

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: 1w

Bond precision: C-C = 0.0128 Å

Wavelength=0.71073

Cell: a=12.5064(12) b=13.6759(12) c=17.5120(16)
 alpha=109.965(4) beta=89.613(4) gamma=114.963(4)
Temperature: 100 K

	Calculated	Reported
Volume	2518.8(4)	2518.8(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H34 Cu2 I2 N6 O2, 2(C6 H7 N)	C44 H34 Cu2 I2 N6 O2, 2(C6 H7 N)
Sum formula	C56 H48 Cu2 I2 N8 O2	C56 H48 Cu2 I2 N8 O2
Mr	1245.93	1245.90
Dx, g cm ⁻³	1.643	1.643
Z	2	2
Mu (mm ⁻¹)	2.121	2.121
F000	1240.0	1240.0
F000'	1239.72	
h,k,lmax	15,16,21	15,16,21
Nref	9236	8943
Tmin,Tmax	0.400,0.428	0.487,0.745
Tmin'	0.370	

Correction method= # Reported T Limits: Tmin=0.487 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.968

Theta(max)= 25.371

R(reflections)= 0.0477(7041)

wR2(reflections)= 0.1148(8943)

S = 1.109

Npar= 636

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

PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01281 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N7 --H7A .	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N7 --H7B .	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N8 --H8A .	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N8 --H8B .	Please Check



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.35 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.004 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Cu1 .	10.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Cu1_d .	7.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Cu2 .	5.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I2 --Cu2_c .	7.5 s.u.
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	12 Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	! Info

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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
6 **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

- 2 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
1 ALERT type 3 Indicator that the structure quality may be low
2 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.

