

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 539_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: 539_sq

Bond precision: C-C = 0.0356 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 H12 Co3 F6 O41 Zn8 [+ solvent]	?
Sum formula	C54 H12 Co3 F6 O41 Zn8 [+ solvent]	C54 H18 Cu3 F6 O41 Zn8
Mr	2130.55	2136.55
Dx, g cm ⁻³	1.147	1.093
Z	4	4
Mu (mm ⁻¹)	1.983	1.974
F000	4156.0	3967.0
F000'	4171.67	
h, k, lmax	30, 30, 30	30, 30, 30
Nref	5186 [2779]	5116
Tmin, Tmax		0.625, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.625 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.99 Theta (max)= 28.358

R(reflections)= 0.1565(4694)

wR2(reflections)=
0.4008(5116)

S = 1.852

Npar= 171

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

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.715
Additional refinement cycles may be required.
PLAT080_ALERT_2_A Maximum Shift/Error 0.71 Why ?

Alert level B

ABSMU01_ALERT_1_B The ratio of given/expected absorption coefficient lies
outside the range 0.95 <> 1.05
Calculated value of mu = 2.097
Value of mu given = 1.974
DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -4.000
Test value = -3.000
PLAT046_ALERT_1_B Reported Z, MW and D(calc) are Inconsistent 1.150 Check
PLAT082_ALERT_2_B High R1 Value 0.16 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.40 Report
PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -4.00 eA-3
PLAT213_ALERT_2_B Atom O3 has ADP max/min Ratio 5.0 prolat
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.03556 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C2 - C6 . 1.64 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C3 - C8 . 1.60 Ang.
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for
compound is greater 1 mass unit. Check that all hydrogen
atoms have been taken into account.
DENSD01_ALERT_1_C The ratio of the submitted crystal density and that
calculated from the formula is outside the range 0.99 <> 1.01
Crystal density given = 1.093
Calculated crystal density = 1.150
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.354
From the CIF: _refine_ls_abs_structure_Flack_su 0.007
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Co1 Check
PLAT368_ALERT_2_C Short C(sp2)-C(sp2) Bond C6 - C7 . 1.22 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
 0 1 27, 0 3 27, 1 4 27, 0 5 27,
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 18 Check

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 H12 Co3 F6 O41 Zn8
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests
 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
 WARNING: Unexpected atom type is in site list: Co
 WARNING: Formula and atom_type_symbol element names mismatch.

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

WARNING: Site labels do not match formula elements

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 . 0.354 Note
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 Calc: C54 H12 Co3 F6 O41 Zn8
 Rep.: C54 H18 Cu3 F6 O41 Zn8

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
 PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C4 -C9 0.23 Ang.
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.38 Ratio
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 2.08 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 2.30 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 2.43 Info
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 PLAT870_ALERT_4_G ALERTS Related to Twinning Effects 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,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 14 Note
 PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.15 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1-1 0) Est.d BASF 0.21 Check
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 11.143 Note
 Predicted wR2: Based on SigI**2 3.60 or SHELX Weight 21.92
 PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
10 ALERT type 4 Improvement, methodology, query or suggestion
7 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.

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