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: Compound6

Bond precision: C-C = 0.0083 A Wavelength=0.71069

Cell: a=7.4297(14) b=8.9152(17) c=10.918(2)
alpha=70.268(6) beta=76.204(6) gamma=81.371(5)
Temperature: 100 K

	Calculated	Reported
Volume	659.2(2)	659.2(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H20 Cu N10 O10, 2(H2 O)	?
Sum formula	C22 H24 Cu N10 O12	C22 H24 Cu N10 O12
Mr	684.06	684.05
Dx,g cm-3	1.723	1.723
Z	1	1
Mu (mm-1)	0.915	0.915
F000	351.0	351.0
F000’	351.49	
h,k,lmax	7,9,11	7,9,11
Nref	1630	1417
Tmin,Tmax	0.858,0.896	0.589,0.745
Tmin’	0.848	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.745
AbsCorr = EMPIRICAL

Data completeness= 0.869 Theta(max)= 22.051

R(reflections)= 0.0466(1171) wR2(reflections)= 0.1137(1417)

S = 1.060 Npar= 205

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5283

Alert level B

REFNR01_ALERT_3_B Ratio of reflections to parameters is < 8 for a
centrosymmetric structure
sine(theta)/lambda 0.5283
Proportion of unique data used 1.0000
Ratio reflections to parameters 6.9122
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.95 Note

---

Alert level C

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.14 Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00833 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O1W - H1W1 .. 1.03 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X H4A .. H52A .. 1.91 Ang.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 5 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 5 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ..... 2.22 Note

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 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 26/02/2017; check.def file version of 21/02/2017

Datablock Compound6 - ellipsoid plot