

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 18zs_boo_so10_0m

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: 18zs_boo_so10_0m

Bond precision:	C-C = 0.0065 A	Wavelength=0.71073
Cell:	a=8.1650(5)	b=15.5778(9) c=16.2365(10)
	alpha=77.700(1)	beta=87.359(2) gamma=83.158(3)
Temperature:	100 K	
	Calculated	Reported
Volume	2002.9(2)	2002.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H46 Ag2 N4 S4	C40 H46 Ag2 N4 S4
Sum formula	C40 H46 Ag2 N4 S4	C40 H46 Ag2 N4 S4
Mr	926.79	926.79
Dx,g cm-3	1.537	1.537
Z	2	2
Mu (mm-1)	1.220	1.220
F000	944.0	944.0
F000'	941.62	
h,k,lmax	10,19,20	10,19,20
Nref	8753	8657
Tmin,Tmax	0.757,0.874	0.683,0.746
Tmin'	0.677	

Correction method= # Reported T Limits: Tmin=0.683 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.999

R(reflections)= 0.0418(6302) wR2(reflections)= 0.1196(8657)

S = 0.983 Npar= 474

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

PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max) / Ueq(min) Range	4.2	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.8	Ratio
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible Voids of .		32	Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	67	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.86A From Agl	1.55	eA-3

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		5	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	2%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H23 ..H42B .	1.99	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H33 ..H42A .	2.06	Ang.
		1+x,y,z =	1_655	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		2	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON		1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		7	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	27	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
4 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.

