

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_BruecknerJK_153F40_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: cu_BruecknerJK_153F40_0m

Bond precision:	C-C = 0.0031 A	Wavelength=1.54178	
Cell:	a=19.678 (3)	b=37.0229 (9)	c=4.7720 (4)
	alpha=90	beta=90	gamma=90
Temperature:	102 K		
	Calculated	Reported	
Volume	3476.6 (6)	3476.6 (7)	
Space group	P 21 21 2	P 21 21 2	
Hall group	P 2 2ab	P 2 2ab	
Moiety formula	2(C38 H38 O12), C H4 O	?	
Sum formula	C77 H80 O25	C38.50 H40 O12.50	
Mr	1405.41	702.70	
Dx, g cm ⁻³	1.343	1.343	
Z	2	4	
Mu (mm ⁻¹)	0.838	0.838	
F000	1484.0	1484.0	
F000'	1489.09		
h, k, lmax	25, 47, 6	24, 47, 5	
Nref	7449 [4339]	7338	
Tmin, Tmax	0.904, 0.967	0.770, 0.929	
Tmin'	0.832		

Correction method= # Reported T Limits: Tmin=0.770 Tmax=0.929
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.99 Theta(max)= 78.476

R(reflections)= 0.0364 (7290)	wR2(reflections)= 0.0919 (7338)
S = 1.198	Npar= 479

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H13 ..H19B . 2.14 Ang.
 x,y,-1+z = 1_554 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O13 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C39 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39C Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3 .	109.2	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C17 .	2.91	Ang.
	-1/2+x, 1/2-y, -z =	4_455	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	6	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	16	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	22	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
2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
18 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
11 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.

