checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4HoFe

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: 4HoFe

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=12.721(2) b=12.661(1) c=17.293(2)
alpha=90 beta=103.04(1) gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	2713.4(6)	2713.4(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H19 Fe Ho N13 O4, 3(H2 O)	C17 H19 Fe Ho N13 O4, 3(H2 O)
Sum formula	C17 H25 Fe Ho N13 O7	C17 H25 Fe Ho N13 O7
Mr	744.28	744.28
Dx,g cm-3	1.822	1.822
Z	4	4
Mu (mm-1)	3.491	3.491
F000	1468.0	1468.0
F000'	1468.99	
h,k,lmax	17,17,23	17,17,23
Nref	7570	6386
Tmin,Tmax	0.904,0.959	0.511,1.000
Tmin'	0.421	

Correction method= # Reported T Limits: Tmin=0.511 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.844 Theta(max)= 29.522

R(reflections)= 0.0519(4584) wR2(reflections)= 0.0902(6386)

S = 1.000 Npar= 399

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

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.00825	Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N2 --H2B .	Please	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	6.381	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	12	Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ho1	1.38	eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From O3 .	0.72	eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From O5 .	0.70	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From O6 .	-0.70	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.50Ang From O4 .	-0.64	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3C .	-0.31	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5WA .	-0.32	eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	25	Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1	Report
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds	1	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT480_ALERT_4_G Long H...A H-Bond Reported H4 ..N13 .	2.71	Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H3B ..O7 .	2.74	Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H6 ..O7 .	2.64	Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H8 ..O2 .	2.62	Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	10	Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) .	2.97	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	27	Note
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	1172	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	29	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.6	Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities	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
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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
9 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 4HoFe - ellipsoid plot