736489	3.550338
C	-2.464485	1.520755	4.724629
C	-3.450634	1.209420	5.705013
C	-4.328884	0.108059	5.500031
C	-4.220825	-0.677248	4.324374
C	-4.023776	-3.960106	2.365073
C	-4.987148	-4.997707	2.422489
C	-6.320199	-4.759335	1.981253
C	-6.682551	-3.474898	1.483556
C	-5.717935	-2.438205	1.424775
C	-3.617996	-0.708813	-0.902356
C	-3.987565	0.128681	-1.987526
C	-4.427089	1.463546	-1.739681
C	-4.512815	1.939262	-0.402768
C	-4.144005	1.097121	0.683913
C	0.037224	-4.816983	3.878325
C	-0.275082	-5.695195	4.947545
C	-1.153935	-5.273945	5.984032
C	-1.717429	-3.965554	5.943339
C	-1.407437	-3.091546	4.873806
C	2.452547	-2.914032	1.463013
C	3.398158	-3.589717	0.649053
C	2.967972	-4.595495	-0.260585
C	1.584128	-4.925592	-0.345661
C	0.642286	-4.250774	0.468733
H	0.735210	-5.164320	3.106060
H	0.172284	-6.699721	4.982599
H	-1.389240	-5.952024	6.818892

H	-2.385842	-3.635376	6.752075
H	-1.845655	-2.085113	4.881371
H	2.817076	-2.148792	2.160404
H	4.466931	-3.339248	0.723596
H	3.701327	-5.121720	-0.891079
H	1.253020	-5.712911	-1.039152
H	-0.410414	-4.555416	0.391204
H	0.788644	0.162746	1.213648
H	2.023328	2.126256	2.125532
H	2.676211	2.199573	4.561840
H	2.082546	0.269960	6.077247
H	0.849133	-1.698149	5.186840
H	-3.008864	-4.171479	2.726405
H	-4.709828	-5.989880	2.807809
H	-7.068602	-5.565832	2.022587
H	-7.711682	-3.290855	1.140535
H	-6.024488	-1.460403	1.030170
H	-3.391259	-1.764131	-1.121128
H	-3.968883	-0.257298	-3.018280
H	-4.718644	2.114004	-2.579056
H	-4.870710	2.961634	-0.207758
H	-4.229075	1.494806	1.703513
H	-1.596190	1.011053	2.809078
H	-1.793580	2.378302	4.879704
H	-3.539279	1.824334	6.614092
H	-5.098334	-0.126434	6.250728
H	-4.916587	-1.515465	4.185842

(AuCl)₂ RI-BP86/SVP

4			
E(SCF) =	-1192.030365		
Au	0.000000	1.391582	0.000000
Cl	-2.148331	0.009516	0.000000
Au	-0.000011	-1.392074	0.000000
Cl	2.148382	-0.007233	0.000000

ReO₃⁺ RI-BP86/SVP

4			
E(SCF) =	-303.610935		
Re	0.669942	0.444670	1.859055
O	1.820335	0.513402	3.130283
O	1.218746	-0.839460	0.862553
O	-0.746183	-0.176102	2.602799

W₂(CO)₂-tp_real RI-BP86/SVP

E(SCF) =	-1231.278831		
W	-3.067179	2.895478	5.055609
C	-5.053124	3.210613	4.975398
O	-6.197193	3.453764	4.998931
C	-3.308366	4.551882	6.172721
O	-3.539279	5.497162	6.822104
N	-0.948652	2.517624	5.463433
N	-0.186389	2.080557	4.406463
N	-1.589441	3.191764	2.578732
N	-2.595805	3.812048	3.345145
N	-2.991518	0.947599	4.056888
N	-1.937211	0.735229	3.200763
B	-0.876419	1.849017	3.042251
H	-0.062401	1.545295	2.199271
C	1.119837	1.969814	4.789056
C	1.189653	2.331198	6.144468
C	-0.116405	2.675351	6.536407
C	-3.005144	4.956983	2.659885
C	-2.263233	5.041438	1.490423
C	-1.384708	3.924135	1.464779
C	-2.069237	-0.480085	2.592232
C	-3.240241	-1.072308	3.092857
C	-3.798633	-0.154379	4.000308
C	-0.606854	3.104996	7.881837
C	2.221307	1.547773	3.869820
C	-4.061966	5.879521	3.160834
C	-0.389942	3.581739	0.405984
C	-1.107325	-1.008927	1.576716
C	-5.031004	-0.295880	4.834885
H	3.178632	1.518848	4.420811
H	2.341047	2.248850	3.019248
H	2.040341	0.539588	3.445898
H	0.228907	3.497089	8.490213
H	-1.053640	2.257062	8.442510
H	-1.376327	3.898558	7.802182
H	-0.080573	-1.092014	1.986325
H	-1.054981	-0.359566	0.679506
H	-1.425246	-2.014653	1.247638
H	-4.787632	-0.618827	5.869018
H	-5.704445	-1.058680	4.402509
H	-5.590543	0.658310	4.902987
H	0.639089	3.542654	0.815503
H	-0.416665	4.340328	-0.396446
H	-0.602423	2.591037	-0.042842
H	-3.793039	6.312858	4.144645
H	-5.031765	5.358586	3.287870

H	-4.202873	6.707225	2.442709
H	-2.334872	5.820606	0.724450
H	-3.639979	-2.054941	2.822320
H	2.088713	2.346170	6.768977

	W_(CO)2tp	RI-BP86/SVP	
31			
E(SCF) =	-995.508996		
W	-3.062673	2.746220	5.224812
C	-3.272916	4.397004	6.374294
O	-3.457374	5.330136	7.047355
N	-0.914896	2.445065	5.521410
C	-0.048367	2.661343	6.547609
C	1.254759	2.323182	6.153061
C	1.131465	1.918610	4.816676
N	-0.176544	1.990167	4.462906
B	-0.883650	1.743726	3.110183
N	-1.937827	0.627744	3.294090
N	-2.987188	0.843155	4.145734
C	-3.802133	-0.242424	4.055845
C	-3.262404	-1.172851	3.155152
C	-2.087661	-0.573218	2.680629
N	-2.627301	3.668001	3.496185
N	-1.642558	3.080316	2.696405
C	-1.494146	3.832368	1.597221
C	-2.380555	4.937973	1.645523
C	-3.066668	4.798691	2.841654
C	-5.067323	3.013019	5.183951
O	-6.216455	3.203094	5.217818
H	-0.087854	1.462529	2.238708
H	-2.492613	5.727232	0.895226
H	-3.676803	-2.143852	2.867202
H	2.171088	2.382772	6.748280
H	-0.765467	3.551691	0.826215
H	-3.847664	5.417453	3.298071
H	-1.361884	-0.914949	1.933667
H	-4.730200	-0.290640	4.638450
H	1.891350	1.604302	4.091894
H	-0.409252	3.051356	7.507171

	WO3	RI-BP86/SVP	
4			
E(SCF) =	-292.791746		
W	0.599571	0.468683	2.156524
O	1.759986	0.701194	3.448981
O	1.148117	-0.947859	1.282784

O	-0.888901	-0.014379	2.945256
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Fragmente/M-Fragmente/Systematisch/BP86_TZ2P

Ag6 BP86/TZ2P

2			
E(SCF) =	-0.133943		
Ag	-1.365432	-1.629912	0.000000
Cl	-2.838882	-3.385967	0.000000

Au3 BP86/TZ2P

2			
E(SCF) =	-0.126965		
Au	-1.383848	-1.651627	0.000000
Cl	-2.820783	-3.363526	0.000000

Cr4 BP86/TZ2P

11			
E(SCF) =	-3.201658		
Cr	0.000059	-0.000064	0.645568
C	-1.903420	0.000794	0.625813
C	0.000148	0.000374	2.469346
C	1.903279	-0.001046	0.625984
C	-0.001376	-1.902975	0.649631
C	0.000975	1.902824	0.649917
O	0.001856	-3.055886	0.707293
O	3.057178	-0.001153	0.658049
O	-3.057306	0.000670	0.657730
O	-0.001932	3.055687	0.708233
O	0.000307	0.000910	3.630393

Cu6 BP86/TZ2P

2			
E(SCF) =	-0.156629		
Cu	0.017901	-0.972258	0.000000
Cl	-0.035239	-3.002682	0.000000

Fe5 BP86/TZ2P

9			
E(SCF) =	-2.591351		
Fe	-1.482707	-1.977193	-0.006068
C	-2.747779	-3.126771	0.513537
C	-2.602584	-0.658449	-0.452432
C	-0.280810	-2.451163	1.228293
C	-0.302212	-1.674070	-1.312867
O	-3.525242	-3.963494	0.692900
O	-3.264374	0.279976	-0.586879

O	0.394640	-1.636368	-2.234637
O	0.457436	-2.592947	2.106687

Hf1 BP86/TZ2P

5			
E(SCF) =	-0.845528		
Hf	-0.000001	-0.000004	-0.968588
Cl	-1.891445	-0.000015	-2.307316
Cl	0.000017	1.892758	0.368708
Cl	1.891401	0.000023	-2.307364
Cl	0.000035	-1.892745	0.368756

Mo4 BP86/TZ2P

11			
E(SCF) =	-3.246647		
Mo	0.000018	0.000026	0.591780
C	-0.000293	-2.054726	0.602985
C	0.000290	-0.000006	2.529857
C	-0.000459	2.054690	0.602980
C	2.054770	-0.000086	0.597403
C	-2.054887	-0.000083	0.597295
O	3.208217	0.000047	0.635290
O	0.000039	3.207865	0.646789
O	-0.000090	-3.207900	0.646809
O	-3.208350	-0.000004	0.634626
O	0.000506	-0.000009	3.692342

Os5 BP86/TZ2P

9			
E(SCF) =	-2.648941		
Os	-1.483417	-1.977797	-0.005900
C	-2.858743	-3.190050	0.599950
C	-2.707467	-0.580392	-0.532160
C	-0.176043	-2.535664	1.300885
C	-0.191777	-1.604678	-1.391809
O	-3.634932	-4.029348	0.776110
O	-3.366239	0.361140	-0.664309
O	0.504164	-1.569077	-2.315040
O	0.562434	-2.673188	2.180471

Ru5 BP86/TZ2P

9			
E(SCF) =	-2.597257		
Ru	-1.500793	-2.000461	-0.038966
C	-2.878554	-3.175623	0.623313
C	-2.727348	-0.621463	-0.595562

C	-0.184122	-2.560002	1.253057
C	-0.212779	-1.634500	-1.426548
O	-3.663288	-3.993327	0.844598
O	-3.390702	0.310196	-0.755516
O	0.485339	-1.595400	-2.345519
O	0.565343	-2.704880	2.119617

Ti1 BP86/TZ2P

5			
E(SCF) =	-0.788637		
Ti	0.000006	-0.000025	-1.074737
Cl	-1.780668	-0.000002	-2.338970
Cl	0.000037	1.784105	0.184752
Cl	1.780639	0.000015	-2.339031
Cl	-0.000016	-1.784083	0.184848

W1 BP86/TZ2P

11			
E(SCF) =	-3.247631		
W	0.000020	-0.000005	0.494234
C	-2.050124	-0.000004	0.485898
C	-0.000049	0.000034	2.433654
C	2.050128	-0.000006	0.485888
C	-0.000050	-2.050133	0.485756
C	-0.000055	2.050115	0.485787
O	-0.000027	-3.204992	0.512625
O	3.205023	-0.000008	0.513332
O	-3.205015	-0.000002	0.513397
O	-0.000033	3.204972	0.512703
O	-0.000063	0.000079	3.597403

Zr1 BP86/TZ2P

5			
E(SCF) =	-0.840055		
Zr	0.000001	-0.000014	-1.050530
Cl	-1.904174	-0.000059	-2.401988
Cl	0.000069	1.906510	0.297388
Cl	1.904186	0.000107	-2.401979
Cl	-0.000083	-1.906523	0.297411
