

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: I

Bond precision:	Se-Cu = 0.0013 A	Wavelength=0.71073	
Cell:	a=11.2936(13)	b=11.2936(13)	c=11.2936(13)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1440.5(5)	1440.4(5)	
Space group	F -4 3 c	F -4 3 c	
Hall group	F -4c 2 3	F -4c 2 3	
Moiety formula	Cu ₁₆ Se ₁₆ Ti ₄	Cu ₄ Se ₄ Ti	
Sum formula	Cu ₁₆ Se ₁₆ Ti ₄	Cu ₄ Se ₄ Ti	
Mr	2471.64	617.90	
Dx,g cm ⁻³	5.698	5.698	
Z	2	8	
Mu (mm ⁻¹)	32.778	32.779	
F000	2192.0	2192.0	
F000'	2203.67		
h,k,lmax	15,15,15	15,15,15	
Nref	184[107]	170	
Tmin,Tmax	0.212,0.194	0.170,0.210	
Tmin'	0.178		

Correction method= # Reported T Limits: Tmin=0.170 Tmax=0.210
AbsCorr = ANALYTICAL

Data completeness= 1.59/0.92 Theta(max)= 29.902

R(reflections)= 0.0405(88) wR2(reflections)= 0.1031(170)

S = 1.063 Npar= 10

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

PLAT019_ALERT_1_B _diffrn_measured_fraction_theta_full/*_max < 1.0 0.953 Report
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group P-43m Check
Note: (Pseudo) Lattice Translation Implemented

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 0.800
From the CIF: _refine_ls_abs_structure_Flack_su 0.200
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Se Check
PLAT742_ALERT_1_C Angle Calc 54.74(3), Rep 54.70 Missing s.u.
SE -CU2 -CU1 1.555 1.555 1.555 # 36 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure needs to be Inverted? . 0.80 Check

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 261.94 Why ?
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem. I 100 %Fit
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Se -- Cu2 .. 7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Se -- Ti .. 9.7 s.u.
PLAT304_ALERT_4_G Non-Integer Number of Atoms (23.25) in Resd. # 1 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ti (IX) 3.24 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 14 Note

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

1 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

