checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: 3111

Bond precision: C-C = 0.0102 A Wavelength=0.71073

Cell: **a=22.0084(17) b=11.8011(5) c=23.1333(18)**
alpha=90 beta=115.664(9) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	5415.5(8)	5415.5(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C46 H52 Br2 Fe4 N2 O3 Si2 Zn, C3 H6 O	C46 H52 Br2 Fe4 N2 O3 Si2 Zn, C3 H6 O
Sum formula	C49 H58 Br2 Fe4 N2 O4 Si2 Zn	C49 H58 Br2 Fe4 N2 O4 Si2 Zn
Mr	1243.75	1243.74
Dx,g cm-3	1.526	1.525
Z	4	4
Mu (mm-1)	3.044	3.044
F000	2520.0	2520.0
F000’	2525.68	
h,k,lmax	27,14,28	28,16,31
Nref	10645	10638
Tmin,Tmax	0.701,0.738	0.642,1.000
Tmin’	0.539	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.999

R(reflections)= 0.0563(7439) wR2(reflections)= 0.1390(10638)

S = 1.066 Npar= 591

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
PLAT213_ALERT_2_A Atom C29 has ADP max/min Ratio ..... 6.5 prolat

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Alert level B

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PLAT213_ALERT_2_B Atom C14            has ADP max/min Ratio .....       4.5 prolat
PLAT213_ALERT_2_B Atom C28            has ADP max/min Ratio .....       4.6 prolat
PLAT220_ALERT_2_B Large Non-Solvent  C     Ueq(max)/Ueq(min) Range      6.8 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C14    --  C15     ..      8.6 su
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....       C29 Check
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Alert level C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.23 Report
PLAT213_ALERT_2_C Atom C7             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C8             has ADP max/min Ratio .....       3.1 prolat
PLAT222_ALERT_3_C Large Non-Solvent  H     Uiso(max)/Uiso(min) ...      5.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C16    --  C20     ..      5.6 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe2    --  C13     ..     0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..     0.16 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C7 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....      C12 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....      C13 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....      C15 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....      C27 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....      C28 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....      Fe2 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....      Fe3 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....      C11 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....      C26 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of       C37 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0102 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C14    -   C15    ...     1.54 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        5 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     5.41 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for      O3    134.3 Degree
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .      376 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........       19 Note
PLAT793_ALERT_4_G The Model has Chirality at Si1     (Centro SPGR)       S Verify
PLAT793_ALERT_4_G The Model has Chirality at Si2     (Centro SPGR)       S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............       42 Note
PLAT868_ALERT_4_G ALERTS Due to the use of _smtbx_masks Suppressed        ! Info
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ        -2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ        -3 Units
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  5 ALERT level B = A potentially serious problem, consider carefully
 20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
  2 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*, 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 20/08/2014; check.def file version of 19/12/2014

Datablock 3111 - ellipsoid plot