

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DR-RAHEJA-IODINE5-A_Mo

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: DR-RAHEJA-IODINE5-A_Mo

Bond precision: C-C = 0.0087 Å Wavelength=0.71073

Cell: a=10.7289(4) b=12.3645(5) c=15.1570(7)
 alpha=113.470(4) beta=99.187(4) gamma=92.543(3)
Temperature: 153 K

	Calculated	Reported
Volume	1807.70(15)	1807.70(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	5(C8 H16 O4), Cu H12 O6, 2(I3), 2(I2)	5(C8 H16 O4), Cu H12 O6, 2(I3), 2(I2)
Sum formula	C40 H92 Cu I10 O26	C40 H92 Cu I10 O26
Mr	2321.69	2321.67
Dx, g cm ⁻³	2.133	2.133
Z	1	1
Mu (mm ⁻¹)	4.638	4.638
F000	1099.0	1099.0
F000'	1095.10	
h, k, lmax	13, 15, 19	13, 15, 19
Nref	7903	7846
Tmin, Tmax	0.579, 0.723	0.782, 1.000
Tmin'	0.494	

Correction method= # Reported T Limits: Tmin=0.782 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 27.000

R(reflections)= 0.0423(5930) wR2(reflections)= 0.0814(7846)

S = 1.046 Npar= 371

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 A

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 57 Note

Author Response: The completeness is > 99%. No individual reflections were omitted. The omit -3 54 command of the SHELX system may result in the removal of some reflections and there are always some reflections in the inner sphere that collide with the beamstop area.

Alert level B

PLAT434_ALERT_2_B Short Inter HL..HL Contact I1 ..I3 3.38 Ang.
x,y,z = 1_555 Check

Author Response: This is a halogen bond and it is in the expected range.

PLAT434_ALERT_2_B Short Inter HL..HL Contact I2 ..I3 3.38 Ang.
x,y,z = 1_555 Check

Author Response: This is a halogen bond and it is in the expected range.

Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0087 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.938 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	10	Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT300_ALERT_4_G Atom Site Occupancy of I5A Constrained at	0.8	Check
PLAT300_ALERT_4_G Atom Site Occupancy of I5B Constrained at	0.2	Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5)	33%	Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	1	Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) .	2.20	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	7	Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.3	Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	1	Info

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

- 1 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
5 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

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_PLAT342_DR-RAHEJA-IODINE5-A_Mo
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.0087 Ang.
RESPONSE: ...
;
_vrf_PLAT906_DR-RAHEJA-IODINE5-A_Mo
;
PROBLEM: Large K Value in the Analysis of Variance .....      2.938 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 05/12/2020; check.def file version of 05/12/2020

