checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sd01

No syntax errors found.  CIF dictionary  Interpreting this report

Datablock: sd01

Bond precision:  C-C = 0.0056 A  Wavelength=0.71073

Cell:  a=11.8343(2)  b=11.8343(2)  c=26.9552(7)
       alpha=90  beta=90  gamma=90

Temperature:  150 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>3775.09(16)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -4 21 c</td>
</tr>
<tr>
<td>Hall group</td>
<td>P -4 2n</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C19 H24 N2 Na O</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C19 H24 N2 Na O</td>
</tr>
<tr>
<td>Mr</td>
<td>319.39</td>
</tr>
<tr>
<td>Dx,g cm^-3</td>
<td>1.124</td>
</tr>
<tr>
<td>Z</td>
<td>8</td>
</tr>
<tr>
<td>Mu (mm^-1)</td>
<td>0.089</td>
</tr>
<tr>
<td>F000</td>
<td>1368.0</td>
</tr>
<tr>
<td>F000'</td>
<td>1368.69</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>15,15,36</td>
</tr>
<tr>
<td>Nref</td>
<td>2718[ 4884]</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.960,0.978</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.958</td>
</tr>
</tbody>
</table>

Correction method= MULTI-SCAN

Data completeness= 1.79/1.00  Theta(max)= 28.700

R(reflections)= 0.0656( 2883)  wr2(reflections)= 0.1930( 4876)

S = 1.007  Npar= 229

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 B
PLAT220_ALERT_2_B Large Non-Solvent  C  Ueq(max)/Ueq(min) ...  4.4 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for  C12 -- C14 ..  8.1 su
```
Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.19
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C19A -- C18A .. 0.16 Ang.
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C9
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C12
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 6
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) ..... 3
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4

Alert level G

REFLT03_ALERT_4_G ALERT: MoKa measured Friedel data cannot be used to determine absolute structure in a light-atom study EXCEPT under VERY special conditions. It is preferred that Friedel data is merged in such cases.

From the CIF: _differn_reflns_theta_max 28.70
From the CIF: _reflns_number_total 4876
Count of symmetry unique reflns 2718
Completeness (_total/calc) 179.40%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2158
Fraction of Friedel pairs measured 0.794
Are heavy atom types Z>Si present no
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 1
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.500
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.11
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by .... 3 Units
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for C18
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for C18A
PLAT301_ALERT_3_G Note: Main Residue Disorder ................... 8 Perc.
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety C1
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety C5
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.24 Ratio
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by . 0.20

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
6 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, 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 30/05/2011; check.def file version of 24/05/2011