Structure factors have been supplied for datablock(s) 14037

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: 14037**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0223 A</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=10.00(2)</td>
<td>b=20.29(5)</td>
</tr>
<tr>
<td></td>
<td>alpha=106.04(2)</td>
<td>beta=94.78(5)</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
<tr>
<td>Volume</td>
<td>5553(22)</td>
<td>5553(22)</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>C2 H2 B22 Cl22 In0.13, 6(C H B11 Cl11), 11.87(C6 H5 Br), 7.87(I C6 H5 Br), 5.93(C6 H5 Br), 4(C H B11 Cl11), 4In</td>
<td></td>
</tr>
<tr>
<td>Sum formula</td>
<td>C79.24 H67.37 B88 Br11.87</td>
<td>C39.62 H33.69 B44 Br5.93</td>
</tr>
<tr>
<td>Mr</td>
<td>6957.80</td>
<td>3478.83</td>
</tr>
<tr>
<td>Dx,g cm^-3</td>
<td>2.081</td>
<td>2.080</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm^-1)</td>
<td>4.051</td>
<td>4.051</td>
</tr>
<tr>
<td>F000</td>
<td>3286.4</td>
<td>3286.0</td>
</tr>
<tr>
<td>F000'</td>
<td>3290.77</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>12,25,35</td>
<td>12,24,35</td>
</tr>
<tr>
<td>Nref</td>
<td>22288</td>
<td>29544</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.242,0.309</td>
<td>0.294,0.386</td>
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<tr>
<td>Tmin’</td>
<td>0.190</td>
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<tr>
<td>Correction method= MULTI-SCAN</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Data completeness= 1.326</td>
<td>Theta(max) = 26.184</td>
<td></td>
</tr>
<tr>
<td>R(reflections)= 0.0874( 22942)</td>
<td>wR2(reflections)= 0.2560( 29544)</td>
<td></td>
</tr>
<tr>
<td>S = 1.007</td>
<td>Npar= Npar =1265</td>
<td></td>
</tr>
</tbody>
</table>
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.

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**Alert level A**

- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ..........        In1 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ..........        In2 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ..........        In3 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ..........       >In4 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ..........    <In4'_B Check
- **PLAT308_ALERT_2_A** Single Bonded Metal Atom (Unusual !) ..........    <In5_B Check

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**Alert level B**

Crystal system given = triclinic

- **PLAT342_ALERT_3_B** Low Bond Precision on C-C Bonds ..........     0.0223 Ang.

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**Alert level C**

- **RFACR01_ALERT_3_C** The value of the weighted R factor is > 0.25
  - Weighted R factor given 0.256
- **PLAT041_ALERT_1_C** Calc. and Reported SumFormula Strings Differ Please Check
- **PLAT068_ALERT_1_C** Reported F000 Differs from Calcd (or Missing)... Please Check
- **PLAT084_ALERT_3_C** High wr2 Value (i.e. > 0.25) ............... 0.26 Why ?
- **PLAT148_ALERT_3_C** su on the a - Axis is (Too) Large ....... 0.020 Ang.
- **PLAT148_ALERT_3_C** su on the b - Axis is (Too) Large ....... 0.050 Ang.
- **PLAT148_ALERT_3_C** su on the c - Axis is (Too) Large ....... 0.070 Ang.
- **PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.2 Note
- **PLAT302_ALERT_3_C** Large Average Phenyl C-C Dist. C1E - C6E ... 1.41 Ang.
- **PLAT301_ALERT_2_C** Small Average Phenyl C-C Dist. C1F_A - C6F_A ... 1.36 Ang.
- **PLAT351_ALERT_3_C** Long C-H (X0.96,N1.08A) C1I - H1I ... 1.12 Ang.
- **PLAT351_ALERT_3_C** Long C-H (X0.96,N1.08A) C1G - H1G ... 1.12 Ang.
- **PLAT351_ALERT_3_C** Long C-H (X0.96,N1.08A) C1H - H1H ... 1.12 Ang.
- **PLAT351_ALERT_3_C** Long C-H (X0.96,N1.08A) C1J - H1J ... 1.12 Ang.
- **PLAT906_ALERT_3_C** Large K value in the Analysis of Variance ...... 6.787 Check
- **PLAT906_ALERT_3_C** Large K value in the Analysis of Variance ...... 2.058 Check
- **PLAT910_ALERT_3_C** Missing # of FCF Reflections Below Th(Min) ..... 5 Why ?
- **PLAT911_ALERT_3_C** Missing # FCF Refl Between Th(min) & STh/L= 0.600 666 Why ?

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**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: C39.62 H33.69 B44 Br5.93 Cl
  - Atom count from _chemical_formula_moiety:C39.58 H33.65 B44 Br5.93 Cl
- **PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite 14 Note
- **PLAT003_ALERT_2_G** Number of Uiso or Uij Restrained non-H Atoms ... 136 Why ?
- **PLAT021_ALERT_4_G** Ratio Unique / Expected Reflections too High ... 1.326
- **PLAT042_ALERT_1_G** Calc. and Reported MoietyFormula Strings Differ Please Check
- **PLAT045_ALERT_1_G** Calculated and Reported Z Differ by ............ 0.50 Ratio
- **PLAT083_ALERT_2_G** SHELXL Second Parameter in WGHT Unusually Large. 164.00 Why ?
- **PLAT232_ALERT_2_G** Hirshfeld Test Diff (M-X) In5_B -- C181_a .. 6.7 su
- **PLAT301_ALERT_3_G** Main Residue Disorder Percentage = 0 Note
- **PLAT302_ALERT_4_G** Anion/Solvent Disorder Percentage = 16 Note
- **PLAT343_ALERT_2_G** Check sp? Angle Range in Main Residue for .. C1I
- **PLAT343_ALERT_2_G** Check sp? Angle Range in Main Residue for .. C1G
- **PLAT343_ALERT_2_G** Check sp? Angle Range in Main Residue for .. C1H
- **PLAT343_ALERT_2_G** Check sp? Angle Range in Main Residue for .. C1J
- **PLAT434_ALERT_2_G** Short Inter HL..HL Contact Br1E .. C16H .. 3.47 Ang.
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, and 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.

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PLATON version of 05/02/2014; check.def file version of 05/02/2014