

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3113

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: 3113

| | | | |
|-----------------|---|---|-------------|
| Bond precision: | C-C = 0.0076 A | Wavelength=0.71073 | |
| Cell: | a=47.515(3) | b=10.31587(19) | c=33.897(2) |
| | alpha=90 | beta=132.838(10) | gamma=90 |
| Temperature: | 173 K | | |
| | Calculated | Reported | |
| Volume | 12183(2) | 12183.5(18) | |
| Space group | C 2/c | C 1 2/c 1 | |
| Hall group | -C 2yc | -C 2yc | |
| Moiety formula | 2(C26 H32 Br2 Fe2 N2 O2 Si Zn), C3 H6 O | 2(C26 H32 Br2 Fe2 N2 O2 Si Zn), C3 H6 O | |
| Sum formula | C55 H70 Br4 Fe4 N4 O5 Si2 Zn2 | C55 H70 Br4 Fe4 N4 O5 Si2 Zn2 | |
| Mr | 1597.11 | 1597.11 | |
| Dx, g cm-3 | 1.742 | 1.741 | |
| Z | 8 | 8 | |
| Mu (mm-1) | 4.414 | 4.414 | |
| F000 | 6400.0 | 6400.0 | |
| F000' | 6409.68 | | |
| h,k,lmax | 62,13,44 | 62,13,44 | |
| Nref | 14728 | 14607 | |
| Tmin,Tmax | 0.430,0.643 | 0.837,1.000 | |
| Tmin' | 0.398 | | |

Correction method= # Reported T Limits: Tmin=0.837 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 28.000

R(reflections)= 0.0437(11920) wR2(reflections)= 0.1265(14607)

S = 1.039 Npar= 693

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

| | | | |
|-------------------|--|---------|--------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density | 2.87 | Report |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C45 -- C46 .. | 6.4 | s.u. |
| 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 | C46 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | N2 | Check |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of | C54 | Check |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds | 0.00761 | Ang. |
| PLAT362_ALERT_2_C | Short C(sp3)-C(sp2) Bond C54 - C55 .. | 1.33 | Ang. |
| PLAT412_ALERT_2_C | Short Intra XH3 .. XHn H53A .. H55A .. | 1.88 | Ang. |
| PLAT906_ALERT_3_C | Large K value in the Analysis of Variance | 2.042 | Check |
| PLAT910_ALERT_3_C | Missing # of FCF Reflection(s) Below Theta(Min) | 6 | Note |
| PLAT911_ALERT_3_C | Missing # FCF Refl Between THmin & STh/L= 0.600 | 2 | Report |
| PLAT934_ALERT_3_C | Number of (Iobs-Icalc)/SigmaW > 10 Outliers | 1 | Check |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 1.93A From C53 | 1.64 | eA-3 |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 0.93A From Br3 | 1.58 | eA-3 |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 1.06A From C53 | 1.52 | eA-3 |
| PLAT975_ALERT_2_C | Check Calcd Residual Density 1.00A From N2 | 0.64 | eA-3 |
| PLAT976_ALERT_2_C | Check Calcd Residual Density 0.71A From O5 | -0.55 | eA-3 |
| PLAT978_ALERT_2_C | Number C-C Bonds with Positive Residual Density. | 0 | Note |



Alert level G

| | | | |
|-------------------|--|-------|--------|
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 24.92 | Why ? |
| PLAT128_ALERT_4_G | Alternate Setting for Input Space Group C2/c | I2/a | Note |
| PLAT152_ALERT_1_G | The Supplied and Calc. Volume s.u. Differ by ... | 2 | Units |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Br3 -- Zn2 .. | 6.0 | s.u. |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety | C53 | Check |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety | C55 | Check |
| PLAT790_ALERT_4_G | Centre of Gravity not Within Unit Cell: Resd. # C26 H32 Br2 Fe2 N2 O2 Si Zn | 2 | 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 |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 113 | Note |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 2 | Note |

- 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
11 **ALERT level G** = General information/check it is not something unexpected

- 1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
16 **ALERT type 2** Indicator that the structure model may be wrong or deficient
5 **ALERT type 3** Indicator that the structure quality may be low
8 **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 24/11/2016; check.def file version of 23/11/2016

