

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nos006a_150k

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: nos006a_150k

Bond precision:	C-C = 0.0073 A	Wavelength=1.34143	
Cell:	a=27.7823(14)	b=15.4445(11)	c=7.9423(4)
	alpha=90	beta=102.301(4)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	3329.7(3)	3329.7(3)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C35 H31 Cu2 N3 O8	C35 H31 Cu2 N3 O8	
Sum formula	C35 H31 Cu2 N3 O8	C35 H31 Cu2 N3 O8	
Mr	748.73	748.71	
Dx,g cm-3	1.494	1.494	
Z	4	4	
Mu (mm-1)	7.209	7.203	
F000	1536.0	1536.0	
F000'	1517.08		
h,k,lmax	35,19,10	34,19,9	
Nref	3530	3485	
Tmin,Tmax	0.296,0.339	0.078,0.398	
Tmin'	0.189		

Correction method= # Reported T Limits: Tmin=0.078 Tmax=0.398
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 58.107

R(reflections)= 0.0656(2756) wR2(reflections)= 0.1526(3485)

S = 1.212 Npar= 222

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**

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00726 Ang.
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by -0.0011 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H15 -0.34 eA-3

● **Alert level G**

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	33.56	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	2.16	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	36	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info
PLAT984_ALERT_1_G	The C-f' = 0.0148 Deviates from the B&C-Value	0.0137	Check
PLAT984_ALERT_1_G	The Cu-f' = -2.9183 Deviates from the B&C-Value	-2.7974	Check
PLAT984_ALERT_1_G	The N-f' = 0.0253 Deviates from the B&C-Value	0.0241	Check
PLAT984_ALERT_1_G	The O-f' = 0.0412 Deviates from the B&C-Value	0.0389	Check
PLAT985_ALERT_1_G	The Cu-f" = 3.6937 Deviates from the B&C-Value	3.6876	Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
3 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
2 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 04/06/2020; check.def file version of 02/06/2020

