checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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

Bond precision:  Si–O = 0.0072 Å  Wavelength=0.7107 Å

Cell:

\[
\begin{align*}
&\text{a} = 10.1951(2) \\
&\text{b} = 14.4697(2) \\
&\text{c} = 14.8556(2) \\
&\text{alpha} = 90 \\
&\text{beta} = 100.3961(8) \\
&\text{gamma} = 90
\end{align*}
\]

Temperature: 293 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2155.52(6)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/m</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yb</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>Mo3 O40 Si W9, 10(3)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>Mo3 O50 Si W9</td>
</tr>
<tr>
<td>Mr</td>
<td>2770.47</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>4.269</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>24.897</td>
</tr>
<tr>
<td>F000</td>
<td>2412.0</td>
</tr>
<tr>
<td>F000'</td>
<td>2390.11</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>13,19,20</td>
</tr>
<tr>
<td>Nref</td>
<td>5740</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.026, 0.019</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.013</td>
</tr>
</tbody>
</table>

Correction method= #  Reported T Limits: Tmin=0.500  Tmax=0.950  AbsCorr = ?

Data completeness= 0.998  Thetamax= 28.620

R(reflections)= 0.0284 (4506)  wR2(reflections)= wR= 0.0448 (5729)

S = 1.920  Npar= 176
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**

- **GEOM006_ALERT_1_A**
  _geom_angle_atom_site_label_2 is missing
  Label identifying the atom site 2.

- **GEOM007_ALERT_1_A**
  _geom_angle_atom_site_label_3 is missing
  Label identifying the atom site 3.

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**Alert level B**

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow1 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow2 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow3 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow4 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow5 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ Ow6 Check

- **PLAT306_ALERT_2_B**
  Isolated Oxygen Atom (H-atoms Missing ?) ........ O20 Check

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**Alert level C**

- **PLAT041_ALERT_1_C**
  Calc. and Reported SumFormula Strings Differ Please Check

- **PLAT043_ALERT_1_C**
  Calculated and Reported Mol. Weight Differ by .... 24.23 Check

- **PLAT052_ALERT_1_C**
  Info on Absorption Correction Method Not Given Please Do !

- **PLAT202_ALERT_3_C**
  Isotropic non-H Atoms in Anion/Solvent ........... 7 Check

- **PLAT601_ALERT_2_C**
  Structure Contains Solvent Accessible VOIDS of .... 58 Ang3

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**Alert level G**

- **FORMU01_ALERT_2_G**
  There is a discrepancy between the atom counts in the
  _chemical_formula_sum and the formula from the _atom_site* data.
  Atom count from _chemical_formula_sum:H24 Mo3 O50 Si1 W9
  Atom count from the _atom_site data: Mo3 O50 Si1 W9

- **CELLZ01_ALERT_1_G**
  Difference between formula and atom_site contents detected.

- **CELLZ01_ALERT_1_G**
  WARNING: H atoms missing from atom site list. Is this intentional?
  From the CIF: _cell_formula_units_Z 2
  From the CIF: _chemical_formula_sum H24 Mo3 O50 Si1 W9
  TEST: Compare cell contents of formula and atom_site data

<table>
<thead>
<tr>
<th>atom</th>
<th>Z*formula</th>
<th>cif sites diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>48.00</td>
<td>0.00 48.00</td>
</tr>
<tr>
<td>Mo</td>
<td>6.00</td>
<td>6.00 0.00</td>
</tr>
<tr>
<td>O</td>
<td>100.00</td>
<td>100.00 0.00</td>
</tr>
<tr>
<td>Si</td>
<td>2.00</td>
<td>2.00 0.00</td>
</tr>
<tr>
<td>W</td>
<td>18.00</td>
<td>18.00 0.00</td>
</tr>
</tbody>
</table>

- **PLAT005_ALERT_5_G**
  No Embedded Refinement Details found in the CIF Please Do !

- **PLAT199_ALERT_1_G**
  Reported _cell_measurement_temperature ..... (K) 293 Check

- **PLAT200_ALERT_1_G**
  Reported _diffrn_ambient_temperature ..... (K) 293 Check

- **PLAT304_ALERT_4_G**
  Non-Integer Number of Atoms ( 0.50) in Resd. # 2 Check

- **PLAT304_ALERT_1_G**
  Non-Integer Number of Atoms ( 0.50) in Resd. # 5 Check

- **PLAT304_ALERT_1_G**
  Non-Integer Number of Atoms ( 0.50) in Resd. # 6 Check

- **PLAT304_ALERT_1_G**
  Non-Integer Number of Atoms ( 0.50) in Resd. # 8 Check

- **PLAT720_ALERT_4_G**
  Number of Unusual/Non-Standard Labels ........... 6 Note

- **PLAT790_ALERT_4_G**
  Centre of Gravity not Within Unit Cell: Resd. # 3 Note

- **PLAT790_ALERT_4_G**
  Centre of Gravity not Within Unit Cell: Resd. # 7 Note

- **PLAT790_ALERT_4_G**
  Centre of Gravity not Within Unit Cell: Resd. # 8 Note
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.

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PLATON version of 08/07/2016; check.def file version of 05/07/2016