checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: nl090_cu

Bond precision: C-C = 0.0366 A Wavelength=1.54186

Cell: a=14.5025(2) b=16.4157(2) c=27.2255(4)
alpha=81.172(1) beta=86.050(1) gamma=67.160(1)
Temperature: 100 K

	Calculated	Reported
Volume	5902.27(15)	5902.27(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	4(C18 H36 K N2 O6), Bi7 Th, 2(C2 H4 N2), 5(Bi)	Bi12 Th, 4(C18 H36 K N2 O6), 4(C H2 N)
Sum formula	C76 H152 Bi12 K4 N12 O24 Th	C72 H0.50 Bi12 K4 N8 O24 Th
Mr	4514.30	4257.50
Dx,g cm-3	2.540	2.396
Z	2	2
Mu (mm-1)	40.103	40.064
F000	4092.0	3685.0
F000’	4002.82	
h,k,lmax	17,19,32	17,19,32
Nref	21506	21352
Tmin,Tmax	0.033,0.548	
Tmin’	0.000	

Correction method= Not given

Data completeness= 0.993 Theta(max)= 67.993

R(reflections)= 0.0725(14810) wR2(reflections)= 0.2128(21352)

S = 1.016 Npar= 1171

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

PLAT058_ALERT_1_A Maximum Transmission Factor Missing	?	
PLAT059_ALERT_1_A Minimum Transmission Factor Missing	?	
PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual)	Bi02	Check
PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual)	Bi03	Check
PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual)	Bi04	Check
PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual)	Bi06	Check
PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual)	Bi0C	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi05	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi07	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi08	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi09	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi0A	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi0B	Check
PLAT308_ALERT_2_A Single Bonded Metal Atom in Structure (Unusual)	Bi0D	Check

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Alert level B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.95 <> 1.05
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 4257.50
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	76.00	912.84
N	14.01	12.00	168.08
O	16.00	24.00	383.98
K	39.10	4.00	156.39
Bi	208.98	12.00	2507.76
Th	232.04	1.00	232.04
H	1.01	152.00	153.22

Calculated formula weight 4514.30

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..	256.80	Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds	0.03658	Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.178

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.178	Report
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ	Please	Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT215_ALERT_3_C Disordered C63# has ADP max/min Ratio	3.3	Note
PLAT234_ALERT_4_C Large Hirshfeld Difference N01O --C48	0.19	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01S --C52	0.20	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5BA --C0EA	0.20	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2DA --C57	0.24	Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C019     --C60             0.22 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O01R Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C0AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C9CA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C6BA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C3AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C4CA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C1EA Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      K00F Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      K00G Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C2CA     - C3CA     .      1.39 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H7CB     ..H4EB            1.93 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C72 H0.5 Bi12 K4 N8 O24 Th1
           Atom count from _chemical_formula_moiety:C76 H152 Bi12 K4 N12 O24 Th
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C72 H0.5 Bi12 K4 N8 O24 Th1
           Atom count from the _atom_site data:  C76 H152 Bi12 K4 N12 O24 Th1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C72 H0.50 Bi12 K4 N8 O24 Th
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        144.00    152.00   -8.00
           H          1.00    304.00 -303.00
           Bi        24.00     24.00    0.00
           K          8.00      8.00    0.00
           N         16.00     24.00   -8.00
           O         48.00     48.00    0.00
           Th         2.00      2.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.14 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.001 Degree
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C3EA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4EA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9CC       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9CD       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9CA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9CB       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3EA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3EB       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4EA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4EB       Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        4% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       242 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.13 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
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 15 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 25 ALERT level G = General information/check it is not something unexpected

 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 27 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock nl090_cu - ellipsoid plot