Supporting Information

Preparation and Crystallography of 1,2-bis(chloromercurio)tetrafluorobenzene Adducts with Nitrobenzene and Nitrotoluenes

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Table 1S. The Shifts of ν_{as}(NO) and ν_s(NO) Vibration Bands in IR Spectras of Complexes of II With Nitrocompounds

Complex	Coordinated		Uncoordinated		$\Delta\nu_{as}$(NO)* cm^{-1}	$\Delta\nu_s$(NO)* cm^{-1}
	ν_{as}(NO); cm^{-1}	ν_s(NO) cm^{-1}	ν_{as}(NO); cm^{-1}	ν_s(NO) cm^{-1}		
II·1	1519	1345	1524	1347	5	2
II·2	1514	1344	1510	1348	-4	4
II·3	1518	1347	1521	1347	3	0
II·4	1523	1344	1525	1350	2	6
2(II)·4	1524	1344	1525	1350	1	6

* $\Delta\nu_{as}(NO) = \nu_{as}(NO)(uncoord.) - \nu_{as}(NO)(coord.)$
$\Delta\nu_s(NO) = \nu_s(NO)(uncoord.) - \nu_s(NO)(coord.)$

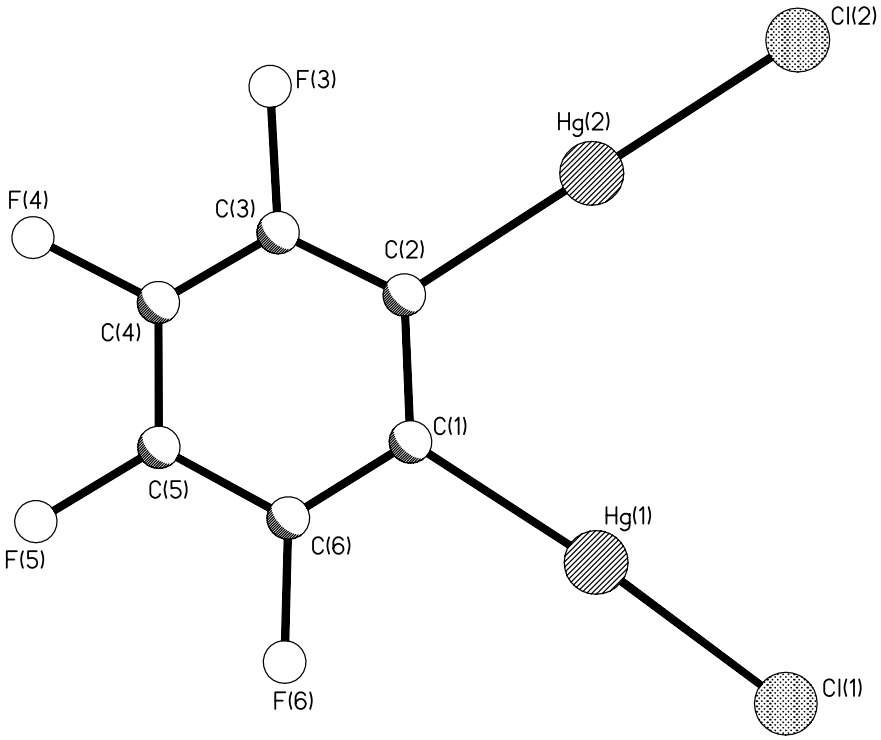


Figure 1S. The molecular structure and the numbering scheme of compound **II** in the complexes with nitrocompounds

Table 2S. Important Geometrical Parameters of Molecule II in Complexes and Compressing of Those Parameters with Previously Investigated Structure of Uncoordinated II.

	Ref[IS] Mol. A	Ref[IS] Mol. B	II·1	II·2	II·3	II·4	2(II)·4 Mol. A	2(II)·4 Mol. B
Bond length, Å								
Hg(1)-Cl(1)	2.336	2.325	2.313(3)	2.316(2)	2.317(2)	2.3128(19)	2.331(3)	2.344(3)
Hg(2)-Cl(2)	2.315	2.316	2.310(3)	2.311(2)	2.313(2)	2.315(2)	2.314(3)	2.328(3)
Hg(1)-C(1)	2.072	2.084	2.054(14)	2.049(8)	2.052(10)	2.040(7)	2.061(13)	2.060(13)
Hg(2)-C(2)	2.075	2.097	2.063(14)	2.067(8)	2.055(9)	2.065(7)	2.051(13)	2.065(13)
F(3)-C(3)	1.383	1.392	1.372(16)	1.360(9)	1.367(11)	1.350(9)	1.342(15)	1.368(15)
F(4)-C(4)	1.32	1.361	1.348(15)	1.340(10)	1.339(11)	1.341(8)	1.338(15)	1.351(15)
F(5)-C(5)	1.43	1.359	1.333(15)	1.346(10)	1.343(11)	1.364(9)	1.336(15)	1.328(15)
F(6)-C(6)	1.353	1.345	1.349(15)	1.364(9)	1.355(11)	1.355(8)	1.371(15)	1.355(16)
C(1)-C(6)	1.407	1.35	1.37(2)	1.378(12)	1.393(13)	1.384(10)	1.363(18)	1.398(19)
C(1)-C(2)	1.378	1.383	1.43(2)	1.405(12)	1.408(14)	1.438(10)	1.423(19)	1.425(19)
C(2)-C(3)	1.333	1.328	1.364(19)	1.384(12)	1.388(14)	1.370(9)	1.384(19)	1.380(19)
C(3)-C(4)	1.441	1.314	1.371(17)	1.382(13)	1.388(14)	1.389(10)	1.391(19)	1.374(19)
C(4)-C(5)	1.358	1.37	1.380(19)	1.378(12)	1.373(15)	1.357(11)	1.413(19)	1.37(2)
C(5)-C(6)	1.325	1.359	1.384(18)	1.394(12)	1.372(14)	1.379(10)	1.385(19)	1.363(19)
Bond angles, deg								
C(1)-Hg(1)-Cl(1)	178.2	173.7	176.9(4)	176.2(2)	177.3(3)	177.0(2)	179.0(4)	175.8(4)
C(2)-Hg(2)-Cl(2)	176.9	178.5	176.4(4)	176.0(2)	176.3(3)	176.6(2)	175.2(4)	177.9(4)
C(6)-C(1)-Hg(1)	118	120.5	120.9(10)	119.9(6)	119.0(7)	120.4(5)	118.9(10)	116.7(9)
C(2)-C(1)-Hg(1)	123.5	120.6	121.0(10)	122.4(6)	123.0(7)	123.0(5)	123.4(9)	126.8(10)
C(3)-C(2)-Hg(2)	116.8	114.8	117.5(10)	116.4(6)	116.9(7)	117.4(5)	119.7(12)	118.3(10)
C(1)-C(2)-Hg(2)	119.5	125.2	124.3(9)	124.0(6)	124.7(7)	123.3(5)	123.9(9)	121.6(10)
mean dev from plane*	0.06	0.09	0.11	0.11	0.12	0.08	0.11	0.08

* mean deviation of atoms from molecular plane

The description of mercury atoms coordination in a "plate" complexes

As shown on Figure 2Sa the coordination of Hg(1) atom is distorted trigonal bipyramidal, and contain C(1) and Cl(1) atoms which are directly bonded to the Hg(1); two chlorine atoms Cl(1A) and Cl(2B), which are laying in equatorial positions of molecule **II,** and one oxygen atom O(1) from the nitro group of the ligand.

The most important geometrical parameters of Hg(1) atom coordination are presented in Table 3S. Deviations of Hg(1) from the equatorial plane (atoms Cl(1A), Cl(2B) and O(1)) for all complexes are small (range 0.19-0.30 Å). The angles between the axial bond vectors Cl(1)-Hg(1), C(1)-Hg(1) and equatorial plane are equal to 82.8-86.3 and 81.2-83.6° respectively. The equatorial distances Hg(1)…Cl(1A), Hg(1)…Cl(2B) and Hg(1)…O(1) are similar to each other and have approximate values 3.1Å. However, the coordination angle Cl(1A)…Hg(1)…Cl(2B) (102.3-105.5°) is smaller then values of angles O(1)…Hg(1)…Cl(1A) (112.6-121.6°) and O(1)…Hg(1)…Cl(2B) (av. 132.3-140.7°). This situation can be explain by strong interaction of chlorine atoms, which laying in a chelate position with two mercury atoms, while the oxygen atom interacts only with one mercury.

The coordination of Hg(2) atom is a distorted tetragonal bipyramid, which contains in axial position atoms Cl(2) and C(2), which directly bonded to central Hg(2) atom, and equantorial plane which built by chlorine atoms Cl(1A), Cl(2B), Cl(1C) and oxygen atom O(2D) (Figure 2Sb). The most important geometrical parameters of Hg(2) atom coordination are presented in Table 4S.

The deviation of mercury atom from the equatorial plane thru chlorines Cl(1A), Cl(2B), Cl(1C) and oxygen O(2D) is small and laying a range 0.00-0.15Å. The angles

between bond vectors Cl(2)-Hg(2), C(2)-Hg(2) and this plane is close to 90°. The Hg(2)…O(2D), Hg(2)…Cl(1A) and Hg(2)…Cl(1C) distances are similar, when Hg(2)…Cl(2B) distance is longer then other approximately on 0.3Å. The coordination angles around atom Hg(2) is clause to 90° except Cl(1C)-Hg(2)-Cl(1A), which have value around 70°.

Table 3S. Coordination of the Hg(1) Atom in a "Plate" Complexes.

Parametr	**II·1**	**II·2**	**II·3**	**II·4**
Hg(1)-Cl(1) (Å)	2.313(3)	2.316(2)	2.317(2)	2.313(2)
Hg(1)-C(1) (Å)	2.054(14)	2.049(8)	2.052(10)	2.040(7)
Hg(1)…Cl(1A) (Å)	3.18	3.21	3.26	3.21
Hg(1)…Cl(2B) (Å)	3.12	3.10	3.07	3.16
Hg(1)…O(1) (Å)	3.04(1)	3.005(6)	3.051(7)	3.089(6)
C(1)-Hg(1)-Cl(1) (deg)	176.9(4)	176.2(2)	177.3(3)	177.0(2)
Cl(1A)-Hg(1)-Cl(2B) (deg)	102.3	103.0	105.5	103.6
O(1)-Hg(1)-Cl(1A) (deg)	117.3	117.4	112.6	121.2
O(1)-Hg(1)-Cl(2B) (deg)	138.5	137.9	140.7	132.3
Deviation of Hg(1)* (Å)	0.24	0.23	0.19	0.30
∠(Cl-Hg;PL) (deg)	85.2	86.3	82.8	83.7
∠(C-Hg;PL) (deg)	83.6	83.5	81.3	81.2

* Mean deviation of Hg(1) atom from the plane of O(1), Cl(1A) and Cl(2B) atoms. ∠(Cl-Hg;PL) angle between vector of the bond Cl(1)-Hg(1) and plane of atoms O(1), Cl(1A) and Cl(2B); ∠(C-Hg;PL) angle between vector of the bond C(1)-Hg(1) and plane of atoms O(1), Cl(1A) and Cl(2B)

For **II·1** :A -*x*+1, *y*-0.5, -*z*+1, B –*x*, *y*+0.5, -*z*; for **II·2**: A –*x*+1.5, *y*-0.5, -*z*+0.5, B -*x*+0.5, *y*-0.5, -*z*+0.5; for **II·3**: A –*x*-0.5, *y*+0.5, -*z*+0.5 B –*x*+0.5, *y*-0.5, -*z*+0.5; for **II·4**: A -*x*+2, *y*-0.5, -*z*+3, B –*x*+1, *y*+0.5, -*z*+3

Table 4S. Coordination of the Hg(2) Atom in a "Plate" Complexes.

Parametr	**II·1**	**II·2**	**II·3**	**II·4**
Hg(2)-Cl(2) (Å)	2.310(3)	2.311(2)	2.313(2)	2.315(2)
Hg(2)-C(2) (Å)	2.063(14)	2.066(8)	2.055(9)	2.065(7)
Hg(2)…Cl(1A) (Å)	3.27	3.26	3.29	3.25
Hg(2)…Cl(2B) (Å)	3.46	3.49	3.52	3.55
Hg(2)…Cl(1C) (Å)	3.17	3.21	3.27	3.21
Hg(2)…O(2D) (Å)	3.11(1)	3.149(6)	3.091(7)	3.115(6)
C(2)-Hg(2)-Cl(2) (deg)	176.4(4)	176.0(2)	176.3(3)	176.6(2)
Cl(1A)-Hg(2)-Cl(2B) (deg)	93.6	93.9	95.3	94.6
Cl(2B)-Hg(2)-O(2D) (deg)	84.0	87.0	90.1	80.5
O(2D)-Hg(2)-Cl(1C) (deg)	111.6	107.0	100.5	112.2
Cl(1C)-Hg(2)-Cl(1A) (deg)	70.7	71.9	73.9	72.7
Deviation of Hg(2)* (Å)	0.15	0.12	0.10	0.00
∠(Cl-Hg;PL) (deg)	85.3	84.6	75.5	81.8
∠(C-Hg;PL) (deg)	82.2	81.7	78.3	83.0

*Mean deviation of Hg(2) atom from the plane of O(2D), Cl(1A), Cl(2B), Cl(1C) atoms. ∠(Cl-Hg;PL) angle between vectror of the bond Cl(2)-Hg(2) and plane of atoms O(2D), Cl(1A), Cl(2B), Cl(1C); ∠(C-Hg;PL) angle between vectror of the bond C(2)-Hg(2) and plane of atoms O(2D), Cl(1A), Cl(2B) and Cl(1C).

For **II·1** : A –*x*+1, *y*-0.5, -*z*+1 B –*x*, *y*+0.5, -*z*+1, C *x*, *y*-1, *z*, D *x*-1, *y*-1, *z*; for **II·2**: A –*x*+1.5, B –*x*+0.5, *y*+0.5, -*z*+0.5, C *x*, *y*-1, *z*, *y*-0.5, -*z*+0.5, D *x*-1, *y*-1, *z*; for **II·3** A –*x*+0.5, *y*+0.5, -*z*+0.5, B –*x*+0.5, *y*-0.5, -*z*+0.5, C *x*, *y*+1, *z*, D *x*+1, *y*+1, *z*; for **II·4** A –*x*+2, *y*-0.5, -*z*+3, B –*x*+1, *y*+0.5, -*z*+3, C *x*, *y*-1, *z*, D *x*-1, *y*-1, *z*

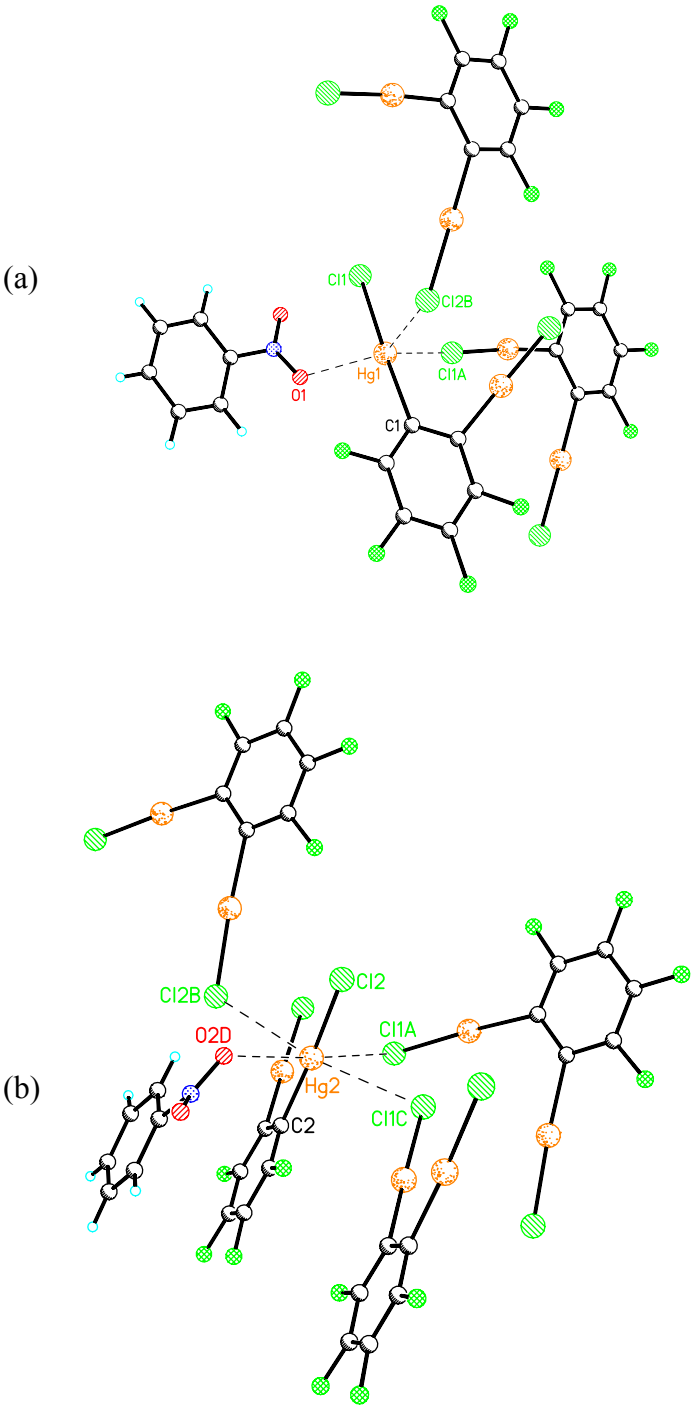


Figure 2S. The coordination of Hg(1) (a) and Hg(2) (b) atoms**.**

The description of mercury atoms coordination in a 2(II)·4 complex

The Hg(1A) atom have distorted tetragonal bipyramidal (Figure3Sa) configuration, which include covalently bonded atoms Cl(1A) and C(1A) in axial positions, and non-bonded atoms Cl(1B), Cl(2A)$^{\#}$, Cl(2B)$^{\#}$ and O(1) in equatorial positions. The distances Hg(1A)…Cl are clouse to each other, when Hg(1A)…O(1) is significantly shorter (Table 5S). The angles in equatorial plane very from 71.0-118.9°. The deviation of mercury atom from the plane of the equatorial atoms is small and equal to 0.21Å. The angles between bond vectors Hg(1A)-Cl(1A), Hg(1A)-C(1A) and equatorial plane are clause to the 90°.

Analogous configuration have mercury atom Hg(1B) (Figure 3Sc). This configuration include Cl(1B) and C(1B) atoms in axial positions, and Cl(2A), Cl(1A)$^{\$}$, Cl(2B)$^{\#}$ and Cl(2B)$^{\%}$ atom, which are laying in equatorial position. The geometrical parameters of those configuration very similar to the parameters of Hg(1A) configuration and presented in Table 7S.

The configuration of mercury atom Hg(2A) is a “see-sow” and it presented on a Figure 3Sb. The most important geometrical parameters of this configuration are presented in Table 6S. How can be seen from Figure 3Sb, the Hg(2A) atom covalently bonded to Cl(2A), C(2A) atoms and non-bonded Cl(1B), Cl(2B)$^{\#}$ atoms. The distance Hg(2A)…Cl(1B) (3.12Å) is less then distance Hg(2A)…Cl(2B)$^{\#}$ (3.38Å) on 0.26Å. The angle between non-bonded chlorine atoms is equal to 75.2°.

Configuration of mercury atom Hg(2B) is presented on Figure 3Sd. The atom Hg(2B) also have “see-sow” configuration, however in to comparison with Hg(2A) atom, Hg(2B) have three chlorine atoms in it equatorial plane (Cl(2A), Cl(1A)$^{\#}$ and Cl(1A)$^{\$}$).

The axial positions are occupied by C(2B) and Cl(2B) atoms, which are directly bonded to the mercury center. The Hg(2B)…Cl distances are deferent from each other (Table 8S). The angles between bond vectors Hg(2B)-Cl(2B), Hg(2B)-C(2B) equatorial plane of atoms Cl(2A), Cl(1A)$^{\#}$ and Cl(1A)$^{\$}$ are clouse to 64°. Other geometrical parameters of Hg(2B) atomic configuration presented in Table 8S.

Table 5S. Coordination of the Hg(1A) Atom in a Complex 2(II)·4.

Parametr	2(II)·4
Hg(1A)-Cl(1A)	2.331(3)
Hg(1A)-C(1A)	2.061(13)
Hg(1A)…Cl(1B)	3.26
Hg(1A)…Cl(2A)$^{\#}$	3.23
Hg(1A)…Cl(2B)$^{\#}$	3.29
Hg(1A)…O(1)	2.95
C(1A)-Hg(1A)-Cl(1A)	179.0(4)
O(1)-Hg(1A)-Cl(1B)	94.3
Cl(1B)-Hg(1A)-Cl(2B)$^{\#}$	74.8
Cl(2B)$^{\#}$-Hg(1A)-Cl(2A)$^{\#}$	71.0
Cl(2A)$^{\#}$-Hg(1A)-O(1)	118.9
Deviation of Hg(1A)* (Å)	0.21
∠(Cl-Hg;PL) (deg)	86.0
∠(C-Hg;PL) (deg)	85.0

* Mean deviation of Hg(1A) atom from the plane of O(1), Cl(1B), Cl(2A)$^{\#}$ and Cl(2B)$^{\#}$ atoms.
∠(Cl-Hg;PL) angle between vectror of the bond Cl(1A)-Hg(1A) and plane of O(1), Cl(1B), Cl(2A)$^{\#}$ and Cl(2B)$^{\#}$ atoms ; ∠(C-Hg;PL) angle between vectror of the bond C(1A)-Hg(1A) and plane of of O(1), Cl(1B), Cl(2A)$^{\#}$ and Cl(2B)$^{\#}$ atoms

$^{\#}$ *x*-1, *y*, *z*;

Table 6S. Coordination of the Hg(2A) Atom in a Complex 2(II)·4

Parametr	2(II)·4
Hg(2A)-Cl(2A)	2.314(3)
Hg(2A)-C(2A)	2.051(13)
Hg(2A)…Cl(1B)	3.12
Hg(2A)…Cl(2B)$^{\#}$	3.38
C(2A)-Hg(2A)-Cl(2A)	175.2(4)
Cl(1B)-Hg(2A)-Cl(2B)$^{\#}$	75.2
∠(Cl-Hg;PL)* (deg)	80.4
∠(C-Hg;PL) (deg)	79.4

*∠(Cl-Hg;PL) angle between vectror of the bond Cl(2A)-Hg(2A) and plane of Cl(1B), Cl(2B)$^{\#}$ and Hg(2A) ; ∠(C-Hg;PL) angle between vectror of the bond C(2A)-Hg(2A) and plane of Cl(1B), Cl(2B)$^{\#}$ and Hg(2A)

$^{\#}$ *x*-1, *y*, *z*;

Table 7S. Coordination of the Hg(1B) Atom in a Complex 2(II)·4

Parametr	**2(II)·4**
Hg(1B)-Cl(1B)	2.344(3)
Hg(1B)-C(1B)	2.060(13)
Hg(1B)…Cl(2A)	3.24
Hg(1B)…Cl(1A)$^{\$}$	3.19
Hg(1B)…Cl(2B)$^{\#}$	3.26
Hg(1B)…Cl(2B)$^{\%}$	3.13
C(1B)-Hg(1B)-Cl(1B)	175.8(4)
Cl(2A)-Hg(1B)-Cl(1A)$^{\$}$	75.0
Cl(1A)$^{\$}$-Hg(1B)-Cl(2B)$^{\%}$	83.7
Cl(2B)$^{\%}$-Hg(1B)-Cl(2B)$^{\#}$	158.5
Cl(2B)$^{\#}$-Hg(1B)-Cl(2A)	70.9
Deviation of Hg(1B)* (Å)	0.08
∠(Cl-Hg;PL) (deg)	86.2
∠(C-Hg;PL) (deg)	82.6

***** Mean deviation of Hg(1B) atom from the plane of Cl(2A), Cl(1A)$^{\$}$, Cl(2B)$^{\#}$ and Cl(2B)$^{\%}$ atoms.
∠(Cl-Hg;PL) angle between vectror of the bond Cl(1B)-Hg(1B) and plane of Cl(2A), Cl(1A)$^{\$}$, Cl(2B)$^{\#}$ and Cl(2B)$^{\%}$ atoms ; ∠(C-Hg;PL) angle between vectror of the bond C(1B)-Hg(1B) and plane of Cl(2A), Cl(1A)$^{\$}$, Cl(2B)$^{\#}$ and Cl(2B)$^{\%}$ atoms.

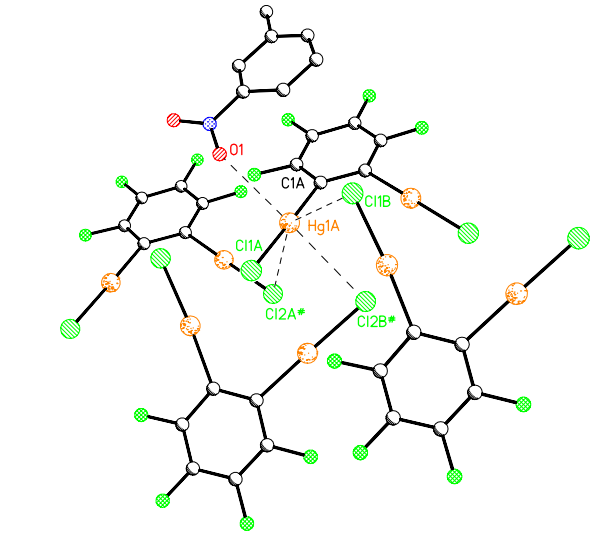
$^{\#}$ x-1, y, z; $^{\$}$ x+1, y, z; $^{\%}$ x-0.5, -y+0.5, z+0.5

Table 8S. Coordination of The Hg(2B) Atom in a Complex 2(II)·4

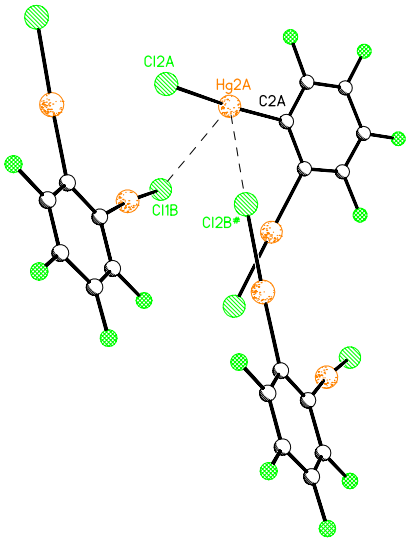
Parametr	**2(II)·4**
Hg(2B)-Cl(2B)	2.328(3)
Hg(2B)-C(2B)	2.060(13)
Hg(2B)…Cl(2A)	3.36
Hg(2B)…Cl(1A)$^{\#}$	3.17
Hg(2B)…Cl(1A)$^{\$}$	3.65
C(2B)-Hg(2B)-Cl(2B)	177.9(4)
Cl(1A)$^{\#}$-Hg(2B)-Cl(2A)	73.6
Cl(2A)-Hg(2B)-Cl(1A)$^{\$}$	58.8
Cl(1A)$^{\$}$-Hg(2B)-Cl(1A)$^{\#}$	230.2
Deviation of Hg(2B)* (Å)	0.74
∠(Cl-Hg;PL) (deg)	64.2
∠(C-Hg;PL) (deg)	63.7

* Mean deviation of Hg(2B) atom from the plane of Cl(2A), Cl(1A)$^{\#}$and Cl(1A)$^{\$}$ atoms. ∠(Cl-Hg;PL) angle between vectror of the bond Cl(1B)-Hg(1B) and plane of Cl(2A), Cl(1A)$^{\#}$and Cl(1A)$^{\$}$ atoms; ∠(C-Hg;PL) angle between vectror of the bond C(1B)-Hg(1B) and plane of Cl(2A), Cl(1A)$^{\#}$and Cl(1A)$^{\$}$ atoms.

$^{\#}$ x+1, y, z; $^{\$}$ x+0.5, -y+0.5, z-0.5



(a)



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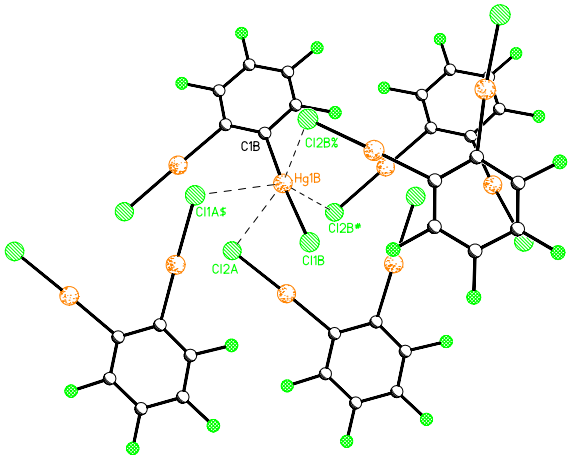

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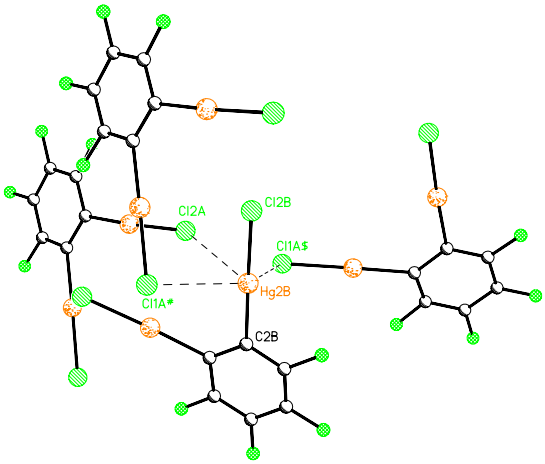

(d)

Figure 3S. The coordination of Hg(1A) (a), Hg(2A) (b), Hg(1B) (c) and Hg(2B) (d) atoms in complex **2(II)·4**

Table 9S. Molecular Geometrical Parametrs of Compounds 1-4 in Complexes With Compound II and its Comparison with Geometrical Parametrs of Uncoordinated Compounds 1-4

	II·1	**1** Ref.[2s]	**II·2**	**2** Ref.[3s]	**II·3**	**3** Ref.[3s]	**II·4**	**2(II)·4**	**4** triclin Ref.[3s].
Bond length, Å									
O(1)-N(1)	1.221(15)	1.225(1)	1.237(10)	1.231(2)	1.216(11)	1.227(3)	1.249(9)	1.229(18)	1.216(4)
O(2)-N(1)	1.241(16)	1.228(1)	1.213(10)	1.227(2)	1.220(11)	1.222(4)	1.220(10)	1.207(19)	1.223(4)
N(1)-C(7)	1.481(19)	1.467(1)	1.473(12)	1.469(2)	1.493(13)	1.472(4)	1.534(14)	1.44(2)	1.471(5)
C(7)-C(8)	1.40(2)	1.387(1)	1.387(13)	1.387(2)	1.393(13)	1.386(5)	1.373(15)	1.34(2)	1.384(5)
C(7)-C(12)	1.37(2)	1.387(1)	1.372(12)	1.389(2)	1.393(14)	1.394(4)	1.351(16)	1.43(3)	1.382(5)
C(8)-C(9)	1.37(2)	1.385(1)	1.379(14)	1.390(2)	1.382(15)	1.403(5)	1.523(15)	1.43(3)	1.381(5)
C(9)-C(10)	1.35(2)	1.388(1)	1.393(14)	1.399(2)	1.387(16)	1.390(5)	1.379(13)	1.35(3)	1.393(5)
C(10)-C(11)	1.37(2)	1.389(1)	1.394(13)	1.403(2)	1.367(15)	1.376(6)	1.279(17)	1.39(3)	1.391(5)
C(11)-C(12)	1.38(2)	1.386(1)	1.379(13)	1.387(2)	1.384(14)	1.378(5)	1.55(2)	1.39(3)	1.379(6)
C(*n*)-C(13)	N/A	N/A	1.515(14)	1.507(2)	1.513(15)	1.513(5)	1.505(15)	1.41(2)	1.516(5)
Bond Angels, deg									
O(1)-N(1)-O(2)	125.3(13)	123.2(1)	124.3(8)	123.2(1)	125.9(9)	123.3(3)	122.8(9)	123.5(16)	122.8(4)
O(1)-N(1)-C(7)	116.6(12)	118.3(1)	118.3(7)	118.5(1)	116.7(9)	118.5(3)	122.0(8)	118.9(15)	118.9(3)
O(2)-N(1)-C(7)	118.1(12)	118.5(1)	117.5(8)	118.3(1)	117.4(8)	118.2(3)	115.2(8)	117.6(16)	118.4(3)
C(8)-C(7)-C(12)	122.2(14)	122.7(1)	121.7(9)	122.5(1)	123.7(10)	123.5(3)	129.2(12)	119(2)	122.3(4)
C(8)-C(7)-N(1)	117.9(13)	118.5(1)	118.6(8)	118.8(1)	121.5(9)	121.0(3)	114.7(12)	121.4(18)	118.9(3)
C(12)-C(7)-N(1)	119.9(14)	118.8(1)	119.7(8)	118.7(1)	114.8(9)	115.5(3)	116.1(9)	118.9(17)	118.8(3)
C(7)-C(8)-C(9)	117.4(14)	118.2(1)	118.7(9)	118.2(1)	115.5(10)	116.0(3)	112.1(11)	122.9(19)	119.4(3)
C(8)-C(9)-C(10)	121.1(14)	120.2(1)	120.7(9)	121.3(1)	122.3(10)	121.4(4)	118.1(9)	122.2(18)	119.1(3)

C(11)-C(10)-C(9)	121.6(15)	120.5(1)	119.0(9)	118.7(1)	120.4(10)	120.5(3)	129.6(15)	128(2)	120.6(4)
C(12)-C(11)-C(10)	119.9(15)	120.3(1)	120.8(10)	121.0(1)	120.1(11)	120.1(3)	114.4(13)	116(2)	120.6(3)
C(11)-C(12)-C(7)	117.8(15)	118.1(1)	120.2(9)	118.4(1)	118.1(10)	118.6(4)	116.6(11)	120.0(19)	118.1(3)
C(*m*)-C(*n*)-C(13)	N/A	N/A	120.5(9)	120.5(1)	123.6(10)	125.4(3)	125.2(10)	122.2(18)	121.1(3)
C(*l*)-C(*n*)-C(13)	N/A	N/A	119.2(8)	120.7(1)	120.8(9)	118.6(3)	124.4(10)	124(2)	119.8(4)
Dihedral angle, deg									
φ(Ph/NO_2)	19.0	2.12	21.2	1.3	34.5	31.8	19.8	14.8	4.3

For compound **2**:*n*=10, *m*=9 and *l*=11; for compound **3** *n*=8, *m*=7 and *l*=9; for compound **4** *n*=9, *m*=8 and *l*=10

References

1S. Beckwith, J.D.; Tschinkl, M.; Picot, A.; Tsunoda, M.; Bachman, R.; Gabbai, F.P., *Organometallics,* **2001**, 20**,** 3169

2S. Boese, R.; Blaser, D.; Nussbaumer, M.; Krygowski, T.M. *Struct. Chem*. **1992**, 3 363.

3S. Yakovenko A.A.; Antipin, M.Yu.; Timofeeva, T. V., *Cryst. Growth Des.* **2008**, *Submitted.*