Supplementary Information

Two reversible transformable mercury(II) coordination polymers as efficient adsorbents for removal of dibenzothiophene

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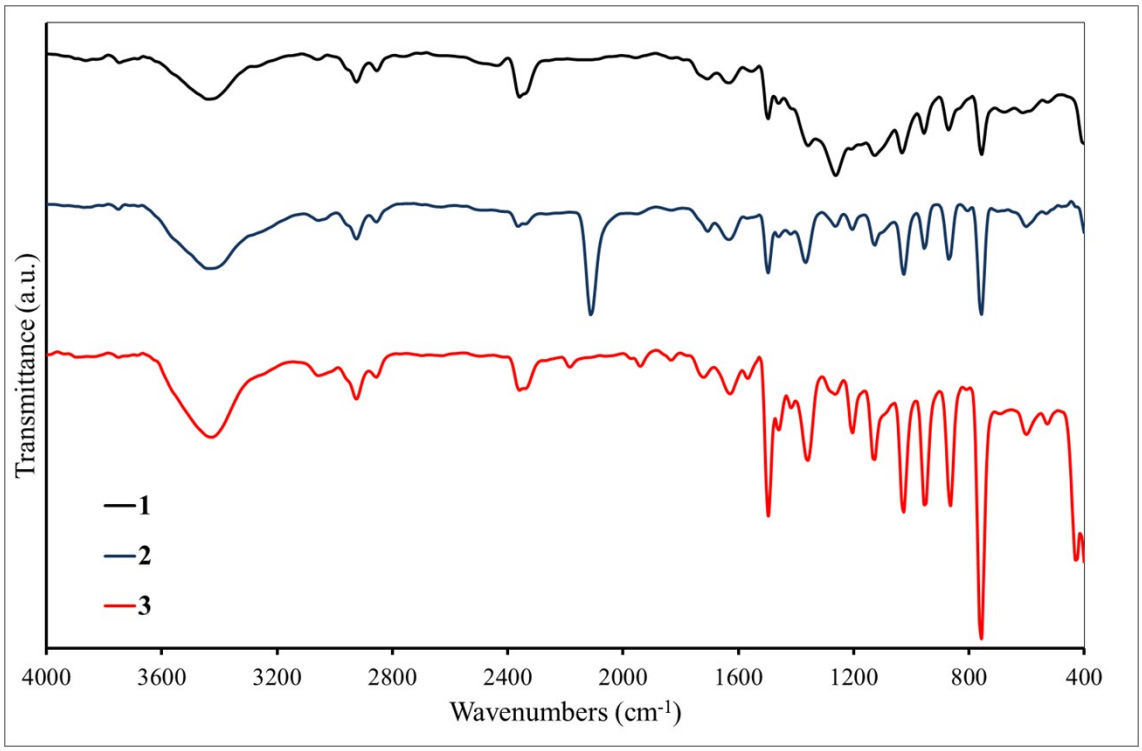

Fig. S1. The IR spectra of compound **1**, **2** and **3**.

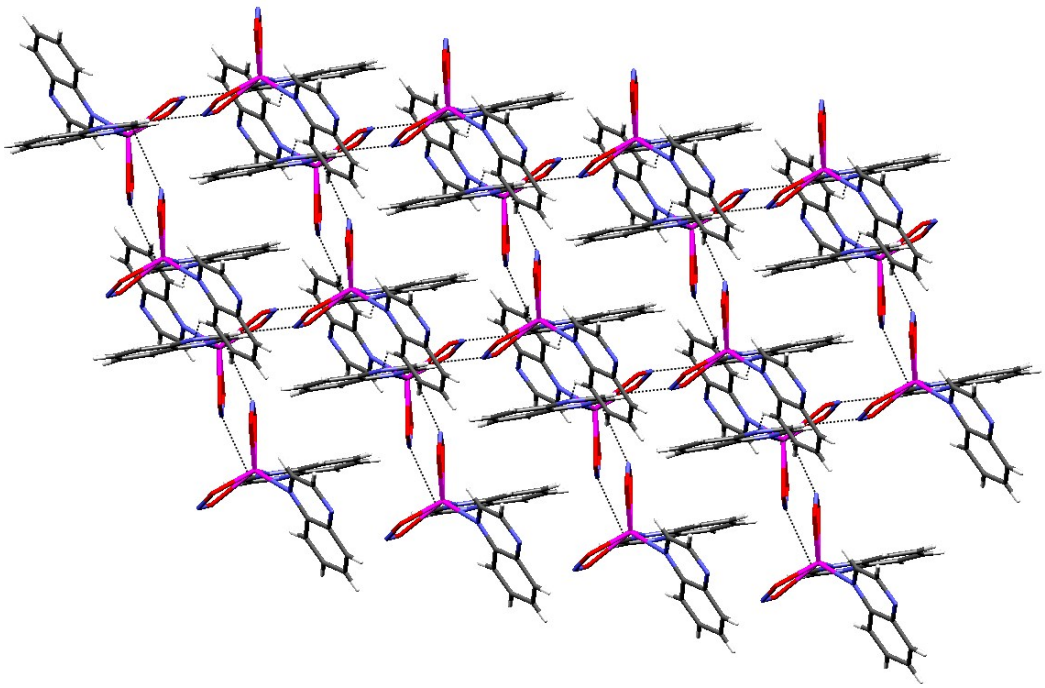

Fig. S2. Showing of the weak hydrogen bonds in the compound **1**. Color code: O: red; N: blue; C: gray and Hg: pink.

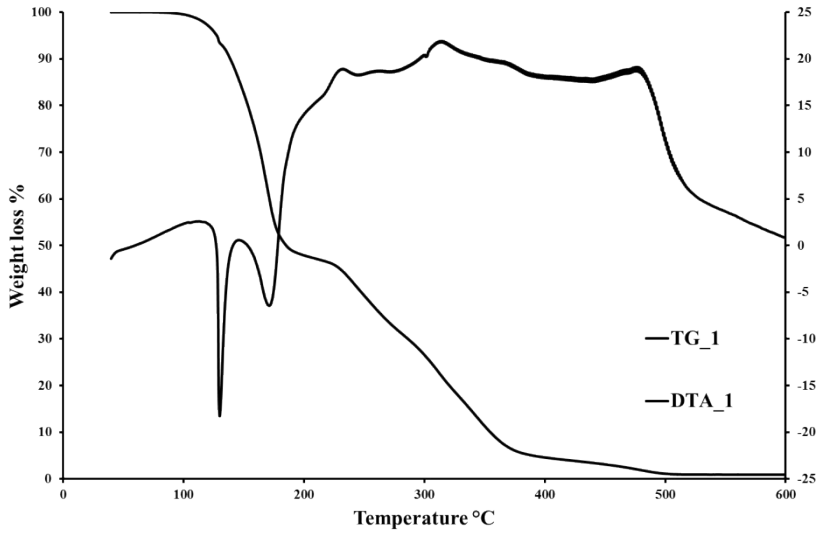

Fig S3. Thermal behaviour of compound $[Hg(quinoxaline)_2(NO_2)_2]$ **(1)**.

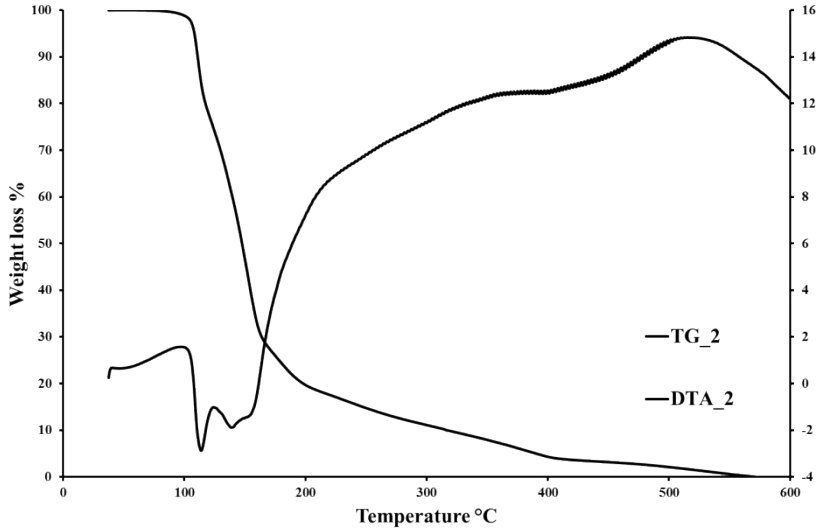

Fig S4. Thermal behaviour of compound $[Hg_3(\mu\text{-quinoxaline})_2(\mu\text{-SCN})_6]_n$ **(2)**.

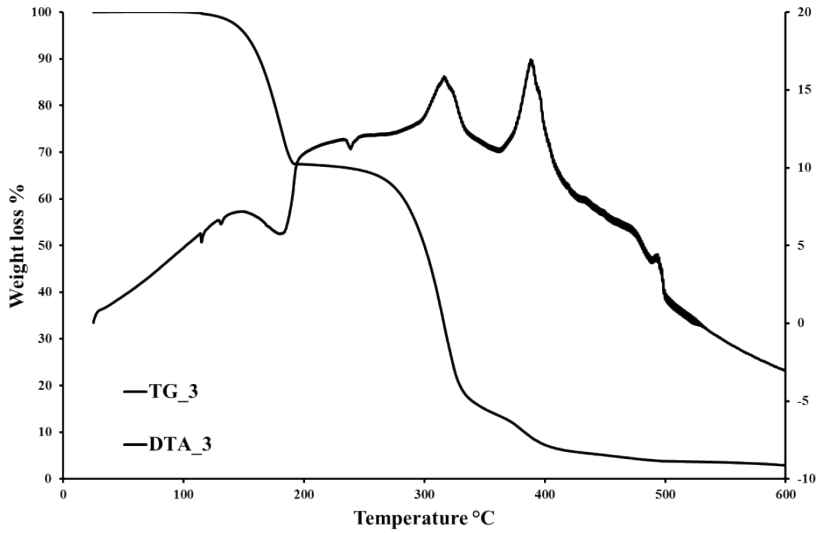

Fig S5. Thermal behaviour of compound $[Hg(\mu\text{-quinoxaline})(\mu\text{-CN})_2]_n$ **(3)**.

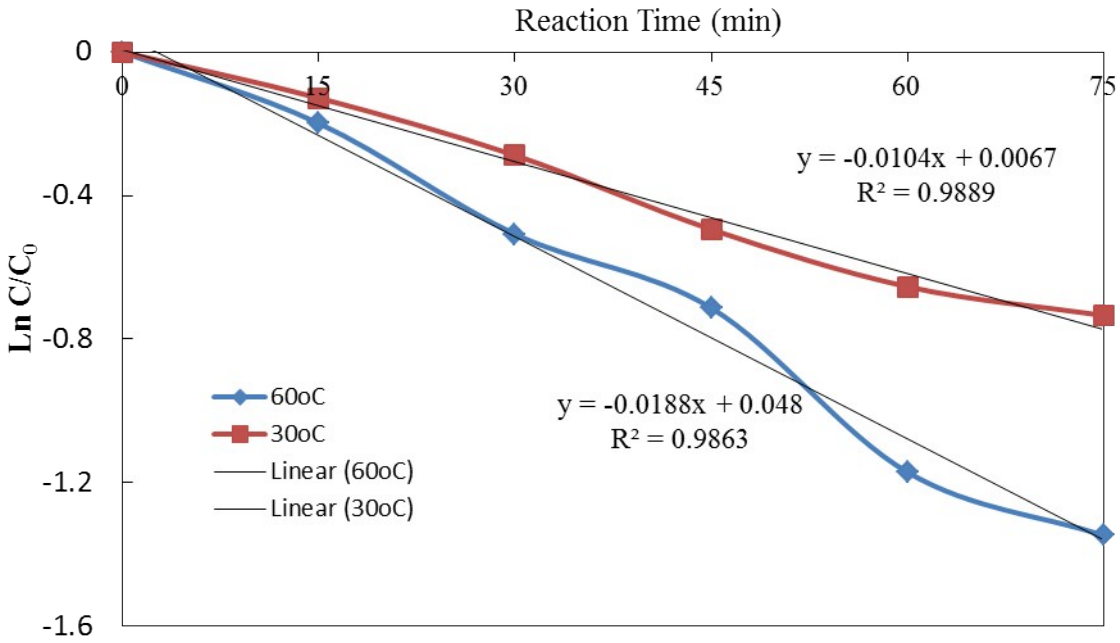

Fig. S6 Reaction kinetics of Removal of DBT over adsorbent of 2 at different temperatures.

Table S1 Crystal data and structure refinement of $[Hg(quinoxaline)_2(NO_2)_2]$ **(1)**, $[Hg_3(\mu\text{-}quinoxaline)_2(\mu\text{-}SCN)_6]_n$ **(2)** and $[Hg(\mu\text{-}quinoxaline)(\mu\text{-}CN)_2]_n$ **(3)**.

	1	**2**	**3**
Empirical formula	$C_{16}H_{12}HgN_6O_4$	$C_{22}H_{12}Hg_3N_{10}S_6$	$C_{10}H_6HgN_4$
Formula weight	552.91	1210.55	382.78
Temperature (ºK)	298(2)	100(2)	180(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal size (mm^3)	0.44 × 0.26 × 0.19	0.22 × 0.14 × 0.12	0.30 × 0.25 × 0.20
Crystal system	Triclinic	Triclinic	Triclinic
space group	Pī	Pī	Pī
a (Å)	8.441(8)	10.6771(13)	10.1350(5)
b (Å)	8.833(9)	11.7810(14)	10.1437(5)
c (Å)	12.787(12)	13.604(2)	11.0965(6)
α (deg)	80.631(17)	105.335(4)	88.561(3)
β (deg)	83.312(17)	110.148(4)	88.606(2)
γ (deg)	73.966(16)	95.645(3)	68.603(2)
Volume ($Å^3$)	901.5(15)	1515.0(3)	1061.69(9)
Z	2	2	4
D_{calc} (Mg/m^{3-})	2.037	2.654	2.395
Absorption coefficient (mm^{-1})	8.572	15.61	14.466
F(000)	524	1100	696
θ range for data collection (deg)	2.42 to 25.02	1.68 to 29.00	2.16 to 26.00
Limiting indices	$-9 \le h \le 9$	$-14 \le h \le 14$	-12<=h<=12
	$-10 \le k \le 10$	$-16 \le k \le 16$	-12<=k<=12
	$-15 \le l \le 11$	$-18 \le l \le 18$	-13<=l<=13
Reflections collected	3176	24644	11907
Independent reflections	3045	8057	4135 [R(int) = 0.0488]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Multi-scan
Completeness to theta	25.02 : 98.9 %	29.00 : 99.9 %	26.00 : 98.8 %

Max. and min. transmission	0.2013 and 0.0812	0.158 and 0.041	0.1600 and 0.0979
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F^2
Data / restraints / parameters	3045 / 0 / 244	8057 / 0 / 371	4135 / 0 / 244
Goodness-of-fit on F^2	1.009	1.02	1.093
Final R indices [I>2σ(I)]	R_1 = 0.0594, wR2 = 0.1463	R_1 = 0.0265, wR_2 = 0.0621	R1 = 0.0451, wR2 = 0.1242
R indices (all data)	R_1 = 0.0679, wR_2 = 0.1509	R_1 = 0.0321, wR_2 = 0.0645	R1 = 0.0478, wR2 = 0.1262
Largest diff. peak and hole ($e.A^{-3}$)	3.101 and -2.606	2.227 and -1.229	2.678 and -5.394

Table S2. Bond lengths /Å and angles /° for $[Hg(quinoxaline)_2(NO_2)_2]$ **(1)**.

Hg(1)-N(3)	2.366(10)	N(3)-Hg(1)-N(1)	117.7(3)
Hg(1)-N(1)	2.378(9)	N(3)-Hg(1)-O(4)	82.5(4)
Hg(1)-O(4)	2.437(16)	N(1)-Hg(1)-O(4)	121.0(7)
Hg(1)-O(2)	2.443(13)	N(3)-Hg(1)-O(2)	83.8(4)
Hg(1)-O(1)	2.453(12)	N(1)-Hg(1)-O(2)	115.0(5)
Hg(1)-O(3)	2.453(14)	O(4)-Hg(1)-O(2)	122.3(8)
		N(3)-Hg(1)-O(1)	133.4(4)
		N(1)-Hg(1)-O(1)	86.7(4)
		O(4)-Hg(1)-O(1)	120.1(6)
		O(2)-Hg(1)-O(1)	49.5(4)
		N(3)-Hg(1)-O(3)	128.6(5)
		N(1)-Hg(1)-O(3)	88.7(6)
		O(4)-Hg(1)-O(3)	46.8(6)
		O(2)-Hg(1)-O(3)	126.2(6)
		O(1)-Hg(1)-O(3)	87.8(6)

Table S3. Bond lengths /Å for $[Hg_3(\mu\text{-quinoxaline})_2(\mu\text{-SCN})_6]_n$ **(2)**.

Hg(1)-S(3)	2.4015(12)	N(1)-Hg(2)	2.496(4)	Hg(3)-S(5)	2.4066(12)
Hg(1)-S(1)	2.4143(12)	Hg(2)-S(4)	2.4068(12)	Hg(3)-S(6)	2.4171(12)
Hg(1)-N(9)	2.569(4)	Hg(2)-S(2)	2.4159(11)	Hg(3)-N(6)#4	2.636(4)
Hg(1)-N(2)	2.622(4)	Hg(2)-N(18)	2.608(4)	Hg(3)-N(11)	2.666(4)
Hg(1)-N(4)#1	2.736(4)	Hg(2)-N(3)#2	2.963(4)	Hg(3)-N(5)#5	2.788(4)
		Hg(2)-S(2)#3	3.2980(11)	Hg(3)-N(21)#4	2.881(4)

Table S4. Angles /° for $[Hg_3(\mu\text{-quinoxaline})_2(\mu\text{-SCN})_6]_n$ **(2)**.

S(3)-Hg(1)-S(1)	160.02(4)	S(4)-Hg(2)-S(2)	160.75(4)	S(5)-Hg(3)-S(6)	172.99(3)
S(3)-Hg(1)-N(9)	103.01(9)	S(4)-Hg(2)-N(1)	94.07(9)	S(5)-Hg(3)-N(6)#4	90.98(9)
S(1)-Hg(1)-N(9)	96.32(9)	S(2)-Hg(2)-N(1)	101.13(9)	S(6)-Hg(3)-N(6)#4	94.46(9)
S(3)-Hg(1)-N(2)	87.78(10)	S(4)-Hg(2)-N(18)	98.61(9)	S(5)-Hg(3)-N(11)	96.50(9)
S(1)-Hg(1)-N(2)	98.59(10)	S(2)-Hg(2)-N(18)	94.53(9)	S(6)-Hg(3)-N(11)	87.71(9)
N(9)-Hg(1)-N(2)	86.21(12)	N(1)-Hg(2)-N(18)	84.74(13)	N(6)#4-Hg(3)-N(11)	92.26(12)
S(3)-Hg(1)-N(4)#1	100.41(8)	S(4)-Hg(2)-N(3)#2	86.96(8)	S(5)-Hg(3)-N(5)#5	94.70(9)
S(1)-Hg(1)-N(4)#1	77.52(8)	S(2)-Hg(2)-N(3)#2	75.40(8)	S(6)-Hg(3)-N(5)#5	80.40(9)
N(9)-Hg(1)-N(4)#1	80.96(11)	N(1)-Hg(2)-N(3)#2	165.68(12)	N(6)#4-Hg(3)-N(5)#5	171.48(12)
N(2)-Hg(1)-N(4)#1	166.04(13)	N(18)-Hg(2)-N(3)#2	109.26(11)	N(11)-Hg(3)-N(5)#5	80.80(11)
		S(4)-Hg(2)-S(2)#3	88.06(4)	S(5)-Hg(3)-N(21)#4	84.39(9)
		S(2)-Hg(2)-S(2)#3	83.22(4)	S(6)-Hg(3)-N(21)#4	91.90(9)
		N(1)-Hg(2)-S(2)#3	79.48(10)	N(6)#4-Hg(3)-N(21)#4	82.85(12)
		N(18)-Hg(2)-S(2)#3	163.28(8)	N(11)-Hg(3)-N(21)#4	175.06(10)
		N(3)#2-Hg(2)-S(2)#3	86.29(8)	N(5)#5-Hg(3)-N(21)#4	104.00(12)

Symmetry transformations used to generate equivalent atoms: #1 x,y-1,z ; #2 x,y+1,z ; #3 -x-3,-y-1,-z-2 ; #4 -x-1,-y-1,-z-1 ; #5 -x-1,-y-2,-z-1

Table S5. Bond lengths /Å and angles /° for [Hg(μ-quinoxaline)(μ-$CN)_2]_n$ **(3)**.

Hg(1)-N(1)	2.832(11)	N(7)-Hg(1)-N(8)#5	172.8(5)
Hg(1)-N(3)	2.851(13)	C(18)-Hg(1)-C(17)	174.6(5)
Hg(1)-N(7)	2.716(13)	N(2)#1-Hg(2)-N(4)#2	176.4(4)
Hg(1)-N(8)#5	2.839(17)	C(20)-Hg(2)-C(19)	176.2(6)
Hg(1)-C(18)	2.036(12)		
Hg(1)-C(17)	2.061(12)		
Hg(2)-N(2)#1	2.826(12)		
Hg(2)-N(4)#2	2.793(11)		
Hg(2)-N(5)#3	2.821(12)		
Hg(2)-N(6)#4	2.862(13)		
Hg(2)-C(20)	2.011(14)		
Hg(2)-C(19)	2.044(15)		

Table S6. Kinetics equation of DBT removal.

compound	**Order(s)**	**$K_1(min^{-1})$**	**R_0**	**R_1**	**R_2**
2	ln (C_0/C)= -0.0188t + 0.048	0.0188	0.9756	0.9863	0.9394