<table>
<thead>
<tr>
<th><strong>Title</strong></th>
<th>Copper-catalysed asymmetric sulfide oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Author(s)</strong></td>
<td>O'Mahony, Graham E.</td>
</tr>
<tr>
<td><strong>Publication date</strong></td>
<td>2013</td>
</tr>
<tr>
<td><strong>Type of publication</strong></td>
<td>Doctoral thesis</td>
</tr>
<tr>
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<td>© 2013, Graham E. O'Mahony</td>
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</tbody>
</table>

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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: 2g

Bond precision:  C-C = 0.0051 A        Wavelength=0.71073

Cell:  a=5.7020(9)      b=8.4251(13)      c=14.510(2)
       alpha=75.881(3)   beta=89.787(3)   gamma=89.329(3)

Temperature:  296 K

Calculated  Reported
Volume       675.96(18)      675.96(18)
Space group  P 1      P 1
Hall group   P 1      P 1
Moiety formula  C17 H14 O S        C17 H14 O S
Sum formula   C17 H14 O S        C17 H14 O S
Mr            266.35        266.34
Dx,g cm-3    1.309        1.309
Z             2              2
Mu (mm-1)    0.227        0.227
F000         280.0        280.0
F000’        280.35
h,k,lmax     6,10,17      6,10,17
Nref          2599[ 5198]  4784
Tmin,Tmax    0.957,0.980  0.840,0.980
Tmin’        0.917

Correction method= MULTI-SCAN

Data completeness= 1.84/0.92        Theta(max)= 25.780
R(reflections)= 0.0433( 3208)        wR2(reflections)= 0.0938( 4784)
S = 0.901        Npar= 343

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**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT029_ALERT_3_C</td>
<td>_diffrn_measured_fraction_theta_full Low</td>
<td>0.965</td>
</tr>
<tr>
<td>PLAT331_ALERT_2_C</td>
<td>Small Average Phenyl C-C Dist. C34 -C39</td>
<td>1.37 Ang.</td>
</tr>
<tr>
<td>PLAT340_ALERT_3_C</td>
<td>Low Bond Precision on C-C Bonds</td>
<td>0.0051 Ang.</td>
</tr>
</tbody>
</table>
Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffrn_reflns_theta_max           25.78
From the CIF: _reflns_number_total               4784
Count of symmetry unique reflns         2599
Completeness (_total/calc)               184.07%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured       2185
Fraction of Friedel pairs measured       0.841
Are heavy atom types Z>Si present        yes

The su’s on the Cell Angles are Equal ............ 0.00300 Deg.

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.

PLATON version of 04/07/2012; check.def file version of 28/06/2012