checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11069a

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: 11069a**

Bond precision:  C-C = 0.0053 Å  Wavelength=0.71073 Å

Cell:          a=13.492(3)  b=21.920(5)  c=24.597(6)
                              alpha=90      beta=97.372(5)  gamma=90

Temperature:  100 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>7214(3)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yn</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C74 H90 Fe2 N8 O4 S, 2(C2 H3 N)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C78 H96 Fe2 N10 O4 S</td>
</tr>
<tr>
<td>Mr</td>
<td>1381.41</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.272</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.488</td>
</tr>
<tr>
<td>F000</td>
<td>2936.0</td>
</tr>
<tr>
<td>F000’</td>
<td>2940.15</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>16,27,30</td>
</tr>
<tr>
<td>Nref</td>
<td>14187</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.810,0.929</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.772</td>
</tr>
</tbody>
</table>

Correction method: # Reported T Limits: Tmin=0.782  Tmax=0.930
AbsCorr = MULTI-SCAN

Data completeness= 1.000  Theta(max)= 25.997

R(reflections)= 0.0585( 9994)  wr2(reflections)= 0.1491( 14186)

S = 0.992  Npar= 856
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**

- **PLAT410_ALERT_2_A** Short Intra H...H Contact \( \text{H42A} \ldots \text{H45B} \) \ldots 1.77 Ang.

---

**Alert level C**

- **PLAT220_ALERT_2_C** Large Non-Solvent C \( \text{Ueq(max)}/\text{Ueq(min)} \) Range 3.7 Ratio
- **PLAT244_ALERT_4_C** Low ‘Solvent’ Ueq as Compared to Neighbors of C2T Check
- **PLAT906_ALERT_3_C** Large K value in the Analysis of Variance ...... 5.456 Check

---

**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: C78 H96 Fe2 N10 O4 S1
  - Atom count from \_chemical_formula_moiety: C76 H96 Fe2 N10 O4 S1
- **PLAT042_ALERT_1_G** Calc. and Reported MoietyFormula Strings Differ Please Check
- **PLAT066_ALERT_1_G** Predicted and Reported Tmin&Tmax Range Identical ? Check
- **PLAT083_ALERT_2_G** SHELXL Second Parameter in WGHT Unusually Large. 7.00 Why ?
- **PLAT720_ALERT_4_G** Number of Unusual/Non-Standard Labels ............ 6 Note
- **PLAT910_ALERT_3_G** Missing # of FCF Reflection(s) Below Th(Min) ... 1 Report

---

1 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
6 ALERT level G = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 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*, 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 21/06/2015; check.def file version of 21/06/2015