checkCIF/PLATON report

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

Datablock: fa-lsogau

Bond precision: C-C = 0.0090 A Wavelength=0.71070

Cell: **a=10.1329(3) b=12.4857(4) c=15.3870(7)**
alpha=110.370(4) beta=96.693(3) gamma=90.526(3)
Temperature: 130 K

	Calculated	Reported
Volume	1809.94(12)	1809.94(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H28 Cl4 Hg2 O4 S2, 2(C2 H6 O S)	C22 H28 Cl4 Hg2 O4 S2, 2(C2 H6 O S)
Sum formula	C26 H40 Cl4 Hg2 O6 S4	C26 H40 Cl4 Hg2 O6 S4
Mr	1119.84	1119.80
Dx,g cm-3	2.055	2.055
Z	2	2
Mu (mm-1)	9.034	9.034
F000	1072.0	1072.0
F000’	1065.43	
h,k,lmax	14,17,21	14,17,20
Nref	10658	9370
Tmin,Tmax	0.407,0.582	0.208,0.637
Tmin’	0.084	

Correction method= GAUSSIAN

Data completeness= 0.879 Theta(max)= 30.080

R(reflections)= 0.0436(7543) wR2(reflections)= 0.1137(9370)

S = 1.057 Npar= 389

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.52
PLAT230_ALERT_2_C Hirshfeld Test Diff for S2 -- C12 .. 7.0 su
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0090 Ang

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Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT022_ALERT_3_G Ratio Unique / Expected Reflections (too) Low ..      0.879
PLAT793_ALERT_4_G The Model has Chirality at C1      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C12     (Verify) ....          S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          6
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 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

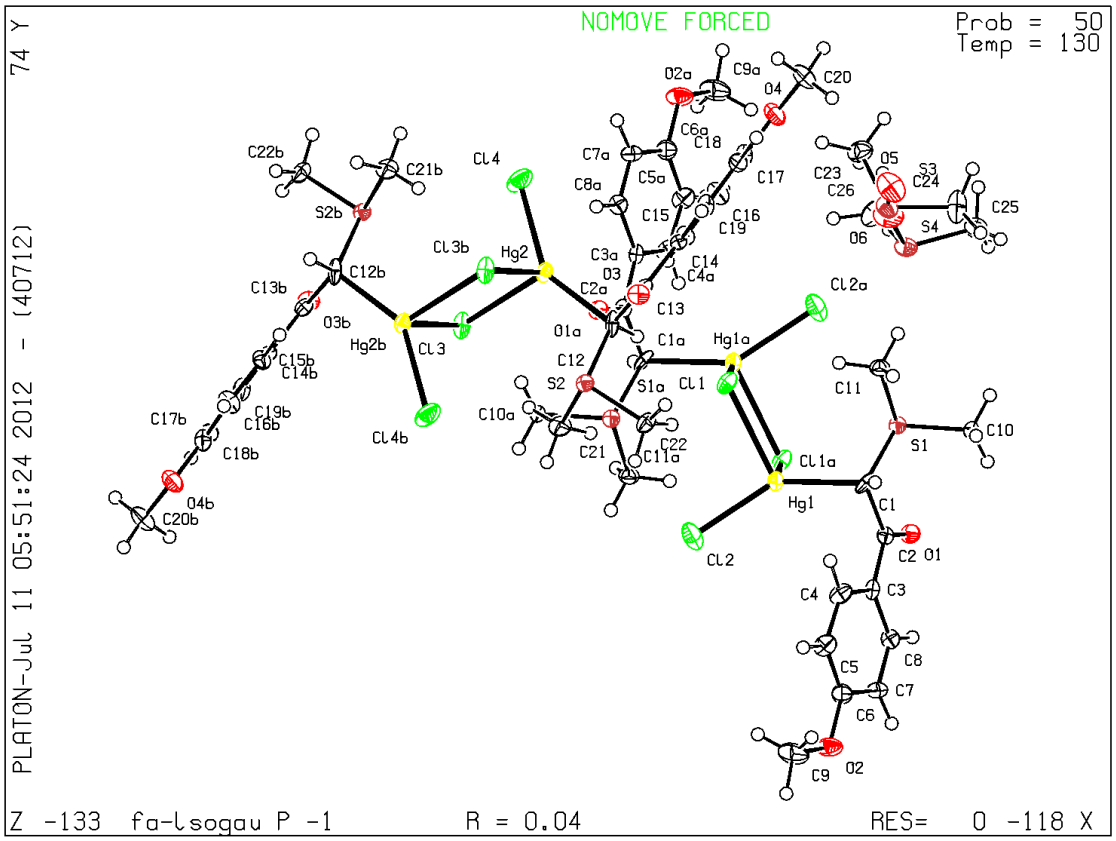
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 04/07/2012; check.def file version of 28/06/2012

Datablock fa-lsogau - ellipsoid plot



checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: h__solution_494_new

```
Bond precision:  C-C = 0.0192 A          Wavelength=0.71073

Cell:            a=15.5940(7)    b=7.3471(4)         c=15.0885(7)
                 alpha=90        beta=115.877(3)     gamma=90
Temperature:     298 K

                 Calculated                Reported
Volume           1555.37(14)               1555.37(13)
Space group      P 21/c                    P21/c
Hall group       -P 2ybc                   ?
Moiety formula   C22 H28 Br4 Hg2 O4 S2     ?
Sum formula      C22 H28 Br4 Hg2 O4 S2     C22 H28 Br4 Hg2 O4 S2
Mr               1141.36                   1141.36
Dx,g cm-3        2.437                     2.437
Z                2                         2
Mu (mm-1)        15.156                    15.156
F000             1048.0                    1048.0
F000'            1038.16
h,k,lmax         19,9,18                   19,9,18
Nref             3051                      3046
Tmin,Tmax        0.006,0.048               0.350,0.720
Tmin'            0.002

Correction method= NUMERICAL

Data completeness= 0.998          Theta(max)= 26.000

R(reflections)= 0.0796( 2543)     wR2(reflections)= 0.2121( 3046)

S = 1.075                 Npar= 155
```

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Alert level C

```
DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =     -6.020
           Test value =     -6.000
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
```

```
            The relevant atom site should be identified.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0192 Ang
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.15
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Hg1    --  Br2     ..       14.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Hg1    --  Br2_a   ..       16.1 su
PLAT793_ALERT_4_G The Model has Chirality at C3     (Verify) ....          S
```

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