checkCIF/PLATON report

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

Datablock: danr129a

Bond precision: C-C = 0.0100 A Wavelength=0.71073

Cell: a=30.433(8) b=6.7319(11) c=28.332(6)
alpha=90 beta=112.54(3) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	5361(2)	5361(2)
Space group	C c	Cc
Hall group	C -2yc	?
Moiety formula	C24 H40 Ag N O4 S2 Si	?
Sum formula	C24 H40 Ag N O4 S2 Si	C24 H42 AG N O4 S2 SI
Mr	606.67	608.67
Dx,g cm-3	1.503	1.508
Z	8	8
Mu (mm-1)	0.983	0.983
F000	2528.0	2544.0
F000’	2524.26	
h,k,lmax	40,8,37	40,8,36
Nref	6600[13196]	9316
Tmin,Tmax	0.838,0.934	0.820,0.934
Tmin’	0.813	

Correction method= MULTI-SCAN

Data completeness= 1.41/0.71 Theta(max)= 28.210

R(reflections)= 0.0473(7311) wR2(reflections)= 0.1015(9316)

S = 1.031 Npar= 600

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
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag1 -- O1 .. 13.25 su

Author Response: Atom identities consistent with synthetic method.

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O5

Author Response: Atom identities consistent with synthetic method.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for N1

Author Response: Atom identities consistent with synthetic method.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for N2

Author Response: Atom identities consistent with synthetic method.

PLAT430_ALERT_2_B Short Inter D...A Contact O3 .. O4 .. 2.68 Ang.

Author Response: Initial solutions show H-bonding interactions however H-atom positions are computationally unstable and were ignored.

PLAT430_ALERT_2_B Short Inter D...A Contact O4 .. O6 .. 2.78 Ang.

Author Response: Initial solutions show H-bonding interactions however H-atom positions are computationally unstable and were ignored.

PLAT430_ALERT_2_B Short Inter D...A Contact O7 .. O8 .. 2.71 Ang.

Author Response: Initial solutions show H-bonding interactions however H-atom positions are computationally unstable and were ignored.

PLAT115_ALERT_5_B ADDSYM Detects Noncrystallographic Inversion ... 96 PerFi

Author Response: Solutions in C2/c (R ~14%) are computationally unstable unless 691 restraints are applied. The current structure in Cc uses only 50 restraints.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.520
From the CIF: _refine_ls_abs_structure_Flack_su 0.020
PLAT213_ALERT_2_C Atom O3 has ADP max/min Ratio ..... 3.30 prola
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1

Author Response: Atom identities consistent with synthetic method.

```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..         10
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT234_ALERT_4_C Large Hirshfeld Difference C4     --  C5      ..       0.16 Ang.
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Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C24 H42 Ag1 N1 O4 S2 Si1
           Atom count from the _atom_site data:  C24 H40 Ag1 N1 O4 S2 Si1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
```

Author Response: See response to PLAT430

```
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C24 H42 Ag N O4 S2 Si
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        192.00    192.00    0.00
          H        336.00    320.00   16.00
          Ag         8.00      8.00    0.00
          N          8.00      8.00    0.00
          O         32.00     32.00    0.00
          S         16.00     16.00    0.00
          Si         8.00      8.00    0.00
```

Author Response: See response to PLAT430

```
REFLT03_ALERT_4_G  WARNING: Large fraction of Friedel related reflns may
                     be needed to determine absolute structure
          From the CIF: _diffrn_reflns_theta_max          28.21
          From the CIF: _reflns_number_total              9316
          Count of symmetry unique reflns         6600
          Completeness (_total/calc)           141.15%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      2716
          Fraction of Friedel pairs measured     0.412
          Are heavy atom types Z>Si present        yes
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         50
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero .....       0.52
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   0 ALERT level A = In general: serious problem
   8 ALERT level B = Potentially serious problem
   7 ALERT level C = Check and explain
   6 ALERT level G = General alerts; check

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 13/08/2009; check.def file version of 12/08/2009

Datablock danr129a - ellipsoid plot