

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision:	C-C = 0.0146 Å	Wavelength=0.71073
Cell:	a=7.4137 (6)	b=21.8314 (13) c=13.5172 (11)
	alpha=90	beta=105.047 (3) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	2112.8 (3)	2112.8 (3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H22 Fe3 N14 O6 Pt3, 8 (H2 O)	C24 H22 Fe3 N14 O6 Pt3, 8 (H2 O)
Sum formula	C24 H38 Fe3 N14 O14 Pt3	C24 H38 Fe3 N14 O14 Pt3
Mr	1499.47	1499.50
Dx, g cm ⁻³	2.357	2.357
Z	2	2
Mu (mm ⁻¹)	10.971	10.971
F000	1408.0	1408.0
F000'	1401.06	
h, k, lmax	8, 26, 16	8, 26, 16
Nref	3860	3842
Tmin, Tmax	0.363, 0.645	0.521, 0.745
Tmin'	0.185	

Correction method= # Reported T Limits: Tmin=0.521 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.341

R(reflections)= 0.0388 (2581)	wR2(reflections)= 0.0627 (3842)
S = 1.022	Npar= 300

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

PLAT213_ALERT_2_C	Atom N4	has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	3.2	prolat
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.0146	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		5.513	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	12	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on	H3A	-0.41	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H3B	-0.37	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H5A	-0.32	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H10	-0.34	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H12A	-0.62	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H5C	-0.53	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		3	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		8	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		14	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		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
PLAT417_ALERT_2_G	Short Inter D-H..H-D	H2B ..H6A .	2.12	Ang.
		-1+x,1/2-y,-1/2+z =	4_465	Check
PLAT417_ALERT_2_G	Short Inter D-H..H-D	H3A ..H6D .	2.13	Ang.
		-1+x,y,z =	1_455	Check
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set			Please Do !
PLAT794_ALERT_5_G	Tentative Bond Valency for Pt1 (II) .		2.20	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON		2	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		92	Note
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).		4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.2	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
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

2 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
6 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
4 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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