checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

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: x

Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=3.9829(1) b=3.9829(1) c=23.2854(6)
alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	319.899(18)	319.899(18)
Space group	P 63/m m c	P 63/m m c
Hall group	-P 6c 2c	-P 6c 2c
Moiety formula	Bi2.80 Cd1.12 S6, 0.047(K6), 0.09(K6), 0.09(K6)	Bi2.80 Cd1.12 S6, 0.047(K6), 0.09(K6), 0.09(K6)
Sum formula	Bi2.80 Cd1.12 K1.36 S6	Bi2.80 Cd1.12 K1.36 S6
Mr	957.13	956.57
Dx,g cm-3	4.968	4.965
Z	1	1
Mu (mm-1)	41.603	41.595
F000	408.2	408.0
F000'	397.94	
h,k,lmax	5,5,33	5,5,32
Nref	240	232
Tmin,Tmax	0.001,0.125	0.090,1.000
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.090 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.967 Theta(max)= 30.805

R(reflections)= 0.0293(215) wR2(reflections)= 0.0923(232)

S = 1.181 Npar= 25

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.56Ang From Bi1 2.93 eA-3

Author Response: This is due to the relatively low quality of the crystal used for X-ray structure determination. Despite many attempts, we have not been able to obtain better-quality crystals for this compound. However, all the residual peaks are near the heavy metal Bi, showing no features.

Alert level C

PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms . Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.28 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.516 Check
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by . 1.07 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.54Ang From Cd1 2.32 eA-3

Author Response: This is due to the relatively low quality of the crystal used for X-ray structure determination. Despite many attempts, we have not been able to obtain better-quality crystals for this compound. However, all the residual peaks are near the heavy metal Bi, showing no features.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.31Ang From K1 1.63 eA-3

Author Response: This is due to the relatively low quality of the crystal used for X-ray structure determination. Despite many attempts, we have not been able to obtain better-quality crystals for this compound. However, all the residual peaks are near the heavy metal Bi, showing no features.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.21Ang From K1 -1.74 eA-3

Alert level G

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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:Bi2.8 Cd1.12 K1.36 S6
           Atom count from the _atom_site data:  Bi2.8 Cd1.1248 K1.899 S6
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    1
           From the CIF: _chemical_formula_sum  Bi2.80 Cd1.12 K1.36 S6
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Bi         2.80      2.80    0.00
           Cd         1.12      1.12   -0.00
           K          1.36      1.90   -0.54
           S          6.00      6.00    0.00
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          3 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Bi1        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cd1        Constrained at     0.2812 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K2         Constrained at     0.0469 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K1         Constrained at       0.09 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K3         Constrained at     0.0898 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        69% 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
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        18 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          8 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      8.089 Note
              Predicted wR2: Based on SigI**2  1.14 or SHELX Weight  7.82
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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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   4 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

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duplicate check

No duplication found

Datablock x - ellipsoid plot

