checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rod146_150k_0m

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: rod146_150k_0m

```
Bond precision:  C-C = 0.0046 A          Wavelength=1.54178

Cell:          a=7.9898(5)       b=9.3656(5)      c=23.6072(13)
               alpha=98.626(2)   beta=96.301(2)   gamma=97.555(2)
Temperature:   150 K
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	Calculated	Reported
Volume	1716.19(17)	1716.19(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C35 H30 Br Cu2 N3 O8	C70 H60 Br2 Cu4 N6 O16
Sum formula	C35 H30 Br Cu2 N3 O8	C70 H60 Br2 Cu4 N6 O16
Mr	827.62	1655.22
Dx,g cm-3	1.602	1.602
Z	2	1
Mu (mm-1)	3.363	3.363
F000	836.0	836.0
F000’	828.88	
h,k,lmax	9,11,28	9,11,28
Nref	6534	6338
Tmin,Tmax	0.508,0.714	0.611,0.753
Tmin’	0.454	

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Correction method= # Reported T Limits: Tmin=0.611 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.970          Theta(max)= 70.224

R(reflections)= 0.0482( 6120)     wR2(reflections)= 0.1328( 6338)

S = 1.072                 Npar= 446
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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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01A From Br1 2.96 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.50 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.78 eA-3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 63 Report

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 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
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) . 2.13 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 132 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 8 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 4 Check

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

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

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock rod146_150k_0m - ellipsoid plot