

Structure factors have been supplied for datablock(s) 4MePy4Ag2_Tos2

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0021 Å	Wavelength=1.54184	
Cell:	a=9.48181(5)	b=11.83720(7)	c=16.98475(10)
	alpha=90	beta=90.0419(5)	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	1906.335(19)	1906.336(18)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C38 H42 Ag2 N4 O6 S2	C24 H28 Ag2 N4, 2(C7 H7 O3 S)	
Sum formula	C38 H42 Ag2 N4 O6 S2	C38 H42 Ag2 N4 O6 S2	
Mr	930.62	930.61	
Dx, g cm-3	1.621	1.621	
Z	2	2	
Mu (mm-1)	9.683	9.683	
F000	944.0	944.0	
F000'	948.17		
h, k, lmax	11, 14, 20	11, 14, 20	
Nref	3374	3375	
Tmin, Tmax	0.548, 0.587	0.676, 0.780	
Tmin'	0.402		

Data completeness= 1.000 Theta (max)= 66.746

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R(reflections)= 0.0160( 3353)      wR2(reflections)=
S = 1.071                        0.0430( 3375)
Npar= 238
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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.



Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check



Alert level G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00007 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag1 --N2 . 5.3 s.u.
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 98% Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 133.5 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 14 Info

- 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
7 **ALERT level G** = General information/check it is not something unexpected

- 1 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
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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* or *IUCrData*, 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.

