

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_Wenzel_SW_487_3_0m_sq

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: mo_Wenzel_SW_487_3_0m_sq

Bond precision: C-C = 0.0229 A Wavelength=0.71073

Cell: a=23.1084 (10) b=23.1084 (10) c=23.1084 (10)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	12339.8 (16)	12339.8 (17)
Space group	I 2 3	I 2 3
Hall group	I 2 2 3	I 2 2 3
Moiety formula	C54 H6 Cu3 F6 O41 Zn8 [+ solvent]	?
Sum formula	C54 H6 Cu3 F6 O41 Zn8 [+ solvent]	C54 H18 Cu3 F6 O41 Zn8
Mr	2138.36	2150.41
Dx, g cm ⁻³	1.151	1.151
Z	4	4
Mu (mm ⁻¹)	2.097	2.097
F000	4156.0	4156.0
F000'	4171.33	
h, k, lmax	30, 30, 30	30, 30, 30
Nref	4918 [2641]	4916
Tmin, Tmax	0.900, 0.900	0.669, 0.746
Tmin'	0.900	

Correction method= # Reported T Limits: Tmin=0.669 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.86/1.00 Theta (max)= 27.837

R(reflections)= 0.1191(3890)

wR2(reflections)=
0.3201(4916)

S = 1.273

Npar= 181

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

PLAT213_ALERT_2_A Atom O3	has ADP max/min Ratio	5.4	prolat
PLAT213_ALERT_2_A Atom O5	has ADP max/min Ratio	6.4	prolat
PLAT213_ALERT_2_A Atom C3	has ADP max/min Ratio	5.2	prolat
PLAT213_ALERT_2_A Atom C6	has ADP max/min Ratio	8.2	prolat
PLAT241_ALERT_2_A High 'MainMol' Ueq as Compared to Neighbors of			O5 Check

Alert level B

PLAT213_ALERT_2_B Atom F1B	has ADP max/min Ratio	4.9	prolat
PLAT213_ALERT_2_B Atom C9	has ADP max/min Ratio	4.1	prolat
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of			Zn1 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of			C2 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds		0.02289	Ang.
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.81Ang From O8		2.87	eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 2.04Ang From O8		2.84	eA-3

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75			
_refine_diff_density_min given =	-2.477		
Test value =	-2.250		
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75			
The relevant atom site should be identified.			
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75			
The relevant atom site should be identified.			
RINTA01_ALERT_3_C The value of Rint is greater than 0.12			
Rint given	0.159		
STRVA01_ALERT_4_C Flack test results are ambiguous.			
From the CIF: _refine_ls_abs_structure_Flack	0.490		
From the CIF: _refine_ls_abs_structure_Flack_su	0.060		
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12		0.159	Report
PLAT082_ALERT_2_C High R1 Value		0.12	Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)		0.32	Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density		2.80	eA-3
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density		-2.48	eA-3
PLAT213_ALERT_2_C Atom O2	has ADP max/min Ratio	3.2	oblate
PLAT213_ALERT_2_C Atom O7	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C Atom C4	has ADP max/min Ratio	3.2	prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range		4.6	Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of			O2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of			O6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of			Cu1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of			O8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of			C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of			C3 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check
 PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.8 Note
 PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C2 - C6 . 1.54 Ang.
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 14 Check
 PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.28Ang From Zn1 -2.32 eA-3
 PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.30Ang From Zn1 -2.29 eA-3
 PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Cu1 1.20 eA-3

● 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: C54 H18 Cu3 F6 O41 Zn8
 Atom count from the _atom_site data: C54 H6 Cu3 F6 O41 Zn8
 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 4
 From the CIF: _chemical_formula_sum C54 H18 Cu3 F6 O41 Zn8
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	216.00	216.00	0.00
H	72.00	24.00	48.00
Cu	12.00	12.00	0.00
F	24.00	24.00	0.00
O	164.00	164.00	0.00
Zn	32.00	32.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
 PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.490 Note
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 Calc: C54 H6 Cu3 F6 O41 Zn8
 Rep.: C54 H18 Cu3 F6 O41 Zn8
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 5% Note
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.27 Ratio
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 2.59 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 2.13 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.20 Info
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
 0 1 1, 0 0 2,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 9.553 Note
 Predicted wR2: Based on SigI**2 3.35 or SHELX Weight 25.31
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

5 **ALERT level A** = Most likely a serious problem - resolve or explain
 7 **ALERT level B** = A potentially serious problem, consider carefully
 28 **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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

34 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
5 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 22/08/2024; check.def file version of 21/08/2024

