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: I

Bond precision: Zn- O = 0.0080 A Wavelength=1.54051

Cell: a=10.94783(7) b=10.94783(7) c=38.3638(3)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	3982.07(7)	3982.06(5)
Space group	R 3 c	R 3 c
Hall group	R 3 -2"c	R 3;-2"c
Moiety formula	Bi6 O168 Pb8.84 V42 Zn6, 39.161(Ca)	?
Sum formula	Bi6 Ca39.16 O168 Pb8.84 V42 Zn6	Bi0.999 Ca6.527 O28 Pb1.474 V7 Zn1.01
Mr	9874.37	1646.40
Dx,g cm-3	4.118	4.119
Z	1	6
Mu (mm-1)	61.554	63.577
F000	4495.9	4498.0
F000’	4461.98	
h,k,lmax	9,9,34	
Nref	674[339]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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 B

POWD004_ALERT_1_B No 'Bragg' R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.067
Additional refinement cycles may be required.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check
PLAT080_ALERT_2_C Maximum Shift/Error ..... 0.07 Why ?
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit R 3;-2"c
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . V2 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . V3 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O2 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O3 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O4 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O5 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O6 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O7 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O8 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O9 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O10 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . V2 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . V3 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O2 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O3 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O4 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O5 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O6 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O7 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O8 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O9 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O10 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . V2 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . V3 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O2 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O3 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O4 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O5 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O6 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O7 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O8 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O9 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O10 Check
PLAT752_ALERT_4_C Angle Calc 108.17, Rep 108.17 ..... Senseless s.u.
O3 -V2 -O4 1.555 1.555 1.555 # 244 Check
PLAT752_ALERT_4_C Angle Calc 94.10, Rep 94.10 ..... Senseless s.u.
O3 -V2 -O5 1.555 1.555 1.555 # 245 Check
PLAT752_ALERT_4_C Angle Calc 108.85, Rep 108.85 ..... Senseless s.u.
O3 -V2 -O6 1.555 1.555 1.555 # 246 Check
PLAT752_ALERT_4_C Angle Calc 120.25, Rep 120.25 ..... Senseless s.u.
O4 -V2 -O5 1.555 1.555 1.555 # 248 Check

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PLAT752_ALERT_4_C Angle   Calc      116.66, Rep      116.66 ......  Senseless s.u.
             O4     -V2     -O6         1.555   1.555   1.555     #  249 Check
PLAT752_ALERT_4_C Angle   Calc      106.15, Rep      106.15 ......  Senseless s.u.
             O5     -V2     -O6         1.555   1.555   1.555     #  251 Check
PLAT752_ALERT_4_C Angle   Calc      108.84, Rep      108.84 ......  Senseless s.u.
             O7     -V3     -O8         1.555   1.555   1.555     #  284 Check
PLAT752_ALERT_4_C Angle   Calc      107.23, Rep      107.23 ......  Senseless s.u.
             O7     -V3     -O9         1.555   1.555   1.555     #  285 Check
PLAT752_ALERT_4_C Angle   Calc       98.25, Rep       98.25 ......  Senseless s.u.
             O7     -V3     -O10        1.555   1.555   1.555     #  286 Check
PLAT752_ALERT_4_C Angle   Calc      111.09, Rep      111.09 ......  Senseless s.u.
             O8     -V3     -O9         1.555   1.555   1.555     #  289 Check
PLAT752_ALERT_4_C Angle   Calc      107.03, Rep      107.03 ......  Senseless s.u.
             O8     -V3     -O10        1.555   1.555   1.555     #  290 Check
PLAT752_ALERT_4_C Angle   Calc       98.61, Rep       98.61 ......  Senseless s.u.
             O1     -V1     -O2         1.555   1.555   1.555     #  299 Check
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ......          ?
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    6
          From the CIF: _chemical_formula_sum  Bi0.999 Ca6.527 O28 Pb1.474 V7 Z
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          Bi         5.99      6.00    0.00
          Ca        39.16     39.16    0.00
          O        168.00    168.00    0.00
          Pb         8.84      8.84    0.00
          V         42.00     42.00    0.00
          Zn         6.06      6.00    0.06
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.17 Check
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka    1.54051 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00030 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          2 Units
PLAT300_ALERT_4_G Atom Site Occupancy of Bi1     is Constrained at     0.1933 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Bi2     is Constrained at     0.1398 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Pb3     is Constrained at     0.4912 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1     is Constrained at     0.8067 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca2     is Constrained at     0.8602 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca3     is Constrained at     0.5087 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          6 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4)..        100 % Note
PLAT984_ALERT_1_G The Bi-f'=    -4.016 Deviates from the B&C-Value     -3.848 Check
PLAT984_ALERT_1_G The  O-f'=     0.052 Deviates from the B&C-Value      0.050 Check
PLAT984_ALERT_1_G The Pb-f'=    -4.084 Deviates from the B&C-Value     -3.929 Check
PLAT984_ALERT_1_G The  V-f'=     0.077 Deviates from the B&C-Value      0.071 Check
PLAT984_ALERT_1_G The Zn-f'=    -1.556 Deviates from the B&C-Value     -1.546 Check
PLAT985_ALERT_1_G The Bi-f"=     9.118 Deviates from the B&C-Value      8.940 Check
PLAT985_ALERT_1_G The Pb-f"=     8.687 Deviates from the B&C-Value      8.514 Check
PLAT985_ALERT_1_G The Zn-f"=     0.695 Deviates from the B&C-Value      0.679 Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
 52 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
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  16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
  58 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_CRYSC01_I
;
PROBLEM: No recognised colour has been given for crystal colour.
RESPONSE: ...
;
_vrf_SHFSU01_I
;
PROBLEM: The absolute value of parameter shift to su ratio > 0.05
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell contains non-integer number of atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT080_I
;
PROBLEM: Maximum Shift/Error ............................       0.07 Why ?
RESPONSE: ...
;
_vrf_PLAT127_I
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit    R 3;-2"c
RESPONSE: ...
;
_vrf_PLAT161_I
;
PROBLEM: Missing or Zero s.u. (esd) on x-coordinate for .         V2 Check
RESPONSE: ...
;
_vrf_PLAT162_I
;
PROBLEM: Missing or Zero s.u. (esd) on y-coordinate for .         V2 Check
RESPONSE: ...
;
_vrf_PLAT163_I
;
PROBLEM: Missing or Zero s.u. (esd) on z-coordinate for .         V2 Check
RESPONSE: ...
;
_vrf_PLAT752_I
;
PROBLEM: Angle   Calc      108.17, Rep      108.17 ......  Senseless s.u.
```

```
RESPONSE: ...
;
_vrf_PLAT799_I
;
PROBLEM: Numeric Label on Displacement Par. Record ......          ?
RESPONSE: ...
;
# end Validation Reply Form
```

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 27/03/2017; check.def file version of 24/03/2017

Datablock I - ellipsoid plot