checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0035 A Wavelength=0.71075

Cell: a=15.4749(7) b=13.9637(6) c=18.8880(9)
alpha=90 beta=103.392(7) gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	3970.5(3)	3970.5(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H26 Fe N4 O2, C24 H20 B	C22 H26 Fe N4 O2, C24 H20 B
Sum formula	C46 H46 B Fe N4 O2	C46 H46 B Fe N4 O2
Mr	753.53	753.53
Dx,g cm-3	1.261	1.261
Z	4	4
Mu (mm-1)	0.423	0.422
F000	1588.0	1588.0
F000’	1589.89	
h,k,lmax	20,18,24	20,18,24
Nref	9074	9057
Tmin,Tmax	0.776,0.959	0.684,0.959
Tmin’	0.713	

Correction method= # Reported T Limits: Tmin=0.684 Tmax=0.959
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.456

R(reflections)= 0.0492(7592) wR2(reflections)= 0.1285(9057)

S = 1.117 Npar= 491

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for C38 --C39 . 6.5 s.u.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.80 mm
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --N2 . 6.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --N3 . 7.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --N4_a . 8.4 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) . 3.11 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ..... Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.1 Low

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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
1 **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

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

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 04/06/2020; check.def file version of 02/06/2020

Datablock I - ellipsoid plot