checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: seab054

Bond precision: C-C = 0.0036 A Wavelength=0.71073

Cell: a=9.022(12) b=9.973(13) c=14.506(19)
alpha=106.661(16) beta=102.324(16) gamma=99.959(16)
Temperature: 200 K

	Calculated	Reported
Volume	1183(3)	1183(3)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C17 H38 Ag N3 Si2	?
Sum formula	C17 H38 Ag N3 Si2	C17 H38 Ag N3 Si2
Mr	448.55	448.55
Dx,g cm-3	1.259	1.259
Z	2	2
Mu (mm-1)	0.957	0.957
F000	472.0	472.0
F000'	470.61	
h,k,lmax	12,13,19	12,13,19
Nref	5871	5830
Tmin,Tmax	0.716,0.850	0.722,0.857
Tmin'	0.702	

Correction method= NONE

Data completeness= 0.993 Theta(max)= 28.290

R(reflections)= 0.0250(5605) wR2(reflections)= 0.0685(5830)

S = 1.039 Npar= 220

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 B

PLAT148_ALERT_3_B su on the a - Axis is Too Large (x 1000) . 12 Ang.
PLAT148_ALERT_3_B su on the b - Axis is Too Large (x 1000) . 13 Ang.
PLAT148_ALERT_3_B su on the c - Axis is Too Large (x 1000) . 19 Ang.
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Si2

Alert level C

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ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
            However values have been given for Tmin and Tmax. Remove
            these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.722
  From the CIF: _exptl_absorpt_correction_T_max   0.857
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.19
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.07
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.12 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Ag     --  Si1     ..      10.00 su
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Alert level G

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PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)       1600 Deg.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         13
            C1  -AG  -N3  -SI2   -89.10  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         14
            C1  -AG  -N3  -SI1    71.80  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         23
            N3  -AG  -C1  -N2    169.70  1.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         24
            N3  -AG  -C1  -N1     -9.50  1.90   1.555   1.555   1.555   1.555
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   4 **ALERT level B** = A potentially serious problem, consider carefully
   7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   5 **ALERT level G** = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 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*, 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 16/02/2011; check.def file version of 16/02/2011

Datablock seab054 - ellipsoid plot