

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: C-C = 0.0088 Å Wavelength=0.71073

Cell: a=4.3887(7) b=19.267(3) c=8.9217(15)
 alpha=90 beta=91.730(3) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	754.1(2)	754.0(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C5 H7 Cu I N2	C10 H14 Cu2 I2 N4
Sum formula	C5 H7 Cu I N2	C10 H14 Cu2 I2 N4
Mr	285.58	571.13
Dx,g cm-3	2.515	2.515
Z	4	2
Mu (mm-1)	6.902	6.902
F000	532.0	532.0
F000'	531.53	
h,k,lmax	6,28,13	6,28,13
Nref	2612	2489
Tmin,Tmax	0.158,0.933	0.495,0.746
Tmin'	0.133	

Correction method= # Reported T Limits: Tmin=0.495 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.953 Theta(max)= 31.927

R(reflections)= 0.0418(2296) wR2(reflections)= 0.0935(2489)

S = 1.294 Npar= 82

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

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00875 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 5.017 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT971_ALERT_2_C Check Calcd Residual Density 0.80A From Cul 1.73 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 -- Cul .. 21.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 -- Cul_a .. 44.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1 -- Cul_c .. 54.4 s.u.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.25 Ratio
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 124 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 1 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 2 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

