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 = 0.0057 A   Wavelength=0.71075

Cell: a=11.5785(4)   b=36.8734(10)   c=16.5868(5)
               alpha=90   beta=103.385(7)   gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	6889.2(4)	6889.2(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H26 Fe N4 O2, 2(C24 H20 B), C5 H4 N, C6 H11 N	C22 H26 Fe N4 O2, 2(C24 H20, B), C5 H4 N, C6 H16 N
Sum formula	C81 H81 B2 Fe N6 O2	C81 H86 B2 Fe N6 O2
Mr	1247.99	1253.03
Dx,g cm-3	1.203	1.208
Z	4	4
Mu (mm-1)	0.271	0.271
F000	2644.0	2664.0
F000'	2646.24	
h,k,lmax	15,47,21	15,47,21
Nref	15789	15732
Tmin,Tmax	0.920,0.987	0.641,0.987
Tmin'	0.867	

Correction method= # Reported T Limits: Tmin=0.641 Tmax=0.987
AbsCorr = MULTI-SCAN

Data completeness= 0.996   Theta(max)= 27.484

R(reflections)= 0.0673(8554)   wR2(reflections)= 0.1747(15732)

S = 1.011   Npar= 844

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

PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   5.04 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for   N3   --C14   .   6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C35   --C36   .   5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6   --C76   .   0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C33 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C43 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   C74 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   C75 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   C76 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   C80 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C73 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   N6 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C78 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   N6   0.155 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C76   - C77   .   1.38 Ang.

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum: C81 H86 B2 Fe1 N6 O2
           Atom count from _chemical_formula_moiety:C81 H86 B1 Fe1 N6 O2
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C81 H86 B2 Fe1 N6 O2
           Atom count from the _atom_site data: C81 H81 B2 Fe1 N6 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z   4
           From the CIF: _chemical_formula_sum C81 H86 B2 Fe N6 O2
           TEST: Compare cell contents of formula and atom_site data

           atom   Z*formula cif sites diff
           C   324.00   324.00   0.00
           H   344.00   324.00   20.00
           B   8.00   8.00   0.00
           Fe   4.00   4.00   0.00
           N   24.00   24.00   0.00
           O   8.00   8.00   0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C76   --C77   .   5.2 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C80   --C81A   .   7.8 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C81A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C81B   Constrained at   0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5)   14% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact C33   ..C81B   3.08 Ang.
                              -1/2+x,3/2-y,-1/2+z   =   4_575 Check

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PLAT794_ALERT_5_G Tentative Bond Valency for Fe1        (III)     .     3.99 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
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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
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

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

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