

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 2-120K

Bond precision:	C-C = 0.0029 A	Wavelength=0.71073
Cell:	a=17.7659(8)	b=9.5962(4) c=14.4516(7)
	alpha=90	beta=110.495(1) gamma=90
Temperature:	120 K	
	Calculated	Reported
Volume	2307.83(18)	2307.83(18)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H28 Fe N4 O4, 2(H N0.50 O2)	C22 H28 Fe N4 O4, N O3, H2 O
Sum formula	C22 H30 Fe N5 O8	C22 H30 Fe N5 O8
Mr	548.36	548.36
Dx,g cm-3	1.578	1.578
Z	4	4
Mu (mm-1)	0.714	0.714
F000	1148.0	1148.0
F000'	1149.90	
h,k,lmax	24,13,19	24,13,19
Nref	6139	6138
Tmin,Tmax	0.813,0.911	0.820,0.913
Tmin'	0.813	

Correction method= # Reported T Limits: Tmin=0.820 Tmax=0.913
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.000

R(reflections)= 0.0390(5239) wR2(reflections)= 0.0930(6138)

S = 1.058 Npar= 364

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

PLAT420_ALERT_2_B D-H Without Acceptor O2X --H3O . Please Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O2A' Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O1A' Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of N1A' Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H3O Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H4O Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O1A Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O2A Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of N1A Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H1O Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H2O Constrained at 0.5 Check
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 60% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 60% Note
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 3.50 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 3.50 Check
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 5 Do !
 N2 -FE1 -O1 -C6 82.70 0.60 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 9 Do !
 N3 -FE1 -O3 -C16 93.80 0.60 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 13 Do !
 N4 -FE1 -N1 -C7 -163.00 6.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 18 Do !
 N4 -FE1 -N1 -C8 22.00 6.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 22 Do !
 O1 -FE1 -N2 -C9 -99.30 0.60 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 27 Do !
 O1 -FE1 -N2 -C10 27.40 0.60 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 31 Do !
 O3 -FE1 -N3 -C11 41.90 0.70 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 36 Do !
 O3 -FE1 -N3 -C12 -86.40 0.60 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 43 Do !
 N1 -FE1 -N4 -C14 -129.00 6.00 1.555 1.555 1.555 1.555
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 48 Do !
 N1 -FE1 -N4 -C13 55.00 6.00 1.555 1.555 1.555 1.555
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
 PLAT793_ALERT_4_G Model has Chirality at N2 (Centro SPGR) R Verify
 PLAT793_ALERT_4_G Model has Chirality at N3 (Centro SPGR) S Verify
 PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

0 ALERT level A = Most likely a serious problem - resolve or explain

1 ALERT level B = A potentially serious problem, consider carefully

0 ALERT level C = Check. Ensure it is not caused by an omission or oversight

32 ALERT level G = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
28 ALERT type 4 Improvement, methodology, query or suggestion
2 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 10/08/2020; check.def file version of 06/08/2020

