

# European Journal of Inorganic Chemistry

## Supporting Information

### A Dibismuthane with Olefin Functional Groups: Towards Tridentate Hybrid Chalcogen/Olefin Ligands

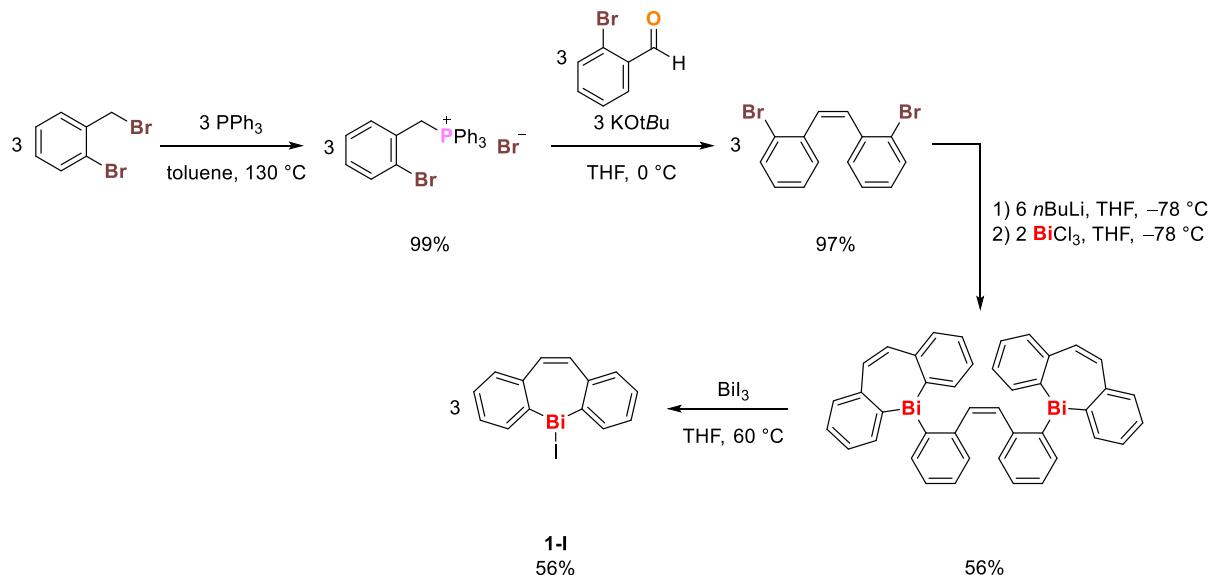
Felix Geist, Sebastián Martínez, Jacqueline Ramler, Kai Oberdorf, Lisa Brändler, Sascha Reith, and Crispin Lichtenberg\*

## Table of Contents

Synthesis of compound <b>1-I</b> .....	2
Single-crystal X-ray diffraction.....	5
UV/vis spectroscopy of compound <b>2</b> .....	12
NMR Spectra .....	13
Density Functional Theory Studies .....	26
Formation of complexes with Co, Rh and Ir.....	26
Ligand preparation energy .....	27
Formation of complexes with Ni, Pd and Pt series.....	29
Insights into the electronic structure of the ligands. ....	31
NBO calculations. ....	32
Cartesian coordinates after optimization with M06-L+GD3/def2SVP/LANL2DZ.....	35

### Synthesis of compound 1-I

The synthesis of halobismepines **1-X** (X = Cl, Br, I) was reported by this group in a previous publication.<sup>[22]</sup> Since then, some changes have been made to the synthetic procedure in order to simplify it and increase batch sizes. An overview over the synthetic route is given in Scheme S1.



**Scheme S1.** Synthetic route to halobismepine **1-I** starting from 2-bromobenzyl bromide.

#### (2-Bromobenzyl)triphenylphosphonium bromide:

The compound was prepared using a modified literature procedure.<sup>[52]</sup>

2-Bromobenzyl bromide (35.1 g, 140 mmol) and PPh<sub>3</sub> (55.3 g, 211 mmol, 1.4 eq.) were dissolved in toluene (500 mL) and refluxed for 3 h, during which the product precipitated from the solution. The product was isolated by filtration, washed with toluene (100 mL) and *n*-pentane (100 mL), and dried in vacuo.

yield: 71.0 g (139 mmol, 99%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 5.72 (d, 2H, <sup>2</sup>J<sub>HP</sub> = 14.3 Hz, CH<sub>2</sub>), 7.11–7.16 (m, 1H, ArH), 7.20 (t, 1H, <sup>3</sup>J<sub>HH</sub> = 7.5 Hz, ArH), 7.37 (d, 1H, <sup>3</sup>J<sub>HH</sub> = 7.8 Hz, ArH), 7.57–7.61 (m, 1H, ArH), 7.61–7.67 (m, 6H, PPh<sub>3</sub>-H<sup>p/m</sup>), 7.68–7.75 (m, 6H, PPh<sub>3</sub>-H<sup>m/o</sup>), 7.77–7.82 (m, 3H, PPh<sub>3</sub>-H<sup>p</sup>) ppm.

### (Z)-1,1'-Dibromostilbene

The compound was prepared using a modified literature procedure.<sup>[53,55]</sup>

A solution of (2-bromobenzyl)triphenylphosphonium bromide (18.2 g, 36 mmol) in THF (400 mL) was cooled to 0 °C, and a solution of potassium *tert*-butoxide (5.2 g, 46 mmol) in THF (150 mL) was slowly added over a period of 30 min. 2-Bromobenzaldehyde (8.3 g, 5.2 mL, 45 mmol) was added to the suspension, resulting in a color change from bright orange to pale yellow. The reaction mixture was stirred at ambient temperature overnight. All volatiles were removed under reduced pressure, the residue extracted with *n*-pentane (4 x 80 mL) and concentrated in vacuo. The crude product was purified by column chromatography (SiO<sub>2</sub>, *n*-pentane) resulting in a 10:1 mixture of the (*Z*)- and (*E*)-isomers, which was used in further reactions without additional purification.

Yield: 11.7 g (35 mmol, 97%).

**<sup>1</sup>H NMR** (400 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 6.51–6.56 (m, 4H, C<sub>6</sub>H<sub>4</sub>), 6.72 (s, 2H, C<sub>2</sub>H<sub>2</sub>), 6.90–6.93 (m, 2H, C<sub>6</sub>H<sub>4</sub>), 7.31–7.35 (m, 2H, C<sub>6</sub>H<sub>4</sub>) ppm.

### (Z)-1,2-Bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene

In contrast to the previously reported procedure,<sup>[22]</sup> (*Z*)-1,2-bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene was prepared directly from (*Z*)-1,1'-dibromostilbene without isolation of the air-sensitive dilithiated stilbene species.

At -78 °C, *n*-butyllithium (1.6 M in hexanes, 11.1 mL, 28 mmol) was added dropwise to a solution of (*Z*)-1,1'-dibromostilbene (4.7 g, 14 mmol) in THF (180 mL). After stirring the red solution for 2 h at -78 °C, a solution of bismuth trichloride (2.9 g, 9 mmol) in THF (8 mL) was added dropwise. The pale yellow suspension was stirred at ambient temperature for 16 h. All volatiles were removed under reduced pressure, and the residue was extracted with toluene (5 x 20 mL). The light-yellow filtrate was layered with *n*-pentane (100 mL) and stored at -30 °C. A colorless solid was obtained after 16 h, isolated by filtration, washed with *n*-pentane (2 x 20 mL) and dried in vacuo.

yield: 2.5 g (2.6 mmol, 56%).

**<sup>1</sup>H NMR** (400 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 6.68 (s, 4H, C<sub>2</sub>H<sub>2</sub>), 6.84–6.89 (m, 4H, C<sub>2</sub>H<sub>2</sub>, C<sub>6</sub>H<sub>4</sub>), 6.96–7.10 (m, 10H, C<sub>6</sub>H<sub>4</sub>), 7.18–7.21 (m, 4H, C<sub>6</sub>H<sub>4</sub>), 7.34–7.39 (m, 6H, C<sub>6</sub>H<sub>4</sub>), 8.24 (dd, 2H, <sup>3</sup>J<sub>HH</sub> = 7.6 Hz, <sup>4</sup>J<sub>HH</sub> = 1.0 Hz, C<sub>6</sub>H<sub>4</sub>) ppm.

**5-Iodo-5H-dibenzo[*b,f*]bismepine (1-I)**

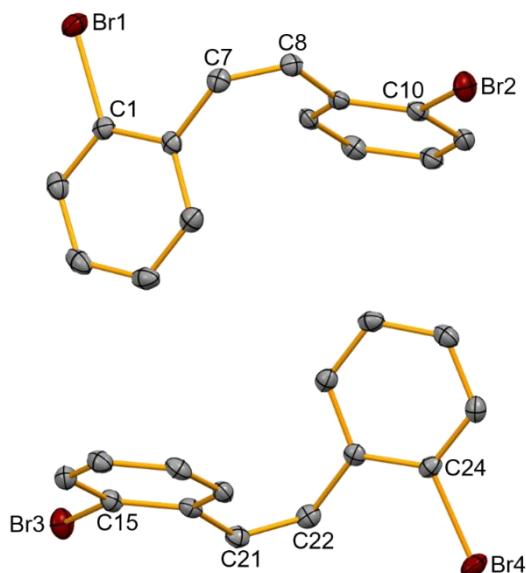
A suspension of bismuth triiodide (867 mg, 1.5 mmol) and (*Z*)-1,2-bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene (1.0 g, 1.1 mmol) in THF (125 mL) was stirred at 60 °C for 16 h. All volatiles were removed under reduced pressure, and the residue was extracted with toluene (5 x 20 mL). The pale yellow solution was layered with *n*-pentane (100 mL) and stored at –30 °C. After 16 h a greyish solid had precipitated, which was isolated by filtration, washed with *n*-pentane (3 x 10 mL) and dried in vacuo.

yield: 906 mg (1.8 mmol, 56%)

**<sup>1</sup>H NMR** (400 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 6.56 (s, 2H, C<sub>2</sub>H<sub>2</sub>), 6.96 (ddd, 2H, <sup>3</sup>J<sub>HH</sub> = 7.5 Hz, <sup>3</sup>J<sub>HH</sub> = 7.5 Hz, <sup>4</sup>J<sub>HH</sub> = 1.2 Hz, C<sub>6</sub>H<sub>4</sub>), 7.10 (dd, 2H, <sup>3</sup>J<sub>HH</sub> = 7.7 Hz, <sup>4</sup>J<sub>HH</sub> = 1.1 Hz, C<sub>6</sub>H<sub>4</sub>), 7.19 (dd, 2H, <sup>3</sup>J<sub>HH</sub> = 7.4 Hz, <sup>4</sup>J<sub>HH</sub> = 1.3 Hz, C<sub>6</sub>H<sub>4</sub>), 9.19 (dd, 2H, <sup>3</sup>J<sub>HH</sub> = 7.6 Hz, <sup>4</sup>J<sub>HH</sub> = 1.0 Hz, C<sub>6</sub>H<sub>4</sub>) ppm.

## Single-crystal X-ray diffraction

The molecular structures of the compounds first reported in this work that have been determined by single-crystal X-ray diffraction analysis are discussed in the main text. Additionally, single-crystal X-ray diffraction analyses of of (*Z*)-1,1'-dibromostilbene (**SI-1**) and (*Z*-1,2-bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene (**SI-2**), intermediate products in the synthesis of starting material **1-I**, have been performed, and the results will be discussed here. (*Z*-1,1'-Dibromostilbene has been used in the synthesis of a broad variety of heteropines,<sup>[53,55]</sup> however, to the best of our knowledge, its molecular structure in the solid state has not been reported so far.

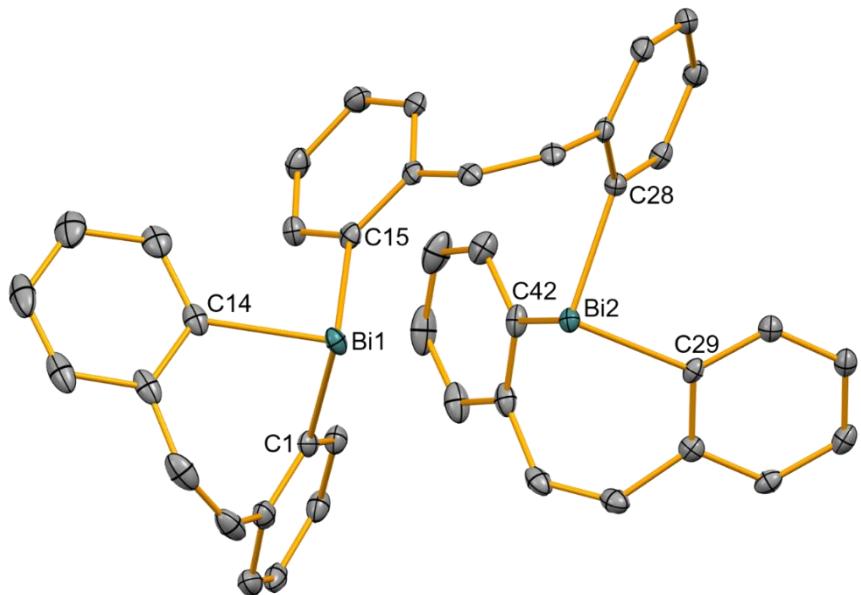


**Figure S1.** Molecular structure of (*Z*)-1,1'-dibromostilbene in the solid state. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å): Br1–C1, 1.8981(17); Br2–C10; 1.9021(17); C7–C8, 1.330(2); Br3–C15, 1.9010(17); Br4–C24, 1.8993(17); C21–C22, 1.334(2).

(*Z*)-1,1'-Dibromostilbene crystallizes in the monoclinic space group *P*2<sub>1</sub>/c with *Z* = 4. The asymmetric unit contains two crystallographically independent, but chemically equivalent molecules with very similar bonding parameters. The data is reported for completeness, but not discussed in detail.

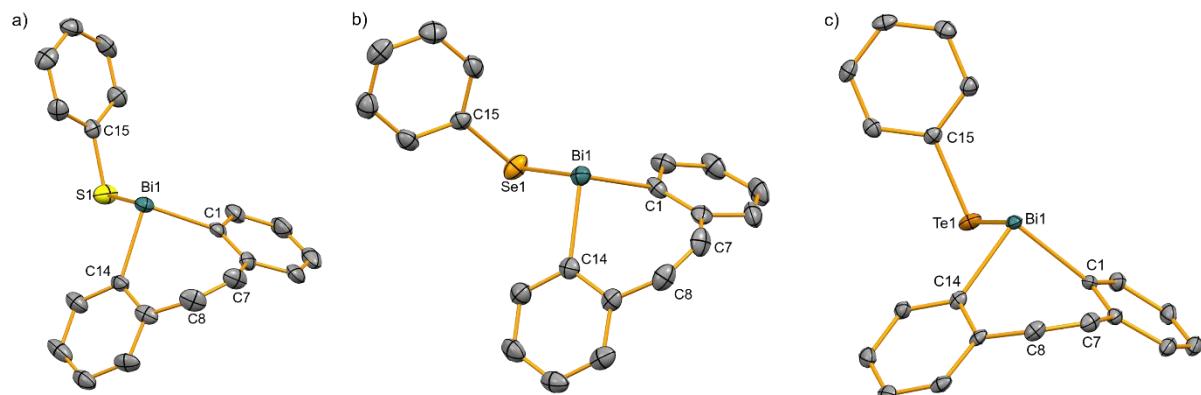
The molecular structure of (*Z*-1,2-bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene containing one toluene molecule in the crystal lattice was reported and discussed in our first publication on dibenzobismepines. Additionally, a range of data sets with varying types of solvent molecules in the crystal lattice (benzene, dichloromethane or tetrahydrofuran; CCDC deposition numbers: 1961408–11) have been reported.<sup>[22]</sup> In the course of our further investigations an additional data set (**SI-2**) containing no solvent molecule in the crystal lattice

was obtained (triclinic space group  $P\bar{1}$ ,  $Z = 2$ ). The data is reported for completeness, but not discussed in detail, because the structural parameters of all data sets obtained so far are highly similar.



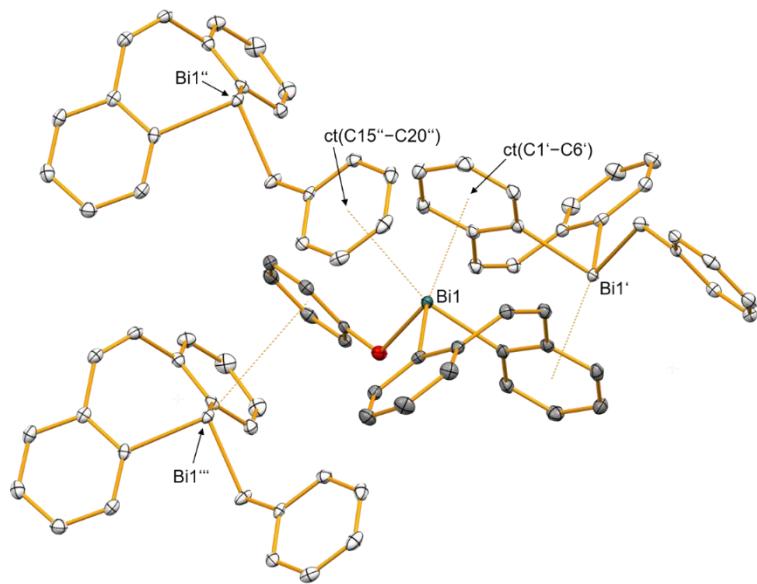
**Figure S2.** Molecular structure of (*Z*)-1,2-bis[2-(5*H*-dibenzo[*b,f*]bismepin-5-yl)phenyl]ethene in the solid state. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å): Bi1–C1, 2.236(2); Bi1–C14; 2.249(3); Bi1–C15, 2.255(2); Bi2–C29, 2.256(2); Bi2–C42, 2.241(2); Bi2–C28, 2.254(2).

A graphical representation of the molecular structure of **3-O** is given in Figure 2 of the main text. Figure S3 shows the molecular structures of compounds **3-S**, **3-Se** and **3-Te**. The bonding parameters are discussed in the main text.

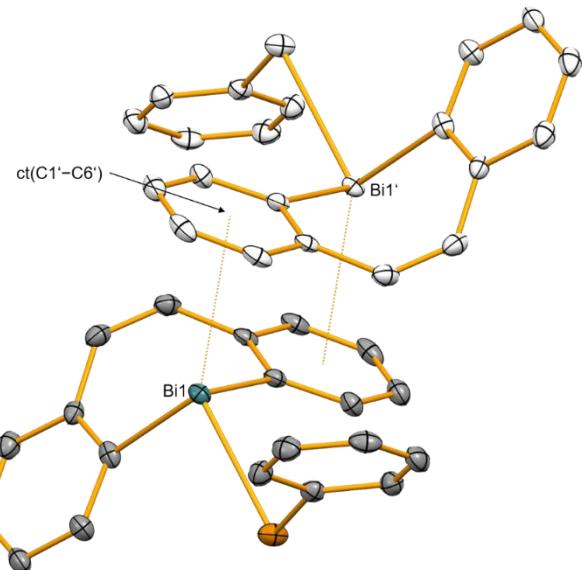


**Figure S3.** Molecular structures of **3-S** (a), **3-Se** (b) and **3-Te** (c) in the solid state. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

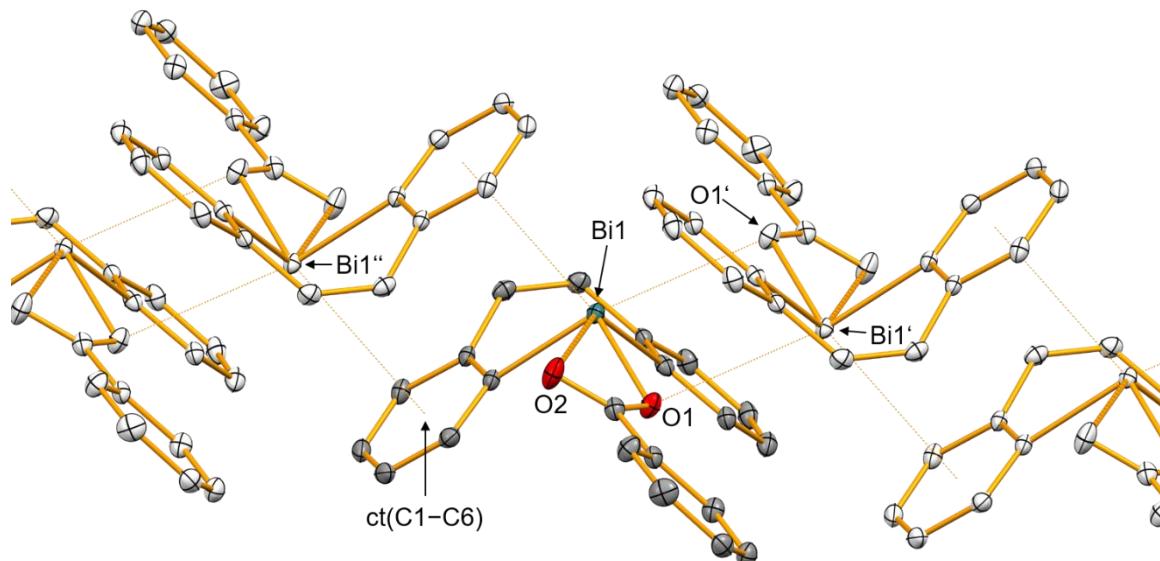
The intermolecular interactions of compounds **3-E** and **4** in the solid state lead to the formation of coordination polymers (**3-O** and **4**) or dimeric structures (**3-S**, **3-Se**, and **3-Te**), as discussed in the main text. Graphical representations are shown in Figures S4–6. As **3-S**, **3-Se** and **3-Te** are isostructural only **3-Te** is shown as a representative example.



**Figure S4.** Intermolecular interactions of **3-O** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms and one lattice-bound benzene molecule are omitted for clarity.

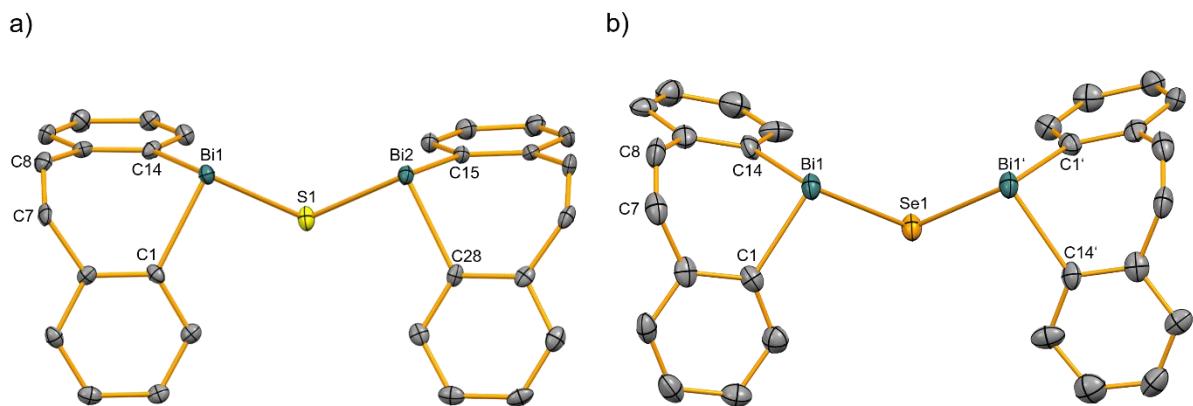


**Figure S5.** Intermolecular interactions of **3-Te** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms are omitted for clarity.



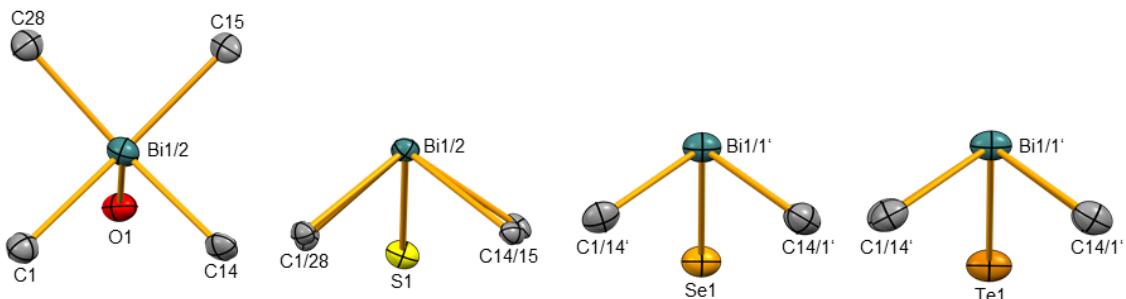
**Figure S6.** Intermolecular interactions of **4** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms are omitted for clarity.

The molecular structures of **5-O** and **5-Te** are depicted in Figure 4 of the main text. Figure S7 shows the molecular structures of compounds **5-S** and **5-Se**. The bonding parameters are discussed in the main text.



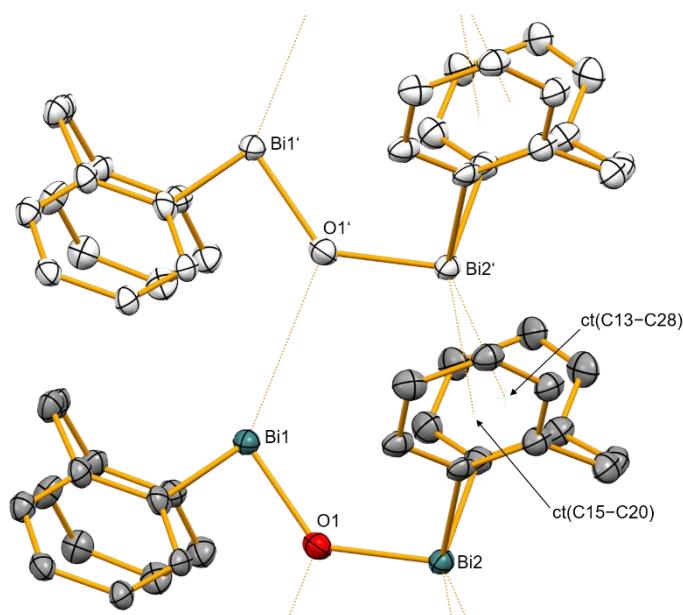
**Figure S7.** Molecular structures of **5-S** (a) and **5-Se** (b) in the solid state. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

The different orientations of the dibenzobismepine units in compounds **5-E** ( $E = O, S, Se, Te$ ) in the solid state are discussed in the main text. Figure S8 contains a simplified representation of the molecular structures of the compounds viewed along the Bi-Bi axis.

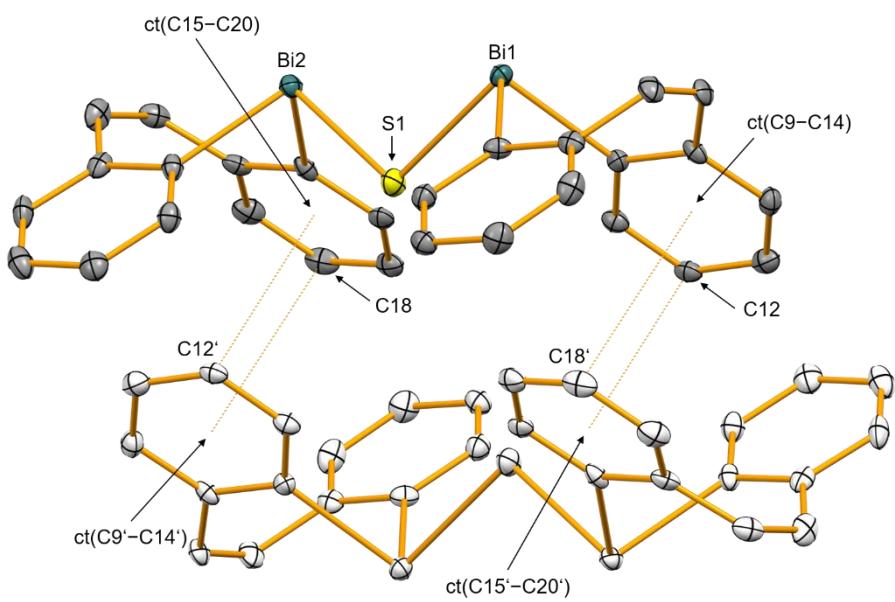


**Figure S8.** View of the molecular structures of compounds **5-E** along a Bi-Bi axis showing the *anti*-periplanar/*syn*-periplanar orientation of the dibenzobismepine units. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms and all carbon atoms not directly bound to bismuth are omitted for clarity.

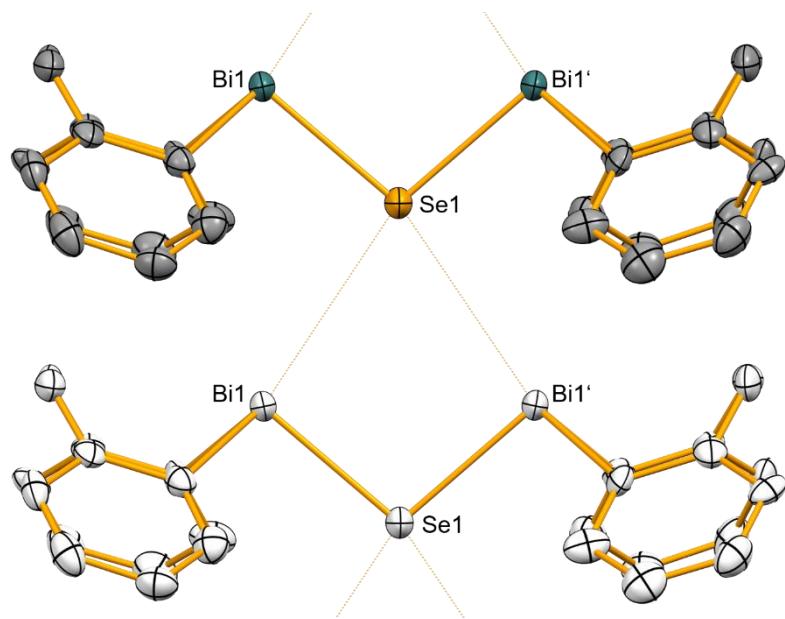
The intermolecular interactions of compounds **5-E** ( $E = O, S, Se, Te$ ) in the solid state lead to the formation of coordination polymers ( $E = O, Se, Te$ ) or dimeric structures ( $E = S$ ), as discussed in the main text. Graphical representations are shown in Figures S9-11. As **5-Se** and **5-Te** are isostructural, only **5-Se** is shown as a representative example.



**Figure S9.** Intermolecular interactions of **5-O** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms are omitted for clarity.



**Figure S10.** Intermolecular interactions of **5-S** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms are omitted for clarity.

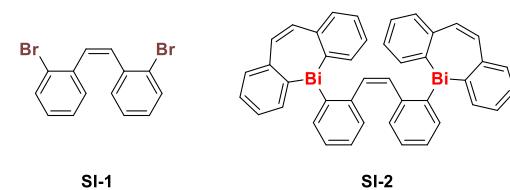


**Figure S11.** Intermolecular interactions of **5-Se** in the solid state. Displacement ellipsoids are drawn at the 50% level. Displacement ellipsoids exceeding one molecular unit are shown in white. Hydrogen atoms are omitted for clarity.

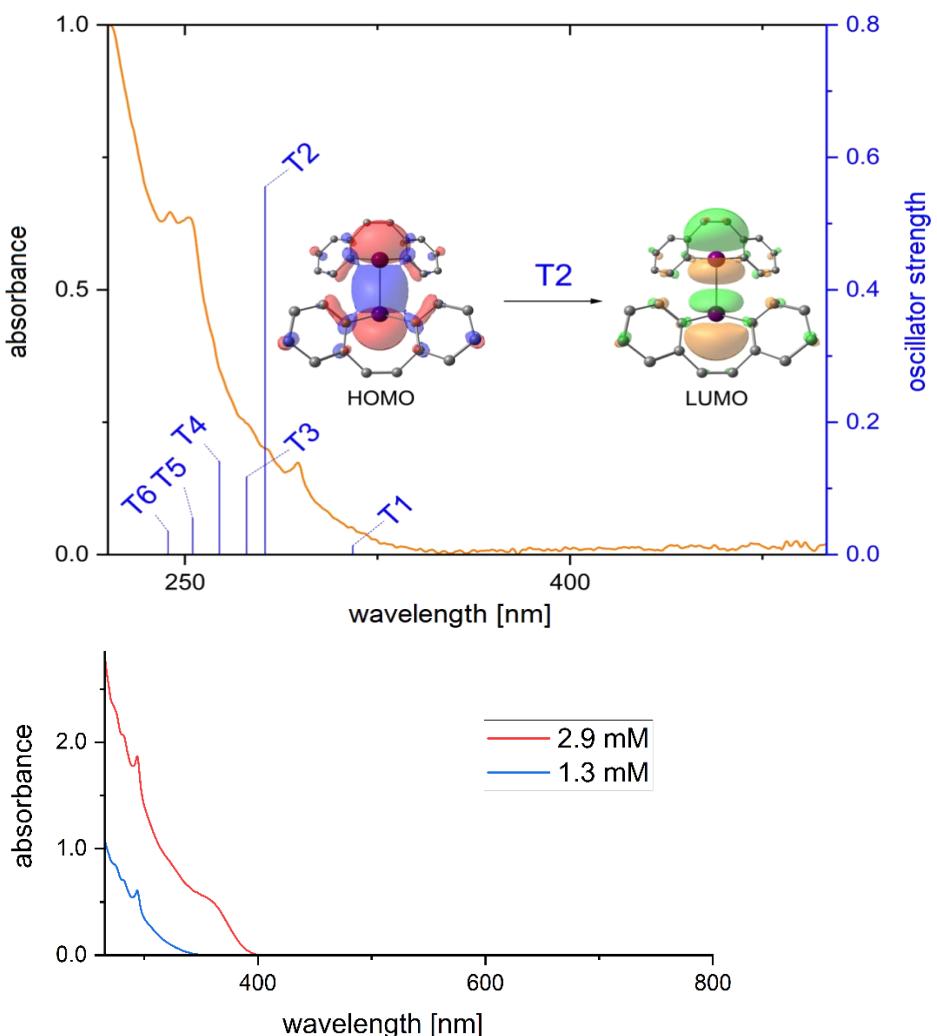
**Table S1.** Selected crystal structure data of the structure determinations.

Data	2	3-O	3-S	3-Se	3-Te	4	5-O	5-S	5-Se	5-Te	SI-1	SI-2
Empirical formula	C <sub>14</sub> H <sub>10</sub> Bi	C <sub>23</sub> H <sub>18</sub> BiO	C <sub>20</sub> H <sub>15</sub> BiS	C <sub>20</sub> H <sub>15</sub> BiSe	C <sub>20</sub> H <sub>15</sub> BiTe	C <sub>21</sub> H <sub>15</sub> BiO <sub>2</sub>	C <sub>56</sub> H <sub>40</sub> O <sub>2</sub> Bi <sub>4</sub>	C <sub>28</sub> H <sub>20</sub> Bi <sub>2</sub> S	C <sub>28</sub> H <sub>20</sub> Bi <sub>2</sub> Se	C <sub>28</sub> H <sub>20</sub> Bi <sub>2</sub> Te	C <sub>28</sub> H <sub>20</sub> Br <sub>4</sub>	C <sub>42</sub> H <sub>30</sub> Bi <sub>2</sub>
Formula weight (g·mol <sup>-1</sup> )	387.20	519.35	496.36	543.26	591.90	508.31	1580.80	806.46	853.36	902.00	676.08	952.62
Temperature (K)	100(2)	100(2)	200(2) <sup>a</sup>	180(2) <sup>a</sup>	100(2)	100	100(2)	100(2)	100(2)	173(2) <sup>a</sup>	100	100
Radiation, $\lambda$ (Å)						MoK <sub>α</sub> , 0.71073						
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	orthorhombic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	Pbca	P <sub>1</sub>	P2 <sub>1</sub> /n	C2/c	C2/c	P2 <sub>1</sub> /c	P <sub>1</sub>
Unit cell dimensions												
<i>a</i> (Å)	9.1902(5)	11.8835(18)	9.5440(5)	9.6440(17)	9.7592(3)	9.430(2)	4.8746(17)	11.7237(10)	19.8041(16)	19.753(4)	15.574(2)	9.3341(16)
<i>b</i> (Å)	14.9075(8)	8.3914(11)	15.8368(8)	15.960(3)	16.0421(4)	16.169(4)	13.049(5)	16.1981(11)	4.7557(4)	4.8206(8)	14.719(3)	13.658(3)
<i>c</i> (Å)	7.8773(4)	18.201(4)	10.8489(5)	10.8721(18)	10.8441(3)	21.324(5)	36.660(12)	11.9567(10)	28.314(2)	29.075(5)	11.1447(16)	13.9881(2)
$\alpha$ (°)	90	90	90	90	90	90	89.432(10)	90	90	90	90	66.633(11)
$\beta$ (°)	90.513(2)	91.409(6)	97.213(3)	97.221(4)	96.8660(10)	90	87.490(9)	93.910(4)	102.903(3)	102.917(4)	108.183(9)	83.945(13)
$\gamma$ (°)	90	90	90	90	90	90	80.294(9)	90	90	90	90	82.056(13)
Volume (Å <sup>3</sup> )	1079.17(10)	1814.4(5)	1626.80(14)	1660.2(5)	1685.56(8)	3251.3(14)	2296.2(14)	2265.3(3)	2599.4(4)	2698.6(8)	2427.1(7)	1618.0(5)
<i>Z</i>	4	4	4	4	4	8	2	4	4	4	4	2
Calculated density (g·cm <sup>-3</sup> )	2.383	1.901	2.027	2.173	2.332	2.077	2.286	2.365	2.181	2.220	1.850	1.955
Absorption coefficient (mm <sup>-1</sup> )	16.297	9.724	10.959	12.806	12.150	10.855	15.324	15.621	14.933	14.096	6.647	10.890
<i>F</i> (000)	708.0	988	936	1008	1080	1920	1448.0	1480	1552	1624	1312	896
Theta range for collection (°)	2.604 to 26.750	2.239 to 26.827	2.151 to 25.119	2.129 to 25.108	2.456 to 31.059	2.677 to 28.704	1.112 to 26.811	2.120 to 31.067	2.074 to 25.227	2.116 to 27.542	2.370 to 28.726	2.603 to 30.099
Reflections collected	11863	79430	10750	10841	24055	34787	21247	42725	14854	15942	63925	66223
Independent reflections	2293	3871	2888	2937	5363	4193	9765	7245 / 280 / 0	2399 / 142 / 0	3110 / 142 / 0	6266 / 289 / 0	9445 / 397 / 0
Minimum/maximum transmission	0.5741/0.7454	0.5089/0.7454	0.0361/0.1016	0.0691/0.1359	0.1766/0.3723	0.5053/0.7458	0.5108/0.7454	0.2084/0.4685	0.0224/0.0608	0.0671/0.1410	0.4762/0.7458	0.4305/0.7460
Refinement method							Full-matrix least-squares on <i>P</i> <sup>2</sup>					
Data / parameters / restraints	2293 / 136 / 300	3871 / 226 / 0	2888 / 200 / 0	2937 / 199 / 0	5363 / 199 / 0	4193 / 217 / 0	9765 / 559 / 854	7245 / 280 / 0	2399 / 142 / 0	3110 / 142 / 0	6266 / 289 / 0	9445 / 397 / 0
Goodness-of-fit on <i>P</i> <sup>2</sup>	0.933	1.103	1.077	1.074	1.037	1.082	0.971	1.050	1.194	1.080	1.046	1.026
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0338$ , $wR_2 = 0.0758$	$R_1 = 0.0117$ , $wR_2 = 0.0273$	$R_1 = 0.0420$ , $wR_2 = 0.1040$	$R_1 = 0.0297$ , $wR_2 = 0.0721$	$R_1 = 0.0232$ , $wR_2 = 0.0568$	$R_1 = 0.0160$ , $wR_2 = 0.0328$	$R_1 = 0.0661$ , $wR_2 = 0.1230$	$R_1 = 0.0311$ , $wR_2 = 0.0628$	$R_1 = 0.0286$ , $wR_2 = 0.0651$	$R_1 = 0.0228$ , $wR_2 = 0.0567$	$R_1 = 0.0209$ , $wR_2 = 0.0457$	$R_1 = 0.0191$ , $wR_2 = 0.0387$
R indices (all data)	$R_1 = 0.0566$ , $wR_2 = 0.0893$	$R_1 = 0.0128$ , $wR_2 = 0.0277$	$R_1 = 0.0469$ , $wR_2 = 0.1072$	$R_1 = 0.0353$ , $wR_2 = 0.0744$	$R_1 = 0.0281$ , $wR_2 = 0.0586$	$R_1 = 0.0180$ , $wR_2 = 0.0333$	$R_1 = 0.1547$ , $wR_2 = 0.1560$	$R_1 = 0.0441$ , $wR_2 = 0.0666$	$R_1 = 0.0306$ , $wR_2 = 0.0662$	$R_1 = 0.0255$ , $wR_2 = 0.0581$	$R_1 = 0.0263$ , $wR_2 = 0.0472$	$R_1 = 0.0237$ , $wR_2 = 0.0399$
Maximum/minimum residual electron density (e·Å <sup>-3</sup> )	1.00 / 0.87	0.452 / -0.581	2.150 / -1.992	1.435 / -1.138	1.743 / -1.619	0.72 / -0.60	2.35 / -2.55	2.011 / -2.398	2.08 / -1.70	2.074 / -1.378	0.65 / -0.55	1.07 / -0.95

a: cooling to 100 K did not give satisfactory results, presumably due to a phase transition.



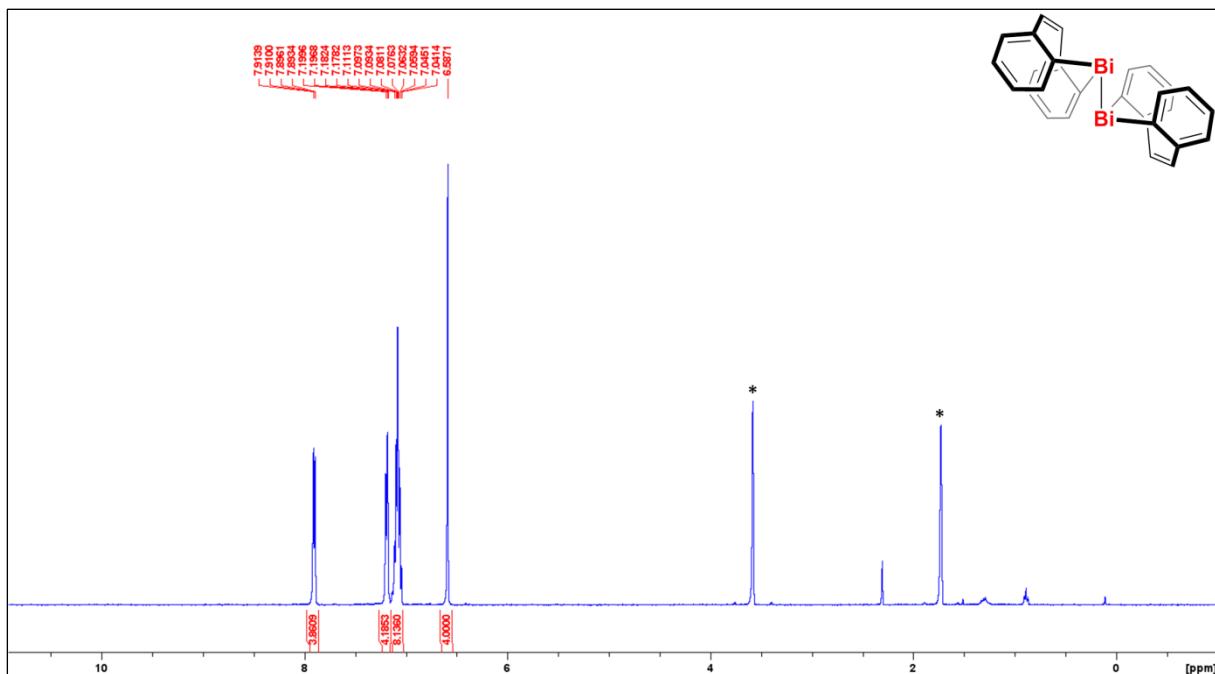
### UV-vis spectroscopy of compound 2



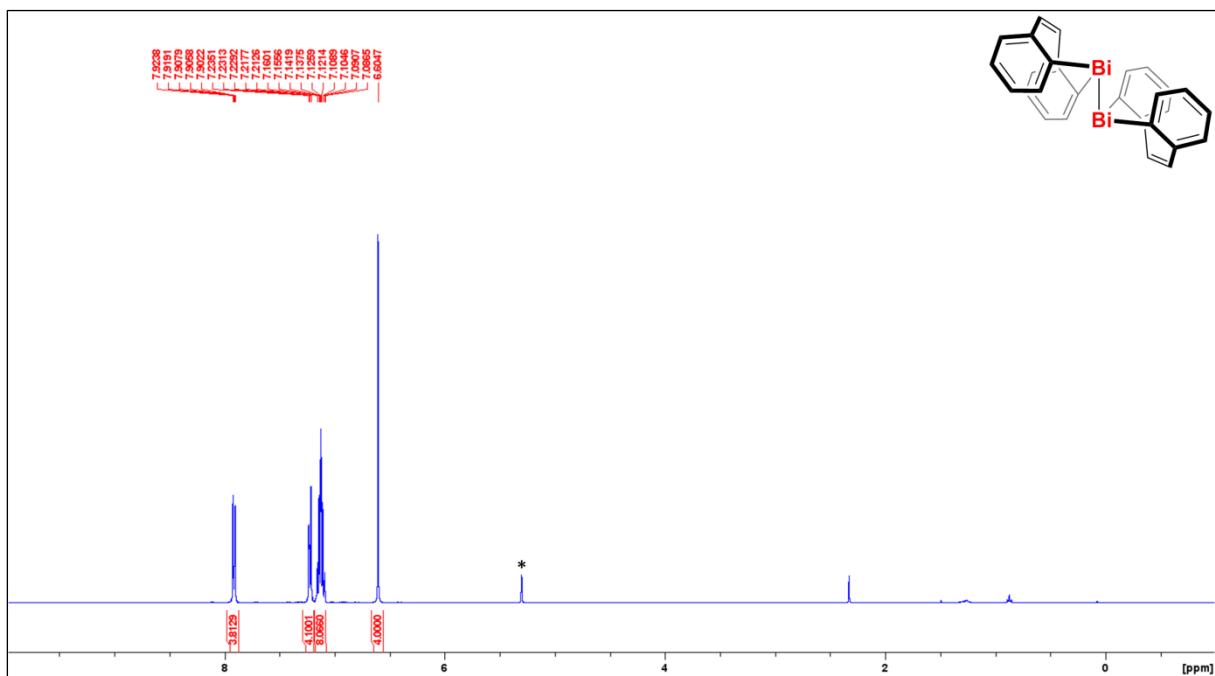
**Figure S12.** Experimental UV-vis spectrum of bis[dibenzobismepine] (**2**). Top: 1.3 mM in THF (orange), calculated transitions (blue) and molecular orbitals with main contributions to transition T<sub>2</sub>. Bottom: 1.3 mM in THF (blue) and 2.9 mM in THF (red).

Due to its orange color, a UV-vis spectrum of dibismuthane **2** was measured using a Mettler Toledo UV5 spectrometer. The UV/Vis absorption spectrum in THF shows weak absorption maxima at 244, 252 and 292 nm and an even weaker shoulder between 270 and 286 nm. Absorptions between 400 and 800 nm which could explain the color of compound **2** could not be detected under these conditions. At higher concentrations, a shoulder reaching into the visible region at ca. 400 nm becomes apparent (Figure S12 bottom). TD-DFT calculations were performed with the B3LYP functional,<sup>[56]</sup> Grimme D3 dispersion corrections,<sup>[57]</sup> and 6-31G(d,p)<sup>[58]</sup> [H,C] and LANL2DZ<sup>[59]</sup> [Bi] basis sets. The theoretical data suggest that the  $\sigma$ -bonding Bi–Bi interactions are primarily present in the HOMO, while the LUMO can be described as  $\sigma^*$ -antibonding. According to the TD-DFT data, these molecular orbitals contribute to the transition with the highest oscillator strength, T<sub>2</sub> ( $\lambda_{\text{calc}} = 291$  nm,  $f = 0.5554$ , HOMO to LUMO; 91%). The molecular orbitals contributing to T<sub>1</sub> and T<sub>3</sub>–T<sub>6</sub> were found to be exclusively centered on the organic dibenzobismepine backbone.

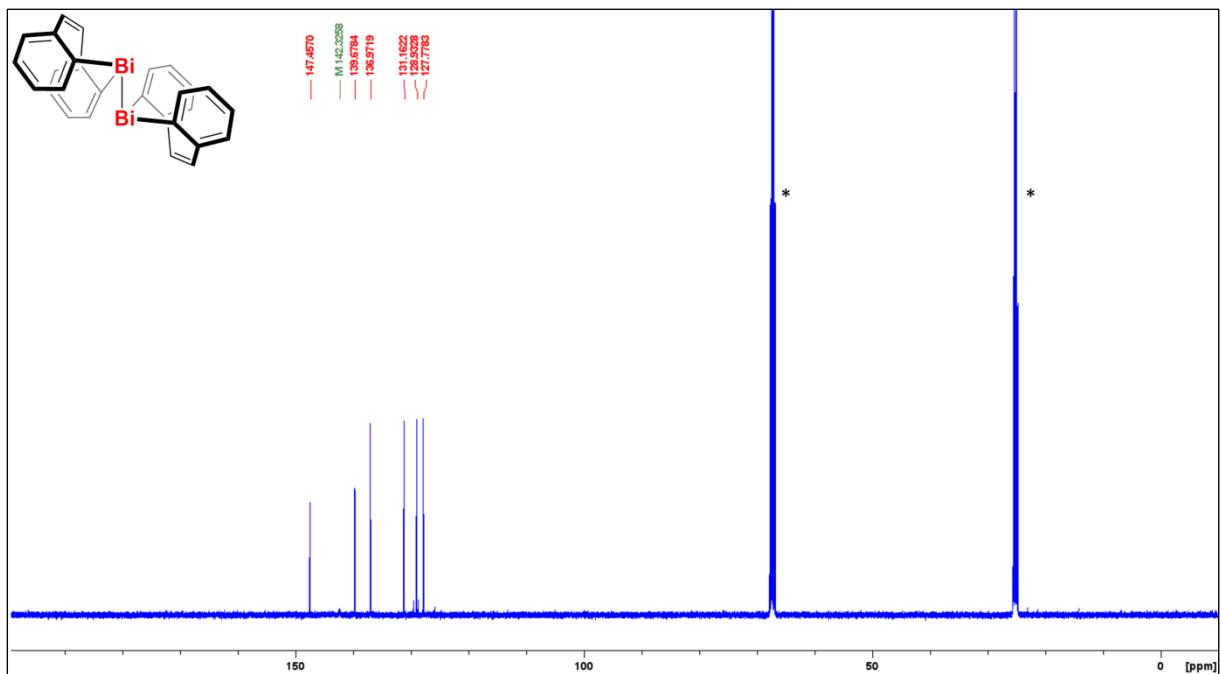
## NMR Spectra



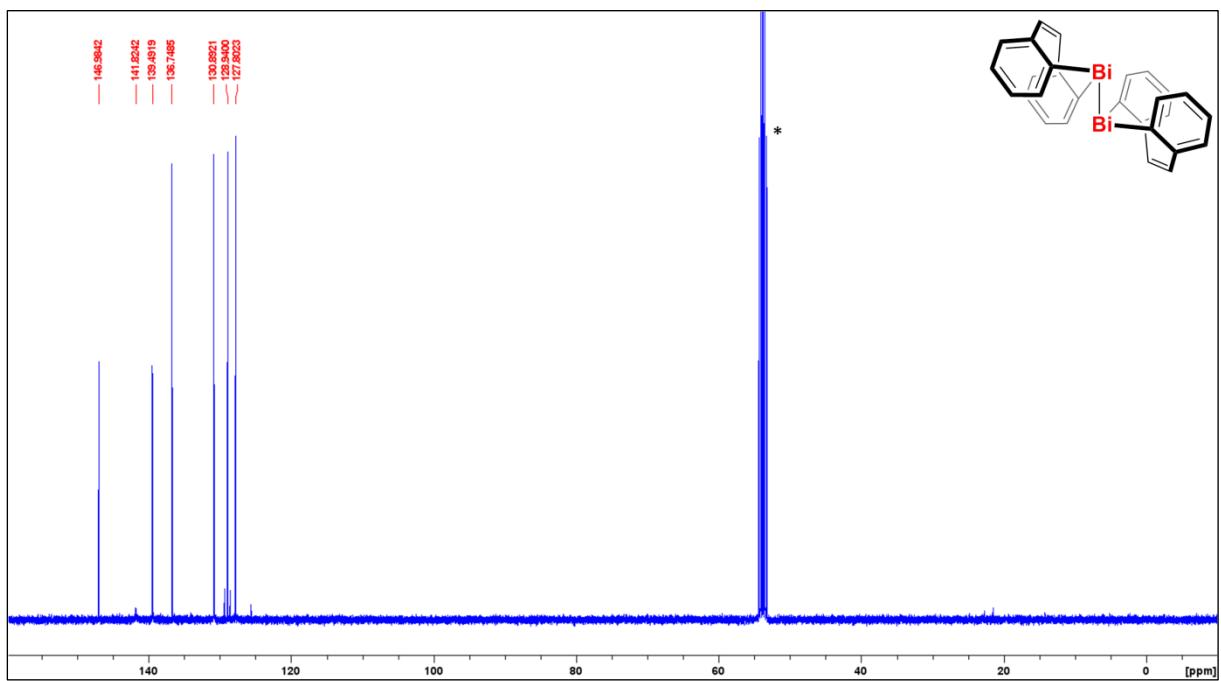
**Figure S13.** <sup>1</sup>H NMR spectrum of **2** in THF-*d*<sub>8</sub> (solvent signals: \*). Traces of toluene were detected.



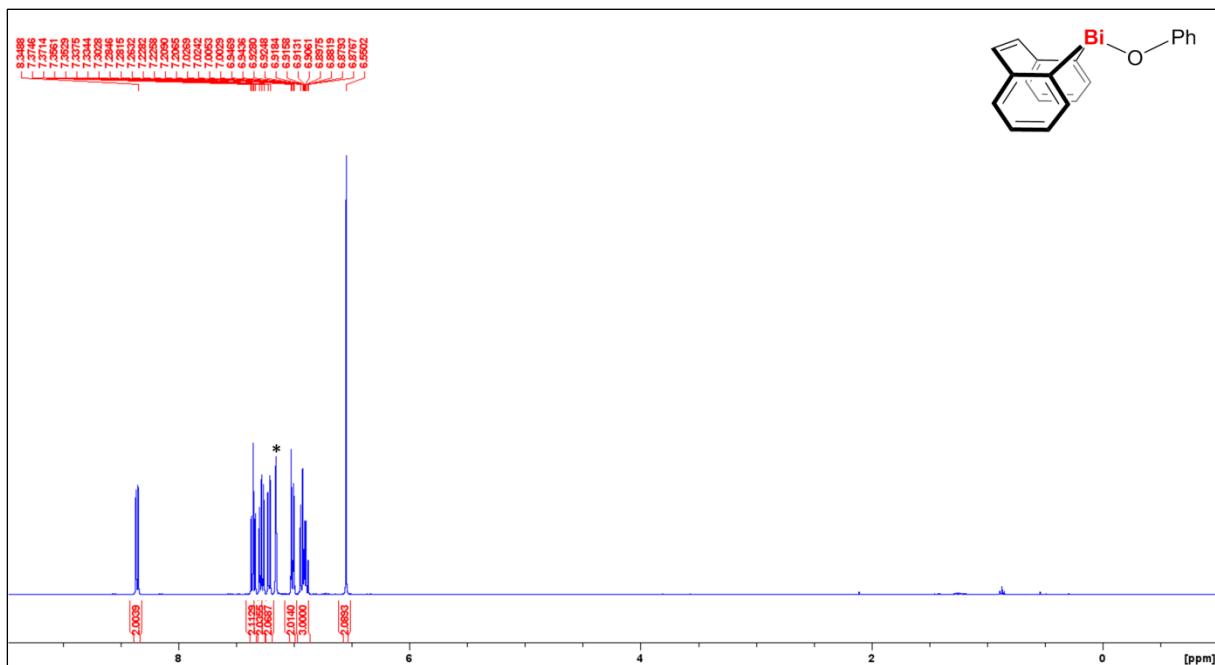
**Figure S14.** <sup>1</sup>H NMR spectrum of **2** in CD<sub>2</sub>Cl<sub>2</sub> (solvent signal: \*). Traces of toluene were detected.



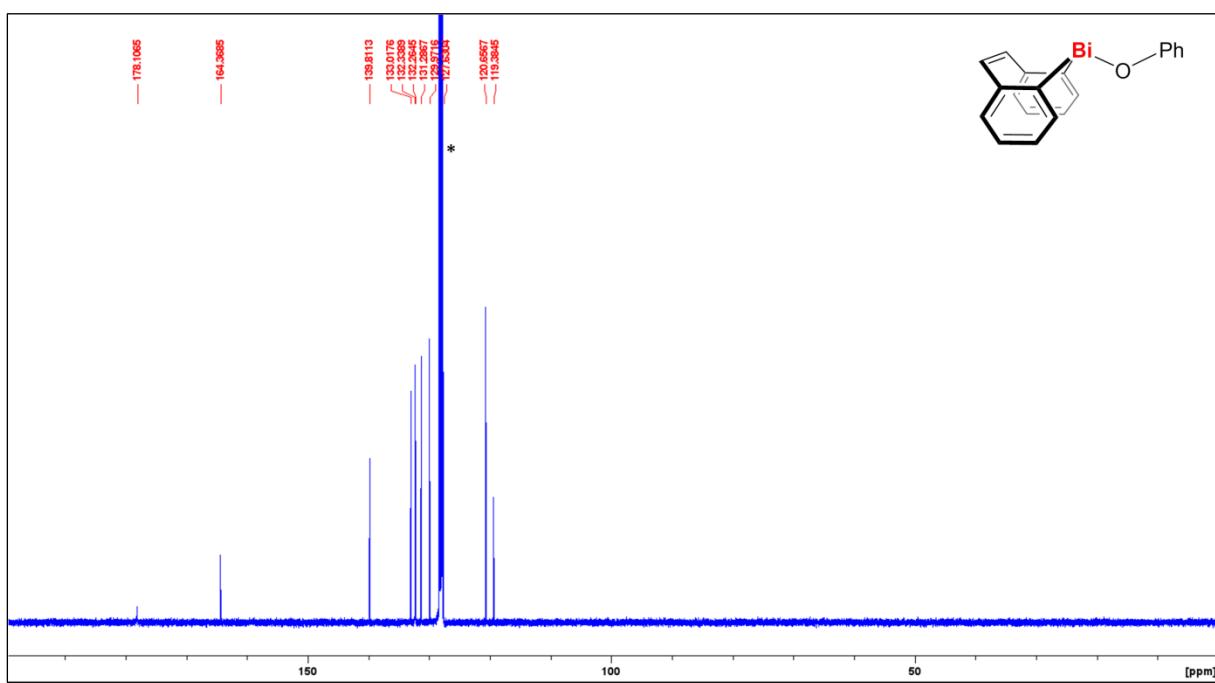
**Figure S15.**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{THF}-d_8$  (solvent signals: \*).



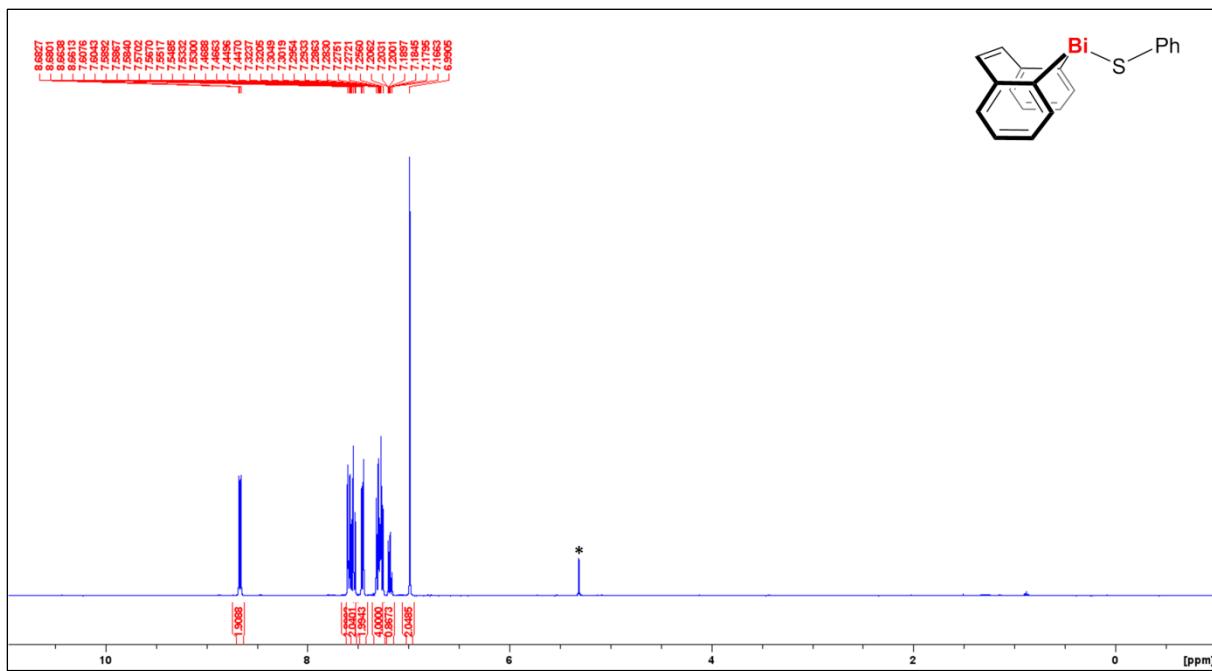
**Figure S16.**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



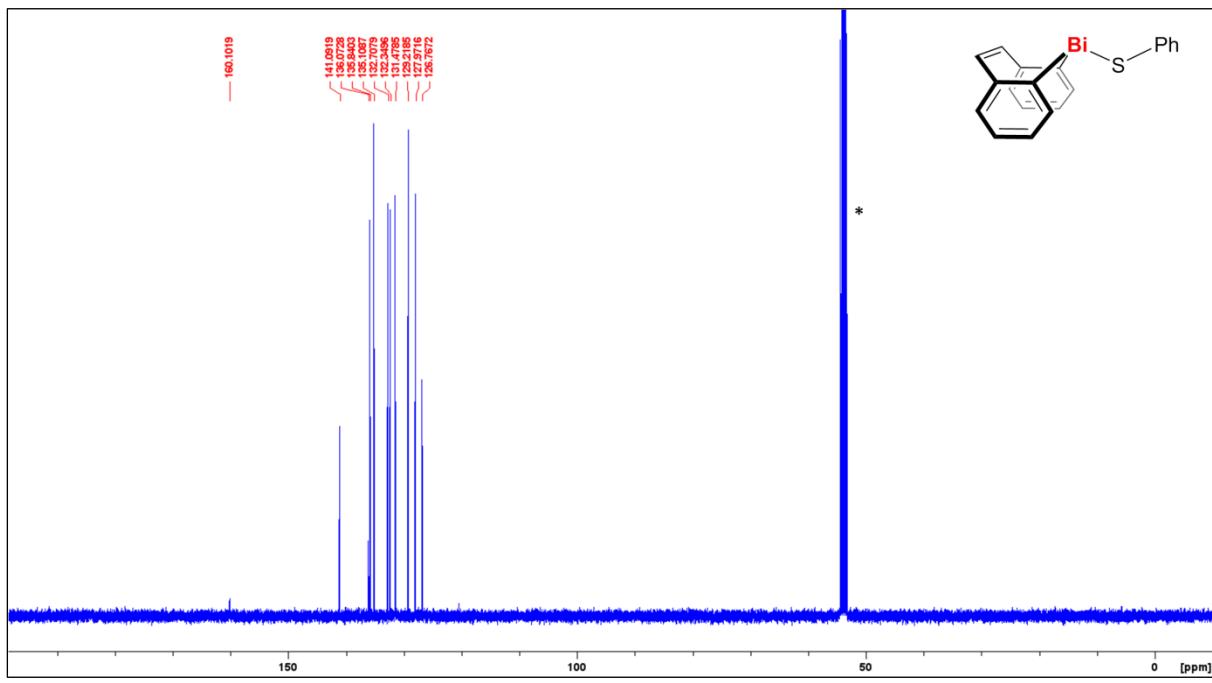
**Figure S17.**  $^1\text{H}$  NMR spectrum of **3-O** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



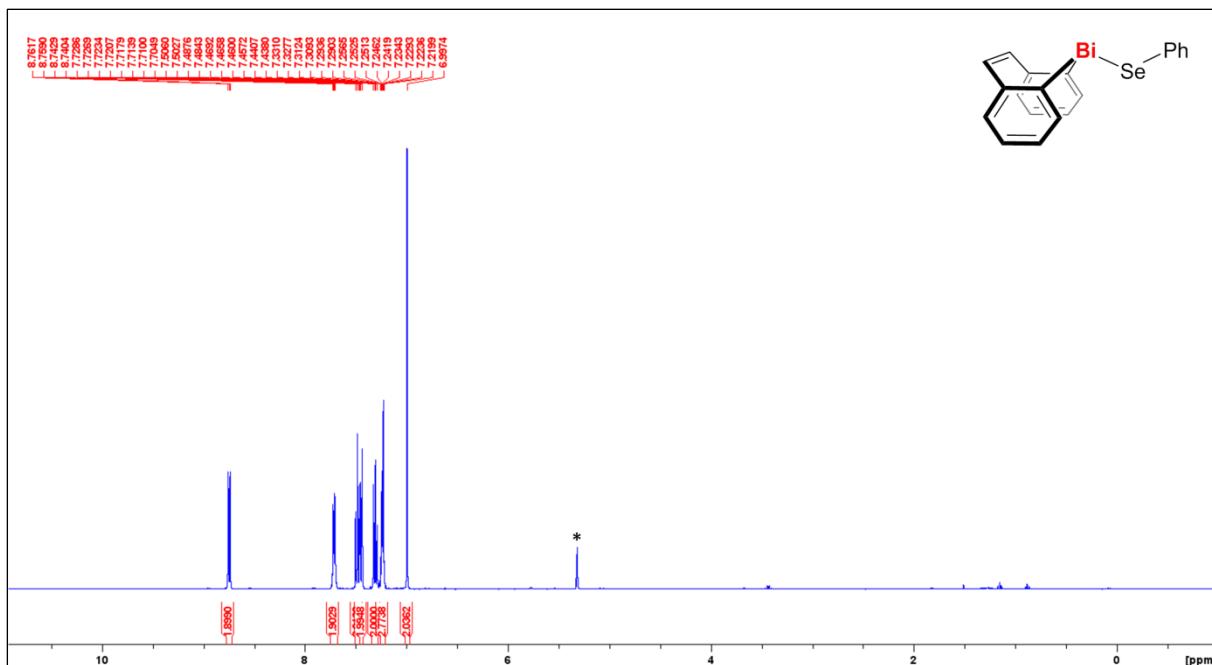
**Figure S18.**  $^{13}\text{C}$  NMR spectrum of **3-O** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



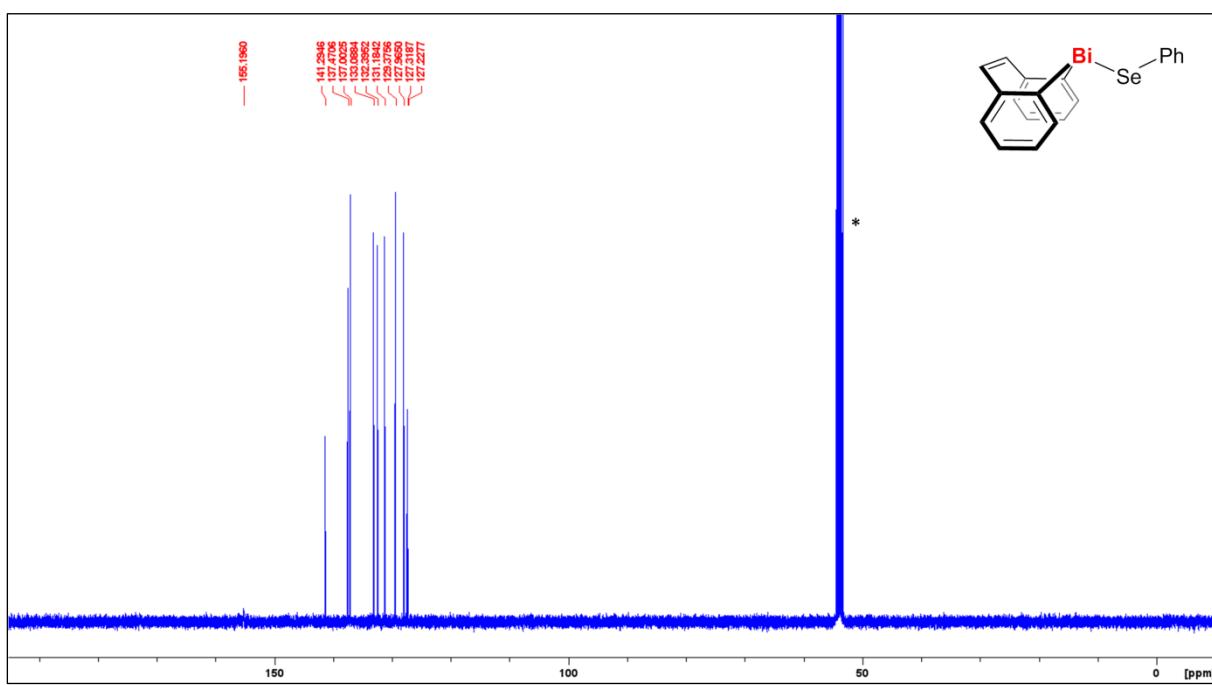
**Figure S19.**  $^1\text{H}$  NMR spectrum of **3-S** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



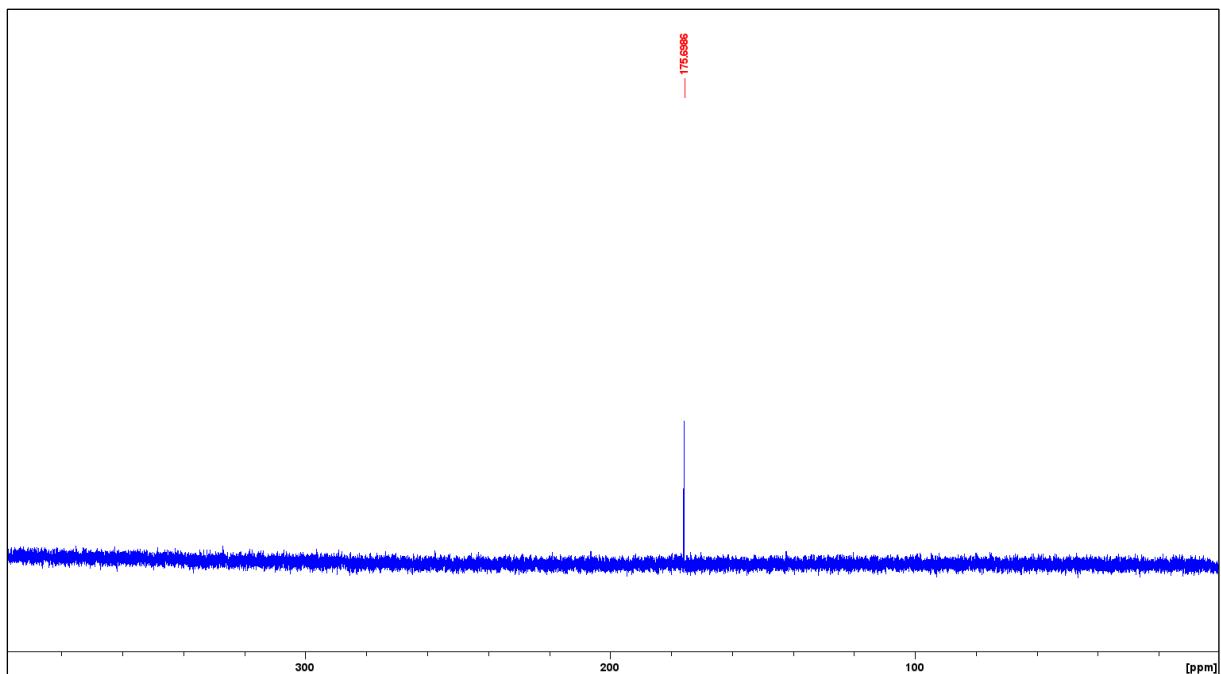
**Figure S20.**  $^{13}\text{C}$  NMR spectrum of **3-S** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



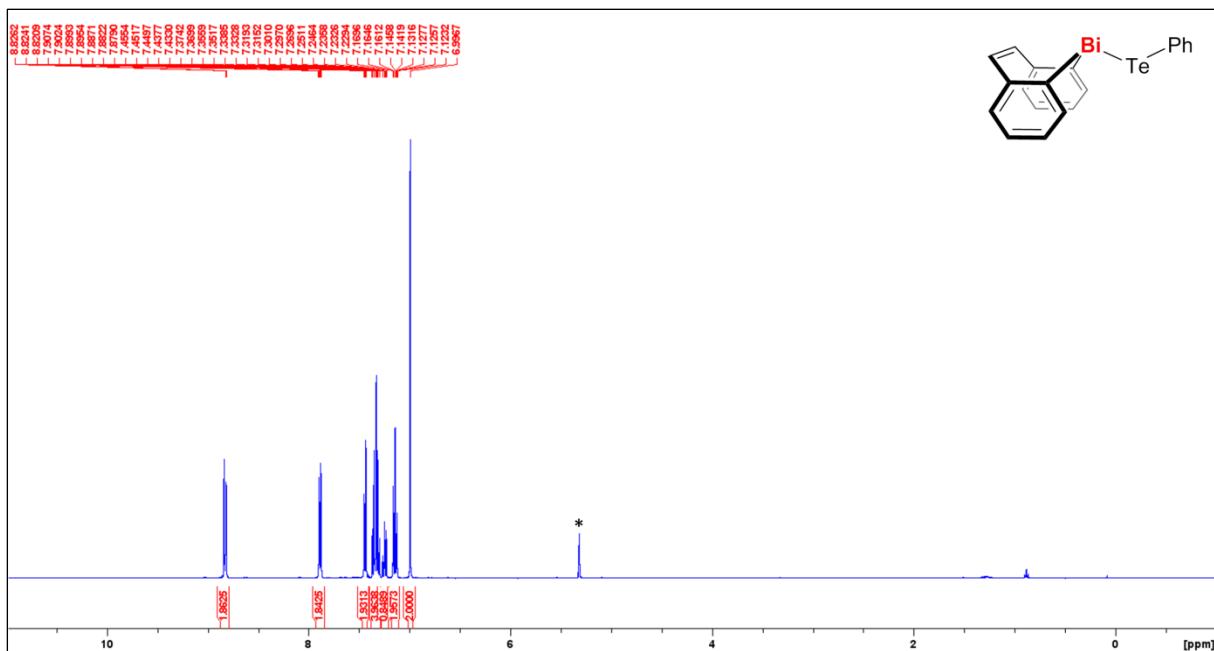
**Figure S21.**  $^1\text{H}$  NMR spectrum of **3-Se** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



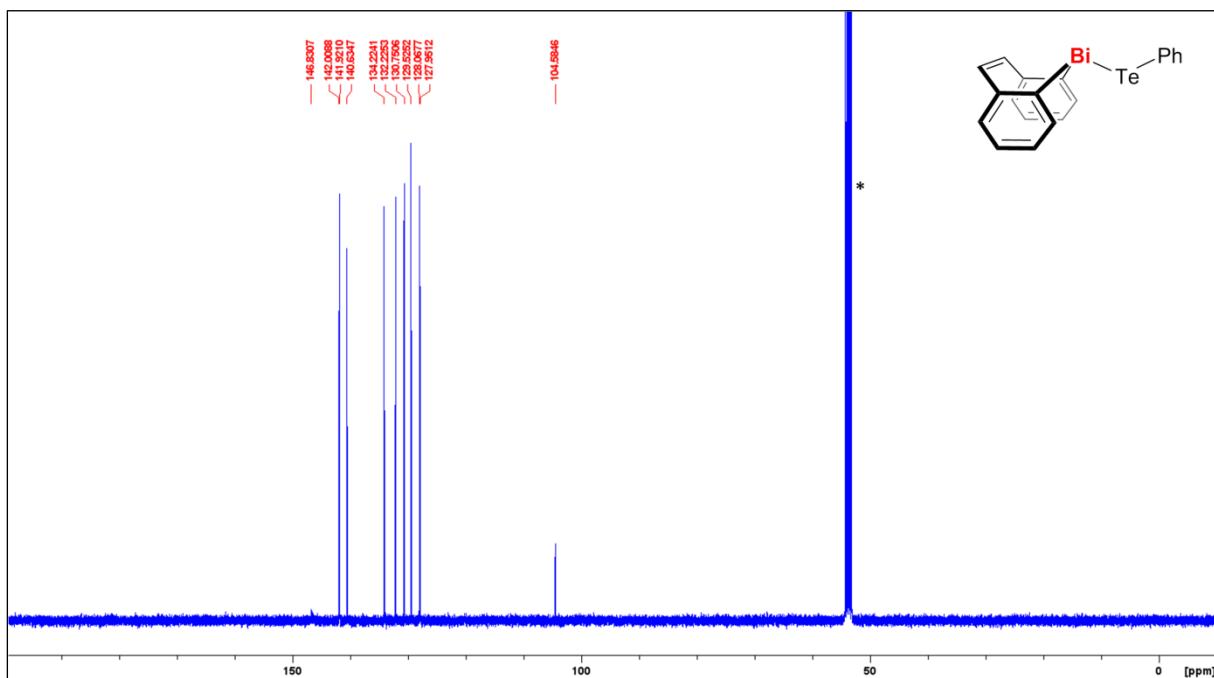
**Figure S22.**  $^{13}\text{C}$  NMR spectrum of **3-Se** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



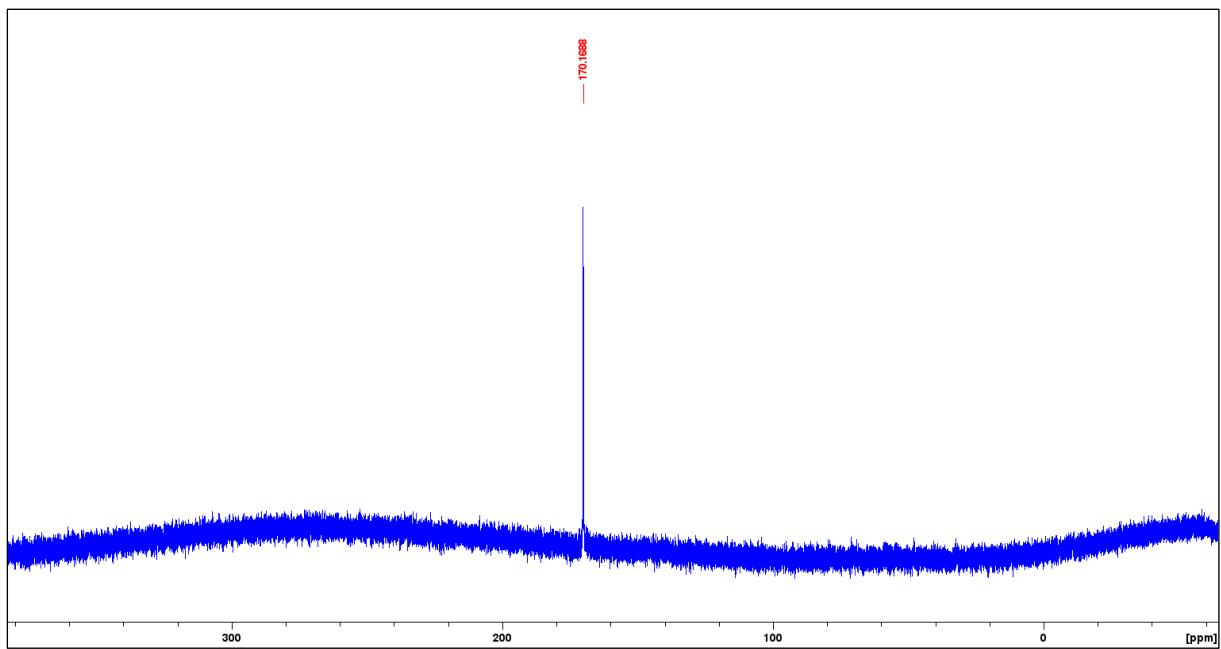
**Figure S23.** <sup>77</sup>Se NMR spectrum of **3-Se** in CD<sub>2</sub>Cl<sub>2</sub>.



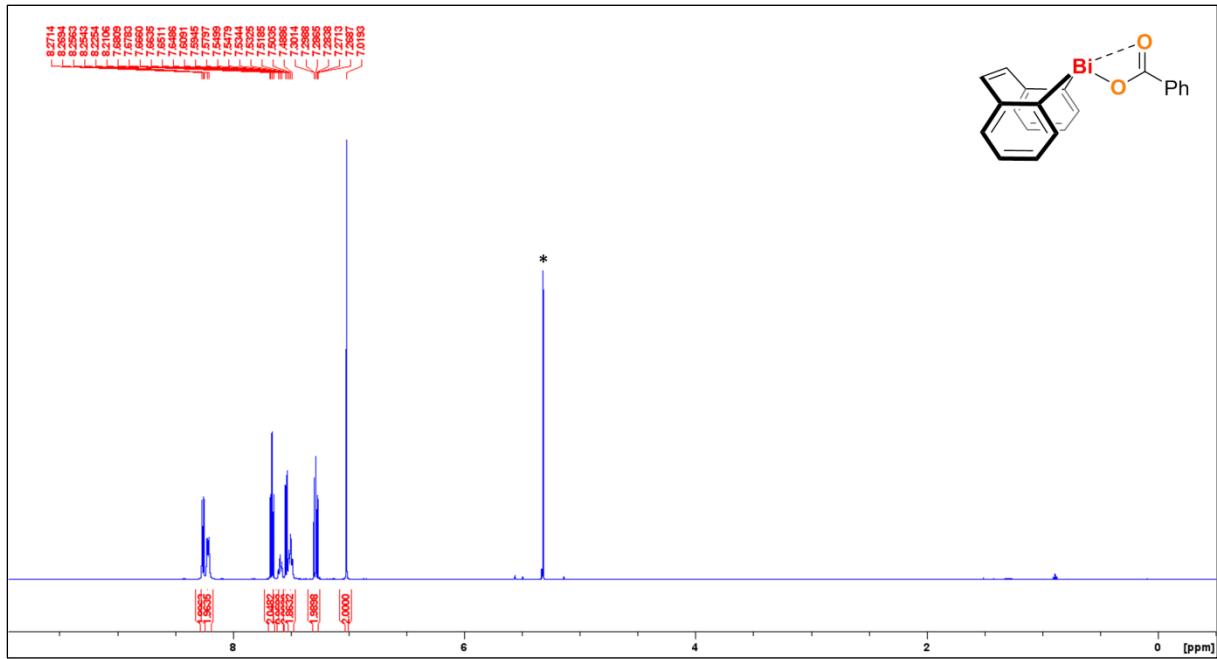
**Figure S24.**  $^1\text{H}$  NMR spectrum of **3-Te** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



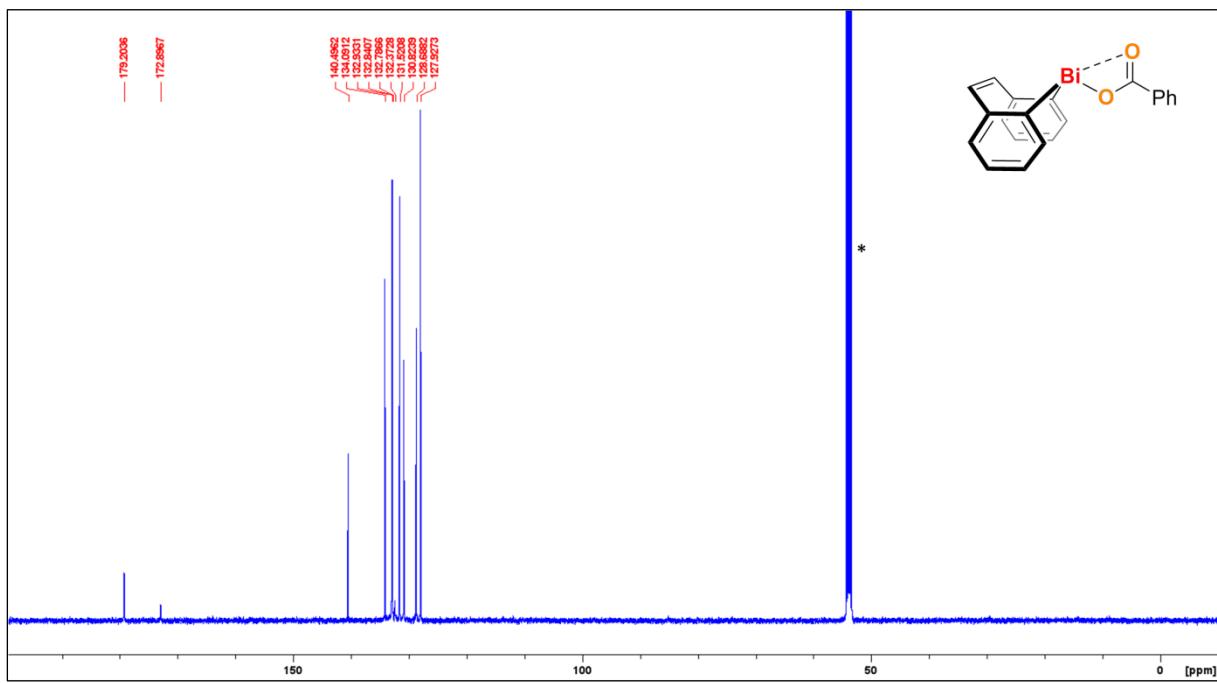
**Figure S25.**  $^{13}\text{C}$  NMR spectrum of **3-Te** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



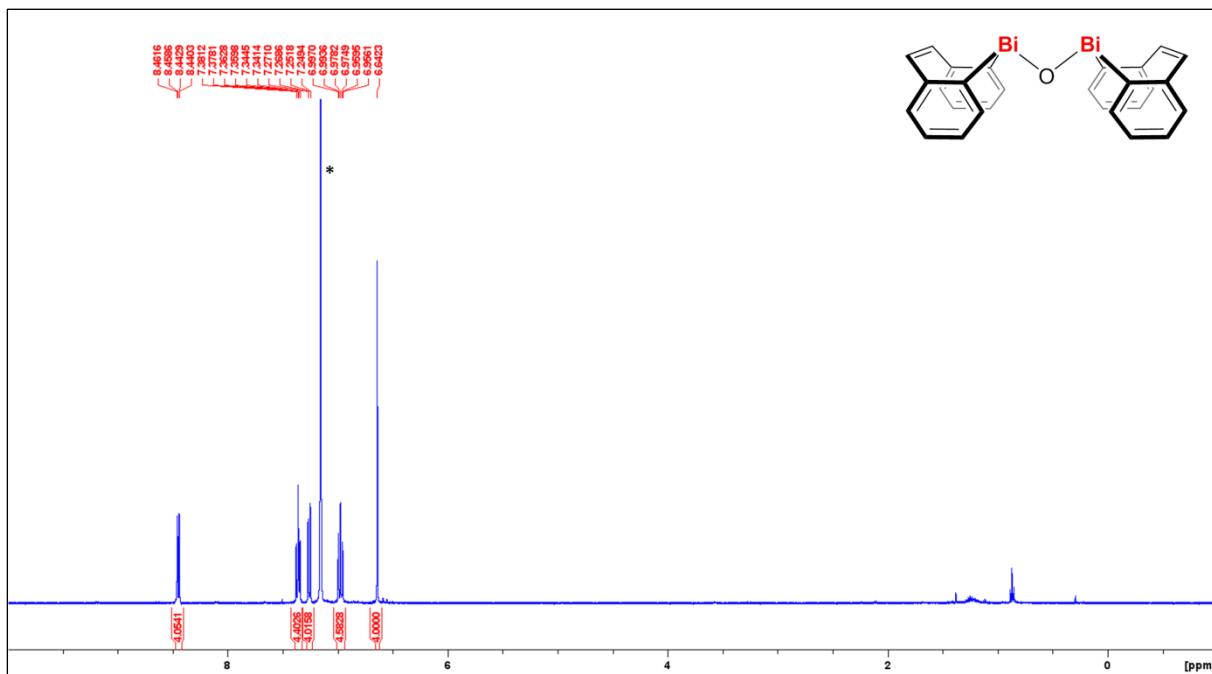
**Figure S26.**  $^{125}\text{Te}$  NMR spectrum of **3-Te** in  $\text{CD}_2\text{Cl}_2$ .



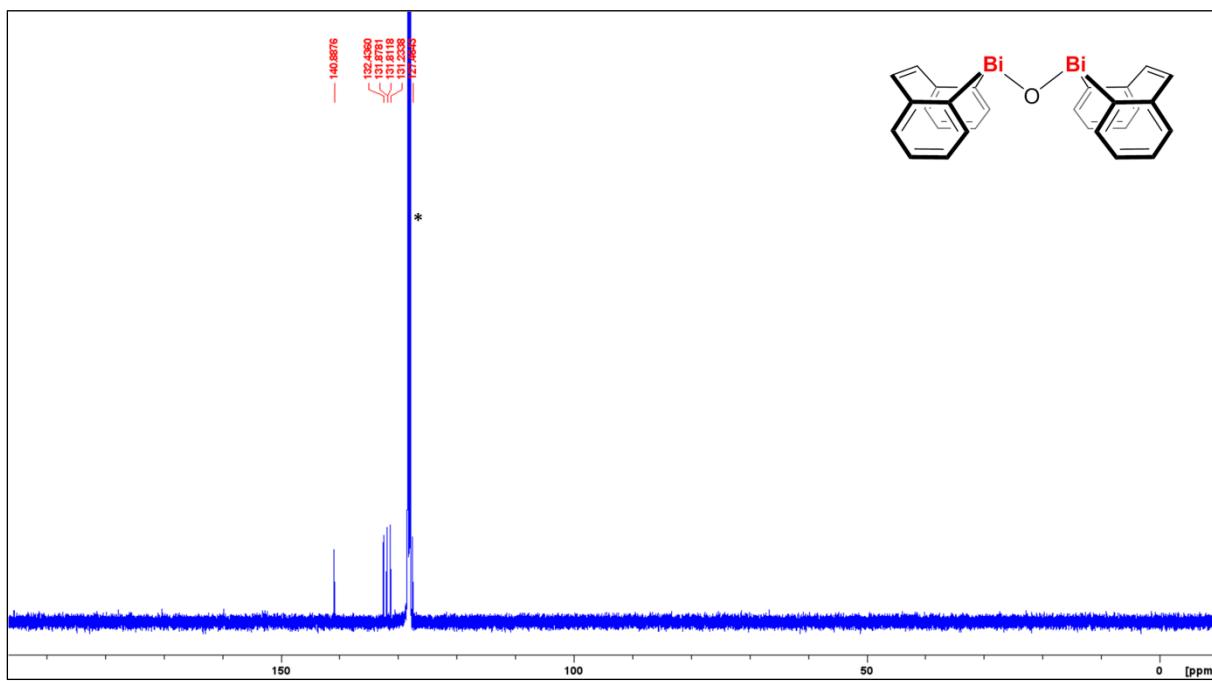
**Figure S27.**  $^1\text{H}$  NMR spectrum of **4** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



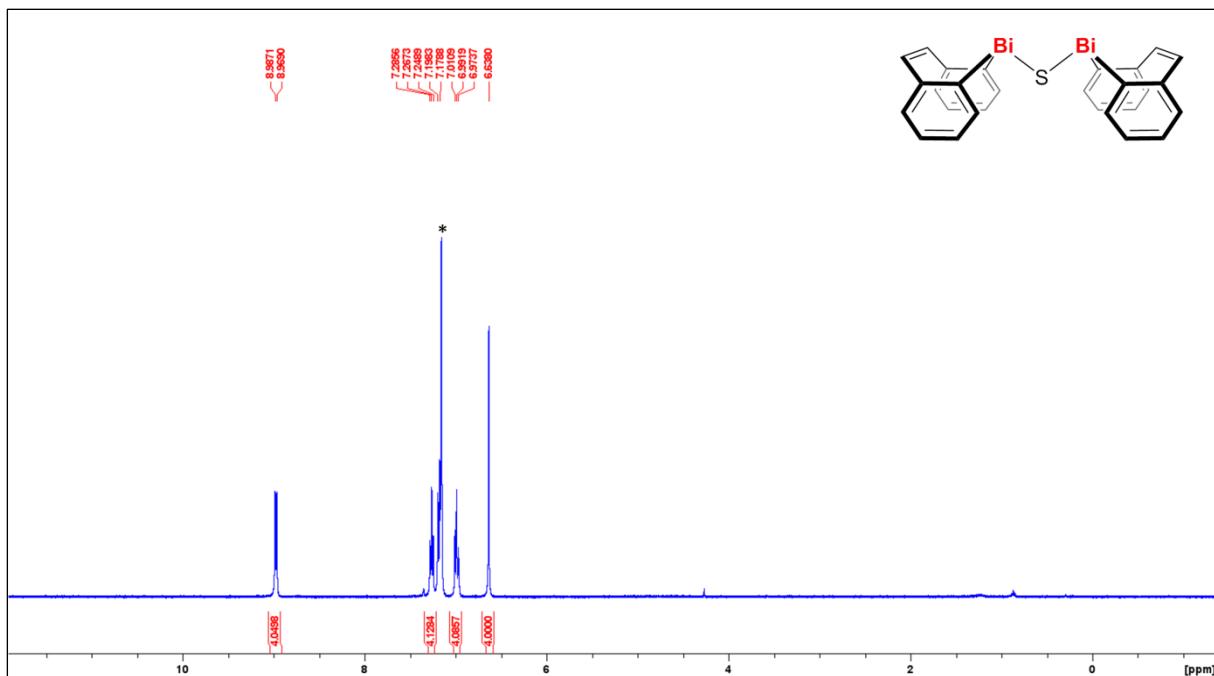
**Figure S28.**  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CD}_2\text{Cl}_2$  (solvent signal: \*).



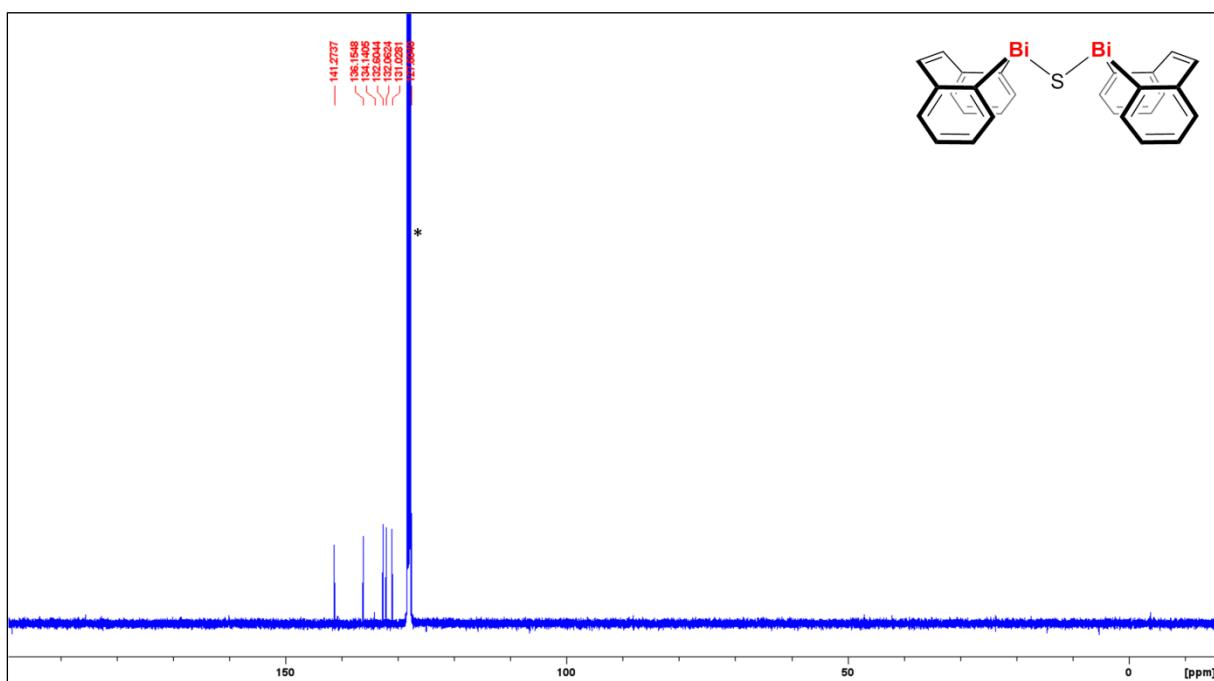
**Figure S29.**  $^1\text{H}$  NMR spectrum of **5-O** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



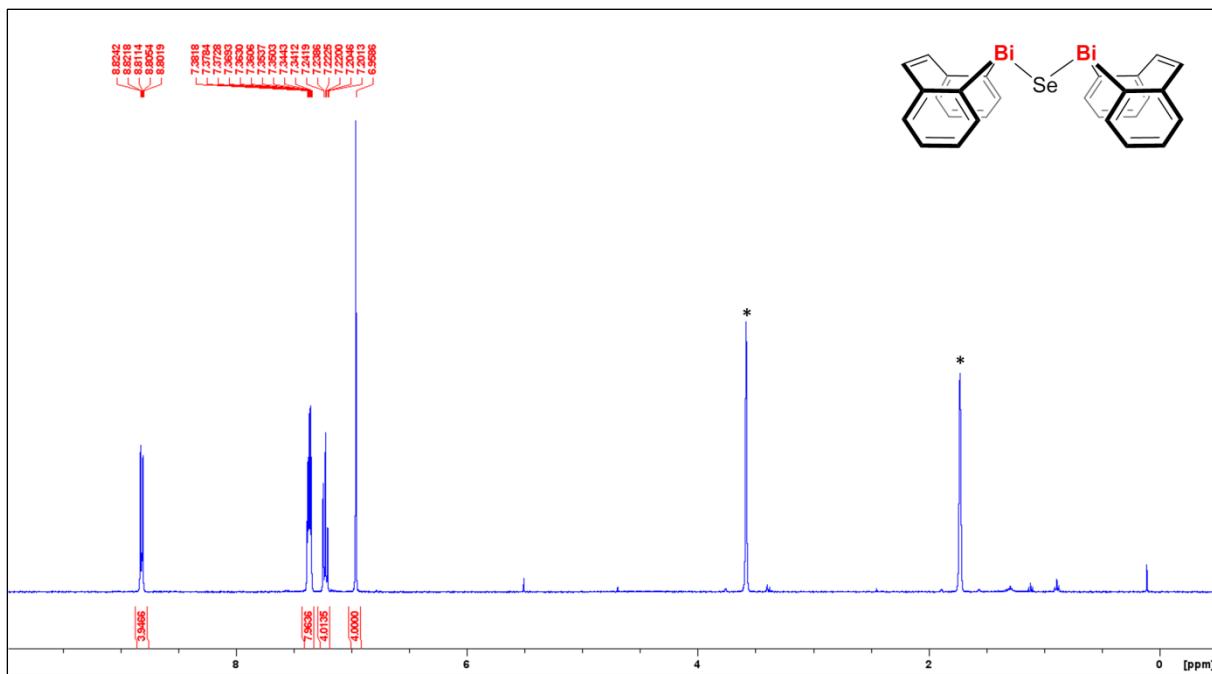
**Figure S30.**  $^{13}\text{C}$  NMR spectrum of **5-O** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



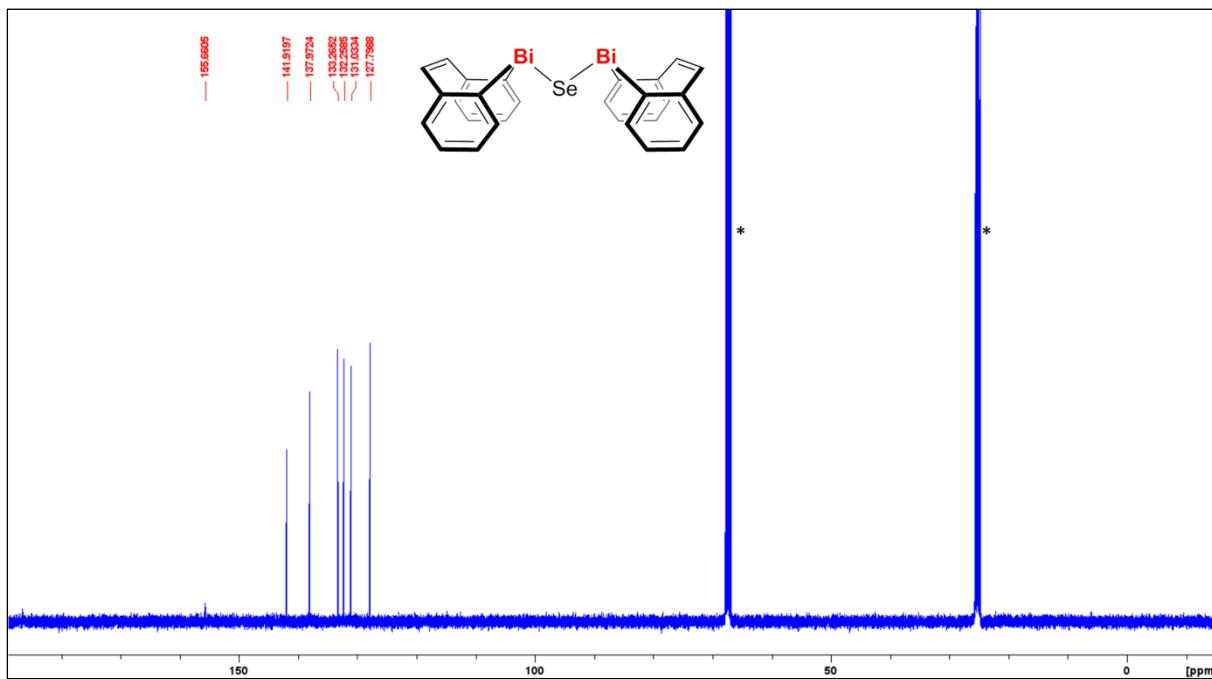
**Figure S31.**  $^1\text{H}$  NMR spectrum of **5-S** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



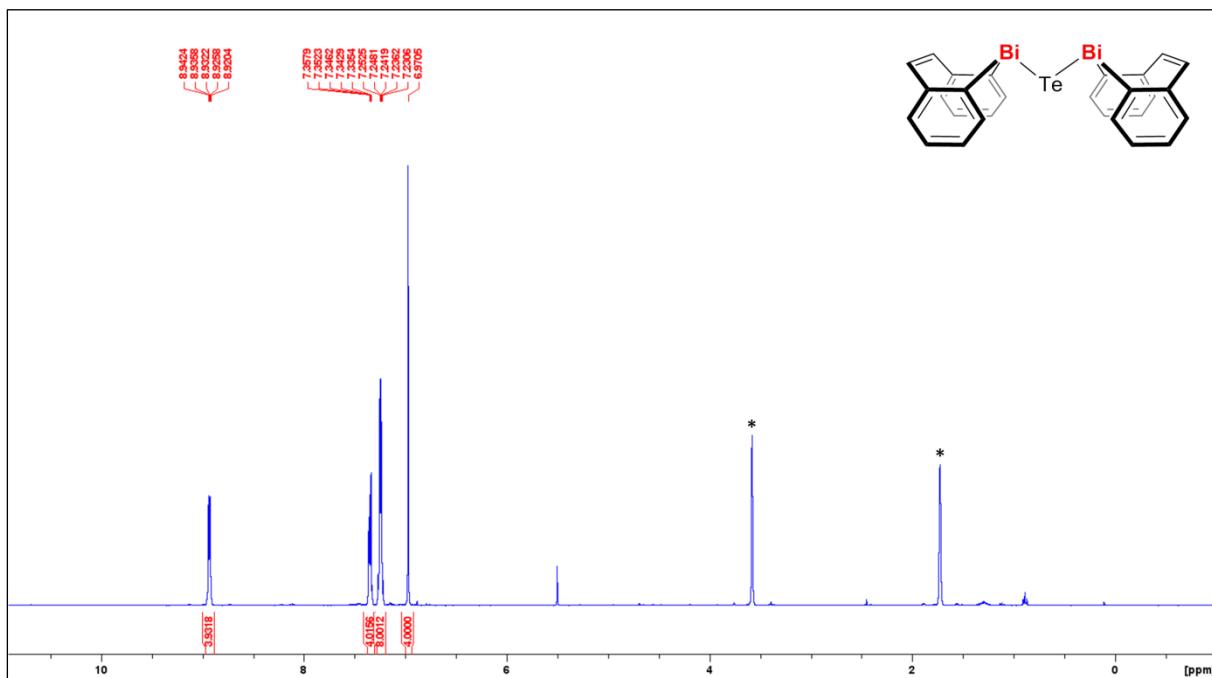
**Figure S32.**  $^{13}\text{C}$  NMR spectrum of **5-S** in  $\text{C}_6\text{D}_6$  (solvent signal: \*).



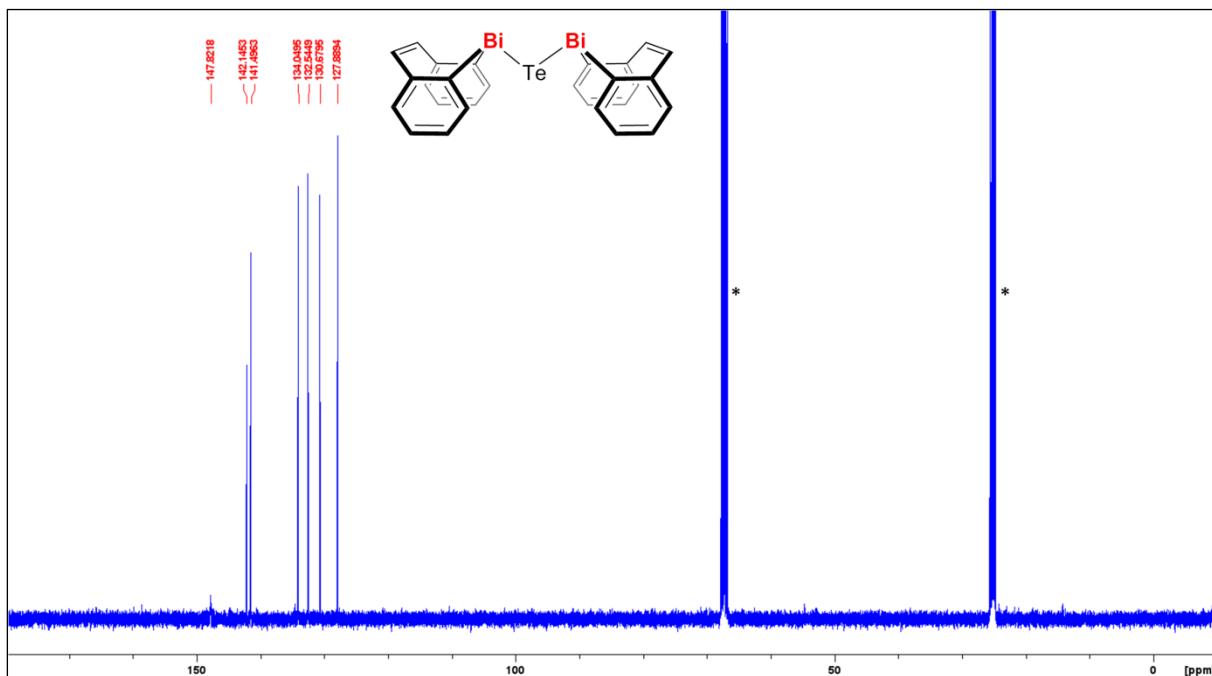
**Figure S33.**  $^1\text{H}$  NMR spectrum of **5-Se** in  $\text{THF}-d_8$  (solvent signals: \*).



**Figure S34.**  $^{13}\text{C}$  NMR spectrum of **5-Se** in  $\text{THF}-d_8$  (solvent signals: \*).



**Figure S35.**  $^1\text{H}$  NMR spectrum of **5-Te** in  $\text{THF}-d_8$  (solvent signals: \*). Traces of dichloromethane were detected.

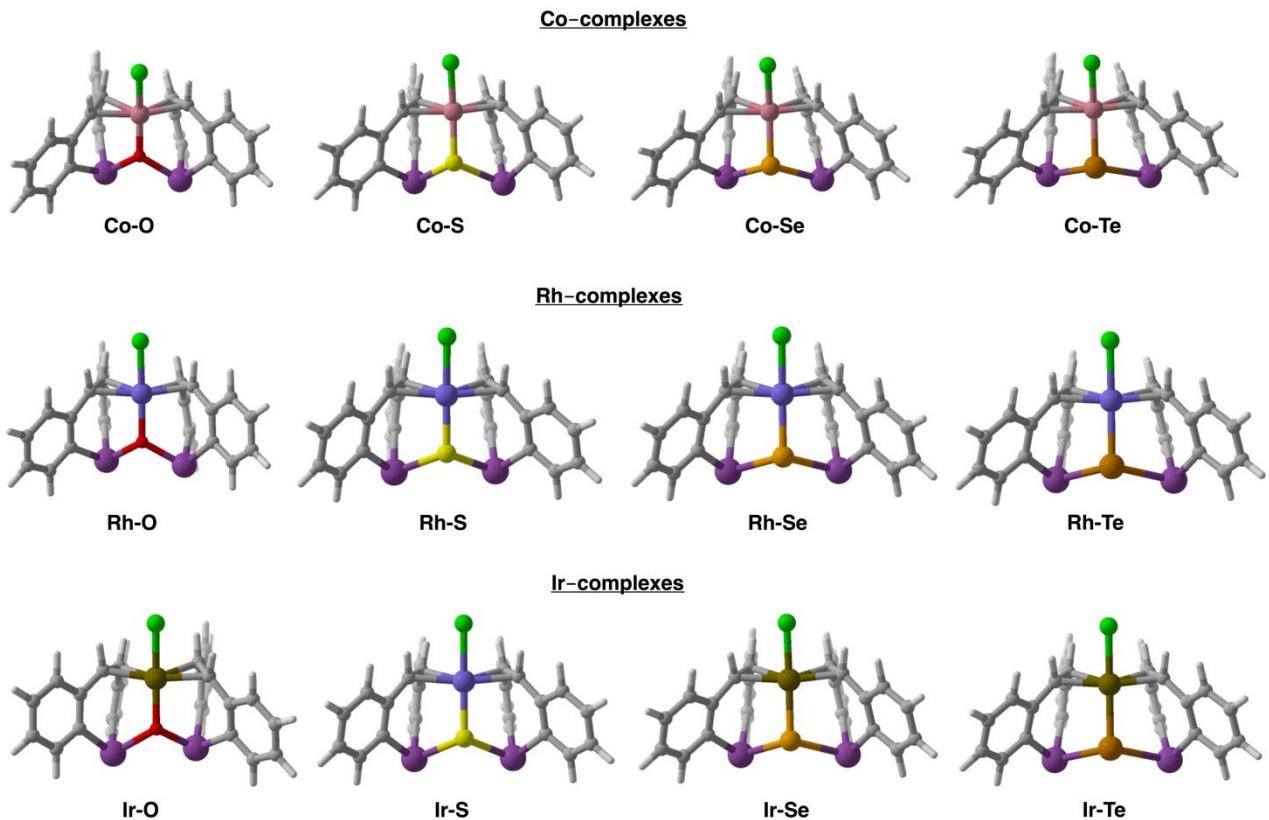


**Figure S36.**  $^{13}\text{C}$  NMR spectrum of **5-Te** in  $\text{THF}-d_8$  (solvent signals: \*).

## Density Functional Theory Studies

### Formation of complexes with Co, Rh and Ir.

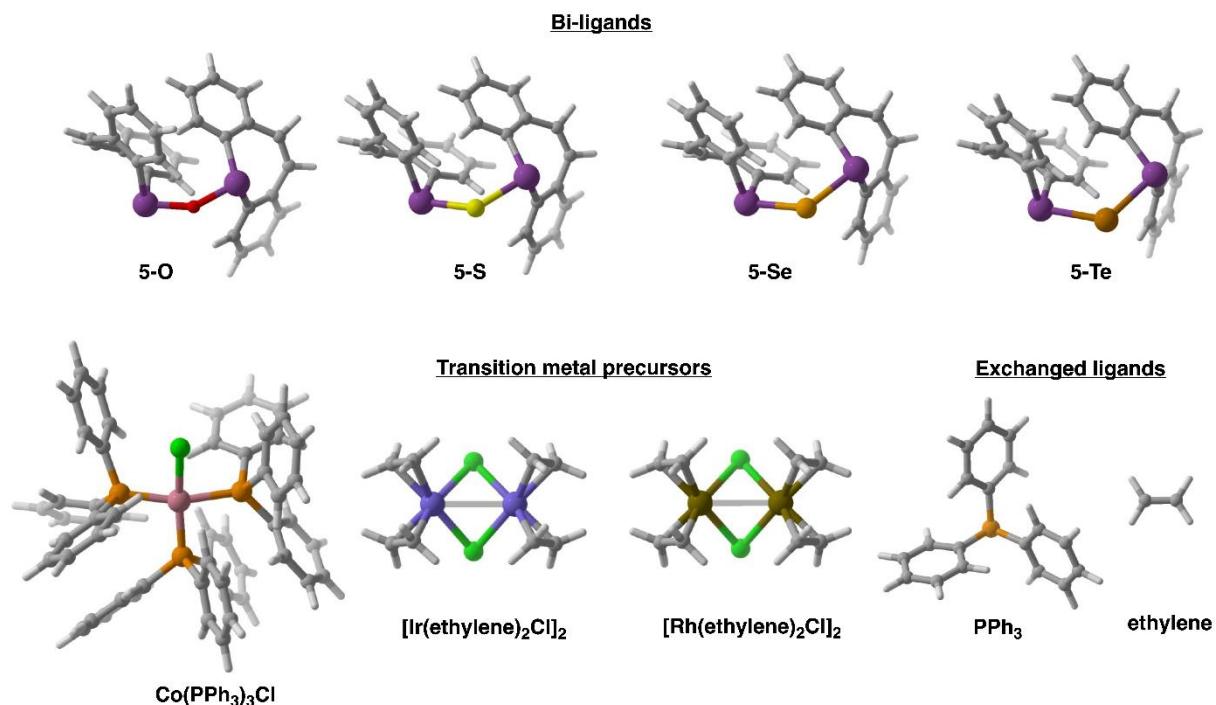
All hypothetical compounds evaluated are shown in Chart S1. Calculated Gibbs energies,  $\Delta G$ , for the reactions shown in Figure 5a (main part) are listed in Table S1.



**Chart S1.** Optimized geometries for the complexes of **5-E** with Co, Rh and Ir.

E	Co	Rh	Ir
O	-0.5	+2.4	+6.5
S	-3.0	-3.2	-2.4
Se	+4.1	+0.9	+4.9
Te	+7.7	+3.6	+6.7

**Table S1.** Gibbs energies,  $\Delta G$ , for the reactions shown in Figure 5a (main part); values are given in  $\text{kcal}\cdot\text{mol}^{-1}$ .

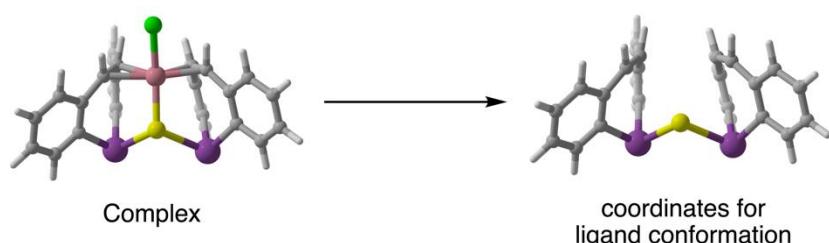


**Chart S2.** Optimized geometries of the ligands **5-E**, transition metal precursors, and exchanged ligands.

### Ligand preparation energy

We estimated the free energy penalty involved in the ligand's preparation energy to form the complexes as follows:  $\Delta G_{\text{preparation}} = G_{\text{ligand conf}} - G_{\text{ligand free}}$ .

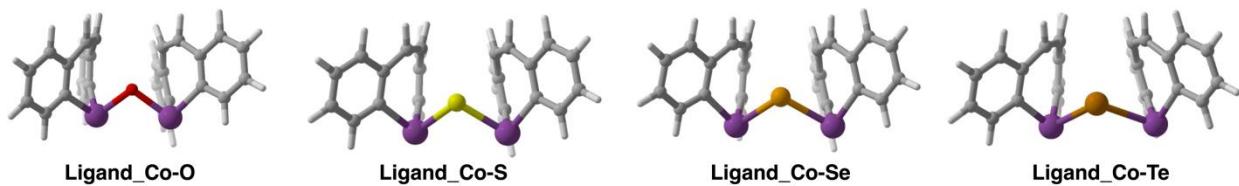
" $G_{\text{ligand conf.}}$ " corresponds to the Gibbs free energy of the ligand in the complex, which was obtained by performing a vibrational analysis on the ligand geometries taken from the complexes coordinates, without further optimization (Scheme S2). The term " $G_{\text{ligand free}}$ " corresponds to the Gibbs free energy of the free ligand after geometry optimization.



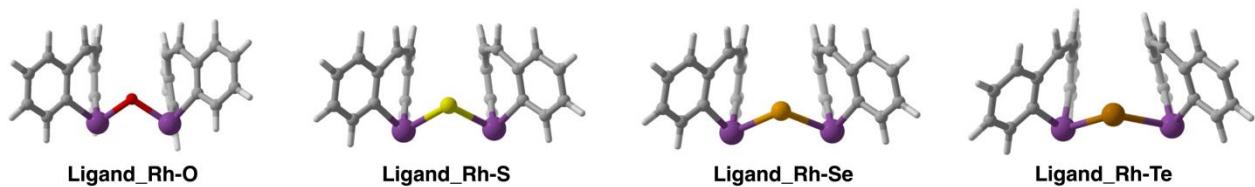
**Scheme S2.** Ligand conformation coordinates imported from coordinates of the complex.

The ligand geometries used for the calculations of " $G_{\text{ligand conf.}}$ " are presented in Chart S3.

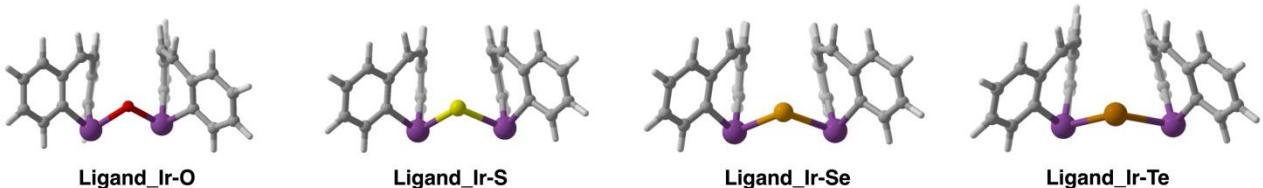
Ligand conformation in Co-complexes



Ligand conformation in Rh-complexes



Ligand conformation in Ir-complexes

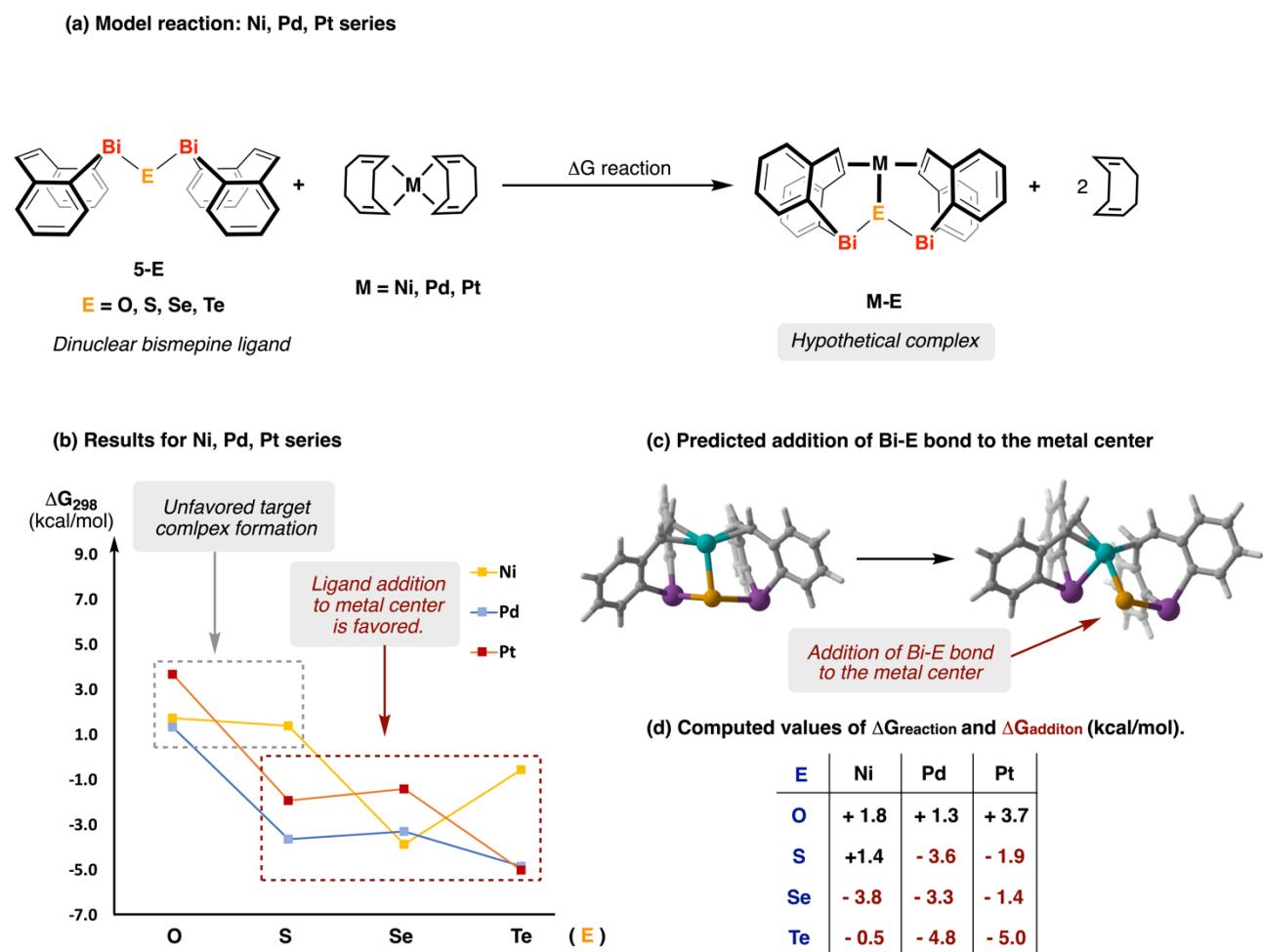


**Chart S3.** Geometries adopted by bismuth-containing ligands in the transition metal complexes.

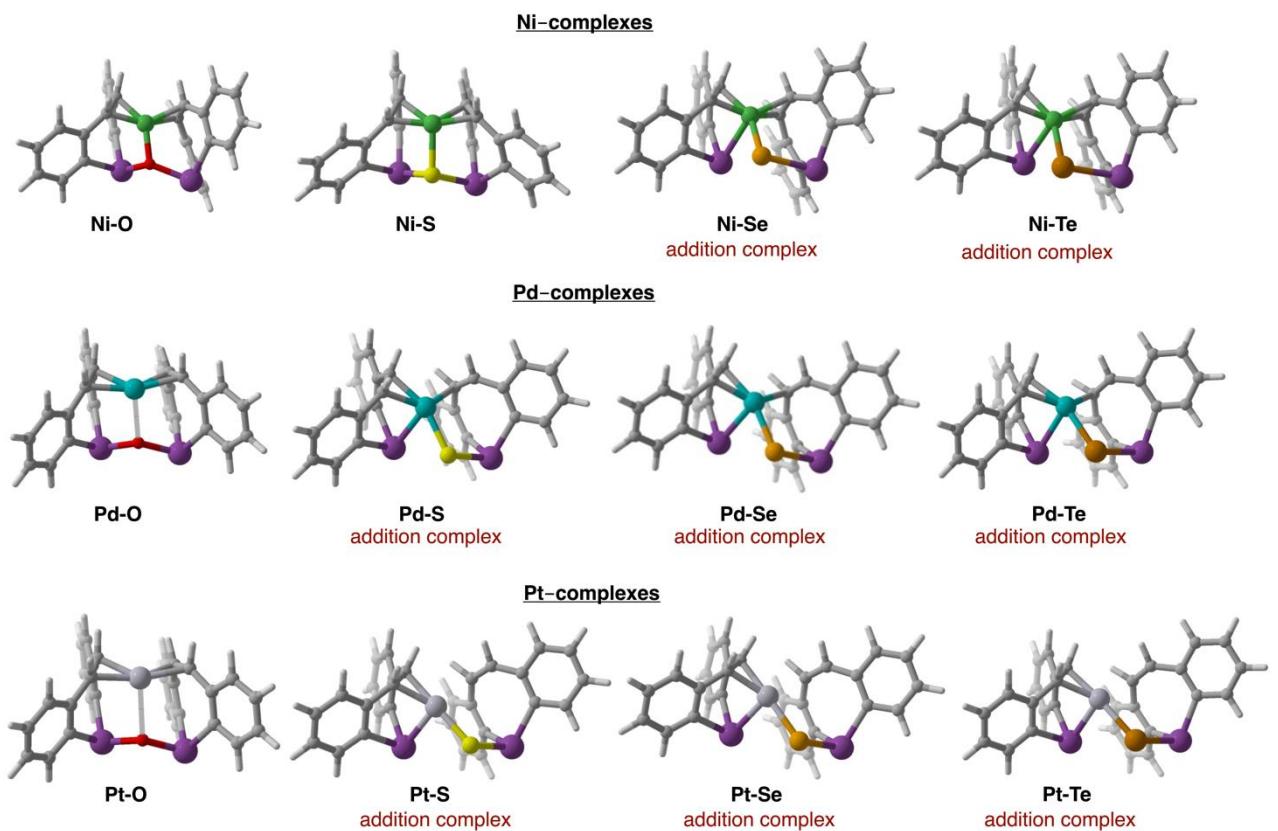
## Formation of complexes with Ni, Pd and Pt series.

We further evaluated the formation of complexes formed by coordination of ligands **5-E** to transition metals of the series Ni<sup>0</sup>, Pd<sup>0</sup>, and Pt<sup>0</sup> (Figure S36a). Our calculations predict that the formation of the targeted complexes is not favored for Ni, Pd or Pt and any given E atom (O, S, Se or Te) (Figure S36b). The complex formation was predicted to be slightly endergonic for reactions between **5-O** and all three transition metal precursors and for the reaction of **5-S** with Ni(cod)<sub>2</sub> (cod = 1,5-cyclo-octadiene). For all other combinations (i.e. reaction of **5-S** with the Pd and Pt precursor and reactions of **5-Se** and **5-Te** with all metal precursors), we found that an addition reaction of the ligand to the metal center is thermodynamically favored (see Figure S36c). Therefore, none of the evaluated combinations could be considered as promising candidates, when targeting the mere coordination of **5-E** to a group 10 central atom in the oxidation state of zero. However, these results suggest that incorporating these oxidative additions into the synthetic strategy might be a valuable approach for the synthesis of complexes of group 10 metals in the oxidation state of two and bismuth-based ligand systems. All computed structures of the complexes are presented in Chart S4. Additional computed structures of the metal precursors and exchanged ligand are presented in Chart S5.

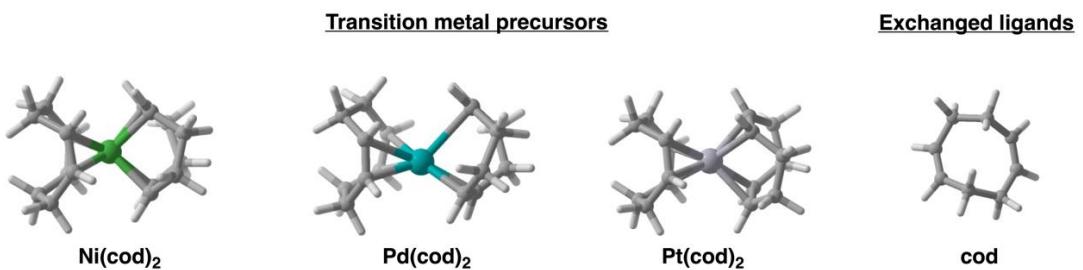
### Evaluation of dinuclear bismepine compounds as ligands for Ni, Pd and Pt complexes.



**Figure S37.** Evaluation of dinuclear bismepine compounds as ligands in transition metal complexes of Ni, Pd and Pt.



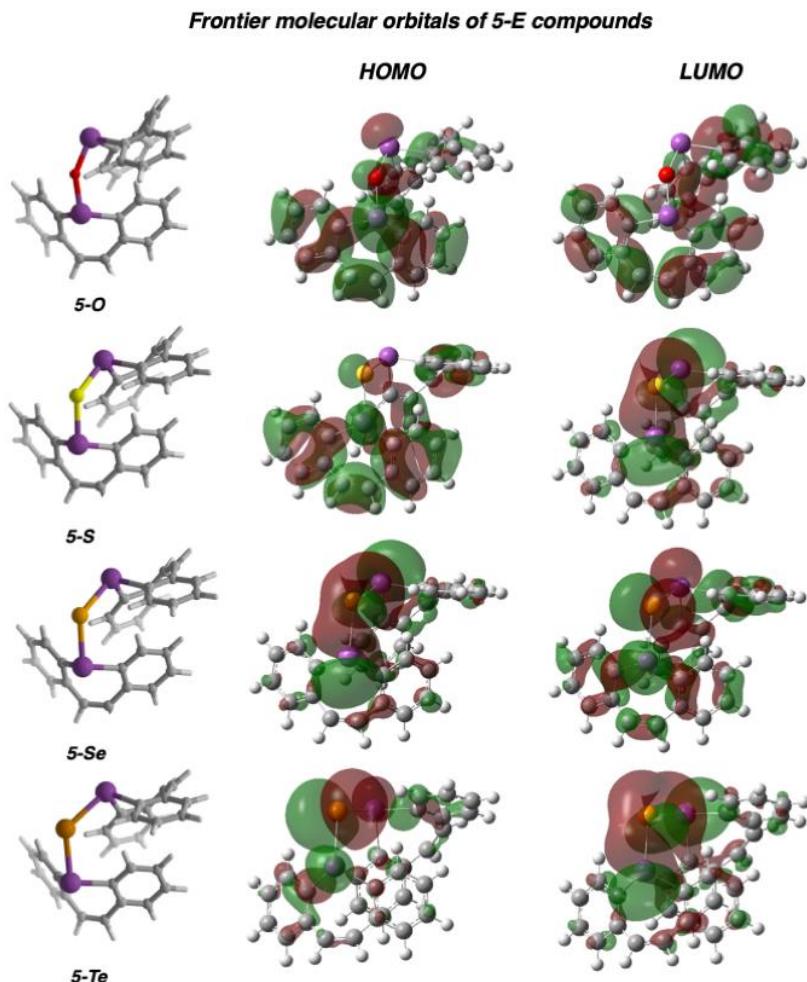
**Chart S4.** Optimized geometries for the complexes of with Ni, Pd and Pt.



**Chart S5.** Optimized geometries of the transition metal precursors and exchanged ligand.

## Insights into the electronic structure of the ligands.

We performed a frontier orbital analysis to gain further insights into the electronic structure of the ligands **5-E**. For the ligands containing E = O, S atoms, we found that the HOMO is highly delocalized, with contributions by the carbon atoms that are part of the aromatic and olefinic functional groups, by the bismuth atom, and by the E atom. In contrast, for ligands containing E = Se, Te atoms, the HOMO is localized at the bismuth and E atoms, with almost no contributions by the hydrocarbon backbone. The LUMO was found to be mainly localized at the bismuth and the E atoms in all cases, with the exception of E = O, which presents a high degree of delocalization.



**Chart S6.** Frontier molecular orbitals of compounds **5-E** (isovalue 0.02).

## NBO calculations.

We performed NBO calculations to investigate a possible correlation of the M–E interaction energies with the predicted stability trend of the complexes **M-E**. All potential E→M interactions of significant strength ( $> 4 \text{ kcal}\cdot\text{mol}^{-1}$ ) were considered. Due to the presence of one chloride ligand and a d<sup>8</sup> electron configuration of the central atom, the most prominent interactions were LP(E)→LP\*(M) interactions. The results show that the M–S interaction energies are not more favorable than the other M–E interaction energies (E = O, Se, Te), making electronic factors unlikely to be the key contributors for the thermodynamically favorable formation of compounds **M-S** (as compared to **M-O**, **M-Se**, and **M-Te**).

## Table of computed values

**Table S2.**  $G_{corr}$  is the thermal correction to the Gibbs free energy and  $G_{298\text{ gas phase}}$  is the sum of electronic and thermal free energies at the M06-L+GD3/def2svp/LANL2DZ level of theory in gas phase (values in hartree);  $E_{0\text{ dcm}}$  is the electronic energy obtained at M06-L+GD3/def2tzvp/LANL2DZ (SMD)//M06-L+GD3/def2svp/LANL2DZ level of theory in dichloromethane as solvent; SMD, solvation model based on density (values in hartree);  $G_{298\text{ dcm}}$  is the sum of  $E_{0\text{ dcm}}$  and  $G_{corr}$  (values in hartree). No imaginary frequencies were found in the optimized structures.

Structure	$G_{corr}$	$G_{298\text{ gas phase}}$	$E_{0\text{ dcm}}$	$G_{298\text{ dcm}}$
<b>5-E compounds</b>				
Bi <sub>2</sub> O	0.326673	-1163.80143	-1165.378166	-1165.051493
Bi <sub>2</sub> S	0.325798	-1486.750116	-1488.362956	-1488.037158
Bi <sub>2</sub> Se	0.324352	-1097.908813	-1099.39387	-1099.069518
Bi <sub>2</sub> Te	0.323263	-1096.729429	-1098.211466	-1097.888203
<b>Transition metal precursors</b>				
Co(PPh <sub>3</sub> )Cl	0.735778	-3711.409296	-3714.870706	-3714.134928
Ir(ethylene) <sub>4</sub> Cl <sub>2</sub>	0.174336	-1443.687438	-1444.538769	-1444.364433
Rh(ethylene) <sub>4</sub> Cl <sub>2</sub>	0.173545	-1453.355097	-1454.193694	-1454.020149
Ni(cod) <sub>2</sub>	0.320695	-792.632982	-793.6241675	-793.3034725
Pd(cod) <sub>2</sub>	0.314698	-750.069996	-751.056579	-750.741881
Pt(cod) <sub>2</sub>	0.320479	-742.451245	-743.4442948	-743.1238158
Ethylene	0.029716	-78.483188	-78.6037015	-78.5739855
PPh <sub>3</sub>	0.227306	-1035.382424	-1036.469305	-1036.241999
cod	0.148655	-311.61514	-312.1029041	-311.9542491
<b>Complexes with Co, Rh, Ir</b>				
Co-O	0.331445	-1769.056656	-1770.792622	-1770.461177
Rh-O	0.330258	-1733.503162	-1735.240002	-1734.909744
Ir-O	0.330973	-1728.660723	-1730.406282	-1730.075309
Co-S	0.328901	-2092.00469	-2093.779845	-2093.450944
Rh-S	0.330766	-2056.455919	-2058.235109	-2057.904343
Ir-S	0.32807	-2051.619412	-2053.403238	-2053.075168
Co-Se	0.326849	-1703.151477	-1704.798763	-1704.471914
Rh-Se	0.324346	-1667.60808	-1669.254582	-1668.930236
Ir-Se	0.326154	-1662.765131	-1664.422121	-1664.095967
Co-Te	0.325593	-1701.966231	-1703.610383	-1703.28479
Rh-Te	0.324523	-1666.424683	-1668.069045	-1667.744522
Ir-Te	0.324842	-1661.58386	-1663.236676	-1662.911834

<b>Ligand preparation energies</b>				
Ligand_Co-O	0.328121	-1163.753344	-1165.339099	-1165.010978
Ligand_Rh-O	0.326454	-1163.757048	-1165.343086	-1165.016632
Ligand_Ir-O	0.326652	-1163.74142	-1165.326783	-1165.000131
Ligand_Co-S	0.325785	-1486.713944	-1488.333644	-1488.007859
Ligand_Rh-S	0.326871	-1486.713211	-1488.335499	-1488.008628
Ligand_Ir-S	0.323886	-1486.701099	-1488.319886	-1487.996
Ligand_Co-Se	0.3226	-1097.869526	-1099.358566	-1099.035966
Ligand_Rh-Se	0.324742	-1097.867265	-1099.359856	-1099.035114
Ligand_Ir-Se	0.321605	-1097.854949	-1099.34382	-1099.022215
Ligand_Co-Te	0.325523	-1096.68469	-1098.173491	-1097.847968
Ligand_Rh-Te	0.32023	-1096.690205	-1098.175136	-1097.854906
Ligand_Ir-Te	0.320816	-1096.673661	-1098.158669	-1097.837853
<b>Complexes with Ni, Pd, Pt</b>				
Ni-O	0.328715	-1333.193242	-1334.772389	-1334.443674
Pd-O	0.328077	-1290.631215	-1292.210812	-1291.882735
Pt-O	0.328013	-1283.005487	-1284.588906	-1284.260893
Ni-S	0.327322	-1656.154967	-1657.77437	-1657.447048
Pd-S	0.327125	-1613.584612	-1615.203375	-1614.87625
Pt-S	0.327665	-1605.961154	-1607.583192	-1607.255527
Ni-Se	0.325399	-1267.309046	-1268.800129	-1268.47473
Pd-Se	0.323589	-1224.745388	-1226.231712	-1225.908123
Pt-Se	0.324454	-1217.12244	-1218.611503	-1218.287049
Ni-Te	0.324065	-1266.130467	-1267.617972	-1267.293907
Pd-Te	0.32278	-1223.56848	-1225.052033	-1224.729253
Pt-Te	0.323981	-1215.948961	-1217.435457	-1217.111476

## **Cartesian coordinates after optimization with M06-L+GD3/def2SVP/LANL2DZ**

The coordinates of the optimized structures are listed below. Additionally, we provide them as a coordinates file ‘coordinates.xyz’ for convenient visualization.

### **Complexes with M = Co, Rh, Ir**

Co-O

O	0.1291290	-0.6124660	-0.3538240
C	-2.7091320	-1.6497480	-0.8110370
C	1.1918850	3.2873830	-0.8016800
H	1.3951860	3.3914800	-1.8741750
C	-2.4759240	1.7555010	2.8359300
H	-2.3898030	1.3880440	3.8629700
C	5.4240080	-1.9261180	-0.4144700
H	6.2554710	-2.3356640	-0.9922610
C	-3.4497750	-2.2768800	-1.8185940
H	-3.5925210	-1.7806960	-2.7854900
C	0.4373160	4.2628000	1.2585770
H	0.0559150	5.1135090	1.8286320
C	-1.6590840	-0.4473920	2.1604320
H	-1.4854700	-0.5112550	3.2406270
C	1.1077340	1.9051530	1.2078550
C	-2.1340950	0.8838910	1.7803560
C	0.6246130	3.0410100	1.8922880
H	0.4004860	2.9489370	2.9589700
C	0.7256820	4.3974720	-0.0985810
H	0.5751140	5.3518020	-0.6087090
C	1.2863450	0.6949590	2.0188060
H	0.9224340	0.8522320	3.0422800
C	1.3872730	2.0527920	-0.1716920
C	-1.7837440	-1.7425440	1.5881370
H	-1.6534100	-2.5124360	2.3540410
C	-3.7832660	-4.1925850	-0.4096120
H	-4.1934770	-5.1911220	-0.2409090
C	-2.4984120	-2.2823340	0.4322210
C	-4.0043420	-3.5398740	-1.6231100
H	-4.5847930	-4.0178570	-2.4154410
C	5.3492440	-2.1242580	0.9655340
H	6.1279810	-2.6914670	1.4807890
C	4.2824540	-1.6114700	1.6898690
H	4.2267400	-1.7827830	2.7682230
C	-3.0363740	3.5262780	1.2972980
H	-3.3741590	4.5471820	1.1037230
C	-3.0389890	-3.5791790	0.5892100
H	-2.8748840	-4.0980840	1.5376140
C	4.4049850	-1.2192270	-1.0482290
H	4.4473200	-1.0923700	-2.1364370
C	-2.2416630	1.3829800	0.4657070
C	3.2537970	-0.8582630	1.0761880
C	2.1938640	-0.3903320	1.9611160

H	2.3254990	-0.8254790	2.9525030
C	-2.6813190	2.6898620	0.2385630
H	-2.7368080	3.0816420	-0.7840870
C	3.3334420	-0.6881270	-0.3208030
C	-2.9299020	3.0487100	2.6023480
H	-3.1958430	3.6901790	3.4461310
Cl	0.4665990	-2.1966620	3.5068660
Bi	-1.6378420	0.1976280	-1.2941020
Bi	1.7473620	0.2905740	-1.4591050
Co	0.2160720	-1.0446780	1.5457530

#### Rh-O

O	0.0933390	-0.5218140	-0.5815940
C	-2.8193540	-1.4962150	-0.9220820
C	1.4395410	3.3314740	-0.5375340
H	1.6029690	3.5149420	-1.6064350
C	-2.4390290	1.8944370	2.7505480
H	-2.4159400	1.5133380	3.7757440
C	5.2574290	-2.2164160	-0.8071370
H	6.0240850	-2.6353230	-1.4626010
C	-3.5534170	-2.0803010	-1.9613150
H	-3.6272860	-1.5744740	-2.9312110
C	0.8285060	4.1715270	1.6267530
H	0.5197670	4.9910120	2.2803340
C	-1.8100200	-0.3685070	2.0949730
H	-1.7067990	-0.4404250	3.1834810
C	1.3599820	1.7932790	1.3526690
C	-2.1533520	1.0005370	1.6967280
C	0.9688630	2.8919490	2.1482430
H	0.7781860	2.7204770	3.2117440
C	1.0731000	4.4036680	0.2743890
H	0.9608500	5.4047400	-0.1486730
C	1.4872780	0.5123590	2.0602590
H	1.2089480	0.6250330	3.1154120
C	1.5842700	2.0373750	-0.0229400
C	-2.0003710	-1.6578830	1.5154060
H	-1.9718430	-2.4291310	2.2943110
C	-4.0605770	-3.9758490	-0.5794590
H	-4.5355250	-4.9487840	-0.4323900
C	-2.7037960	-2.1450450	0.3267600
C	-4.1875310	-3.3100050	-1.7985570
H	-4.7574180	-3.7515360	-2.6191300
C	5.2310290	-2.5310690	0.5517730
H	5.9842240	-3.1995330	0.9755190
C	4.2439070	-2.0025800	1.3724580
H	4.2289120	-2.2609620	2.4347120
C	-2.7716200	3.7235870	1.2172440
H	-2.9959290	4.7753650	1.0241230
C	-3.3284280	-3.4064250	0.4538270
H	-3.2390140	-3.9349680	1.4069400

C	4.2733420	-1.3744390	-1.3199030
H	4.2803150	-1.1491770	-2.3930780
C	-2.1776670	1.5131720	0.3817180
C	3.2503550	-1.1236150	0.8828850
C	2.2718940	-0.6596360	1.8659480
H	2.4149150	-1.1824160	2.8165550
C	-2.4775230	2.8614610	0.1610110
H	-2.4718700	3.2641200	-0.8591620
C	3.2796930	-0.8299580	-0.4969570
C	-2.7535720	3.2282890	2.5196060
H	-2.9765350	3.8867950	3.3626500
Cl	0.2289070	-2.0628060	3.6690870
Bi	-1.6874880	0.3198080	-1.4155520
Bi	1.7829950	0.4112980	-1.5080990
Rh	0.1389380	-1.1053270	1.4815240

#### Ir-O

O	-0.0908770	-0.3022790	-0.7846990
C	-3.2974970	-0.5396500	-0.7499970
C	2.4963760	2.7969970	0.8351070
H	2.4854590	3.4545820	-0.0426530
C	-0.9094960	2.3941090	2.6720490
H	-0.7195620	1.9746900	3.6645070
C	4.2988790	-2.5775250	-2.6102020
H	4.9043590	-2.7720390	-3.4982200
C	-4.3305430	-0.8217770	-1.6532620
H	-4.3373630	-0.3502050	-2.6433230
C	2.8197440	2.5218470	3.2000830
H	3.0727920	2.9293180	4.1818960
C	-1.4025330	0.0933210	2.0147670
H	-1.1670910	-0.0264610	3.0808500
C	2.1499320	0.6041470	1.8331700
C	-1.2956310	1.5166130	1.6378140
C	2.4773680	1.1793700	3.0769120
H	2.4599430	0.5414360	3.9655840
C	2.8261890	3.3437610	2.0756320
H	3.0715520	4.4049690	2.1622410
C	1.7534440	-0.8145110	1.8588470
H	1.7065360	-1.1728760	2.8950900
C	2.1684610	1.4441780	0.7002420
C	-2.2320420	-0.9951500	1.5516950
H	-2.4270920	-1.6919420	2.3738790
C	-5.3319180	-2.3268110	-0.0770310
H	-6.1192210	-3.0318530	0.2003550
C	-3.2661080	-1.1488870	0.5215640
C	-5.3556210	-1.7056560	-1.3260310
H	-6.1533410	-1.9181670	-2.0410590
C	4.1704690	-3.5401790	-1.6090280
H	4.6806800	-4.5018820	-1.7028850
C	3.3929910	-3.2829350	-0.4872090

H	3.3025840	-4.0447450	0.2921990
C	-1.0049890	4.3086720	1.2110730
H	-0.8902790	5.3813270	1.0380020
C	-4.3054180	-2.0589410	0.8189170
H	-4.2935520	-2.5585100	1.7914330
C	3.6230200	-1.3682950	-2.4673900
H	3.7016090	-0.6230110	-3.2676790
C	-1.5216710	2.0816410	0.3613830
C	2.7201160	-2.0549510	-0.3030030
C	1.9494570	-1.9195510	0.9415720
H	1.9767170	-2.8611230	1.5049510
C	-1.3730860	3.4609680	0.1678600
H	-1.5375080	3.8933450	-0.8266300
C	2.8438250	-1.1000320	-1.3349180
C	-0.7663450	3.7614120	2.4701790
H	-0.4598010	4.4013960	3.3011610
Cl	-0.2512850	-2.8629140	2.9190560
Bi	-1.7722930	0.8590760	-1.4629860
Bi	1.6894340	0.7647940	-1.3502750
Ir	-0.1450070	-1.3588940	1.0615560

#### Co-S

S	0.1372840	-1.0135320	-0.7150370
C	-3.1051440	-1.3007880	-0.8768010
C	1.5298870	3.2630610	-0.0652810
H	1.7492850	3.5869720	-1.0899420
C	-2.2759460	1.7023720	2.9397290
H	-2.2251250	1.2358900	3.9282110
C	5.4487550	-2.2047280	-0.7117620
H	6.2991700	-2.5185400	-1.3212070
C	-4.0114130	-1.7461570	-1.8456430
H	-4.1846030	-1.1496120	-2.7483070
C	0.8562470	3.8193270	2.1688960
H	0.5467550	4.5502280	2.9199120
C	-1.7230480	-0.5076300	2.0878430
H	-1.5347530	-0.6622390	3.1555540
C	1.3300030	1.4812510	1.5884360
C	-2.0340810	0.8956780	1.8067890
C	0.9434650	2.4762480	2.5124750
H	0.7123740	2.1690950	3.5367130
C	1.1544790	4.2259340	0.8707560
H	1.0834870	5.2777900	0.5840800
C	1.4013040	0.1169080	2.1269680
H	1.0764940	0.0970430	3.1750810
C	1.6184670	1.9071760	0.2715370
C	-2.0297200	-1.7274100	1.4426450
H	-1.9722050	-2.5658700	2.1445900
C	-4.4440790	-3.7382760	-0.5777120
H	-4.9526280	-4.6967730	-0.4508250
C	-2.8664810	-2.0686100	0.2868660

C	-4.6937100	-2.9526690	-1.7018180
H	-5.3967480	-3.2836050	-2.4695320
C	5.2123910	-2.7822740	0.5353870
H	5.8800080	-3.5570230	0.9194710
C	4.1252380	-2.3747960	1.2953740
H	3.9521350	-2.8296730	2.2745610
C	-2.6337360	3.6560850	1.5790650
H	-2.8506550	4.7224130	1.4805270
C	-3.5462340	-3.3037750	0.3880670
H	-3.3664670	-3.9209350	1.2726030
C	4.5673200	-1.2330530	-1.1795070
H	4.7400670	-0.8017990	-2.1723160
C	-2.0989540	1.5160540	0.5408670
C	3.2290000	-1.3697290	0.8595810
C	2.1747160	-1.0327300	1.8188030
H	2.2587740	-1.6775800	2.6967460
C	-2.3850850	2.8820270	0.4451890
H	-2.4120840	3.3692090	-0.5370660
C	3.4687450	-0.8154270	-0.4180780
C	-2.5861140	3.0524790	2.8334110
H	-2.7784210	3.6382100	3.7356220
Cl	0.1421280	-2.5407380	3.4490900
Bi	-1.8781730	0.4619650	-1.4008180
Bi	2.0738430	0.5568010	-1.4255600
Co	0.1023760	-1.3759640	1.4899420

#### Rh-S

C	-3.3107000	-1.0486300	-0.7761750
C	2.0475790	3.1605690	0.2640200
H	2.1512530	3.5890610	-0.7402200
C	-1.7464530	2.1241180	2.8007140
H	-1.6240700	1.7137800	3.8075590
C	5.0389140	-2.6239760	-1.4724090
H	5.7706620	-2.9533170	-2.2134470
C	-4.2608870	-1.4923580	-1.7048740
H	-4.3931040	-0.9535940	-2.6502320
C	1.8448730	3.4968620	2.6322720
H	1.7923580	4.1556340	3.5023910
C	-1.7124090	-0.1958310	2.0829330
H	-1.5021310	-0.2996370	3.1535780
C	1.8143450	1.2207190	1.7167940
C	-1.8118270	1.2228940	1.7161610
C	1.7513040	2.1212470	2.8020640
H	1.6297220	1.7103360	3.8087720
C	1.9929660	4.0288530	1.3540350
H	2.0522350	5.1091130	1.2021020
C	1.7136270	-0.1981360	2.0826630
H	1.5038760	-0.3024550	3.1533550
C	1.9604560	1.7729690	0.4249990
C	-2.2331620	-1.4087710	1.5562860

H	-2.2933000	-2.1707690	2.3417180
C	-4.8558360	-3.3313520	-0.2836540
H	-5.4455080	-4.2278980	-0.0788070
C	-3.1295040	-1.7425520	0.4432950
C	-5.0417210	-2.6215820	-1.4687250
H	-5.7740490	-2.9509360	-2.2091840
C	4.8530030	-3.3345310	-0.2878140
H	5.4420710	-4.2316960	-0.0839310
C	3.9158070	-2.9023060	0.6403460
H	3.7837630	-3.4612130	1.5708240
C	-1.9878960	4.0309910	1.3516780
H	-2.0462420	5.1112080	1.1990830
C	-3.9178910	-2.8991330	0.6437510
H	-3.7858550	-3.4574280	1.5745970
C	4.2588400	-1.4939700	-1.7073410
H	4.3910420	-0.9545900	-2.6523480
C	-1.9588670	1.7744350	0.4241600
C	3.1282370	-1.7449550	0.4411440
C	2.2327390	-1.4112440	1.5548400
H	2.2924780	-2.1739180	2.3396550
C	-2.0447670	3.1620150	0.2623340
H	-2.1492310	3.5899190	-0.7420750
C	3.3094080	-1.0502290	-0.7778800
C	-1.8387110	3.4997170	2.6300850
H	-1.7843330	4.1590290	3.4996800
Cl	-0.0003320	-2.4157290	3.5563040
Bi	-2.0414310	0.6234740	-1.4706420
Bi	2.0407810	0.6231220	-1.4706090
Rh	-0.0003040	-1.3821550	1.3786920
S	-0.0004460	-0.8686730	-0.8894840

#### Ir-S

C	-3.24056900	-0.78711000	-1.15405500
C	1.87583000	3.22160400	0.82464700
H	2.02430000	3.83818300	-0.07021800
C	-1.99805400	1.35793500	3.16594300
H	-1.91608800	0.69832200	4.03512500
C	5.22557300	-1.97807600	-1.82678300
H	6.00523800	-2.12436100	-2.57759600
C	-4.17656900	-0.98125900	-2.17889100
H	-4.31429400	-0.20957400	-2.94509600
C	1.50987200	3.08864500	3.19213300
H	1.37081500	3.56437100	4.16587900
C	-1.70782100	-0.67752500	1.86467500
H	-1.58465400	-1.04241500	2.89183100
C	1.64253700	1.03095400	1.86196200
C	-1.91528900	0.78234300	1.88137600
C	1.47343500	1.70304200	3.09004900
H	1.30861100	1.10282800	3.98998800
C	1.71334700	3.86184800	2.05269100

H	1.73381800	4.95245300	2.11361400
C	1.58041200	-0.44148700	1.94328100
H	1.39757300	-0.74354000	2.98262900
C	1.84188900	1.82636100	0.71283400
C	-2.15773300	-1.74493600	1.00687800
H	-2.26484800	-2.66996900	1.58655300
C	-4.74618000	-3.14140000	-1.30826700
H	-5.32165100	-4.06889700	-1.35528900
C	-3.05172700	-1.77941500	-0.16400600
C	-4.93727300	-2.14463400	-2.26335200
H	-5.65925000	-2.27517700	-3.07251400
C	5.03959200	-2.90181700	-0.79973600
H	5.67738100	-3.78614800	-0.73042800
C	4.04084400	-2.70009300	0.14301000
H	3.90864100	-3.42786400	0.94837200
C	-2.26998100	3.56995200	2.25764300
H	-2.39338600	4.64730600	2.39062400
C	-3.82224500	-2.95742600	-0.28843300
H	-3.68772100	-3.74208100	0.46129100
C	4.38636900	-0.86870400	-1.88932200
H	4.52311500	-0.15472500	-2.70986300
C	-2.01763800	1.64972100	0.77342400
C	3.18637200	-1.57429600	0.11677600
C	2.20802700	-1.51783800	1.21656100
H	2.35063200	-2.37890800	1.87968600
C	-2.18820500	3.02416400	0.97662900
H	-2.25399800	3.70057700	0.11574400
C	3.37493300	-0.65706100	-0.94228400
C	-2.18036300	2.72237900	3.35821400
H	-2.24184800	3.12447100	4.37230200
Cl	0.03805400	-3.07589600	2.80810900
Bi	-2.00895700	1.03780200	-1.36015500
Bi	2.07322600	1.07664600	-1.36031300
Ir	0.03222600	-1.55059200	0.93697000
S	0.04616400	-0.54584400	-1.14374700

#### Co-Se

Se	0.1344360	-1.0454170	-0.8186000
C	-3.2052330	-1.2682570	-0.7844760
C	1.6375100	3.3031120	-0.0140690
H	1.8863460	3.6334570	-1.0298860
C	-2.2212870	1.8307300	2.9401900
H	-2.1394030	1.3832520	3.9353730
C	5.4252270	-2.3248340	-0.6363490
H	6.2711200	-2.6720760	-1.2337680
C	-4.1305330	-1.7486280	-1.7187500
H	-4.3421180	-1.1707400	-2.6253880
C	0.9196380	3.8511930	2.2078030
H	0.6025050	4.5797530	2.9578690
C	-1.7355400	-0.4045430	2.1241910

H	-1.5360750	-0.5345640	3.1931620
C	1.3820890	1.5112370	1.6205140
C	-2.0331110	0.9964220	1.8164510
C	0.9868010	2.5050420	2.5426120
H	0.7312250	2.1929140	3.5594540
C	1.2487120	4.2633100	0.9191370
H	1.1947520	5.3175550	0.6377740
C	1.4255860	0.1451510	2.1572510
H	1.0995800	0.1340120	3.2049950
C	1.7073560	1.9433350	0.3136390
C	-2.0614780	-1.6384360	1.5161860
H	-2.0018770	-2.4563300	2.2420480
C	-4.4893100	-3.7260260	-0.4065500
H	-4.9751040	-4.6916810	-0.2487840
C	-2.9202710	-2.0113970	0.3856540
C	-4.7844470	-2.9654880	-1.5366200
H	-5.5014810	-3.3225800	-2.2792190
C	5.1262230	-2.9162570	0.5904280
H	5.7387070	-3.7367590	0.9713350
C	4.0468160	-2.4625310	1.3348700
H	3.8254740	-2.9273770	2.2994990
C	-2.6005200	3.7626620	1.5561250
H	-2.8060130	4.8298150	1.4435710
C	-3.5750950	-3.2562670	0.5266510
H	-3.3606650	-3.8533490	1.4172120
C	4.6125230	-1.2930790	-1.0997680
H	4.8359990	-0.8484300	-2.0763490
C	-2.1419220	1.5918270	0.5404590
C	3.2176800	-1.3998860	0.9027570
C	2.1673040	-1.0258650	1.8537830
H	2.2285590	-1.6698140	2.7345690
C	-2.4101460	2.9613110	0.4303010
H	-2.4742940	3.4288090	-0.5597500
C	3.5192370	-0.8303400	-0.3561160
C	-2.5147250	3.1829410	2.8195580
H	-2.6638950	3.7885670	3.7168030
Cl	0.1012410	-2.4341030	3.5568860
Bi	-2.0561780	0.5205880	-1.4034290
Bi	2.2415150	0.6358880	-1.3956500
Co	0.0784170	-1.3306160	1.5612300

#### Rh-Se

C	-3.3562600	-1.0865970	-0.7200520
C	2.0441020	3.2358950	0.2216110
H	2.2035120	3.6396630	-0.7855590
C	-1.8123040	2.1509650	2.8223950
H	-1.6727280	1.7434430	3.8281480
C	5.1066270	-2.6647910	-1.2548220
H	5.8521910	-3.0316100	-1.9637280
C	-4.2945090	-1.5797440	-1.6365390

H	-4.4765850	-1.0412070	-2.5737060
C	1.6781440	3.6320630	2.5597520
H	1.5491670	4.3122530	3.4050990
C	-1.7486140	-0.1679830	2.1152470
H	-1.5453130	-0.2561880	3.1882680
C	1.7758570	1.3294330	1.7131930
C	-1.8765740	1.2461190	1.7402360
C	1.6179010	2.2595380	2.7637620
H	1.4451770	1.8735440	3.7728600
C	1.8914990	4.1328080	1.2783520
H	1.9288000	5.2095920	1.0976860
C	1.6982320	-0.0788470	2.1240370
H	1.4731840	-0.1465310	3.1945230
C	1.9899480	1.8503230	0.4169790
C	-2.2281790	-1.4012960	1.5988380
H	-2.2686210	-2.1546030	2.3943150
C	-4.7535840	-3.4634980	-0.2245310
H	-5.2842830	-4.3958480	-0.0183710
C	-3.1135710	-1.7790700	0.4904000
C	-5.0014560	-2.7563000	-1.3995720
H	-5.7249380	-3.1222500	-2.1314450
C	4.8590650	-3.3433520	-0.0628800
H	5.4122820	-4.2535350	0.1798980
C	3.9063990	-2.8612860	0.8238900
H	3.7270610	-3.3947370	1.7613730
C	-2.0915970	4.0525130	1.3746670
H	-2.1645700	5.1315960	1.2204580
C	-3.8294560	-2.9817120	0.6921590
H	-3.6504990	-3.5375510	1.6166320
C	4.3714520	-1.5161530	-1.5379370
H	4.5547910	-0.9998980	-2.4873560
C	-2.0519530	1.7933990	0.4493790
C	3.1599480	-1.6862500	0.5744570
C	2.2420190	-1.3053000	1.6548050
H	2.2974690	-2.0313440	2.4739650
C	-2.1534150	3.1806410	0.2880320
H	-2.2799360	3.6062490	-0.7148080
C	3.4044830	-1.0230310	-0.6517010
C	-1.9240830	3.5248800	2.6521280
H	-1.8701490	4.1855700	3.5207570
Cl	0.0099860	-2.2676330	3.6791990
Bi	-2.2122100	0.6622050	-1.4523460
Bi	2.2382970	0.6799340	-1.4500490
Rh	0.0102440	-1.3282770	1.4635870
Se	0.0187440	-0.8991820	-0.9907560

#### Ir-Se

C	-3.3094540	-0.8347930	-1.0643340
C	1.9256670	3.2730350	0.7881340
H	2.1163570	3.8671460	-0.1139030

C	-1.9693970	1.4774910	3.1663840
H	-1.8554300	0.8428850	4.0504730
C	5.2265000	-2.1338630	-1.6895910
H	6.0066560	-2.3321910	-2.4277850
C	-4.2457000	-1.0978010	-2.0742690
H	-4.4324350	-0.3489090	-2.8526630
C	1.4588550	3.2007210	3.1394360
H	1.2787950	3.7002450	4.0944040
C	-1.7185860	-0.5957130	1.9239300
H	-1.5971630	-0.9231350	2.9637640
C	1.6485700	1.1081670	1.8688750
C	-1.9282450	0.8639510	1.8969350
C	1.4293430	1.8132290	3.0707090
H	1.2279010	1.2360440	3.9782170
C	1.7082850	3.9450580	1.9901610
H	1.7257830	5.0368840	2.0232340
C	1.5837730	-0.3611650	1.9949550
H	1.3985110	-0.6243330	3.0443800
C	1.8996430	1.8745970	0.7097370
C	-2.1622570	-1.6980530	1.1082320
H	-2.2638890	-2.5980790	1.7275690
C	-4.6949710	-3.2659460	-1.1563410
H	-5.2222290	-4.2225470	-1.1786130
C	-3.0601370	-1.7963660	-0.0567160
C	-4.9461570	-2.2998950	-2.1288010
H	-5.6685230	-2.4825820	-2.9273910
C	4.9760420	-3.0321220	-0.6537970
H	5.5621970	-3.9497130	-0.5644550
C	3.9792710	-2.7612780	0.2733550
H	3.7977870	-3.4689330	1.0870700
C	-2.2757040	3.6626960	2.2076740
H	-2.3971300	4.7432220	2.3138780
C	-3.7730970	-3.0131260	-0.1497640
H	-3.5928900	-3.7737890	0.6149410
C	4.4518000	-0.9803210	-1.7758150
H	4.6411560	-0.2844880	-2.6015810
C	-2.0765870	1.6996460	0.7691820
C	3.1867260	-1.5915310	0.2217630
C	2.2049120	-1.4702430	1.3138500
H	2.3386470	-2.3026970	2.0147290
C	-2.2403420	3.0799650	0.9411250
H	-2.3434750	3.7315670	0.0649050
C	3.4403240	-0.6996070	-0.8461100
C	-2.1474930	2.8461990	3.3275270
H	-2.1754200	3.2757890	4.3318310
Cl	0.0290020	-2.9308600	2.9902530
Bi	-2.1913710	1.0544360	-1.3502650
Bi	2.2598550	1.1032810	-1.3359340
Ir	0.0273620	-1.5119730	1.0446600
Se	0.0512100	-0.5659990	-1.2547090

## Co-Te

Te	0.1459660	-1.1423130	-0.9064130
C	-3.2916500	-1.2296640	-0.6888940
C	1.6499870	3.3466900	-0.0400200
H	1.9227310	3.6633310	-1.0540110
C	-2.2259180	1.9367440	2.9415660
H	-2.1312020	1.5059260	3.9429700
C	5.4922900	-2.2990410	-0.4457150
H	6.3577320	-2.6558220	-1.0085380
C	-4.2440370	-1.7290450	-1.5855620
H	-4.4860030	-1.1666590	-2.4942720
C	0.8765670	3.9256740	2.1548200
H	0.5364340	4.6632450	2.8857170
C	-1.7502980	-0.3114850	2.1638260
H	-1.5402660	-0.4173970	3.2332600
C	1.3761070	1.5800170	1.6180320
C	-2.0510160	1.0828230	1.8300550
C	0.9522290	2.5864060	2.5138450
H	0.6797120	2.2892300	3.5306960
C	1.2269600	4.3184130	0.8660030
H	1.1671280	5.3666280	0.5640370
C	1.4157580	0.2254070	2.1834740
H	1.0753150	0.2378260	3.2266390
C	1.7289620	1.9933960	0.3122630
C	-2.0821700	-1.5583540	1.5872660
H	-2.0111970	-2.3603730	2.3303160
C	-4.5594870	-3.6841890	-0.2296720
H	-5.0381160	-4.6477140	-0.0403090
C	-2.9718510	-1.9523110	0.4856850
C	-4.8883770	-2.9445360	-1.3639610
H	-5.6258640	-3.3155840	-2.0791860
C	5.1403850	-2.8827060	0.7703900
H	5.7292160	-3.7075280	1.1782120
C	4.0385600	-2.4132240	1.4711120
H	3.7769620	-2.8695530	2.4297720
C	-2.6200880	3.8451520	1.5310000
H	-2.8266360	4.9102920	1.4023400
C	-3.6208270	-3.1947270	0.6686250
H	-3.3807860	-3.7741170	1.5643630
C	4.7089070	-1.2603330	-0.9433720
H	4.9771810	-0.8197850	-1.9104520
C	-2.1783820	1.6557840	0.5453940
C	3.2361570	-1.3456110	1.0025830
C	2.1586520	-0.9539610	1.9179210
H	2.2016450	-1.5785860	2.8139330
C	-2.4460900	3.0240690	0.4168440
H	-2.5273760	3.4742530	-0.5798800
C	3.5905260	-0.7842710	-0.2466250
C	-2.5205580	3.2867630	2.8028140

H	-2.6592520	3.9069210	3.6917730
Cl	0.0766600	-2.2957830	3.6798450
Bi	-2.1837810	0.5642480	-1.3914290
Bi	2.3802830	0.6932350	-1.3644040
Co	0.0648790	-1.2677910	1.6386940

Rh-Te

C	-3.3879180	-1.1330010	-0.6823140
C	1.9681240	3.3362400	0.1101070
H	2.1938420	3.6992830	-0.8998100
C	-1.9800500	2.1384720	2.8612390
H	-1.8429200	1.7276150	3.8659890
C	5.2658950	-2.5938150	-0.9128090
H	6.0469060	-2.9875260	-1.5670290
C	-4.3158190	-1.6586580	-1.5913720
H	-4.5369940	-1.1174320	-2.5184300
C	1.3866010	3.8246270	2.3857170
H	1.1508100	4.5358080	3.1809930
C	-1.8057730	-0.1676140	2.1423280
H	-1.6049020	-0.2480710	3.2158570
C	1.6749420	1.4915100	1.6729230
C	-1.9873150	1.2409780	1.7706570
C	1.3838900	2.4623480	2.6562780
H	1.1506920	2.1171800	3.6679560
C	1.6808400	4.2738210	1.1016080
H	1.6790230	5.3409750	0.8677680
C	1.6443800	0.1046710	2.1581370
H	1.3772910	0.0882960	3.2211420
C	1.9674880	1.9606260	0.3722410
C	-2.2236390	-1.4199660	1.6238590
H	-2.2302750	-2.1761060	2.4183990
C	-4.6692160	-3.5789810	-0.1979660
H	-5.1536100	-4.5371870	0.0034210
C	-3.0992240	-1.8287540	0.5168140
C	-4.9640390	-2.8699480	-1.3606830
H	-5.6797030	-3.2595040	-2.0880640
C	4.9644590	-3.2173360	0.2964230
H	5.5094010	-4.1111350	0.6087210
C	3.9685300	-2.6993020	1.1124670
H	3.7469840	-3.1882100	2.0651100
C	-2.3047200	4.0392770	1.4238160
H	-2.4159870	5.1159550	1.2755450
C	-3.7575320	-3.0643840	0.7135390
H	-3.5431420	-3.6205070	1.6303290
C	4.5415720	-1.4632460	-1.2835850
H	4.7723410	-0.9880600	-2.2440610
C	-2.1643180	1.7904810	0.4813630
C	3.2271240	-1.5442300	0.7707850
C	2.2547430	-1.1244090	1.7885020
H	2.3054270	-1.7932960	2.6550850

C	-2.3141670	3.1744220	0.3295720
H	-2.4424910	3.6033750	-0.6715040
C	3.5286310	-0.9357610	-0.4710860
C	-2.1441360	3.5082130	2.7005320
H	-2.1357130	4.1626730	3.5755100
Cl	0.0243320	-2.0961050	3.8140770
Bi	-2.3341710	0.6755010	-1.4320650
Bi	2.4163260	0.7334810	-1.4205920
Rh	0.0279340	-1.2623330	1.5439200
Te	0.0601410	-0.9836270	-1.0527430

#### Ir-Te

C	-3.3754220	-0.8760420	-0.9637960
C	1.9554730	3.3412830	0.7117400
H	2.1877680	3.9011100	-0.2022870
C	-1.9783150	1.6091530	3.1548320
H	-1.8413940	1.0038620	4.0560830
C	5.2726430	-2.2407550	-1.4720740
H	6.0636540	-2.4863290	-2.1840720
C	-4.3189530	-1.1991590	-1.9495380
H	-4.5445160	-0.4786310	-2.7442230
C	1.3838270	3.3585140	3.0404800
H	1.1594240	3.8930980	3.9666170
C	-1.7365810	-0.5014820	1.9819640
H	-1.6051060	-0.7863460	3.0327060
C	1.6393750	1.2184300	1.8617470
C	-1.9564950	0.9548370	1.9049780
C	1.3659170	1.9693500	3.0243860
H	1.1293100	1.4266430	3.9445610
C	1.6794220	4.0587630	1.8749270
H	1.6905690	5.1511320	1.8652350
C	1.5781160	-0.2443910	2.0500200
H	1.3740420	-0.4582940	3.1070450
C	1.9394600	1.9407230	0.6862400
C	-2.1717850	-1.6414990	1.2176640
H	-2.2603580	-2.5145940	1.8767670
C	-4.6841470	-3.3534710	-0.9641540
H	-5.1804790	-4.3266060	-0.9502620
C	-3.0807590	-1.8006290	0.0664230
C	-4.9798450	-2.4247710	-1.9598430
H	-5.7078150	-2.6527920	-2.7415340
C	4.9672530	-3.0983650	-0.4170550
H	5.5192690	-4.0319180	-0.2855780
C	3.9592360	-2.7646780	0.4768770
H	3.7353910	-3.4393020	1.3079380
C	-2.3201150	3.7597940	2.1345060
H	-2.4481890	4.8422830	2.2079720
C	-3.7573160	-3.0406360	0.0208300
H	-3.5429570	-3.7712920	0.8057830
C	4.5409970	-1.0643100	-1.6106060

H	4.7772450	-0.3990660	-2.4493410
C	-2.1379010	1.7523340	0.7547840
C	3.2064740	-1.5726070	0.3693130
C	2.2059800	-1.3873160	1.4367620
H	2.3261220	-2.1818020	2.1828880
C	-2.3085480	3.1362500	0.8869770
H	-2.4401760	3.7582220	-0.0066550
C	3.5155950	-0.7215010	-0.7173500
C	-2.1639250	2.9807660	3.2769400
H	-2.1757260	3.4414560	4.2677020
Cl	0.0216780	-2.7528970	3.1952690
Bi	-2.3368580	1.0516940	-1.3423720
Bi	2.4193200	1.1119140	-1.3134950
Ir	0.0249070	-1.4539610	1.1551190
Te	0.0618300	-0.6462990	-1.3298450

### Ligands

#### Bi2O

Bi	1.6701300	-1.5914120	0.5771990
C	1.1795560	0.1842200	1.8511160
C	-0.1635260	0.3873830	2.1742770
H	-0.9233260	-0.2840960	1.7630110
C	4.5520070	1.2768930	-1.4422690
H	5.3663460	1.9416010	-1.1382850
C	4.1987480	1.1929830	-2.7841030
H	4.7400980	1.7837360	-3.5269720
C	3.1595390	0.3496690	-3.1785830
H	2.8856890	0.2673120	-4.2335180
C	2.4880980	-0.4018780	-2.2155580
H	1.6807020	-1.0786960	-2.5189580
C	2.8232710	-0.3103620	-0.8613340
C	-0.5599390	1.4467530	2.9867870
H	-1.6201120	1.5975390	3.2089740
C	0.4085940	2.3013610	3.5130470
H	0.1177620	3.1327870	4.1592120
C	1.7516350	2.0920820	3.2196370
H	2.5082620	2.7637060	3.6371850
C	4.2962020	0.7478040	0.9394880
H	5.3826050	0.8659740	1.0389840
C	2.1653260	1.0507190	2.3635080
C	3.6038250	0.9547190	2.0851830
H	4.2294980	1.2094630	2.9501440
C	3.8617340	0.5491350	-0.4504300
Bi	-1.4698620	-0.4421650	-1.4839320
C	-1.0810640	1.6513130	-0.7421780
C	0.2277530	2.1068220	-0.5610060
H	1.0647980	1.4176060	-0.6966030
C	-5.0102250	-0.4060830	1.3365420

H	-5.9070780	0.2056220	1.4779480
C	-4.8062680	-1.5250680	2.1345090
H	-5.5457200	-1.7941780	2.8927270
C	-3.6622180	-2.3058060	1.9594080
H	-3.5001860	-3.1929260	2.5766210
C	-2.7399290	-1.9582510	0.9734750
H	-1.8447710	-2.5696790	0.8117200
C	-2.9303320	-0.8269030	0.1753840
C	0.4973790	3.4241540	-0.1989560
H	1.5316870	3.7464370	-0.0490000
C	-0.5596530	4.3222070	-0.0494450
H	-0.3681020	5.3633200	0.2219400
C	-1.8628750	3.8933230	-0.2667610
H	-2.6900660	4.6030860	-0.1664890
C	-4.3612950	1.1995060	-0.4026130
H	-5.4317000	1.3440710	-0.5955480
C	-2.1577150	2.5518030	-0.5935440
C	-3.5795770	2.2359810	-0.7899800
H	-4.1354750	3.0667790	-1.2426100
C	-4.0688730	-0.0182140	0.3599010
O	-0.0230280	-1.5750150	-0.5655880

### Bi2S

Bi	2.02535000	-1.49156500	0.76103500
C	1.16694500	0.34712200	1.79541900
C	-0.20551200	0.41842100	2.03186200
H	-0.85839700	-0.38515700	1.68050300
C	4.74354400	1.49464800	-1.34999400
H	5.46873300	2.25042300	-1.03288300
C	4.54041200	1.26180100	-2.70463800
H	5.10824200	1.83028600	-3.44489400
C	3.61796200	0.29769700	-3.11288900
H	3.45869400	0.10140500	-4.17613900
C	2.91309600	-0.42782000	-2.15366800
H	2.19290300	-1.19083900	-2.47112100
C	3.09858900	-0.18699100	-0.78967000
C	-0.76743900	1.50710600	2.69538400
H	-1.84915200	1.54988900	2.85277100
C	0.06455500	2.52654300	3.15796000
H	-0.35714300	3.38630000	3.68404400
C	1.43838800	2.44449700	2.95937300
H	2.08833900	3.24106900	3.33448100
C	4.28942500	1.15791700	1.03306100
H	5.34630300	1.39080300	1.21399300
C	2.01972000	1.36972300	2.25514100
C	3.47922200	1.39739700	2.09211500
H	3.99996800	1.78951800	2.97490800
C	4.01292800	0.79777000	-0.36434600
Bi	-1.86342000	-0.58794900	-1.52133400
C	-1.16095900	1.51333100	-0.96885900

C	0.19646300	1.83378200	-0.94191500
H	0.94344300	1.05192700	-1.09953600
C	-5.01543100	0.05276600	1.69435100
H	-5.82133500	0.77509300	1.85661500
C	-4.84876400	-1.00377000	2.58116000
H	-5.52514400	-1.11097400	3.43247200
C	-3.82422500	-1.92854700	2.37449700
H	-3.69263400	-2.76888600	3.06078400
C	-2.98214900	-1.78638900	1.27242700
H	-2.18551300	-2.51942100	1.09854500
C	-3.13076800	-0.71608700	0.38692900
C	0.62502300	3.13925300	-0.70920800
H	1.69491300	3.36424100	-0.67799600
C	-0.32187300	4.14897600	-0.53601600
H	-0.00377700	5.18035400	-0.36547300
C	-1.67642800	3.84425100	-0.59389300
H	-2.41692300	4.64022600	-0.46874700
C	-4.40484400	1.40304000	-0.25727100
H	-5.47331900	1.62714500	-0.36724100
C	-2.12920900	2.52154500	-0.78540600
C	-3.58491200	2.32703200	-0.81460300
H	-4.11387900	3.16086100	-1.29324500
C	-4.14895500	0.23586900	0.59578600
S	0.03291700	-2.16937000	-0.73409500

### Bi2Se

Bi	2.0719910	-1.0036480	1.1931530
C	1.1901200	1.0230990	1.5287620
C	-0.1874680	1.1635160	1.6982800
H	-0.8373380	0.2909730	1.5933980
C	4.8930180	1.0371450	-1.6712850
H	5.6320140	1.8403630	-1.5929440
C	4.7365950	0.3612510	-2.8745630
H	5.3549050	0.6297560	-3.7342250
C	3.7957520	-0.6638770	-2.9753410
H	3.6703460	-1.2093810	-3.9137480
C	3.0300290	-1.0054810	-1.8619270
H	2.3025470	-1.8218200	-1.9400590
C	3.1671310	-0.3196970	-0.6513450
C	-0.7593900	2.4000980	1.9883310
H	-1.8440850	2.4838400	2.1013870
C	0.0662070	3.5134210	2.1435350
H	-0.3628900	4.4904110	2.3791870
C	1.4429270	3.3774210	2.0093410
H	2.0891260	4.2506940	2.1421000
C	4.3350570	1.5480350	0.6541500
H	5.3866570	1.8375350	0.7728160
C	2.0358630	2.1416940	1.6769420
C	3.4972350	2.1255400	1.5486130
H	3.9948200	2.7979400	2.2585250

C	4.0989920	0.7344680	-0.5446080
Bi	-2.0562150	-0.9570670	-1.2295760
C	-1.1923550	1.0902830	-1.4776750
C	0.1847490	1.2551920	-1.6273310
H	0.8458380	0.3886250	-1.5453940
C	-4.9193840	0.9447070	1.6857920
H	-5.6682750	1.7407030	1.6294390
C	-4.7624670	0.2294930	2.8661590
H	-5.3902200	0.4605080	3.7300270
C	-3.8091450	-0.7864790	2.9385540
H	-3.6832150	-1.3621690	3.8587720
C	-3.0314300	-1.0799260	1.8196680
H	-2.2942570	-1.8894450	1.8748060
C	-3.1689880	-0.3544640	0.6325360
C	0.7418860	2.5088490	-1.8691080
H	1.8262690	2.6116250	-1.9680650
C	-0.0977050	3.6153980	-1.9956400
H	0.3198630	4.6052030	-2.1939970
C	-1.4734250	3.4566000	-1.8797220
H	-2.1307830	4.3243960	-1.9902190
C	-4.3516980	1.5412470	-0.6173310
H	-5.4064170	1.8188770	-0.7360280
C	-2.0521370	2.2017980	-1.5962490
C	-3.5144400	2.1608820	-1.4834810
H	-4.0151140	2.8496820	-2.1754200
C	-4.1136460	0.6909150	0.5553720
Se	0.0061600	-2.2901680	-0.0367590

### Bi2Te

Bi	2.1691810	-0.8488750	1.2315990
C	1.1808850	1.1383780	1.5077880
C	-0.1999820	1.2224740	1.6901020
H	-0.8135710	0.3208240	1.6155880
C	4.8838200	1.2231260	-1.7065810
H	5.5845810	2.0616630	-1.6509030
C	4.7652310	0.5031580	-2.8882830
H	5.3743530	0.7728390	-3.7541490
C	3.8733560	-0.5670540	-2.9585270
H	3.7766620	-1.1480480	-3.8788700
C	3.1190630	-0.9072750	-1.8369210
H	2.4324310	-1.7598070	-1.8960360
C	3.2163070	-0.1783790	-0.6476440
C	-0.8237570	2.4386870	1.9593080
H	-1.9097030	2.4754190	2.0847840
C	-0.0480220	3.5913670	2.0788850
H	-0.5181720	4.5529860	2.2971980
C	1.3315320	3.5136450	1.9305280
H	1.9397250	4.4172220	2.0356560
C	4.2960980	1.7833580	0.5977060
H	5.3320140	2.1290160	0.7009490

C	1.9762710	2.2980200	1.6204240
C	3.4350220	2.3479810	1.4784740
H	3.9037610	3.0667960	2.1619960
C	4.0992050	0.9206530	-0.5729560
Bi	-2.1751750	-0.8635260	-1.2250920
C	-1.1743250	1.1136790	-1.5278460
C	0.2070810	1.1819740	-1.7121750
H	0.8102600	0.2737950	-1.6361310
C	-4.8842050	1.2651150	1.6795430
H	-5.5805860	2.1064650	1.6115470
C	-4.7725600	0.5590580	2.8701160
H	-5.3828870	0.8419530	3.7308520
C	-3.8853840	-0.5140670	2.9561170
H	-3.7933110	-1.0837320	3.8838380
C	-3.1301970	-0.8718110	1.8405440
H	-2.4475480	-1.7265760	1.9123560
C	-3.2215070	-0.1579410	0.6417820
C	0.8447210	2.3904940	-1.9837450
H	1.9309900	2.4145240	-2.1099010
C	0.0820180	3.5520020	-2.1031830
H	0.5632250	4.5080050	-2.3210230
C	-1.2986940	3.4891050	-1.9568170
H	-1.8960860	4.3994500	-2.0629910
C	-4.2854330	1.7968580	-0.6281620
H	-5.3181790	2.1494680	-0.7389370
C	-1.9569260	2.2813990	-1.6452660
C	-3.4157850	2.3465630	-1.5099410
H	-3.8750180	3.0631920	-2.2020950
C	-4.0980910	0.9450800	0.5517370
Te	-0.0059610	-2.3834640	0.0255020

### Transition metal precursors

Co(PPh <sub>3</sub> )Cl			
Co	-0.06366800	0.57183000	0.23083900
Cl	0.07687600	2.67516300	1.09803300
P	2.24637900	0.79434900	0.03284100
P	-0.03484600	-1.56378600	0.00005700
P	-2.23832900	0.88771000	0.05991500
C	3.44382100	-0.57143100	-0.36083600
C	4.02557100	-0.69866600	-1.63243600
C	3.72660200	-1.57500200	0.58180500
C	4.87660200	-1.75989500	-1.93504200
H	3.80206900	0.02960700	-2.41419700
C	4.58294800	-2.63256400	0.28217800
H	3.26273200	-1.56233800	1.56640200
C	5.16899900	-2.72865600	-0.97738600
H	5.30734000	-1.82951900	-2.93739100
H	4.77971600	-3.39131000	1.04431800
H	5.83765300	-3.55921700	-1.21623300

C	3.11479400	1.70672700	1.38791200
C	3.56972200	1.05285600	2.54165200
C	3.23418000	3.10459300	1.33108300
C	4.15095900	1.76461000	3.59025700
H	3.47196200	-0.02728000	2.64682000
C	3.82147100	3.81375400	2.37556000
H	2.84741100	3.65165500	0.46998200
C	4.28537000	3.14868100	3.50970700
H	4.50041500	1.22628800	4.47552500
H	3.90303100	4.90104900	2.30335500
H	4.74222600	3.70756900	4.32977000
C	2.45286200	1.93344900	-1.39408000
C	1.32150200	2.30550200	-2.12886700
C	3.70087100	2.46465900	-1.75274900
C	1.43220400	3.17943300	-3.20988100
H	0.34387100	1.90983200	-1.81941600
C	3.81238800	3.33786200	-2.83190600
H	4.59166100	2.19497700	-1.17682500
C	2.67799800	3.69494900	-3.56394500
H	0.53829800	3.46637200	-3.76949800
H	4.78951300	3.74693000	-3.10068100
H	2.76735500	4.38357100	-4.40783300
C	0.93533800	-2.19133200	-1.44631200
C	1.52880000	-3.45502300	-1.55107100
C	0.98657000	-1.33716900	-2.55681500
C	2.13287300	-3.85646400	-2.74175800
H	1.53048300	-4.13935400	-0.70038600
C	1.56720100	-1.74502500	-3.75607000
H	0.58269900	-0.32353300	-2.45439700
C	2.13815200	-3.01232900	-3.85260300
H	2.60162100	-4.84196300	-2.80179900
H	1.58870700	-1.06019000	-4.60789600
H	2.60210600	-3.33874000	-4.78655100
C	0.67547800	-2.23074900	1.56959200
C	0.93754500	-1.30792500	2.59346900
C	0.86691200	-3.59513600	1.82936500
C	1.43015800	-1.73238300	3.82737400
H	0.75277000	-0.23997900	2.40901300
C	1.37674900	-4.01837300	3.05577000
H	0.58811800	-4.34179600	1.08137000
C	1.66723600	-3.08763500	4.05473000
H	1.63072400	-0.99613600	4.61031300
H	1.53218300	-5.08427600	3.23925100
H	2.05929700	-3.42314500	5.01795900
C	-1.51644500	-2.66350400	-0.11979900
C	-1.92678800	-3.24452700	-1.32810800
C	-2.28892700	-2.88999400	1.02865700
C	-3.08792500	-4.01190200	-1.39064800
H	-1.33857900	-3.09221600	-2.23716200
C	-3.44292300	-3.66849100	0.96774400

H	-1.98641900	-2.45291800	1.98564200
C	-3.85093300	-4.22544800	-0.24332600
H	-3.39634900	-4.44645500	-2.34475300
H	-4.02926900	-3.83186000	1.87552100
H	-4.75917100	-4.83077500	-0.29225200
C	-3.20579300	0.19428800	-1.34312100
C	-4.59180700	0.38816800	-1.45854300
C	-2.52458100	-0.40040000	-2.40738700
C	-5.27606200	-0.05651600	-2.58687000
H	-5.13656700	0.91567900	-0.67029100
C	-3.20295500	-0.82990500	-3.54717400
H	-1.44077200	-0.52109900	-2.33158400
C	-4.58362100	-0.67005000	-3.63323900
H	-6.35584100	0.09390400	-2.65930300
H	-2.64623400	-1.29382300	-4.36617200
H	-5.12246900	-1.00811600	-4.52165900
C	-3.04756900	0.31183600	1.60691000
C	-2.36430000	0.61874800	2.79694700
C	-4.21808700	-0.45197200	1.67897800
C	-2.84874300	0.17836600	4.02584100
H	-1.44221200	1.20822600	2.73960600
C	-4.69920100	-0.89354600	2.91261200
H	-4.74524600	-0.74485800	0.76860900
C	-4.01842800	-0.58178500	4.08734600
H	-2.30420000	0.42540300	4.94042200
H	-5.60933900	-1.49799400	2.94979600
H	-4.39502000	-0.93483000	5.05044100
C	-2.79019400	2.63565600	-0.09610800
C	-2.56927700	3.27345900	-1.32426900
C	-3.36222400	3.36013300	0.95234000
C	-2.90660300	4.61170500	-1.49830900
H	-2.12704500	2.71335700	-2.15534500
C	-3.70419900	4.70096800	0.77510200
H	-3.53390300	2.88279100	1.92039000
C	-3.47441000	5.33131300	-0.44571300
H	-2.72447500	5.09692900	-2.46042000
H	-4.14832000	5.25758900	1.60387700
H	-3.73775000	6.38320400	-0.57912900

### [Rh(ethylene)2Cl]2

Cl	10.8058860	11.8473380	5.5634760
Cl	8.5233650	11.5739130	3.1036760
C	10.6924740	8.6164960	5.7438280
C	11.7081620	8.8140370	4.7945000
C	9.6926590	8.5728610	2.6213660
C	8.6918370	8.3765380	3.5865980
C	8.2975140	11.8196610	7.6104380
C	8.4345810	13.1918430	7.3454850
C	6.4183900	12.9501970	5.1730410
C	6.2960990	11.5797550	5.4536900

Rh	8.3379120	12.1318980	5.5178740
Rh	9.9947790	9.9162410	4.2266840
H	6.1918800	10.8572130	4.6374450
H	5.9155790	11.2381720	6.4210230
H	6.4091120	13.3076070	4.1378780
H	6.1409690	13.7003120	5.9200030
H	9.4199820	13.6683140	7.3821820
H	7.5896800	13.8740410	7.4808340
H	9.1772210	11.2149730	7.8545610
H	7.3461330	11.4097800	7.9626730
H	10.5126200	7.8562470	2.5131190
H	9.4949470	9.1821420	1.7330700
H	8.7107830	7.5010080	4.2425680
H	7.7050300	8.8335390	3.4581140
H	12.5052900	9.5422350	4.9781270
H	11.9604690	8.0292010	4.0748150
H	10.6897300	9.1916870	6.6756830
H	10.1402770	7.6727810	5.7848090

[Ir(ethylene)2Cl]2

Cl	0.0000960	-1.6785020	-1.1795040
Cl	-0.0000500	1.6784760	-1.1794130
C	-2.1355920	-1.4570760	1.2549850
C	-2.9864150	-1.4695680	0.1185100
C	-2.9865590	1.4691790	0.1182940
C	-2.1359430	1.4567960	1.2548990
C	2.1357960	-1.4569660	1.2549760
C	2.9865330	-1.4692470	0.1184530
C	2.9863250	1.4695010	0.1188340
C	2.1354370	1.4569070	1.2552510
H	1.3567250	2.2209450	1.3631680
H	2.4901100	1.0487900	2.2076690
H	2.8677890	2.2455690	-0.6466010
H	4.0025750	1.0662260	0.1873300
H	2.8679920	-2.2452070	-0.6470720
H	4.0027280	-1.0658360	0.1868770
H	1.3572130	-2.2211520	1.3628930
H	2.4905340	-1.0489280	2.2074070
H	-4.0027610	1.0657810	0.1865790
H	-2.8679220	2.2451870	-0.6471550
H	-2.4907820	1.0486970	2.2072610
H	-1.3573590	2.2209540	1.3629490
H	-2.8678490	-2.2455890	-0.6469800
H	-4.0026700	-1.0662800	0.1869780
H	-1.3569000	-2.2211420	1.3628970
H	-2.4903210	-1.0490180	2.2074140
Ir	-1.5074060	-0.0001090	-0.1211720
Ir	1.5073670	0.0000270	-0.1210510

Ni(cod)2

C	-0.9682910	-1.6585990	0.3350930
C	-1.9548070	-0.7520480	1.0763220
H	-0.6199340	-2.4470500	1.0231090
H	-1.6076740	-0.6158170	2.1121820
H	-1.9515530	0.2611570	0.6473090
C	-2.8994490	-0.3128050	-1.7692920
H	-3.0155760	0.0366670	-2.8068110
H	-2.1146280	0.3316840	-1.3458400
C	-4.2233650	-0.1158890	-1.0257440
H	-4.3625900	0.9518010	-0.7649320
H	-5.0564960	-0.3475520	-1.7102560
C	-2.4343120	-1.7506600	-1.7820340
H	-2.5706380	-2.2836320	-2.7285270
C	-1.5556750	-2.3290350	-0.8752170
H	-1.0517320	-3.2495200	-1.1924660
C	-4.3692080	-0.9877110	0.1899870
H	-5.4003610	-1.1761240	0.5111140
C	-3.3635450	-1.2988680	1.0958970
H	-3.6883380	-1.7355940	2.0457700
H	-0.0531780	-1.0939110	0.0684740
C	-2.7947390	-5.6786670	-0.7572070
C	-4.0175480	-5.5355830	-1.6675260
H	-1.8835710	-5.4886480	-1.3488320
H	-3.7774030	-5.9510780	-2.6583650
H	-4.8506140	-6.1543960	-1.3018730
C	-5.2995940	-4.9165530	1.0075480
H	-5.7706950	-4.9867610	2.0001220
H	-5.2546350	-5.9554290	0.6478770
C	-6.1850180	-4.0638520	0.0946480
H	-7.0631670	-4.6482180	-0.2441080
H	-6.6112970	-3.2338280	0.6826260
C	-3.9015550	-4.3640170	1.1628670
H	-3.6930100	-3.8653230	2.1148620
C	-2.7944030	-4.7292610	0.4081160
H	-1.8092330	-4.5163270	0.8393850
C	-5.4521260	-3.4709870	-1.0761330
H	-5.9100960	-2.5750170	-1.5113330
C	-4.4719990	-4.1034360	-1.8299220
H	-4.2194690	-3.6324050	-2.7853540
H	-2.6925830	-6.7266400	-0.4126820
Ni	-3.5428560	-2.8792450	-0.3383070

#### Pd(cod)2

C	2.4543640	-1.6977490	0.8466510
C	2.9440960	-0.3920110	1.4858090
H	1.8249850	-2.2357940	1.5776730
H	3.3095570	-0.6240020	2.4984390
H	3.8257800	-0.0170240	0.9477040
C	2.7839940	0.5603730	-1.4153970
H	2.9936330	0.8468490	-2.4575970

H	3.7558120	0.2095290	-1.0335690
C	2.3494000	1.8311330	-0.6739460
H	3.2174160	2.5098550	-0.5663870
H	1.6480230	2.3850680	-1.3201730
C	1.7886390	-0.5838510	-1.4216540
H	1.4078100	-0.8571030	-2.4124750
C	1.6690380	-1.5735860	-0.4325830
H	1.2150810	-2.5205560	-0.7527200
C	1.6781180	1.6483170	0.6563660
H	0.9310460	2.4092270	0.9117060
C	1.9124310	0.6916360	1.5789070
H	1.3068630	0.7188460	2.4931560
H	3.3281650	-2.3612230	0.6921130
C	-2.6258330	-1.7594340	-0.7823460
C	-2.9835740	-0.4285560	-1.4620380
H	-2.1142870	-2.4048710	-1.5143770
H	-3.3389470	-0.6507640	-2.4798220
H	-3.8471290	0.0343710	-0.9623490
C	-2.7341490	0.4837990	1.4262330
H	-2.9327990	0.7433450	2.4775330
H	-3.7099260	0.1613860	1.0334950
C	-2.2629520	1.7541670	0.7046290
H	-3.1158480	2.4512210	0.5901940
H	-1.5555150	2.2886350	1.3610930
C	-1.7636010	-0.6694740	1.3841180
H	-1.1605690	-0.8340220	2.2844440
C	-1.7410140	-1.6630700	0.4298700
H	-1.1696360	-2.5692950	0.6611560
C	-1.5807120	1.5404810	-0.6164810
H	-0.8797910	2.3292850	-0.9145510
C	-1.8615590	0.5768360	-1.5515930
H	-1.3524100	0.6576980	-2.5175800
H	-3.5593010	-2.3006670	-0.5327150
Pd	-0.0546970	-0.2466260	-0.2212660

#### Pt(cod)2

C	2.4104560	-1.9010270	0.2316770
C	2.7417500	-0.8196180	1.2646120
H	1.9060580	-2.7398260	0.7381620
H	3.0025240	-1.3026470	2.2186770
H	3.6509090	-0.2697540	0.9772270
C	2.7411130	0.8199920	-1.2648220
H	3.0008040	1.3035480	-2.2189120
H	3.6508700	0.2705940	-0.9783870
C	2.4100250	1.9009470	-0.2312700
H	3.3432870	2.3351300	0.1787580
H	1.9057410	2.7401320	-0.7372360
C	1.6100990	-0.1647840	-1.5047000
H	1.1226830	-0.0803230	-2.4830450
C	1.5075010	-1.4276450	-0.8763930

H	0.9716230	-2.2161380	-1.4171070
C	1.5071420	1.4273010	0.8767490
H	0.9709430	2.2155820	1.4174620
C	1.6102690	0.1644710	1.5049310
H	1.1228940	0.0794910	2.4832580
H	3.3436050	-2.3355750	-0.1782420
C	-2.4105320	-1.9009500	-0.2315150
C	-2.7415050	-0.8197470	-1.2648210
H	-1.9062610	-2.7399730	-0.7377070
H	-3.0016170	-1.3030400	-2.2189310
H	-3.6509700	-0.2700300	-0.9780860
C	-2.7414090	0.8199020	1.2645900
H	-3.0017990	1.3031470	2.2186420
H	-3.6508660	0.2704310	0.9774190
C	-2.4098740	1.9010940	0.2314980
H	-3.3429430	2.3357890	-0.1784760
H	-1.9052810	2.7399040	0.7378140
C	-1.6103190	-0.1646900	1.5047960
H	-1.1229750	-0.0800150	2.4831630
C	-1.5076120	-1.4275750	0.8765870
H	-0.9717470	-2.2160490	1.4173600
C	-1.5070750	1.4273860	-0.8765610
H	-0.9708610	2.2156580	-1.4172600
C	-1.6101380	0.1645700	-1.5048190
H	-1.1227080	0.0797980	-2.4831330
H	-3.3438080	-2.3351990	0.1783580
Pt	-0.0000130	-0.0003040	0.0000620

## Others

### Ethylene

C	8.2624860	11.7444210	7.4692870
C	8.3264410	13.0596130	7.2843120
H	9.2259910	13.6341700	7.5220330
H	9.1063100	11.1746210	7.8681650
H	7.4825420	13.6294460	6.8856400
H	7.3630110	11.1698320	7.2313610

### PPh<sub>3</sub>

P	0.0637590	0.0509650	-1.2711690
C	-1.4497850	-0.6984700	-0.5454110
C	-1.4456700	-1.6273450	0.5039380
C	-2.6825990	-0.3154780	-1.0978580
C	-2.6432960	-2.1494500	0.9927870
H	-0.4986940	-1.9454710	0.9484870
C	-3.8782700	-0.8257320	-0.5992350
H	-2.7016850	0.3980590	-1.9278340
C	-3.8616410	-1.7480830	0.4478460
H	-2.6220650	-2.8735320	1.8109060
H	-4.8283380	-0.5099720	-1.0369230

H	-4.7981210	-2.1570530	0.8340840
C	1.3914590	-0.8897380	-0.4138550
C	1.8419290	-2.0694210	-1.0264280
C	1.9636280	-0.5055100	0.8072610
C	2.8230420	-2.8553670	-0.4253350
H	1.4154520	-2.3735810	-1.9879960
C	2.9526110	-1.2871610	1.4031300
H	1.6319810	0.4129500	1.3004230
C	3.3815550	-2.4651090	0.7919400
H	3.1598740	-3.7726030	-0.9150640
H	3.3877700	-0.9746930	2.3555570
H	4.1570460	-3.0755560	1.2608560
C	0.1428370	1.6619370	-0.3879190
C	-0.7600840	2.0709590	0.6022110
C	1.1814040	2.5348200	-0.7515730
C	-0.6222120	3.3165020	1.2163070
H	-1.5765890	1.4096640	0.9051530
C	1.3273340	3.7701840	-0.1270580
H	1.8898580	2.2338750	-1.5302750
C	0.4220810	4.1670490	0.8583900
H	-1.3349310	3.6195290	1.9873380
H	2.1477490	4.4313050	-0.4168930
H	0.5297610	5.1397970	1.3440710

cod

C	-1.2188970	-1.2165700	-0.4932400
C	0.0043860	-1.6878310	-0.2119040
C	1.0753890	-1.0981050	0.6613910
C	1.9148720	-0.0217520	-0.0262890
C	1.2198910	1.2172440	-0.4914460
C	-0.0037980	1.6884970	-0.2118690
C	-1.0760580	1.0987450	0.6598630
C	-1.9145430	0.0224330	-0.0290970
H	1.8264270	1.8309820	-1.1686780
H	-0.2791000	2.6260800	-0.7100520
H	0.2803940	-2.6254150	-0.7096930
H	-1.8244580	-1.8303020	-1.1713490
H	-2.4188040	0.4716860	-0.9035910
H	-2.7496250	-0.2674420	0.6357930
H	-1.7578180	1.9063730	0.9672820
H	-0.6649940	0.7101040	1.6013310
H	0.6629630	-0.7095140	1.6022840
H	1.7567090	-1.9057430	0.9697580
H	2.4204770	-0.4709670	-0.9000260
H	2.7489340	0.2681370	0.6398770

## Ligand Conformations

Ligand\_Co-O

O	0.12912900	-0.61246600	-0.35382400
---	------------	-------------	-------------

C	-2.70913200	-1.64974800	-0.81103700
C	1.19188500	3.28738300	-0.80168000
H	1.39518600	3.39148000	-1.87417500
C	-2.47592400	1.75550100	2.83593000
H	-2.38980300	1.38804400	3.86297000
C	5.42400800	-1.92611900	-0.41447000
H	6.25547100	-2.33566500	-0.99226100
C	-3.44977500	-2.27688000	-1.81859400
H	-3.59252100	-1.78069600	-2.78549000
C	0.43731600	4.26280000	1.25857700
H	0.05591500	5.11350900	1.82863200
C	-1.65908400	-0.44739200	2.16043200
H	-1.48547000	-0.51125500	3.24062700
C	1.10773400	1.90515300	1.20785500
C	-2.13409500	0.88389100	1.78035600
C	0.62461300	3.04101000	1.89228800
H	0.40048600	2.94893700	2.95897000
C	0.72568200	4.39747200	-0.09858100
H	0.57511500	5.35180200	-0.60870900
C	1.28634500	0.69495900	2.01880600
H	0.92243400	0.85223200	3.04228000
C	1.38727300	2.05279200	-0.17169200
C	-1.78374400	-1.74254400	1.58813700
H	-1.65341000	-2.51243600	2.35404100
C	-3.78326600	-4.19258500	-0.40961200
H	-4.19347800	-5.19112200	-0.24090900
C	-2.49841200	-2.28233400	0.43222100
C	-4.00434200	-3.53987400	-1.62311000
H	-4.58479300	-4.01785700	-2.41544100
C	5.34924400	-2.12425900	0.96553400
H	6.12798100	-2.69146800	1.48078900
C	4.28245400	-1.61147100	1.68986900
H	4.22674000	-1.78278400	2.76822300
C	-3.03637400	3.52627800	1.29729800
H	-3.37415900	4.54718200	1.10372300
C	-3.03898900	-3.57917900	0.58921000
H	-2.87488400	-4.09808400	1.53761400
C	4.40498500	-1.21922800	-1.04822900
H	4.44732000	-1.09237100	-2.13643700
C	-2.24166300	1.38298000	0.46570700
C	3.25379700	-0.85826300	1.07618800
C	2.19386400	-0.39033200	1.96111600
H	2.32549900	-0.82547900	2.95250300
C	-2.68131900	2.68986200	0.23856300
H	-2.73680800	3.08164200	-0.78408700
C	3.33344200	-0.68812700	-0.32080300
C	-2.92990200	3.04871000	2.60234800
H	-3.19584300	3.69017900	3.44613100
Bi	-1.63784200	0.19762800	-1.29410200
Bi	1.74736200	0.29057400	-1.45910500

Ligand\_Rh-O

O	0.09333900	-0.52181400	-0.58159400
C	-2.81935400	-1.49621400	-0.92208200
C	1.43954200	3.33147400	-0.53753400
H	1.60297000	3.51494200	-1.60643500
C	-2.43902900	1.89443700	2.75054800
H	-2.41594000	1.51333800	3.77574400
C	5.25742900	-2.21641700	-0.80713700
H	6.02408400	-2.63532400	-1.46260100
C	-3.55341700	-2.08030000	-1.96131500
H	-3.62728600	-1.57447300	-2.93121100
C	0.82850700	4.17152700	1.62675300
H	0.51976800	4.99101200	2.28033400
C	-1.81002000	-0.36850700	2.09497300
H	-1.70679900	-0.44042500	3.18348100
C	1.35998200	1.79327900	1.35266900
C	-2.15335200	1.00053700	1.69672800
C	0.96886300	2.89194900	2.14824300
H	0.77818600	2.72047700	3.21174400
C	1.07310100	4.40366800	0.27438900
H	0.96085100	5.40474000	-0.14867300
C	1.48727800	0.51235900	2.06025900
H	1.20894800	0.62503300	3.11541200
C	1.58427000	2.03737500	-0.02294000
C	-2.00037100	-1.65788300	1.51540600
H	-1.97184400	-2.42913100	2.29431100
C	-4.06057800	-3.97584800	-0.57945900
H	-4.53552600	-4.94878300	-0.43239000
C	-2.70379600	-2.14504400	0.32676000
C	-4.18753200	-3.31000400	-1.79855700
H	-4.75741900	-3.75153500	-2.61913000
C	5.23102800	-2.53107000	0.55177300
H	5.98422300	-3.19953400	0.97551900
C	4.24390700	-2.00258100	1.37245800
H	4.22891200	-2.26096300	2.43471200
C	-2.77161900	3.72358800	1.21724400
H	-2.99592800	4.77536600	1.02412300
C	-3.32842900	-3.40642400	0.45382700
H	-3.23901500	-3.93496700	1.40694000
C	4.27334200	-1.37444000	-1.31990300
H	4.28031500	-1.14917800	-2.39307800
C	-2.17766700	1.51317200	0.38171800
C	3.25035500	-1.12361600	0.88288500
C	2.27189400	-0.65963600	1.86594800
H	2.41491500	-1.18241600	2.81655500
C	-2.47752300	2.86146200	0.16101100
H	-2.47186900	3.26412100	-0.85916200
C	3.27969300	-0.82995900	-0.49695700
C	-2.75357100	3.22829000	2.51960600

H	-2.97653400	3.88679600	3.36265000
Bi	-1.68748800	0.31980800	-1.41555200
Bi	1.78299500	0.41129800	-1.50809900

#### Ligand\_Ir-O

O	-0.09087700	-0.30227900	-0.78469900
C	-3.29749700	-0.53965000	-0.74999700
C	2.49637600	2.79699700	0.83510700
H	2.48545900	3.45458200	-0.04265300
C	-0.90949600	2.39410900	2.67204900
H	-0.71956200	1.97469000	3.66450700
C	4.29887900	-2.57752500	-2.61020200
H	4.90435900	-2.77203900	-3.49822000
C	-4.33054300	-0.82177700	-1.65326200
H	-4.33736300	-0.35020500	-2.64332300
C	2.81974400	2.52184700	3.20008300
H	3.07279200	2.92931800	4.18189600
C	-1.40253300	0.09332100	2.01476700
H	-1.16709100	-0.02646100	3.08085000
C	2.14993200	0.60414700	1.83317000
C	-1.29563100	1.51661300	1.63781400
C	2.47736800	1.17937000	3.07691200
H	2.45994300	0.54143600	3.96558400
C	2.82618900	3.34376100	2.07563200
H	3.07155200	4.40496900	2.16224100
C	1.75344400	-0.81451100	1.85884700
H	1.70653600	-1.17287600	2.89509000
C	2.16846100	1.44417800	0.70024200
C	-2.23204200	-0.99515000	1.55169500
H	-2.42709200	-1.69194200	2.37387900
C	-5.33191800	-2.32681100	-0.07703100
H	-6.11922100	-3.03185300	0.20035500
C	-3.26610800	-1.14888700	0.52156400
C	-5.35562100	-1.70565600	-1.32603100
H	-6.15334100	-1.91816700	-2.04105900
C	4.17046900	-3.54017900	-1.60902800
H	4.68068000	-4.50188200	-1.70288500
C	3.39299100	-3.28293500	-0.48720900
H	3.30258400	-4.04474500	0.29219900
C	-1.00498900	4.30867200	1.21107300
H	-0.89027900	5.38132700	1.03800200
C	-4.30541800	-2.05894100	0.81891700
H	-4.29355200	-2.55851000	1.79143300
C	3.62302000	-1.36829500	-2.46739000
H	3.70160900	-0.62301100	-3.26767900
C	-1.52167100	2.08164100	0.36138300
C	2.72011600	-2.05495100	-0.30300300
C	1.94945700	-1.91955100	0.94157200
H	1.97671700	-2.86112300	1.50495100
C	-1.37308600	3.46096800	0.16786000

H	-1.53750800	3.89334500	-0.82663000
C	2.84382500	-1.10003200	-1.33491800
C	-0.76634500	3.76141200	2.47017900
H	-0.45980100	4.40139600	3.30116100
Bi	-1.77229300	0.85907600	-1.46298600
Bi	1.68943400	0.76479400	-1.35027500

#### Ligand\_Co-S

S	0.13728400	-1.01353200	-0.71503700
C	-3.10514400	-1.30078800	-0.87680100
C	1.52988700	3.26306100	-0.06528100
H	1.74928500	3.58697200	-1.08994200
C	-2.27594600	1.70237200	2.93972900
H	-2.22512500	1.23589000	3.92821100
C	5.44875500	-2.20472800	-0.71176200
H	6.29917000	-2.51854000	-1.32120700
C	-4.01141300	-1.74615700	-1.84564300
H	-4.18460300	-1.14961200	-2.74830700
C	0.85624700	3.81932700	2.16889600
H	0.54675500	4.55022800	2.91991200
C	-1.72304800	-0.50763000	2.08784300
H	-1.53475300	-0.66223900	3.15555400
C	1.33000300	1.48125100	1.58843600
C	-2.03408100	0.89567800	1.80678900
C	0.94346500	2.47624800	2.51247500
H	0.71237400	2.16909500	3.53671300
C	1.15447900	4.22593400	0.87075600
H	1.08348700	5.27779000	0.58408000
C	1.40130400	0.11690800	2.12696800
H	1.07649400	0.09704300	3.17508100
C	1.61846700	1.90717600	0.27153700
C	-2.02972000	-1.72741000	1.44264500
H	-1.97220500	-2.56587000	2.14459000
C	-4.44407900	-3.73827600	-0.57771200
H	-4.95262800	-4.69677300	-0.45082500
C	-2.86648100	-2.06861000	0.28686600
C	-4.69371000	-2.95266900	-1.70181800
H	-5.39674800	-3.28360500	-2.46953200
C	5.21239100	-2.78227400	0.53538700
H	5.88000800	-3.55702300	0.91947100
C	4.12523800	-2.37479600	1.29537400
H	3.95213500	-2.82967300	2.27456100
C	-2.63373600	3.65608500	1.57906500
H	-2.85065500	4.72241300	1.48052700
C	-3.54623400	-3.30377500	0.38806700
H	-3.36646700	-3.92093500	1.27260300
C	4.56732000	-1.23305300	-1.17950700
H	4.74006700	-0.80179900	-2.17231600
C	-2.09895400	1.51605400	0.54086700
C	3.22900000	-1.36972900	0.85958100

C	2.17471600	-1.03273000	1.81880300
H	2.25877400	-1.67758000	2.69674600
C	-2.38508500	2.88202700	0.44518900
H	-2.41208400	3.36920900	-0.53706600
C	3.46874500	-0.81542700	-0.41807800
C	-2.58611400	3.05247900	2.83341100
H	-2.77842100	3.63821000	3.73562200
Bi	-1.87817300	0.46196500	-1.40081800
Bi	2.07384300	0.55680100	-1.42556000

#### Ligand\_Rh-S

C	-3.31070000	-1.04863000	-0.77617500
C	2.04757900	3.16056900	0.26402000
H	2.15125300	3.58906100	-0.74022000
C	-1.74645300	2.12411800	2.80071400
H	-1.62407000	1.71378000	3.80755900
C	5.03891400	-2.62397600	-1.47240900
H	5.77066200	-2.95331700	-2.21344700
C	-4.26088700	-1.49235800	-1.70487400
H	-4.39310400	-0.95359400	-2.65023200
C	1.84487300	3.49686200	2.63227200
H	1.79235800	4.15563400	3.50239100
C	-1.71240900	-0.19583100	2.08293300
H	-1.50213100	-0.29963700	3.15357800
C	1.81434500	1.22071900	1.71679400
C	-1.81182700	1.22289400	1.71616100
C	1.75130400	2.12124700	2.80206400
H	1.62972200	1.71033600	3.80877200
C	1.99296600	4.02885300	1.35403500
H	2.05223500	5.10911300	1.20210200
C	1.71362700	-0.19813600	2.08266300
H	1.50387600	-0.30245500	3.15335500
C	1.96045600	1.77296900	0.42499900
C	-2.23316200	-1.40877100	1.55628600
H	-2.29330000	-2.17076900	2.34171800
C	-4.85583600	-3.33135200	-0.28365400
H	-5.44550800	-4.22789700	-0.07880700
C	-3.12950400	-1.74255200	0.44329500
C	-5.04172100	-2.62158100	-1.46872500
H	-5.77404900	-2.95093500	-2.20918400
C	4.85300300	-3.33453100	-0.28781400
H	5.44207100	-4.23169600	-0.08393100
C	3.91580700	-2.90230600	0.64034600
H	3.78376300	-3.46121300	1.57082400
C	-1.98789600	4.03099100	1.35167800
H	-2.04624200	5.11120800	1.19908300
C	-3.91789100	-2.89913300	0.64375100
H	-3.78585500	-3.45742800	1.57459700
C	4.25884000	-1.49397000	-1.70734100
H	4.39104200	-0.95459000	-2.65234800

C	-1.95886700	1.77443500	0.42416000
C	3.12823700	-1.74495500	0.44114400
C	2.23273900	-1.41124400	1.55484000
H	2.29247800	-2.17391800	2.33965500
C	-2.04476700	3.16201500	0.26233400
H	-2.14923100	3.58991900	-0.74207500
C	3.30940800	-1.05022900	-0.77788000
C	-1.83871100	3.49971700	2.63008500
H	-1.78433300	4.15902900	3.49968000
Bi	-2.04143100	0.62347400	-1.47064200
Bi	2.04078100	0.62312200	-1.47060900
S	-0.00044600	-0.86867300	-0.88948400

#### Ligand\_Ir-S

C	-3.24056900	-0.78711000	-1.15405500
C	1.87583000	3.22160400	0.82464700
H	2.02430000	3.83818300	-0.07021800
C	-1.99805400	1.35793500	3.16594300
H	-1.91608800	0.69832200	4.03512500
C	5.22557300	-1.97807600	-1.82678300
H	6.00523800	-2.12436100	-2.57759600
C	-4.17656900	-0.98125900	-2.17889100
H	-4.31429400	-0.20957400	-2.94509600
C	1.50987200	3.08864500	3.19213300
H	1.37081500	3.56437100	4.16587900
C	-1.70782100	-0.67752500	1.86467500
H	-1.58465400	-1.04241500	2.89183100
C	1.64253700	1.03095400	1.86196200
C	-1.91528900	0.78234300	1.88137600
C	1.47343500	1.70304200	3.09004900
H	1.30861100	1.10282800	3.98998800
C	1.71334700	3.86184800	2.05269100
H	1.73381800	4.95245300	2.11361400
C	1.58041200	-0.44148700	1.94328100
H	1.39757300	-0.74354000	2.98262900
C	1.84188900	1.82636100	0.71283400
C	-2.15773300	-1.74493600	1.00687800
H	-2.26484800	-2.66996900	1.58655300
C	-4.74618000	-3.14140000	-1.30826700
H	-5.32165100	-4.06889700	-1.35528900
C	-3.05172700	-1.77941500	-0.16400600
C	-4.93727300	-2.14463400	-2.26335200
H	-5.65925000	-2.27517700	-3.07251400
C	5.03959200	-2.90181700	-0.79973600
H	5.67738100	-3.78614800	-0.73042800
C	4.04084400	-2.70009300	0.14301000
H	3.90864100	-3.42786400	0.94837200
C	-2.26998100	3.56995200	2.25764300
H	-2.39338600	4.64730600	2.39062400
C	-3.82224500	-2.95742600	-0.28843300

H	-3.68772100	-3.74208100	0.46129100
C	4.38636900	-0.86870400	-1.88932200
H	4.52311500	-0.15472500	-2.70986300
C	-2.01763800	1.64972100	0.77342400
C	3.18637200	-1.57429600	0.11677600
C	2.20802700	-1.51783800	1.21656100
H	2.35063200	-2.37890800	1.87968600
C	-2.18820500	3.02416400	0.97662900
H	-2.25399800	3.70057700	0.11574400
C	3.37493300	-0.65706100	-0.94228400
C	-2.18036300	2.72237900	3.35821400
H	-2.24184800	3.12447100	4.37230200
Bi	-2.00895700	1.03780200	-1.36015500
Bi	2.07322600	1.07664600	-1.36031300
S	0.04616400	-0.54584400	-1.14374700

#### Ligand\_Co-Se

Se	0.13443600	-1.04541700	-0.81860000
C	-3.20523300	-1.26825700	-0.78447600
C	1.63751000	3.30311200	-0.01406900
H	1.88634600	3.63345700	-1.02988600
C	-2.22128700	1.83073000	2.94019000
H	-2.13940300	1.38325200	3.93537300
C	5.42522700	-2.32483400	-0.63634900
H	6.27112000	-2.67207600	-1.23376800
C	-4.13053300	-1.74862800	-1.71875000
H	-4.34211800	-1.17074000	-2.62538800
C	0.91963800	3.85119300	2.20780300
H	0.60250500	4.57975300	2.95786900
C	-1.73554000	-0.40454300	2.12419100
H	-1.53607500	-0.53456400	3.19316200
C	1.38208900	1.51123700	1.62051400
C	-2.03311100	0.99642200	1.81645100
C	0.98680100	2.50504200	2.54261200
H	0.73122500	2.19291400	3.55945400
C	1.24871200	4.26331000	0.91913700
H	1.19475200	5.31755500	0.63777400
C	1.42558600	0.14515100	2.15725100
H	1.09958000	0.13401200	3.20499500
C	1.70735600	1.94333500	0.31363900
C	-2.06147800	-1.63843600	1.51618600
H	-2.00187700	-2.45633000	2.24204800
C	-4.48931000	-3.72602600	-0.40655000
H	-4.97510400	-4.69168100	-0.24878400
C	-2.92027100	-2.01139700	0.38565400
C	-4.78444700	-2.96548800	-1.53662000
H	-5.50148100	-3.32258000	-2.27921900
C	5.12622300	-2.91625700	0.59042800
H	5.73870700	-3.73675900	0.97133500
C	4.04681600	-2.46253100	1.33487000

H	3.82547400	-2.92737700	2.29949900
C	-2.60052000	3.76266200	1.55612500
H	-2.80601300	4.82981500	1.44357100
C	-3.57509500	-3.25626700	0.52665100
H	-3.36066500	-3.85334900	1.41721200
C	4.61252300	-1.29307900	-1.09976800
H	4.83599900	-0.84843000	-2.07634900
C	-2.14192200	1.59182700	0.54045900
C	3.21768000	-1.39988600	0.90275700
C	2.16730400	-1.02586500	1.85378300
H	2.22855900	-1.66981400	2.73456900
C	-2.41014600	2.96131100	0.43030100
H	-2.47429400	3.42880900	-0.55975000
C	3.51923700	-0.83034000	-0.35611600
C	-2.51472500	3.18294100	2.81955800
H	-2.66389500	3.78856700	3.71680300
Bi	-2.05617800	0.52058800	-1.40342900
Bi	2.24151500	0.63588800	-1.39565000

#### Ligand\_Rh-Se

C	-3.35626000	-1.08659700	-0.72005200
C	2.04410200	3.23589500	0.22161100
H	2.20351200	3.63966300	-0.78555900
C	-1.81230400	2.15096500	2.82239500
H	-1.67272800	1.74344300	3.82814800
C	5.10662700	-2.66479100	-1.25482200
H	5.85219100	-3.03161000	-1.96372800
C	-4.29450900	-1.57974400	-1.63653900
H	-4.47658500	-1.04120700	-2.57370600
C	1.67814400	3.63206300	2.55975200
H	1.54916700	4.31225300	3.40509900
C	-1.74861400	-0.16798300	2.11524700
H	-1.54531300	-0.25618800	3.18826800
C	1.77585700	1.32943300	1.71319300
C	-1.87657400	1.24611900	1.74023600
C	1.61790100	2.25953800	2.76376200
H	1.44517700	1.87354400	3.77286000
C	1.89149900	4.13280800	1.27835200
H	1.92880000	5.20959200	1.09768600
C	1.69823200	-0.07884700	2.12403700
H	1.47318400	-0.14653100	3.19452300
C	1.98994800	1.85032300	0.41697900
C	-2.22817900	-1.40129600	1.59883800
H	-2.26862100	-2.15460300	2.39431500
C	-4.75358400	-3.46349800	-0.22453100
H	-5.28428300	-4.39584800	-0.01837100
C	-3.11357100	-1.77907000	0.49040000
C	-5.00145600	-2.75630000	-1.39957200
H	-5.72493800	-3.12225000	-2.13144500
C	4.85906500	-3.34335200	-0.06288000

H	5.41228200	-4.25353500	0.17989800
C	3.90639900	-2.86128600	0.82389000
H	3.72706100	-3.39473700	1.76137300
C	-2.09159700	4.05251300	1.37466700
H	-2.16457000	5.13159600	1.22045800
C	-3.82945600	-2.98171200	0.69215900
H	-3.65049900	-3.53755100	1.61663200
C	4.37145200	-1.51615300	-1.53793700
H	4.55479100	-0.99989800	-2.48735600
C	-2.05195300	1.79339900	0.44937900
C	3.15994800	-1.68625000	0.57445700
C	2.24201900	-1.30530000	1.65480500
H	2.29746900	-2.03134400	2.47396500
C	-2.15341500	3.18064100	0.28803200
H	-2.27993600	3.60624900	-0.71480800
C	3.40448300	-1.02303100	-0.65170100
C	-1.92408300	3.52488000	2.65212800
H	-1.87014900	4.18557000	3.52075700
Bi	-2.21221000	0.66220500	-1.45234600
Bi	2.23829700	0.67993400	-1.45004900
Se	0.01874400	-0.89918200	-0.99075600

#### Ligand\_Ir-Se

C	-3.30945400	-0.83479300	-1.06433400
C	1.92566700	3.27303500	0.78813400
H	2.11635700	3.86714600	-0.11390300
C	-1.96939700	1.47749100	3.16638400
H	-1.85543000	0.84288500	4.05047300
C	5.22650000	-2.13386300	-1.68959100
H	6.00665600	-2.33219100	-2.42778500
C	-4.24570000	-1.09780100	-2.07426900
H	-4.43243500	-0.34890900	-2.85266300
C	1.45885500	3.20072100	3.13943600
H	1.27879500	3.70024500	4.09440400
C	-1.71858600	-0.59571300	1.92393000
H	-1.59716300	-0.92313500	2.96376400
C	1.64857000	1.10816700	1.86887500
C	-1.92824500	0.86395100	1.89693500
C	1.42934300	1.81322900	3.07070900
H	1.22790100	1.23604400	3.97821700
C	1.70828500	3.94505800	1.99016100
H	1.72578400	5.03688400	2.02323400
C	1.58377300	-0.36116500	1.99495500
H	1.39851100	-0.62433300	3.04438000
C	1.89964300	1.87459700	0.70973700
C	-2.16225700	-1.69805300	1.10823200
H	-2.26388900	-2.59807900	1.72756900
C	-4.69497100	-3.26594600	-1.15634100
H	-5.22222900	-4.22254700	-1.17861300
C	-3.06013700	-1.79636600	-0.05671600

C	-4.94615700	-2.29989500	-2.12880100
H	-5.66852300	-2.48258100	-2.92739100
C	4.97604200	-3.03212200	-0.65379700
H	5.56219700	-3.94971300	-0.56445500
C	3.97927100	-2.76127800	0.27335500
H	3.79778700	-3.46893300	1.08707000
C	-2.27570400	3.66269600	2.20767400
H	-2.39712900	4.74322200	2.31387800
C	-3.77309700	-3.01312600	-0.14976400
H	-3.59289000	-3.77378900	0.61494100
C	4.45180000	-0.98032100	-1.77581500
H	4.64115600	-0.28448800	-2.60158100
C	-2.07658700	1.69964600	0.76918200
C	3.18672600	-1.59153100	0.22176300
C	2.20491200	-1.47024300	1.31385000
H	2.33864700	-2.30269700	2.01472900
C	-2.24034200	3.07996500	0.94112500
H	-2.34347500	3.73156700	0.06490500
C	3.44032400	-0.69960700	-0.84611000
C	-2.14749300	2.84619900	3.32752700
H	-2.17542000	3.27578900	4.33183100
Bi	-2.19137100	1.05443600	-1.35026500
Bi	2.25985500	1.10328100	-1.33593400
Se	0.05121000	-0.56599900	-1.25470900

#### Ligand\_Co-Te

Te	0.14596600	-1.14231300	-0.90641300
C	-3.29165000	-1.22966400	-0.68889400
C	1.64998700	3.34669000	-0.04002000
H	1.92273100	3.66333100	-1.05401100
C	-2.22591800	1.93674400	2.94156600
H	-2.13120200	1.50592600	3.94297000
C	5.49229000	-2.29904100	-0.44571500
H	6.35773200	-2.65582200	-1.00853800
C	-4.24403700	-1.72904500	-1.58556200
H	-4.48600300	-1.16665900	-2.49427200
C	0.87656700	3.92567400	2.15482000
H	0.53643400	4.66324500	2.88571700
C	-1.75029800	-0.31148500	2.16382600
H	-1.54026600	-0.41739700	3.23326000
C	1.37610700	1.58001700	1.61803200
C	-2.05101600	1.08282300	1.83005500
C	0.95222900	2.58640600	2.51384500
H	0.67971200	2.28923000	3.53069600
C	1.22696000	4.31841300	0.86600300
H	1.16712800	5.36662800	0.56403700
C	1.41575800	0.22540700	2.18347400
H	1.07531500	0.23782600	3.22663900
C	1.72896200	1.99339600	0.31226300
C	-2.08217000	-1.55835400	1.58726600

H	-2.01119700	-2.36037300	2.33031600
C	-4.55948700	-3.68418900	-0.22967200
H	-5.03811600	-4.64771400	-0.04030900
C	-2.97185100	-1.95231100	0.48568500
C	-4.88837700	-2.94453600	-1.36396100
H	-5.62586400	-3.31558400	-2.07918600
C	5.14038500	-2.88270600	0.77039000
H	5.72921600	-3.70752800	1.17821200
C	4.03856000	-2.41322400	1.47111200
H	3.77696200	-2.86955300	2.42977200
C	-2.62008800	3.84515200	1.53100000
H	-2.82663600	4.91029200	1.40234000
C	-3.62082700	-3.19472700	0.66862500
H	-3.38078600	-3.77411700	1.56436300
C	4.70890700	-1.26033300	-0.94337200
H	4.97718100	-0.81978500	-1.91045200
C	-2.17838200	1.65578400	0.54539400
C	3.23615700	-1.34561100	1.00258300
C	2.15865200	-0.95396100	1.91792100
H	2.20164500	-1.57858600	2.81393300
C	-2.44609000	3.02406900	0.41684400
H	-2.52737600	3.47425300	-0.57988000
C	3.59052600	-0.78427100	-0.24662500
C	-2.52055800	3.28676300	2.80281400
H	-2.65925200	3.90692100	3.69177300
Bi	-2.18378100	0.56424800	-1.39142900
Bi	2.38028300	0.69323500	-1.36440400

#### Ligand\_Rh-Te

C	-3.38791800	-1.13300100	-0.68231400
C	1.96812400	3.33624000	0.11010700
H	2.19384200	3.69928300	-0.89981000
C	-1.98005000	2.13847200	2.86123900
H	-1.84292000	1.72761500	3.86598900
C	5.26589500	-2.59381400	-0.91280900
H	6.04690600	-2.98752500	-1.56702900
C	-4.31581900	-1.65865800	-1.59137200
H	-4.53699400	-1.11743200	-2.51843000
C	1.38660100	3.82462700	2.38571700
H	1.15081000	4.53580800	3.18099300
C	-1.80577300	-0.16761400	2.14232800
H	-1.60490200	-0.24807100	3.21585700
C	1.67494200	1.49151000	1.67292300
C	-1.98731500	1.24097800	1.77065700
C	1.38389000	2.46234800	2.65627800
H	1.15069200	2.11718000	3.66795600
C	1.68084000	4.27382100	1.10160800
H	1.67902300	5.34097500	0.86776800
C	1.64438000	0.10467100	2.15813700
H	1.37729100	0.08829600	3.22114200

C	1.96748800	1.96062600	0.37224100
C	-2.22363900	-1.41996600	1.62385900
H	-2.23027500	-2.17610600	2.41839900
C	-4.66921600	-3.57898100	-0.19796600
H	-5.15361000	-4.53718700	0.00342100
C	-3.09922400	-1.82875400	0.51681400
C	-4.96403900	-2.86994800	-1.36068300
H	-5.67970300	-3.25950400	-2.08806400
C	4.96445900	-3.21733500	0.29642300
H	5.50940100	-4.11113400	0.60872100
C	3.96853000	-2.69930200	1.11246700
H	3.74698400	-3.18821000	2.06511000
C	-2.30472000	4.03927700	1.42381600
H	-2.41598700	5.11595500	1.27554500
C	-3.75753200	-3.06438400	0.71353900
H	-3.54314200	-3.62050700	1.63032900
C	4.54157200	-1.46324600	-1.28358500
H	4.77234100	-0.98805900	-2.24406100
C	-2.16431800	1.79048100	0.48136300
C	3.22712400	-1.54423000	0.77078500
C	2.25474300	-1.12440900	1.78850200
H	2.30542700	-1.79329600	2.65508500
C	-2.31416700	3.17442200	0.32957200
H	-2.44249100	3.60337500	-0.67150400
C	3.52863100	-0.93576100	-0.47108600
C	-2.14413600	3.50821300	2.70053200
H	-2.13571300	4.16267300	3.57551000
Bi	-2.33417100	0.67550100	-1.43206500
Bi	2.41632600	0.73348100	-1.42059200
Te	0.06014100	-0.98362700	-1.05274300

#### Ligand\_Ir-Te

C	-3.37542200	-0.87604200	-0.96379600
C	1.95547300	3.34128300	0.71174000
H	2.18776800	3.90111000	-0.20228700
C	-1.97831500	1.60915300	3.15483200
H	-1.84139400	1.00386200	4.05608300
C	5.27264300	-2.24075500	-1.47207400
H	6.06365400	-2.48632900	-2.18407200
C	-4.31895300	-1.19915900	-1.94953800
H	-4.54451600	-0.47863100	-2.74422300
C	1.38382700	3.35851400	3.04048000
H	1.15942400	3.89309800	3.96661700
C	-1.73658100	-0.50148200	1.98196400
H	-1.60510600	-0.78634600	3.03270600
C	1.63937500	1.21843000	1.86174700
C	-1.95649500	0.95483700	1.90497800
C	1.36591700	1.96935000	3.02438600
H	1.12931000	1.42664300	3.94456100
C	1.67942200	4.05876300	1.87492700

H	1.69056900	5.15113200	1.86523500
C	1.57811600	-0.24439100	2.05002000
H	1.37404200	-0.45829400	3.10704500
C	1.93946000	1.94072300	0.68624000
C	-2.17178500	-1.64149900	1.21766400
H	-2.26035800	-2.51459400	1.87676700
C	-4.68414700	-3.35347100	-0.96415400
H	-5.18047900	-4.32660600	-0.95026200
C	-3.08075900	-1.80062900	0.06642300
C	-4.97984500	-2.42477100	-1.95984300
H	-5.70781500	-2.65279200	-2.74153400
C	4.96725300	-3.09836500	-0.41705500
H	5.51926900	-4.03191800	-0.28557800
C	3.95923600	-2.76467800	0.47687700
H	3.73539100	-3.43930200	1.30793800
C	-2.32011500	3.75979400	2.13450600
H	-2.44818900	4.84228300	2.20797200
C	-3.75731600	-3.04063600	0.02083000
H	-3.54295700	-3.77129200	0.80578300
C	4.54099700	-1.06431000	-1.61060600
H	4.77724500	-0.39906600	-2.44934100
C	-2.13790100	1.75233400	0.75478400
C	3.20647400	-1.57260700	0.36931300
C	2.20598000	-1.38731600	1.43676200
H	2.32612200	-2.18180200	2.18288800
C	-2.30854800	3.13625000	0.88697700
H	-2.44017600	3.75822200	-0.00665500
C	3.51559500	-0.72150100	-0.71735000
C	-2.16392500	2.98076600	3.27694000
H	-2.17572600	3.44145600	4.26770200
Bi	-2.33685800	1.05169400	-1.34237200
Bi	2.41932000	1.11191400	-1.31349500
Te	0.06183000	-0.64629900	-1.32984500

### Complexes with M = Ni, Pd, Pt

#### Ni-O

O	0.3535080	-0.9549840	-0.6487860
C	-2.7273460	-1.5616800	-0.7850020
C	1.9133310	2.7689250	-1.6103390
H	2.4394340	2.5267820	-2.5413710
C	-3.0089800	1.4176870	3.0766000
H	-3.0357300	0.9982380	4.0871840
C	5.0881410	-2.0887890	1.6979950
H	6.0166670	-2.6516830	1.5781650
C	-3.5813000	-2.0340220	-1.7845200
H	-3.6526450	-1.5096160	-2.7441570
C	0.6929280	4.3620620	-0.2903010
H	0.2663420	5.3582090	-0.1503240

C	-1.7857570	-0.6259390	2.3727630
H	-1.5994040	-0.7764480	3.4451760
C	1.0584790	2.0928540	0.5693920
C	-2.4331510	0.6520600	2.0452600
C	0.5227390	3.3971180	0.6920930
H	-0.0375480	3.6445680	1.5989370
C	1.4049880	4.0561970	-1.4510300
H	1.5425320	4.8057600	-2.2338530
C	0.7942900	1.2056100	1.7032420
H	0.0726400	1.6627540	2.3900770
C	1.7451510	1.7796580	-0.6316050
C	-1.7325610	-1.8051410	1.5515540
H	-1.3617660	-2.6694670	2.1227130
C	-4.2272090	-3.8791430	-0.3834010
H	-4.8032830	-4.7932770	-0.2190530
C	-2.6228540	-2.2348460	0.4473490
C	-4.3392370	-3.1894950	-1.5891690
H	-4.9981770	-3.5571120	-2.3795250
C	4.5438090	-1.8764070	2.9630840
H	5.0447310	-2.2661010	3.8523410
C	3.3555360	-1.1688660	3.0949510
H	2.9367870	-1.0017740	4.0918260
C	-3.4865240	3.2361490	1.5623260
H	-3.8896950	4.2336200	1.3701660
C	-3.3788830	-3.4089370	0.6158210
H	-3.2989710	-3.9565130	1.5598580
C	4.4146780	-1.5933230	0.5818750
H	4.8352060	-1.7913230	-0.4114610
C	-2.3833770	1.2213540	0.7472390
C	2.6727700	-0.6330590	1.9811870
C	1.4427020	0.1055850	2.2853380
H	1.1309620	-0.0501790	3.3252450
C	-2.8987060	2.5013500	0.5289750
H	-2.8326510	2.9579700	-0.4670260
C	3.2180860	-0.8772940	0.7002960
C	-3.5333230	2.6864940	2.8419970
H	-3.9740710	3.2522100	3.6667240
Bi	-1.4613490	0.2345700	-1.0957580
Bi	2.2665630	-0.3013860	-1.2249680
Ni	-0.1725970	-0.6524280	1.2380400

#### Pd-O

O	0.2211920	-0.8764160	-0.6995850
C	-2.7836340	-1.6941520	-0.4699110
C	1.4338440	3.0074830	-1.2049930
H	1.6706800	2.8921290	-2.2705520
C	-2.5939380	2.3688580	2.4458930
H	-2.6737240	2.2281950	3.5285890
C	5.1813220	-2.4607810	0.4295490
H	5.9794600	-3.0627740	-0.0106350

C	-3.5065110	-2.4632520	-1.3892620
H	-3.5113620	-2.1816950	-2.4490240
C	0.6637670	4.4027080	0.5875220
H	0.2942940	5.3596500	0.9643240
C	-1.9538250	0.0089640	2.3653910
H	-1.8998070	0.1602910	3.4500610
C	1.2569920	2.0620380	1.0300530
C	-2.2320800	1.2619880	1.6512200
C	0.7933910	3.3263700	1.4556670
H	0.5288520	3.4554760	2.5095170
C	0.9929810	4.2530750	-0.7572320
H	0.8936360	5.0890180	-1.4538520
C	1.3466180	1.0470830	2.0848870
H	0.9422440	1.4365720	3.0260300
C	1.5690910	1.9110930	-0.3437190
C	-2.0906280	-1.3535000	1.9995820
H	-2.0478120	-1.9985880	2.8879940
C	-4.1769600	-3.9860090	0.3379390
H	-4.7082060	-4.8817800	0.6688480
C	-2.7674390	-2.0553550	0.8963280
C	-4.2112520	-3.6015500	-1.0007480
H	-4.7628610	-4.1900470	-1.7374920
C	4.9994380	-2.4174330	1.8104610
H	5.6594730	-2.9826660	2.4727740
C	3.9733530	-1.6531990	2.3497760
H	3.8431650	-1.6218420	3.4354990
C	-2.7631730	3.8067430	0.5213190
H	-2.9592790	4.7848300	0.0750130
C	-3.4649120	-3.2285280	1.2598410
H	-3.4529200	-3.5367280	2.3095350
C	4.3115110	-1.7366130	-0.3839170
H	4.4467110	-1.7931660	-1.4709410
C	-2.1118880	1.4651010	0.2550640
C	3.0926840	-0.8923030	1.5465660
C	2.0748760	-0.1370000	2.2849140
H	2.0908150	-0.4146140	3.3462420
C	-2.3810130	2.7289080	-0.2802750
H	-2.2767430	2.8961540	-1.3602660
C	3.2713010	-0.9624420	0.1453330
C	-2.8625160	3.6188640	1.8968380
H	-3.1479330	4.4482410	2.5489630
Bi	-1.5967110	-0.0382410	-1.3369030
Bi	1.9930250	-0.0112670	-1.3939860
Pd	0.0012890	-0.7549810	1.7966380

#### Pt-O

O	0.2820600	-0.7463470	-1.0387780
C	-2.7440910	-1.5568410	-0.8881560
C	1.4132470	3.2004070	-0.9740490
H	1.6813340	3.2155770	-2.0383010

C	-2.7854280	1.9778840	2.6019720
H	-2.9108460	1.6715120	3.6453810
C	5.2219250	-2.3612680	0.1315920
H	6.0473280	-2.8896000	-0.3508850
C	-3.4890140	-2.1545820	-1.9113330
H	-3.4812530	-1.7185650	-2.9173680
C	0.5920920	4.3708000	0.9522590
H	0.2103080	5.2753550	1.4319580
C	-1.9670700	-0.3016530	2.2123820
H	-2.0291130	-0.3282640	3.3077570
C	1.1847410	1.9959540	1.1242030
C	-2.3166820	1.0282890	1.6756740
C	0.7091420	3.1981400	1.6886030
H	0.4168920	3.1988250	2.7431390
C	0.9504810	4.3814410	-0.3928260
H	0.8613590	5.2934540	-0.9880180
C	1.2386490	0.8555510	2.0557160
H	0.8715090	1.1683800	3.0406480
C	1.5358770	2.0091930	-0.2464810
C	-2.0270390	-1.6086540	1.5974160
H	-2.0245500	-2.3810330	2.3809170
C	-4.2239000	-3.8872310	-0.4245430
H	-4.7900280	-4.8010200	-0.2278610
C	-2.7452490	-2.1160380	0.4071440
C	-4.2345710	-3.3122120	-1.6929670
H	-4.8029140	-3.7668220	-2.5077470
C	4.9990620	-2.4852180	1.5011660
H	5.6528500	-3.1106070	2.1135930
C	3.9393520	-1.8105130	2.0929540
H	3.7761910	-1.9108200	3.1699460
C	-2.9223440	3.6815620	0.9069100
H	-3.1437530	4.7068330	0.5996670
C	-3.4893700	-3.2984060	0.5987940
H	-3.4930300	-3.7573870	1.5920540
C	4.3603820	-1.5620480	-0.6174450
H	4.5318260	-1.4830400	-1.6980360
C	-2.1400670	1.4375680	0.3326110
C	3.0640170	-0.9802050	1.3570750
C	2.0016620	-0.3440540	2.1538950
H	2.0675270	-0.6788210	3.1964300
C	-2.4489260	2.7534630	-0.0244100
H	-2.3036560	3.0856840	-1.0606400
C	3.2854020	-0.8778590	-0.0350790
C	-3.0888130	3.2852380	2.2298510
H	-3.4511160	3.9939500	2.9786220
Bi	-1.5384350	0.2084630	-1.4691520
Bi	2.0575210	0.2384410	-1.5068610
Pt	-0.0290800	-0.8848480	1.6209040

Ni-S

C	-2.9902730	-1.3835860	-0.9030210
C	1.8859310	2.8127230	-1.4924600
H	2.4806810	2.6544510	-2.3996040
C	-3.0947330	1.1638930	3.2110980
H	-3.0836960	0.6482360	4.1763650
C	5.2403600	-1.8796110	1.9979850
H	6.2325160	-2.3364010	1.9761630
C	-3.9194870	-1.7012570	-1.8952050
H	-3.9920420	-1.0907190	-2.8017040
C	0.4841410	4.2587230	-0.1792770
H	-0.0200870	5.2151600	-0.0223890
C	-1.8879380	-0.7857140	2.2537010
H	-1.5934200	-1.0216830	3.2855570
C	0.9730980	1.9857380	0.6032460
C	-2.5446750	0.5165810	2.0889600
C	0.3404960	3.2421530	0.7549720
H	-0.2787540	3.4079770	1.6419270
C	1.2673830	4.0497210	-1.3136700
H	1.3827010	4.8361580	-2.0632260
C	0.6998420	1.0293270	1.6763560
H	-0.1026170	1.3938980	2.3266990
C	1.7443650	1.7726100	-0.5649270
C	-1.9299790	-1.8922360	1.3545320
H	-1.5474990	-2.8165980	1.8136740
C	-4.6479080	-3.6116850	-0.6224450
H	-5.2851870	-4.4921440	-0.5095460
C	-2.8902790	-2.1703590	0.2579180
C	-4.7532770	-2.8126860	-1.7591430
H	-5.4698480	-3.0619030	-2.5456440
C	4.4917800	-1.8633480	3.1729230
H	4.8906890	-2.3029870	4.0898750
C	3.2290350	-1.2854560	3.1764100
H	2.6513480	-1.2644200	4.1053150
C	-3.6602890	3.1050660	1.8914130
H	-4.0883600	4.1074100	1.8102520
C	-3.7250420	-3.2947090	0.3714850
H	-3.6473710	-3.9264590	1.2615360
C	4.6943320	-1.3275510	0.8395040
H	5.2800340	-1.3742900	-0.0860010
C	-2.5433230	1.2063610	0.8534690
C	2.6693080	-0.6933320	2.0220500
C	1.3622930	-0.0651760	2.2250780
H	0.9402190	-0.3450540	3.1980340
C	-3.0968280	2.4863900	0.7723220
H	-3.0757510	3.0355880	-0.1773610
C	3.4221010	-0.7447520	0.8274880
C	-3.6495040	2.4376980	3.1153070
H	-4.0706690	2.9143690	4.0039640
Bi	-1.6008150	0.3596090	-1.0413190
Bi	2.6718120	-0.1647940	-1.1889920

Ni	-0.2756080	-0.8409890	1.0234430
S	0.5122370	-1.5084790	-0.9400600

Pd-S

C	-3.2778000	-1.2876350	-0.7415310
C	1.7621670	2.7260600	-1.6250280
H	2.2645870	2.5376900	-2.5810530
C	-2.9693970	1.7211610	3.0028090
H	-2.9815270	1.3313820	4.0255240
C	5.6553290	-1.6281950	1.7777530
H	6.6523440	-2.0636970	1.6779140
C	-4.2399280	-1.5747640	-1.7112440
H	-4.1936160	-1.0921970	-2.6936050
C	0.4349460	4.1896470	-0.2541130
H	-0.1034270	5.1280570	-0.1004780
C	-2.0721380	-0.4747510	2.2959060
H	-1.7473580	-0.5984900	3.3374300
C	1.1167410	1.9946610	0.5987610
C	-2.5275630	0.8860860	1.9597350
C	0.4379430	3.2256100	0.7448790
H	-0.1037120	3.4151820	1.6766730
C	1.1056940	3.9445820	-1.4509700
H	1.1037220	4.6876130	-2.2521100
C	1.0106900	1.0979130	1.7499100
H	0.1723610	1.3847610	2.3955460
C	1.7737900	1.7406300	-0.6291730
C	-2.3637190	-1.6779170	1.6118200
H	-2.1713570	-2.5791110	2.2102560
C	-5.3126070	-3.1368310	-0.2245650
H	-6.0960200	-3.8698710	-0.0182670
C	-3.3350280	-1.9185460	0.5153550
C	-5.2600570	-2.4950240	-1.4593070
H	-5.9984370	-2.7220070	-2.2322100
C	5.0395390	-1.5446230	3.0255840
H	5.5482080	-1.9119170	3.9197670
C	3.7687980	-0.9964210	3.1285120
H	3.2905440	-0.9291710	4.1102250
C	-3.3961540	3.5216030	1.4546970
H	-3.7299470	4.5427870	1.2530390
C	-4.3570200	-2.8534030	0.7488000
H	-4.4009850	-3.3637370	1.7158070
C	4.9711010	-1.1733900	0.6517420
H	5.4538110	-1.2777830	-0.3271850
C	-2.4919250	1.4079130	0.6463450
C	3.0744550	-0.4928960	2.0045860
C	1.7790620	0.1077850	2.2997770
H	1.3939100	-0.2213910	3.2731560
C	-2.9343750	2.7129520	0.4140490
H	-2.8948410	3.1324000	-0.5986700
C	3.6908440	-0.6115750	0.7375610

C	-3.4013620	3.0217870	2.7561300
H	-3.7418180	3.6474770	3.5847600
Bi	-1.6348920	0.2096760	-1.0971040
Bi	2.7546610	-0.1813870	-1.2464780
S	0.7148190	-1.6741550	-1.0390720
Pd	-0.3953600	-1.0290000	0.9694190

#### Pt-S

C	-3.5919920	-0.9821440	-0.6372610
C	1.7173830	2.8396380	-1.4310510
H	2.1644080	2.7261420	-2.4258060
C	-2.4664240	1.6513330	3.0986100
H	-2.3148110	1.1806790	4.0753640
C	5.9911270	-1.5416250	1.5090310
H	6.9931870	-1.9378540	1.3284280
C	-4.7426450	-1.0921050	-1.4196980
H	-4.8293470	-0.5310010	-2.3564240
C	0.4264450	4.1650670	0.1038610
H	-0.1393900	5.0681430	0.3458610
C	-1.7523880	-0.4927200	2.0818690
H	-1.2578300	-0.6900770	3.0430930
C	1.2520740	1.9591510	0.7851800
C	-2.2182120	0.9042830	1.9338500
C	0.5333440	3.1477010	1.0427580
H	0.0396310	3.2591080	2.0138030
C	1.0237600	4.0164340	-1.1462400
H	0.9390550	4.8018940	-1.9012360
C	1.2590530	0.9952350	1.8838760
H	0.4226620	1.1812960	2.5674310
C	1.8388940	1.8059550	-0.4932480
C	-2.3037100	-1.6533020	1.4535500
H	-2.1408270	-2.5849040	2.0136230
C	-5.6880980	-2.6684380	0.1400380
H	-6.4973930	-3.3364350	0.4437590
C	-3.4870080	-1.7167850	0.5597880
C	-5.7933100	-1.9281050	-1.0354890
H	-6.6844210	-2.0126340	-1.6623950
C	5.4462320	-1.5481340	2.7923750
H	6.0163970	-1.9491280	3.6335150
C	4.1682010	-1.0484310	2.9980740
H	3.7441090	-1.0549090	4.0066430
C	-3.1153430	3.5702010	1.7874200
H	-3.4620210	4.6049940	1.7256240
C	-4.5423060	-2.5671910	0.9251790
H	-4.4596170	-3.1554250	1.8442860
C	5.2299090	-1.0463700	0.4519530
H	5.6583030	-1.0792020	-0.5570250
C	-2.3919000	1.5295620	0.6820750
C	3.3953300	-0.5043230	1.9465340
C	2.0972470	0.0252180	2.3408570

H	1.7653710	-0.3958210	3.2984150
C	-2.8496730	2.8474920	0.6232390
H	-2.9775350	3.3421920	-0.3462310
C	3.9415300	-0.5293660	0.6426200
C	-2.9118550	2.9690340	3.0290730
H	-3.1000880	3.5281820	3.9486800
Bi	-1.8561050	0.3576040	-1.1722720
Bi	2.9056020	-0.0051630	-1.2698290
Pt	-0.4570940	-1.1812900	0.4870070
S	0.9919550	-1.6700480	-1.2640340

#### Ni-Se

C	-3.0757590	-1.3714840	-0.8033030
C	1.8951280	2.7645840	-1.6836380
H	2.5338070	2.5531960	-2.5490100
C	-3.1754890	1.3743430	3.1756000
H	-3.1462020	0.9070550	4.1648490
C	5.1698300	-1.6091600	2.3664160
H	6.1640830	-2.0566170	2.4347520
C	-4.0104500	-1.7460080	-1.7700950
H	-4.0926310	-1.1853690	-2.7074230
C	0.3916620	4.2656560	-0.5573190
H	-0.1490030	5.2136620	-0.5025320
C	-1.9479080	-0.5997160	2.2998310
H	-1.6314180	-0.7771120	3.3371440
C	0.9248160	2.0868870	0.4386230
C	-2.6257630	0.6828570	2.0798360
C	0.2462360	3.3288160	0.4566150
H	-0.4116010	3.5484030	1.3033570
C	1.2237150	3.9867400	-1.6403620
H	1.3402210	4.7071290	-2.4533940
C	0.6279620	1.2163350	1.5767390
H	-0.2087000	1.6149240	2.1604910
C	1.7558940	1.8050580	-0.6726210
C	-1.9898690	-1.7544400	1.4642550
H	-1.5912000	-2.6493610	1.9661450
C	-4.7207440	-3.5879560	-0.3890760
H	-5.3540090	-4.4629840	-0.2231410
C	-2.9612460	-2.0963530	0.3955300
C	-4.8368260	-2.8528530	-1.5670490
H	-5.5576470	-3.1480900	-2.3336780
C	4.3444040	-1.5367010	3.4865530
H	4.6827200	-1.9230370	4.4504500
C	3.0817320	-0.9701110	3.3736570
H	2.4426060	-0.9037320	4.2594530
C	-3.7909600	3.2372930	1.7683510
H	-4.2372360	4.2272700	1.6433980
C	-3.7904410	-3.2154200	0.5789160
H	-3.7030880	-3.7977970	1.5009280
C	4.6998360	-1.1246360	1.1459530

H	5.3479160	-1.2141830	0.2661920
C	-2.6495020	1.3104910	0.8122230
C	2.5962280	-0.4476370	2.1536650
C	1.2779940	0.1821060	2.2404900
H	0.8090690	-0.0295870	3.2093030
C	-3.2302250	2.5736440	0.6739330
H	-3.2313900	3.0738500	-0.3025660
C	3.4276370	-0.5558560	1.0157950
C	-3.7540610	2.6322580	3.0237150
H	-4.1734580	3.1453490	3.8928240
Bi	-1.6990460	0.3747910	-1.0271280
Bi	2.8262320	-0.1157650	-1.0837700
Se	0.5754800	-1.6512100	-0.9037160
Ni	-0.3420910	-0.7169070	1.0626400

#### Pd-Se

C	-3.4042410	-1.2761750	-0.5795020
C	1.7800410	2.6192850	-1.8779640
H	2.3347570	2.3534390	-2.7852700
C	-3.0325360	2.0464050	2.8626500
H	-3.0262410	1.7486920	3.9158380
C	5.6258420	-1.2687370	2.1729550
H	6.6336920	-1.6904230	2.1725170
C	-4.3848610	-1.6449300	-1.5017260
H	-4.3594540	-1.2475190	-2.5221480
C	0.3309600	4.1589480	-0.7322970
H	-0.2515830	5.0830570	-0.7039860
C	-2.1367750	-0.2000860	2.3375500
H	-1.7832100	-0.2269080	3.3768190
C	1.0650180	2.1025610	0.3846230
C	-2.6023200	1.1244960	1.8902140
C	0.3308510	3.3104090	0.3665870
H	-0.2575520	3.5754790	1.2503570
C	1.0630760	3.8159130	-1.8673570
H	1.0650160	4.4653960	-2.7459990
C	0.9361850	1.3308660	1.6202950
H	0.0634830	1.6600260	2.1963680
C	1.7902210	1.7504190	-0.7788960
C	-2.4444760	-1.4608520	1.7785100
H	-2.2389490	-2.3028290	2.4537720
C	-5.4233360	-3.0769690	0.1335830
H	-6.2005120	-3.7907130	0.4166570
C	-3.4348830	-1.7988760	0.7268660
C	-5.3975070	-2.5409970	-1.1515740
H	-6.1511570	-2.8326990	-1.8871020
C	4.9327080	-1.0882490	3.3688330
H	5.3901710	-1.3648100	4.3213890
C	3.6502350	-0.5590190	3.3449220
H	3.1108100	-0.4155540	4.2858540
C	-3.4970510	3.6994390	1.1677420

H	-3.8416420	4.6966180	0.8820230
C	-4.4487440	-2.7122780	1.0597610
H	-4.4709940	-3.1397750	2.0668400
C	5.0066100	-0.9282780	0.9716440
H	5.5515670	-1.1065880	0.0372120
C	-2.5894500	1.5287970	0.5363550
C	3.0182300	-0.1715550	2.1408540
C	1.6987970	0.4251940	2.3056370
H	1.2717980	0.1890880	3.2886510
C	-3.0466430	2.8045340	0.1952070
H	-3.0275340	3.1310240	-0.8515160
C	3.7147700	-0.3877790	0.9291030
C	-3.4770830	3.3175140	2.5085410
H	-3.8082980	4.0126250	3.2838040
Bi	-1.7597570	0.1734440	-1.0905400
Bi	2.9094580	-0.1572980	-1.1405990
Se	0.7864630	-1.8439670	-0.9204260
Pd	-0.4763250	-0.8904970	1.0467010

#### Pt-Se

C	-3.6490760	-1.0096760	-0.5652330
C	1.7748760	2.7640910	-1.6993820
H	2.2911220	2.5716920	-2.6471320
C	-2.6641890	2.0209630	2.9149720
H	-2.5446630	1.6594300	3.9413160
C	5.9438010	-1.2078870	1.9194190
H	6.9626680	-1.5948220	1.8431650
C	-4.7713360	-1.2119320	-1.3700220
H	-4.8280970	-0.7550320	-2.3638960
C	0.3444510	4.1840110	-0.3883230
H	-0.2615290	5.0860520	-0.2725810
C	-1.9120080	-0.2163110	2.1579140
H	-1.4618690	-0.3096520	3.1562010
C	1.1857010	2.0839930	0.5576660
C	-2.3770580	1.1533690	1.8465410
C	0.4171450	3.2659260	0.6509180
H	-0.1421890	3.4532490	1.5734450
C	1.0296890	3.9372010	-1.5762780
H	0.9737770	4.6429200	-2.4086510
C	1.1447410	1.2307300	1.7434380
H	0.2682900	1.4646140	2.3582500
C	1.8622670	1.8303540	-0.6587080
C	-2.4294430	-1.4419790	1.6263340
H	-2.2794500	-2.3100660	2.2840270
C	-5.7628260	-2.6194920	0.3175020
H	-6.5791340	-3.2575610	0.6638140
C	-3.5816660	-1.6110220	0.7059860
C	-5.8307620	-2.0105460	-0.9337170
H	-6.6993620	-2.1692360	-1.5775880
C	5.3133120	-1.1082990	3.1590310

H	5.8320740	-1.4155890	4.0699290
C	4.0156660	-0.6228920	3.2319960
H	3.5241780	-0.5464150	4.2064220
C	-3.2717660	3.7840960	1.3836170
H	-3.6174370	4.8045120	1.1991410
C	-4.6450420	-2.4255900	1.1254510
H	-4.5912950	-2.9114880	2.1045590
C	5.2480680	-0.8310470	0.7724770
H	5.7447010	-0.9458180	-0.1982460
C	-2.5099170	1.6391050	0.5291930
C	3.3054920	-0.1976310	2.0854950
C	1.9743170	0.3321470	2.3436890
H	1.5917040	-0.0005340	3.3170130
C	-2.9678110	2.9406390	0.3137440
H	-3.0652490	3.3267920	-0.7073110
C	3.9404350	-0.3300380	0.8286920
C	-3.1075030	3.3217220	2.6889030
H	-3.3253080	3.9764110	3.5360470
Bi	-1.9058380	0.2855520	-1.1775470
Bi	3.0263550	-0.0069070	-1.1820930
Se	1.0066800	-1.8272000	-1.0858820
Pt	-0.5530810	-1.0466190	0.6977480

#### Ni-Te

C	-3.1515610	-1.3788400	-0.6226140
C	1.8844170	2.6481610	-1.9532400
H	2.5577450	2.3594940	-2.7685720
C	-3.2379390	1.7610590	3.0415480
H	-3.2070660	1.3972520	4.0731530
C	5.1138100	-1.1951550	2.6918170
H	6.1098260	-1.6164450	2.8465130
C	-4.0952080	-1.8554740	-1.5342770
H	-4.1949840	-1.3907930	-2.5209850
C	0.3049590	4.2210160	-1.0527950
H	-0.2646490	5.1505430	-1.1242590
C	-2.0070220	-0.2886640	2.3728430
H	-1.6825890	-0.3535990	3.4204420
C	0.8734910	2.1928430	0.2084740
C	-2.6874730	0.9617300	2.0219120
C	0.1609930	3.4070950	0.0625320
H	-0.5244000	3.7049290	0.8620420
C	1.1734840	3.8419900	-2.0746790
H	1.2911310	4.4633370	-2.9655250
C	0.5648150	1.4542140	1.4333900
H	-0.2867170	1.9080120	1.9518810
C	1.7458500	1.8109560	-0.8387810
C	-2.0432230	-1.5233630	1.6642950
H	-1.6404640	-2.3582730	2.2577070
C	-4.7699840	-3.5585310	0.0303510
H	-5.3913070	-4.4192590	0.2893170

C	-3.0184280	-1.9786850	0.6420070
C	-4.9083070	-2.9437820	-1.2125300
H	-5.6354400	-3.3193050	-1.9367200
C	4.2387170	-1.0284120	3.7624900
H	4.5385030	-1.3129030	4.7735410
C	2.9759180	-0.4955210	3.5398150
H	2.2979570	-0.3525220	4.3865320
C	-3.8605580	3.4672690	1.4510390
H	-4.3094220	4.4378250	1.2254610
C	-3.8339400	-3.0818100	0.9450520
H	-3.7301200	-3.5686290	1.9195120
C	4.6932690	-0.8376760	1.4108780
H	5.3823870	-0.9978160	0.5735830
C	-2.7140910	1.4560200	0.6967380
C	2.5376040	-0.1039790	2.2546040
C	1.2096180	0.5111860	2.2271390
H	0.7172680	0.4073410	3.2016520
C	-3.3000600	2.6958370	0.4298690
H	-3.3046370	3.0919830	-0.5931350
C	3.4207350	-0.3071710	1.1701680
C	-3.8200510	2.9946350	2.7620000
H	-4.2400380	3.5929340	3.5743030
Bi	-1.7802970	0.3402220	-1.0448780
Bi	2.9258180	-0.0829790	-0.9920760
Ni	-0.3922310	-0.5228180	1.1448080
Te	0.5908130	-1.8195780	-0.7618110

#### Pd-Te

C	-3.4511180	-1.2821180	-0.4249370
C	1.7721000	2.4780270	-2.1545890
H	2.3619510	2.1213870	-3.0068370
C	-3.1370100	2.4108350	2.6385680
H	-3.1425510	2.2311120	3.7181070
C	5.5504750	-0.8385760	2.4811940
H	6.5628530	-1.2394170	2.5705500
C	-4.4176100	-1.7694210	-1.3064700
H	-4.3922400	-1.4848070	-2.3638910
C	0.2547750	4.1059040	-1.2433460
H	-0.3481200	5.0119580	-1.3419760
C	-2.2292000	0.1248710	2.3740170
H	-1.8820960	0.2137890	3.4118100
C	1.0032140	2.2187690	0.1341050
C	-2.6934090	1.3879950	1.7789480
C	0.2440260	3.3972870	-0.0495740
H	-0.3727420	3.7531310	0.7812740
C	1.0248980	3.6456760	-2.3096090
H	1.0361580	4.1824350	-3.2612110
C	0.8485760	1.5970870	1.4487220
H	-0.0433430	1.9806750	1.9578680
C	1.7725930	1.7500220	-0.9574170

C	-2.5086540	-1.1902750	1.9482580
H	-2.2948700	-1.9520540	2.7104360
C	-5.4403760	-3.0347080	0.4697720
H	-6.2057270	-3.7285450	0.8253110
C	-3.4816940	-1.6585330	0.9309820
C	-5.4150170	-2.6423630	-0.8663060
H	-6.1571400	-3.0277930	-1.5697060
C	4.7990790	-0.5481850	3.6186740
H	5.2139800	-0.7164100	4.6149710
C	3.5127800	-0.0467480	3.4801410
H	2.9274710	0.1841740	4.3750990
C	-3.5874440	3.8644770	0.7662600
H	-3.9317650	4.8224370	0.3682460
C	-4.4806370	-2.5505460	1.3556280
H	-4.5029490	-2.8650060	2.4035110
C	4.9853260	-0.6338660	1.2237600
H	5.5777310	-0.8949140	0.3390630
C	-2.6651780	1.6414300	0.3890710
C	2.9324830	0.2013610	2.2146900
C	1.5993660	0.7892220	2.2597200
H	1.1427500	0.6665910	3.2500500
C	-3.1234290	2.8693830	-0.0961410
H	-3.0938540	3.0773940	-1.1724980
C	3.6892950	-0.1257960	1.0654220
C	-3.5806860	3.6331100	2.1413220
H	-3.9223590	4.4082970	2.8314300
Bi	-1.8303230	0.1303000	-1.0888040
Bi	2.9906190	-0.1272350	-1.0548700
Pd	-0.5253460	-0.6808750	1.1680460
Te	0.7819820	-2.0085490	-0.7136910

#### Pt-Te

C	-3.6507720	-1.0425280	-0.5150770
C	1.8037670	2.6229450	-2.0392010
H	2.3779310	2.3285440	-2.9252570
C	-2.9130910	2.3422880	2.7042370
H	-2.8469080	2.0863660	3.7663960
C	5.8280720	-0.7545630	2.3063350
H	6.8580060	-1.1170420	2.3447260
C	-4.7259240	-1.3536430	-1.3489380
H	-4.7423270	-0.9982830	-2.3849010
C	0.2732280	4.1574640	-0.9970840
H	-0.3543390	5.0516290	-1.0283550
C	-2.0804260	0.0591690	2.2149010
H	-1.6916520	0.0703470	3.2426030
C	1.1040740	2.2165810	0.2511100
C	-2.5518920	1.3789860	1.7452410
C	0.3102670	3.3820210	0.1540760
H	-0.2950320	3.6731430	1.0181840
C	1.0256970	3.7788250	-2.1072830

H	0.9993910	4.3698350	-3.0259470
C	1.0038580	1.5136720	1.5284530
H	0.0920660	1.8056610	2.0617980
C	1.8541330	1.8310840	-0.8845660
C	-2.5331930	-1.2248280	1.7650170
H	-2.3952970	-2.0254860	2.5058930
C	-5.7698850	-2.6141700	0.4209620
H	-6.5881270	-3.2370730	0.7896350
C	-3.6341940	-1.5130340	0.8114280
C	-5.7877540	-2.1344030	-0.8868350
H	-6.6185690	-2.3799830	-1.5529010
C	5.1088300	-0.5347370	3.4803960
H	5.5674310	-0.7219560	4.4539500
C	3.7995060	-0.0821410	3.4076300
H	3.2381130	0.0899990	4.3306910
C	-3.4614840	3.9330950	0.9743630
H	-3.8119930	4.9228620	0.6707750
C	-4.6993700	-2.3102990	1.2586400
H	-4.6848050	-2.6951420	2.2830100
C	5.2088800	-0.5295070	1.0785990
H	5.7766610	-0.7364210	0.1639470
C	-2.6187160	1.7303080	0.3803420
C	3.1638500	0.1894640	2.1738040
C	1.8083550	0.7092050	2.2808520
H	1.3699140	0.4884370	3.2624480
C	-3.0849780	2.9944110	0.0122700
H	-3.1314450	3.2754680	-1.0462270
C	3.8896530	-0.0655670	0.9868520
C	-3.3631630	3.6046430	2.3260620
H	-3.6382590	4.3347080	3.0909720
Bi	-1.9144770	0.2401210	-1.1695460
Bi	3.1112490	-0.0066170	-1.1037280
Pt	-0.6169380	-0.8686770	0.9018230
Te	0.9897000	-1.9984260	-0.8572580