

Title	Copper-catalysed asymmetric sulfide oxidation
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# UCC

**University College Cork, Ireland**  
Coláiste na hOllscoile Corcaigh

# 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: 2f

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Bond precision:    C-C = 0.0038 A                      Wavelength=0.71073  
Cell:                      a=5.6554(8)              b=14.536(2)              c=16.378(2)  
                                    alpha=90                      beta=90                      gamma=90  
Temperature:              300 K

	Calculated	Reported
Volume	1346.4(3)	1346.4(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
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	1.314	1.314
Z	4	4
Mu (mm-1)	0.228	0.228
F000	560.0	560.0
F000'	560.71	
h,k,lmax	7,18,20	7,18,20
Nref	1651[ 2809]	2764
Tmin,Tmax	0.962,0.971	0.689,0.745
Tmin'	0.962	

Correction method= MULTI-SCAN

Data completeness= 1.67/0.98                      Theta(max)= 26.580

R(reflections)= 0.0396( 2122)                      wR2(reflections)= 0.0884( 2764)

S = 1.023    Npar= 172


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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 C**  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for    C7    --    C8    ..    5.5 su

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 **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: <code>_diffrn_reflns_theta_max</code>	26.58
From the CIF: <code>_reflns_number_total</code>	2764
Count of symmetry unique reflns	1651
Completeness ( <code>_total/calc</code> )	167.41%
TEST3: Check Friedels for noncentro structure	
Estimate of Friedel pairs measured	1113
Fraction of Friedel pairs measured	0.674
Are heavy atom types Z>Si present	yes

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

0 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  
0 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

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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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