checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: = 0.0000 A Wavelength=0.02510

Cell: a=10.65(2) b=10.65(2) c=10.65(2)
alpha=90 beta=90 gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	1208(7)	1208(4)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4;2;3
Moiety formula	Ag6 As0.46 Cd3 Cu15 S26 Sb7.54	?
Sum formula	Ag6 As0.46 Cd3 Cu15 S26 Sb7.54	Ag3 As0.231 Cd1.5 Cu7.5 S13 Sb3.769
Mr	3723.58	1861.80
Dx,g cm-3	5.120	5.119
Z	1	2
Mu (mm-1)	0.000	0.000
F000	0.0	1677.0
F000'	1676.39	
h,k,lmax		14,15,15
Nref		4573
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= Theta(max)= 1.010

R(reflections)= 0.0890(2317) wR2(reflections)= wR= 0.0943(4573)

S = 2.050 Npar= 119

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

PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ... Please Do !

Author Response: The internal R-factor is not applicable for dynamical refinement from electron diffraction data because reflections from different frames are not merged

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Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.050

Author Response: Electron diffraction data do not often reach low GOF values

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Author Response: .checked

PLAT076_ALERT_1_C Occupancy 0.250 Less Than 1.0 for Sp.pos . CD1

Author Response: substitutional disorder, Cu1/Cd1, Cu2/Ag2 and Sb1/As1

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

Author Response: substitutional disorder, Cu1/Cd1, Cu2/Ag2 and Sb1/As1

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit I -4;2;3 Check

Author Response: Checked

PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.020 Ang.

Author Response: electron diffraction data do not give accurate lattice parameters

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S2 Check

Author Response: Ueq of S2 lower because Cu2/Ag2 neighbors tend to have positional disorder with U22 and U33 = 0.095, and thus, a high Ueq

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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          3 Units
PLAT300_ALERT_4_G Atom Site Occupancy of Sb1        Constrained at     0.9421 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ag2        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cd1        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As1        Constrained at     0.0578 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cu1        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cu2        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         79% Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of         3.0 Sig(I)
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   8 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
   2 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 09/05/2022; check.def file version of 21/03/2022

Datablock I - ellipsoid plot