checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 120321d_0m

Bond precision:  C-C = 0.0050 Å  Wavelength=0.7107 Å

Cell:  
a=5.444(3)  b=10.883(5)  c=10.373(5)
alpha=90  beta=98.308(7)  gamma=90

Temperature:  293 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>608.1(5)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ybc</td>
</tr>
<tr>
<td>Moleity formula</td>
<td>C10 H10 Cu N4 O6</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C10 H10 Cu N4 O6</td>
</tr>
<tr>
<td>Mr</td>
<td>345.77</td>
</tr>
<tr>
<td>Dx, g cm^-3</td>
<td>1.888</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm^-1)</td>
<td>1.833</td>
</tr>
<tr>
<td>F000</td>
<td>350.0</td>
</tr>
<tr>
<td>F000’</td>
<td>350.80</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>7,14,13</td>
</tr>
<tr>
<td>Nref</td>
<td>1391</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.680,0.817</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.541</td>
</tr>
</tbody>
</table>

Correction method= MULTI-SCAN

Data completeness= 0.986  Theta(max)= 27.490

R(reflections)= 0.0521( 995)  wr2(reflections)= 0.1166( 1371)

S = 0.955  Npar= 103

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

ABSTY02_ALERT_1_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
The word below has not been recognised as a standard identifier.
little
The value of Rint is greater than 0.12
Rint given 0.133
Large U3/U1 Ratio for Average U(i,j) Tensor ....     2.2

**Alert level G**

- PLAT002_ALERT_2_G: Number of Distance or Angle Restraints on AtSite 3
- PLAT005_ALERT_5_G: No _iucr_refine_instructions_details in CIF ....  ?
- PLAT194_ALERT_1_G: Missing _cell_measurement_reflns_used datum ....  ?
- PLAT195_ALERT_1_G: Missing _cell_measurement_theta_max datum ....  ?
- PLAT196_ALERT_1_G: Missing _cell_measurement_theta_min datum ....  ?
- PLAT199_ALERT_1_G: Check the Reported _cell_measurement_temperature 293 K
- PLAT200_ALERT_1_G: Check the Reported _diffrn_ambient_temperature 293 K
- PLAT710_ALERT_4_G: Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 1
  O2 -CU1 -O2 -C5  17.00  0.00   3.665   1.555   1.555   1.555
- PLAT710_ALERT_4_G: Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 8
  N1 -CU1 -N1 -C1  14.00  0.00   3.665   1.555   1.555   1.555
- PLAT710_ALERT_4_G: Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 13
  N1 -CU1 -N1 -C3  4.00  0.00   3.665   1.555   1.555   1.555
- PLAT720_ALERT_4_G: Number of Unusual/Non-Standard Labels ........... 2
- PLAT794_ALERT_5_G: Note: Tentative Bond Valency for Cu1 (II) 2.24
- PLAT860_ALERT_3_G: Note: Number of Least-Squares Restraints ........ 3

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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 12/03/2012; check.def file version of 10/02/2012**