checkCIF/PLATON report

Structure factors have been supplied for datablock(s) am81_100

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.

**Datablock: am81_100**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1847.03(18)</td>
<td>1847.03(18)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>O40 Si W12, 5(C10 H10 Fe), Si W12 O40, 5(C10 H10 Fe), 2(C H4 O)</td>
<td>2(C H4 O)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C52 H58 Fe5 O42 Si W12</td>
<td>C52 H58 Fe5 O42 Si W12</td>
</tr>
<tr>
<td>Mr</td>
<td>3868.40</td>
<td>3868.40</td>
</tr>
<tr>
<td>DxF, g cm⁻³</td>
<td>3.478</td>
<td>3.478</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>19.651</td>
<td>19.651</td>
</tr>
<tr>
<td>F000</td>
<td>1738.0</td>
<td>1738.0</td>
</tr>
<tr>
<td>F000'</td>
<td>1731.74</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>16,17,17</td>
<td>16,17,17</td>
</tr>
<tr>
<td>Nref</td>
<td>8922</td>
<td>8904</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.248, 0.608</td>
<td>0.230, 0.621</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.034</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.230 Tmax=0.621
AbsCorr = ANALYTICAL

Data completeness= 0.998
Theta(max) = 28.000

R(reflections) = 0.0358 (6061)
wr2(reflections) = 0.0719 (8904)

S = 0.862
Npar= 505
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 O10 has ADP max/min Ratio ..... 5.8 prolat

### Alert level B
- **PLAT213_ALERT_2_B** Atom O9 has ADP max/min Ratio ..... 4.1 prolat
- **PLAT213_ALERT_2_B** Atom O17 has ADP max/min Ratio ..... 4.8 prolat
- **PLAT220_ALERT_2_B** Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 8.0 Ratio
- **PLAT241_ALERT_2_B** High ‘MainMol’ Ueq as Compared to Neighbors of O18 Check
- **PLAT242_ALERT_2_B** Low ‘MainMol’ Ueq as Compared to Neighbors of Fe2 Check
- **PLAT973_ALERT_2_B** Check Calcd Positive Residual Density on W5 1.58 eA^{-3}
- **PLAT975_ALERT_2_B** Check Calcd Residual Density 0.60A From O18 1.61 eA^{-3}
- **PLAT975_ALERT_2_B** Check Calcd Residual Density 0.44A From O10 1.54 eA^{-3}

### Alert level C
- **PLAT213_ALERT_2_C** Atom O3 has ADP max/min Ratio ..... 3.5 prolat
- **PLAT213_ALERT_2_C** Atom O5 has ADP max/min Ratio ..... 3.1 prolat
- **PLAT213_ALERT_2_C** Atom O7 has ADP max/min Ratio ..... 3.8 prolat
- **PLAT213_ALERT_2_C** Atom O11 has ADP max/min Ratio ..... 3.8 prolat
- **PLAT213_ALERT_2_C** Atom O12 has ADP max/min Ratio ..... 3.8 prolat
- **PLAT213_ALERT_2_C** Atom O13 has ADP max/min Ratio ..... 3.3 prolat
- **PLAT213_ALERT_2_C** Atom O14 has ADP max/min Ratio ..... 3.1 prolat
- **PLAT213_ALERT_2_C** Atom O16 has ADP max/min Ratio ..... 3.7 prolat
- **PLAT213_ALERT_2_C** Atom O18 has ADP max/min Ratio ..... 4.0 prolat
- **PLAT214_ALERT_2_C** Atom C15 (Anion/Solvent) ADP max/min Ratio 4.3 prolat
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O7 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O8 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O9 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O12 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O13 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O14 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of O17 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C13 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C14 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C15 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C17 Check
- **PLAT241_ALERT_2_C** High ‘MainMol’ Ueq as Compared to Neighbors of C18 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W1 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W2 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W3 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W4 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W5 Check
- **PLAT242_ALERT_2_C** Low ‘MainMol’ Ueq as Compared to Neighbors of W6 Check
- **PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor ..... 3.0 Note
- **PLAT342_ALERT_3_C** Low Bond Precision on C-C Bonds ............... 0.0137 Ang.
- **PLAT413_ALERT_2_C** Short Inter XH3 .. XHn H1M2 .. H24A .. 2.11 Ang.
- **PLAT731_ALERT_1_C** Bond Calc 1.34(2), Rep 1.34(6) ...... C13 -C14 1.555 1.555 ............ 3 su-Rat
- **PLAT731_ALERT_1_C** Bond Calc 1.34(19), Rep 1.34(6) ...... C14 -C15 1.555 1.555 ............ 3 su-Rat
- **PLAT731_ALERT_1_C** Bond Calc 1.371(16), Rep 1.370(5) ...... C16 -C17 1.555 1.555 ............ 3 su-Rat
- **PLAT906_ALERT_3_C** Large K value in the Analysis of Variance ..... 4.368 Check
- **PLAT910_ALERT_3_C** Missing # of FCF Reflection(s) Below Theta(Min) 8 Note
- **PLAT911_ALERT_3_C** Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report
Alert level G

Number of Uiso or Uij Restrained non-H Atoms ... 30 Report
Calc. and Reported MoietyFormula Strings ................. 1 Report
The CIF-Embedded .res File Contains DELU Records 6 Report
The CIF-Embedded .res File Contains ISOR Records 1 Report
Atom Site Occupancy of *O19 is Constrained at 0.5 Check
Atom Site Occupancy of *O20 is Constrained at 0.5 Check
Atom Site Occupancy of *O21 is Constrained at 0.5 Check
Atom Site Occupancy of *O22 is Constrained at 0.5 Check
Main Residue Disorder ..................(Resd 1) .. 8 % Note
Anion/Solvent/Minor-Residue Disorder (Resd 2) .. 91 % Note
Short Inter X...Y Contact O3 .. C5 .. 2.98 Ang.
Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 125 Do !
O19 -S11 -O19 -W3 3.00 0.00 2.656 1.555 1.555 1.555
Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 132 Do !
O19 -S11 -O19 -W2 15.00 0.00 2.656 1.555 1.555 1.555
Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 139 Do !
O19 -S11 -O19 -W1 9.00 0.00 2.656 1.555 1.555 1.555
Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 197 Do !
O20 -S11 -O20 -O21 13.00 0.00 2.656 1.555 1.555 1.555
Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 204 Do !
O20 -S11 -O20 -W5 13.00 0.00 2.656 1.555 1.555 1.555
O20 -SI1 -O20 -W2      0.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 218 Do !
O20 -SI1 -O20 -W6     12.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 294 Do !
O21 -SI1 -O21 -O20    13.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 300 Do !
O21 -SI1 -O21 -W3     1.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 307 Do !
O21 -SI1 -O21 -W5     13.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 314 Do !
O21 -SI1 -O21 -W4     11.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 317 Do !
O22 -SI1 -O22 -W4      5.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 375 Do !
O22 -SI1 -O22 -W6      8.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 382 Do !
O22 -SI1 -O22 -W1     17.00  0.00   2.656   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 389 Do !

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        120 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
76 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
23 ALERT type 4 Improvement, methodology, query or suggestion
1 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**