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: 1

Bond precision: C-C = 0.0217 A Wavelength=0.71073

Cell: a=20.7845(5) b=20.7845(5) c=23.8369(12)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	10297.4(7)	10297.4(7)
Space group	I 41/a	I4(1)/a
Hall group	-I 4ad	-I4ad
Moiety formula	C6 H16 Cu2 N4 O44 P W12, 2(C2 H8 N2), 2(O)	C6 H17 Cu2 N4 O44 P W12, 2(C2 H8 N2), 2(H2O)
Sum formula	C10 H32 Cu2 N8 O46 P W12	C10 H37 Cu2 N8 O46 P W12
Mr	3364.59	3369.57
Dx,g cm-3	4.341	4.341
Z	8	8
Mu (mm-1)	27.639	27.639
F000	11816.0	11816.0
F000’	11759.37	
h,k,lmax	27,27,31	27,27,31
Nref	6412	6412
Tmin,Tmax	0.001,0.003	0.001,0.003
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.001 Tmax=0.003
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 28.290

R(reflections)= 0.0422(5030) wR2(reflections)= 0.1181(6404)

S = 1.096 Npar= 354

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

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 13.61 eA-3
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 1 Report
PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 7.0 Ratio
PLAT220_ALERT_2_B Non-Solvent Resd 1 P Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1W Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02167 Ang.
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 4.99 Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.41 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 44 Ang3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C10 H37 Cu2 N8 O46 P1 W12
Atom count from the _atom_site data: C10 H32 Cu2 N8 O46 P1 W12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C10 H37 Cu2 N8 O46 P W12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	80.00	80.00	0.00
H	296.00	256.00	40.00
Cu	16.00	16.00	0.00
N	64.00	64.00	0.00
O	368.00	368.00	0.00
P	8.00	8.00	0.00
W	96.00	96.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 13 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 8 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 847.72 Why ?
PLAT093_ALERT_1_G No s.u.’s on H-positions, Refinement Reported as mixed Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W1 -- O19 .. 5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W1 -- O20 .. 8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W2 -- O3 .. 5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W3 -- O16 .. 6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W4 -- O20 .. 7.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W4 -- O16_c .. 6.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W4 -- O19_e .. 7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W6 -- O12 .. 8.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W6 -- O3_d .. 5.6 s.u.

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PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.15 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1     (II)    .....       2.09 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         91 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 27/03/2017; check.def file version of 24/03/2017

Datablock 1 - ellipsoid plot