

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4CNPY4Ag2_Heps2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4CNPY4Ag2_Heps2

Bond precision: C-C = 0.0021 Å Wavelength=1.54184

Cell: a=8.3444(2) b=10.8479(2) c=12.5798(3)
 alpha=99.107(2) beta=100.320(2) gamma=107.639(2)
Temperature: 120 K

	Calculated	Reported
Volume	1039.82(4)	1039.82(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H46 Ag2 N8 O6 S2	2(C19 H23 Ag N4 O3 S)
Sum formula	C38 H46 Ag2 N8 O6 S2	C38 H46 Ag2 N8 O6 S2
Mr	990.69	990.69
Dx, g cm ⁻³	1.582	1.582
Z	1	1
Mu (mm ⁻¹)	8.943	8.943
F000	504.0	504.0
F000'	506.18	
h, k, lmax	9, 12, 14	9, 12, 14
Nref	3670	3664
Tmin, Tmax	0.278, 0.374	0.588, 0.932
Tmin'	0.134	

Correction method= # Reported T Limits: Tmin=0.588 Tmax=0.932
AbsCorr = GAUSSIAN

Data completeness= 0.998 Theta(max)= 66.740

R(reflections)= 0.0150(3650)	wR2(reflections)= 0.0387(3664)
S = 1.093	Npar= 254

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
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.596	6 Report



Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C3 --C6 .	5.2 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C9 --C12 .	6.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --O1 .	12.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --N1 .	5.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --O1_a .	5.2 s.u.
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	99% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.5 Low
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
2 **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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
0 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.

