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

Bond precision:  O - B = 0.0030 A
Wavelength=0.71073

Cell:

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>11.0685(2)</td>
<td>11.0685(2)</td>
</tr>
<tr>
<td>b</td>
<td>11.0685(2)</td>
<td>11.0685(2)</td>
</tr>
<tr>
<td>c</td>
<td>40.5755(19)</td>
<td>40.5755(19)</td>
</tr>
<tr>
<td>alpha</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>beta</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>gamma</td>
<td>120</td>
<td>120</td>
</tr>
</tbody>
</table>

Temperature: 293 K

Volume: 4305.0(3) 4305.0(3)
Space group: R -3 c
Hall group: -R 3 2"c
Moiety formula: C2 H19 B12 K6 Na O29
Sum formula: C2 H19 B12 K6 Na O29
Mr: 894.49 894.48
Dx,g cm-3: 2.070 2.070
Z: 6 6
Mu (mm-1): 1.041 1.041
F000: 2688.0 2688.0
F000': 2697.19
h,k,lmax: 13,13,50 13,13,50
Nref: 988 978
Tmin, Tmax: 0.829, 0.864 0.666, 0.745
Tmin': 0.829

Correction method: # Reported T Limits: Tmin=0.666 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness: 0.990
Theta(max): 26.391
R(reflections): 0.0351(904)
wr2(reflections): 0.1067(978)
S: 1.112
Npar: 110

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

An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

Alert level G

Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
Polymeric Structure Found with Maximum Dimension 3 Info
Number of Unrefined Donor-H Atoms ............. 4 Report
SHELXL Second Parameter in WGHT Unusually Large 15.67 Why?
The CIF-Embedded .res File Contains ISOR Records 2 Report
The CIF-Embedded .res File Contains RIGU Records 1 Report
Reported _cell_measurement_temperature ..... (K) 293 Check
Reported _diffrn_ambient_temperature ..... (K) 293 Check

Atom Site Occupancy of <O6     is Constrained at 0.1667 Check
Atom Site Occupancy of <O7     is Constrained at 0.1667 Check
Atom Site Occupancy of <C1     is Constrained at 0.1667 Check
Atom Site Occupancy of <C2     is Constrained at 0.1667 Check
Atom Site Occupancy of <H1A    is Constrained at 0.1667 Check
Atom Site Occupancy of <H1B    is Constrained at 0.1667 Check
Atom Site Occupancy of <H2A    is Constrained at 0.1667 Check
Atom Site Occupancy of <H2B    is Constrained at 0.1667 Check
Atom Site Occupancy of <H2C    is Constrained at 0.1667 Check
Atom Site Occupancy of <H6     is Constrained at 0.1667 Check
Atom Site Occupancy of <H7     is Constrained at 0.1667 Check
Main Residue Disorder ............... Percentage = 8 Note
Short Inter X...Y Contact  B2     ..  C2      ..  3.02 Ang.
Bond Calc 0.97000, Rep 0.96000 Dev... 0.01 Ang.

Atoms with Negative _atom_site_disorder_group  # 9 Check
Number of Least-Squares Restraints ............. 33 Note
Missing # of FCF Reflection(s) Below Theta(Min) 3 Note
Number of OMIT records in Embedded RES .......... 3 Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
15 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

checkCIF publication errors
**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 level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```plaintext
# start Validation Reply Form  
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
_RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
```
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 you wish to submit your CIF for publication in IUCrData, 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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