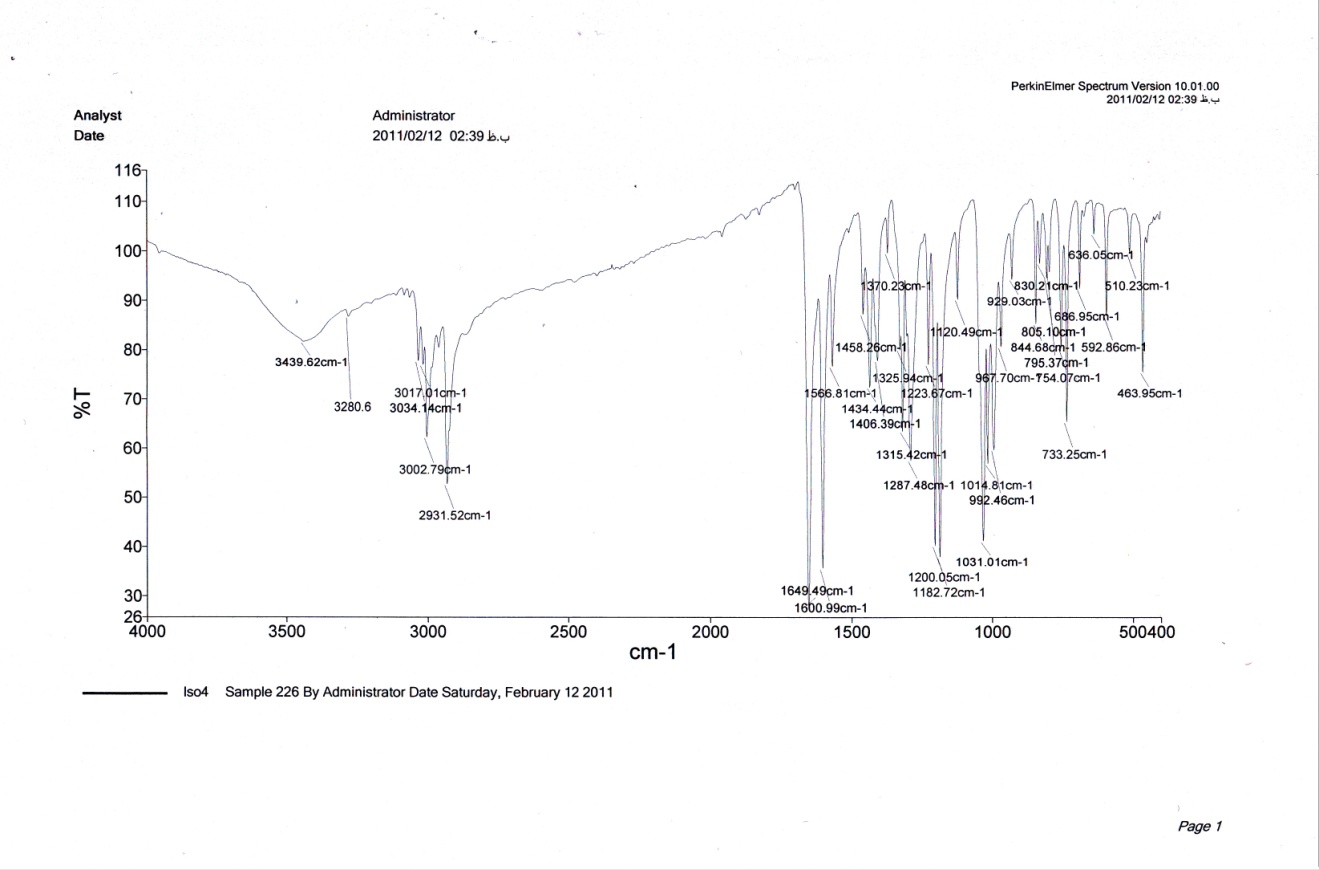
**X-ray Crystal Structure and Spectral Characterization of Pseudo Five-Coordinate Hg(II) Polymeric and Four-Coordinate Binuclear Complexes of an Ambidentate Sulfonium Ylide**

Seyyed Javad Sabounchei\*a, Fateme Akhlaghi Bagherjeria, Marjan Hosseinzadeha, Colette Boskovicb, Robert W. Gableb

aFaculty of Chemistry, Bu-Ali Sina University, Hamedan, 65174, Iran, Tel: +98811828280, Fax: +988118257408

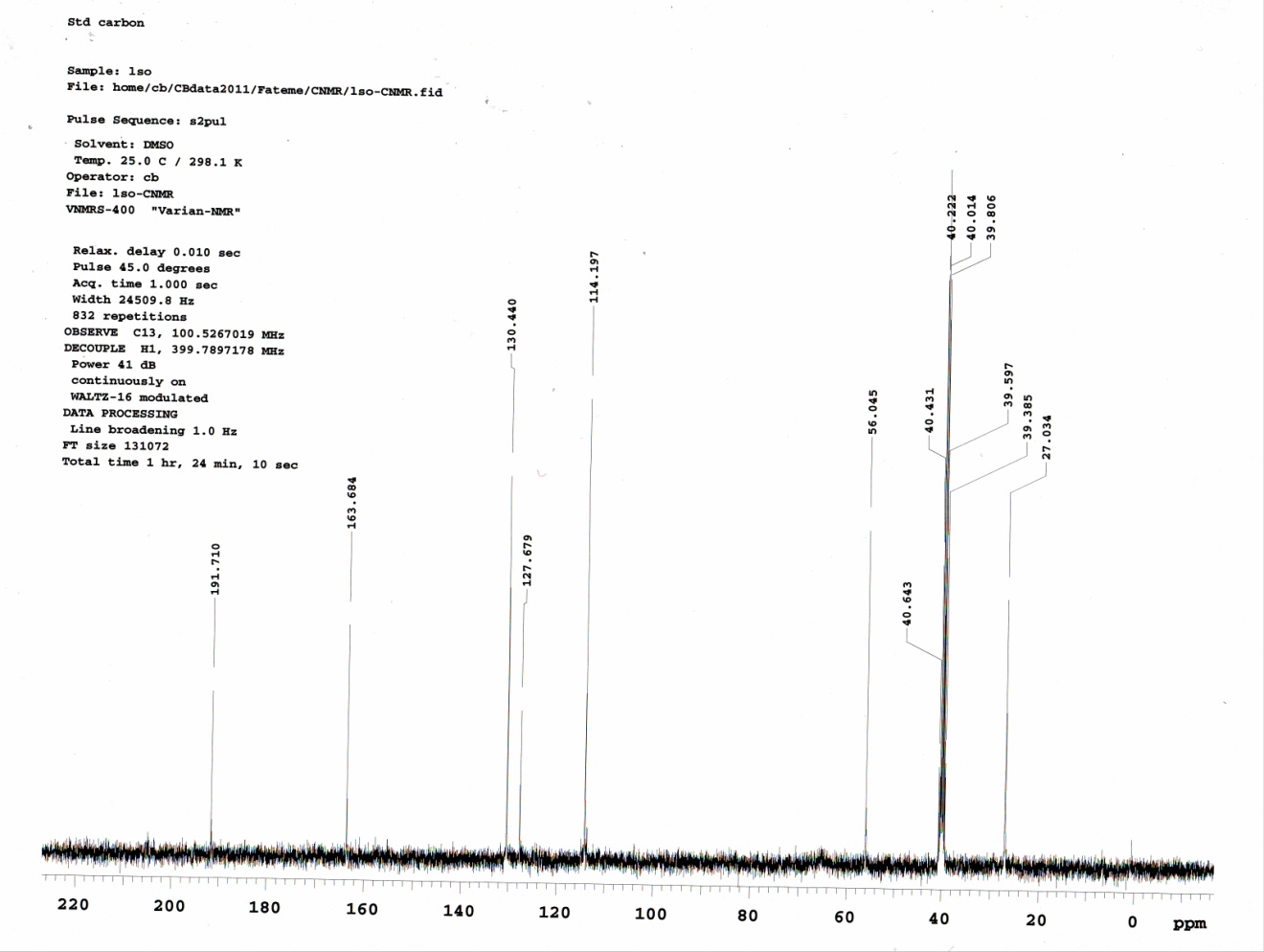
bSchool of Chemistry, University of Melbourne, Victoria, 3010, Australia



IR spectrum of complex **1**



1HNMR spectrum of complex **1**



13CNMR spectrum of complex **1**

**Response to checkcif 881011**

Alert level C

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.52

Due to the approx 7% disorder of the Hg atoms

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for S2 -- C12 .. 7.0 su

One of the residual electron density peaks arising from the disorder of the Hg atoms lies close to C12

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ............... 0.0090 Ang

Due to refining light atoms in the presence of many heavy atoms

Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained Atom Sites .... 1

C1 was restrained to near ideal values, as it was affected by the peaks due to the disordered Hg atoms

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in CIF .... ? ?

PLAT022\_ALERT\_3\_G Ratio Unique / Expected Reflections (too) Low .. 0.879

A full data set was collected to theta = 27.50°. The data collection measures some, but not all, reflections beyond this value (here theta max = 30.08°). The parameter diffrn\_measured\_fraction\_theta\_full 0.999 should be used instead.

PLAT793\_ALERT\_4\_G The Model has Chirality at C1 (Verify) .... S

PLAT793\_ALERT\_4\_G The Model has Chirality at C12 (Verify) .... S

Compound is racemic mixture

PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ....... 6

See PLAT003\_ALERT\_2\_G above

**CIFs**

data\_h:\solution\494\new

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

;

?

;

\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

'C22 H28 Br4 Hg2 O4 S2'

\_chemical\_formula\_weight 1141.36

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scat\_dispersion\_real

\_atom\_type\_scat\_dispersion\_imag

\_atom\_type\_scat\_source

'C' 'C' 0.0033 0.0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'H' 'H' 0.0000 0.0000

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'N' 'N' 0.0061 0.0033

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'P' 'P' 0.1023 0.0942

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Hg' 'Hg' -2.3894 9.2266

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Br' 'Br' -0.2901 2.4595

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'S' 'S' 0.1246 0.1234

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting Monoclinic

\_symmetry\_space\_group\_name\_H-M P21/c

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-x, y+1/2, -z+1/2'

'-x, -y, -z'

'x, -y-1/2, z-1/2'

\_cell\_length\_a 15.5940(7)

\_cell\_length\_b 7.3471(4)

\_cell\_length\_c 15.0885(7)

\_cell\_angle\_alpha 90.00

\_cell\_angle\_beta 115.877(3)

\_cell\_angle\_gamma 90.00

\_cell\_volume 1555.37(13)

\_cell\_formula\_units\_Z 2

\_cell\_measurement\_temperature 298(2)

\_cell\_measurement\_reflns\_used 8130

\_cell\_measurement\_theta\_min 2.70

\_cell\_measurement\_theta\_max 26

\_exptl\_crystal\_description Prism

\_exptl\_crystal\_colour Colorless

\_exptl\_crystal\_size\_max 0.40

\_exptl\_crystal\_size\_mid 0.30

\_exptl\_crystal\_size\_min 0.20

\_exptl\_crystal\_density\_meas ?

\_exptl\_crystal\_density\_diffrn 2.437

\_exptl\_crystal\_density\_method 'not measured'

\_exptl\_crystal\_F\_000 1048

\_exptl\_absorpt\_coefficient\_mu 15.156

\_exptl\_absorpt\_correction\_type numerical

\_exptl\_absorpt\_correction\_T\_min 0.350

\_exptl\_absorpt\_correction\_T\_max 0.720

\_exptl\_absorpt\_process\_details 'shape of crystal determined optically'

\_exptl\_special\_details

;

?

;

\_diffrn\_ambient\_temperature 298(2)

\_diffrn\_radiation\_wavelength 0.71073

\_diffrn\_radiation\_type MoK\a

\_diffrn\_radiation\_source 'fine-focus sealed tube'

\_diffrn\_radiation\_monochromator graphite

\_diffrn\_measurement\_device\_type 'STOE IPDS II'

\_diffrn\_measurement\_method 'rotation method'

\_diffrn\_detector\_area\_resol\_mean '0.15 mm'

\_diffrn\_standards\_number 0

\_diffrn\_standards\_interval\_count ?

\_diffrn\_standards\_interval\_time ?

\_diffrn\_standards\_decay\_% ?

\_diffrn\_reflns\_number 8130

\_diffrn\_reflns\_av\_R\_equivalents 0.1154

\_diffrn\_reflns\_av\_sigmaI/netI 0.0821

\_diffrn\_reflns\_limit\_h\_min -19

\_diffrn\_reflns\_limit\_h\_max 19

\_diffrn\_reflns\_limit\_k\_min -8

\_diffrn\_reflns\_limit\_k\_max 9

\_diffrn\_reflns\_limit\_l\_min -18

\_diffrn\_reflns\_limit\_l\_max 18

\_diffrn\_reflns\_theta\_min 2.70

\_diffrn\_reflns\_theta\_max 26.00

\_reflns\_number\_total 3046

\_reflns\_number\_gt 2543

\_reflns\_threshold\_expression >2sigma(I)

\_computing\_data\_collection 'X-Area 1.31 (Stoe & Cie GmbH, 2005)'

\_computing\_cell\_refinement 'X-Area 1.31 (Stoe & Cie GmbH, 2005)'

\_computing\_data\_reduction 'X-Area 1.31 (Stoe & Cie GmbH, 2005)'

\_computing\_structure\_solution 'SHELXS-97 (Sheldrick, 1990)'

\_computing\_structure\_refinement 'SHELXL-97 (Sheldrick, 1997)'

\_computing\_molecular\_graphics 'ORTEP-3 for Windows (Farrugia, 1997)'

\_computing\_publication\_material 'WinGX (Farrugia, 1999)'

\_refine\_special\_details

;

Refinement of F^2^ against ALL reflections. The weighted R-factor wR and

goodness of fit S are based on F^2^, conventional R-factors R are based

on F, with F set to zero for negative F^2^. The threshold expression of

F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is

not relevant to the choice of reflections for refinement. R-factors based

on F^2^ are statistically about twice as large as those based on F, and R-

factors based on ALL data will be even larger.

;

\_refine\_ls\_structure\_factor\_coef Fsqd

\_refine\_ls\_matrix\_type full

\_refine\_ls\_weighting\_scheme calc

\_refine\_ls\_weighting\_details

'calc w=1/[\s^2^(Fo^2^)+(0.1459P)^2^+0.2503P] where P=(Fo^2^+2Fc^2^)/3'

\_atom\_sites\_solution\_primary direct

\_atom\_sites\_solution\_secondary difmap

\_atom\_sites\_solution\_hydrogens geom

\_refine\_ls\_hydrogen\_treatment constr

\_refine\_ls\_extinction\_method SHELXL

\_refine\_ls\_extinction\_coef 0.0026(6)

\_refine\_ls\_extinction\_expression

'Fc^\*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'

\_refine\_ls\_number\_reflns 3046

\_refine\_ls\_number\_parameters 155

\_refine\_ls\_number\_restraints 0

\_refine\_ls\_R\_factor\_all 0.0903

\_refine\_ls\_R\_factor\_gt 0.0796

\_refine\_ls\_wR\_factor\_ref 0.2121

\_refine\_ls\_wR\_factor\_gt 0.2016

\_refine\_ls\_goodness\_of\_fit\_ref 1.075

\_refine\_ls\_restrained\_S\_all 1.075

\_refine\_ls\_shift/su\_max 0.005

\_refine\_ls\_shift/su\_mean 0.000

loop\_

\_atom\_site\_label

\_atom\_site\_type\_symbol

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_U\_iso\_or\_equiv

\_atom\_site\_adp\_type

\_atom\_site\_occupancy

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_calc\_flag

\_atom\_site\_refinement\_flags

\_atom\_site\_disorder\_assembly

\_atom\_site\_disorder\_group

C1 C 0.0338(9) 0.136(2) 1.1531(10) 0.055(3) Uani 1 1 d . . .

H1A H 0.0454 0.0352 1.1192 0.066 Uiso 1 1 calc R . .

H1B H 0.0025 0.2317 1.1070 0.066 Uiso 1 1 calc R . .

H1C H -0.0060 0.0967 1.1833 0.066 Uiso 1 1 calc R . .

C2 C 0.2049(14) 0.010(2) 1.3088(15) 0.073(5) Uani 1 1 d . . .

H2A H 0.2716 0.0327 1.3474 0.088 Uiso 1 1 calc R . .

H2B H 0.1967 -0.0818 1.2604 0.088 Uiso 1 1 calc R . .

H2C H 0.1772 -0.0315 1.3509 0.088 Uiso 1 1 calc R . .

C3 C 0.2045(8) 0.2789(19) 1.1725(9) 0.044(3) Uani 1 1 d . . .

H3 H 0.2017 0.1776 1.1291 0.053 Uiso 1 1 calc R . .

C4 C 0.3070(8) 0.3271(18) 1.2394(9) 0.041(2) Uani 1 1 d . . .

C5 C 0.3773(8) 0.3275(16) 1.1970(8) 0.040(2) Uani 1 1 d . . .

C6 C 0.3557(8) 0.2704(18) 1.1016(9) 0.044(3) Uani 1 1 d . . .

H6 H 0.2941 0.2323 1.0607 0.053 Uiso 1 1 calc R . .

C7 C 0.4259(10) 0.2692(18) 1.0654(10) 0.048(3) Uani 1 1 d . . .

H7 H 0.4111 0.2312 1.0016 0.057 Uiso 1 1 calc R . .

C8 C 0.5162(10) 0.3259(19) 1.1276(11) 0.051(3) Uani 1 1 d . . .

C9 C 0.5767(13) 0.250(3) 1.0124(15) 0.076(5) Uani 1 1 d . . .

H9A H 0.5243 0.3065 0.9587 0.091 Uiso 1 1 calc R . .

H9B H 0.5636 0.1223 1.0140 0.091 Uiso 1 1 calc R . .

H9C H 0.6337 0.2644 1.0038 0.091 Uiso 1 1 calc R . .

C10 C 0.5388(10) 0.387(2) 1.2239(10) 0.053(3) Uani 1 1 d . . .

H10 H 0.6000 0.4266 1.2653 0.064 Uiso 1 1 calc R . .

C11 C 0.4690(9) 0.387(2) 1.2543(10) 0.050(3) Uani 1 1 d . . .

H11 H 0.4836 0.4294 1.3174 0.061 Uiso 1 1 calc R . .

O1 O 0.3317(8) 0.3590(18) 1.3250(7) 0.064(3) Uani 1 1 d . . .

O2 O 0.5891(7) 0.3320(18) 1.1024(8) 0.068(3) Uani 1 1 d . . .

Hg1 Hg 0.14414(4) 0.52147(8) 1.08745(4) 0.0526(3) Uani 1 1 d . . .

Br1 Br 0.19782(10) 0.8140(2) 1.04280(12) 0.0612(4) Uani 1 1 d . . .

Br2 Br -0.02038(9) 0.63483(19) 1.10234(9) 0.0495(4) Uani 1 1 d . . .

S1 S 0.1462(2) 0.2186(5) 1.2473(2) 0.0453(7) Uani 1 1 d . . .

loop\_

\_atom\_site\_aniso\_label

\_atom\_site\_aniso\_U\_11

\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33

\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

C1 0.039(6) 0.070(9) 0.057(8) 0.007(6) 0.021(6) -0.016(6)

C2 0.064(10) 0.090(12) 0.082(11) 0.045(9) 0.047(9) 0.029(8)

C3 0.039(6) 0.058(7) 0.044(6) 0.013(5) 0.026(5) 0.015(6)

C4 0.033(5) 0.052(7) 0.040(6) -0.001(5) 0.017(5) 0.007(5)

C5 0.034(5) 0.037(6) 0.039(6) -0.005(5) 0.008(5) -0.003(5)

C6 0.025(5) 0.052(7) 0.055(7) 0.003(5) 0.017(5) -0.005(5)

C7 0.050(7) 0.052(7) 0.045(6) -0.005(5) 0.025(6) -0.007(6)

C8 0.044(7) 0.053(7) 0.061(7) -0.003(6) 0.028(6) -0.008(6)

C9 0.071(11) 0.078(11) 0.109(14) -0.020(10) 0.066(11) -0.018(9)

C10 0.042(7) 0.055(8) 0.062(8) -0.018(6) 0.022(6) -0.023(6)

C11 0.036(6) 0.061(8) 0.050(7) -0.008(6) 0.014(5) -0.007(6)

O1 0.055(6) 0.093(8) 0.044(5) -0.005(5) 0.022(4) -0.002(6)

O2 0.050(5) 0.089(8) 0.078(7) -0.021(6) 0.039(5) -0.025(6)

Hg1 0.0502(4) 0.0547(4) 0.0547(4) 0.0118(2) 0.0246(3) 0.0066(2)

Br1 0.0517(8) 0.0590(9) 0.0783(10) 0.0024(7) 0.0333(7) -0.0105(6)

Br2 0.0495(7) 0.0582(8) 0.0520(7) -0.0097(5) 0.0324(6) -0.0016(6)

S1 0.0417(15) 0.0560(17) 0.0462(16) 0.0048(13) 0.0265(13) 0.0047(13)

\_geom\_special\_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

C1 S1 1.813(13) . ?

C1 H1A 0.9600 . ?

C1 H1B 0.9600 . ?

C1 H1C 0.9600 . ?

C2 S1 1.819(15) . ?

C2 H2A 0.9600 . ?

C2 H2B 0.9600 . ?

C2 H2C 0.9600 . ?

C3 C4 1.514(17) . ?

C3 S1 1.786(11) . ?

C3 Hg1 2.158(12) . ?

C3 H3 0.9800 . ?

C4 O1 1.199(15) . ?

C4 C5 1.490(16) . ?

C5 C11 1.379(17) . ?

C5 C6 1.393(17) . ?

C6 C7 1.419(16) . ?

C6 H6 0.9300 . ?

C7 C8 1.372(19) . ?

C7 H7 0.9300 . ?

C8 O2 1.348(15) . ?

C8 C10 1.411(19) . ?

C9 O2 1.42(2) . ?

C9 H9A 0.9600 . ?

C9 H9B 0.9600 . ?

C9 H9C 0.9600 . ?

C10 C11 1.354(18) . ?

C10 H10 0.9300 . ?

C11 H11 0.9300 . ?

Hg1 Br1 2.5031(16) . ?

Hg1 Br2 2.7981(13) . ?

Hg1 Br2 2.9016(14) 3\_567 ?

Br2 Hg1 2.9016(14) 3\_567 ?

loop\_

\_geom\_angle\_atom\_site\_label\_1

\_geom\_angle\_atom\_site\_label\_2

\_geom\_angle\_atom\_site\_label\_3

\_geom\_angle

\_geom\_angle\_site\_symmetry\_1

\_geom\_angle\_site\_symmetry\_3

\_geom\_angle\_publ\_flag

S1 C1 H1A 109.5 . . ?

S1 C1 H1B 109.5 . . ?

H1A C1 H1B 109.5 . . ?

S1 C1 H1C 109.5 . . ?

H1A C1 H1C 109.5 . . ?

H1B C1 H1C 109.5 . . ?

S1 C2 H2A 109.5 . . ?

S1 C2 H2B 109.5 . . ?

H2A C2 H2B 109.5 . . ?

S1 C2 H2C 109.5 . . ?

H2A C2 H2C 109.5 . . ?

H2B C2 H2C 109.5 . . ?

C4 C3 S1 108.6(8) . . ?

C4 C3 Hg1 105.2(9) . . ?

S1 C3 Hg1 111.7(6) . . ?

C4 C3 H3 110.4 . . ?

S1 C3 H3 110.4 . . ?

Hg1 C3 H3 110.4 . . ?

O1 C4 C5 120.7(11) . . ?

O1 C4 C3 120.8(11) . . ?

C5 C4 C3 118.4(10) . . ?

C11 C5 C6 117.4(11) . . ?

C11 C5 C4 119.1(11) . . ?

C6 C5 C4 123.5(10) . . ?

C5 C6 C7 121.3(11) . . ?

C5 C6 H6 119.3 . . ?

C7 C6 H6 119.3 . . ?

C8 C7 C6 118.0(12) . . ?

C8 C7 H7 121.0 . . ?

C6 C7 H7 121.0 . . ?

O2 C8 C7 123.9(12) . . ?

O2 C8 C10 114.6(12) . . ?

C7 C8 C10 121.4(12) . . ?

O2 C9 H9A 109.5 . . ?

O2 C9 H9B 109.5 . . ?

H9A C9 H9B 109.5 . . ?

O2 C9 H9C 109.5 . . ?

H9A C9 H9C 109.5 . . ?

H9B C9 H9C 109.5 . . ?

C11 C10 C8 118.2(12) . . ?

C11 C10 H10 120.9 . . ?

C8 C10 H10 120.9 . . ?

C10 C11 C5 123.7(12) . . ?

C10 C11 H11 118.2 . . ?

C5 C11 H11 118.2 . . ?

C8 O2 C9 118.3(12) . . ?

C3 Hg1 Br1 139.4(3) . . ?

C3 Hg1 Br2 112.0(3) . . ?

Br1 Hg1 Br2 101.08(5) . . ?

C3 Hg1 Br2 100.9(4) . 3\_567 ?

Br1 Hg1 Br2 103.34(5) . 3\_567 ?

Br2 Hg1 Br2 87.64(4) . 3\_567 ?

Hg1 Br2 Hg1 92.36(4) . 3\_567 ?

C3 S1 C1 100.0(6) . . ?

C3 S1 C2 104.4(7) . . ?

C1 S1 C2 102.5(9) . . ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1

\_geom\_torsion\_atom\_site\_label\_2

\_geom\_torsion\_atom\_site\_label\_3

\_geom\_torsion\_atom\_site\_label\_4

\_geom\_torsion

\_geom\_torsion\_site\_symmetry\_1

\_geom\_torsion\_site\_symmetry\_2

\_geom\_torsion\_site\_symmetry\_3

\_geom\_torsion\_site\_symmetry\_4

\_geom\_torsion\_publ\_flag

S1 C3 C4 O1 -16.1(17) . . . . ?

Hg1 C3 C4 O1 103.7(13) . . . . ?

S1 C3 C4 C5 161.8(9) . . . . ?

Hg1 C3 C4 C5 -78.4(12) . . . . ?

O1 C4 C5 C11 -8(2) . . . . ?

C3 C4 C5 C11 174.2(12) . . . . ?

O1 C4 C5 C6 172.0(13) . . . . ?

C3 C4 C5 C6 -5.9(18) . . . . ?

C11 C5 C6 C7 1.5(19) . . . . ?

C4 C5 C6 C7 -178.4(12) . . . . ?

C5 C6 C7 C8 0(2) . . . . ?

C6 C7 C8 O2 -179.7(14) . . . . ?

C6 C7 C8 C10 -1(2) . . . . ?

O2 C8 C10 C11 179.3(14) . . . . ?

C7 C8 C10 C11 1(2) . . . . ?

C8 C10 C11 C5 1(2) . . . . ?

C6 C5 C11 C10 -2(2) . . . . ?

C4 C5 C11 C10 177.8(14) . . . . ?

C7 C8 O2 C9 -10(2) . . . . ?

C10 C8 O2 C9 171.4(15) . . . . ?

C4 C3 Hg1 Br1 16.9(10) . . . . ?

S1 C3 Hg1 Br1 134.5(4) . . . . ?

C4 C3 Hg1 Br2 -125.3(6) . . . . ?

S1 C3 Hg1 Br2 -7.7(8) . . . . ?

C4 C3 Hg1 Br2 142.8(6) . . . 3\_567 ?

S1 C3 Hg1 Br2 -99.6(6) . . . 3\_567 ?

C3 Hg1 Br2 Hg1 -100.9(4) . . . 3\_567 ?

Br1 Hg1 Br2 Hg1 103.13(5) . . . 3\_567 ?

Br2 Hg1 Br2 Hg1 0.0 3\_567 . . 3\_567 ?

C4 C3 S1 C1 -171.9(10) . . . . ?

Hg1 C3 S1 C1 72.5(8) . . . . ?

C4 C3 S1 C2 -66.1(12) . . . . ?

Hg1 C3 S1 C2 178.3(9) . . . . ?

\_diffrn\_measured\_fraction\_theta\_max 0.998

\_diffrn\_reflns\_theta\_full 26.00

\_diffrn\_measured\_fraction\_theta\_full 0.998

\_refine\_diff\_density\_max 2.758

\_refine\_diff\_density\_min -6.020

\_refine\_diff\_density\_rms 0.405

#===END

data\_fa-lsogau

\_audit\_creation\_date 2012-07-11

\_audit\_creation\_method

;

Olex2 1.2

(compiled 2012.05.09 svn.r2324, GUI svn.r4230)

;

\_publ\_contact\_author\_address ?

\_publ\_contact\_author\_email ?

\_publ\_contact\_author\_name ''

\_publ\_contact\_author\_phone ?

\_chemical\_name\_common ?

\_chemical\_name\_systematic

;

?

;

\_chemical\_formula\_moiety 'C22 H28 Cl4 Hg2 O4 S2, 2(C2 H6 O S)'

\_chemical\_formula\_sum 'C26 H40 Cl4 Hg2 O6 S4'

\_chemical\_formula\_weight 1119.80

\_chemical\_melting\_point ?

\_chemical\_oxdiff\_formula 'Hg2 S4 O6 Cl4 C26 H40'

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scat\_dispersion\_real

\_atom\_type\_scat\_dispersion\_imag

\_atom\_type\_scat\_source

'C' 'C' 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'H' 'H' 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'S' 'S' 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Cl' 'Cl' 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Hg' 'Hg' -2.3894 9.2266

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_space\_group\_crystal\_system 'triclinic'

\_space\_group\_IT\_number 2

\_space\_group\_name\_H-M\_alt 'P -1'

\_space\_group\_name\_Hall '-P 1'

loop\_

\_space\_group\_symop\_id

\_space\_group\_symop\_operation\_xyz

1 'x, y, z'

2 '-x, -y, -z'

\_cell\_length\_a 10.1329(3)

\_cell\_length\_b 12.4857(4)

\_cell\_length\_c 15.3870(7)

\_cell\_angle\_alpha 110.370(4)

\_cell\_angle\_beta 96.693(3)

\_cell\_angle\_gamma 90.526(3)

\_cell\_volume 1809.94(11)

\_cell\_formula\_units\_Z 2

\_cell\_measurement\_reflns\_used 8301

\_cell\_measurement\_temperature 130.00(10)

\_cell\_measurement\_theta\_max 30.0138

\_cell\_measurement\_theta\_min 2.7372

\_exptl\_absorpt\_coefficient\_mu 9.034

\_exptl\_absorpt\_correction\_T\_max 0.637

\_exptl\_absorpt\_correction\_T\_min 0.208

\_exptl\_absorpt\_correction\_type gaussian

\_exptl\_absorpt\_process\_details

;

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(compiled Jan 23 2012,18:06:46)

Numerical absorption correction based on gaussian integration over

a multifaceted crystal model

;

\_exptl\_crystal\_colour colourless

\_exptl\_crystal\_colour\_primary colourless

\_exptl\_crystal\_density\_diffrn 2.055

\_exptl\_crystal\_density\_meas ?

\_exptl\_crystal\_density\_method 'not measured'

\_exptl\_crystal\_description needle

\_exptl\_crystal\_F\_000 1072

\_exptl\_crystal\_size\_max 0.2703

\_exptl\_crystal\_size\_mid 0.0866

\_exptl\_crystal\_size\_min 0.0600

\_exptl\_special\_details

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?

;

\_diffrn\_reflns\_av\_R\_equivalents 0.0401

\_diffrn\_reflns\_av\_unetI/netI 0.0656

\_diffrn\_reflns\_limit\_h\_max 14

\_diffrn\_reflns\_limit\_h\_min -13

\_diffrn\_reflns\_limit\_k\_max 16

\_diffrn\_reflns\_limit\_k\_min -17

\_diffrn\_reflns\_limit\_l\_max 20

\_diffrn\_reflns\_limit\_l\_min -19

\_diffrn\_reflns\_number 17790

\_diffrn\_reflns\_theta\_full 27.50

\_diffrn\_reflns\_theta\_max 30.08

\_diffrn\_reflns\_theta\_min 2.74

\_diffrn\_ambient\_temperature 130.00(10)

\_diffrn\_detector\_area\_resol\_mean 10.2273

\_diffrn\_measured\_fraction\_theta\_full 0.999

\_diffrn\_measured\_fraction\_theta\_max 0.879

\_diffrn\_measurement\_details

;

#\_\_ type\_ start\_\_ end\_\_\_\_ width\_\_\_ exp.time\_

1 omega -60.00 41.00 1.0000 8.0500

omega\_\_\_\_ theta\_\_\_\_ kappa\_\_\_\_ phi\_\_\_\_\_\_ frames

- 13.6163 -57.0000 -30.0000 101

#\_\_ type\_ start\_\_ end\_\_\_\_ width\_\_\_ exp.time\_

2 omega 43.00 102.00 1.0000 8.0500

omega\_\_\_\_ theta\_\_\_\_ kappa\_\_\_\_ phi\_\_\_\_\_\_ frames

- 13.6163 -178.0000 -30.0000 59

#\_\_ type\_ start\_\_ end\_\_\_\_ width\_\_\_ exp.time\_

3 omega 35.00 98.00 1.0000 8.0500

omega\_\_\_\_ theta\_\_\_\_ kappa\_\_\_\_ phi\_\_\_\_\_\_ frames

- 13.6163 -178.0000 -120.0000 63

#\_\_ type\_ start\_\_ end\_\_\_\_ width\_\_\_ exp.time\_

4 omega 0.00 90.00 1.0000 8.0500

omega\_\_\_\_ theta\_\_\_\_ kappa\_\_\_\_ phi\_\_\_\_\_\_ frames

- 13.6163 37.0000 120.0000 90

#\_\_ type\_ start\_\_ end\_\_\_\_ width\_\_\_ exp.time\_

5 omega -19.00 28.00 1.0000 8.0500

omega\_\_\_\_ theta\_\_\_\_ kappa\_\_\_\_ phi\_\_\_\_\_\_ frames

- -13.6945 -99.0000 -120.0000 47

;

\_diffrn\_measurement\_device\_type 'SuperNova, Dual, Cu at zero, Atlas'

\_diffrn\_measurement\_method '\w scans'

\_diffrn\_orient\_matrix\_UB\_11 0.0675678000

\_diffrn\_orient\_matrix\_UB\_12 -0.0091603000

\_diffrn\_orient\_matrix\_UB\_13 -0.0069154000

\_diffrn\_orient\_matrix\_UB\_21 -0.0174478000

\_diffrn\_orient\_matrix\_UB\_22 -0.0131107000

\_diffrn\_orient\_matrix\_UB\_23 -0.0487163000

\_diffrn\_orient\_matrix\_UB\_31 0.0105753000

\_diffrn\_orient\_matrix\_UB\_32 0.0585395000

\_diffrn\_orient\_matrix\_UB\_33 0.0060760000

\_diffrn\_radiation\_monochromator mirror

\_diffrn\_radiation\_type 'Mo K\a'

\_diffrn\_radiation\_wavelength 0.7107

\_diffrn\_source 'SuperNova (Mo) X-ray Source'

\_diffrn\_standards\_decay\_% ?

\_diffrn\_standards\_interval\_count ?

\_diffrn\_standards\_interval\_time ?

\_diffrn\_standards\_number ?

\_reflns\_number\_gt 7543

\_reflns\_number\_total 9370

\_reflns\_odcompleteness\_completeness 99.87

\_reflns\_odcompleteness\_iscentric 1

\_reflns\_odcompleteness\_theta 27.50

\_reflns\_threshold\_expression >2\s(I)

\_computing\_cell\_refinement

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\_computing\_data\_collection

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Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET)

(compiled Jan 23 2012,18:06:46)

;

\_computing\_data\_reduction

;

CrysAlisPro, Agilent Technologies,

Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET)

(compiled Jan 23 2012,18:06:46)

;

\_computing\_molecular\_graphics

;

O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann,

OLEX2: a complete structure solution, refinement and analysis program.

J. Appl. Cryst. (2009). 42, 339-341.

;

\_computing\_publication\_material

;

O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann,

OLEX2: a complete structure solution, refinement and analysis program.

J. Appl. Cryst. (2009). 42, 339-341.

;

\_computing\_structure\_refinement

;

SHELXL, G.M. Sheldrick, Acta Cryst.

(2008). A64, 112-122

;

\_computing\_structure\_solution

;

SHELXS, G.M. Sheldrick, Acta Cryst.

(2008). A64, 112-122

;

\_refine\_diff\_density\_max 5.862

\_refine\_diff\_density\_min -1.664

\_refine\_diff\_density\_rms 0.264

\_refine\_ls\_extinction\_coef ?

\_refine\_ls\_extinction\_method none

\_refine\_ls\_goodness\_of\_fit\_ref 1.057

\_refine\_ls\_hydrogen\_treatment constr

\_refine\_ls\_matrix\_type full

\_refine\_ls\_number\_parameters 389

\_refine\_ls\_number\_reflns 9370

\_refine\_ls\_number\_restraints 6

\_refine\_ls\_R\_factor\_all 0.0601

\_refine\_ls\_R\_factor\_gt 0.0436

\_refine\_ls\_restrained\_S\_all 1.057

\_refine\_ls\_shift/su\_max 0.002

\_refine\_ls\_shift/su\_mean 0.000

\_refine\_ls\_structure\_factor\_coef Fsqd

\_refine\_ls\_weighting\_details

'calc w=1/[\s^2^(Fo^2^)+(0.0560P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'

\_refine\_ls\_weighting\_scheme calc

\_refine\_ls\_wR\_factor\_gt 0.1029

\_refine\_ls\_wR\_factor\_ref 0.1137

\_refine\_special\_details

;

Refinement of F^2^ against ALL reflections. The weighted R-factor wR and

goodness of fit S are based on F^2^, conventional R-factors R are based

on F, with F set to zero for negative F^2^. The threshold expression of

F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is

not relevant to the choice of reflections for refinement. R-factors based

on F^2^ are statistically about twice as large as those based on F, and R-

factors based on ALL data will be even larger.

Hydrogen atoms were constrained at geometrical estimates, all were

assigned isotropic displacement parameters which were 1.5 (methyl) or

1.2 (other) times the parent carbon atom.

The final difference map showed 4 peaks (range 5.86 - 4.42 eA-3) close to

the Hg atoms, two peaks for each Hg atom, suggesting some disorder of the

structure. Assigning these peaks as mercury atoms gave, after refinement,

occupancy factors of around 0.03 - 0.04, indicating the disorder was only

around 7%. Accordingly no attempt was made to model this disorder; the

refinement was completed with the assigned Hg atoms given full occupancy.

It was also noted that one of these peaks was close to C1, and another

close to C12. The CIFCHECK reported showed an anomalous ADP for C1 and

slightly large Hirshfeld test difference for the C-S1 & C12-S2 bonds.

In the final refinement C1 was constrained to near ideal geometry; as C12

did not show an anomalous ADP, no restraints were applied, so the slightly

large Hirshfeld test difference for C12-S2 remained.

;

\_atom\_sites\_solution\_hydrogens geom

\_atom\_sites\_solution\_primary heavy

\_atom\_sites\_solution\_secondary difmap

loop\_

\_atom\_site\_label

\_atom\_site\_type\_symbol

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_U\_iso\_or\_equiv

\_atom\_site\_adp\_type

\_atom\_site\_occupancy

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_calc\_flag

\_atom\_site\_refinement\_flags

\_atom\_site\_disorder\_assembly

\_atom\_site\_disorder\_group

Hg1 Hg 0.06088(2) 0.556631(17) 0.409486(16) 0.01780(7) Uani 1 1 d . . .

S1 S 0.00719(15) 0.79619(12) 0.57212(10) 0.0161(3) Uani 1 1 d . . .

Cl1 Cl 0.18708(15) 0.47337(12) 0.53016(11) 0.0218(3) Uani 1 1 d . . .

Cl2 Cl 0.0502(2) 0.38634(13) 0.27582(12) 0.0355(4) Uani 1 1 d . . .

O1 O -0.1574(4) 0.7999(3) 0.4186(3) 0.0210(9) Uani 1 1 d . . .

O2 O 0.0022(5) 0.6697(4) 0.0126(3) 0.0306(11) Uani 1 1 d . . .

C1 C 0.0546(6) 0.7401(5) 0.4557(4) 0.0185(12) Uani 1 1 d U . .

H1 H 0.1428 0.7753 0.4539 0.022 Uiso 1 1 calc R . .

C2 C -0.0495(6) 0.7668(4) 0.3916(4) 0.0158(12) Uani 1 1 d . . .

C3 C -0.0258(6) 0.7466(4) 0.2946(4) 0.0170(12) Uani 1 1 d . . .

C4 C 0.0911(7) 0.7017(5) 0.2590(5) 0.0237(14) Uani 1 1 d . . .

H4 H 0.1623 0.6899 0.3001 0.028 Uiso 1 1 calc R . .

C5 C 0.1055(7) 0.6742(5) 0.1656(5) 0.0254(14) Uani 1 1 d . . .

H5 H 0.1847 0.6422 0.1425 0.030 Uiso 1 1 calc R . .

C6 C 0.0023(7) 0.6941(5) 0.1060(4) 0.0235(14) Uani 1 1 d . . .

C7 C -0.1107(7) 0.7468(5) 0.1420(4) 0.0207(13) Uani 1 1 d . . .

H7 H -0.1773 0.7670 0.1025 0.025 Uiso 1 1 calc R . .

C8 C -0.1256(6) 0.7693(5) 0.2337(4) 0.0188(12) Uani 1 1 d . . .

H8 H -0.2051 0.8010 0.2564 0.023 Uiso 1 1 calc R . .

C9 C 0.1148(9) 0.6153(7) -0.0284(5) 0.0396(19) Uani 1 1 d . . .

H9A H 0.1013 0.6003 -0.0958 0.059 Uiso 1 1 calc R . .

H9B H 0.1253 0.5429 -0.0175 0.059 Uiso 1 1 calc R . .

H9C H 0.1950 0.6654 0.0001 0.059 Uiso 1 1 calc R . .

C10 C 0.0158(7) 0.9493(5) 0.6035(4) 0.0207(13) Uani 1 1 d . . .

H10A H 0.0998 0.9738 0.5886 0.031 Uiso 1 1 calc R . .

H10B H 0.0112 0.9855 0.6707 0.031 Uiso 1 1 calc R . .

H10C H -0.0589 0.9721 0.5684 0.031 Uiso 1 1 calc R . .

C11 C 0.1562(7) 0.7820(5) 0.6409(4) 0.0218(13) Uani 1 1 d . . .

H11A H 0.2310 0.8217 0.6277 0.033 Uiso 1 1 calc R . .

H11B H 0.1735 0.7008 0.6253 0.033 Uiso 1 1 calc R . .

H11C H 0.1459 0.8158 0.7074 0.033 Uiso 1 1 calc R . .

Hg2 Hg 0.43576(2) 0.133990(18) 0.585937(16) 0.01889(8) Uani 1 1 d . . .

Cl3 Cl 0.31150(15) -0.05492(12) 0.46693(12) 0.0245(3) Uani 1 1 d . . .

Cl4 Cl 0.4481(2) 0.08034(17) 0.72040(14) 0.0426(5) Uani 1 1 d . . .

S2 S 0.49314(15) 0.23233(12) 0.42252(10) 0.0168(3) Uani 1 1 d . . .

O3 O 0.6599(4) 0.3664(3) 0.5799(3) 0.0211(9) Uani 1 1 d . . .

O4 O 0.4381(5) 0.6011(4) 0.9681(3) 0.0289(11) Uani 1 1 d . . .

C12 C 0.4462(6) 0.2777(5) 0.5384(5) 0.0210(14) Uani 1 1 d . . .

H12 H 0.3590 0.3147 0.5400 0.025 Uiso 1 1 calc R . .

C13 C 0.5502(6) 0.3575(5) 0.6033(4) 0.0168(12) Uani 1 1 d . . .

C14 C 0.5201(6) 0.4230(5) 0.7000(4) 0.0159(12) Uani 1 1 d . . .

C15 C 0.3927(6) 0.4157(5) 0.7269(4) 0.0205(13) Uani 1 1 d . . .

H15 H 0.3233 0.3683 0.6832 0.025 Uiso 1 1 calc R . .

C16 C 0.3699(7) 0.4767(5) 0.8154(5) 0.0248(14) Uani 1 1 d . . .

H16 H 0.2837 0.4728 0.8329 0.030 Uiso 1 1 calc R . .

C17 C 0.4720(7) 0.5457(5) 0.8816(5) 0.0258(15) Uani 1 1 d . . .

C18 C 0.5972(7) 0.5546(5) 0.8543(4) 0.0220(14) Uani 1 1 d . . .

H18 H 0.6664 0.6025 0.8979 0.026 Uiso 1 1 calc R . .

C19 C 0.6205(7) 0.4936(5) 0.7638(5) 0.0228(14) Uani 1 1 d . . .

H19 H 0.7055 0.5001 0.7453 0.027 Uiso 1 1 calc R . .

C20 C 0.5383(8) 0.6771(6) 1.0354(5) 0.0350(18) Uani 1 1 d . . .

H20A H 0.5039 0.7094 1.0956 0.052 Uiso 1 1 calc R . .

H20B H 0.5621 0.7391 1.0139 0.052 Uiso 1 1 calc R . .

H20C H 0.6173 0.6348 1.0427 0.052 Uiso 1 1 calc R . .

C21 C 0.3445(6) 0.1578(5) 0.3535(5) 0.0245(14) Uani 1 1 d . . .

H21A H 0.2700 0.2081 0.3662 0.037 Uiso 1 1 calc R . .

H21B H 0.3263 0.0899 0.3691 0.037 Uiso 1 1 calc R . .

H21C H 0.3555 0.1344 0.2871 0.037 Uiso 1 1 calc R . .

C22 C 0.4850(7) 0.3586(5) 0.3923(5) 0.0228(14) Uani 1 1 d . . .

H22A H 0.5629 0.4100 0.4246 0.034 Uiso 1 1 calc R . .

H22B H 0.4039 0.3973 0.4112 0.034 Uiso 1 1 calc R . .

H22C H 0.4838 0.3373 0.3246 0.034 Uiso 1 1 calc R . .

S3 S 0.90046(17) 0.91424(14) 0.83359(12) 0.0258(4) Uani 1 1 d . . .

O5 O 1.0468(5) 0.9464(4) 0.8538(4) 0.0397(13) Uani 1 1 d . . .

C23 C 0.8605(8) 0.8497(6) 0.9133(5) 0.0319(16) Uani 1 1 d . . .

H23A H 0.9073 0.7787 0.9026 0.048 Uiso 1 1 calc R . .

H23B H 0.7643 0.8322 0.9042 0.048 Uiso 1 1 calc R . .

H23C H 0.8878 0.9021 0.9773 0.048 Uiso 1 1 calc R . .

C24 C 0.8168(8) 1.0445(5) 0.8806(6) 0.0380(19) Uani 1 1 d . . .

H24A H 0.8466 1.0797 0.9478 0.057 Uiso 1 1 calc R . .

H24B H 0.7205 1.0273 0.8705 0.057 Uiso 1 1 calc R . .

H24C H 0.8379 1.0974 0.8492 0.057 Uiso 1 1 calc R . .

S4 S 0.40130(17) 0.87128(13) 0.82752(11) 0.0231(3) Uani 1 1 d . . .

O6 O 0.5452(5) 0.8580(5) 0.8559(4) 0.0380(13) Uani 1 1 d . . .

C25 C 0.3590(7) 1.0078(5) 0.9011(5) 0.0279(15) Uani 1 1 d . . .

H25A H 0.3775 1.0136 0.9665 0.042 Uiso 1 1 calc R . .

H25B H 0.2642 1.0176 0.8862 0.042 Uiso 1 1 calc R . .

H25C H 0.4120 1.0675 0.8910 0.042 Uiso 1 1 calc R . .

C26 C 0.3063(8) 0.7882(6) 0.8745(6) 0.0353(17) Uani 1 1 d . . .

H26A H 0.3186 0.7067 0.8425 0.053 Uiso 1 1 calc R . .

H26B H 0.2119 0.8032 0.8652 0.053 Uiso 1 1 calc R . .

H26C H 0.3362 0.8091 0.9414 0.053 Uiso 1 1 calc R . .

loop\_

\_atom\_site\_aniso\_label

\_atom\_site\_aniso\_U\_11

\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33

\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

Hg1 0.01856(14) 0.01453(12) 0.02107(13) 0.00622(9) 0.00551(9) 0.00253(8)

S1 0.0123(7) 0.0174(6) 0.0184(7) 0.0061(5) 0.0013(6) 0.0007(5)

Cl1 0.0142(7) 0.0235(7) 0.0335(9) 0.0169(6) 0.0045(6) 0.0032(5)

Cl2 0.0470(12) 0.0234(8) 0.0306(9) -0.0004(7) 0.0155(8) -0.0055(7)

O1 0.018(2) 0.025(2) 0.021(2) 0.0083(17) 0.0039(18) 0.0069(17)

O2 0.031(3) 0.046(3) 0.019(2) 0.015(2) 0.010(2) 0.009(2)

C1 0.012(3) 0.020(3) 0.034(3) 0.022(2) 0.002(2) -0.002(2)

C2 0.012(3) 0.015(3) 0.019(3) 0.005(2) -0.000(2) -0.002(2)

C3 0.016(3) 0.012(3) 0.023(3) 0.006(2) 0.005(2) 0.002(2)

C4 0.016(3) 0.031(3) 0.030(4) 0.017(3) 0.004(3) 0.005(3)

C5 0.023(4) 0.032(3) 0.028(4) 0.016(3) 0.012(3) 0.007(3)

C6 0.028(4) 0.024(3) 0.021(3) 0.009(2) 0.008(3) 0.002(3)

C7 0.021(4) 0.026(3) 0.017(3) 0.010(2) -0.001(2) -0.001(2)

C8 0.013(3) 0.021(3) 0.022(3) 0.006(2) 0.003(2) 0.003(2)

C9 0.043(5) 0.057(5) 0.021(4) 0.013(3) 0.014(3) 0.005(4)

C10 0.030(4) 0.015(3) 0.017(3) 0.006(2) 0.003(3) 0.008(2)

C11 0.021(3) 0.025(3) 0.017(3) 0.007(2) -0.001(3) 0.003(2)

Hg2 0.02028(14) 0.01647(12) 0.02303(14) 0.00933(9) 0.00736(10) 0.00307(9)

Cl3 0.0154(8) 0.0169(7) 0.0408(9) 0.0086(6) 0.0071(7) 0.0011(5)

Cl4 0.0631(14) 0.0467(10) 0.0351(10) 0.0289(8) 0.0262(10) 0.0287(10)

S2 0.0149(8) 0.0186(7) 0.0175(7) 0.0068(5) 0.0027(6) 0.0024(5)

O3 0.014(2) 0.027(2) 0.023(2) 0.0094(18) 0.0030(18) -0.0005(17)

O4 0.032(3) 0.026(2) 0.022(2) -0.0009(19) 0.002(2) 0.002(2)

C12 0.008(3) 0.011(3) 0.041(4) 0.005(2) 0.004(3) 0.003(2)

C13 0.011(3) 0.020(3) 0.023(3) 0.012(2) 0.002(2) 0.002(2)

C14 0.019(3) 0.016(3) 0.014(3) 0.007(2) 0.002(2) 0.001(2)

C15 0.016(3) 0.019(3) 0.021(3) 0.002(2) -0.004(2) 0.001(2)

C16 0.016(3) 0.027(3) 0.025(3) 0.002(3) 0.003(3) -0.001(2)

C17 0.035(4) 0.016(3) 0.026(4) 0.006(2) 0.005(3) 0.003(3)

C18 0.024(4) 0.019(3) 0.021(3) 0.006(2) -0.002(3) -0.000(2)

C19 0.018(3) 0.017(3) 0.032(4) 0.007(3) 0.001(3) 0.002(2)

C20 0.039(5) 0.030(4) 0.024(4) -0.004(3) -0.000(3) -0.006(3)

C21 0.015(3) 0.029(3) 0.027(4) 0.010(3) -0.005(3) -0.001(2)

C22 0.023(4) 0.020(3) 0.029(4) 0.014(3) 0.001(3) -0.000(2)

S3 0.0195(9) 0.0279(8) 0.0247(8) 0.0036(6) -0.0007(7) 0.0013(6)

O5 0.019(3) 0.046(3) 0.044(3) 0.003(2) 0.003(2) -0.002(2)

C23 0.028(4) 0.039(4) 0.031(4) 0.016(3) 0.001(3) 0.007(3)

C24 0.026(4) 0.022(3) 0.063(6) 0.010(3) 0.007(4) 0.002(3)

S4 0.0178(8) 0.0297(8) 0.0209(8) 0.0084(6) 0.0008(6) -0.0001(6)

O6 0.018(3) 0.058(3) 0.036(3) 0.014(2) 0.003(2) 0.007(2)

C25 0.030(4) 0.033(3) 0.022(3) 0.009(3) 0.007(3) 0.002(3)

C26 0.027(4) 0.040(4) 0.049(5) 0.027(4) 0.009(3) 0.004(3)

\_geom\_special\_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Hg1 Cl1 2.8433(16) 2\_566 ?

Hg1 Cl1 2.6417(15) . ?

Hg1 Cl2 2.3795(15) . ?

Hg1 C1 2.153(5) . ?

S1 C1 1.806(7) . ?

S1 C10 1.800(6) . ?

S1 C11 1.787(6) . ?

Cl1 Hg1 2.8433(16) 2\_566 ?

O1 C2 1.238(7) . ?

O2 C6 1.361(8) . ?

O2 C9 1.430(9) . ?

C1 H1 1.0000 . ?

C1 C2 1.479(8) . ?

C2 C3 1.474(9) . ?

C3 C4 1.402(8) . ?

C3 C8 1.397(8) . ?

C4 H4 0.9500 . ?

C4 C5 1.382(9) . ?

C5 H5 0.9500 . ?

C5 C6 1.392(9) . ?

C6 C7 1.399(9) . ?

C7 H7 0.9500 . ?

C7 C8 1.366(9) . ?

C8 H8 0.9500 . ?

C9 H9A 0.9800 . ?

C9 H9B 0.9800 . ?

C9 H9C 0.9800 . ?

C10 H10A 0.9800 . ?

C10 H10B 0.9800 . ?

C10 H10C 0.9800 . ?

C11 H11A 0.9800 . ?

C11 H11B 0.9800 . ?

C11 H11C 0.9800 . ?

Hg2 Cl3 2.8579(15) 2\_656 ?

Hg2 Cl3 2.6274(15) . ?

Hg2 Cl4 2.3772(18) . ?

Hg2 C12 2.166(6) . ?

Cl3 Hg2 2.8579(15) 2\_656 ?

S2 C12 1.796(7) . ?

S2 C21 1.782(6) . ?

S2 C22 1.791(6) . ?

O3 C13 1.223(7) . ?

O4 C17 1.356(8) . ?

O4 C20 1.434(8) . ?

C12 H12 1.0000 . ?

C12 C13 1.465(8) . ?

C13 C14 1.497(8) . ?

C14 C15 1.411(9) . ?

C14 C19 1.387(8) . ?

C15 H15 0.9500 . ?

C15 C16 1.358(9) . ?

C16 H16 0.9500 . ?

C16 C17 1.406(9) . ?

C17 C18 1.396(10) . ?

C18 H18 0.9500 . ?

C18 C19 1.384(9) . ?

C19 H19 0.9500 . ?

C20 H20A 0.9800 . ?

C20 H20B 0.9800 . ?

C20 H20C 0.9800 . ?

C21 H21A 0.9800 . ?

C21 H21B 0.9800 . ?

C21 H21C 0.9800 . ?

C22 H22A 0.9800 . ?

C22 H22B 0.9800 . ?

C22 H22C 0.9800 . ?

S3 O5 1.500(5) . ?

S3 C23 1.765(8) . ?

S3 C24 1.799(6) . ?

C23 H23A 0.9800 . ?

C23 H23B 0.9800 . ?

C23 H23C 0.9800 . ?

C24 H24A 0.9800 . ?

C24 H24B 0.9800 . ?

C24 H24C 0.9800 . ?

S4 O6 1.500(5) . ?

S4 C25 1.776(6) . ?

S4 C26 1.786(8) . ?

C25 H25A 0.9800 . ?

C25 H25B 0.9800 . ?

C25 H25C 0.9800 . ?

C26 H26A 0.9800 . ?

C26 H26B 0.9800 . ?

C26 H26C 0.9800 . ?

loop\_

\_geom\_angle\_atom\_site\_label\_1

\_geom\_angle\_atom\_site\_label\_2

\_geom\_angle\_atom\_site\_label\_3

\_geom\_angle

\_geom\_angle\_site\_symmetry\_1

\_geom\_angle\_site\_symmetry\_3

\_geom\_angle\_publ\_flag

Cl1 Hg1 Cl1 91.03(4) . 2\_566 ?

Cl2 Hg1 Cl1 96.97(6) . . ?

Cl2 Hg1 Cl1 99.04(6) . 2\_566 ?

C1 Hg1 Cl1 93.90(17) . 2\_566 ?

C1 Hg1 Cl1 115.91(17) . . ?

C1 Hg1 Cl2 144.39(17) . . ?

C10 S1 C1 105.5(3) . . ?

C11 S1 C1 101.3(3) . . ?

C11 S1 C10 98.8(3) . . ?

Hg1 Cl1 Hg1 88.97(4) . 2\_566 ?

C6 O2 C9 117.6(5) . . ?

Hg1 C1 H1 110.4 . . ?

S1 C1 Hg1 110.6(3) . . ?

S1 C1 H1 110.4 . . ?

C2 C1 Hg1 107.1(4) . . ?

C2 C1 S1 107.9(4) . . ?

C2 C1 H1 110.4 . . ?

O1 C2 C1 119.8(6) . . ?

O1 C2 C3 121.0(5) . . ?

C3 C2 C1 119.1(5) . . ?

C4 C3 C2 123.1(5) . . ?

C8 C3 C2 118.9(5) . . ?

C8 C3 C4 117.9(6) . . ?

C3 C4 H4 119.1 . . ?

C5 C4 C3 121.7(6) . . ?

C5 C4 H4 119.1 . . ?

C4 C5 H5 120.5 . . ?

C4 C5 C6 118.9(6) . . ?

C6 C5 H5 120.5 . . ?

O2 C6 C5 125.2(6) . . ?

O2 C6 C7 114.9(6) . . ?

C5 C6 C7 119.9(6) . . ?

C6 C7 H7 119.9 . . ?

C8 C7 C6 120.3(6) . . ?

C8 C7 H7 119.9 . . ?

C3 C8 H8 119.5 . . ?

C7 C8 C3 121.1(6) . . ?

C7 C8 H8 119.5 . . ?

O2 C9 H9A 109.5 . . ?

O2 C9 H9B 109.5 . . ?

O2 C9 H9C 109.5 . . ?

H9A C9 H9B 109.5 . . ?

H9A C9 H9C 109.5 . . ?

H9B C9 H9C 109.5 . . ?

S1 C10 H10A 109.5 . . ?

S1 C10 H10B 109.5 . . ?

S1 C10 H10C 109.5 . . ?

H10A C10 H10B 109.5 . . ?

H10A C10 H10C 109.5 . . ?

H10B C10 H10C 109.5 . . ?

S1 C11 H11A 109.5 . . ?

S1 C11 H11B 109.5 . . ?

S1 C11 H11C 109.5 . . ?

H11A C11 H11B 109.5 . . ?

H11A C11 H11C 109.5 . . ?

H11B C11 H11C 109.5 . . ?

Cl3 Hg2 Cl3 91.77(5) . 2\_656 ?

Cl4 Hg2 Cl3 97.07(7) . . ?

Cl4 Hg2 Cl3 96.50(6) . 2\_656 ?

C12 Hg2 Cl3 94.28(16) . 2\_656 ?

C12 Hg2 Cl3 116.53(17) . . ?

C12 Hg2 Cl4 144.29(17) . . ?

Hg2 Cl3 Hg2 88.23(5) . 2\_656 ?

C21 S2 C12 101.9(3) . . ?

C21 S2 C22 98.8(3) . . ?

C22 S2 C12 104.1(3) . . ?

C17 O4 C20 116.8(6) . . ?

Hg2 C12 H12 110.5 . . ?

S2 C12 Hg2 110.5(3) . . ?

S2 C12 H12 110.5 . . ?

C13 C12 Hg2 105.7(4) . . ?

C13 C12 S2 109.2(5) . . ?

C13 C12 H12 110.5 . . ?

O3 C13 C12 120.7(6) . . ?

O3 C13 C14 121.4(5) . . ?

C12 C13 C14 117.9(5) . . ?

C15 C14 C13 121.8(5) . . ?

C19 C14 C13 118.4(6) . . ?

C19 C14 C15 119.8(6) . . ?

C14 C15 H15 120.1 . . ?

C16 C15 C14 119.7(6) . . ?

C16 C15 H15 120.1 . . ?

C15 C16 H16 119.5 . . ?

C15 C16 C17 121.0(7) . . ?

C17 C16 H16 119.5 . . ?

O4 C17 C16 115.7(6) . . ?

O4 C17 C18 125.1(6) . . ?

C18 C17 C16 119.2(6) . . ?

C17 C18 H18 120.0 . . ?

C19 C18 C17 120.0(6) . . ?

C19 C18 H18 120.0 . . ?

C14 C19 H19 119.9 . . ?

C18 C19 C14 120.3(6) . . ?

C18 C19 H19 119.9 . . ?

O4 C20 H20A 109.5 . . ?

O4 C20 H20B 109.5 . . ?

O4 C20 H20C 109.5 . . ?

H20A C20 H20B 109.5 . . ?

H20A C20 H20C 109.5 . . ?

H20B C20 H20C 109.5 . . ?

S2 C21 H21A 109.5 . . ?

S2 C21 H21B 109.5 . . ?

S2 C21 H21C 109.5 . . ?

H21A C21 H21B 109.5 . . ?

H21A C21 H21C 109.5 . . ?

H21B C21 H21C 109.5 . . ?

S2 C22 H22A 109.5 . . ?

S2 C22 H22B 109.5 . . ?

S2 C22 H22C 109.5 . . ?

H22A C22 H22B 109.5 . . ?

H22A C22 H22C 109.5 . . ?

H22B C22 H22C 109.5 . . ?

O5 S3 C23 107.8(4) . . ?

O5 S3 C24 106.6(3) . . ?

C23 S3 C24 97.6(4) . . ?

S3 C23 H23A 109.5 . . ?

S3 C23 H23B 109.5 . . ?

S3 C23 H23C 109.5 . . ?

H23A C23 H23B 109.5 . . ?

H23A C23 H23C 109.5 . . ?

H23B C23 H23C 109.5 . . ?

S3 C24 H24A 109.5 . . ?

S3 C24 H24B 109.5 . . ?

S3 C24 H24C 109.5 . . ?

H24A C24 H24B 109.5 . . ?

H24A C24 H24C 109.5 . . ?

H24B C24 H24C 109.5 . . ?

O6 S4 C25 107.5(3) . . ?

O6 S4 C26 106.9(4) . . ?

C25 S4 C26 97.0(4) . . ?

S4 C25 H25A 109.5 . . ?

S4 C25 H25B 109.5 . . ?

S4 C25 H25C 109.5 . . ?

H25A C25 H25B 109.5 . . ?

H25A C25 H25C 109.5 . . ?

H25B C25 H25C 109.5 . . ?

S4 C26 H26A 109.5 . . ?

S4 C26 H26B 109.5 . . ?

S4 C26 H26C 109.5 . . ?

H26A C26 H26B 109.5 . . ?

H26A C26 H26C 109.5 . . ?

H26B C26 H26C 109.5 . . ?

loop\_

\_exptl\_crystal\_face\_index\_h

\_exptl\_crystal\_face\_index\_k

\_exptl\_crystal\_face\_index\_l

\_exptl\_crystal\_face\_perp\_dist

\_exptl\_oxdiff\_crystal\_face\_indexfrac\_h

\_exptl\_oxdiff\_crystal\_face\_indexfrac\_k

\_exptl\_oxdiff\_crystal\_face\_indexfrac\_l

\_exptl\_oxdiff\_crystal\_face\_x

\_exptl\_oxdiff\_crystal\_face\_y

\_exptl\_oxdiff\_crystal\_face\_z

0 -1 0 0.0300 -0.0000 -1.0000 -0.0000 0.0092 0.0131 -0.0585

0 1 0 0.0300 0.0000 1.0000 0.0000 -0.0092 -0.0131 0.0585

-1 0 0 0.1300 -1.0000 -0.0000 0.0000 -0.0676 0.0174 -0.0106

1 0 0 0.1300 1.0000 0.0000 -0.0000 0.0676 -0.0174 0.0106

0 0 -1 0.0300 -0.0000 -0.0000 -1.0000 0.0069 0.0487 -0.0061

0 0 1 0.0300 0.0000 0.0000 1.0000 -0.0069 -0.0487 0.0061