

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 = 0.0148 A	Wavelength=0.71075
Cell:	a=20.5365(14)	b=13.5405(9) c=13.5727(9)
	alpha=90	beta=92.588(4) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	3770.4(4)	3770.4(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	F13 Fe3, 1.5(C4 H12 N2), C2 H6 N, O	?
Sum formula	C8 H24 F13 Fe3 N4 O	C8 H26 F13 Fe3 N4 O
Mr	606.86	608.88
Dx,g cm-3	2.138	2.145
Z	8	8
Mu (mm-1)	2.410	2.410
F000	2424.0	2440.0
F000'	2434.14	
h,k,lmax	24,16,16	24,16,16
Nref	3321	3321
Tmin,Tmax	0.845,0.930	0.734,1.000
Tmin'	0.845	

Correction method= # Reported T Limits: Tmin=0.734 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 24.998

R(reflections)= 0.0608(1790) wR2(reflections)= 0.1790(3321)

S = 1.014 Npar= 264

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

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) O1S Check
 PLAT430_ALERT_2_B Short Inter D...A Contact O1S ..O1S . 2.83 Ang.
 $1-x,y,1/2-z = 2_655$ Check

Author respond: O1S is a non-coordinated solvent water molecule with enlarged thermal motion, which position and the corresponding hydrogen atoms' positions can not be located accurately based on the data.

● Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
 Rint given 0.153
 PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.02 Check
 PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
 PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of F12 Check
 PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of F13 Check
 PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of N2 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1S 0.187 Check
 PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01475 Ang.
 PLAT420_ALERT_2_C D-H Without Acceptor N2 --H2A . Please Check
 PLAT431_ALERT_2_C Short Inter HL..A Contact F14 ..O1S . 2.77 Ang.
 $x,1+y,z = 1_565$ Check
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -3.441 Report
 PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.67A From O1S 0.44 eA-3
 PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.75A From O1S -0.46 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: C8 H26 F13 Fe3 N4 O1
 Atom count from the _atom_site data: C8 H24 F13 Fe3 N4 O1
 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 8
 From the CIF: _chemical_formula_sum C8 H26 F13 Fe3 N4 O
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	64.00	64.00	0.00
H	208.00	192.00	16.00
F	104.00	104.00	0.00
Fe	24.00	24.00	0.00
N	32.00	32.00	0.00
O	8.00	8.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Report
 PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.153 Report
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.31 Why ?
 PLAT432_ALERT_2_G Short Inter X...Y Contact F3 ..C1 2.71 Ang.
 $x,y,z = 1_555$ Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact F4 ..C1 2.79 Ang.
 $3/2-x,1/2+y,1/2-z = 4_655$ Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact F6 ..C1 2.86 Ang.
 $3/2-x,1/2-y,1-z = 7_656$ Check
 PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) . 3.08 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Fe2 (III) . 3.03 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Fe3 (III) . 3.07 Info

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check
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
 2 **ALERT level B** = A potentially serious problem, consider carefully
 14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 16 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 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
 1 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 18/09/2020; check.def file version of 20/08/2020

