checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>As– C = 0.0080 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=11.6328(11)</td>
<td>b=14.0632(12)</td>
</tr>
<tr>
<td></td>
<td>alpha=90</td>
<td>beta=90</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1958.6(3)</td>
</tr>
<tr>
<td>Space group</td>
<td>P n m a</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ac 2n</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C21 H21 As Au Cl</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C21 H21 As Au Cl</td>
</tr>
<tr>
<td>Mr</td>
<td>580.72</td>
</tr>
<tr>
<td>Dx,g cm⁻³</td>
<td>1.969</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>9.324</td>
</tr>
<tr>
<td>F000</td>
<td>1104.0</td>
</tr>
<tr>
<td>F000’</td>
<td>1097.59</td>
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<tr>
<td>h,k,lmax</td>
<td>16,19,16</td>
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<tr>
<td>Nref</td>
<td>2967</td>
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<tr>
<td>Tmin,Tmax</td>
<td>0.232,0.479</td>
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<tr>
<td>Tmin’</td>
<td>0.008</td>
</tr>
</tbody>
</table>

Correction method= MULTI-SCAN

Data completeness= 0.994  Theta(max)= 30.000

R(reflections)= 0.0375( 2413)  wR2(reflections)= 0.0911( 2949)

S = 1.148  Npar= 194

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

PLAT048_ALERT_1_C Moiety Formula Not Given ........................ Please Do!
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & Sh/L= 0.600 17 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT971_ALERT_2_C Check Calcd Residual Density 0.80A From Au1 2.03 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.82A From Au1 1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.84A From Au1 -2.49 eA-3

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 14.42 Report
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as mixed
PLAT171_ALERT_4_G The CIF-Embedded.res File Contains EADP Records 2 Report
PLAT301_ALERT_3_G Main Residue Disorder Percentage = 79 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .... C14 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C2 .. C13X .. 2.50 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C2 .. C12X .. 2.85 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C2 .. C14X .. 3.04 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 .. C13X .. 2.69 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 .. C14X .. 3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C7 .. C12 .. 2.74 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C7 .. C14 .. 2.89 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C7 .. C13 .. 3.03 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 1 Do!
  CL1 -AU1 -AS1 -C8X  -56.80  1.10  1.555  1.555  1.555  8.565
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 2 Do!
  CL1 -AU1 -AS1 -C8X  56.80  1.10  1.555  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 3 Do!
  CL1 -AU1 -AS1 -C1  180.00  0.00  1.555  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 4 Do!
  CL1 -AU1 -AS1 -C8  -62.90  1.10  1.555  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 5 Do!
  CL1 -AU1 -AS1 -C8  62.90  1.10  1.555  1.555  1.555  1.555
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ............. 1 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.35 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2     --  C5      1.96 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3     --  C6      1.77 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C5     --  C2      1.96 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C6     --  C3      1.77 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C6     --  C6      1.96 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 5 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 9 Check
  C8X  -AS1  -C8  1.555  1.555  1.555  7.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 32 Check
  C3  -C2  -C5  1.555  1.555  8.565  38.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 41 Check
  C2  -C3  -C6  1.555  1.555  8.565  44.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 64 Check
  C4  -C5  -C6  1.555  1.555  8.565  43.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 69 Check
  C6  -C5  -C2  1.555  1.555  8.565  39.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 77 Check
  C5  -C6  -C3  1.555  1.555  8.565  43.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 79 Check
  C1  -C6  -C6  1.555  1.555  8.565  44.00 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflections Below TH(Min) .... 1 Report
checkCIF publication errors

### Alert level A

**PUBL024_ALERT_1_A** The number of authors is greater than 5. Please specify the role of each of the co-authors for your paper.

**Author Response:** The design of experiment and synthesis and spectral characterization work was conducted by the visiting scholar Tariq with Khan assistance. The crystal structures solving and refinement were carried out by both Goh and Rosli. Final verification and justification of work were confirmed by both Shawkataly and Fun.

### Alert level G

**PUBL017_ALERT_1_G** The _publ_section_references section is missing or empty.

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1 **ALERT level A** = Data missing that is essential or data in wrong format  
1 **ALERT level G** = General alerts. Data that may be required is missing
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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PLATON version of 24/07/2014; check.def file version of 24/07/2014

Datablock I - ellipsoid plot