checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2-Br123K

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-Br123K

Bond precision: C-C = 0.0071 A Wavelength=0.71075

Cell: a=12.683(7) b=30.984(14) c=9.633(5)
alpha=90 beta=95.330(11) gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	3769(3)	3769(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C26 H20 Br2 Fe N8 O6, C8 H Br4 O4	C34 H21 Br6 Fe N8 O10
Sum formula	C34 H21 Br6 Fe N8 O10	C34 H21 Br6 Fe N8 O10
Mr	1236.84	1236.86
Dx,g cm-3	2.180	2.179
Z	4	4
Mu (mm-1)	6.832	6.850
F000	2388.0	2388.0
F000’	2383.81	
h,k,lmax	16,40,12	16,39,12
Nref	4341	4309
Tmin,Tmax	0.277,0.254	0.174,0.254
Tmin’	0.233	

Correction method= # Reported T Limits: Tmin=0.174 Tmax=0.254
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 27.483

R(reflections)= 0.0579(3973) wR2(reflections)= 0.1615(4309)

S = 1.116 Npar= 270

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 A

PLAT482_ALERT_4_A Small D-H..A Angle Rep for N2 .. N3 .. 35.40 Degree

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Alert level B

PLAT431_ALERT_2_B Short Inter HL..A Contact Br1 .. O3 .. 2.99 Ang.

Alert level C

PLAT303_ALERT_2_C Full Occupancy H-Atom H11 with # Connections 2.00 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00706 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.049 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 7 Note
PLAT972_ALERT_2_C Check Calcd Residual Density 0.62A From Br1 -2.28 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.58A From Br1 -2.04 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.69A From Br1 -1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.72A From Br2 -1.67 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.75A From Br3 -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.61A From Br1 -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.90A From Br2 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.72A From Br3 -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.50A From Br3 -1.54 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H3 -0.59 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H5 -0.34 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

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Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.
From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or
From the CIF: _chemical_formula_sum:C34 H21 Br6 Fe1 N8 O10
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.46 Why ?
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br3 .. Br3 .. 3.58 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 83 Check
N2 -H5 -N3 1.555 1.555 1.555 35.40 Deg.
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI . Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 24 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

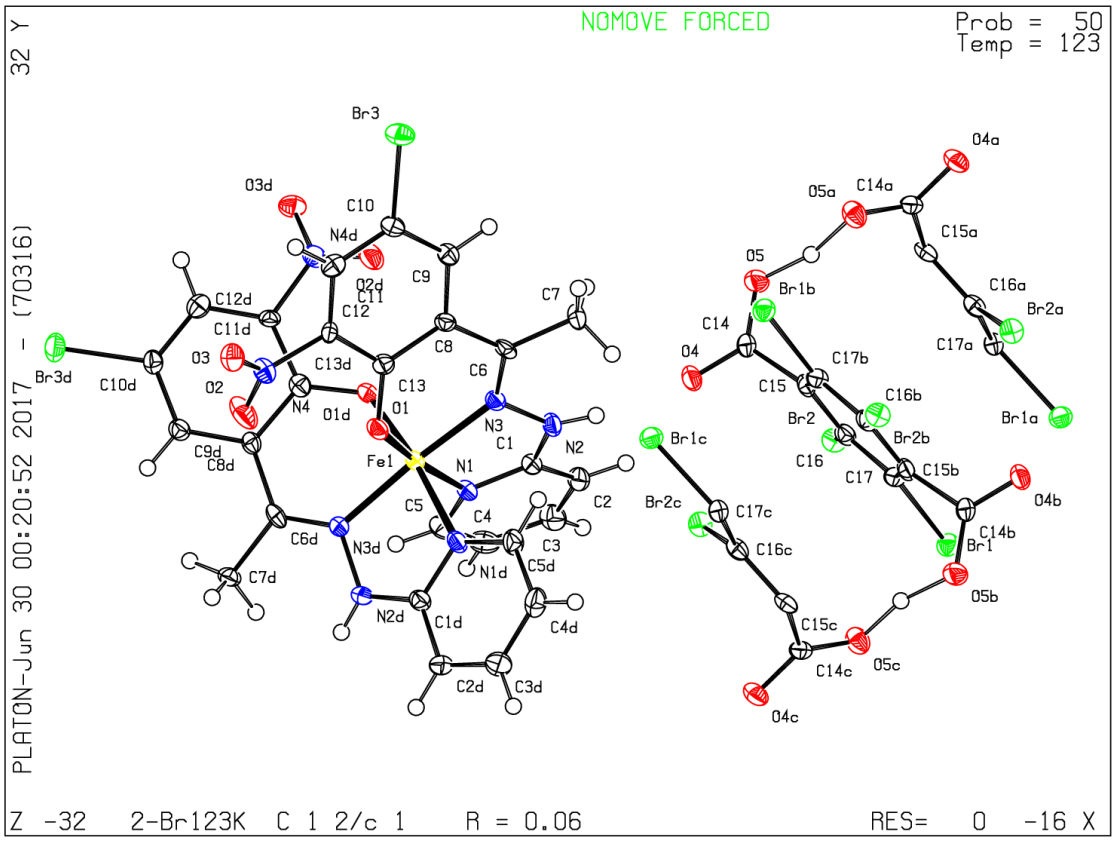
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 27/03/2017; check.def file version of 24/03/2017

Datablock 2-Br123K - ellipsoid plot