

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0032 A	Wavelength=0.71073	
Cell:	a=10.901(2)	b=16.032(3)	c=23.843(5)
	alpha=90	beta=90	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	4166.9(14)	4167.0(15)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C44 H30 Cu2 Mn N6 O12	C44 H30 Cu2 Mn N6 O12	
Sum formula	C44 H30 Cu2 Mn N6 O12	C44 H30 Cu2 Mn N6 O12	
Mr	1016.78	1016.78	
Dx,g cm-3	1.621	1.621	
Z	4	4	
Mu (mm-1)	1.384	1.383	
F000	2060.0	2060.0	
F000'	2064.74		
h,k,lmax	13,19,29	13,19,29	
Nref	4101	4096	
Tmin,Tmax	0.713,0.813	0.936,1.000	
Tmin'	0.562		

Correction method= # Reported T Limits: Tmin=0.936 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.021

R(reflections)= 0.0269(3729) wR2(reflections)= 0.0702(4096)

S = 1.049 Npar= 299

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1 -- O1 .. 14.1 s.u.
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1 -- O2 .. 14.9 s.u.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT352_ALERT_3_C Short N-H (X0.87,N1.01A) N3 - H3A .. 0.74 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- O5 .. 6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- N2 .. 5.5 s.u.

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **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
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

