Supplementary Information

Influence of the ligand frameworks on the coordination environment and properties of new phenylmercury(II) β-oxodithioester complexes.

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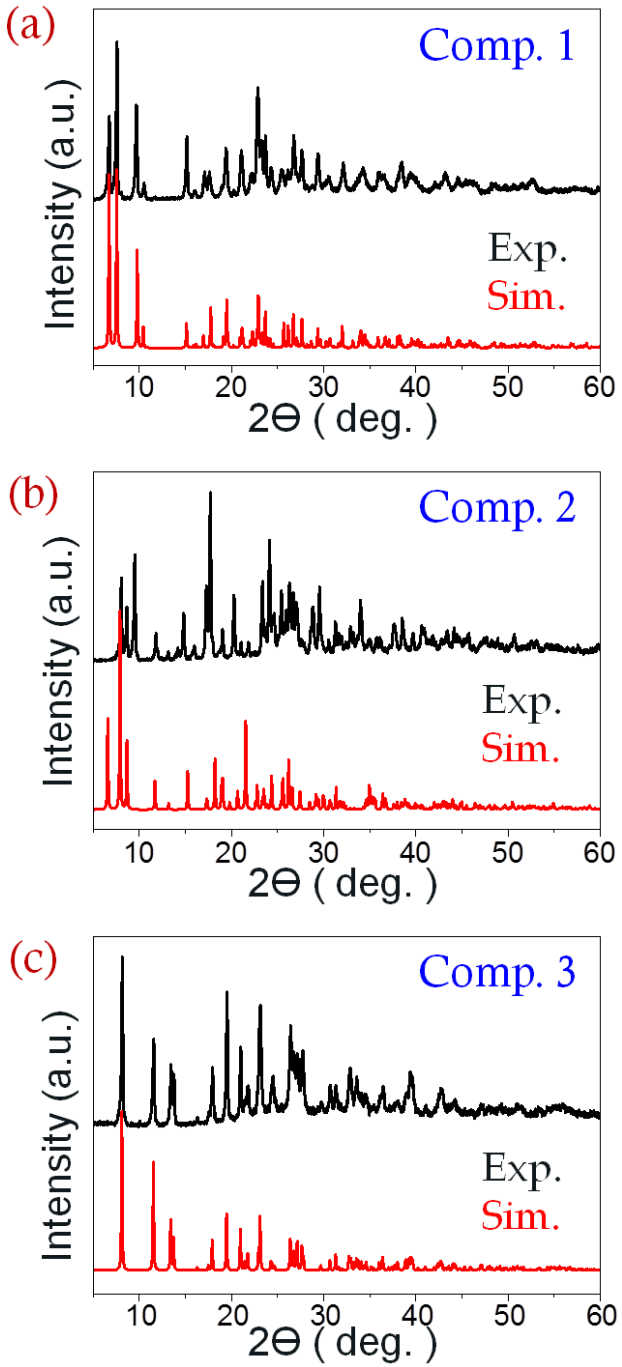
Contents

S1: Figure S1. Simulated (in red, generated from single crystal data) and experimental (in black) PXRD patterns of **1-3**



S2: Table S2. Selected non-conventional hydrogen bonding interactions and their parameters

Compound	D–H···A	d(H···A) (Å)	d(D···A) (Å)	∠ D–H···A (°)
1	C–H26 ···S13[a]	2.97	3.86(3)	160

	C–H28B···O27[b]	2.59	3.53(3)	165
3	C–H15···O17[c]	2.65	3.53(5)	159
	C–H24 ···S11[d]	3.00	3.63(3)	127
Symmetry code: [a]1-x,-1/2+y,-z; [b] 1-x,-1/2+y,1-z; [c] x,-y,-1/2+z ; [d] -1+x,y,-1+z				
Other weak interactions				
Compound	Interaction Type	Distance (Å)		
2	Br24···π[a] (-x, 1.5+y, 0.5-z)	3.65		
	S13···S13(1-x, -y, 1-z)	3.554(4)		

[a] Ring C41···C46 inclusive

S3: Table S3. Selected Wiberg Bond Orders for **1** and **3**

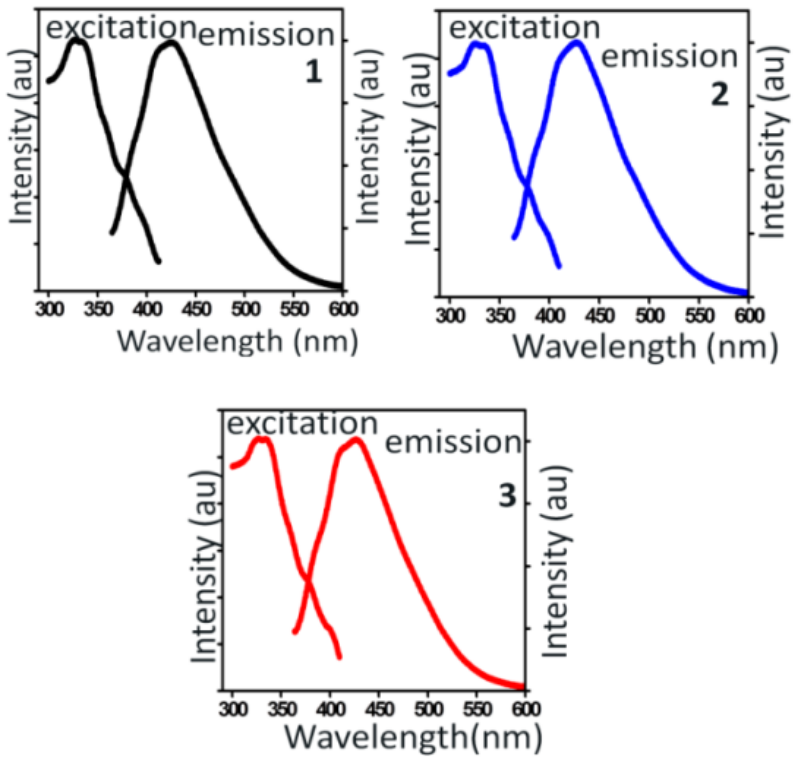
Compound	P(Hg-X)	P (Hg-S)	P(Hg···S)	P(Hg-C)
1 (X=O)	0.117	0.405	---	0.665
3 (X=N)	0.093	0.496(A) 0.486(B)	0.089(A) 0.092(B)	0.473(A) 0.491(B)

S4: Table S4. Charge distribution given by Natural Bond Orbital Analysis for **1** and **3**

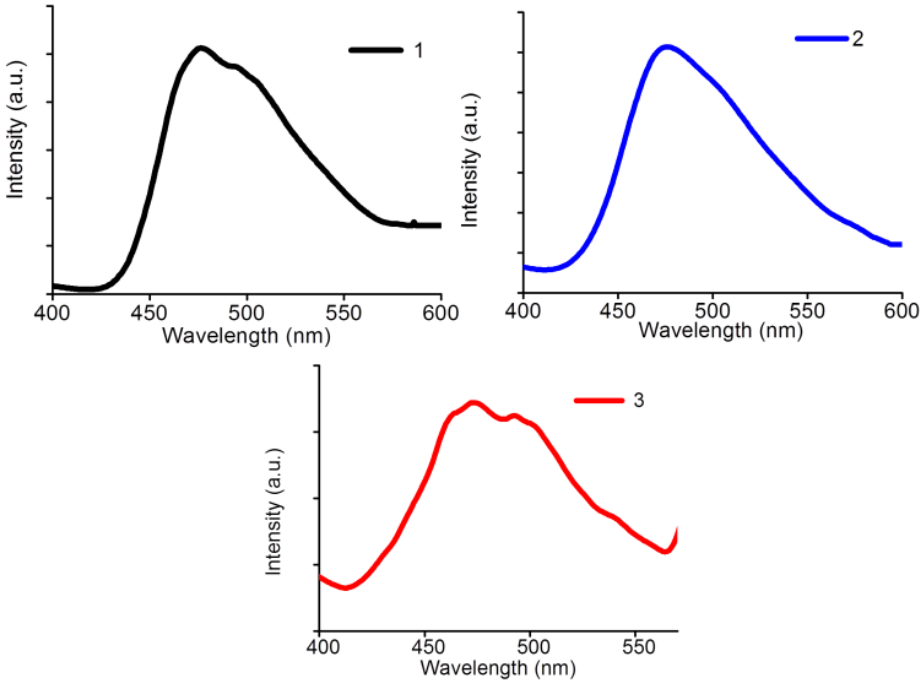
Charge on atoms	**1** (X=O)	**3** (X=N)
Hg	1.077	0.948(A) 0.991(B)
X	-0.718	-0.511
S(11)	-0.271	-0.211(A)

		-0.187(B)
S(13)	0.300	0.299(A) 0.283(B)
X#	-0.535	-0.457(B)
# for O/N not involved in interaction with metal		

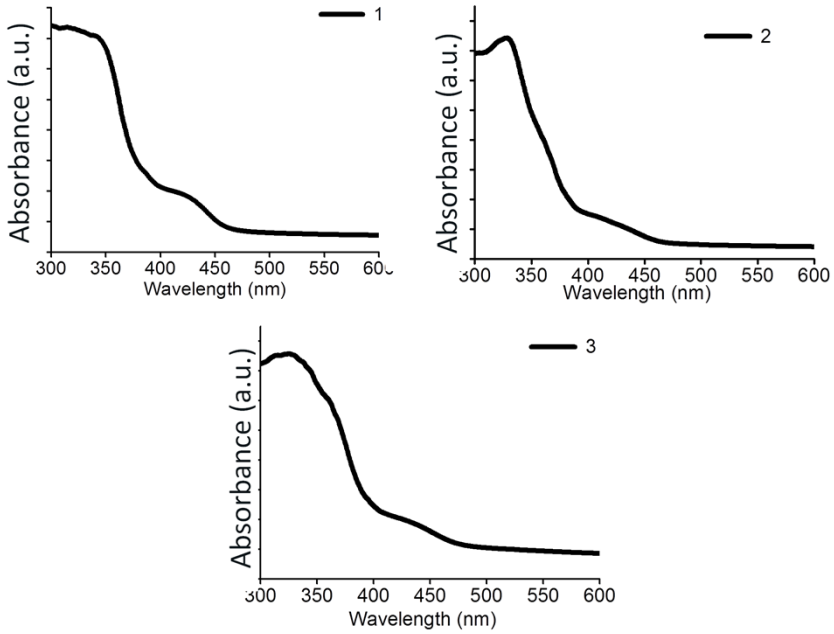
S5: Figure S5. Excitation and emission spectra of **1-3** in CH_2Cl_2 solution at room temperature showing λ_{em}^{max} at ~ 420 nm.



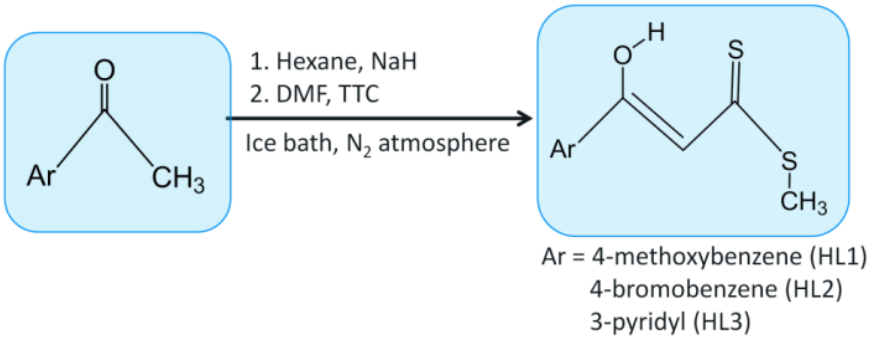
S6: Figure S6. Solid phase emission spectra of **1-3** at room temperature, λ_{em}^{max} at ~ 480 nm.



S7: Figure S7. Solid state absorption spectra of **1-3** in Nujol.



S8. Scheme S8. Generalized methodology for the synthesis of ligands H**L1**-H**L3**



S9. Scheme S9. Generalized methodology for the synthesis of complexes **1-3**