

## 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: hanauerite\_Friedrichsseggen\_Mine

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Bond precision:	Hg- S = 0.0050 A	Wavelength=0.71073	
Cell:	a=9.9276 (8)	b=4.6209 (2)	c=9.9006 (4)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	454.19 (5)	454.19 (5)	
Space group	P m m a	P m m a	
Hall group	-P 2a 2a	?	
Moiety formula	Ag4 Br0.06 Hg4 I3.02 S4, 0.92 (Br)	?	
Sum formula	Ag4 Br0.98 Hg4 I3.02 S4	Ag Br0.25 Hg I0.75 S	
Mr	1823.62	455.67	
Dx, g cm-3	6.667	6.664	
Z	1	4	
Mu (mm-1)	45.600	45.610	
F000	766.4	766.0	
F000'	753.45		
h,k,lmax	13,6,13	13,6,13	
Nref	669	667	
Tmin,Tmax	0.354,0.473	0.274,0.521	
Tmin'	0.121		

Correction method= # Reported T Limits: Tmin=0.274 Tmax=0.521  
AbsCorr = GAUSSIAN

Data completeness= 0.997      Theta(max)= 28.280

R(reflections)= 0.0544 ( 635)	wR2(reflections)= 0.0995 ( 667)
S = 1.447	Npar= 37

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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.

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### 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 gaussian

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
PLAT199_ALERT_1_C	Reported _cell_measurement_temperature .....	(K) 293	Check
PLAT200_ALERT_1_C	Reported _diffrn_ambient_temperature .....	(K) 293	Check

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### Alert level G

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 ...	0.250	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	7.79	Why ?
PLAT300_ALERT_4_G	Atom Site Occupancy of Ag	Constrained at 0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ag'	Constrained at 0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 ) 66%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		! Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL-	2019/2	Note

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

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
5 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

