

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0087 Å Wavelength=0.71073

Cell: a=18.1059(8) b=18.6900(8) c=19.5380(8)
 alpha=79.916(1) beta=66.223(2) gamma=83.277(2)

Temperature: 295 K

	Calculated	Reported
Volume	5949.1(4)	5949.1(4)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C99 H75 Cl12 Fe3 N9 O13, 0.167(C10 H10 N2), 0.667(C5 H5 N), Cl	C104.00 H80.00 Cl13 Fe3 N10.00 O13
Sum formula	C104 H80 Cl13 Fe3 N10 O13	C104.00 H80.00 Cl13 Fe3 N10.00 O13
Mr	2306.18	2306.27
Dx, g cm ⁻³	1.287	1.287
Z	2	2
Mu (mm ⁻¹)	0.711	0.711
F000	2354.0	2354.0
F000'	2360.69	
h, k, lmax	21, 22, 23	21, 22, 23
Nref	22111	21983
Tmin, Tmax	0.865, 0.892	0.890, 0.890
Tmin'	0.837	

Correction method= # Reported T Limits: Tmin=0.890 Tmax=0.890
AbsCorr = NUMERICAL

Data completeness= 0.994

Theta(max)= 25.476

R(reflections)= 0.0483(13266)

wR2(reflections)=
0.1309(13266)

S = 1.000

Npar= 1321

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 C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0087 Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N4 --H41 .	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L= 0.600	84 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N12 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C110 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C111 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C112 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C113 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C114 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1101 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1111 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1121 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1131 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1141 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N10 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C100 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C101 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C102 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C103 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C104 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1001 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1011 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1021 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1031 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1041 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N11 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C105 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C106 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C107 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C108 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C109 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1051 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1061 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1071 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1081 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1091 Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C113 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C114 Constrained at	0.25	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of Cl15	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl16	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl17	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl18	Constrained at	0.125	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 8)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 9)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 10)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)		7.33	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)		3.67	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)		3.67	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)		0.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)		0.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 7)		0.12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 8)		0.12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 9)		0.12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 10)		0.12	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl10 ..Cl10 .		3.38	Ang.
	2-x,-y,1-z =		2_756	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		19	Note
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data			Please Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .		3.02	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2 (III) .		3.05	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe3 (III) .		3.00	Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found			Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		48	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI			Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		113	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked			! Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		1	Check

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 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
 60 ALERT type 4 Improvement, methodology, query or suggestion
 6 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.

