


Title	Copper-catalysed asymmetric sulfide oxidation
Author(s)	O'Mahony, Graham E.
Publication date	2013
Original citation	O'Mahony, G. E. 2013. Copper-catalysed asymmetric sulfide oxidation. Ph.D. Thesis, University College Cork.
Type of publication	Doctoral thesis
Rights	<p>© 2013, Graham E. O'Mahony</p> <p>http://creativecommons.org/licenses/by-nc-nd/3.0/</p> 
Item downloaded from	http://hdl.handle.net/10468/1173

Downloaded on 2019-01-19T10:36:09Z

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	Low	0.965
PLAT331_ALERT_2_C	Small Average Phenyl	C-C Dist.	C34 -C39	1.37 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.0051 Ang

● Alert level G

REFLT03_ALERT_4_G 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_reflms_theta_max      25.78
From the CIF: _reflms_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
```

PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00300 Deg.

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

