checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 13002

No syntax errors found.  CIF dictionary  Interpreting this report

Datablock: 13002

Bond precision:  C-C = 0.0063 Å  Wavelength=0.7107 Å

Cell:

a=22.041(3)  b=9.2035(14)  c=22.084(3)

alpha=90  beta=98.579(3)  gamma=90

Temperature:  100 K

Volume  4429.7(11)  Reported  4429.7(11)

Space group  P 21/n

Hall group  -P 2yn

Moiety formula  C₁₃ H₁₄ F₆ N₄ O₈ S₂ Zn

Sum formula  C₁₃ H₁₄ F₆ N₄ O₈ S₂ Zn

Mr  597.81  597.77

Dx, g cm⁻³  1.793  1.793

Z  8  8

Mu (mm⁻¹)  1.396  1.396

F000  2400.0  2400.0

F000'  2405.89

h,k,lmax  29,12,29  29,12,28

Nref  11046  10840

Tmin,Tmax  0.735,0.778  0.619,0.787

Tmin'  0.582

Correction method= MULTI-SCAN

Data completeness= 0.981  Theta(max)= 28.327

R(reflections)= 0.0510( 9951)  wR²(reflections)= 0.1486( 10840)

S = 1.005  Npar= 627

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 B

Crystal system given = monoclinic

PLAT922_ALERT_1_B  wr2 in the CIF and FCF Differ by ...............  0.0073

PLAT927_ALERT_1_B  Reported and Calculated  wr2 Differ by ...........  0.0072
### Alert level C

<table>
<thead>
<tr>
<th>Alert Code</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT341_ALERT_3_C</td>
<td>Low Bond Precision on C-C Bonds</td>
<td>0.0063 Ang</td>
</tr>
<tr>
<td>PLAT353_ALERT_3_C</td>
<td>Long N-H Bond (0.87A) N2A - H2A</td>
<td>1.05 Ang.</td>
</tr>
<tr>
<td>PLAT431_ALERT_2_C</td>
<td>Short Inter HL..A Contact F3B .. O1A</td>
<td>2.88 Ang.</td>
</tr>
<tr>
<td>PLAT910_ALERT_3_C</td>
<td>Missing # of FCF Reflections Below Th(Min)</td>
<td>2</td>
</tr>
<tr>
<td>PLAT911_ALERT_3_C</td>
<td>Missing # FCF Refl Between Thmin &amp; STh/L= 0.600</td>
<td>63</td>
</tr>
<tr>
<td>PLAT921_ALERT_1_C</td>
<td>R1 in the CIF and FCF Differ by</td>
<td>0.0023</td>
</tr>
<tr>
<td>PLAT923_ALERT_1_C</td>
<td>S values in the CIF and FCF Differ by</td>
<td>0.129</td>
</tr>
<tr>
<td>PLAT926_ALERT_1_C</td>
<td>Reported and Calculated R1 Differ by</td>
<td>0.0023</td>
</tr>
<tr>
<td>PLAT928_ALERT_1_C</td>
<td>Reported and Calculated S value Differ by</td>
<td>0.128</td>
</tr>
<tr>
<td>PLAT973_ALERT_2_C</td>
<td>Large Calcd. Positive Residual Density on Zn1A</td>
<td>1.45 eA-3</td>
</tr>
<tr>
<td>PLAT973_ALERT_2_C</td>
<td>Large Calcd. Positive Residual Density on Zn1B</td>
<td>1.32 eA-3</td>
</tr>
</tbody>
</table>

### Alert level G

<table>
<thead>
<tr>
<th>Alert Code</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT003_ALERT_2_G</td>
<td>Number of Uiso or Uij Restrained Atom Sites</td>
<td>28</td>
</tr>
<tr>
<td>PLAT083_ALERT_2_G</td>
<td>No _iucr_refine_instructions_details in the CIF</td>
<td>?</td>
</tr>
<tr>
<td>PLAT128_ALERT_4_G</td>
<td>Alternate Setting of Space-group P21/c</td>
<td>P21/n</td>
</tr>
<tr>
<td>PLAT720_ALERT_4_G</td>
<td>Number of Unusual/Non-Standard Labels</td>
<td>16</td>
</tr>
<tr>
<td>PLAT912_ALERT_4_G</td>
<td>Missing # of FCF Reflections Above STh/L= 0.600</td>
<td>122</td>
</tr>
</tbody>
</table>

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 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 05/11/2012; check.def file version of 05/11/2012**