checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 6

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Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:          a=8.8804(3)       b=12.4215(4)     c=25.7892(7)
               alpha=96.136(2)   beta=92.641(2)   gamma=107.740(3)
Temperature:   123 K
```

	Calculated	Reported
Volume	2684.65(15)	2684.65(14)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C54 H54 Ag2 N6 P2 S4), C3 H6 O	2(C54 H54 Ag2 N6 P2 S4), C3 H6 O
Sum formula	C111 H114 Ag4 N12 O P4 S8	C111 H114 Ag4 N12 O P4 S8
Mr	2443.98	2443.98
Dx,g cm-3	1.512	1.512
Z	1	1
Mu (mm-1)	0.989	0.989
F000	1248.0	1248.0
F000’	1246.11	
h,k,lmax	13,18,39	13,18,39
Nref	19845	17860
Tmin,Tmax	0.779,0.888	0.983,1.000
Tmin’	0.714	

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Correction method= # Reported T Limits: Tmin=0.983 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.900          Theta(max)= 32.740

R(reflections)= 0.0367( 11618)    wR2(reflections)= 0.0642( 17860)

S = 0.867                 Npar= 653
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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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C3D -- C4D .. 8.3 s.u.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C4D -- C5D .. 7.0 s.u.
PLAT420_ALERT_2_C D-H Without Acceptor N13 -- H13B ... Please Check
PLAT420_ALERT_2_C D-H Without Acceptor N23 -- H23B ... Please Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H23B .. S1B .. 2.93 Ang.

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag1 -- S1A_a .. 39.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag2 -- N21 .. 5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag2 -- S1B_b .. 27.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of *O1S is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C1S is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C2S is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C3S is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2SA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2SB is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2SC is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H3SA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H3SB is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H3SC is Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 100 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C3S Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O1S .. C3S .. 2.23 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C1S .. C3S .. 1.13 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C1S .. C1S .. 2.26 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C1S .. C2S .. 2.64 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C2S .. C3S .. 1.04 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C3S .. C3S .. 1.68 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 36 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 237 Check
C3S -C1S -C2S 2.555 1.555 1.555 42.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 256 Check
C1S -C3S -C3S 1.555 1.555 2.555 39.80 Deg.
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
17 ALERT type 4 Improvement, methodology, query or suggestion
2 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 19/11/2015; check.def file version of 17/11/2015

Datablock 6 - ellipsoid plot