checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1-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: 1-Br123K

Bond precision: C-C = 0.0063 A Wavelength=0.71075

Cell: a=12.595(3) b=30.851(7) c=9.607(2)
alpha=90 beta=95.945(5) gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	3712.9(14)	3713.2(16)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C26 H20 Cl2 Fe N8 O6, C8 H Br4 O4	C34 H21 Br4 Cl2 Fe N8 O10
Sum formula	C34 H21 Br4 Cl2 Fe N8 O10	C34 H21 Br4 Cl2 Fe N8 O10
Mr	1147.94	1147.96
Dx,g cm-3	2.054	2.053
Z	4	4
Mu (mm-1)	4.927	4.939
F000	2244.0	2244.0
F000’	2242.99	
h,k,lmax	16,40,12	16,40,12
Nref	4278	4242
Tmin,Tmax	0.387,0.372	0.282,0.372
Tmin’	0.358	

Correction method= # Reported T Limits: Tmin=0.282 Tmax=0.372
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 27.485

R(reflections)= 0.0513(3785) wR2(reflections)= 0.0932(4242)

S = 1.128 Npar= 274

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 .. 39.00 Degree

---

Alert level B

PLAT431_ALERT_2_B Short Inter HL..A Contact Br2 .. O3 .. 2.91 Ang.

Alert level C

PLAT303_ALERT_2_C Full Occupancy H-Atom H12 with # Connections 2.00 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00631 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C26 H20 Cl2 Fe N8 O6
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 4.840 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on H3 -0.31 eA-3

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 Br4 Cl2 Fe1 N8 O10
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 30.92 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... -2 Units
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 83 Check
N2 -H6 -N3 1.555 1.555 1.555 39.00 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 25 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Note

---

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

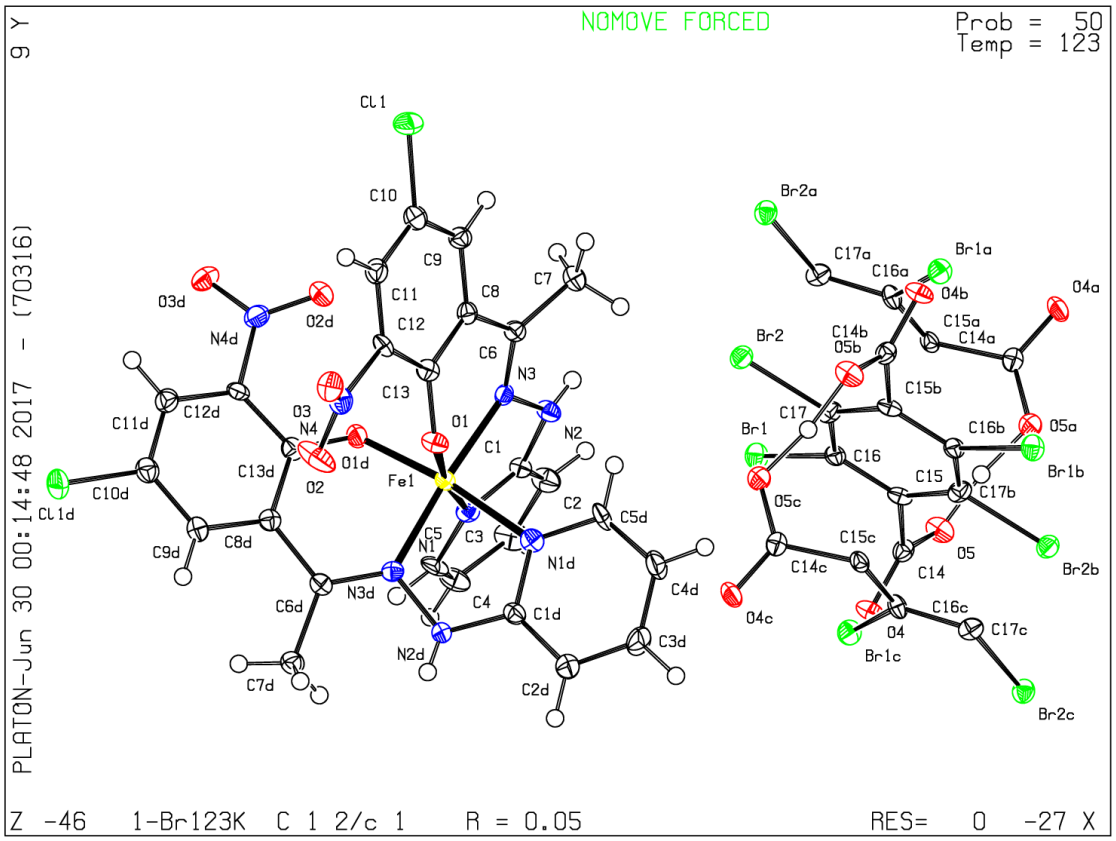
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 1-Br123K - ellipsoid plot