

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_Wenzel_SW663_0m_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_SW663_0m_a_sq

Bond precision:	C-C = 0.0067 A	Wavelength=0.71073		
Cell:	a=19.9908 (5)	b=19.9908 (5)	c=19.9908 (5)	
	alpha=90	beta=90	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	7989.0 (6)	7989.0 (6)
Space group	I -4 3 d	I -4 3 d
Hall group	I -4bd 2c 3	I -4bd 2c 3
Moiety formula	C36 F4 Ga3 O24 [+ solvent]	?
Sum formula	C36 F4 Ga3 O24 [+ solvent]	C36 H8 F4 Ga3 O24
Mr	1101.51	1109.60
Dx, g cm ⁻³	0.916	0.916
Z	4	4
Mu (mm ⁻¹)	1.061	1.061
F000	2148.0	2148.0
F000'	2152.15	
h, k, l _{max}	26, 26, 26	26, 26, 26
Nref	1664 [901]	1662
Tmin, Tmax	0.767, 0.767	0.682, 0.746
Tmin'	0.751	

```
Correction method= # Reported T Limits: Tmin=0.682 Tmax=0.746
AbsCorr = MULTI-SCAN
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Data completeness= 1.84/1.00 Theta (max)= 28.273

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R(reflections)= 0.0260( 1396)      wR2(reflections)=
S = 1.092                        0.0909( 1662)
Npar= 57
```

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

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement [Please Check](#)

Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of [C3 Check](#)
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) [2.7 Note](#)
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ga1 [0.133 Check](#)
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds [0.00667 Ang.](#)
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. [1 Check](#)
0 2 6,

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: C36 H8 F4 Ga3 O24
Atom count from the _atom_site data: C36 F4.0046 Ga3 O24
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 C36 H8 F4 Ga3 O24
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	144.00	144.00	0.00
H	32.00	0.00	32.00
F	16.00	16.00	0.00
Ga	12.00	12.00	0.00
O	96.00	96.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension [3 Info](#)
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. [Please Check](#)
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ [Please Check](#)
Calc: C36 F4 Ga3 O24
Rep.: C36 H8 F4 Ga3 O24
PLAT300_ALERT_4_G Atom Site Occupancy of F1 Constrained at [0.3333 Check](#)
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) [6% Note](#)
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure [! Info](#)
PLAT794_ALERT_5_G Tentative Bond Valency for Ga1 (III) . [2.94 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 !](#)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value [8.518 Note](#)
Predicted wR2: Based on SigI**2 1.07 or SHELX Weight [8.41](#)
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. [0 Info](#)

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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

