Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information for MS:

Counter-ions Influence on Coordination Mode of 2,5-Bis(4-pyridyl)-1,3,4-oxadiazole (bpo) Ligand in Mercury(II) Coordination Polymers, $[Hg(bpo)_nX_2]$: X = I^-, Br^-, SCN^-, N_3^- and NO_2^-; Spectroscopic, Thermal, Fluorescence and Structural Studies

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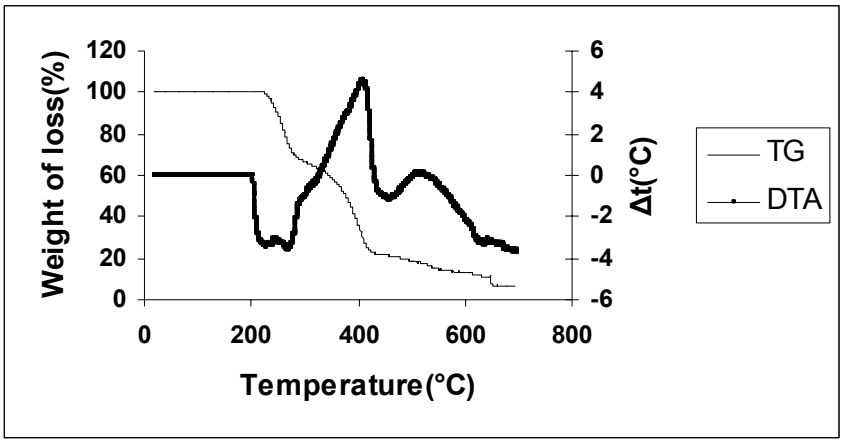

Figure S1. Thermal behaviour of $[Hg(bpo)(SCN)_2]_n$ (**1**).

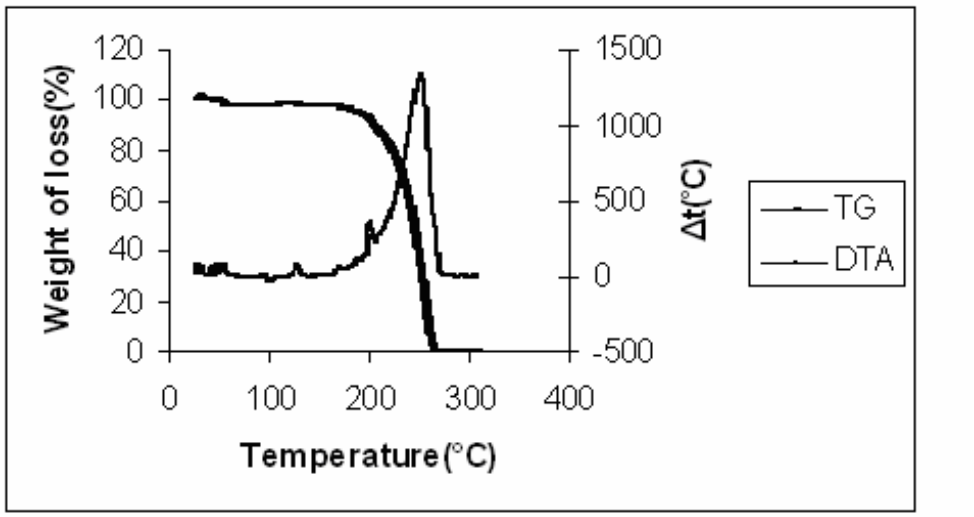

Figure S2. Thermal behaviour of $[Hg_2(\mu\text{-bpo})I_4]_2$ (**2**).

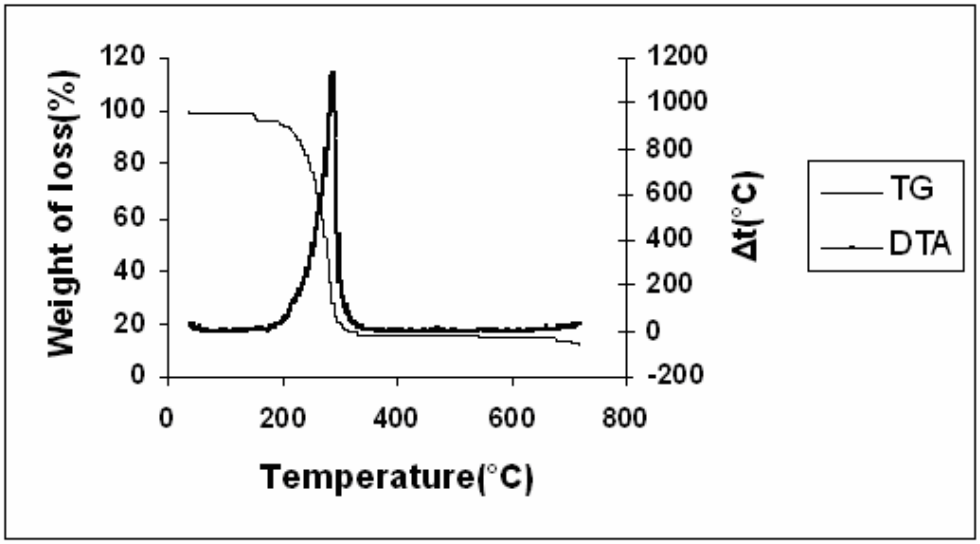

Figure S3. Thermal behaviour of $[Hg(\mu\text{-bpo})Br_2]_n$ (**3**).

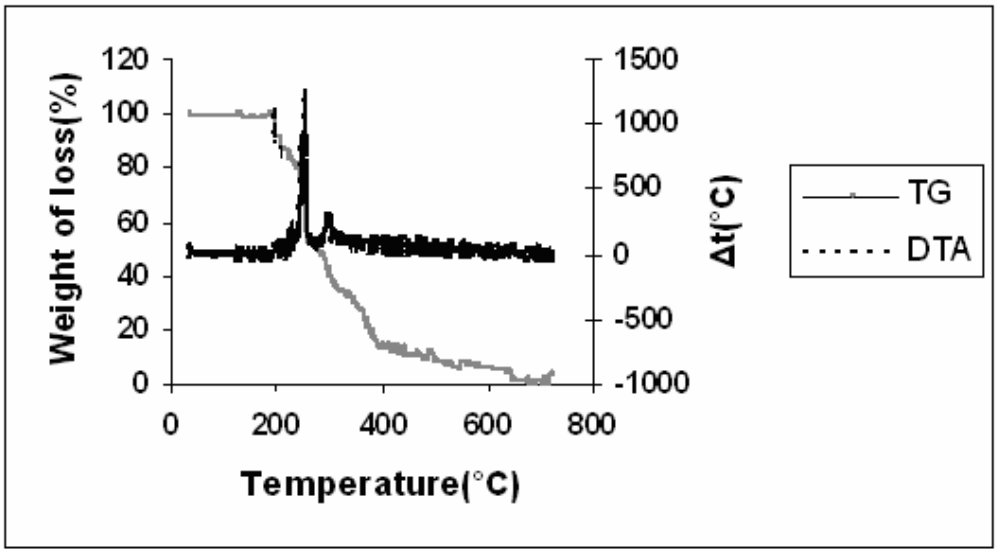

Figure S4. Thermal behaviour of $[Hg(\mu\text{-bpo})(NO_2)_2]_n$ (**4**).

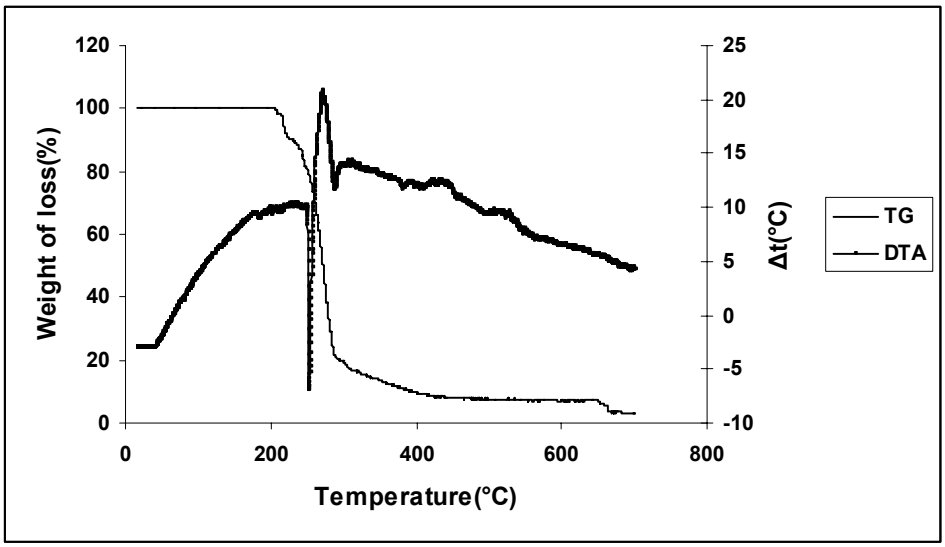

Figure S5. Thermal behaviour of $[Hg(\mu\text{-bpo})_2(N_3)_2]_n$ (**5**).

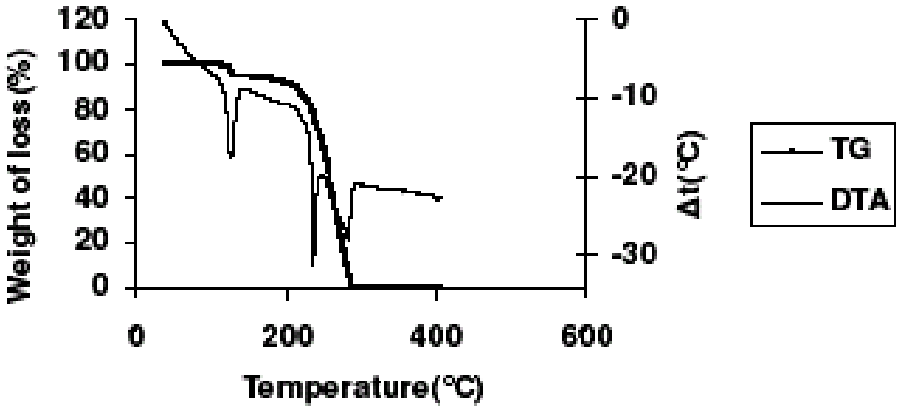

Figure S6. Thermal behaviour of $[Hg(\mu\text{-bpo})I_2]\cdot CH_3CN$ (**6**).

Table S1. Selected bond lengths /Å and angles /° for $[Hg(bpo)(\mu\text{-}SCN)_2]_n$ (**1**)

Hg1-S1	2.4046(15)
Hg1-S2	2.4158(17)
Hg1-N1	2.430(5)
Hg1-N6	2.548(6)
S1-Hg1-S2	149.60(6)
S1-Hg1-N1	110.12(13)
S2-Hg1-N1	98.66(13)
S1-Hg1-N6	98.38(14)
S2-Hg1-N6	92.67(15)

Table S2. Selected bond lengths /Å and angles /° for $[Hg_2(\mu\text{-}bpo)I_4]_2$ (**2**)

Hg1-N1	2.445(10)
Hg1-I1	2.6027(12)
Hg1- I2	2.6712(10)
Hg1-I3	3.1038(11)
Hg2-N4^{i}	2.388(10)
Hg2-I4	2.6262(10)
Hg2-I3	2.6442(11)
N1-Hg1-I1	106.5(3)
N1-Hg1-I2	99.3(3)
I1-Hg1-I2	145.55(4)
N1-Hg1-I3	92.4(3)
I1-Hg1-I3	103.53(3)
I2-Hg1-I3	97.72(3)
N4^{i}-Hg2-I4	106.1(3)
N4^{i}-Hg2-I3	105.0(3)
I4-Hg2-I3	148.77(4)

i: -x, -y, -z

Table S3. Selected bond lengths /Å and angles /° for $[Hg(\mu\text{-bpo})Br_2]_n$ (**3**)

Hg1-Br1	2.4754(6)
Hg1-Br2	2.4878(6)
Hg1-N1	2.425(4)
Hg1-N4^{i}	2.459(4)
N1-Hg1-N4^{i}	101.91(15)
N1-Hg1-Br1	104.24(10)
N4^{i} -Hg1-Br1	100.00(10)
N1-Hg1-Br2	95.38(10)
N4^{i} -Hg1-Br2	96.80(10)
Br1-Hg1-Br2	150.79(2)

i: -x, y+1/2, -z+1/2

Table S4. Selected bond lengths /Å and angles /° for $[Hg(\mu\text{-bpo})(NO_2)_2]_n$ (**4**)

Hg1-N4^{i}	2.291(3)
Hg1-O3	2.319(3)
Hg1-O5	2.333(3)
Hg1-N1	2.339(3)
Hg1-O4	2.529(3)
Hg1-O2	2.622(3)
N4^{i}-Hg1-O3	129.70(10)
N4^{i}-Hg1-O5	122.96(11)
O3-Hg1-O5	88.15(11)
N4^{i}-Hg1-N1	98.92(10)
O3-Hg1-N1	99.20(10)
O5-Hg1-N1	117.24(11)
N4^{i}-Hg1-O4	92.52(10)
O3-Hg1-O4	135.04(10)
O5-Hg1-O4	51.13(10)
N1-Hg1-O4	86.57(10)
N4^{i}-Hg1-O2	83.08(9)
O3-Hg1-O2	50.06(9)
O5-Hg1-O2	133.94(9)
N1-Hg1-O2	91.25(9)
O4-Hg1-O2	174.74(8)

i: -x+2,y-1/2,-z+1/2

Table S5. Selected bond lengths /Å and angles /° for $[Hg(\mu\text{-bpo})_2(N_3)_2]_n$ (**5**)

Hg1-N5	2.091(3)
Hg1-N3	2.698(3)
Hg1-N1^{ii}	2.757(3)
Hg1-N1^{iii}	2.757(3)
N5-Hg1-N5^{i}	180.00(18)
N5^{i}-Hg1-N3	86.09(10)
N5-Hg1-N3	93.91(10)
N3^{i}-Hg1-N3	180.00(11)
N5i-Hg1-N1^{ii}	92.20(10)
N5-Hg1-N1^{ii}	87.80(10)
N3^{i}-Hg1-N1^{ii}	95.57(9)
N3-Hg1-N1^{ii}	84.43(9),
N1^{ii}-Hg1-N1^{iii}	180.00(15).

i: -x, -y, -z ii: -x, y+1/2, -z+1/2 iii: x, -y+1/2, z+1/2