checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ad2102

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: ad2102

Bond precision: C-C = 0.0068 A Wavelength=0.71073

Cell: a=17.0583(7) b=15.3458(6) c=14.6767(6)
alpha=90 beta=90 gamma=90
Temperature: 65 K

	Calculated	Reported
Volume	3842.0(3)	3842.0(3)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C20 H24 Fe N6 O4, C24 H20 B	C20 H24 Fe N6 O4, C24 H20 B
Sum formula	C44 H44 B Fe N6 O4	C44 H44 B Fe N6 O4
Mr	787.51	787.51
Dx,g cm-3	1.362	1.361
Z	4	4
Mu (mm-1)	0.445	0.445
F000	1652.0	1652.0
F000’	1653.96	
h,k,lmax	21,18,18	21,18,17
Nref	3783	3742
Tmin,Tmax	0.958,0.965	0.610,0.746
Tmin’	0.852	

Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.022

R(reflections)= 0.0689(2011) wR2(reflections)= 0.1314(3742)

S = 1.119 Npar= 259

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.198

Author Response: The observed high Rint is attributed to the structural changes that the crystal structure underwent when cooling from 120 K down to 65 K. This structural change included a thermally induced excited spin state trapping (TIEEST) accompanied by a slight elongation of the crystallographic a axis while the crystallographic b and c axes shortened in the expected range for this temperature change.

Alert level C

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00684 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report

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Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.198 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.14 Why ?
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 10 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 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 16/05/2021; check.def file version of 13/05/2021

Datablock ad2102 - ellipsoid plot