

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	= 0.0000 A	Wavelength=0.71073		
Cell:	a=10.3545 (6)	b=10.3545 (6)	c=10.3545 (6)	
	alpha=90	beta=90	gamma=90	
Temperature:	293 K			
	Calculated	Reported		
Volume	1110.17 (19)	1110.16 (19)		
Space group	I -4 3 m	I -4 3 m		
Hall group	I -4 2 3	I -4 2 3		
Moiety formula	As _{4.48} Bi _{3.52} Cu ₂₀ S ₂₆ Zn ₄	?		
Sum formula	As _{4.48} Bi _{3.52} Cu ₂₀ S ₂₆ Zn ₄	As _{2.24} Bi _{1.76} Cu ₁₀ S ₁₃ Zn ₂		
Mr	3437.37	1718.69		
Dx, g cm ⁻³	5.141	5.141		
Z	1	2		
Mu (mm ⁻¹)	29.894	29.894		
F000	1556.0	1556.0		
F000'	1553.99			
h, k, lmax		13, 13, 13		
Nref		278		
Tmin, Tmax	0.248, 0.302	0.258, 0.302		
Tmin'	0.216			

Correction method= # Reported T Limits: Tmin=0.258 Tmax=0.302
AbsCorr = MULTI-SCAN

Data completeness= Theta (max)= 28.234

R(reflections)= 0.0493 (278)	wR2(reflections)= 0.1291 (278)
S = 1.166	Npar= 23

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 C

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.370
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.070
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 7.00 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
 0 3 3, 0 8 8,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.56Ang From M2A 2.17 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From X3AS 1.69 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.21Ang From S2 1.58 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A as CU
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B as CU
PLAT019_ALERT_1_G `_diffrn_measured_fraction_theta_full/*_max` < 1.0 0.996 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 67.17 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 3 Report
PLAT199_ALERT_1_G Reported `_cell_measurement_temperature` (K) 293 Check
PLAT200_ALERT_1_G Reported `_diffrn_ambient_temperature` (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M1CU Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M1ZN Constrained at 0.3333 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 79% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
 M2A M2B M1CU M1ZN X3BI X3AS
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 !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT940_ALERT_3_G Fsqd Refinement With I > n * Sigma(I) Only Please Check
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

0 **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
21 **ALERT level G** = General information/check it is not something unexpected

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

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.

