Supporting Information for

Formation and Structures of Mercury Complexes of 18-Membered

Unsaturated and Saturated Thiacrown Ethers

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**X-Ray Structure
of
 $\text{Hg}^{\text{II}}(18\text{-UT-6})\text{Cl}_2\cdot\text{Me}_2\text{CO}$ (4)**

Figure S1. ORTEP drawing of $\text{Hg}^{\text{II}}(18\text{-UT-6})\text{Cl}_2 \cdot \text{Me}_2\text{CO}$ (**4**)

data_General

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Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.

Single Crystal Structure Analysis Software. Version 1.11.

MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Rigaku, 3-9-12 Akishima, Tokyo, Japan.

North, A.C.T., Phillips, D. C. & Mathews, F. S. (1968).

Acta Cryst. A24, 351-359.

Zachariasen, W. H. (1967). Acta Cryst. 23, 558-564.

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CHEMICAL DATA

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_chemical_formula_moiety '?'

_chemical_formula_weight 339.08

_chemical_melting_point ?

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CRYSTAL DATA

_symmetry_cell_setting orthorhombic

_symmetry_space_group_name_H-M	'P 21/n 21/m 21/a'
_symmetry_Int_Tables_number	62
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_symmetry_equiv_pos_as_xyz	
x,y,z	
1/2+x,1/2-y,1/2-z	
-x,1/2+y,-z	
1/2-x,-y,1/2+z	
-x,-y,-z	
1/2-x,1/2+y,1/2+z	
x,1/2-y,z	
1/2+x,y,1/2-z	
_cell_length_a	16.746(5)
_cell_length_b	12.028(8)
_cell_length_c	11.574(9)
_cell_angle_alpha	89
_cell_angle_beta	89
_cell_angle_gamma	90
_cell_volume	2331(3)
_cell_formula_units_Z	8
_cell_measurement_reflns_used	25
_cell_measurement_theta_min	14.8
_cell_measurement_theta_max	15.0
_cell_measurement_temperature	193.2
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_exptl_crystal_size_min	0.300
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_exptl_crystal_density_diffn	1.932
_exptl_crystal_density_meas	?
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_exptl_absorpt_coefficient_mu	7.389
_exptl_absorpt_correction_type	psi-scan
_exptl_absorpt_process_details	'(North, Phillips & Mathews, 1968)'

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_diffn_measurement_device_type        'Rigaku AFC7R'
_diffn_measurement_method              $\Psi$ w-2 $\Psi$ q
_diffn_reflns_number                  3032
_diffn_reflns_av_R_equivalents        ?
_diffn_reflns_theta_max                27.50
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Refinement using reflections with  $F^2 > 0.0 \sigma(F^2)$ . The weighted
R-factor (wR) and goodness of fit (S) are based on  $F^2$ . R-factor (gt) are
based on F. The threshold expression of  $F^2 > 2.0 \sigma(F^2)$  is used only
for calculating R-factor (gt).
;
_reflns_number_total                   2795
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_reflns_threshold_expression            $F^2 > 2.0 \sigma(F^2)$ 
_refine_ls_structure_factor_coef       Fsqd
_refine_ls_R_factor_gt                 0.0698

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_refine_ls_number_parameters       122
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  'w = 1/[ $\sigma^2(F_o^2) + (0.11700(\text{Max}(F_o^2, 0) + 2F_c^2)/3)^2$ ]'
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;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'H' 'H'  0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
  'S' 'S'  0.125 0.123
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)

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'Cl' 'Cl' 0.148 0.159

;International Tables for Crystallography

(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)

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'O' 'O' 0.011 0.006

;International Tables for Crystallography

(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)

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ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_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_calc_flag

_atom_site_refinement_flags

_atom_site_disorder_assembly

_atom_site_disorder_group

Hg(1)	Hg	0.15057(4)	0.2500	-0.14143(6)	0.0382(3)	Uiso 1.00 d S . .
Cl(1)	Cl	0.2165(2)	0.2500	-0.3233(4)	0.0358(10)	Uani 1.00 d S . .
Cl(2)	Cl	0.0866(3)	0.2500	0.0384(4)	0.043(1)	Uani 1.00 d S . .
S(1)	S	0.3170(3)	0.2500	-0.0230(4)	0.040(1)	Uani 1.00 d S . .
S(2)	S	0.2426(2)	0.4832(3)	-0.0939(3)	0.0439(8)	Uani 1.00 d . . .
S(3)	S	0.0708(2)	0.4766(3)	-0.2156(3)	0.0422(8)	Uani 1.00 d . . .
S(4)	S	-0.0147(3)	0.2500	-0.2772(4)	0.045(1)	Uani 1.00 d S . .
O(1)	O	0.486(1)	0.2500	0.188(2)	0.070(5)	Uani 1.00 d S . .
C(1)	C	0.3130(9)	0.361(1)	0.074(2)	0.057(4)	Uani 1.00 d . . .
C(2)	C	0.2838(9)	0.459(1)	0.043(2)	0.062(5)	Uani 1.00 d . . .
C(3)	C	0.1660(8)	0.576(1)	-0.059(1)	0.050(4)	Uani 1.00 d . . .
C(4)	C	0.0943(8)	0.573(1)	-0.111(1)	0.048(4)	Uani 1.00 d . . .
C(5)	C	-0.0311(6)	0.457(1)	-0.192(1)	0.047(4)	Uani 1.00 d . . .

C(6)	C	-0.0673(6)	0.363(1)	-0.218(1)	0.051(4)	Uani 1.00 d ...
C(7)	C	0.538(2)	0.2500	0.126(4)	0.15(2)	Uani 1.00 d S ...
C(8)	C	0.573(4)	0.171(7)	0.089(6)	0.69(6)	Uani 1.00 d ...
H(1)	H	0.3323	0.3511	0.1505	0.0688	Uiso 1.00 calc ...
H(2)	H	0.2853	0.5188	0.0975	0.0739	Uiso 1.00 calc ...
H(3)	H	0.1755	0.6307	-0.0020	0.0597	Uiso 1.00 calc ...
H(4)	H	0.0550	0.6256	-0.0883	0.0580	Uiso 1.00 calc ...
H(5)	H	-0.0615	0.5162	-0.1592	0.0566	Uiso 1.00 calc ...
H(6)	H	-0.1231	0.3555	-0.2053	0.0613	Uiso 1.00 calc ...
H(7)	H	0.5389	0.1293	0.0397	0.8317	Uiso 1.00 calc ...
H(8)	H	0.6183	0.1954	0.0462	0.8317	Uiso 1.00 calc ...
H(9)	H	0.5903	0.1251	0.1510	0.8317	Uiso 1.00 calc ...

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_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

Cl(1)	0.033(2)	0.035(2)	0.039(2)	0.0000	0.005(2)	0.0000
Cl(2)	0.047(2)	0.045(2)	0.038(2)	0.0000	0.013(2)	0.0000
S(1)	0.037(2)	0.042(2)	0.043(3)	0.0000	0.000(2)	0.0000
S(2)	0.045(2)	0.036(1)	0.051(2)	-0.001(1)	-0.004(2)	-0.004(1)
S(3)	0.042(1)	0.039(2)	0.046(2)	0.006(1)	0.004(1)	0.006(1)
S(4)	0.038(2)	0.062(3)	0.036(3)	0.0000	0.002(2)	0.0000
O(1)	0.069(10)	0.07(1)	0.07(1)	0.0000	0.020(9)	0.0000
C(1)	0.065(9)	0.043(7)	0.06(1)	-0.004(6)	-0.025(8)	-0.004(7)
C(2)	0.072(10)	0.038(7)	0.07(1)	-0.003(6)	-0.040(8)	-0.005(7)
C(3)	0.065(8)	0.034(6)	0.050(9)	0.007(5)	-0.001(6)	-0.007(6)
C(4)	0.044(7)	0.037(6)	0.065(9)	0.011(5)	0.001(6)	-0.002(6)
C(5)	0.028(5)	0.051(7)	0.062(9)	0.013(5)	0.002(6)	0.007(7)
C(6)	0.028(5)	0.073(9)	0.052(8)	0.009(6)	0.002(5)	0.017(7)
C(7)	0.06(2)	0.28(7)	0.10(3)	0.0000	0.03(2)	0.0000
C(8)	0.7(1)	0.8(1)	0.53(9)	0.7(1)	0.58(10)	0.6(1)

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_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

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Hg(1)	Cl(1)	2.377(4)	.. yes
Hg(1)	Cl(2)	2.341(4)	.. yes
Hg(1)	S(1)	3.106(4)	.. yes
Hg(1)	S(2)	3.247(3)	.. yes
Hg(1)	S(2)	3.247(3)	. 7_555 yes
Hg(1)	S(3)	3.154(3)	.. yes
Hg(1)	S(3)	3.154(3)	. 7_555 yes
Hg(1)	S(4)	3.182(5)	.. yes
S(1)	C(1)	1.75(2)	.. yes
S(1)	C(1)	1.75(2)	. 7_555 yes
S(2)	C(2)	1.76(2)	.. yes
S(2)	C(3)	1.75(1)	.. yes
S(3)	C(4)	1.72(2)	.. yes
S(3)	C(5)	1.74(1)	.. yes
S(4)	C(6)	1.75(2)	.. yes
S(4)	C(6)	1.75(2)	. 7_555 yes
O(1)	C(7)	1.12(3)	.. yes
C(1)	C(2)	1.33(2)	.. yes

C(1)	H(1)	0.950	.. no
C(2)	H(2)	0.950	.. no
C(3)	C(4)	1.34(2)	.. yes
C(3)	H(3)	0.950	.. no
C(4)	H(4)	0.950	.. no
C(5)	C(6)	1.33(2)	.. yes
C(5)	H(5)	0.950	.. no
C(6)	H(6)	0.950	.. no
C(7)	C(8)	1.21(6)	.. yes
C(7)	C(8)	1.21(6)	.. 7_555 yes
C(8)	H(7)	0.950	.. no
C(8)	H(8)	0.950	.. no
C(8)	H(9)	0.950	.. no

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Cl(1)	Hg(1)	Cl(2)	179.6(2)	... yes
Cl(1)	Hg(1)	S(1)	88.5(1)	... yes
Cl(1)	Hg(1)	S(2)	85.97(8)	... yes
Cl(1)	Hg(1)	S(2)	85.97(8)	.. 7_555 yes
Cl(1)	Hg(1)	S(3)	87.45(8)	... yes
Cl(1)	Hg(1)	S(3)	87.45(8)	.. 7_555 yes
Cl(1)	Hg(1)	S(4)	88.1(1)	... yes
Cl(2)	Hg(1)	S(1)	91.1(1)	... yes
Cl(2)	Hg(1)	S(2)	93.81(9)	... yes
Cl(2)	Hg(1)	S(2)	93.81(9)	.. 7_555 yes
Cl(2)	Hg(1)	S(3)	92.76(8)	... yes
Cl(2)	Hg(1)	S(3)	92.76(8)	.. 7_555 yes
Cl(2)	Hg(1)	S(4)	92.4(1)	... yes
S(1)	Hg(1)	S(2)	59.97(6)	... yes

S(1)	Hg(1)	S(2)	59.97(6)	.. 7_555 yes
S(1)	Hg(1)	S(3)	120.01(6)	... yes
S(1)	Hg(1)	S(3)	120.01(6)	.. 7_555 yes
S(1)	Hg(1)	S(4)	176.6(1)	... yes
S(2)	Hg(1)	S(2)	119.5(1)	.. 7_555 yes
S(2)	Hg(1)	S(3)	60.04(8)	... yes
S(2)	Hg(1)	S(3)	173.43(9)	.. 7_555 yes
S(2)	Hg(1)	S(4)	119.74(6)	... yes
S(2)	Hg(1)	S(3)	173.43(9)	7_555 .. yes
S(2)	Hg(1)	S(3)	60.04(8)	7_555 .. 7_555 yes
S(2)	Hg(1)	S(4)	119.74(6)	7_555 .. yes
S(3)	Hg(1)	S(3)	119.5(1)	.. 7_555 yes
S(3)	Hg(1)	S(4)	59.82(6)	... yes
S(3)	Hg(1)	S(4)	59.82(6)	7_555 .. yes
Hg(1)	S(1)	C(1)	104.4(5)	... yes
Hg(1)	S(1)	C(1)	104.4(5)	.. 7_555 yes
C(1)	S(1)	C(1)	99(1)	.. 7_555 yes
Hg(1)	S(2)	C(2)	101.5(5)	... yes
Hg(1)	S(2)	C(3)	104.0(5)	... yes
C(2)	S(2)	C(3)	100.7(8)	... yes
Hg(1)	S(3)	C(4)	107.0(5)	... yes
Hg(1)	S(3)	C(5)	104.9(5)	... yes
C(4)	S(3)	C(5)	101.7(7)	... yes
Hg(1)	S(4)	C(6)	104.2(5)	... yes
Hg(1)	S(4)	C(6)	104.2(5)	.. 7_555 yes
C(6)	S(4)	C(6)	101.1(9)	.. 7_555 yes
S(1)	C(1)	C(2)	121(1)	... yes
S(1)	C(1)	H(1)	119.2	... no
C(2)	C(1)	H(1)	119.2	... no
S(2)	C(2)	C(1)	122(1)	... yes
S(2)	C(2)	H(2)	118.9	... no
C(1)	C(2)	H(2)	119.0	... no
S(2)	C(3)	C(4)	122(1)	... yes
S(2)	C(3)	H(3)	118.7	... no
C(4)	C(3)	H(3)	118.7	... no
S(3)	C(4)	C(3)	122(1)	... yes
S(3)	C(4)	H(4)	118.8	... no

C(3)	C(4)	H(4)	118.8	... no
S(3)	C(5)	C(6)	121.6(10)	... yes
S(3)	C(5)	H(5)	119.2	... no
C(6)	C(5)	H(5)	119.2	... no
S(4)	C(6)	C(5)	121.6(9)	... yes
S(4)	C(6)	H(6)	119.2	... no
C(5)	C(6)	H(6)	119.2	... no
O(1)	C(7)	C(8)	127(3)	... yes
O(1)	C(7)	C(8)	127(3)	.. 7_555 yes
C(8)	C(7)	C(8)	104(6)	.. 7_555 yes
C(7)	C(8)	H(7)	109.5	... no
C(7)	C(8)	H(8)	109.5	... no
C(7)	C(8)	H(9)	109.5	... no
H(7)	C(8)	H(8)	109.5	... no
H(7)	C(8)	H(9)	109.5	... no
H(8)	C(8)	H(9)	109.5	... no

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Hg(1)	S(1)	C(1)	C(2)	-45(1)	 yes
Hg(1)	S(1)	C(1)	C(2)	45(1)	.. 7_555 7_555 yes
Hg(1)	S(2)	C(2)	C(1)	37(1)	 yes
Hg(1)	S(2)	C(3)	C(4)	-36(1)	 yes
Hg(1)	S(2)	C(2)	C(1)	-37(1)	. 7_555 7_555 7_555 yes
Hg(1)	S(2)	C(3)	C(4)	36(1)	. 7_555 7_555 7_555 yes
Hg(1)	S(3)	C(4)	C(3)	38(1)	 yes
Hg(1)	S(3)	C(5)	C(6)	-41(1)	 yes
Hg(1)	S(3)	C(4)	C(3)	-38(1)	. 7_555 7_555 7_555 yes

Hg(1)	S(3)	C(5)	C(6)	41(1)	. 7_555 7_555 7_555 yes
Hg(1)	S(4)	C(6)	C(5)	39(1)	 yes
Hg(1)	S(4)	C(6)	C(5)	-39(1)	.. 7_555 7_555 yes
Cl(1)	Hg(1)	S(1)	C(1)	127.8(6)	 yes
Cl(1)	Hg(1)	S(1)	C(1)	-127.8(6)	... 7_555 yes
Cl(1)	Hg(1)	S(2)	C(2)	-130.3(6)	 yes
Cl(1)	Hg(1)	S(2)	C(3)	125.4(6)	 yes
Cl(1)	Hg(1)	S(2)	C(2)	130.3(6)	.. 7_555 7_555 yes
Cl(1)	Hg(1)	S(2)	C(3)	-125.4(6)	.. 7_555 7_555 yes
Cl(1)	Hg(1)	S(3)	C(4)	-123.8(5)	 yes
Cl(1)	Hg(1)	S(3)	C(5)	128.8(6)	 yes
Cl(1)	Hg(1)	S(3)	C(4)	123.8(5)	.. 7_555 7_555 yes
Cl(1)	Hg(1)	S(3)	C(5)	-128.8(6)	.. 7_555 7_555 yes
Cl(1)	Hg(1)	S(4)	C(6)	-127.2(5)	 yes
Cl(1)	Hg(1)	S(4)	C(6)	127.2(5)	... 7_555 yes
Cl(2)	Hg(1)	S(1)	C(1)	-52.2(6)	 yes
Cl(2)	Hg(1)	S(1)	C(1)	52.2(6)	... 7_555 yes
Cl(2)	Hg(1)	S(2)	C(2)	49.3(6)	 yes
Cl(2)	Hg(1)	S(2)	C(3)	-55.0(6)	 yes
Cl(2)	Hg(1)	S(2)	C(2)	-49.3(6)	.. 7_555 7_555 yes
Cl(2)	Hg(1)	S(2)	C(3)	55.0(6)	.. 7_555 7_555 yes
Cl(2)	Hg(1)	S(3)	C(4)	55.9(5)	 yes
Cl(2)	Hg(1)	S(3)	C(5)	-51.6(6)	 yes
Cl(2)	Hg(1)	S(3)	C(4)	-55.9(5)	.. 7_555 7_555 yes
Cl(2)	Hg(1)	S(3)	C(5)	51.6(6)	.. 7_555 7_555 yes
Cl(2)	Hg(1)	S(4)	C(6)	52.8(5)	 yes
Cl(2)	Hg(1)	S(4)	C(6)	-52.8(5)	... 7_555 yes
S(1)	Hg(1)	S(2)	C(2)	-39.7(6)	 yes
S(1)	Hg(1)	S(2)	C(3)	-144.0(6)	 yes
S(1)	Hg(1)	S(2)	C(2)	39.7(6)	.. 7_555 7_555 yes
S(1)	Hg(1)	S(2)	C(3)	144.0(6)	.. 7_555 7_555 yes
S(1)	Hg(1)	S(3)	C(4)	-37.0(5)	 yes
S(1)	Hg(1)	S(3)	C(5)	-144.4(6)	 yes
S(1)	Hg(1)	S(3)	C(4)	37.0(5)	.. 7_555 7_555 yes
S(1)	Hg(1)	S(3)	C(5)	144.4(6)	.. 7_555 7_555 yes
S(1)	Hg(1)	S(4)	C(6)	-127.2(5)	 yes
S(1)	Hg(1)	S(4)	C(6)	127.2(5)	... 7_555 yes

S(1)	C(1)	C(2)	S(2)	3(2)	 yes
S(1)	C(1)	C(2)	S(2)	-3(2)	.. 7_555 7_555 7_555 yes
S(2)	Hg(1)	S(1)	C(1)	41.6(6)	 yes
S(2)	Hg(1)	S(1)	C(1)	146.0(6)	... 7_555 yes
S(2)	Hg(1)	S(2)	C(2)	47.3(6)	.. 7_555 7_555 yes
S(2)	Hg(1)	S(2)	C(3)	151.5(5)	.. 7_555 7_555 yes
S(2)	Hg(1)	S(3)	C(4)	-37.0(5)	 yes
S(2)	Hg(1)	S(3)	C(5)	-144.4(6)	 yes
S(2)	Hg(1)	S(3)	C(4)	124.9(8)	.. 7_555 7_555 yes
S(2)	Hg(1)	S(3)	C(5)	-127.7(8)	.. 7_555 7_555 yes
S(2)	Hg(1)	S(4)	C(6)	-42.9(5)	 yes
S(2)	Hg(1)	S(4)	C(6)	-148.6(5)	... 7_555 yes
S(2)	C(3)	C(4)	S(3)	0(1)	 yes
S(3)	Hg(1)	S(1)	C(1)	41.6(6)	 yes
S(3)	Hg(1)	S(1)	C(1)	146.0(6)	... 7_555 yes
S(3)	Hg(1)	S(2)	C(2)	140.3(6)	 yes
S(3)	Hg(1)	S(2)	C(3)	36.0(5)	 yes
S(3)	Hg(1)	S(2)	C(2)	131.5(9)	.. 7_555 7_555 yes
S(3)	Hg(1)	S(2)	C(3)	-124.3(9)	.. 7_555 7_555 yes
S(3)	Hg(1)	S(3)	C(4)	-150.6(5)	.. 7_555 7_555 yes
S(3)	Hg(1)	S(3)	C(5)	-43.2(6)	.. 7_555 7_555 yes
S(3)	Hg(1)	S(4)	C(6)	-39.0(5)	 yes
S(3)	Hg(1)	S(4)	C(6)	-144.6(5)	... 7_555 yes
S(3)	C(5)	C(6)	S(4)	0(1)	 yes
S(4)	Hg(1)	S(1)	C(1)	127.8(6)	 yes
S(4)	Hg(1)	S(1)	C(1)	-127.8(6)	... 7_555 yes
S(4)	Hg(1)	S(2)	C(2)	144.2(6)	 yes
S(4)	Hg(1)	S(2)	C(3)	39.9(6)	 yes
S(4)	Hg(1)	S(2)	C(2)	-144.2(6)	.. 7_555 7_555 yes
S(4)	Hg(1)	S(2)	C(3)	-39.9(6)	.. 7_555 7_555 yes
S(4)	Hg(1)	S(3)	C(4)	147.0(5)	 yes
S(4)	Hg(1)	S(3)	C(5)	39.6(6)	 yes
S(4)	Hg(1)	S(3)	C(4)	-147.0(5)	.. 7_555 7_555 yes
S(4)	Hg(1)	S(3)	C(5)	-39.6(6)	.. 7_555 7_555 yes
C(1)	S(1)	C(1)	C(2)	153(1)	.. 7_555 7_555 yes
C(1)	C(2)	S(2)	C(3)	144(1)	 yes
C(2)	S(2)	C(3)	C(4)	-141(1)	 yes

C(3)	C(4)	S(3)	C(5)	148(1)	 yes
C(4)	S(3)	C(5)	C(6)	-152(1)	 yes
C(5)	C(6)	S(4)	C(6)	147(1)	... 7_555 yes
C(5)	C(6)	S(4)	C(6)	147(1)	... 7_555 yes

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Hg(1)	S(1)	3.106(4)	.. ?
Hg(1)	S(2)	3.247(3)	.. ?
Hg(1)	S(2)	3.247(3)	. 7_555 ?
Hg(1)	S(3)	3.154(3)	.. ?
Hg(1)	S(3)	3.154(3)	. 7_555 ?
Hg(1)	S(4)	3.182(5)	.. ?
Cl(2)	O(1)	3.59(2)	. 2_455 ?
O(1)	C(4)	3.43(2)	. 4_565 ?
O(1)	C(4)	3.43(2)	. 6_545 ?
O(1)	C(1)	3.45(2)	.. ?
O(1)	C(1)	3.45(2)	. 7_555 ?

#-----

#-----

X-Ray Structure

of

Hg^{II}(18S6)Cl₂ (5)

Figure S2. ORTEP drawing of $\text{Hg}^{\text{II}}(18\text{S}6)\text{Cl}_2$ (5)

data_General

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_audit_creation_method 'by teXsan'

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_journal_coeditor_code ?

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_publ_contact_author_fax '+81 426 (77) 2525'

_publ_contact_author_phone '+81 426 (77) 2556'

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_publ_requested_category 'CHOOSE FI FM FO CI CM CO or AD'

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Formation and Structures of Mercury Complexes of 18-Membered Unsaturated and Saturated
Thiacrown Ethers

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_publ_section_title_footnote

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_publ_author_name

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_publ_author_address

'Takahiro Tsuchiya'

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FIRST AUTHORS FOOTNOTES

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Minami-ohsawa, Hachioji, Tokyo 192-0397, Japan

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Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan.

Single Crystal Structure Analysis Software. Version 1.11.

MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Rigaku, 3-9-12 Akishima, Tokyo, Japan.

Zachariasen, W. H. (1967). Acta Cryst. 23, 558-564.

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ENTER COMPOUND PREPARATION DETAILS

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data_Hg(18S6)Cl2_

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CHEMICAL DATA

_chemical_formula_sum 'C12 H24 Cl2 Hg S6 '

_chemical_formula_moiety '?'

_chemical_formula_weight 632.18

_chemical_melting_point ?

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CRYSTAL DATA

_symmetry_cell_setting triclinic

_symmetry_space_group_name_H-M 'P -1 '

_symmetry_Int_Tables_number 2

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_symmetry_equiv_pos_as_xyz
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-x,-y,-z
_cell_length_a          7.554(2)
_cell_length_b          7.928(2)
_cell_length_c          17.259(3)
_cell_angle_alpha       95.436(8)
_cell_angle_beta        97.41(1)
_cell_angle_gamma       93.569(10)
_cell_volume            1017.4(4)
_cell_formula_units_Z   2
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_cell_measurement_theta_min 3.9
_cell_measurement_theta_max 27.4
_cell_measurement_temperature 296.2
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_exptl_crystal_description 'block'
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_diffn_measurement_method  'w'

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_diffn_detector_area_resol_mean	10.00
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REFINEMENT DATA

_refine_special_details

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Refinement using reflections with $F^2 > 3.0 \sigma(F^2)$. The weighted R-factor (wR) and goodness of fit (S) are based on F^2 . R-factor (gt) are based on F. The threshold expression of $F^2 > 3.0 \sigma(F^2)$ is used only for calculating R-factor (gt).

;

_reflns_number_total	4631
_reflns_number_gt	2589
_reflns_threshold_expression	$F^2 > 3.0 \sigma(F^2)$
_refine_ls_structure_factor_coef	Fsqd
_refine_ls_R_factor_gt	0.0862
_refine_ls_wR_factor_ref	0.1896
_refine_ls_hydrogen_treatment	noref
_refine_ls_number_reflns	2589
_refine_ls_number_parameters	184
_refine_ls_goodness_of_fit_ref	2.515
_refine_ls_weighting_scheme	calc
_refine_ls_weighting_details	
'w = 1/[$\sigma^2(F_o^2) + (0.05000(\text{Max}(F_o^2, 0) + 2F_c^2)/3)^2$]	
_refine_ls_shift/su_max	0.0002
_refine_diff_density_max	7.87

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_refine_diff_density_min          -7.65
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    'Zachariasen(1967) type 2 Gaussian isotropic'
_refine_ls_extinction_coef        0.0016(9)
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
    'S' 'S'  0.125 0.123
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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    'Cl' 'Cl'  0.148 0.159
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<u>_atom_site_refinement_flags</u>					
<u>_atom_site_disorder_assembly</u>					
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Hg(1)	Hg	1.0000	0.0000	0.0000	0.0362(4) Uiso 1.00 d S . .
Hg(2)	Hg	1.0000	-0.5000	-0.5000	0.0342(4) Uiso 1.00 d S . .
Cl(1)	Cl	1.1510(8)	-0.2769(8)	-0.0618(4)	0.049(2) Uani 1.00 d . . .
Cl(2)	Cl	1.1861(7)	-0.2271(7)	-0.5355(4)	0.040(2) Uani 1.00 d . . .
S(1)	S	1.3324(7)	0.1342(7)	0.0263(3)	0.033(1) Uani 1.00 d . . .
S(2)	S	1.0091(8)	0.1182(7)	-0.1435(3)	0.034(1) Uani 1.00 d . . .
S(3)	S	0.6153(9)	0.4737(8)	-0.2263(4)	0.042(2) Uani 1.00 d . . .
S(4)	S	0.6845(7)	-0.3787(7)	-0.5472(3)	0.030(1) Uani 1.00 d . . .
S(5)	S	0.9374(7)	-0.3530(7)	-0.3563(3)	0.035(1) Uani 1.00 d . . .
S(6)	S	1.3990(9)	0.0154(8)	-0.2743(4)	0.041(2) Uani 1.00 d . . .
C(1)	C	1.359(3)	0.186(3)	-0.072(1)	0.036(6) Uani 1.00 d . . .
C(2)	C	1.201(3)	0.265(3)	-0.113(1)	0.030(6) Uani 1.00 d . . .
C(3)	C	0.825(3)	0.257(3)	-0.147(1)	0.037(6) Uani 1.00 d . . .
C(4)	C	0.817(3)	0.365(3)	-0.215(1)	0.040(7) Uani 1.00 d . . .
C(5)	C	0.670(3)	0.669(3)	-0.162(1)	0.035(6) Uani 1.00 d . . .
C(6)	C	0.657(3)	0.654(3)	-0.079(1)	0.039(7) Uani 1.00 d . . .
C(7)	C	0.682(3)	-0.221(3)	-0.466(1)	0.036(6) Uani 1.00 d . . .
C(8)	C	0.714(3)	-0.296(3)	-0.387(1)	0.041(7) Uani 1.00 d . . .
C(9)	C	1.066(3)	-0.148(3)	-0.338(1)	0.041(7) Uani 1.00 d . . .
C(10)	C	1.250(3)	-0.178(3)	-0.309(1)	0.043(7) Uani 1.00 d . . .
C(11)	C	1.409(3)	0.119(3)	-0.365(1)	0.034(6) Uani 1.00 d . . .
C(12)	C	1.268(3)	0.243(3)	-0.378(1)	0.028(5) Uani 1.00 d . . .
H(1)	H	1.4615	0.2630	-0.0681	0.0433 Uiso 1.00 calc . . .
H(2)	H	1.3771	0.0838	-0.1024	0.0433 Uiso 1.00 calc . . .
H(3)	H	1.1686	0.3547	-0.0788	0.0363 Uiso 1.00 calc . . .
H(4)	H	1.2367	0.3095	-0.1586	0.0363 Uiso 1.00 calc . . .
H(5)	H	0.8392	0.3306	-0.0991	0.0448 Uiso 1.00 calc . . .

H(6)	H	0.7154	0.1888	-0.1512	0.0448	Uiso 1.00 calc ...
H(7)	H	0.9172	0.4466	-0.2062	0.0479	Uiso 1.00 calc ...
H(8)	H	0.8226	0.2933	-0.2620	0.0479	Uiso 1.00 calc ...
H(9)	H	0.7901	0.7082	-0.1665	0.0425	Uiso 1.00 calc ...
H(10)	H	0.5914	0.7505	-0.1798	0.0425	Uiso 1.00 calc ...
H(11)	H	0.7346	0.5721	-0.0604	0.0472	Uiso 1.00 calc ...
H(12)	H	0.5370	0.6179	-0.0734	0.0472	Uiso 1.00 calc ...
H(13)	H	0.7727	-0.1332	-0.4671	0.0430	Uiso 1.00 calc ...
H(14)	H	0.5683	-0.1744	-0.4701	0.0430	Uiso 1.00 calc ...
H(15)	H	0.6846	-0.2152	-0.3478	0.0489	Uiso 1.00 calc ...
H(16)	H	0.6363	-0.3961	-0.3909	0.0489	Uiso 1.00 calc ...
H(17)	H	1.0176	-0.0763	-0.3002	0.0490	Uiso 1.00 calc ...
H(18)	H	1.0630	-0.0957	-0.3856	0.0490	Uiso 1.00 calc ...
H(19)	H	1.2476	-0.2448	-0.2660	0.0516	Uiso 1.00 calc ...
H(20)	H	1.2995	-0.2389	-0.3499	0.0516	Uiso 1.00 calc ...
H(21)	H	1.5234	0.1777	-0.3621	0.0413	Uiso 1.00 calc ...
H(22)	H	1.3928	0.0333	-0.4085	0.0413	Uiso 1.00 calc ...
H(23)	H	1.2838	0.3297	-0.3352	0.0341	Uiso 1.00 calc ...
H(24)	H	1.1525	0.1850	-0.3809	0.0341	Uiso 1.00 calc ...

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_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

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Cl(1)	0.047(3)	0.032(3)	0.064(4)	0.009(3)	0.005(3)	-0.007(3)
Cl(2)	0.034(3)	0.026(3)	0.058(4)	-0.005(2)	0.006(3)	0.007(3)
S(1)	0.029(3)	0.022(3)	0.047(3)	0.005(2)	0.002(2)	-0.001(2)
S(2)	0.039(3)	0.024(3)	0.038(3)	0.006(2)	0.002(2)	0.004(2)
S(3)	0.045(4)	0.038(4)	0.038(4)	0.005(3)	-0.007(3)	0.001(3)
S(4)	0.029(3)	0.024(3)	0.035(3)	-0.006(2)	0.001(2)	0.004(2)
S(5)	0.035(3)	0.027(3)	0.039(3)	-0.007(2)	0.001(2)	0.006(2)
S(6)	0.037(4)	0.043(4)	0.039(3)	-0.006(3)	-0.006(3)	0.005(3)
C(1)	0.03(1)	0.04(1)	0.04(1)	0.004(10)	0.012(10)	0.00(1)

C(2)	0.05(1)	0.03(1)	0.02(1)	0.01(1)	0.012(9)	0.020(9)
C(3)	0.04(1)	0.04(1)	0.04(1)	0.01(1)	0.00(1)	0.02(1)
C(4)	0.03(1)	0.04(1)	0.04(1)	0.01(1)	-0.01(1)	0.01(1)
C(5)	0.05(1)	0.03(1)	0.02(1)	0.00(1)	-0.01(1)	0.002(9)
C(6)	0.05(1)	0.02(1)	0.04(1)	0.00(1)	0.02(1)	-0.01(1)
C(7)	0.04(1)	0.03(1)	0.03(1)	0.00(1)	0.003(10)	-0.006(10)
C(8)	0.04(1)	0.04(1)	0.04(1)	0.00(1)	0.01(1)	0.00(1)
C(9)	0.04(1)	0.02(1)	0.06(2)	-0.01(1)	0.00(1)	-0.01(1)
C(10)	0.03(1)	0.04(1)	0.06(2)	-0.01(1)	0.00(1)	0.02(1)
C(11)	0.04(1)	0.04(1)	0.02(1)	-0.01(1)	0.000(9)	0.009(10)
C(12)	0.03(1)	0.04(1)	0.015(10)	-0.007(10)	0.004(8)	-0.008(9)

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_computing_data_collection      'PROCESS-AUTO'
_computing_cell_refinement      'PROCESS-AUTO'
_computing_data_reduction       'teXsan Ver. 1.11'
_computing_structure_solution   SIR92
_computing_structure_refinement 'teXsan Ver. 1.10'
_computing_publication_material 'teXsan Ver. 1.11'
_computing_molecular_graphics   ?

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_geom_special_details

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?

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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

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Hg(1)   Cl(1)   2.728(6)  .. yes
Hg(1)   Cl(1)   2.728(6)  . 2_755 yes
Hg(1)   S(1)    2.632(5)  .. yes
Hg(1)   S(1)    2.632(5)  . 2_755 yes
Hg(1)   S(2)    2.738(6)  .. yes
Hg(1)   S(2)    2.738(6)  . 2_755 yes

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Hg(2)	Cl(2)	2.670(5)	.. yes
Hg(2)	Cl(2)	2.670(5)	. 2_744 yes
Hg(2)	S(4)	2.684(6)	.. yes
Hg(2)	S(4)	2.684(6)	. 2_744 yes
Hg(2)	S(5)	2.749(6)	.. yes
Hg(2)	S(5)	2.749(6)	. 2_744 yes
S(1)	C(1)	1.81(2)	.. yes
S(1)	C(6)	1.83(2)	. 2_765 yes
S(2)	C(2)	1.79(2)	.. yes
S(2)	C(3)	1.83(2)	.. yes
S(3)	C(4)	1.80(2)	.. yes
S(3)	C(5)	1.81(2)	.. yes
S(4)	C(7)	1.80(2)	.. yes
S(4)	C(12)	1.82(2)	. 2_754 yes
S(5)	C(8)	1.80(2)	.. yes
S(5)	C(9)	1.82(2)	.. yes
S(6)	C(10)	1.84(2)	.. yes
S(6)	C(11)	1.84(2)	.. yes
C(1)	C(2)	1.51(3)	.. yes
C(3)	C(4)	1.52(3)	.. yes
C(5)	C(6)	1.47(3)	.. yes
C(7)	C(8)	1.53(3)	.. yes
C(9)	C(10)	1.46(3)	.. yes
C(11)	C(12)	1.51(3)	.. yes

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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_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

Cl(1)	Hg(1)	Cl(1)	180.0	.. 2_755 yes
Cl(1)	Hg(1)	S(1)	83.7(2)	... yes
Cl(1)	Hg(1)	S(1)	96.3(2)	.. 2_755 yes

Cl(1)	Hg(1)	S(2)	85.7(2)	... yes
Cl(1)	Hg(1)	S(2)	94.3(2)	.. 2_755 yes
Cl(1)	Hg(1)	S(1)	96.3(2)	2_755 ... yes
Cl(1)	Hg(1)	S(1)	83.7(2)	2_755 . 2_755 yes
Cl(1)	Hg(1)	S(2)	94.3(2)	2_755 ... yes
Cl(1)	Hg(1)	S(2)	85.7(2)	2_755 . 2_755 yes
S(1)	Hg(1)	S(1)	180.0	.. 2_755 yes
S(1)	Hg(1)	S(2)	82.8(2)	... yes
S(1)	Hg(1)	S(2)	97.2(2)	.. 2_755 yes
S(1)	Hg(1)	S(2)	97.2(2)	2_755 .. yes
S(1)	Hg(1)	S(2)	82.8(2)	2_755 . 2_755 yes
S(2)	Hg(1)	S(2)	180.0	.. 2_755 yes
Cl(2)	Hg(2)	Cl(2)	180.0	.. 2_744 yes
Cl(2)	Hg(2)	S(4)	92.8(2)	... yes
Cl(2)	Hg(2)	S(4)	87.2(2)	.. 2_744 yes
Cl(2)	Hg(2)	S(5)	94.9(2)	... yes
Cl(2)	Hg(2)	S(5)	85.1(2)	.. 2_744 yes
Cl(2)	Hg(2)	S(4)	87.2(2)	2_744 .. yes
Cl(2)	Hg(2)	S(4)	92.8(2)	2_744 . 2_744 yes
Cl(2)	Hg(2)	S(5)	85.1(2)	2_744 .. yes
Cl(2)	Hg(2)	S(5)	94.9(2)	2_744 . 2_744 yes
S(4)	Hg(2)	S(4)	180.0	.. 2_744 yes
S(4)	Hg(2)	S(5)	82.2(2)	... yes
S(4)	Hg(2)	S(5)	97.8(2)	.. 2_744 yes
S(4)	Hg(2)	S(5)	97.8(2)	2_744 .. yes
S(4)	Hg(2)	S(5)	82.2(2)	2_744 . 2_744 yes
S(5)	Hg(2)	S(5)	180.0	.. 2_744 yes
Hg(1)	S(1)	C(1)	99.4(7)	... yes
Hg(1)	S(1)	C(6)	110.4(8)	.. 2_765 yes
C(1)	S(1)	C(6)	100(1)	.. 2_765 yes
Hg(1)	S(2)	C(2)	95.8(6)	... yes
Hg(1)	S(2)	C(3)	101.1(8)	... yes
C(2)	S(2)	C(3)	102(1)	... yes
C(4)	S(3)	C(5)	103(1)	... yes
Hg(2)	S(4)	C(7)	98.3(8)	... yes
Hg(2)	S(4)	C(12)	104.4(7)	.. 2_754 yes
C(7)	S(4)	C(12)	100.0(10)	.. 2_754 yes

Hg(2)	S(5)	C(8)	96.8(8)	... yes
Hg(2)	S(5)	C(9)	107.2(8)	... yes
C(8)	S(5)	C(9)	102(1)	... yes
C(10)	S(6)	C(11)	102(1)	... yes
S(1)	C(1)	C(2)	114(1)	... yes
S(2)	C(2)	C(1)	113(1)	... yes
S(2)	C(3)	C(4)	112(1)	... yes
S(3)	C(4)	C(3)	111(1)	... yes
S(3)	C(5)	C(6)	114(1)	... yes
S(1)	C(6)	C(5)	109(1)	2_765 ... yes
S(4)	C(7)	C(8)	111(1)	... yes
S(5)	C(8)	C(7)	117(1)	... yes
S(5)	C(9)	C(10)	107(1)	... yes
S(6)	C(10)	C(9)	115(1)	... yes
S(6)	C(11)	C(12)	112(1)	... yes
S(4)	C(12)	C(11)	111(1)	2_754 ... yes

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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

Hg(1)	S(1)	C(1)	C(2)	43(1)	 yes
Hg(1)	S(1)	C(6)	C(5)	77(1)	.. 2_765 2_765 yes
Hg(1)	S(1)	C(1)	C(2)	-43(1)	. 2_755 2_755 2_755 yes
Hg(1)	S(2)	C(2)	C(1)	51(1)	 yes
Hg(1)	S(2)	C(3)	C(4)	170(1)	 yes
Hg(1)	S(2)	C(2)	C(1)	-51(1)	. 2_755 2_755 2_755 yes
Hg(1)	S(2)	C(3)	C(4)	-170(1)	. 2_755 2_755 2_755 yes
Hg(2)	S(4)	C(7)	C(8)	-52(1)	 yes
Hg(2)	S(4)	C(12)	C(11)	-160(1)	.. 2_754 2_754 yes

Hg(2)	S(4)	C(7)	C(8)	52(1)	. 2_744 2_744 2_744 yes
Hg(2)	S(5)	C(8)	C(7)	-42(1)	 yes
Hg(2)	S(5)	C(9)	C(10)	-81(1)	 yes
Hg(2)	S(5)	C(8)	C(7)	42(1)	. 2_744 2_744 2_744 yes
Hg(2)	S(5)	C(9)	C(10)	81(1)	. 2_744 2_744 2_744 yes
Cl(1)	Hg(1)	S(1)	C(1)	77.9(7)	 yes
Cl(1)	Hg(1)	S(1)	C(6)	-176.6(9)	... 2_765 yes
Cl(1)	Hg(1)	S(1)	C(1)	102.1(7)	.. 2_755 2_755 yes
Cl(1)	Hg(1)	S(1)	C(6)	-3.4(9)	.. 2_755 1_545 yes
Cl(1)	Hg(1)	S(2)	C(2)	-102.2(7)	 yes
Cl(1)	Hg(1)	S(2)	C(3)	153.7(8)	 yes
Cl(1)	Hg(1)	S(2)	C(2)	-77.8(7)	.. 2_755 2_755 yes
Cl(1)	Hg(1)	S(2)	C(3)	26.3(8)	.. 2_755 2_755 yes
Cl(2)	Hg(2)	S(4)	C(7)	-74.4(8)	 yes
Cl(2)	Hg(2)	S(4)	C(12)	28.1(6)	... 2_754 yes
Cl(2)	Hg(2)	S(4)	C(7)	-105.6(8)	.. 2_744 2_744 yes
Cl(2)	Hg(2)	S(5)	C(8)	98.8(8)	 yes
Cl(2)	Hg(2)	S(5)	C(9)	-6.8(9)	 yes
Cl(2)	Hg(2)	S(5)	C(8)	81.2(8)	.. 2_744 2_744 yes
Cl(2)	Hg(2)	S(5)	C(9)	-173.2(9)	.. 2_744 2_744 yes
S(1)	Hg(1)	S(2)	C(2)	-18.1(7)	 yes
S(1)	Hg(1)	S(2)	C(3)	-122.1(8)	 yes
S(1)	Hg(1)	S(2)	C(2)	-161.9(7)	.. 2_755 2_755 yes
S(1)	Hg(1)	S(2)	C(3)	-57.9(8)	.. 2_755 2_755 yes
S(1)	C(1)	C(2)	S(2)	-71(1)	 yes
S(1)	C(6)	C(5)	S(3)	167(1)	. 2_765 2_765 2_765 yes
S(2)	Hg(1)	S(1)	C(1)	-8.5(7)	 yes
S(2)	Hg(1)	S(1)	C(6)	97.0(8)	... 2_765 yes
S(2)	Hg(1)	S(1)	C(1)	-171.5(7)	.. 2_755 2_755 yes
S(2)	Hg(1)	S(1)	C(6)	83.0(8)	.. 2_755 1_545 yes
S(2)	C(3)	C(4)	S(3)	170(1)	 yes
S(4)	Hg(2)	S(5)	C(8)	6.7(8)	 yes
S(4)	Hg(2)	S(5)	C(9)	-99.0(9)	 yes
S(4)	Hg(2)	S(5)	C(8)	173.3(8)	.. 2_744 2_744 yes
S(4)	Hg(2)	S(5)	C(9)	-81.0(9)	.. 2_744 2_744 yes
S(4)	C(7)	C(8)	S(5)	71(1)	 yes
S(4)	C(12)	C(11)	S(6)	-165.7(10)	. 2_754 2_754 2_754 yes

S(5)	Hg(2)	S(4)	C(7)	20.2(7)	 yes
S(5)	Hg(2)	S(4)	C(12)	122.7(6)	... 2_754 yes
S(5)	Hg(2)	S(4)	C(7)	159.8(7)	.. 2_744 2_744 yes
S(5)	C(9)	C(10)	S(6)	-172(1)	 yes
C(1)	S(1)	C(6)	C(5)	-178(1)	.. 2_765 2_765 yes
C(1)	C(2)	S(2)	C(3)	154(1)	 yes
C(2)	S(2)	C(3)	C(4)	71(1)	 yes
C(2)	C(1)	S(1)	C(6)	-69(1)	... 2_765 yes
C(3)	C(4)	S(3)	C(5)	87(1)	 yes
C(4)	S(3)	C(5)	C(6)	-81(2)	 yes
C(7)	S(4)	C(12)	C(11)	-58(1)	.. 2_754 2_754 yes
C(7)	C(8)	S(5)	C(9)	66(1)	 yes
C(8)	S(5)	C(9)	C(10)	177(1)	 yes
C(8)	C(7)	S(4)	C(12)	-158(1)	... 2_754 yes
C(9)	C(10)	S(6)	C(11)	-64(2)	 yes
C(10)	S(6)	C(11)	C(12)	91(1)	 yes
C(10)	S(6)	C(11)	C(12)	91(1)	 yes

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loop_

_geom_contact_atom_site_label_1_geom_contact_atom_site_label_2_geom_contact_distance_geom_contact_site_symmetry_1_geom_contact_site_symmetry_2_geom_contact_publ_flag

Hg(1)	Cl(1)	2.728(6)	.. ?
Hg(1)	Cl(1)	2.728(6)	. 2_755 ?
Hg(1)	S(1)	2.632(5)	.. ?
Hg(1)	S(1)	2.632(5)	. 2_755 ?
Hg(1)	S(2)	2.738(6)	.. ?
Hg(1)	S(2)	2.738(6)	. 2_755 ?
Hg(2)	Cl(2)	2.670(5)	.. ?
Hg(2)	Cl(2)	2.670(5)	. 2_744 ?
Hg(2)	S(4)	2.684(6)	.. ?
Hg(2)	S(4)	2.684(6)	. 2_744 ?
Hg(2)	S(5)	2.749(6)	.. ?
Hg(2)	S(5)	2.749(6)	. 2_744 ?

Hg(2) C(12) 3.60(2) . 1_545 ?

S(1) S(1) 3.56(1) . 2_855 ?

S(3) C(8) 3.60(3) . 1_565 ?

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