checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ao_ao_au2p2ccr2_colorless_2_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: ao_ao_au2p2ccr2_colorless_2_0m

Bond precision: C-C = 0.0085 A Wavelength=0.71073

Cell: a=10.8708(5) b=11.0738(5) c=11.7702(5)
alpha=76.6130(13) beta=83.5313(14) gamma=74.0031(14)
Temperature: 180 K

	Calculated	Reported
Volume	1323.22(10)	1323.22(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C52 H44 Au2 P4, 2(C F3 O3 S)	C52 H44 Au2 P4, 2(C1 F3 O3 S1)
Sum formula	C54 H44 Au2 F6 O6 P4 S2	C54 H44 Au2 F6 O6 P4 S2
Mr	1484.83	1484.82
Dx,g cm-3	1.863	1.863
Z	1	1
Mu (mm-1)	5.808	5.808
F000	720.0	720.0
F000'	717.07	
h,k,lmax	15,15,16	15,15,16
Nref	7517	7504
Tmin,Tmax	0.438,0.559	0.539,0.746
Tmin'	0.414	

Correction method= # Reported T Limits: Tmin=0.539 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 29.696

R(reflections)= 0.0386(6495) wR2(reflections)= 0.0745(7504)

S = 1.134 Npar= 411

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C52 H44 Au2 P4, 2(C F3 O3 S)
              Rep.: C52 H44 Au2 P4, 2(C1 F3 O3 S1)
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00852 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.180 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.34Ang From P1            1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.99Ang From C30          -1.84 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        16 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        19 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Au1      --P1        .     18.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Au1      --P2_a      .     26.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Au1A     --P1        .     19.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Au1A     --P2_a      .     27.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)      5.83 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)      2.17 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       125 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        13 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........       1.86 Note
              Predicted wR2: Based on SigI**2  4.01 or SHELX Weight  6.76
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
```

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

2 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
 16 ALERT type 3 Indicator that the structure quality may be low
  9 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 06/01/2024; check.def file version of 05/01/2024

Datablock ao_ao_au2p2ccr2_colorless_2_0m - ellipsoid plot