checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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 = 0.0034 A Wavelength=1.54180

Cell: a=10.400(1) b=10.355(2) c=33.277(2)
alpha=90 beta=99.033(8) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	3539.2(8)	3539.2(8)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C56 H68 Cu4 O23 P8, 7(H2 O)	?
Sum formula	C56 H82 Cu4 O30 P8	C56 H84 Cu4 O30 P8
Mr	1737.18	1739.15
Dx,g cm-3	1.630	1.632
Z	2	2
Mu (mm-1)	3.793	3.793
F000	1788.0	1792.0
F000’	1781.79	
h,k,lmax	12,12,41	12,12,41
Nref	7017	6660
Tmin,Tmax	0.572,0.634	0.474,1.000
Tmin’	0.519	

Correction method= # Reported T Limits: Tmin=0.474 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.949 Theta(max)= 72.397

R(reflections)= 0.0287(5864) wR2(reflections)= 0.0847(6660)

S = 1.067 Npar= 484

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H2WA ..H21B . 2.09 Ang.
x,y,z = 1_555 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

---

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 1.97 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu3 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report

---

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:C56 H84 Cu4 O30 P8
Atom count from the _atom_site data: C56 H82 Cu4 O30 P8
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 2
From the CIF: _chemical_formula_sum C56 H84 Cu4 O30 P8
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	112.00	112.00	0.00
H	168.00	164.00	4.00
Cu	8.00	8.00	0.00
O	60.00	60.00	0.00
P	16.00	16.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 17 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P2/c P2/n Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 7 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) . 2.13 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu3 (II) . 2.13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 11 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 333 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

---

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
4 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 17/03/2019; check.def file version of 04/03/2019

Datablock shelx - ellipsoid plot