

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_Wenzel_SW735_0ma_a_a_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_SW735_0ma_a_a_sq

Bond precision: C-C = 0.0067 Å Wavelength=0.71073

Cell: a=12.0022(11) b=13.1723(12) c=27.801(2)
 alpha=90 beta=92.847(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4389.8(6)	4389.8(7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H2 Co F2 O15 Zn2 [+ solvent]	?
Sum formula	C18 H2 Co F2 O15 Zn2 [+ solvent]	C30 H31 Co F2 O15 Zn2
Mr	685.91	85923.00
Dx, g cm ⁻³	1.038	1.038
Z	4	4
Mu (mm ⁻¹)	1.506	1.506
F000	1340.0	1340.0
F000'	1344.51	
h, k, lmax	16, 17, 37	16, 17, 37
Nref	11221	11160
Tmin, Tmax	0.633, 0.798	0.623, 0.746
Tmin'	0.621	

Correction method= # Reported T Limits: Tmin=0.623 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 28.599

R(reflections)= 0.0718(8447)

wR2(reflections)=
0.3036(11160)

S = 1.304

Npar= 363

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

TYPE017_ALERT_1_A _chemical_formula_weight is not data type numb.

DENSD01_ALERT_1_A The ratio of the submitted crystal density and that
calculated from the formula is outside the range 0.90 <> 1.10

Crystal density given = 1.038

Calculated crystal density = 1.300

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 0.405

Additional refinement cycles may be required.

PLAT046_ALERT_1_A Reported Z, MW and D(calc) are Inconsistent 130.010 Check

PLAT080_ALERT_2_A Maximum Shift/Error 0.41 Why ?

Alert level B

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 6 Check

0 3 1, -2 0 2, 3 0 3, 2 2 3, -1 3 3, -7 2 7,

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Col 1.61 eA-3

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.30 Report

PLAT234_ALERT_4_C Large Hirshfeld Difference F2A --C18 . 0.16 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 04 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 08 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zn1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zn2 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Co1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00667 Ang.

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.155 Report

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 4 Check

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.11Ang From O13 2.08 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.15Ang From O15 1.74 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From O6 . 0.72 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From O14 . 0.54 eA-3

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.67Ang From O6 . -0.51 eA-3

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From O14 . -0.46 eA-3

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From O14 . -0.41 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: C30 H31 Co1 F2 O15 Zn2
 Atom count from the _atom_site data: C18 H2 Co1 F2 O15 Zn2
 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 C30 H31 Co F2 O15 Zn2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	120.00	72.00	48.00
H	124.00	8.00	116.00
Co	4.00	4.00	0.00
F	8.00	8.00	0.00
O	60.00	60.00	0.00
Zn	8.00	8.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 Calc: C18 H2 Co F2 O15 Zn2
 Rep.: C30 H31 Co F2 O15 Zn2

PLAT230_ALERT_2_G Hirshfeld Test Diff for F1B --C5 . 5.9 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Zn2 --O6_f . 5.5 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --O13 . 5.3 s.u.
 PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 5% Note
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 2.19 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 2.06 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 2.12 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). 3 Note
 -1 0 1, 0 1 1, 0 0 2,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 57 Note
 PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 13.116 Note
 Predicted wR2: Based on SigI**2 2.31 or SHELX Weight 23.49
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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- 5 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 20 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 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
 5 ALERT type 4 Improvement, methodology, query or suggestion
 5 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.

Datablock mo_Wenzel_SW735_0ma_a_a_sq - ellipsoid plot

