Supporting Information

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

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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 A_1 , A_2 , A_4 , A_5 and A_6 , (b) Type I X... π interaction in A_3 and (c) Type I X...X interaction in B_1 and B_2 .

	\mathbf{A}_1	A ₂	A ₃	A ₄	A ₅	A ₆ ⁱ
formula	C24H18Cl4HgN4O2	$C_{24}H_{18}Br_2Cl_2HgN_4O_2$	$C_{24}H_{18}Cl_2HgI_2N_4O_2$	$C_{24}H_{18}Br_2Cl_2HgN_4O_2$	$\mathrm{C}_{24}\mathrm{H}_{18}\mathrm{Br}_{4}\mathrm{HgN}_{4}\mathrm{O}_{2}$	$C_{24}H_{18}Br_2HgI_2N_4O_2$
fw	736.81	825.71	919.71	825.71	914.61	1008.61
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	C2/c	C2/c	C2/c	C2/c	C2/c	C2/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)
$D_{\rm calc}/{\rm Mg.m^{-3}}$	1.952	2.124	2.261	2.124	2.293	2.427
Ζ	4	4	4	4	4	4
μ (mm ⁻¹)	6.595	9.293	17.266	9.291	11.870	10.735
<i>F</i> (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
$R_1^a(I \ge 2\sigma(I))$	0.0697	0.0763	0.0719	0.0701	0.0705	0.0489
$wR_2^b(I \ge 2\sigma(I))$	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	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O	$\frac{C_{1}}{C_{24}H_{18}Cl_{2}Hg_{3}I_{6}N_{4}O_{2}}$	$\frac{C_2}{C_{24}H_{18}Br_2Hg_3I_6N_4O_2}$	$\frac{C_{3}}{C_{24}H_{18}Hg_{3}I_{8}N_{4}O_{2}}$	
formula	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05	B2ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50	C ₁ C ₂₄ H ₁₈ Cl ₂ Hg ₃ I ₆ N ₄ O ₂ 1828.49	C ₂ C ₂₄ H ₁₈ Br ₂ Hg ₃ I ₆ N ₄ O ₂ 1917.39	C ₃ C ₂₄ H ₁₈ Hg ₃ I ₈ N ₄ O ₂ 2011.39	
formula fw crystal system	B ₁ C ₁₂ H ₉ CIHgI ₂ N ₂ O 687.05 monoclinic	B2ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic	C ₁ C ₂₄ H ₁₈ Cl ₂ Hg ₃ I ₆ N ₄ O ₂ 1828.49 Monoclinic	C ₂ C ₂₄ H ₁₈ Br ₂ Hg ₃ I ₆ N ₄ O ₂ 1917.39 monoclinic	C ₃ C ₂₄ H ₁₈ Hg ₃ I ₈ N ₄ O ₂ 2011.39 monoclinic	
formula fw crystal system space group	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c	B2 ⁱ C ₁₂ H9BrHgI2N2O 731.50 monoclinic C2/c	C_1 $C_{24}H_{18}Cl_2Hg_3I_6N_4O_2$ 1828.49 Monoclinic $P2_1/n$	$\frac{C_2}{C_{24}H_{18}Br_2Hg_3I_6N_4O_2}$ 1917.39 monoclinic $P2_1/n$	$\frac{C_{3}}{C_{24}H_{18}Hg_{3}I_{8}N_{4}O_{2}}$ 2011.39 monoclinic $P2_{1}/n$	
formula fw crystal system space group <i>a</i> /Å	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6)	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic C2/c 25.3903(15)	$\frac{C_{1}}{C_{24}H_{18}Cl_{2}Hg_{3}I_{6}N_{4}O_{2}}$ 1828.49 Monoclinic $P2_{1}/n$ 4.5347(4)	$\frac{C_2}{C_{24}H_{18}Br_2Hg_3I_6N_4O_2}$ 1917.39 monoclinic $\frac{P2_1/n}{4.5326(4)}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3)	
formula fw crystal system space group <i>a</i> /Å <i>b</i> /Å	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4)	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C</i> 2/ <i>c</i> 25.3903(15) 14.1304(6)	$\frac{C_1}{C_{24}H_{18}Cl_2Hg_3I_6N_4O_2}$ 1828.49 Monoclinic $P2_1/n$ 4.5347(4) 21.3006(12)	$\begin{array}{c} C_2 \\ C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \end{array}$	C ₃ C ₂₄ H ₁₈ Hg ₃ I ₈ N ₄ O ₂ 2011.39 monoclinic <i>P</i> 2 ₁ / <i>n</i> 4.5421(3) 21.7134(19)	
formula fw crystal system space group <i>a</i> /Å <i>b</i> /Å <i>c</i> /Å	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2)	B2 ⁱ C12H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6)	$\begin{array}{c} C_{1} \\ C_{24}H_{18}Cl_{2}Hg_{3}I_{6}N_{4}O_{2} \\ 1828.49 \\ Monoclinic \\ P2_{1}/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \end{array}$	C ₃ C ₂₄ H ₁₈ Hg ₃ I ₈ N ₄ O ₂ 2011.39 monoclinic <i>P</i> 2 ₁ / <i>n</i> 4.5421(3) 21.7134(19) 19.3708(13)	
formula fw crystal system space group <i>a</i> /Å <i>b</i> /Å <i>c</i> /Å β/°	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2) 100.394(18)	B2 ⁱ C12H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5)	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \end{array}$	$\frac{C_2}{C_{24}H_{18}Br_2Hg_3I_6N_4O_2}$ 1917.39 monoclinic $P2_{1/n}$ 4.5326(4) 21.4340(12) 19.1582(16) 92.076(7)	$\begin{array}{c} C_{3} \\ \hline C_{24}H_{18}Hg_{3}I_{8}N_{4}O_{2} \\ 2011.39 \\ monoclinic \\ P2_{1}/n \\ 4.5421(3) \\ 21.7134(19) \\ 19.3708(13) \\ 92.541(6) \end{array}$	
formula fw crystal system space group a/Å b/Å c/Å β/° V/Å ³	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13)	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C</i> 2/ <i>c</i> 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3)	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1}/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \end{array}$	C_3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2)	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853	B2 ⁱ C12H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \end{array}$	$\begin{array}{c} C_{3} \\ \hline C_{24}H_{18}Hg_{3}I_{8}N_{4}O_{2} \\ 2011.39 \\ monoclinic \\ P2_{1}/n \\ 4.5421(3) \\ 21.7134(19) \\ 19.3708(13) \\ 92.541(6) \\ 1908.6(2) \\ 3.500 \end{array}$	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$ Z	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C2/c</i> 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \end{array}$	$\begin{array}{c} C_2 \\ C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1\prime}/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \end{array}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹)	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641	B2 ⁱ C12H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ \end{array}$	C_3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000)	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C</i> 2/ <i>c</i> 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_{1/n} \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \end{array}$	$\begin{array}{c} C_{3} \\ \hline C_{24}H_{18}Hg_{3}I_{8}N_{4}O_{2} \\ 2011.39 \\ monoclinic \\ P2_{1}/n \\ 4.5421(3) \\ 21.7134(19) \\ 19.3708(13) \\ 92.541(6) \\ 1908.6(2) \\ 3.500 \\ 2 \\ 18.534 \\ 1740 \end{array}$	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000) 2θ (°)	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448 54	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C</i> 2/ <i>c</i> 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592 52	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ Monoclinic \\ P2_{1/n} \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \\ 58.50 \\ \end{array}$	$\begin{array}{c} C_2 \\ C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1/n} \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \\ 58.40 \end{array}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534 1740 58.58	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000) 2θ (°) R (int)	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448 54 0.0992	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592 52 0.0985	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \\ 58.50 \\ 0.0915 \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ \hline monoclinic \\ P2_1/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \\ 58.40 \\ 0.0998 \\ \end{array}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534 1740 58.58 0.0998	
formula fw crystal system space group a/Å b/Å c/Å $\beta/°$ $V/Å^3$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000) 2θ (°) R (int) GOOF	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic <i>C</i> 2/ <i>c</i> 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448 54 0.0992 0.895	B ₂ ⁱ C ₁₂ H ₉ BrHgI ₂ N ₂ O 731.50 monoclinic <i>C</i> 2/ <i>c</i> 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592 52 0.0985 1.023	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \\ 58.50 \\ 0.0915 \\ 0.939 \\ \end{array}$	$\begin{array}{c} C_2 \\ \hline C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1}/n \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \\ 58.40 \\ 0.0998 \\ 1.028 \end{array}$	C_3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.71134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534 1740 58.58 0.0998 0.912	
formula fw crystal system space group a/Å b/Å c/Å $\beta/^{\circ}$ $V/Å^{3}$ $D_{cale}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000) 2θ (°) R (int) GOOF $R_1^a(I>2\sigma(I))$	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448 54 0.0992 0.895 0.0861	B2 ⁱ C ₁₂ H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592 52 0.0985 1.023 0.0640	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_{1/n} \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \\ 58.50 \\ 0.0915 \\ 0.939 \\ 0.0906 \\ \end{array}$	$\begin{array}{c} C_2 \\ C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1/n} \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \\ 58.40 \\ 0.0998 \\ 1.028 \\ 0.0528 \end{array}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534 1740 58.58 0.0998 0.912 0.0640	
formula fw crystal system space group a/Å b/Å c/Å $\beta/°$ $V/Å^3$ $D_{calc}/Mg.m^{-3}$ Z μ (mm ⁻¹) F(000) 2θ (°) R (int) GOOF $R_1^a(I>2\sigma(I))$ $wR_2^b(I>2\sigma(I))$	B ₁ C ₁₂ H ₉ ClHgI ₂ N ₂ O 687.05 monoclinic C2/c 25.080(6) 14.097(4) 9.200(2) 100.394(18) 3199.4(13) 2.853 8 13.641 2448 54 0.0992 0.895 0.0861 0.1658	B2i C12H9BrHgI2N2O 731.50 monoclinic C2/c 25.3903(15) 14.1304(6) 9.1996(6) 99.658(5) 3253.8(3) 2.987 8 15.705 2592 52 0.0985 1.023 0.0640 0.1406	$\begin{array}{c} C_1 \\ \hline C_{24}H_{18}Cl_2Hg_3I_6N_4O_2 \\ 1828.49 \\ \hline Monoclinic \\ P2_1/n \\ 4.5347(4) \\ 21.3006(12) \\ 19.0448(15) \\ 91.533(7) \\ 1838.9(2) \\ 3.302 \\ 2 \\ 17.703 \\ 1596 \\ 58.50 \\ 0.0915 \\ 0.939 \\ 0.0906 \\ 0.1101 \\ \end{array}$	$\begin{array}{c} C_2 \\ C_{24}H_{18}Br_2Hg_3I_6N_4O_2 \\ 1917.39 \\ monoclinic \\ P2_{1/n} \\ 4.5326(4) \\ 21.4340(12) \\ 19.1582(16) \\ 92.076(7) \\ 1860.0(2) \\ 3.424 \\ 2 \\ 19.507 \\ 1668 \\ 58.40 \\ 0.0998 \\ 1.028 \\ 0.0528 \\ 0.1174 \end{array}$	C3 $C_{24}H_{18}Hg_3I_8N_4O_2$ 2011.39 monoclinic $P2_1/n$ 4.5421(3) 21.7134(19) 19.3708(13) 92.541(6) 1908.6(2) 3.500 2 18.534 1740 58.58 0.0998 0.912 0.0640 0.1055	

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

 ${}^{a}R_{1} = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|. {}^{b}wR_{2} = [\Sigma(w(F_{o}^{2} - F_{c}^{2})^{2}) / \Sigma w(F_{o}^{2})2]^{\frac{1}{2}}. {}^{i} \text{ From reference [1]}.$

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

Complexes	D-HA	d(D-H)/Å	d(HA)/Å	d(DA)/Å	<d-ha th="" °<=""><th>Sym. Code</th></d-ha>	Sym. Code
A ₁	N2-H2AO1=C6	0.860(8)	2.071(7)	2.89(1)	160.2(7)	x,-1+y,z
A_2	N2-H2AO1=C6	0.86(1)	2.069(1)	2.90(1)	161.5(9)	x, 1+y,z
A_3	N2-H2AO1=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
A_4	N2-H2AO1=C6	0.860(9)	2.86(1)	2.016(9)	167.8(8)	x,-1+y,z
A ₅	N2-H2AO1=C6	0.86(1)	2.039(8)	2.87(1)	163.3(8)	x,1+y,z
A_6	N2-H2AO1=C6	0.860(8)	2.048(7)	2.88(1)	161.1(6)	x,1+y,z
\mathbf{B}_1	N2-H2AO1=C6	0.86(1)	2.08(1)	2.88(2)	155(1)	x,1-y,-1/2+z
	C12-H12O1=C6	0.93(2)	2.59(1)	3.22(2)	126(1)	x,1-y,-1/2+z
	C2-H2I2-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-H2AO1=C6	0.859(7)	2.118(8)	2.91(1)	152.5(6)	x,1-y,1/2+z
	C12-H12O1=C6	0.93(1)	2.540(8)	3.19(1)	127.0(8)	x,1-y,1/2+z
	C2-H2I2-Hg	0.93(1)	3.139(9)	3.92(1)	143.1(7)	1/2-x,1/2+y,1/2-z
C ₁	N2-H2AO1 = 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
C ₂	N2-H2AO1=C6	0.860(7)	2.115(7)	2.84(1)	142.1(6)	1+x,y,z
	C11-H11O1=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
C ₃	N2-H2AO1 = C6	0.862(9)	2.15(1)	2.85(1)	137.9(7)	1+x,y,z
	C11-H11O1=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							
		$[Hg_3I_6(L^{3-Cl-nic})_2]_n, C_1$		$[Hg_{3}I_{6}(L^{3-Br-nic})_{2}]_{n}, C_{2}$		$[Hg_3I_6(L^{3-1-nic})_2]_n, C_3$		Sym. Code	
		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				
	$[HgI_2(L^{3-Cl-nic})], B_1$		$[HgI_2(L^{3-Br-nic})], B_2$						
Bond distance	Hg1-X1	2.6	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	5.0(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.