



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wd2022015_pl

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: wd2022015_pl

Bond precision:	Cu- S = 0.0050 Å		Wavelength=0.71073
Cell:	a=7.6087(9)	b=7.6087(9)	c=11.970(2)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	600.13(17)	600.13(17)	
Space group	P -3 m 1	P -3 m 1	
Hall group	-P 3 2"	-P 3 2"	
Moiety formula	Ag14.99 Cu S9.64 Sb2 Te1.36	Ag15.004 Cu1 S9.64 Sb2 Te1.36	
Sum formula	Ag14.99 Cu S9.64 Sb2 Te1.36	Ag15 Cu S9.64 Sb2 Te1.36	
Mr	2406.42	2407.68	
Dx, g cm-3	6.659	6.662	
Z	1	1	
Mu (mm-1)	17.434	17.444	
F000	1060.4	1061.0	
F000'	1046.83		
h,k,lmax	10,10,16	10,9,16	
Nref	676	626	
Tmin,Tmax	0.738,0.840	0.547,1.000	
Tmin'	0.698		

Correction method= # Reported T Limits: Tmin=0.547 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.926

Theta(max)= 29.275

R(reflections)= 0.0667(548)

wR2(reflections)=
0.1085(626)

S = 1.286

Npar= 65

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

PLAT242_ALERT_2_B	Low	MainResAtom	Ueq as Compared to Neighbours	S3	Check
PLAT971_ALERT_2_B	Check	Calcd Resid. Dens.	0.96Ang From Sb	2.76	eA-3

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ	Please	Check
	Calc:	Ag14.99 Cu S9.64 Sb2 Te1.36			
	Rep.:	Ag15 Cu S9.64 Sb2 Te1.36			
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings	Differ	Please	Check
	Calc:	Ag14.99 Cu S9.64 Sb2 Te1.36			
	Rep.:	Ag15.004 Cu1 S9.64 Sb2 Te1.36			
PLAT077_ALERT_4_C	Unit-Cell Contains Non-integer Number of Atoms	.		Please	Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio			9.63	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density			2.39	Report
PLAT213_ALERT_2_C	Atom Ag3	has ADP max/min Ratio		3.5	prolat
PLAT213_ALERT_2_C	Atom Ag4	has ADP max/min Ratio		3.3	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 S Ueq(max)/Ueq(min) Range		4.3	Ratio
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			14.040	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2.773	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.00Ang From S2		-1.54	eA-3

Alert level G

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:Ag15 Cu1 S9.64 Sb2 Te1.36
Atom count from the _atom_site data: Ag14.98799 Cu1 S9.64 Sb2 Te1.36

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.97	Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffraction_ambient_temperature	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder	57%	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	7	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note

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PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..      Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]=      3.09 Note
      0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      48 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.513 Note
      Predicted wR2: Based on SigI**2 4.32 or SHELX Weight 8.43
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..      ! Note

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0 ALERT level A = Most likely a serious problem - resolve or explain
2 ALERT level B = A potentially serious problem, consider carefully
12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
17 ALERT level G = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
4 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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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_ABSTY02_wd2022015_pl
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT242_wd2022015_pl
;
PROBLEM: Low    MainResAtom    Ueq as Compared to Neighbours      S3 Check
RESPONSE: ...
;
_vrf_PLAT971_wd2022015_pl
;
PROBLEM: Check Calcd Resid. Dens. 0.96Ang From Sb      2.76 eA-3
RESPONSE: ...
;
_vrf_PLAT041_wd2022015_pl
;
PROBLEM: Calc. and Reported SumFormula    Strings    Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT042_wd2022015_pl
;
PROBLEM: Calc. and Reported MoietyFormula Strings    Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT077_wd2022015_pl
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .      Please Check
RESPONSE: ...
;
_vrf_PLAT088_wd2022015_pl

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;
PROBLEM: Poor Data / Parameter Ratio ..... 9.63 Note
RESPONSE: ...
;
_vrf_PLAT094_wd2022015_pl
;
PROBLEM: Ratio of Maximum / Minimum Residual Density .... 2.39 Report
RESPONSE: ...
;
_vrf_PLAT213_wd2022015_pl
;
PROBLEM: Atom Ag3          has ADP max/min Ratio ..... 3.5 prolat
RESPONSE: ...
;
_vrf_PLAT220_wd2022015_pl
;
PROBLEM: NonSolvent   Resd 1   S   Ueq(max)/Ueq(min) Range      4.3 Ratio
RESPONSE: ...
;
_vrf_PLAT906_wd2022015_pl
;
PROBLEM: Large K Value in the Analysis of Variance ..... 14.040 Check
RESPONSE: ...
;
_vrf_PLAT972_wd2022015_pl
;
PROBLEM: Check Calcd Resid. Dens.  0.00Ang From S2          -1.54 eA-3
RESPONSE: ...
;
# end Validation Reply Form

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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 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

