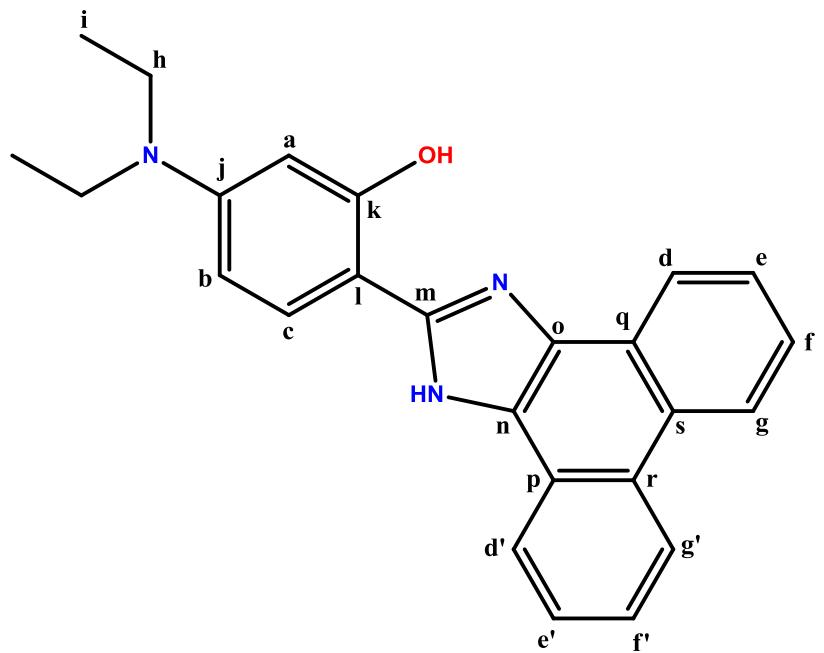


Supporting Information
For
**A Highly Sensitive ESIPT Based Ratiometric
Fluorescence Sensor for Selective Detection of Al³⁺**

Sanghamitra Sinha, Bijit Chowdhury and Pradyut Ghosh†*

†Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Kolkata 700032, India. *E-mail:* icpg@iacs.res.in

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1H

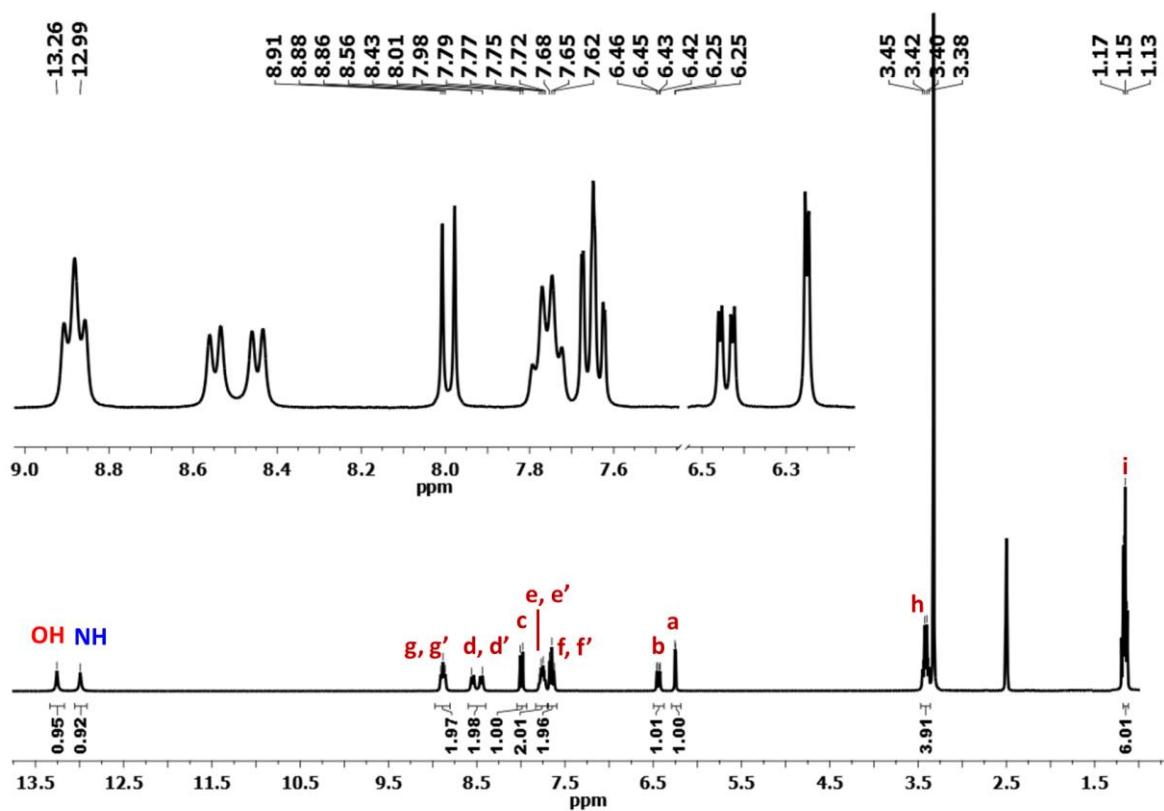


Figure S1: ^1H -NMR (300 MHz) spectrum of **1H** in $\text{DMSO}-d_6$.

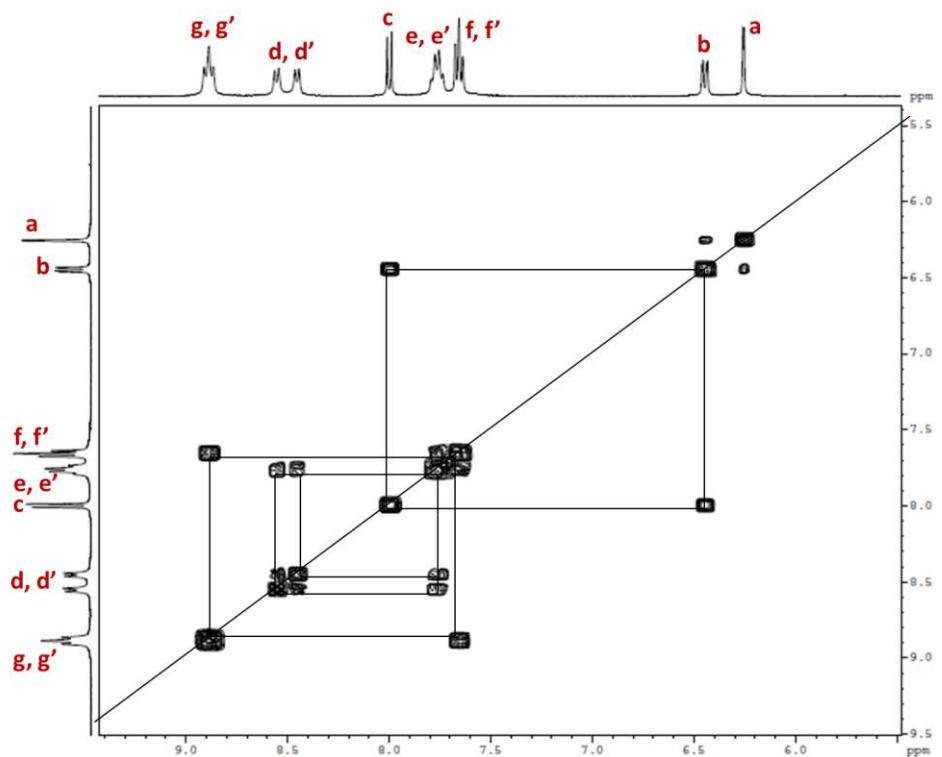


Figure S2: ^1H - ^1H COSY-NMR (400 MHz) spectrum of **1H** in $\text{DMSO}-d_6$.

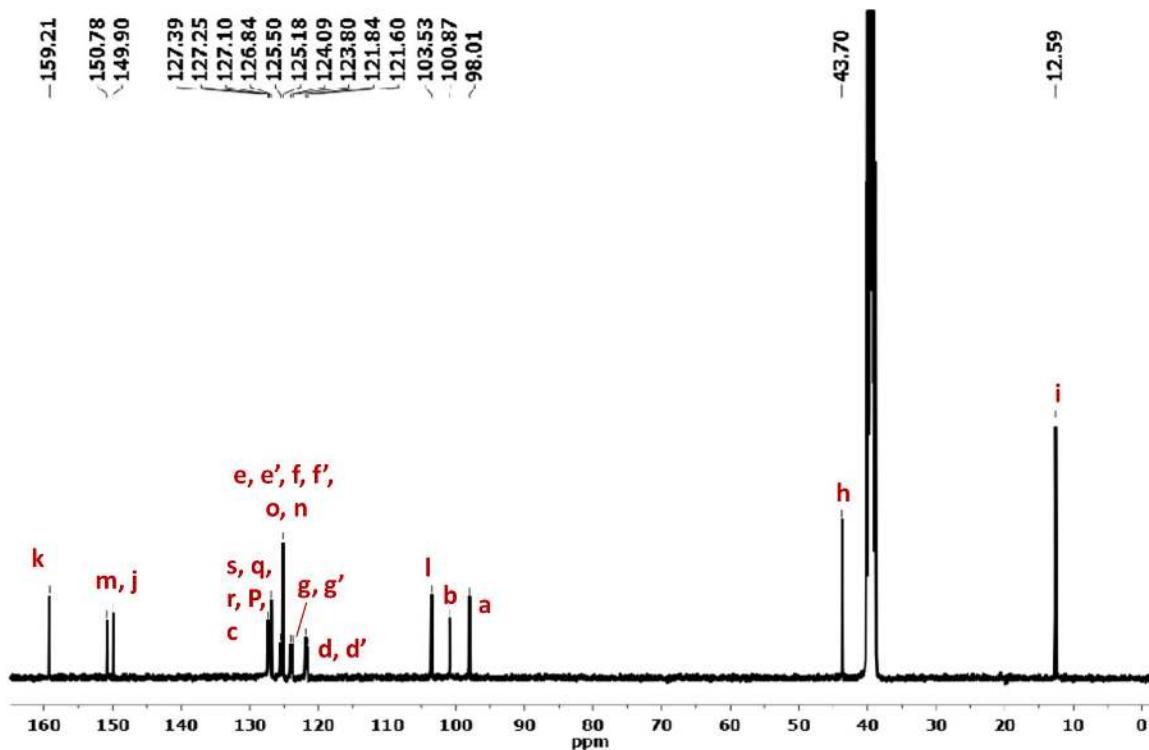


Figure S3: ^{13}C -NMR (100 MHz) spectrum of **1H** in $\text{DMSO}-d_6$.

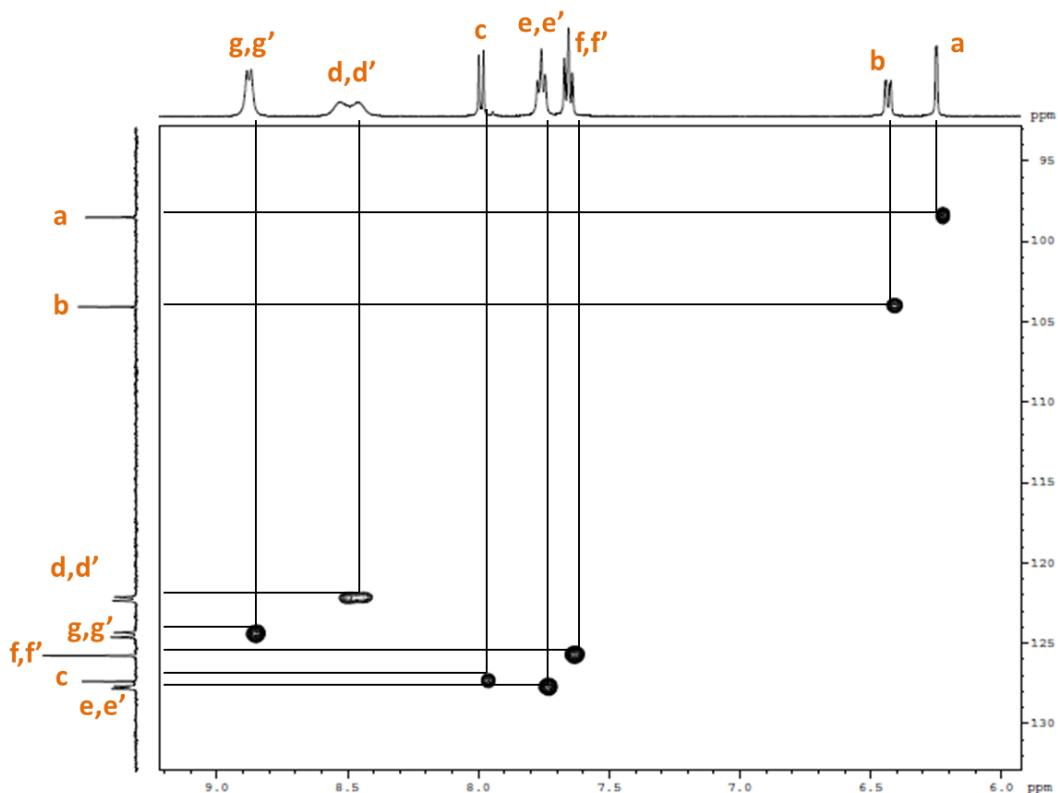


Figure S4: ^1H -DEPT-135 HSQC-NMR (400 MHz) spectrum of **1H** in $\text{DMSO}-d_6$.

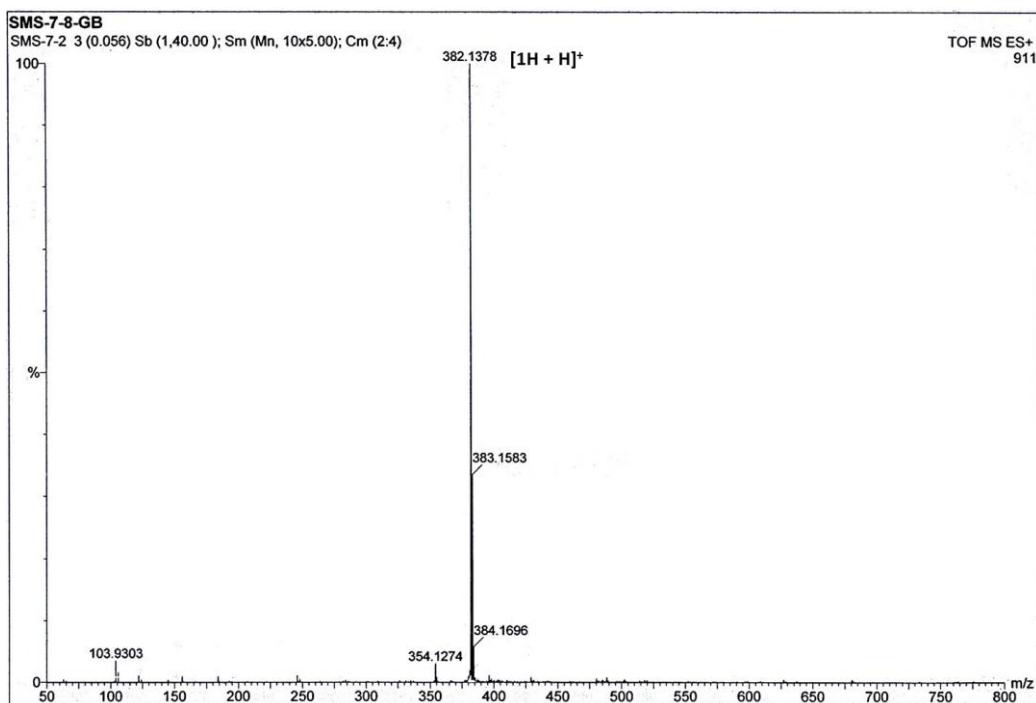
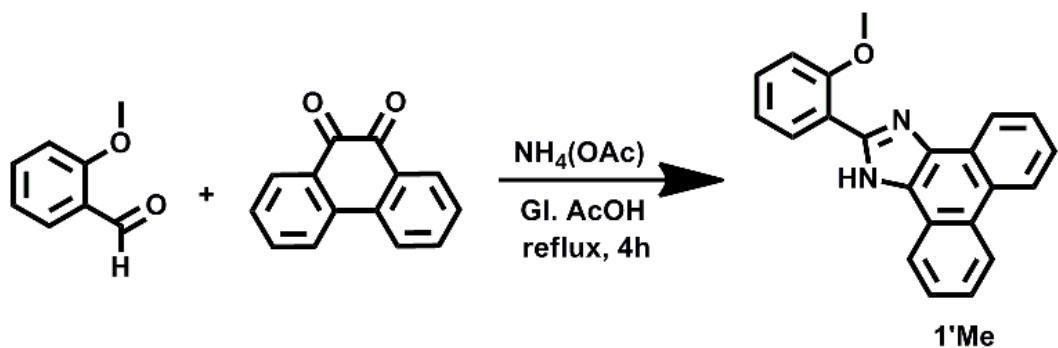


Figure S5: ESI-MS spectrum of **1H**.



Scheme S1. Synthetic scheme of $1'\text{Me}$.

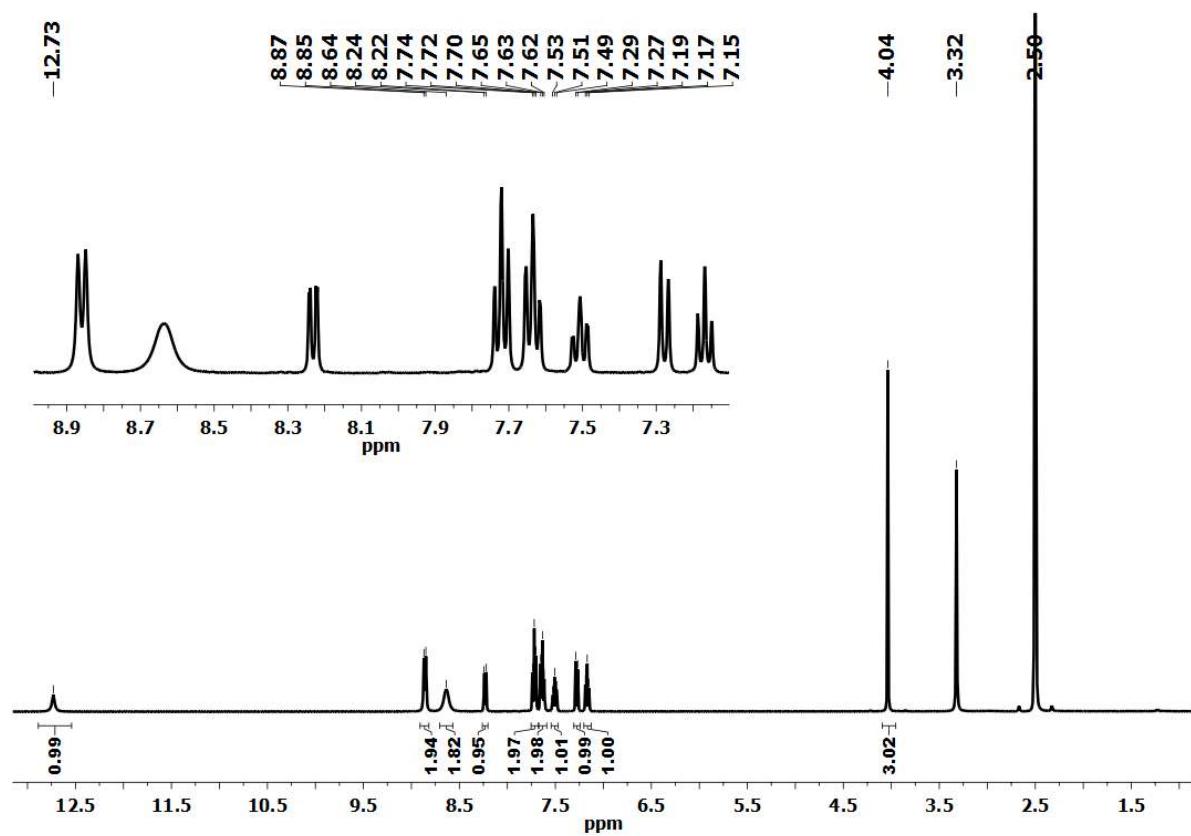


Figure S6: ^1H -NMR (500 MHz) spectrum of $1'\text{Me}$ in $\text{DMSO}-d_6$.

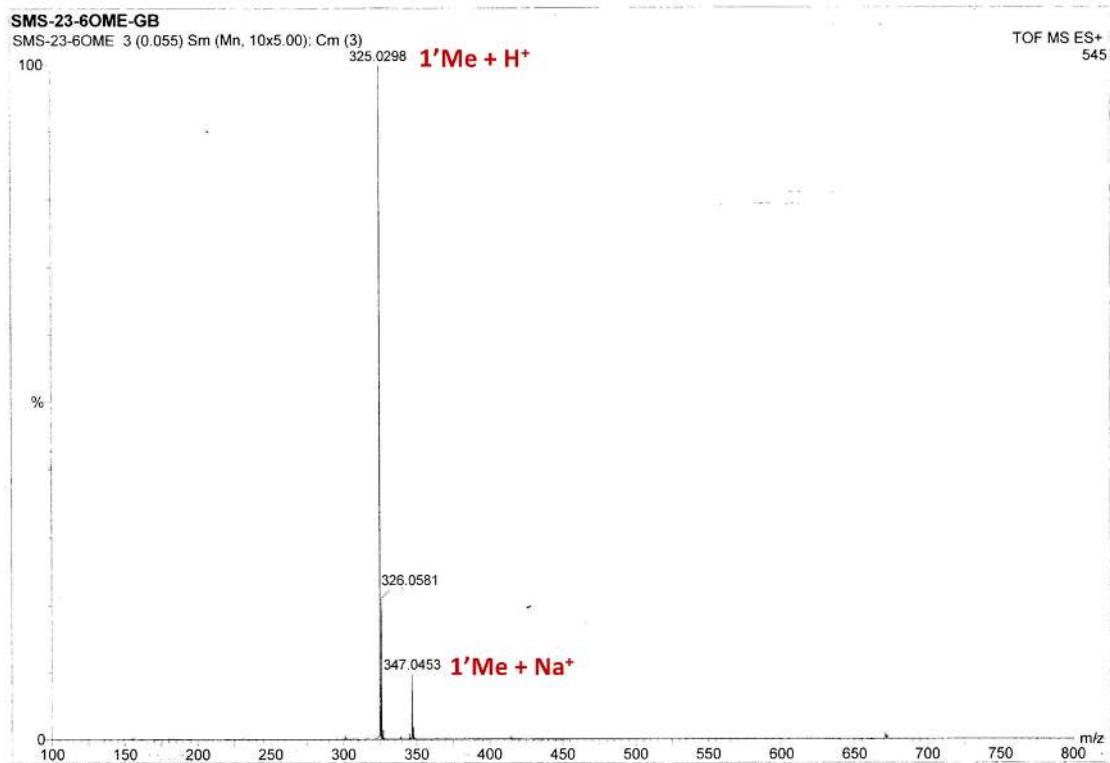


Figure S7: ESI-MS spectrum of **1'Me**.

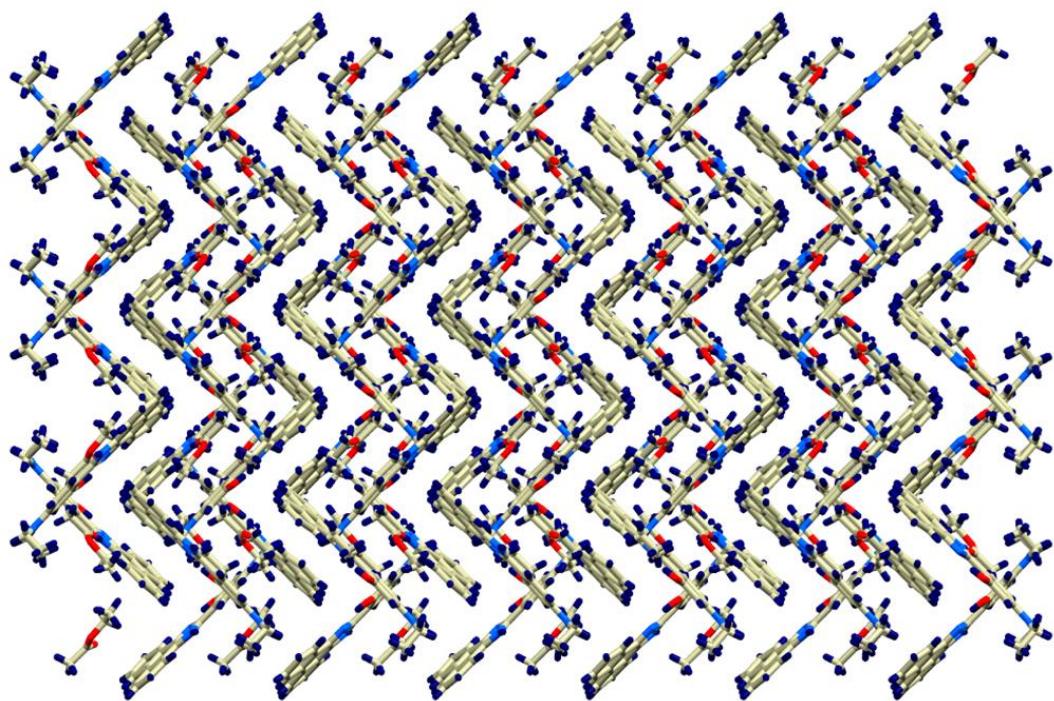


Figure S8: A slice of three-dimensional (3-D) crystal packing of **1H** obtained from ethyl acetate, along the crystallographic c axis.

Table S1: List of crystallographic parameter details of ligand **1H**.

Compound reference	1H
Chemical formula	C ₂₉ H ₃₁ N ₃ O ₃
Formula Mass	469.57
Crystal system	Orthorhombic
<i>a</i> /Å	20.07(3)
<i>b</i> /Å	12.235(16)
<i>c</i> /Å	20.36(3)
$\alpha/^\circ$	90.00
$\beta/^\circ$	90.00
$\gamma/^\circ$	90.00
Unit cell volume/Å³	4999(12)
Temperature/K	150(2)
Space group	<i>Pbca</i>
No. of formula units per unit cell, Z	8
Radiation type	MoKα
Absorption coefficient, μ/mm^{-1}	0.081
No. of reflections measured	21876
No. of independent reflections	2661
R_{int}	0.0923
Final R_I values ($I > 2\sigma(I)$)	0.0455
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1204
Final R_I values (all data)	0.0808
Final $wR(F^2)$ values (all data)	0.1477
Goodness of fit on F^2	0.960
CCDC number	1475692

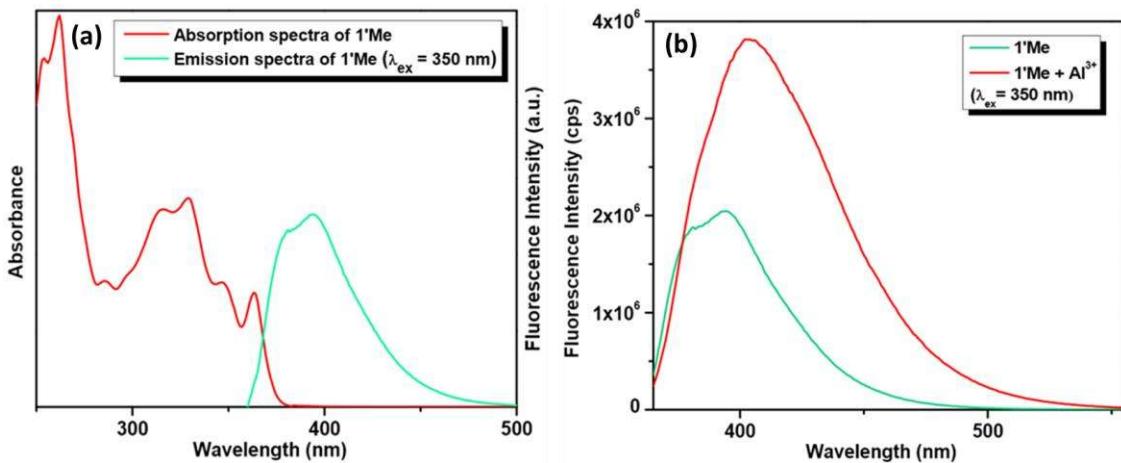


Figure S9: (a) UV-vis and PL spectra of **1'Me** and (b) emission spectral changes of **1'Me** in presence of Al^{3+} in acetonitrile at room temperature.

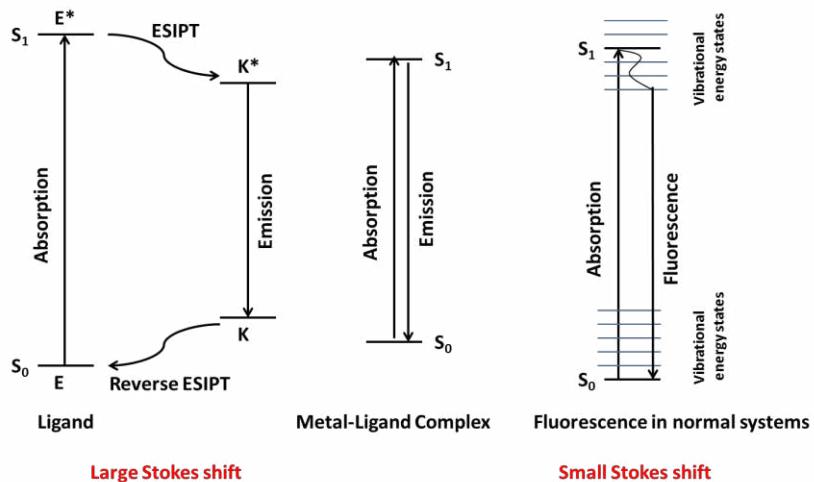


Chart S1: Schematic representation of ESIPT mechanism.

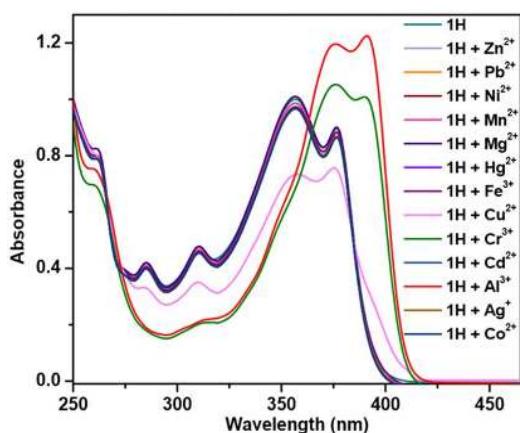


Figure S10: Changes in absorption spectrum of **1H** (20 μM) upon addition of various metal ions (10 equiv) in acetonitrile at room temperature.

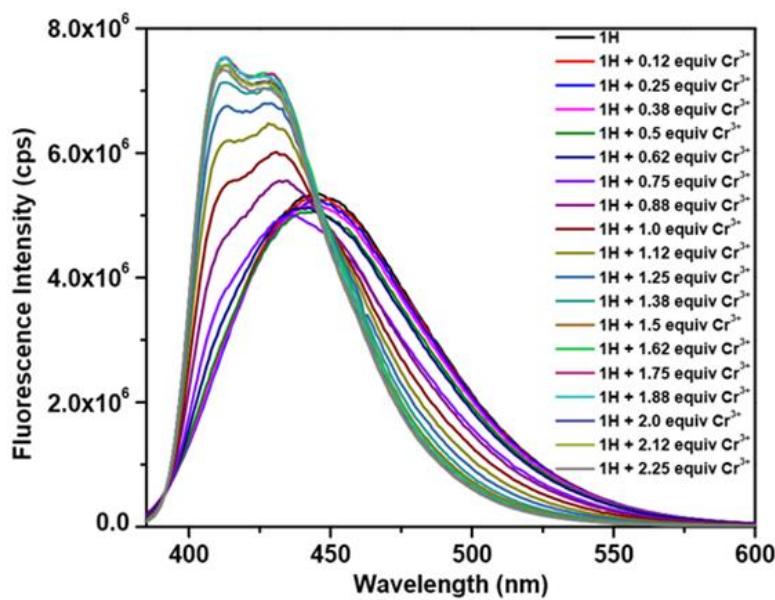


Figure S11: Fluorescence titration profile for **1H** (2.5 μM) with Cr^{3+} in acetonitrile at room temperature.

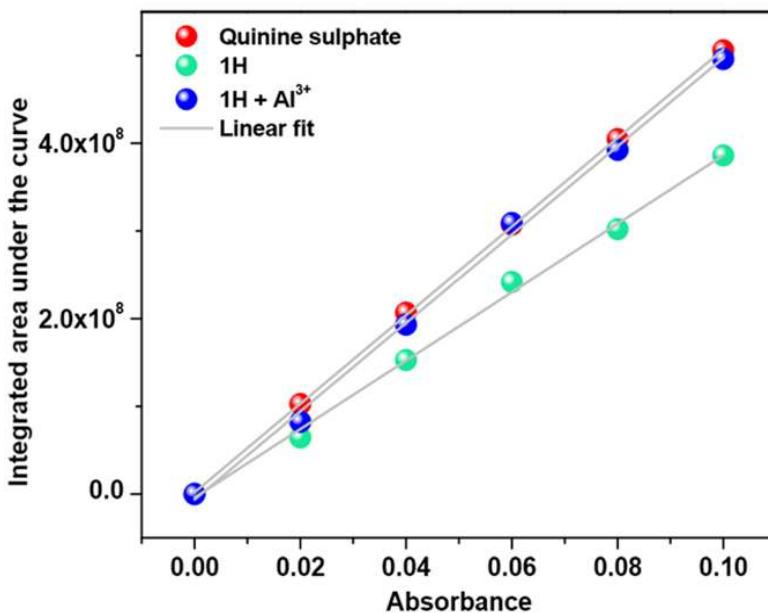


Figure S12: Plot of integrated emission intensity versus absorbance for calculation of quantum yield (ϕ_f) of **1H** and its Al^{3+} adduct in acetonitrile using quinine sulphate as standard (Considering the ϕ_f of quinine sulphate in 0.1M H_2SO_4 as 0.55 when the excitation wavelength is 366 nm).

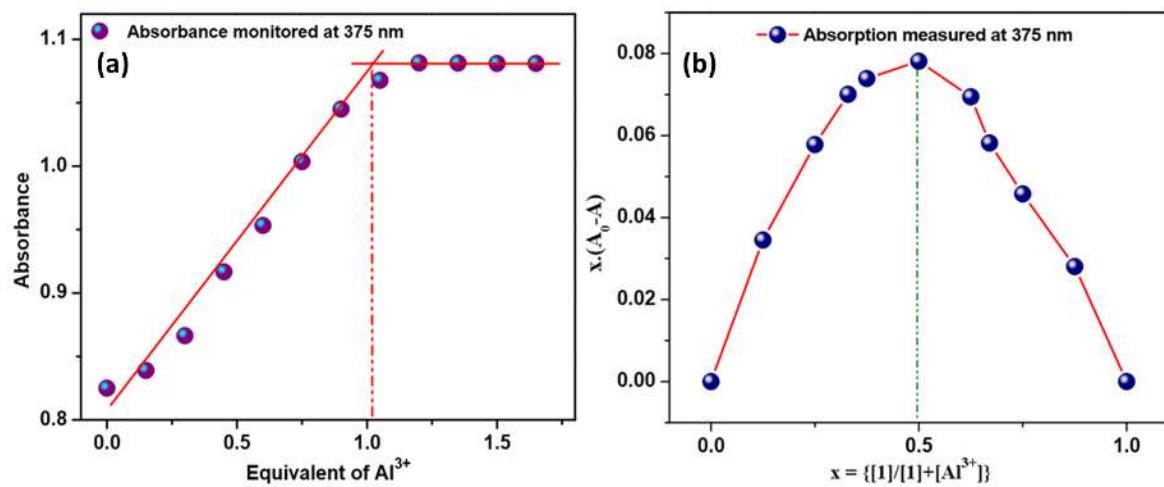


Figure S13: (a) An equivalent plot from UV-vis titration data and (b) Jobs plot of **1H** (20 μM) with Al^{3+} (20 μM) in acetonitrile at room temperature.

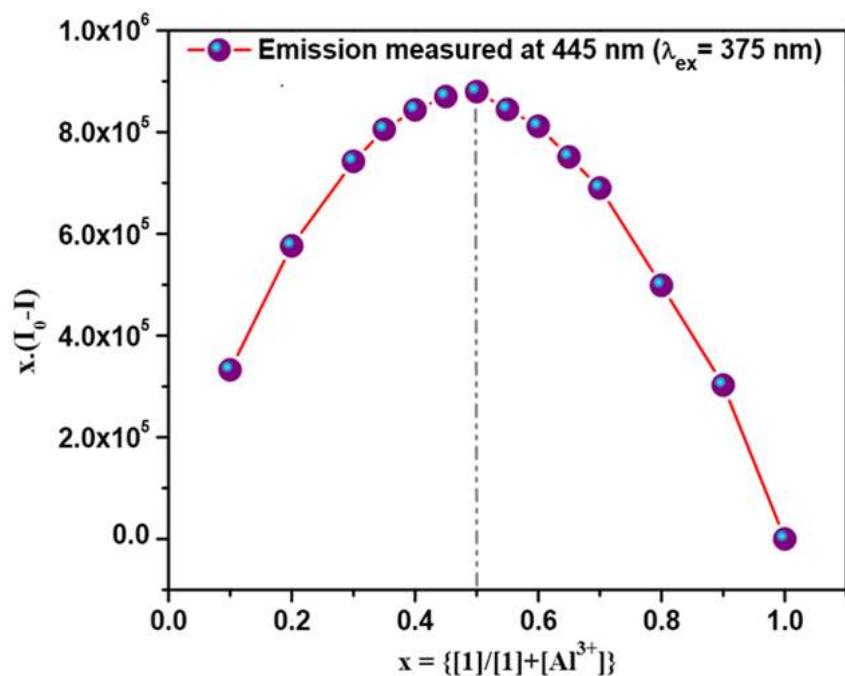


Figure S14. Fluorescence Jobs plot for **1H** (2.5 μM) with Al^{3+} (2.5 μM) in acetonitrile at room temperature.

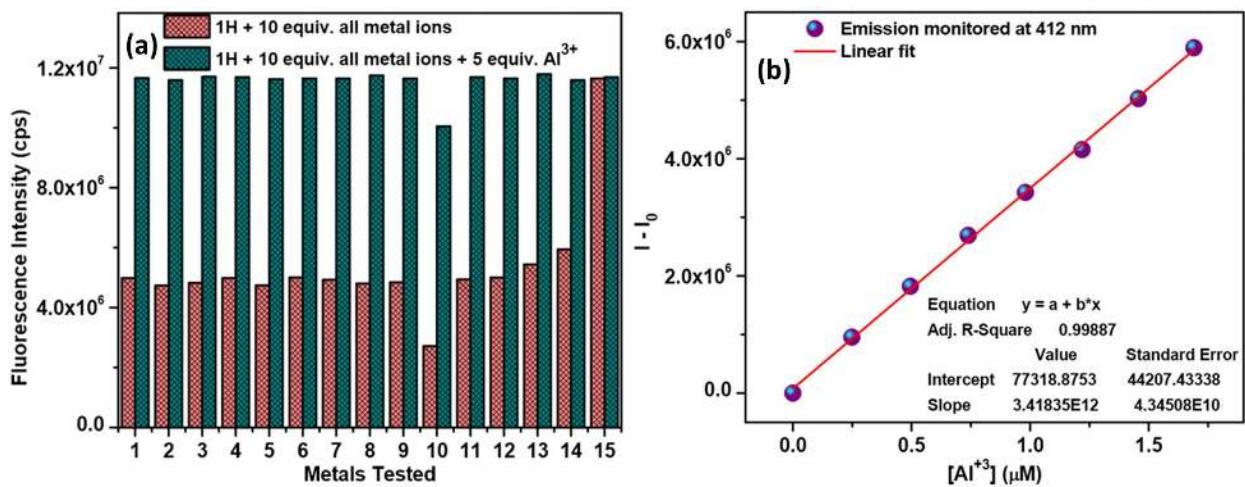


Figure S15: (a) Selectivity graph of **1H** with Al^{3+} in presence of other metal ions in acetonitrile ($\lambda_{\text{em}} = 412 \text{ nm}$ for Al^{3+} , Cr^{3+} , In^{3+} and 445 nm for other metal ions). Orange bars represent the fluorescence intensities of **1H** in presence of all metal ions (10 equiv) and green bars correspond to the same in presence of all metal ions and Al^{3+} . Codes used: (1) Only **1H** (2) Mg^{2+} (3) Ni^{2+} (4) Mn^{2+} (5) Cd^{2+} (6) Pb^{2+} (7) Zn^{2+} (8) Co^{2+} (9) Fe^{3+} (10) Cu^+ (11) Ag^+ (12) Hg^{2+} (13) In^{3+} (14) Cr^{3+} (15) Al^{3+} and (b) the calibration curve for Al^{3+} over the concentration range between 0 and $1.6 \mu\text{M}$ derived from the PL titration with **1H** ($2.5 \mu\text{M}$) in acetonitrile at room temperature.

Table S2: List of lifetimes of **1H** ($2.5 \mu\text{M}$, $\lambda_{\text{em}} = 445 \text{ nm}$) and in presence of various metal ions (1 equiv) in acetonitrile.

Entry	Life Time (ns)	Entry	Life Time (ns)
1H	5.37	1H + 1 equiv Cd^{2+}	5.33
1H + 1 equiv Al^{3+}	1.14	1H + 1 equiv Cr^{3+}	5.56
1H + 1 equiv Cu^{2+}	5.50	1H + 1 equiv Fe^{3+}	5.61
1H + 1 equiv Zn^{2+}	5.46	1H + 1 equiv Mg^{2+}	5.38
1H + 1 equiv Co^{2+}	5.39	1H + 1 equiv Hg^{2+}	5.57
1H + 1 equiv Ni^{2+}	5.38	1H + 1 equiv Ag^+	5.40
1H + 1 equiv Pb^{2+}	5.42		

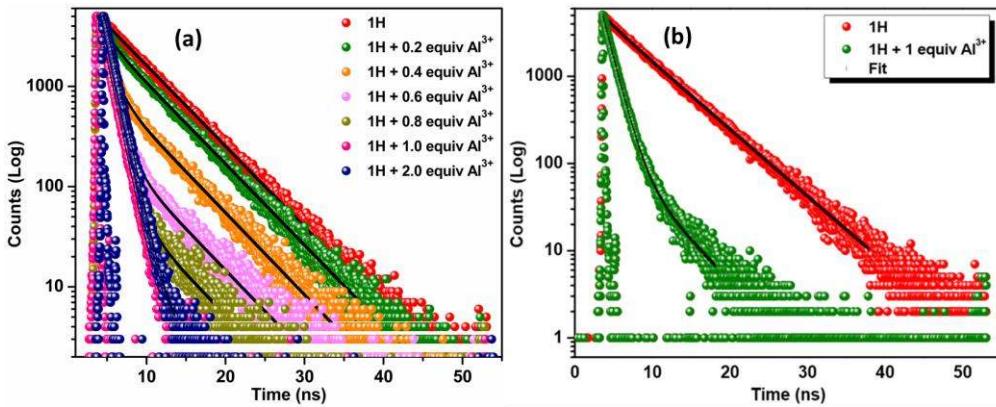


Figure S16: Time-resolved luminescence decays of **1H** ($2.5 \mu\text{M}$) (a) at $\lambda_{\text{em}} = 412 \text{ nm}$ and (b) at $\lambda_{\text{em}} = 525 \text{ nm}$, upon addition of increasing amount of Al³⁺ in acetonitrile at room temperature.

Table S3: List of lifetimes of **1H** with increasing amount Al³⁺.

Equiv of Al ³⁺	λ_{em}	A ₁ (%)	t ₁ (ns)	A ₂ (%)	t ₂ (ns)	T _{avg} (ns)	χ^2
1	445	100	5.37	-	-	5.37	1.14
	412	100	5.38	-	-	5.38	1.15
1 + 0.2 equiv Al³⁺	445	11.7	1.62	88.3	5.43	4.98	1.03
	412	37.9	1.17	62.1	5.36	3.40	1.11
1 + 0.4 equiv Al³⁺	445	58.8	1.17	41.2	5.37	2.90	1.12
	412	80.0	1.12	20.0	5.3	1.96	1.12
1 + 0.6 equiv Al³⁺	445	77.8	1.14	22.2	5.37	2.08	1.07
	412	91.9	1.13	8.1	5.32	1.47	1.04
1 + 0.8 equiv Al³⁺	445	88.7	1.13	11.3	5.35	1.61	1.13
	412	94.9	1.13	5.1	5.3	1.34	1.18
1 + 1.0 equiv Al³⁺	445	98.2	1.13	1.8	5.36	1.20	1.19
	412	96.1	1.10	3.9	2.02	1.14	1.06
1 + 2.0 equiv Al³⁺	445	100	1.14	-	-	1.14	1.19
	412	100	1.13	-	-	1.13	1.11

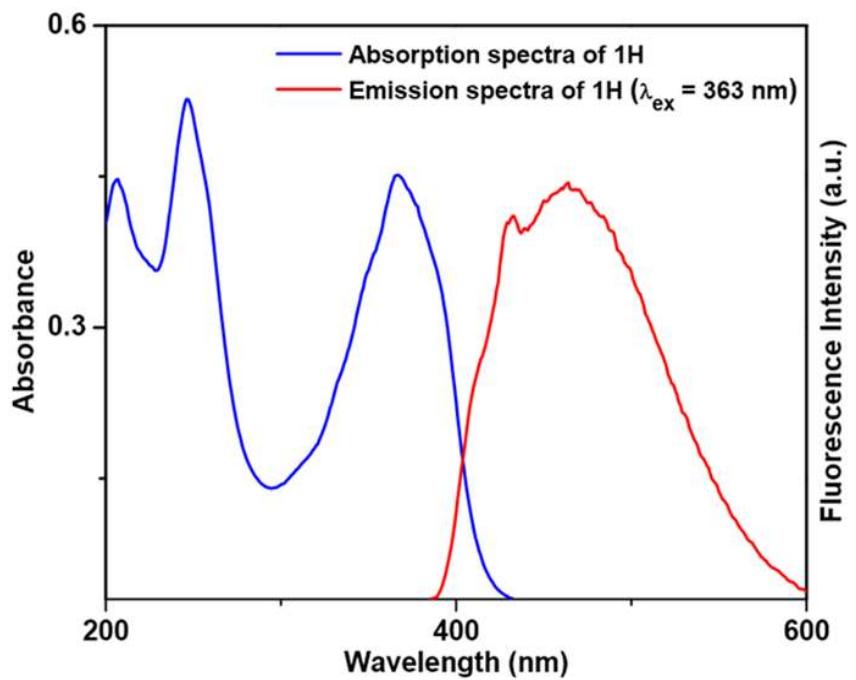


Figure S17: UV-vis and fluorescence spectra of **1H**, measured in H₂O/acetonitrile (9:1 v/v) solvent at room temperature (concentrations: 20 μ M and 2.5 μ M respectively).

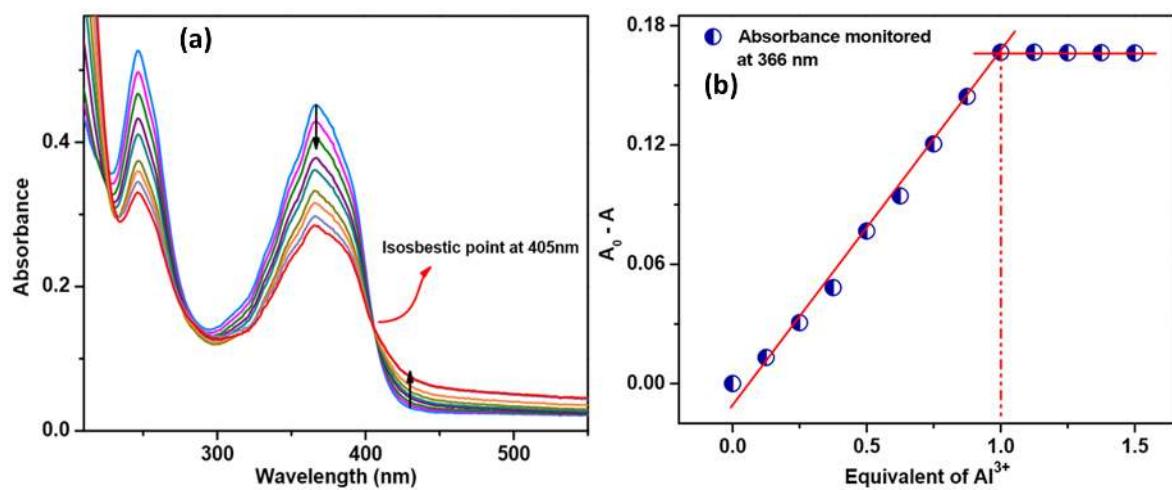


Figure S18: UV-vis (a) titration profile and (b) corresponding equivalent plot for **1H** (20 μ M) with Al³⁺ in H₂O/acetonitrile (9:1 v/v) solvent at room temperature.

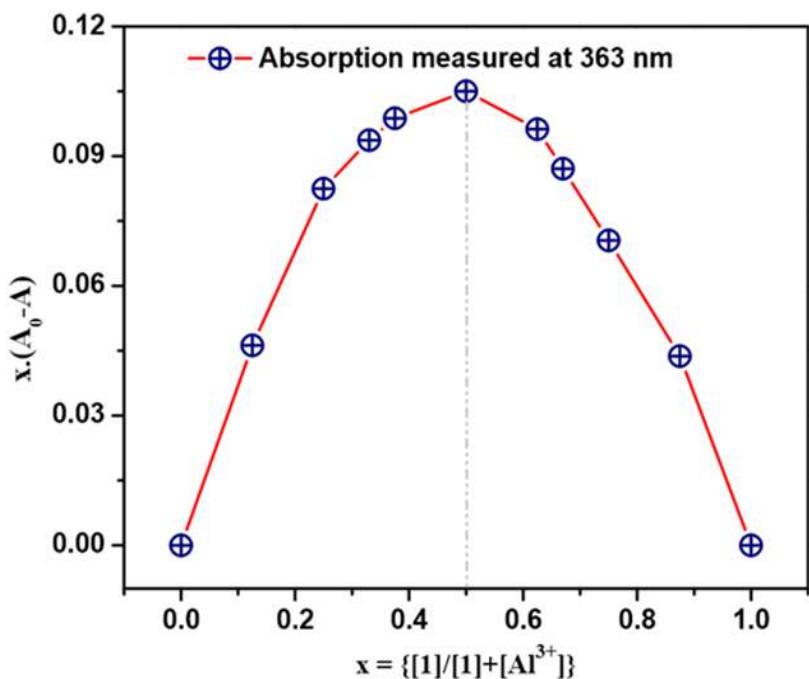


Figure S19: UV-vis Job's plot for **1H** (20 μM) with Al^{3+} (20 μM) in $\text{H}_2\text{O}/\text{acetonitrile}$ (9:1 v/v) solvent at room temperature.

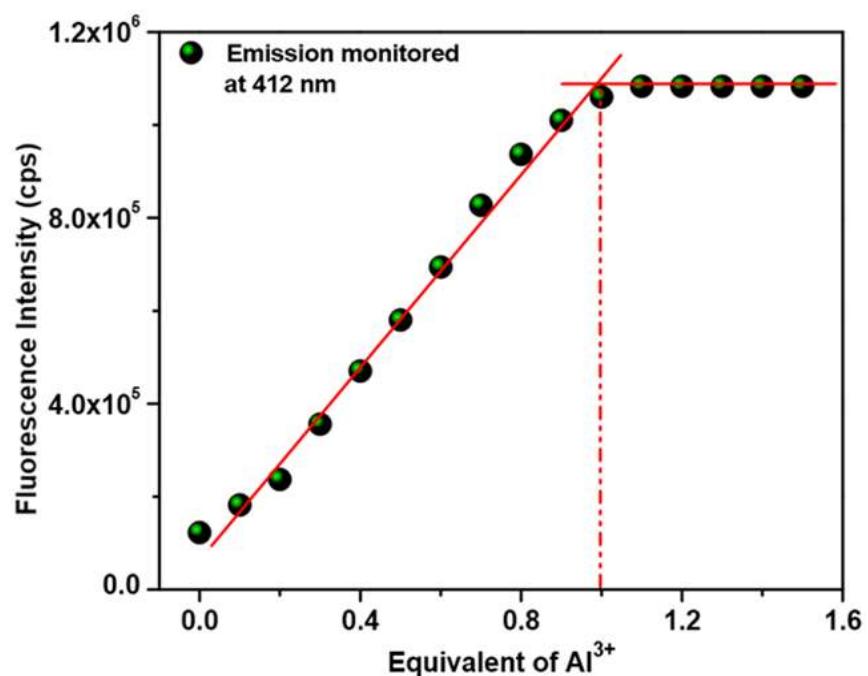


Figure S20: An equivalent plot from fluorescence titration data of **1H** (2.5 μM) with Al^{3+} in $\text{H}_2\text{O}/\text{acetonitrile}$ (9:1 v/v) solvent at room temperature.

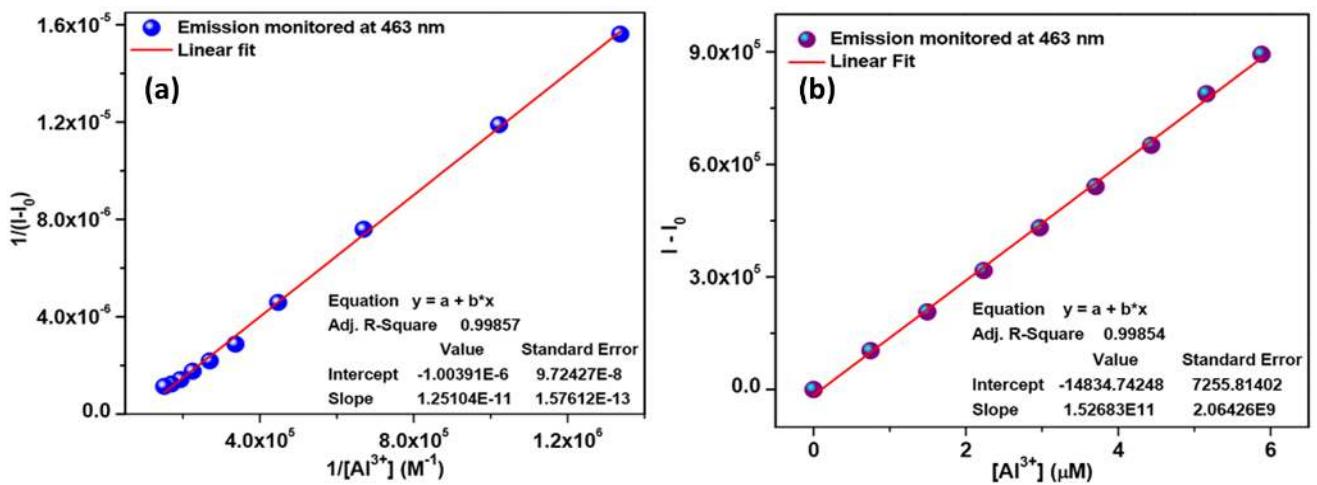


Figure S21: (a) Benesi-Hildebrand Plot and (b) calibration curve for fluorescence titration of **1H** with Al^{3+} in H_2O /acetonitrile (9:1 v/v) solvent at room temperature.

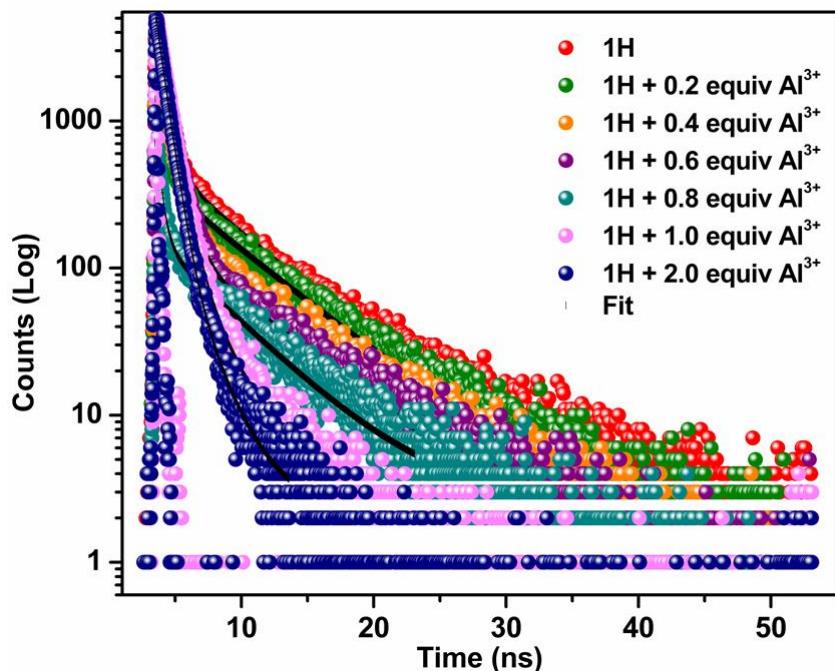


Figure S22: Time-resolved luminescence decays of **1H** ($\lambda_{em} = 465$ nm) upon addition of increasing amount of Al^{3+} in H_2O /acetonitrile (9:1 v/v) at room temperature.

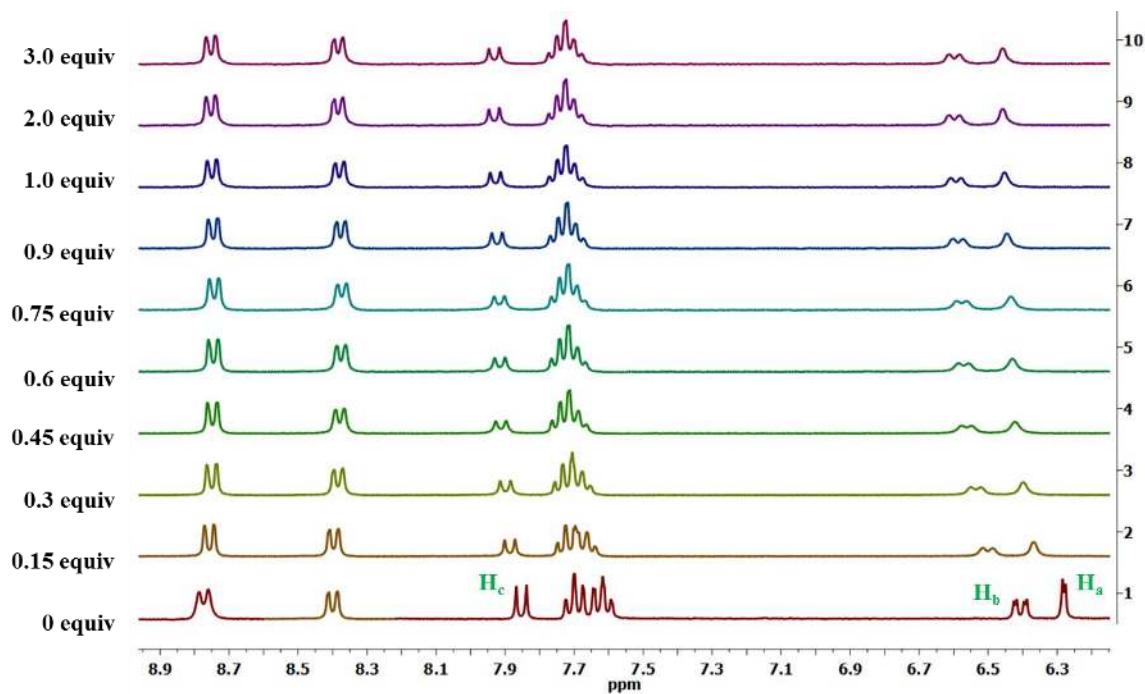


Figure S23: Changes in ^1H -NMR spectra (300 MHz) of **1H** (8 mM) upon addition of increasing amounts of Al^{3+} in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (1:1 v/v) solvent at room temperature.

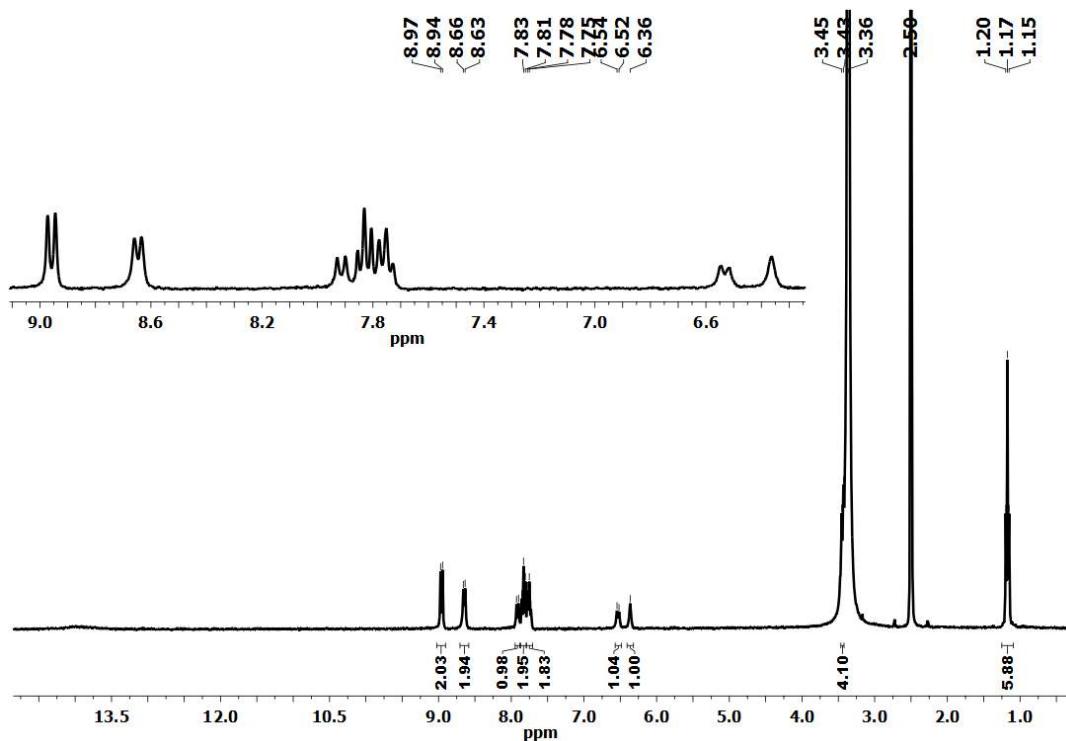


Figure S24: ^1H -NMR spectrum of $[\text{Al}(1)(\text{OH})]_2^{2+}$ in $\text{DMSO}-d_6$ (300 MHz).

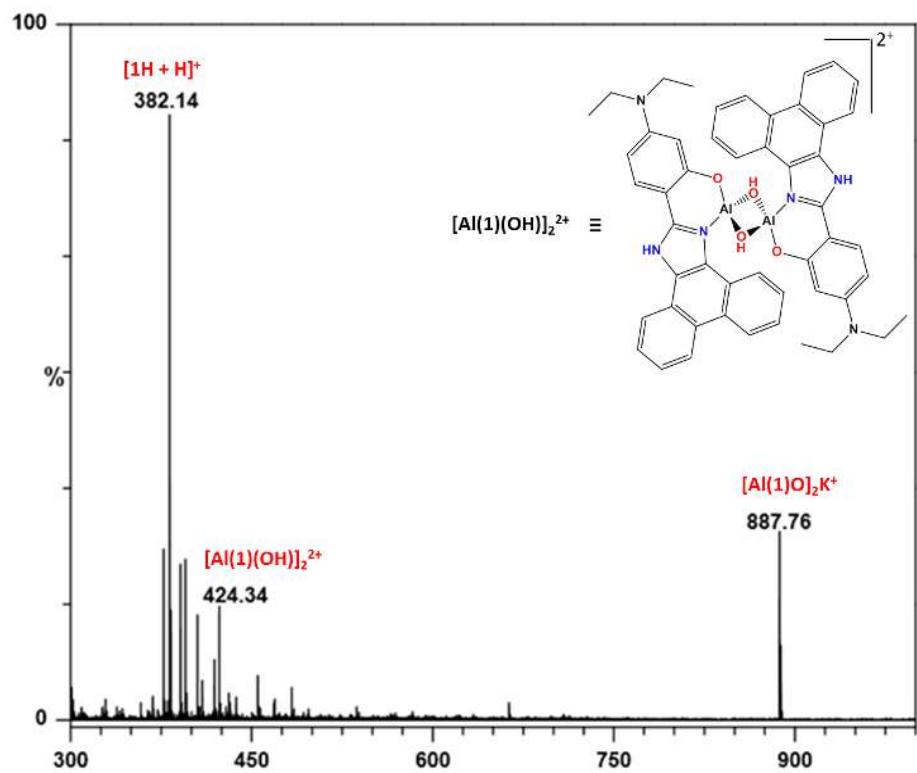


Figure S25: ESI-MS spectra of the Al^{3+} adduct of **1H**.

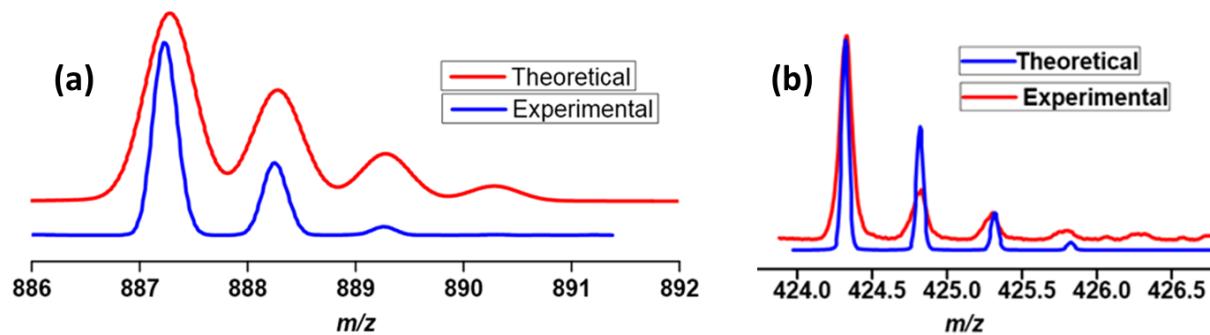


Figure S26: Isotopic distribution pattern of (a) $[\text{Al}(1)\text{O}]_2\text{K}^+$ and (b) $[\text{Al}(1)(\text{OH})]_2^{2+}$ species (in the ESI-MS spectra of the isolated Al^{3+} adduct of **1H**) with its corresponding simulated pattern.

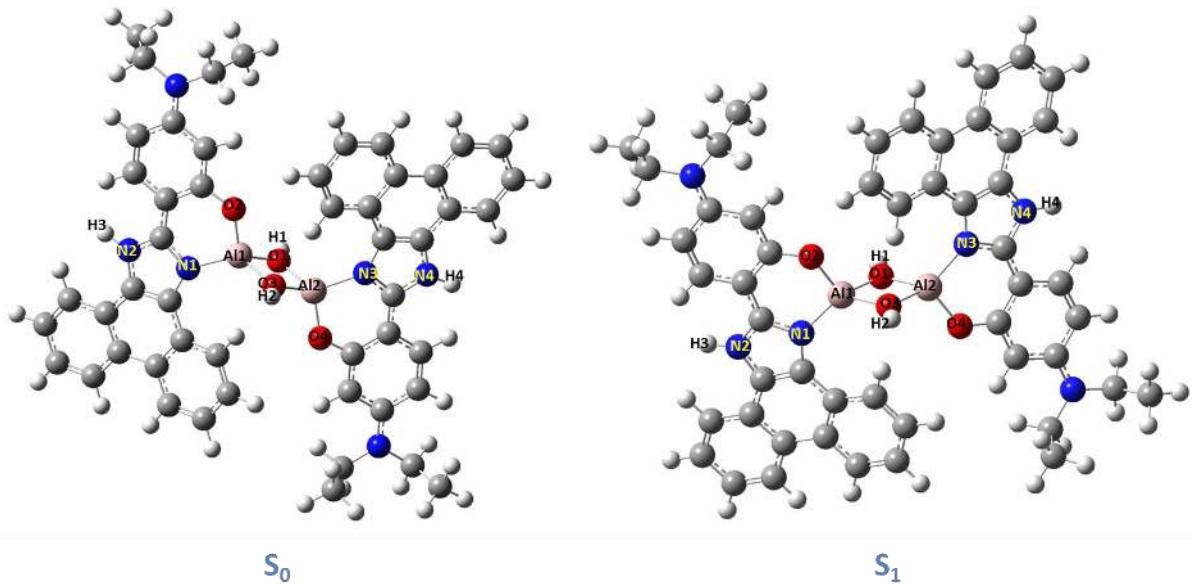


Figure S27. Theoretically (DFT B3LYP/6-311G(d); CPCM for acetonitrile) optimized structures of the ground state (S_0) and first excited state (S_1) of $[\text{Al}(\mathbf{1})(\text{OH})]_2^{2+}$.

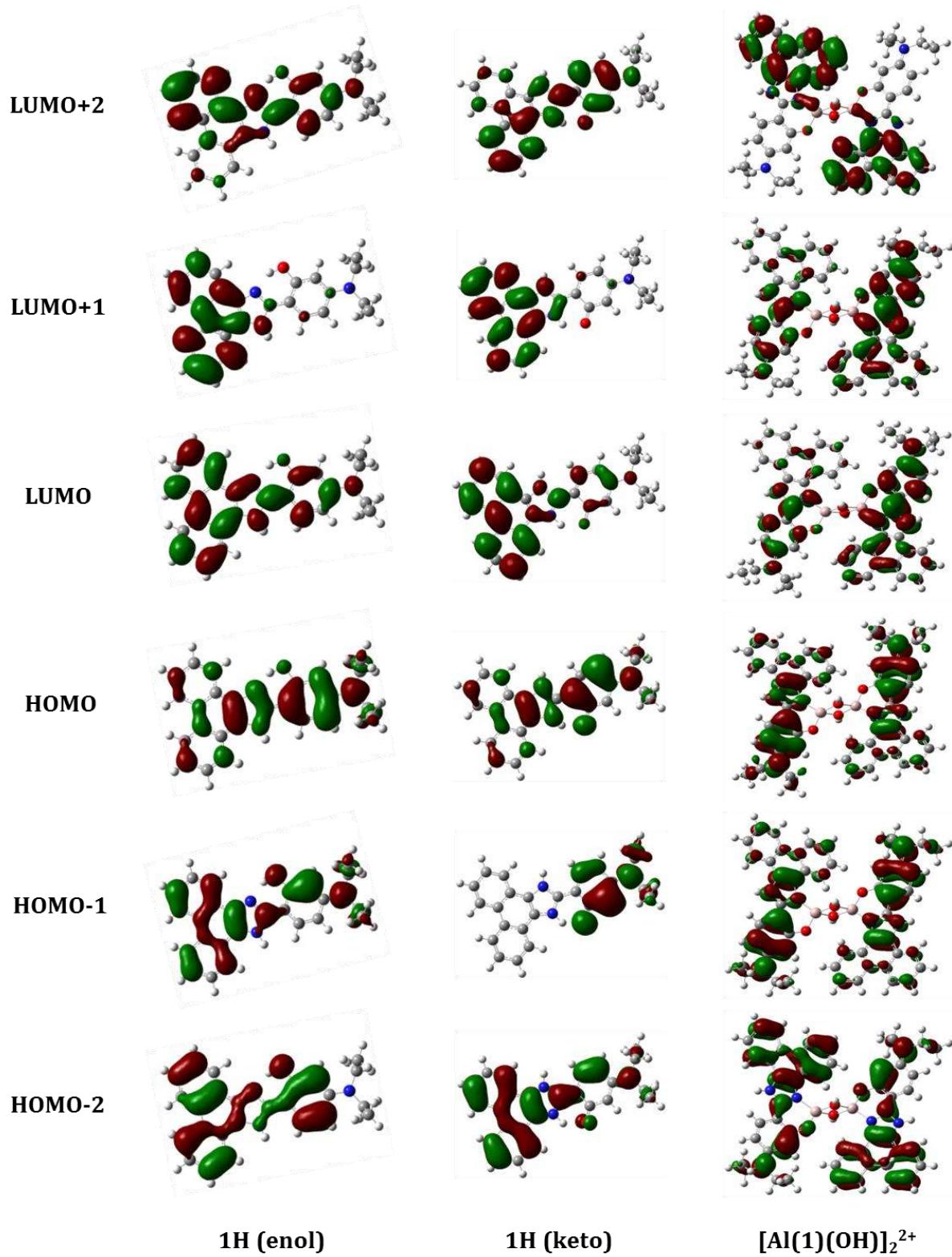


Figure S28. Selected MOs of **1H(enol)**, **1H(keto)** and **[Al(1)(OH)]₂²⁺** as obtained from the DFT B3LYP/6-311G(d) level of computation using CPCM model to encounter the solvent effect of acetonitrile [isovalue = 0.02].

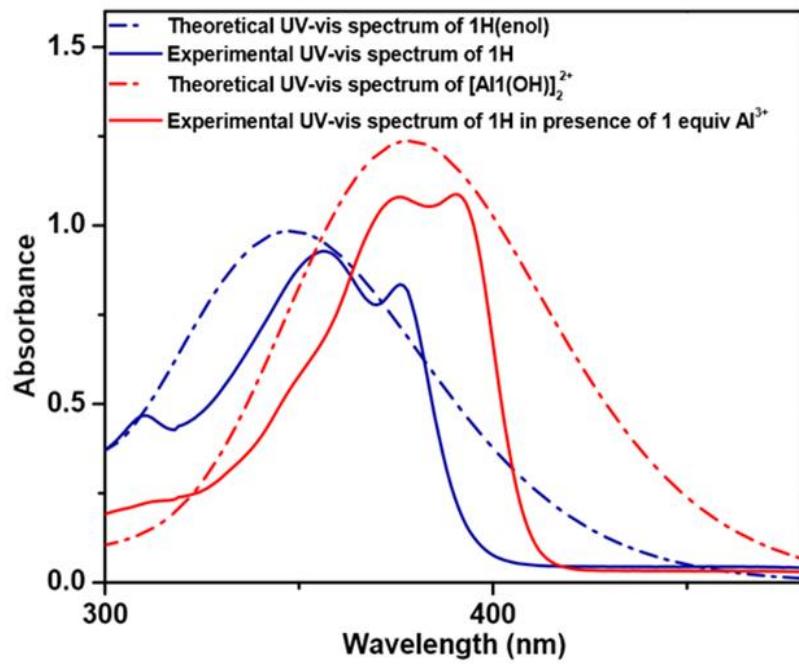


Figure S29: Theoretical (energy calculation by TD-DFT B3LYP/6-311G(d) level of computation (no of states = 26) using CPCM model for acetonitrile) and experimental UV-vis ($20 \mu M$) spectra of **1H** and $[Al(1)(OH)]_2^{2+}$.

Table S4. Main calculated optical transitions for **1H** and $[Al(1)(OH)]_2^{2+}$.

Entry	Computed vertical excitation		Experimentally observed transition		Corresponding MOs	Oscillator strength (<i>f</i>)
	Energy (eV)	λ_{ex} (nm)	Energy (eV)	λ_{ex} (nm)		
1H (enol)	3.5540	348.9	3.4925	355	HOMO \rightarrow LUMO+1	0.6789
	3.3075	374.9	3.3062	375	HOMO \rightarrow LUMO	0.3298
$[Al(1)(OH)]_2^{2+}$	3.3041	375.2	3.1791	390	HOMO \rightarrow LUMO	0.7542
	3.2456	382.0	3.1791	390	HOMO \rightarrow LUMO+1	0.0035
	3.3756	367.3	3.3062	375	HOMO-1 \rightarrow LUMO+1	0.0270
	3.3729	367.6	3.3062	375	HOMO-1 \rightarrow LUMO	0.0162

Table S5. The main geometric parameters for ground state (S_0) and first excited state (S_1) of $[Al(1)(OH)]_2^{2+}$.

Entry	Bond angles (degree)		Entry	Bond lengths (Å)	
	S_0	S_1		S_0	S_1
Al1-O1-Al2	101.23	101.23	Al1-O1	1.832	1.83
Al1-O3-Al2	100.61	100.61	Al1-O3	1.837	1.84
O1-Al1-O3	79.08	79.08	Al1-O2	1.723	1.72
O1-Al2-O3	79.06	79.07	Al2-O1	1.829	1.83
H1-O1-Al1	129.32	129.3	Al2-O3	1.840	1.84
H2-O3-Al2	129.58	129.6	Al2-O4	1.722	1.72
O2-Al1-N1	101.96	101.96	O1-H1	0.963	0.963
O4-Al2-N3	102.15	102.15	O3-H2	0.964	0.964
O2-Al1-O1	116.482	116.5	N2-H3	1.007	1.0074
O2-Al1-O3	113.2	113.2	N4-H4	1.0075	1.0075
O4-Al2-O3	113.1	113.1	N1-Al1	1.870	1.87
O4-Al2-O1	115.8	115.8	N3-Al2	1.870	1.87
N1-Al1-O1	118.66	118.66			
N1-Al1-O3	127.5	127.5			
N3-Al2-O1	119.9	119.9			
N3-Al2-O3	126.7	126.7			

Table S6: The (x,y,z) Cartesian coordinates of **1H**(enol), **1H**(keto) and $[\text{Al}(\mathbf{1})(\text{OH})]_2^{2+}$ calculated from Gaussian-09 at B3LYP/6-311G(d) computational level using CPCM for acetonitrile.

1H (enol)							
Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	x	y	z		x	y	z
C	4.31668	0.145	-0.18208	C	-4.59293	-3.45215	-0.11507
C	3.53706	1.32877	-0.09678	C	-5.79097	-2.72273	-0.0605
C	2.15684	1.26997	-0.06637	C	-5.76379	-1.34086	-0.0026
C	1.44046	0.06276	-0.10485	H	4.00532	2.30018	-0.0403
C	2.21506	-1.11326	-0.16811	H	1.58949	2.19096	-0.00204
C	3.60289	-1.07586	-0.19753	H	4.12485	-2.02303	-0.24021
N	5.69658	0.18165	-0.26468	H	6.04215	-1.85748	-0.57951
C	6.47528	-1.034	-0.00999	H	7.46716	-0.89288	-0.43443
C	6.3705	1.48606	-0.14669	H	5.862	2.18018	-0.81838
C	7.8491	1.4893	-0.52276	H	6.25277	1.89044	0.86921
C	6.59321	-1.40946	1.47125	H	8.20004	2.52401	-0.52055
O	1.55311	-2.3144	-0.19592	H	8.47331	0.93546	0.18097
C	-0.01693	0.08499	-0.06709	H	8.0121	1.086	-1.52545
N	-0.80657	-1.04072	-0.09536	H	7.18383	-2.32299	1.58424
C	-2.1195	-0.63145	-0.04785	H	7.08796	-0.61781	2.04031
C	-2.061	0.75438	0.00863	H	5.61268	-1.58412	1.92036
N	-0.75767	1.18795	-0.00383	H	2.1767	-3.0493	-0.24042
C	-3.33826	-1.37407	-0.05278	H	-0.43635	-1.97823	-0.14293
C	-4.551	-0.61738	0.00406	H	-6.65744	1.16107	0.12696
C	-4.51119	0.84971	0.06599	H	-6.55524	3.58677	0.22658
C	-3.26123	1.53926	0.06806	H	-4.35826	4.76461	0.22783
C	-5.68429	1.63606	0.12498	H	-2.26161	3.44059	0.12694
C	-5.63287	3.01703	0.18215	H	-2.46008	-3.34951	-0.15454
C	-4.39532	3.68101	0.18311	H	-4.61482	-4.53589	-0.16011
C	-3.22708	2.9471	0.12688	H	-6.74367	-3.24166	-0.06357
C	-3.38499	-2.78368	-0.11144	H	-6.70855	-0.81346	0.03781

1H (keto)							
Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	x	y	z		x	y	z
C	-4.35853	-0.12484	0.00759	C	4.61765	-3.55692	0.23184
C	-3.643	-1.36991	0.05484	C	5.79973	-2.80065	0.18979
C	-2.2721	-1.3798	0.04992	C	5.74503	-1.4224	0.1004
C	-1.50329	-0.19493	-0.00501	H	-4.16934	-2.31328	0.07365
C	-2.18568	1.09383	-0.06312	H	-1.77496	-2.34579	0.07946
C	-3.60938	1.05691	-0.04677	H	-4.09001	2.02645	-0.06117
O	-1.54928	2.20356	-0.11593	H	-6.02945	-2.00216	0.88651
N	-5.73617	-0.11609	0.00944	H	-7.46529	-1.04547	0.67076
C	-6.53047	-1.33426	0.18356	H	-5.97832	1.77504	-0.85865
C	-6.4956	1.12409	-0.15074	H	-7.44707	0.86633	-0.62287
C	-6.84096	-2.06554	-1.12602	H	-7.46122	-2.94593	-0.93355
C	-6.76003	1.86509	1.16398	H	-7.38479	-1.41657	-1.81783
C	-0.08618	-0.20972	-0.00299	H	-5.92715	-2.39672	-1.62458
N	0.77557	-1.26558	0.06155	H	-7.34748	2.76933	0.97967
C	2.08623	-0.80154	0.03991	H	-7.32078	1.23717	1.86174
C	2.01781	0.57133	-0.04148	H	-5.82768	2.1598	1.65021
N	0.67664	0.90784	-0.06632	H	0.49118	-2.22973	0.11872
C	3.32171	-1.5123	0.09101	H	0.14952	1.79676	-0.11096
C	4.51626	-0.72756	0.04788	H	6.58294	1.09432	-0.06821
C	4.44534	0.73368	-0.0455	H	6.42617	3.51378	-0.2199
C	3.18063	1.39678	-0.08883	H	4.20484	4.64019	-0.29087
C	5.5999	1.5464	-0.09599	H	2.14498	3.29175	-0.2087
C	5.51698	2.92343	-0.18274	H	2.48515	-3.5069	0.21817
C	4.26567	3.55944	-0.22312	H	4.66329	-4.63817	0.3028
C	3.11271	2.80291	-0.17674	H	6.76297	-3.29774	0.22836
C	3.39562	-2.91836	0.18328	H	6.67825	-0.87491	0.0723

$[\text{Al}(\text{1})(\text{OH})_2]^{2+}$							
Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	x	y	z		x	y	z
C	6.24224	-1.24051	0.15304	C	2.56636	8.3289	-1.16671
C	6.69114	0.08714	-0.12215	C	1.46596	7.63427	-0.70106
C	5.81041	1.13761	-0.16102	Al	1.33278	0.48772	0.45611
C	4.42045	0.98003	0.05753	O	-0.03092	0.04931	1.61147
C	3.97044	-0.34003	0.32691	O	0.00961	0.03745	-0.72387
C	4.85432	-1.4075	0.36402	Al	-1.34706	-0.41988	0.41874
N	7.11397	-2.28886	0.22123	C	-6.20027	1.2546	-0.42469
C	6.64433	-3.65107	0.50636	C	-6.59145	-0.07118	-0.78371
C	8.54975	-2.10835	-0.03854	C	-5.70087	-1.11218	-0.72172
C	8.93125	-2.06281	-1.52132	C	-4.36037	-0.94977	-0.29624
C	6.10508	-4.40981	-0.71019	C	-3.96777	0.36868	0.05944
O	2.66476	-0.60002	0.53963	C	-4.86415	1.42474	0.00478
C	3.53047	2.10728	0.01288	N	-7.06934	2.3038	-0.51039
N	3.91599	3.35519	-0.33229	C	-6.66229	3.66119	-0.1227
C	2.84865	4.22688	-0.24591	C	-8.45834	2.11281	-0.95202
C	1.77114	3.48683	0.17747	C	-9.41405	1.61866	0.13824
N	2.18653	2.14519	0.31206	C	-6.71421	3.9384	1.38308
C	2.80027	5.62094	-0.5469	O	-2.70702	0.63674	0.45836
C	1.5417	6.26327	-0.37009	C	-3.47047	-2.07453	-0.20471
C	0.39971	5.51134	0.15616	N	-3.81886	-3.33789	-0.53346
C	0.51002	4.11456	0.45171	C	-2.7606	-4.19773	-0.31627
C	-0.83651	6.13831	0.42298	C	-1.72941	-3.43433	0.17526
C	-1.90321	5.4511	0.96978	N	-2.16104	-2.09215	0.22084
C	-1.7734	4.09273	1.28714	C	-2.68037	-5.60232	-0.55538
C	-0.58358	3.44242	1.02991	C	-1.44426	-6.23028	-0.2303
C	3.91594	6.34288	-1.01775	C	-0.35789	-5.4502	0.36783
C	3.80263	7.68335	-1.32375	C	-0.49723	-4.04234	0.58928

C	0.84941	-6.05758	0.77542	H	4.66373	8.23274	-1.68734
C	1.86046	-5.34038	1.38601	H	2.47053	9.381	-1.41162
C	1.7011	-3.96927	1.6259	H	0.53163	8.16969	-0.59635
C	0.53868	-3.33839	1.23156	H	-7.59915	-0.2832	-1.10842
C	-3.74295	-6.34854	-1.10468	H	-6.07013	-2.08886	-1.01217
C	-3.59882	-7.70015	-1.34109	H	-4.481	2.39068	0.29807
C	-2.38432	-8.33302	-1.03401	H	-5.66004	3.85606	-0.5114
C	-1.33565	-7.61393	-0.49236	H	-7.32332	4.35413	-0.64448
H	7.73591	0.29326	-0.30065	H	-8.80539	3.0736	-1.33398
H	6.22707	2.11884	-0.35687	H	-8.47092	1.43258	-1.80643
H	4.42049	-2.37824	0.55232	H	-10.4138	1.47876	-0.28203
H	7.48651	-4.19715	0.93342	H	-9.0904	0.66432	0.55936
H	5.88855	-3.60763	1.2938	H	-9.49121	2.33901	0.9553
H	8.89516	-1.20625	0.47145	H	-6.07577	3.25321	1.94493
H	9.06614	-2.93785	0.44562	H	-6.37139	4.95731	1.5832
H	10.00872	-1.90486	-1.62081	H	-7.73166	3.84459	1.76781
H	8.68122	-2.99908	-2.02442	H	-4.73067	-3.60961	-0.86447
H	8.42356	-1.25107	-2.04686	H	0.99623	-7.11882	0.6254
H	5.746	-5.39558	-0.40185	H	2.77001	-5.84532	1.69183
H	5.27331	-3.88239	-1.18229	H	2.47842	-3.40403	2.12672
H	6.88265	-4.55649	-1.4627	H	0.41955	-2.28981	1.4652
H	4.84829	3.60245	-0.62342	H	-4.68047	-5.86251	-1.35196
H	-0.96298	7.19184	0.21229	H	-4.41891	-8.26813	-1.76579
H	-2.83441	5.97049	1.167	H	-2.26443	-9.3942	-1.22262
H	-2.59508	3.55259	1.74249	H	-0.41588	-8.13948	-0.27253
H	-0.49098	2.40665	1.32561	H	0.02644	0.02587	-1.68626
H	4.87159	5.84673	-1.14719	H	-0.04691	0.06094	2.57488