checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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: 1_a

Bond precision: C-C = 0.0087 Å
Wavelength=0.71073 Å

Cell:
\[
\begin{align*}
    & a=10.4461(3) & b=15.7690(5) & c=18.4599(7) \\
    & \alpha=84.440(1) & \beta=73.937(1) & \gamma=78.725(1)
\end{align*}
\]

Temperature: 193 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2862.73(16)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>2(C41 H75 Ir3 N13 P2 U), 3(C7 H8)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C103 H174 Ir6 N26 P4 U2</td>
</tr>
<tr>
<td>Mr</td>
<td>3529.95</td>
</tr>
<tr>
<td>Dx, g cm(^{-3})</td>
<td>2.048</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
</tr>
<tr>
<td>Mu (mm(^{-1}))</td>
<td>9.873</td>
</tr>
<tr>
<td>F000</td>
<td>1680.0</td>
</tr>
<tr>
<td>F000’</td>
<td>1653.70</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>13,20,23</td>
</tr>
<tr>
<td>Nref</td>
<td>13170</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.387,0.373</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.358</td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.366 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.990
Theta(max) = 27.520

R(reflections)= 0.0270( 11570)
wr2(reflections)= 0.0625( 13033)

S = 1.051
Npar= 666
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

- **PLAT220_ALERT_2_C** NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.5 Ratio
- **PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor ... 3.0 Note
- **PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor ... 2.4 Note
- **PLAT260_ALERT_2_C** Large Average Ueq of Residue Including C49 0.101 Check
- **PLAT342_ALERT_3_C** Low Bond Precision on C-C Bonds ... 0.00873 Ang.
- **PLAT910_ALERT_3_C** Missing # of FCF Reflections Below Theta(Min). 7 Note
- **PLAT911_ALERT_3_C** Missing FCF Refl Between Thmin & Sth/L= 0.600 87 Report
- **PLAT917_ALERT_2_C** Check Negative Difference Density on H6 -0.32 eA-3
- **PLAT977_ALERT_2_C** Check Negative Difference Density on H41B -0.33 eA-3
- **PLAT977_ALERT_2_C** Check Negative Difference Density on H47 -0.43 eA-3

### Alert level G

- **PLAT003_ALERT_2_G** Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
- **PLAT042_ALERT_1_G** Calc. and Reported Moiety Formula Strings Differ Please Check
- **PLAT045_ALERT_1_G** Calculated and Reported Z Differ by a Factor ... 0.50 Check
- **PLAT154_ALERT_1_G** The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
- **PLAT178_ALERT_4_G** The CIF-Embedded .res File Contains SIMU Records 2 Report
- **PLAT186_ALERT_4_G** The CIF-Embedded .res File Contains ISOR Records 2 Report
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C49 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C50 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C51 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C52 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C53 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C54 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of C55 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H49A Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H49B Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H49C Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H51 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H52 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H53 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H54 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Atom Site Occupancy of H55 Constrained at 0.5 Check
- **PLAT300_ALERT_4_G** Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
- **PLAT304_ALERT_4_G** Non-Integer Number of Atoms in ..... (Resd 3) 7.50 Check
- **PLAT779_ALERT_4_G** Suspect or Irrelevant (Bond) Angle(s) in CIF ... 39.34 Deg.
- **PLAT789_ALERT_4_G** Centre of Gravity not Within Unit Cell: Resd. # 110 Check
- **PLAT790_ALERT_4_G** Centre of Gravity not Within Unit Cell: Resd. # 2 Note
- **PLAT794_ALERT_5_G** Tentative Bond Valency for U1 (IV) 4.76 Info
- **PLAT860_ALERT_3_G** Number of Least-Squares Restraints ............. 168 Note
- **PLAT912_ALERT_4_G** Missing # of FCF Reflections Above Sth/L= 0.600 43 Note
- **PLAT913_ALERT_3_G** Missing # of Very Strong Reflections in FCF .... 2 Note
- **PLAT941_ALERT_3_G** Number of OMIT Records in Embedded .res File ... 2 Note
- **PLAT978_ALERT_2_G** Number C-C Bonds with Positive Residual Density. 2 Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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 16/05/2021; check.def file version of 13/05/2021