Supplementary Information

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Phenylmercury(II) sulfanylpropenoates: an example of symmetrization with the 3-(2-methoxyphenyl-2-sulfanylpropenoato ligand

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Table S1 Crystal and structure data refinement for [[HQ][PhHg(*o*-mpspa)]·0.5$HgPh_2$ (**2**), [HQ][PhHg(*o*-mpspa)] (**3**), [HQ] [PhHg(*p*-mpspa)] (**4**) and [HQ][PhHg(*o*-tfmpspa)](**5**)

Compound	**[HQ][PhHg(*o*-mpspa)] ·0.5$HgPh_2$ (2)**	**[HQ][PhHg(*o*-mpspa)] (3)**	**[HQ][PhHg(*p*-mpspa)] (4)**	**[HQ][PhHg(*o*-tfmpspa)] (5)**
Empirical formula	$C_{28}H_{34}NO_3SHg_{1.50}$	$C_{22}H_{29}NO_3SHg$	$C_{22}H_{29}NO_3SHg$	$C_{44}H_{52}F_6N_2O_6S_2Hg_2$
Formula weight	765.51	588.11	588.11	1284.18
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, *P-1*	Triclinic, *P-1*	Triclinic, P-*1*
CCDC reference	1455629	1455630	1455631	1455632
Unit cell dimensions				
a (Å)	10.9653(8)	9.977(3)	10.1999(8)	10.9515(9)
b (Å)	24.1931(17)	10.614(3)	11.0816(8)	15.1588(12)
c (Å)	10.7357(7)	12.809(7)	12.1792(10)	16.0378(13)
α (°)		111.613 (4)	101.7130 (10)	91.515(2)
β (°)	93.070(2)	95.65(4)	103.418(2)	109.962(2)
γ (°)		109.288(4)	113.8760(10)	92.162(2)
Volume ($Å^3$)	2843.9 (3)	1154.21(16)	1154.21(16)	2498.5(3)
Z, ρ_c (Mg/m^3)	4, 1.788	2, 1.695	2, 1.692	2/ 1.707
μ(Mo-Kα) (mm^{-1})	8.199	6.791	6.779	6.287
F (000)	1476	576	576	1248
Crystal size (mm)	0.25 x 0.17 x 0.07	0.41 x 0.23 x 0.06	0.41 x 0.17 x 0.09	0.33 x 0.29 x 0.11
θ range (°)	1.68 - 28.01	1.77 - 25.18	1.82 - 28.02	1.87 - 25.00
Index ranges h,k,l	−14, 12; −31,25; −14,14	−11, 11; −12, 12; −15, 15	−10, 13; −14, 13; −13, 15	−13, 12; −18, 17; −15, 19
Reflections collected/unique/R_{int}	14325/5536/ 0.0722	8905/4102/0.0316	7138/4985/0.0330	13253/ 8613/0.0392
Data / parameters	5536/319	4102/258	4985/261	8613/567
Goodness-of-fit on F^2	0.684	1.033	0.891	0.895
R_1, wR_2 indices [I>2σ (I)]	0.0381, 0.0455	0.0279, 0.0621	0.0418, 0.0841	0.0443, 0.1018
R_1, wR_2 indices (all data)	0.1357, 0.0568	0.0384, 0.0676	0.0582, 0.0880	0.1022, 0.1340

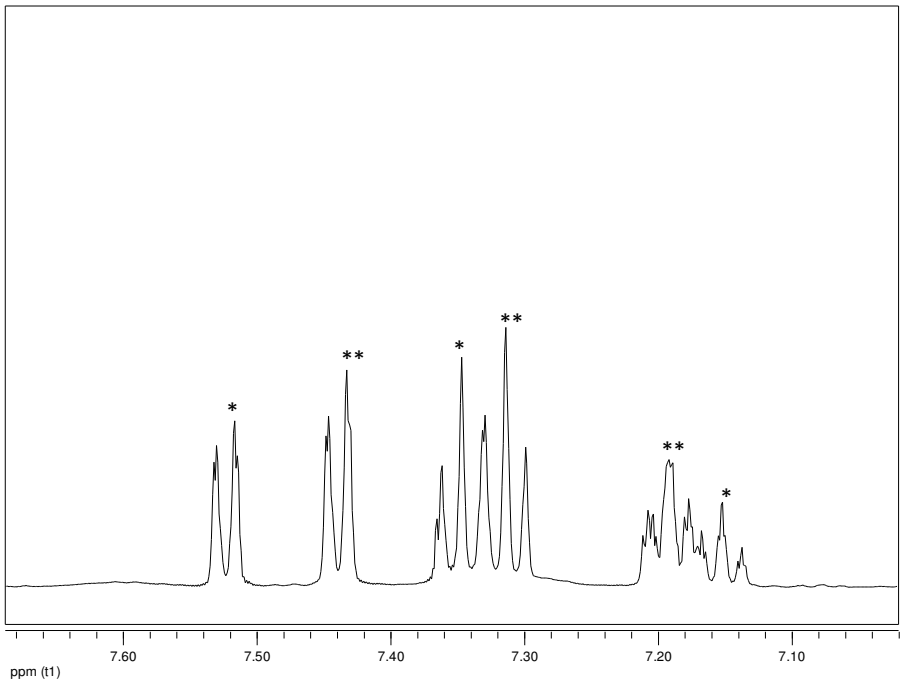

Fig. S1 ^{1}H NMR spectrum of [HQ][PhHg(*o*-mpspa)]·0.5$HgPh_2$ (**2**) in DMSO-d_6. The peaks marked with * indicate $HgPh_2$ signals and ** indicate $HgPh^+$ signals.

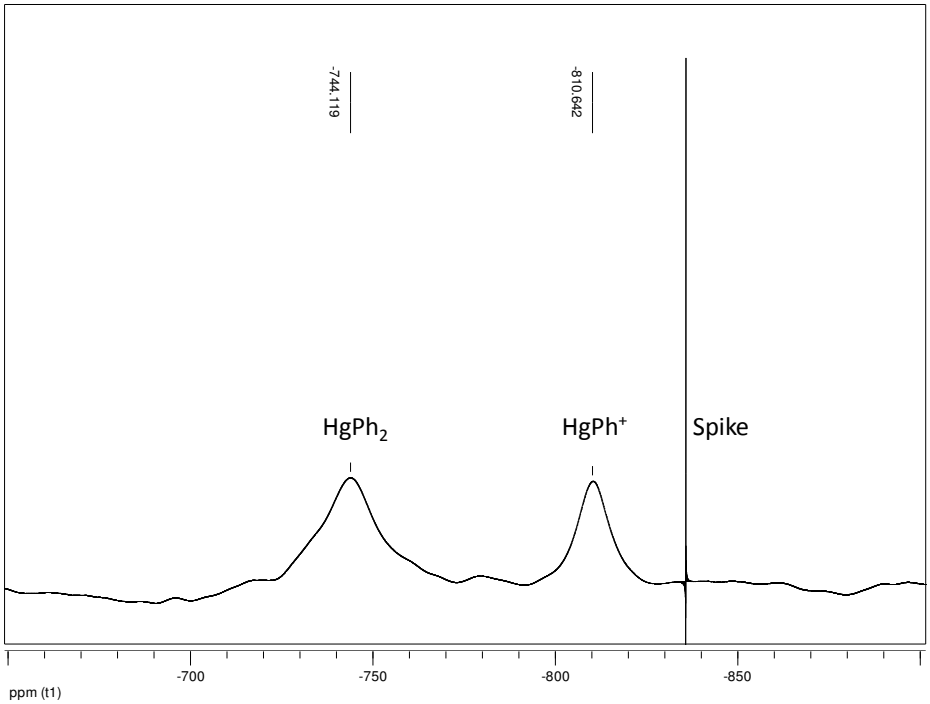

Fig. S2 ^{199}Hg NMR spectrum of [HQ][PhHg(*o*-mpspa)]·0.5$HgPh_2$ (**2**) in DMSO-d_6.