SUPPLEMENTARY INFORMATION (SI)

Aza Crown Ether Appended Hetarylazo Dye–Single Molecular Dual Analyte Chemosensor for Hg^{2+} and Pb^{2+}

Paramjit Kaur[*,a], Divya Sareen[a] and Kamaljit Singh[*,b]

[a]Department of Chemistry, UGC-Centre of Advance Studies-I, [b]Organic Synthesis Laboratory,
Department of Applied Chemical Sciences and Technology, Guru Nanak Dev University,
Amritsar-143 005, India

S1. Experimental

1. General

Mass spectrum was recorded on UPLC-Q-TOF mass spectrometer. ^{1}H NMR and ^{13}C NMR spectra have been recorded on BRUKER Avance II 400 MHz and 100 MHz, respectively with TMS as internal standard using CD_3CN as deuterated solvent. Data are reported as follows: chemical shift in ppm (δ), integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, dd=double doublet), coupling constant J (Hz) and assignment. The purity of the solid products was checked by elemental analysis performed on Thermoelectron FLASH EA1112, CHNS analyzer. UV-visible spectral studies were conducted on Shimadzu 1601 PC spectrophotometer with a quartz cuvette (path length, 1cm). The absorption spectra have been recorded between 1100 and 200 nm. The cell holder of the spectrophotometer was thermostatted at 25°C for consistency in the recordings. The pH titrations have been performed with the Equip-Tronics Digital pH meter model-EQ 610. The electrochemical behavior was determined by cyclic voltammetry on a CHI 660C Electrochemical Workstation with a conventional three-electrode configuration consisting of a platinum working (2 mm diameter) and counter electrodes and Ag/AgCl as the reference electrode. The experiments were carried out in 10^{-4} M solutions of samples in acetonitrile containing 0.01 M tetrabutylammonium hexafluorophosphate as supporting electrolyte at room temperature. Deoxygenation of the solutions was achieved by bubbling nitrogen for 10 min and the working electrode was cleaned after each run. The voltammograms were recorded with a scan rate of 100 mVs^{-1}.

2. Computational Methods

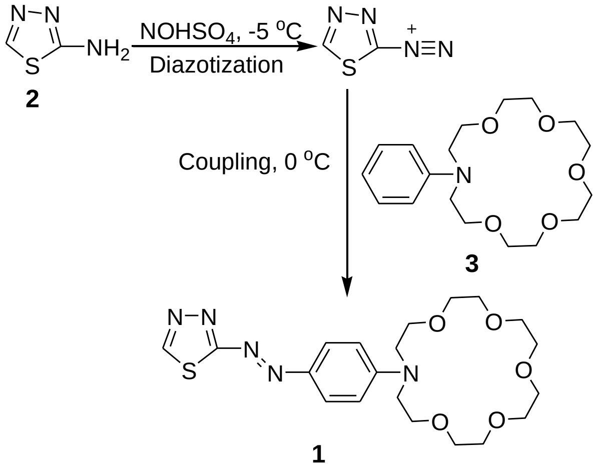
All theoretical calculations were carried out by using the Gaussian 09 suite of programs.

The molecular geometry of **1** was optimized by DFT/B3LYP[1]/6-31G* method. **1**+Hg^{2+} and **1**+Pb^{2+} geometries were optimized by DFT/MPW1PW91/GEN method in which 6-311G basis set was used for C, H, N, O and S with additional diffuse function for the donor atoms (N, O and S) and Stuttgart-Dresden basis set (SDD) for Hg and Pb. Energy values and properties of the systems were computed at the same level and considering solvent (acetonitrile) effects by using the Cossi and Barone's CPCM (conductor-like polarizable continuum model) modification[2] of the Tomasi's PCM formalism.[3] The first 50 excited states were calculated by using time-dependent density functional theory (TD-DFT) calculations. The molecular orbital contours were plotted using Gauss view 5.0.9.

3. Chemicals

Metal salts used in the spectrophotometric studies were of analytical grade and bought from Sigma-Aldrich. The solvents used were also of analytical grade purchased from Thomas Baker.

4. Synthetic Procedure for 1



Scheme S1. Preparation of compound **1**.

(a) Synthesis of 2[4]

Thiosemicarbazide (6.07 g, 1.0 mol) was added (below 25ºC) portion wise, to a stirred mixture of formic acid (4.06 g, 3.4 ml, 1.32 mol, 98-100%) and sulphuric acid (12.27 g, 6.7 ml,

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[1] Bartolottiand, L. J.; Fluchick, K. *Reviews in Computational Chemistry* Lipkowitz, K. B.; Boyd, B. D. Eds., VCH, New York, **1996**, *7*, 187.

[2] (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comp. Chem.* **2003**, *24*, 669.

[3] Miertus, S.; Scrocco, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117. (b) Cammi, R.; Mennucci, B.; Tomasi, J. *J. Phys. Chem. A* **2000**, *104*, 5631.

[4] https://scifinder.cas.org.

sp. gr. 1.84) and the resulting mixture was heated for 3 hours at 90ºC and then drowned in ice/water mixture (150 ml). The pH was adjusted in the range 7.5-8.0 with ammonium hydroxide, whereupon precipitation occurred. The temperature was maintained in the range 10-15ºC during the addition. The precipitates were filtered, dried and crystallized from hot methanol.

(b) Synthesis of 3[5]

A mortar was charged with dry K_2CO_3 (5.0 g), tetraethylene glycol (10 mmol, 8.5 ml), TsCl (15 mmol, 23.85 g), and grinded vigorously for 15 min. After the completion of tosylation, remaining tosyl chloride was removed by addition of powdered KOH (50 mmol, 14.0 g) and vigorously grinded for 5 min. The product was extracted by addition of ether (50 ml), filtered, and finally by the evaporation of organic solvent. Further purification of the ditosylated product was done by column chromatography over silica gel G (60-120 mesh) using 80% ethyl acetate/ hexane as eluent.

A two-necked flask equipped with a dropping funnel was evacuated and refilled with nitrogen, and then 300 ml dry THF and NaH (60% suspension in paraffin oil, 6.40 g, 0.16 mol) were added and refluxed. N-phenyldiethanolamine (14.5 g, 0.08 mol) and tetraethyleneglycol ditosylate (40.2 g, 0.08 mol) were dissolved in 300 ml dry THF and then slowly added dropwise to the reaction mixture. The addition was completed in 3 hours, and refluxing was continued for another 5 hours. After cooling, the solid was filtered and washed with THF, and the filtrate was concentrated under reduced pressure. The residue was dissolved in 10 ml methanol. To this solution, a solution of sodium perchlorate monohydrate (11.3 g, 0.08 mol) in 15 ml methanol was added. The mixture was refluxed for 10 min after which the mixture was concentrated to a small volume followed by the addition of ethyl acetate. The mixture was finally evaporated and the residue was recrystallized from ethyl acetate to give the sodium perchlorate complex.

N-phenylaza-18-crown-6 sodium perchlorate monohydrate (19.2 g) was decomposed by treatment with a mixture of CH_2Cl_2:H_2O (1:1); the organic layer was separated, dried and evaporated to give N-phenylaza-18-crown-6 **3**.

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[5] (a) Kazemi, F.; Massah, A. R.; Javaherian, M. *Tetrahedron* **2007**, *63*, 5083. (b) Deveci, P.; Taner, B.; Ustundag, Z.; Ozcan, E.; Solak, A. O.; Kilic, Z. *J. Mol. Struct.* **2010**, *982*, 162.

(c) Synthesis of 1[6]

Diazotization mixture was prepared by adding sodium nitrite (0.83 g, 0.012 mol) to sulphuric acid (14.7 g, 8 ml, 0.12 mol, 98%) at 30ºC and heating the stirred mixture to 60-65ºC to ensure complete dissolution. The reaction mixture was cooled to 5ºC and acetic acid (8 ml) and propionic acid (2 ml) were added and stirred. The temperature was then reduced to -5ºC, **2** (2.02 g, 0.01 mol) was added slowly and the whole reaction mixture stirred at the same low temperature for at least 2 hours. The completion of diazotization was checked by TLC.

A solution of **3** (3.39 g, 0.015 mol) in acetic anhydride and acetic acid was added to ice/water mixture (200 g) in a beaker equipped with mechanical stirrer and pH meter. A pinch of sulphamic acid was added followed by the addition of diazonium salt liquor at 0-5ºC over 1 hour and the mixture stirred for 3 hours at ambient temperature. The pH was maintained in the range 1.5-2.0 during the addition using aqueous sodium hydroxide solution. The completion of reaction was checked by spotting the reaction mixture on a filter paper close to a spot of an alkaline aqueous solution of H-acid and detecting any color appearance at the interface of the two boundaries. No color indicated the completion of reaction. Finally the pH was raised to 4.0-4.5. The dye was extracted with dichloromethane, dried over anhydrous sodium sulphate, the solvent removed and the residue purified by column chromatography with silica gel G (60-120 mesh) using 50% ethyl acetate/hexane as eluent. Semi-solid. Yield: 80%. Found: C, 53.36; H, 6.58; N, 15.62; S, 7.18. Calc. for $C_{20}H_{29}N_5O_5S$: C, 53.20; H, 6.47; N, 15.51; S, 7.10%. ^{1}H NMR (400 MHz; CD_3CN; Me_4Si; ppm) δ_H: 3.46-3.49 (24H, m, aza crown ether *H*), 6.78 (2H, dd, J=8 Hz, J=12 Hz, aromatic *H*), 7.75 (2H, dd, J=8 Hz, J=12 Hz, aromatic *H*), 9.02 (1H, s, thiadiazolic *H*). ^{13}C NMR (100 MHz; CD_3CN; Me_4Si; ppm) δ_C: 52.51, 69.08, 71.26, 71.27, 71.30, 71.32, 71.43, 71.57, 113.36, 130.35, 143.57, 153.06, 154.80. *m/z* (EI): 474 (M+23).

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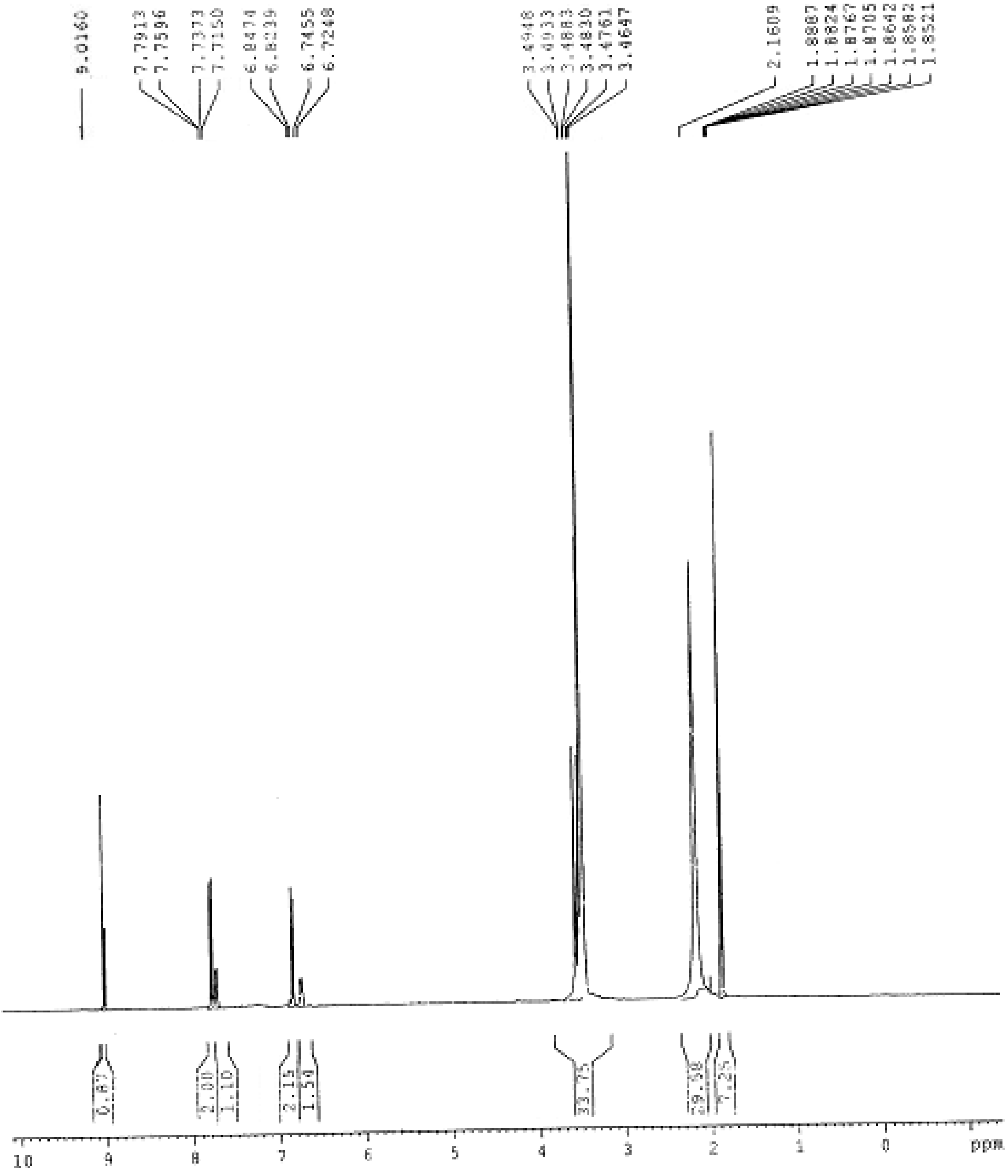
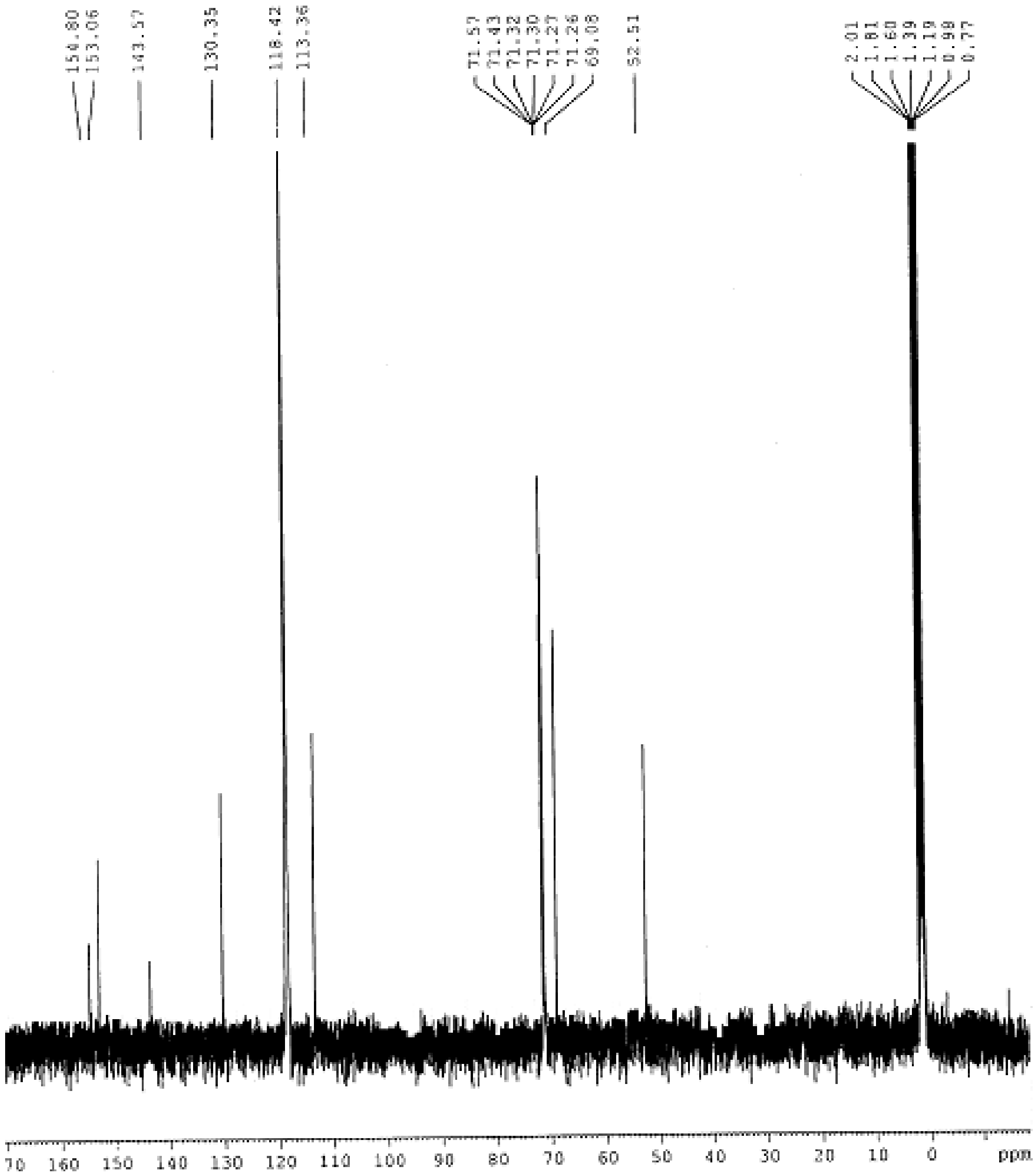
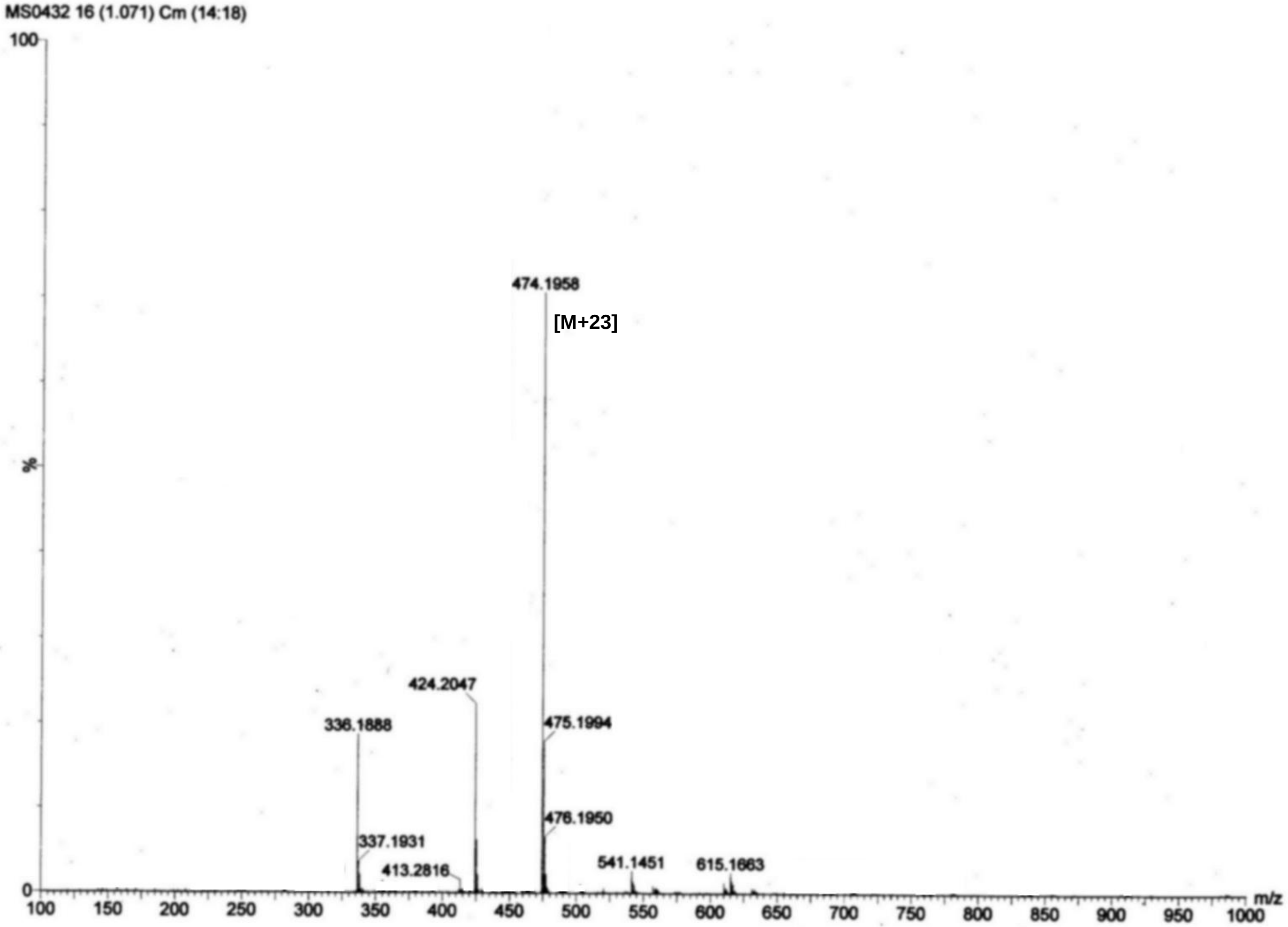
[6] Zollinger, H. *Color chemistry, syntheses, properties and application of organic dyes and pigments* 3rd revised ed., pp.166.



^{1}H NMR spectrum of **1**



^{13}C NMR spectrum of **1**



Mass spectrum of **1**

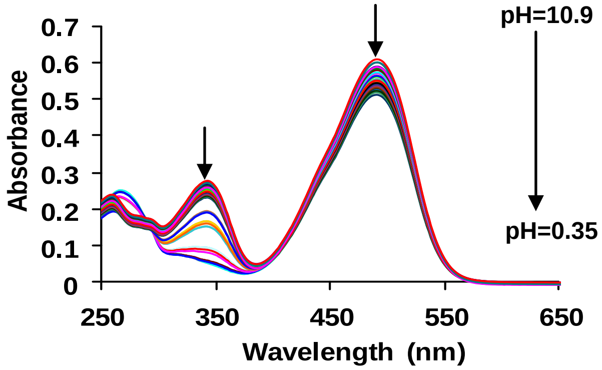


Fig. S2. Changes in the UV-vis spectrum of **1** (3x10^{-5} M, in CH_3CN) upon pH titrations with HCl (0.01 and 0.1 M, in distilled H_2O) and $NaHCO_3$ (0.01 and 0.1 M, in distilled H_2O).

Table S3. **(a)** Selected data of electronic transitions in **1** by TD-DFT method at the B3LYP/6-31G* level.[a][b]

State	λ [nm (eV)]	f	Composition of band and CI coefficiencies
2	455.07 (2.72)	0.8975	H-2→L, 0.11; H-1→L, 0.22; H→L, 0.66
9	298.34 (4.16)	0.0521	H-7→L, 0.66; H-6→L, -0.11; H→L+1, -0.14
11	273.70 (4.53)	0.0349	H-6→L, -0.11; H→L+1, 0.53; H→L+2, 0.42

[a] Calculations were carried out for the lowest 50 excited states, and only energies above 250 nm with f > 0.03 are shown. [b] f = oscillator strength; CI = configuration interaction; H = HOMO; L = LUMO.

(b) Cartesian coordinates from the optimized structure of **1** at B3LYP/6-31G*.

E= -1827.5014 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.956287	-2.187859	-1.471951
2	6	0	2.642946	-3.354046	-0.925709
3	1	0	3.570825	-3.482286	-1.488758
4	6	0	2.986173	-3.255659	0.561278
5	1	0	3.490383	-4.189041	0.867058
6	8	0	3.820549	-2.131487	0.765531
7	6	0	4.127364	-1.889434	2.128779
8	1	0	5.030937	-2.448098	2.424006

9	6	0	4.346215	-0.405439	2.361658
10	1	0	5.105597	-0.011592	1.667681
11	8	0	3.110741	0.264372	2.195735
12	6	0	3.058739	1.544951	2.800858
13	1	0	3.824638	2.218900	2.385490
14	6	0	1.680604	2.139644	2.574082
15	8	0	1.605215	2.699631	1.275699
16	6	0	0.273460	2.978771	0.867780
17	6	0	0.262159	3.829782	-0.394402
18	8	0	0.640770	3.141075	-1.575618
19	6	0	1.941711	3.392209	-2.088547
20	6	0	2.981693	2.381520	-1.629625
21	8	0	2.684728	1.132602	-2.235110
22	6	0	3.248866	0.017203	-1.560400
23	1	0	2.050846	-4.263648	-1.089117
24	1	0	2.070390	-3.157615	1.162729
25	1	0	3.299273	-2.218567	2.773270
26	1	0	4.726907	-0.272135	3.388547
27	1	0	3.241340	1.455422	3.885360
28	1	0	0.931161	1.344831	2.706490
29	1	0	1.485631	2.917516	3.331877
30	1	0	-0.277231	2.042134	0.695021
31	1	0	-0.253908	3.542360	1.656749
32	1	0	-0.769885	4.173282	-0.545774
33	1	0	0.894063	4.716637	-0.237922
34	1	0	1.856795	3.343369	-3.180463
35	1	0	2.276346	4.405254	-1.817639
36	1	0	3.986462	2.724759	-1.935497
37	1	0	2.957000	2.299364	-0.537126
38	1	0	4.349445	0.068036	-1.598430
39	1	0	2.953813	0.006665	-0.504333
40	6	0	2.741033	-1.252384	-2.280115
41	1	0	3.582108	-1.819047	-2.686368
42	1	0	2.139829	-0.924603	-3.134892
43	6	0	0.645434	-1.911254	-1.145239
44	6	0	-0.179364	-2.869661	-0.497811
45	6	0	0.066220	-0.645816	-1.458219
46	6	0	-1.498568	-2.582138	-0.198673
47	1	0	0.207915	-3.848041	-0.241385
48	6	0	-1.248788	-0.369347	-1.147409
49	1	0	0.665966	0.138692	-1.904840
50	6	0	-2.062420	-1.331254	-0.507669
51	1	0	-2.127266	-3.321269	0.289108
52	1	0	-1.667238	0.603107	-1.383429
53	7	0	-3.386093	-1.145394	-0.131352
54	7	0	-3.879080	0.004666	-0.368311

55	6	0	-5.195748	0.121377	0.033004
56	16	0	-6.136299	-1.192939	0.780265
57	6	0	-7.427426	-0.030390	0.835229
58	1	0	-8.402167	-0.272294	1.242553
59	7	0	-5.865416	1.237324	-0.106359
60	7	0	-7.148130	1.150346	0.355512

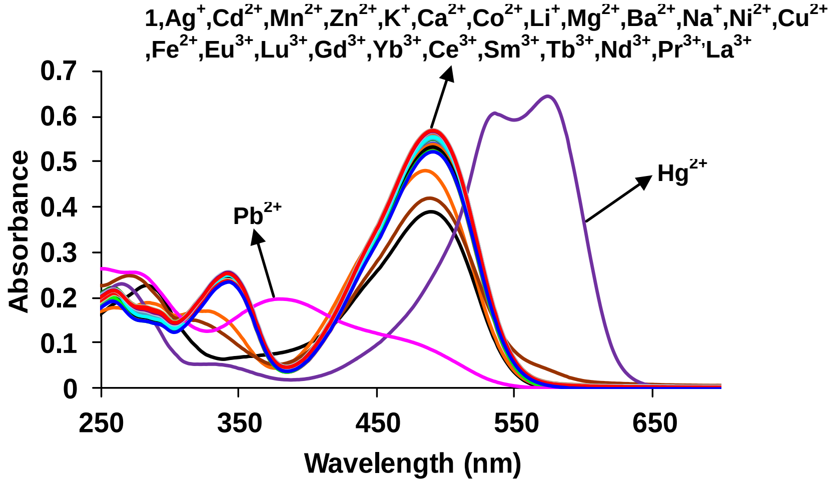


Fig. S4. UV-vis spectra of **1** ($3x10^{-5}$ M, in CH_3CN) in the presence of different metal ions ($3x10^{-5}$ M, in H_2O).

Table S5. (a) Selected data of electronic transitions in **1**+Hg^{2+} by TD-DFT method at the MPW1PW91/GEN level.[a][b]

State	λ [nm (eV)]	f	Composition of band and CI coefficiencies
1	606.88 (2.04)	0.1333	H→L, 0.61; H→L+1, 0.35
10	344.10 (3.60)	0.0591	H-7→L, 0.42; H-7→L+1, -0.12; H-6→L, -0.36; H-6→L+1, -0.40

[a] Calculations were carried out for the lowest 50 excited states, and only energies above 300 nm with f > 0.04 are shown. [b] f = oscillator strength; CI = configuration interaction; H = HOMO; L = LUMO.

(b) Cartesian coordinates from the optimized structure of **1**+Hg^{2+} at MPW1PW91/GEN.

E= -1980.4907 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.580874	-1.623167	-1.772977
2	6	0	3.149921	-2.891646	-1.310664
3	1	0	3.646520	-3.361994	-2.159776
4	6	0	4.160542	-2.770424	-0.181250
5	1	0	4.278410	-3.756064	0.282341
6	8	0	5.406613	-2.350353	-0.741224
7	6	0	6.493372	-2.340868	0.190741
8	1	0	7.376760	-2.680243	-0.351825
9	6	0	6.779640	-0.971421	0.762502
10	1	0	7.019537	-0.264765	-0.039521
11	8	0	5.647710	-0.511774	1.497087
12	6	0	5.956323	0.597554	2.341738
13	1	0	6.504245	1.367244	1.788323
14	6	0	4.677381	1.186852	2.877544
15	8	0	4.088510	2.015415	1.875989
16	6	0	2.812932	2.522019	2.259915
17	6	0	2.401172	3.651756	1.343423
18	8	0	2.033530	3.220161	0.030263
19	6	0	2.928529	3.571020	-1.028454
20	6	0	3.960642	2.509376	-1.329676
21	8	0	3.297567	1.384993	-1.913530
22	6	0	4.175796	0.294003	-2.156908
23	1	0	2.349379	-3.562344	-1.014999
24	1	0	3.816831	-2.069576	0.581330
25	1	0	6.299961	-3.048741	1.001545
26	1	0	7.657062	-1.050409	1.416289
27	1	0	6.586260	0.264208	3.173781
28	1	0	3.996594	0.379105	3.166642
29	1	0	4.895369	1.783299	3.770743
30	1	0	2.061999	1.724592	2.236947
31	1	0	2.858143	2.915669	3.283043
32	1	0	1.524136	4.135897	1.779583
33	1	0	3.205856	4.390600	1.296550
34	1	0	2.310445	3.728999	-1.913081
35	1	0	3.438819	4.511828	-0.800440
36	1	0	4.698573	2.913802	-2.034225
37	1	0	4.472258	2.213459	-0.411214
38	1	0	4.945533	0.582077	-2.884051
39	1	0	4.674196	-0.018866	-1.237151

40	6	0	3.393090	-0.872921	-2.739639
41	1	0	4.108628	-1.577192	-3.155799
42	1	0	2.770580	-0.526311	-3.564355
43	6	0	1.355267	-1.214940	-1.388581
44	6	0	0.587063	-1.925112	-0.412273
45	6	0	0.738664	-0.059573	-1.969534
46	6	0	-0.686167	-1.541955	-0.078378
47	1	0	1.004520	-2.773354	0.101309
48	6	0	-0.523648	0.320675	-1.623394
49	1	0	1.287919	0.544217	-2.667919
50	6	0	-1.287970	-0.404825	-0.666917
51	1	0	-1.196090	-2.126307	0.670972
52	1	0	-0.968107	1.186122	-2.088180
53	7	0	-2.553449	0.008097	-0.338630
54	7	0	-2.887377	1.173534	-0.698034
55	6	0	-4.189770	1.573262	-0.680577
56	16	0	-5.568460	0.603737	-1.201732
57	6	0	-6.515344	2.004530	-0.864645
58	1	0	-7.583175	2.015994	-1.002625
59	7	0	-4.514718	2.805927	-0.363398
60	7	0	-5.834724	3.037473	-0.453659
61	80	0	-4.030951	-1.310069	0.991648

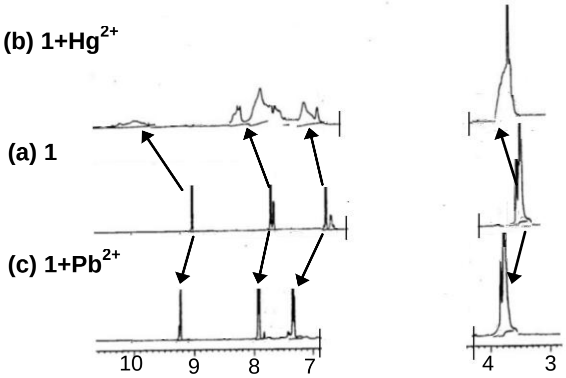
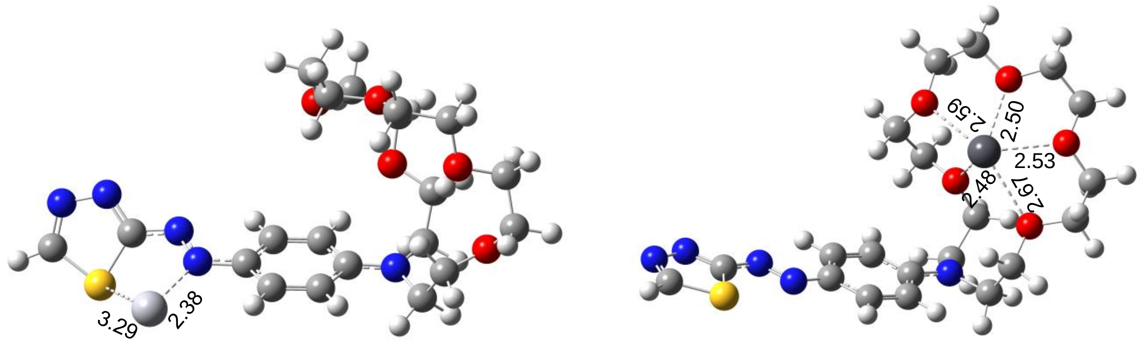


Fig. S6. Partial ^{1}H NMR (CD$_3$CN) of **1** **(a)** before and after addition of **(b)** Hg^{2+} ion and **(c)** Pb^{2+} ion.



(a) **(b)**

Fig. S7. Optimized structures of **(a)** **1**+Hg^{2+} and **(b)** **1**+Pb^{2+} using Gaussian 09 program. All the bond distances are in Å (angstrom).

Table S8. **(a)** Selected data of electronic transitions in **1**+Pb^{2+} by TD-DFT method at the MPW1PW91/GEN level.[a][b]

State	λ [nm (eV)]	f	Composition of band and CI coefficiencies
2	425.00 (2.92)	1.1307	H→L, 0.70
11	246.55 (5.03)	0.1362	H-6→L, 0.49; H→L+5, 0.37; H→L+4, -0.31

[a] Calculations were carried out for the lowest 50 excited states, and only energies above 200 nm with f > 0.10 are shown. [b] f = oscillator strength; CI = configuration interaction; H = HOMO; L = LUMO.

(b) Cartesian coordinates from the optimized structure of **1**+Pb^{2+} at MPW1PW91/GEN.

E= -1830.4568 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.076197	2.413848	1.296403
2	6	0	0.541300	3.495996	0.534191
3	1	0	1.334207	3.925991	1.143234
4	6	0	1.136303	3.069481	-0.799067
5	1	0	1.447644	3.958344	-1.347015
6	8	0	2.291793	2.216942	-0.582207
7	6	0	3.474972	2.647767	-1.291420
8	1	0	3.659357	3.702585	-1.085947
9	6	0	4.643498	1.842473	-0.800159

10	1	0	4.811373	1.993920	0.266993
11	8	0	4.372313	0.445676	-1.049738
12	6	0	5.488713	-0.415851	-0.734557
13	1	0	5.734270	-0.314222	0.323153
14	6	0	5.082171	-1.827394	-1.056442
15	8	0	3.873883	-2.080038	-0.308935
16	6	0	3.451681	-3.459470	-0.219507
17	6	0	2.484683	-3.525346	0.931155
18	8	0	1.436327	-2.566738	0.667603
19	6	0	0.627417	-2.227316	1.811808
20	6	0	1.273545	-1.122053	2.612802
21	8	0	1.539284	-0.014221	1.716270
22	6	0	1.828539	1.245076	2.381027
23	1	0	-0.178931	4.298942	0.358588
24	1	0	0.418752	2.527311	-1.413190
25	1	0	3.331925	2.514109	-2.364794
26	1	0	5.540501	2.134655	-1.347096
27	1	0	6.349354	-0.125659	-1.337226
28	1	0	4.897225	-1.963713	-2.122346
29	1	0	5.860762	-2.518233	-0.734743
30	1	0	2.992935	-3.770169	-1.158529
31	1	0	4.315074	-4.091763	-0.015973
32	1	0	2.051143	-4.521771	1.011666
33	1	0	2.995448	-3.276269	1.861200
34	1	0	-0.331882	-1.906494	1.412730
35	1	0	0.467116	-3.106266	2.435245
36	1	0	0.593984	-0.801101	3.402281
37	1	0	2.213630	-1.433475	3.068137
38	1	0	2.301517	1.042339	3.341503
39	1	0	2.536461	1.766269	1.744990
40	6	0	0.568551	2.074643	2.561587
41	1	0	0.851346	2.999219	3.072468
42	1	0	-0.135615	1.576055	3.219532
43	6	0	-1.312053	1.935708	0.946648
44	6	0	-2.035985	2.494122	-0.140503
45	6	0	-1.925330	0.854477	1.643658
46	6	0	-3.278438	2.008041	-0.491619
47	1	0	-1.635305	3.318488	-0.704917
48	6	0	-3.163098	0.376871	1.284451
49	1	0	-1.420651	0.381863	2.468796
50	6	0	-3.871280	0.943293	0.205292
51	1	0	-3.819579	2.449657	-1.315964
52	1	0	-3.602078	-0.445549	1.827619
53	7	0	-5.116322	0.531507	-0.231827
54	7	0	-5.642980	-0.423323	0.398910
55	6	0	-6.881936	-0.778483	-0.091054

56	16	0	-7.686478	-0.006961	-1.448247
57	6	0	-8.957629	-1.136138	-1.158089
58	1	0	-9.852163	-1.155421	-1.757615
59	7	0	-7.567865	-1.754327	0.445740
60	7	0	-8.756421	-1.958028	-0.166747
61	82	0	2.026973	-0.435419	-0.678090

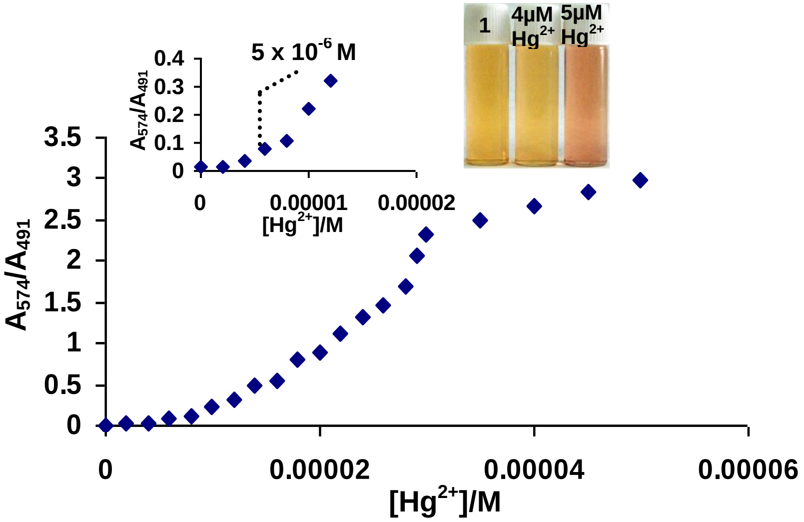


Fig. S9. Changes in the absorbance ratio (A_{574}/A_{491}) of **1** ($3x10^{-5}$ M, in CH_3CN) with increasing Hg^{2+} concentrations ($1x10^{-6}$ M to $5x10^{-5}$ M, in H_2O).

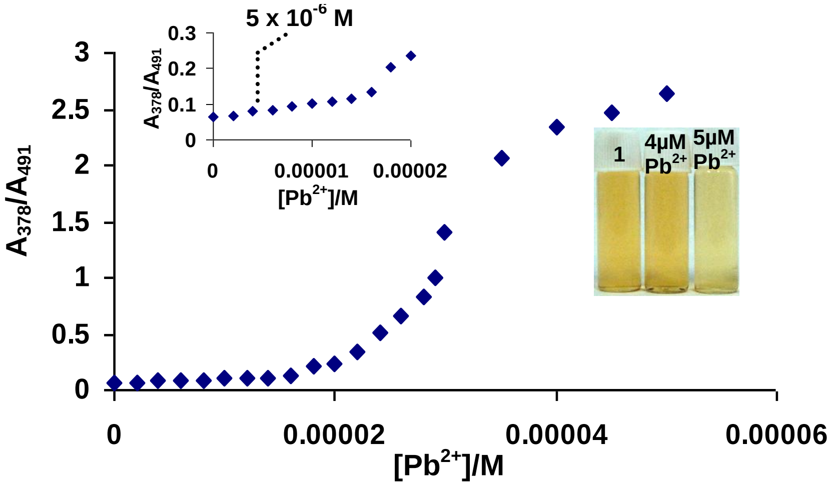


Fig. S10. Changes in the absorbance ratio (A_{378}/A_{491}) of **1** ($3x10^{-5}$ M, in CH_3CN) with increasing Pb^{2+} concentrations ($1x10^{-6}$ M to $5x10^{-5}$ M, in H_2O).

S11. Estimation of metal ions[7]

The estimation of the two metal ions from their mixtures can be done by the use of absorbance measurements defined by the Beer-Lambert law. First we take separate solutions of known concentrations of Hg^{2+} and Pb^{2+} added in the solution of known concentration of **1**.

Hg^{2+} solution:	**Pb^{2+} solution:**
Concentration = c_{Hg}	Concentration = c_{Pb}
$\lambda_{max} = \lambda_{Hg}$	$\lambda_{max} = \lambda_{Pb}$
$A_{574} = A_{Hg}$	$A_{378} = A_{Pb}$
$A_{378} = a_{Hg}$	$A_{574} = a_{Pb}$

Next, we take unknown mixture of the two metal ions and note its absorbances at 574 and 378 nm.

$A_{574} = A_1$

$A_{378} = A_2$

Unknown concentration of Hg^{2+} = x

Unknown concentration of Pb^{2+} = y

Then since the two absorbances are additive, A_1 and A_2 are given by

$A_1 = (x/c_{Hg})\, A_{Hg} + (y/c_{Pb})\, a_{Pb}$ ---------------------- Eq. 1

$A_2 = (x/c_{Hg})\, a_{Hg} + (y/c_{Pb})\, A_{Pb}$ ---------------------- Eq. 2

These are simultaneous equations which can be solved to give the unknown concentrations, x and y of the respective metal ions in their mixture solution.

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[7] McDonald, R. *Colour Physics for Industry* 2nd Ed., Society of Dyers and Colourists, **1997**.

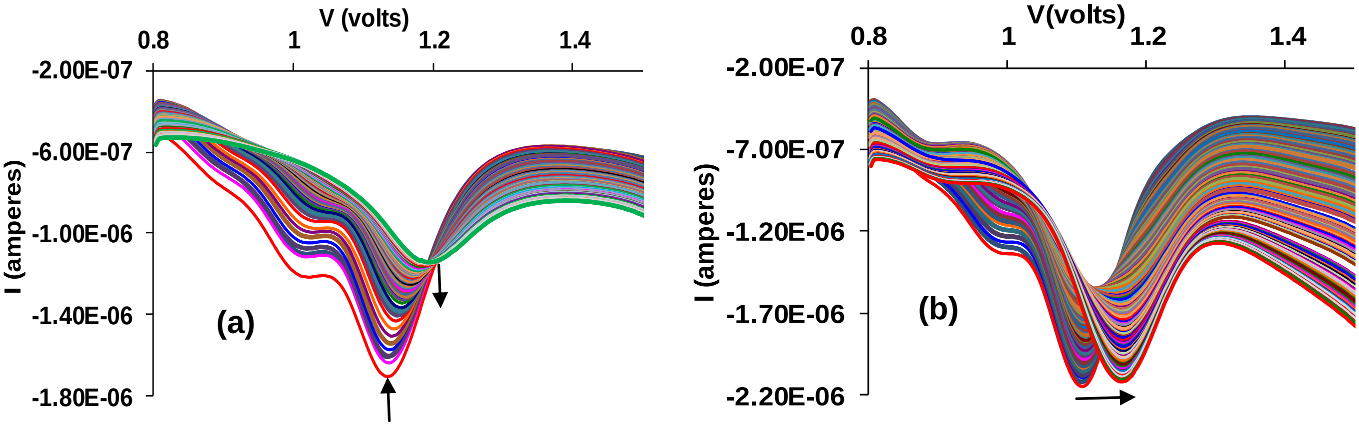

Fig. S12. Osteryoung square-wave voltammetry of **1**($1x10^{-4}$ M, in CH_3CN) upon addition of increased concentrations of **(a)** Hg^{2+} solution ($2x10^{-6}$ M to $1.2x10^{-4}$ M, in H_2O) and **(b)** Pb^{2+} solution ($2x10^{-6}$ M to $2x10^{-4}$ M, in H_2O).

Complete Reference for Gaussian (Reference 13 in manuscript)

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