

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Silvercyanoguanidine

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: Silvercyanoguanidine

Bond precision: N- C = 0.0115 A Wavelength=0.71073

Cell: a=10.670(3) b=18.236(5) c=3.5078(9)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	682.5(3)	682.5(3)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	2(C2 H4 Ag N5 O3), H2 O	?
Sum formula	C4 H10 Ag2 N10 O7	C4 H10 Ag2 N10 O7
Mr	525.96	525.96
Dx,g cm-3	2.559	2.559
Z	2	2
Mu (mm-1)	2.929	2.929
F000	508.0	508.0
F000'	504.60	
h,k,lmax	13,23,4	13,23,4
Nref	1532[948]	1533
Tmin,Tmax	0.839,0.864	0.189,0.746
Tmin'	0.093	

Correction method= # Reported T Limits: Tmin=0.189 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.62/1.00 Theta(max)= 27.139

R(reflections)= 0.0453(1080) wR2(reflections)= 0.0911(1533)

S = 0.993 Npar= 121

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**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.84	Note
PLAT353_ALERT_3_C	Long N-H (N0.87,N1.01A) N4 - H4B .	1.01	Ang.
PLAT353_ALERT_3_C	Long N-H (N0.87,N1.01A) N5 - H5B .	1.01	Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.81	mm
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --N3_b .	5.8	s.u.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	8	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.8	Low

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

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

PLATON version of 18/09/2020; check.def file version of 20/08/2020

