checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0009_0m

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: mo_b0009_0m

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Bond precision:  C-C = 0.0093 A          Wavelength=0.71073

Cell:         a=15.6617(9)     b=16.037(1)       c=25.3913(15)
              alpha=84.162(2)  beta=81.2451(19)  gamma=78.6115(19)
Temperature:  100 K
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	Calculated	Reported
Volume	6162.1(6)	6162.1(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H68 Br2 Fe4 N2 O4 Si4 Zn2, C3 H6 O	C52 H68 Br2 Fe4 N2 O4 Si4 Zn2, C3 H6 O
Sum formula	C55 H74 Br2 Fe4 N2 O5 Si4 Zn2	C55 H74 Br2 Fe4 N2 O5 Si4 Zn2
Mr	1469.51	1469.48
Dx,g cm-3	1.584	1.584
Z	4	4
Mu (mm-1)	3.103	3.103
F000	2992.0	2992.0
F000’	2999.53	
h,k,lmax	21,21,34	21,21,34
Nref	32081	32013
Tmin,Tmax	0.280,0.512	0.628,0.746
Tmin’	0.259	

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Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 28.772

R(reflections)= 0.0624( 20914)    wR2(reflections)= 0.1396( 32013)

S = 1.040                 Npar= 1382
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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

PLAT414_ALERT_2_A Short Intra D-H..H-X H4 .. H32 .. 1.79 Ang.

Alert level B

PLAT213_ALERT_2_B Atom C72 has ADP max/min Ratio ..... 4.1 prolat
PLAT213_ALERT_2_B Atom C73 has ADP max/min Ratio ..... 4.4 prolat
PLAT213_ALERT_2_B Atom C74 has ADP max/min Ratio ..... 5.0 prolat
PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.5 Ratio
PLAT220_ALERT_2_B Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 9.5 Ratio
PLAT420_ALERT_2_B D-H Without Acceptor O4 -- H4 ... Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O6 -- H6A ... Please Check
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 150 Ang3
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min) 14 Note
PLAT971_ALERT_2_B Check Calcd Residual Density 0.88A From Br3 2.85 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density 0.85A From Br2 2.53 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density 0.85A From Br2 2.51 eA-3

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.134
PLAT213_ALERT_2_C Atom Fe6 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C68 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C71 has ADP max/min Ratio ..... 3.8 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.9 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2 H Uiso(max)/Uiso(min) Range 9.2 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C71 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C72 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C73 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C74 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C98 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Fe6 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C106 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00931 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H71 .. H1BB .. 2.12 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C52 H68 Br2 Fe4 N2 O4 Si4 Zn2
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 6.577 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 0.85A From Br2 2.15 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.26A From O9 1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.78A From C109 1.62 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.80A From Br3 -2.23 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.95A From O4 0.69 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 1.01A From O4 -0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.65A From O9 -0.70 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H6A -0.32 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H75 -0.51 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H101 -0.34 eA-3

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         12 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT020_ALERT_3_G The value of Rint is greater than 0.12 .........      0.134 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      38.04 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          3 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4)..        100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)..        100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   5.83) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   4.17) in Resd. #          5 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O10B   ..  C75     ..       2.89 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
            C3 H6 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
            C3 H6 O
PLAT793_ALERT_4_G The Model has Chirality at Si1     (Centro SPGR)          S Verify
PLAT793_ALERT_4_G The Model has Chirality at Si3     (Centro SPGR)          S Verify
PLAT793_ALERT_4_G The Model has Chirality at Si5     (Centro SPGR)          S Verify
PLAT793_ALERT_4_G The Model has Chirality at Si7     (Centro SPGR)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        120 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         48 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Note
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 12 ALERT level B = A potentially serious problem, consider carefully
 31 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 26 ALERT level G = General information/check it is not something unexpected

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT414_mo_b0009_0m
;
PROBLEM: Short Intra D-H..H-X       H4     ..  H32     ..       1.79 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 26/02/2017; check.def file version of 21/02/2017

Datablock mo_b0009_0m - ellipsoid plot