checkCIF/PLATON report

Structure factors have been supplied for datablock(s) KM4

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: KM4

Bond precision: C-C = 0.0065 A   Wavelength=0.71073

Cell: a=13.629(3)   b=20.677(4)   c=26.759(5)
                   alpha=90   beta=90   gamma=90
Temperature: 193 K

	Calculated	Reported
Volume	7541(3)	7541(3)
Space group	F d d d	F d d d
Hall group	-F 2uv 2vw	-F 2uv 2vw
Moiety formula	C34 H34 Fe N10, 2(C2 H3 N), 2(Br)	?
Sum formula	C38 H40 Br2 Fe N12	C38 H40 Br2 Fe N12
Mr	880.47	880.49
Dx,g cm-3	1.551	1.551
Z	8	8
Mu (mm-1)	2.566	2.566
F000	3584.0	3584.0
F000'	3583.06	
h,k,lmax	18,27,35	17,27,35
Nref	2299	2273
Tmin,Tmax	0.623,0.836	0.958,1.050
Tmin'	0.593	

Correction method= # Reported T Limits: Tmin=0.958 Tmax=1.050
AbsCorr = MULTI-SCAN

Data completeness= 0.989   Theta(max)= 28.037

R(reflections)= 0.0547(1520)   wR2(reflections)= 0.1828(2273)

S = 1.059   Npar= 122

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**
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.10 Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0065 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn   H3   ..H10C   2.13 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.434 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.09A   From C101   1.58 eA-3

⚪ **Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   3 Note
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT   Unusually Large   0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large   7.68 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N100   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C101   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C102   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10C   Constrained at   0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 3   0.50 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C9 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #   6 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   2 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   3 Note
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   22 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   5 **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
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 30/01/2018; check.def file version of 30/01/2018

NOMOVE FORCED

Prob = 50
Temp = 193

-17 Y

Br1

PLATON-Mar 27 14:26:46 2018 — (70316)

C9

C4

C3

C102

C7

C8

N3

C5

C6

C7a

C3b

C2b

C1b

N1

N2

C6a

C101

N100

C4b

C9b

C2

C5b

N1b

C1c

C4a

N3b

C5b

N1b

N3a

C2c

Fe1

C9a

N3b

C6b

N2b

N1c

C5a

C3c

N1a

C5c

C3a

C4a

C7b

C1a

N3c

C4c

C6c

C2a

C8b

C7c

C9c

Z -43   KM4   F d d d   R = 0.05   RES=   0   -2 X