Supporting Information

A strategy for obtaining isostructurality in spite of structural diversity in coordination compounds

Vahid Amani,[1]* Maryam Esmaeili,[2] Fataneh Norouzi,[2] Hamid Reza Khavasi[2]*

[1]*Department of Chemistry Education, Farhangian University, P.O. Box 14665-889, Tehran, Iran*
[2]*Department of Inorganic Chemistry and Catalysis, Shahid Beheshti University, General Campus, Evin, Tehran 1983963113, Iran*

E-mail: (V. Amani) *v.amani@cfu.ac.ir*, *v_amani2002@yahoo.com*

Figure S1. The ORTEP diagram of coordination compound in **A**, **B** and **C** series. page 2
Figure S2. Fragments selected for calculation of dimer binding energies in **A** and **B** series. page 3
Table S1. Crystallographic data Page 4
Table S2. Geometrical parameters of hydrogen bonding in **A**, **B** and **C** series. page 5
Table S3. Geometrical parameters around central metal in **B** and **C** series. page 6
References Page 6

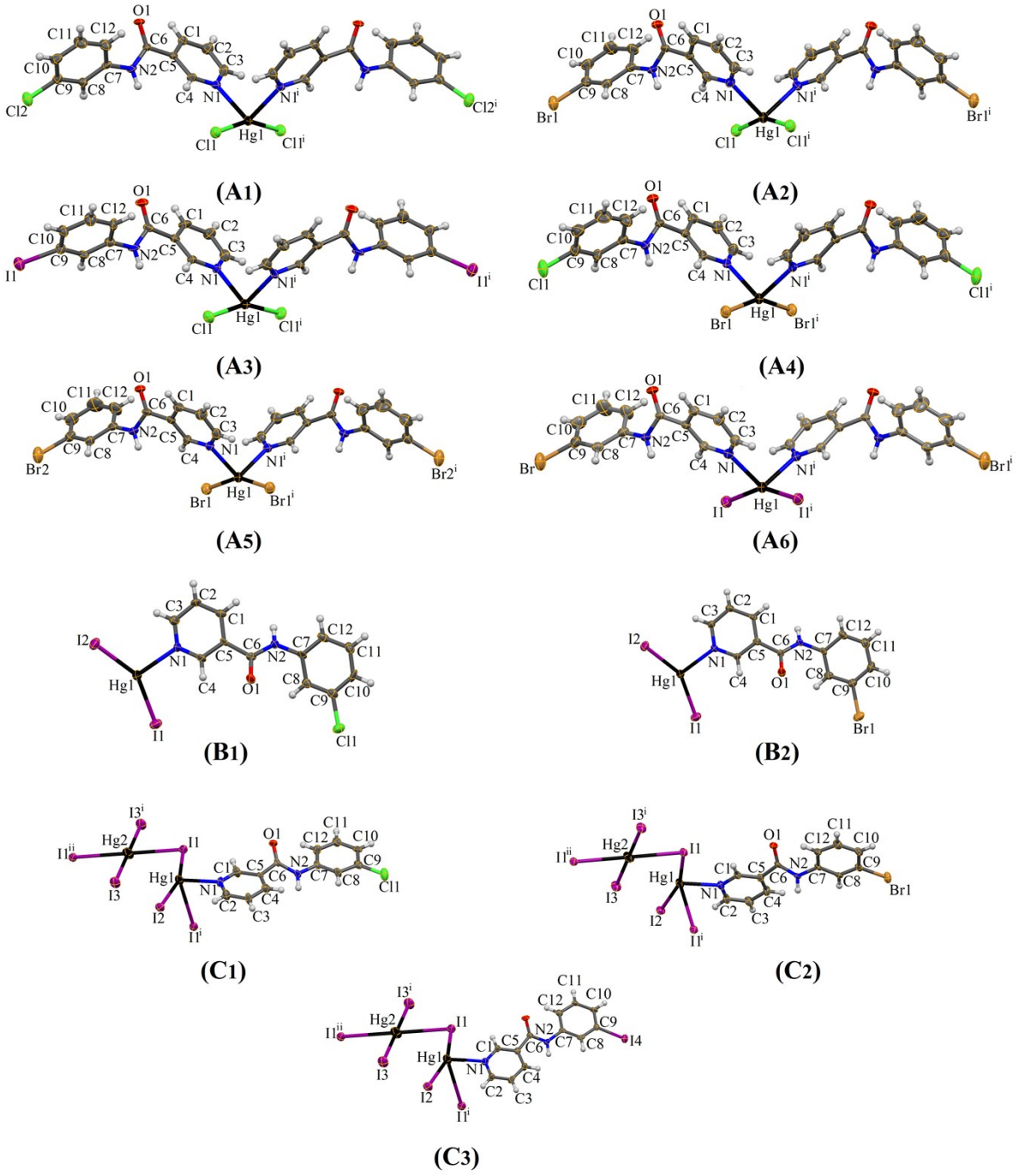

Figure S1. The ORTEP diagram of coordination compounds **A, B** and **C** series, showing coordination geometry around central metal. Ellipsoids are drawn at 30% probability level.

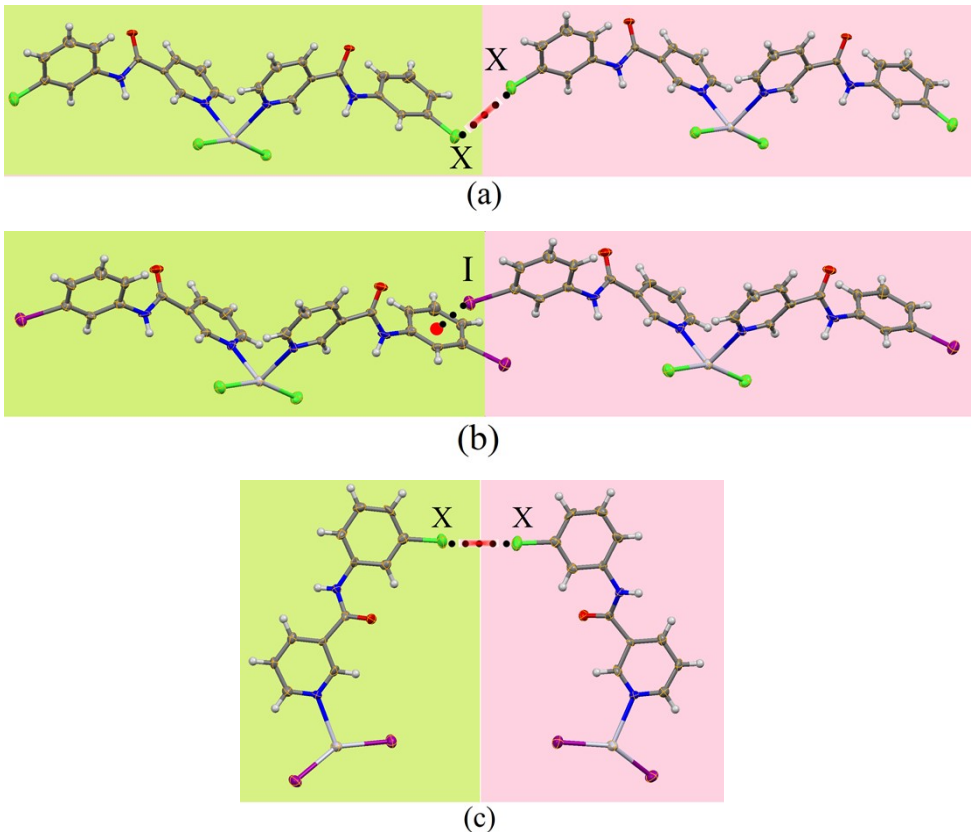

Figure S2. Selected fragments for calculating energy of (a) X...X interaction in $\mathbf{A_1}$, $\mathbf{A_2}$, $\mathbf{A_4}$, $\mathbf{A_5}$ and $\mathbf{A_6}$, (b) Type I X...π interaction in $\mathbf{A_3}$ and (c) Type I X...X interaction in $\mathbf{B_1}$ and $\mathbf{B_2}$.

Table S1. Structural data and refinement parameters for **A**, **B** and **C** series.

	A_1	**A_2**	**A_3**	**A_4**	**A_5**	**A_6**[i]
formula	$C_{24}H_{18}Cl_4HgN_4O_2$	$C_{24}H_{18}Br_2Cl_2HgN_4O_2$	$C_{24}H_{18}Cl_2HgI_2N_4O_2$	$C_{24}H_{18}Br_2Cl_2HgN_4O_2$	$C_{24}H_{18}Br_4HgN_4O_2$	$C_{24}H_{18}Br_2HgI_2N_4O_2$
fw	736.81	825.71	919.71	825.71	914.61	1008.61
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*
a/Å	22.366(2)	22.680(2)	38.520(7)	23.266(3)	23.569(3)	24.3489(18)
b/Å	4.9665(5)	4.9699(3)	4.8018(8)	4.9212(4)	4.9189(4)	4.9200(6)
c/Å	27.267(3)	27.573(3)	14.841(2)	27.288(3)	27.722(3)	28.395(2)
β/°	124.115(7)	123.819(7)	100.118(13)	124.251(8)	124.465(7)	125.751(4)
V/Å^3	2507.6(4)	2582.1(4)	2702.4(8)	2582.5(5)	2649.8(5)	2760.6(4)
D_{calc}/Mg.m^{-3}	1.952	2.124	2.261	2.124	2.293	2.427
Z	4	4	4	4	4	4
μ (mm^{-1})	6.595	9.293	17.266	9.291	11.870	10.735
F(000)	1416	1560	1704	1560	1704	1848
2θ (˚)	58.54	54	58.52	58.60	58.42	52
R (int)	0.1221	0.0895	0.0945	0.0984	0.1032	0.1053
GOOF	1.042	1.004	0.909	0.971	1.011	0.885
R_1[a](I>2σ(I))	0.0697	0.0763	0.0719	0.0701	0.0705	0.0489
wR_2[b](I>2σ(I))	0.1615	0.1102	0.1196	0.1680	0.1562	0.1203
CCDC No.	1016912	1016668	1016669	1016675	1016674	991771
	B_1	**B_2**[i]	**C_1**	**C_2**	**C_3**	
formula	$C_{12}H_9ClHgI_2N_2O$	$C_{12}H_9BrHgI_2N_2O$	$C_{24}H_{18}Cl_2Hg_3I_6N_4O_2$	$C_{24}H_{18}Br_2Hg_3I_6N_4O_2$	$C_{24}H_{18}Hg_3I_8N_4O_2$	
fw	687.05	731.50	1828.49	1917.39	2011.39	
crystal system	monoclinic	monoclinic	Monoclinic	monoclinic	monoclinic	
space group	*C*2/*c*	*C*2/*c*	*P*2$_1$/*n*	*P*2$_1$/*n*	*P*2$_1$/*n*	
a/Å	25.080(6)	25.3903(15)	4.5347(4)	4.5326(4)	4.5421(3)	
b/Å	14.097(4)	14.1304(6)	21.3006(12)	21.4340(12)	21.7134(19)	
c/Å	9.200(2)	9.1996(6)	19.0448(15)	19.1582(16)	19.3708(13)	
β/°	100.394(18)	99.658(5)	91.533(7)	92.076(7)	92.541(6)	
V/Å^3	3199.4(13)	3253.8(3)	1838.9(2)	1860.0(2)	1908.6(2)	
D_{calc}/Mg.m^{-3}	2.853	2.987	3.302	3.424	3.500	
Z	8	8	2	2	2	
μ (mm^{-1})	13.641	15.705	17.703	19.507	18.534	
F(000)	2448	2592	1596	1668	1740	
2θ (˚)	54	52	58.50	58.40	58.58	
R (int)	0.0992	0.0985	0.0915	0.0998	0.0998	
GOOF	0.895	1.023	0.939	1.028	0.912	
R_1[a](I>2σ(I))	0.0861	0.0640	0.0906	0.0528	0.0640	
wR_2[b](I>2σ(I))	0.1658	0.1406	0.1101	0.1174	0.1055	
CCDC No.	1016676	991770	1016677	991767	1016672	

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma w(F_o^2)2]^{½}$. [i] From reference [1].

Table S2. Geometrical parameters of hydrogen bonding in complexes **A-C** series**.**

Complexes	D-H…A	d(D-H)/Å	d(H…A)/Å	d(D…A)/Å	<D-H…A/°	Sym. Code
$\mathbf{A_1}$	N2-H2A …O1= C6	0.860(8)	2.071(7)	2.89(1)	160.2(7)	x,-1+y,z
$\mathbf{A_2}$	N2-H2A …O1= C6	0.86(1)	2.069(1)	2.90(1)	161.5(9)	x, 1+y,z
$\mathbf{A_3}$	N2-H2A …O1= C6	0.860(9)	2.087(9)	2.88(1)	153.2(7)	x,-1+y,z
	C2-H2… Cl1-Hg1	0.93(2)	2.869(3)	3.48(1)	124.7(9)	x,2-y,-1/2+z
$\mathbf{A_4}$	N2-H2A …O1= C6	0.860(9)	2.86(1)	2.016(9)	167.8(8)	x,-1+y,z
$\mathbf{A_5}$	N2-H2A …O1= C6	0.86(1)	2.039(8)	2.87(1)	163.3(8)	x,1+y,z
$\mathbf{A_6}$	N2-H2A …O1= C6	0.860(8)	2.048(7)	2.88(1)	161.1(6)	x,1+y,z
$\mathbf{B_1}$	N2-H2A …O1= C6	0.86(1)	2.08(1)	2.88(2)	155(1)	x,1-y,-1/2+z
	C12-H12 …O1= C6	0.93(2)	2.59(1)	3.22(2)	126(1)	x,1-y,-1/2+z
	C2-H2…I2-Hg	0.93(1)	3.107(2)	3.91(2)	146(1)	1/2-x,1/2+y,1.5-z
$\mathbf{B_2}$	N2-H2A …O1= C6	0.859(7)	2.118(8)	2.91(1)	152.5(6)	x,1-y,1/2+z
	C12-H12 …O1= C6	0.93(1)	2.540(8)	3.19(1)	127.0(8)	x,1-y,1/2+z
	C2-H2…I2-Hg	0.93(1)	3.139(9)	3.92(1)	143.1(7)	1/2-x,1/2+y,1/2-z
$\mathbf{C_1}$	N2-H2A …O1= C6	0.86(1)	2.15(1)	2.84(2)	138(1)	1+x,y,z
	C10-H10… I1-Hg1	0.93(2)	3.225(1)	4.05(2)	149(1)	2-x,-y,1-z
	C4-H4… I2-Hg1	0.93(2)	3.259(1)	4.11(2)	154(1)	1/2+x,1/2-y,1/2+z
$\mathbf{C_2}$	N2-H2A …O1= C6	0.860(7)	2.115(7)	2.84(1)	142.1(6)	1+x,y,z
	C11-H11 …O1= C6	0.93(1)	2.746(8)	3.55(1)	145.6(8)	-x,-y,1-z
	C10-H10… I1-Hg1	0.93(1)	3.239(7)	4.07(1)	149.0(6)	-x,-y,1-z
	C4-H4… I2-Hg1	0.93(1)	3.242(8)	4.11(1)	155.8(7)	-1/2+x,1/2-y,-1/2+z
$\mathbf{C_3}$	N2-H2A …O1= C6	0.862(9)	2.15(1)	2.85(1)	137.9(7)	1+x,y,z
	C11-H11 …O1= C6	0.93(1)	2.63(1)	3.45(2)	147.3(9)	2-x,-y,1-z
	C10-H10… I1-Hg1	0.93(2)	3.321(1)	4.17(1)	152.2(9)	2-x,-y,1-z
	C4-H4… I2-Hg1	0.93(2)	3.286(1)	4.16(1)	157.8(9)	-1/2+x,1/2-y,-1/2+z

Table S3. Geometrical parameters of central atom in B- and C-series complexes.

		Complex						Sym. Code
		$[Hg_3I_6(L^{3\text{-Cl-nic}})_2]_n$, C_1		$[Hg_3I_6(L^{3\text{-Br-nic}})_2]_n$, C_2		$[Hg_3I_6(L^{3\text{-I-nic}})_2]_n$, C_3		
		Hg1	Hg2	Hg1	Hg2	Hg1	Hg2	
Bond distance	**Hg-X1**	2.633(2)	3.499(2)	2.6339(8)	3.5160(6)	2.639(1)	3.576(1)	-
	Hg-X2	2.621(2)	-	2.6230(8)	-	2.620(1)	-	-
	Hg-X3	-	2.592(2)	-	2.5897(9)	-	2.588(1)	-
	Hg-X1	3.430(2)[b]	-	3.4264(8)[a]	-	3.420(1)[b]	-	a=1+x,y,z , b=-1+x,y,z
	Hg-X3	-	3.598(2)[b]	-	3.5976(9)[a]	-	3.615(1)[b]	a=-1+x,y,z , b=1+x,y,z
	Hg-N1	2.45(2)	-	2.488(8)	-	2.50(1)	-	-
Bond angle	**X1-Hg-X2**	159.98(6)	-	159.75(3)	-	159.29(4)	-	-
	X1-Hg-X3	-	91.99(5)	-	91.07(2)	-	91.10(3)	-
	N1-Hg-X1	97.7(4)	-	90.34(2)	-	98.6(3)	-	-
	N1-Hg-X2	102.0(4)	-	100.8(2)	-	101.5(3)	-	-
	N1-Hg-X1	82.7(4)[b]	-	83.9(2)[a]	-	83.7(3)[b]	-	a=1+x,y,z , b=-1+x,y,z
	X1-Hg-X1	95.92(5)[b]	-	95.94(2)[a]	-	96.27(3)[b]	-	a=1+x,y,z , b=-1+x,y,z
	X2-Hg-X1	90.19(5)[b]	-	90.34(2)[a]	-	90.74(3)[b]	-	a=1+x,y,z , b=-1+x,y,z
	X1-Hg-X3	-	88.01(5)[b]	-	88.93(2)[a]	-	88.90(4)[b]	a=-x,-y,-z , b=2-x,-y,2-z
	X1-Hg-X1	-	180.00(3)[b]	-	180.00(1)[a]	-	180.00(2)[b]	a=-x,-y,-z , b=2-x,-y,2-z
	X3-Hg-X3	-	180.00(6)[b]	-	180.00(3)[a]	-	180.00(4)[b]	a=-x,-y,-z , b=2-x,-y,2-z

		Complex		Sym.code
		$[HgI_2(L^{3\text{-Cl-nic}})]$, B_1	$[HgI_2(L^{3\text{-Br-nic}})]$, B_2	
Bond distance	**Hg1-X1**	2.612(2)	2.618(1)	-
	Hg1-X2	2.634(2)	2.636(1)	-
	Hg1-N1	2.43(1)	2.40(1)	-
Bond angle	**X1-Hg1-X2**	148.43(4)	148.48(4)	-
	N1-Hg1-X1	106.0(4)	107.6(2)	-
	N1-Hg1-X2	104.7(4)	102.9(2)	-

References:

[S1] Khavasi, H. R.; Esmaeili, M.*CrystEngComm* **2014**, *16*, 8479−8485.