RSC Advance

Electronic Supplementary Information

Photophysical Property *vs* Medium: Mononuclear, Dinuclear and Trinuclear Zn(II) Complexes†

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Mass spectra

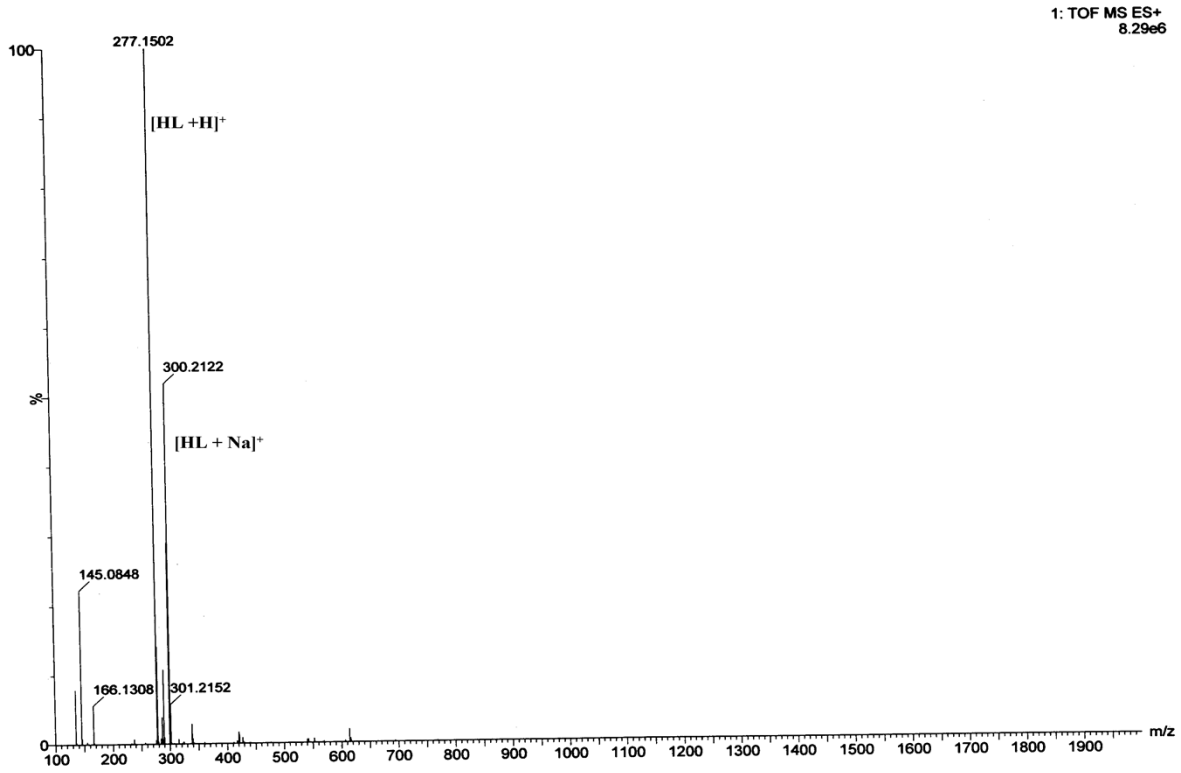


Fig. S1 High-resolution mass spectrum of a solution containing **HL** in acetonitrile. The solution was diluted with acetonitrile prior to spectral acquisition.

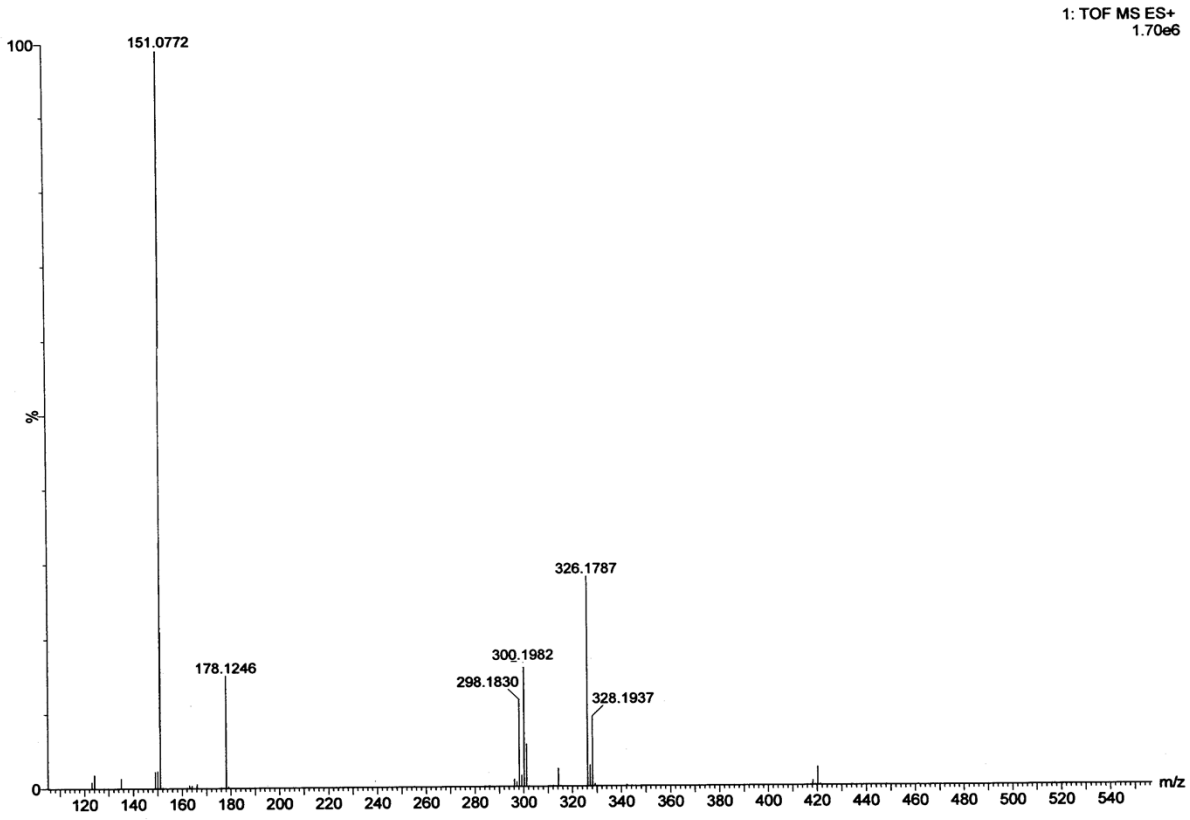


Fig. S2 High-resolution mass spectrum of a solution containing (**A**) in acetonitrile. The solution was diluted with acetonitrile prior to spectral acquisition.

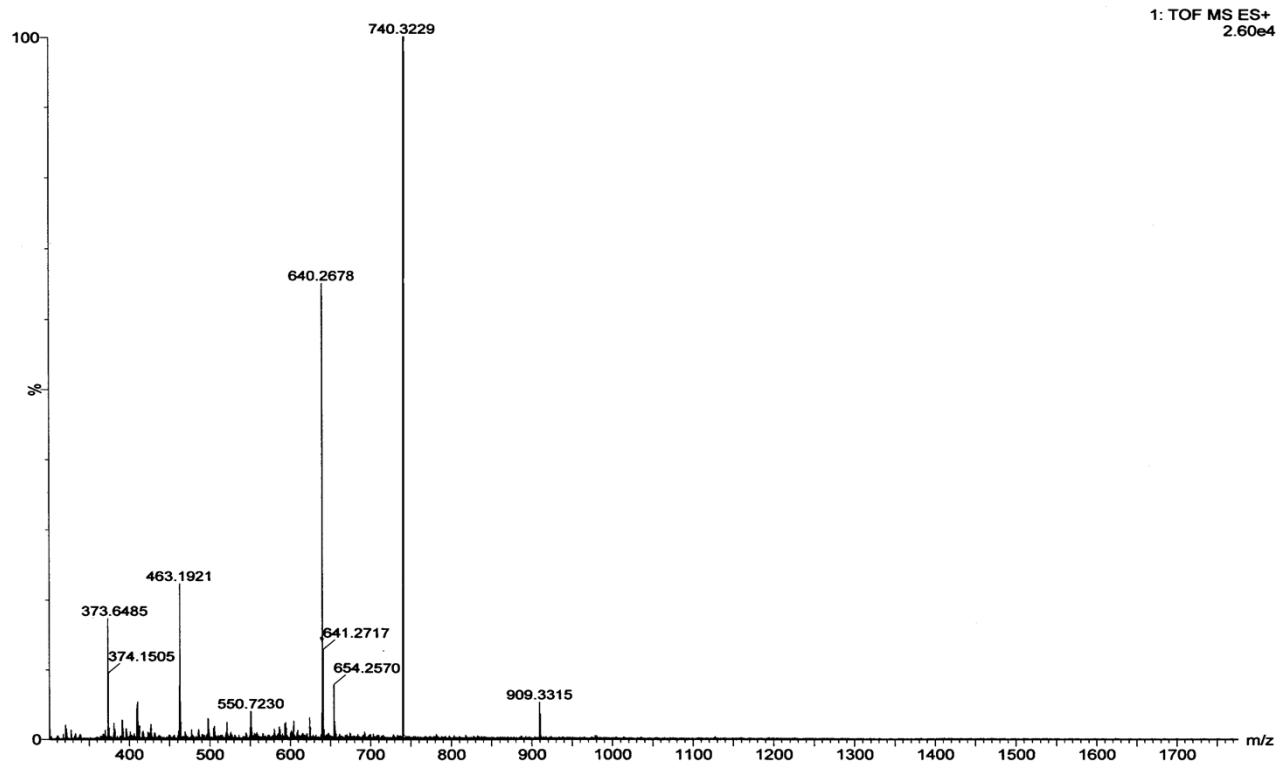


Fig. S3 High-resolution mass spectrum of a solution containing dinuclear complex **1** in acetonitrile. The solution was diluted with acetonitrile prior to spectral acquisition.

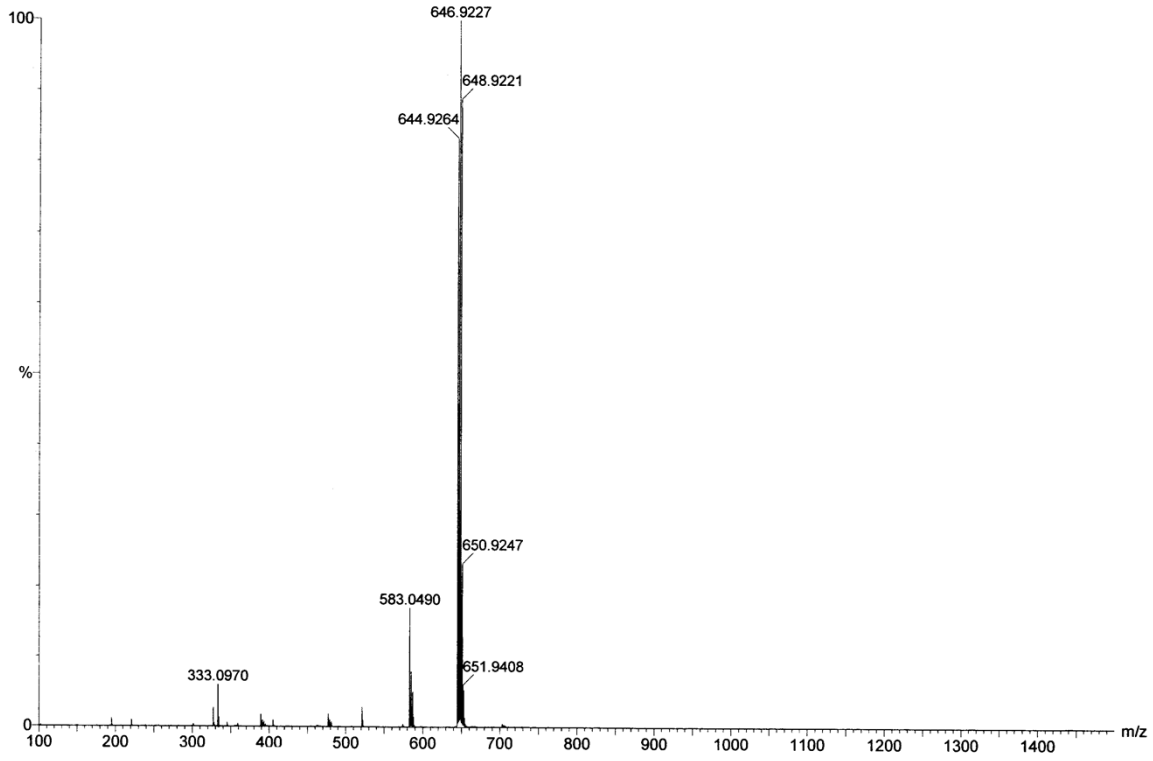


Fig. S4 High-resolution mass spectrum of a solution containing tri-nuclear complex **2** in acetonitrile. The solution was diluted with acetonitrile prior to spectral acquisition.

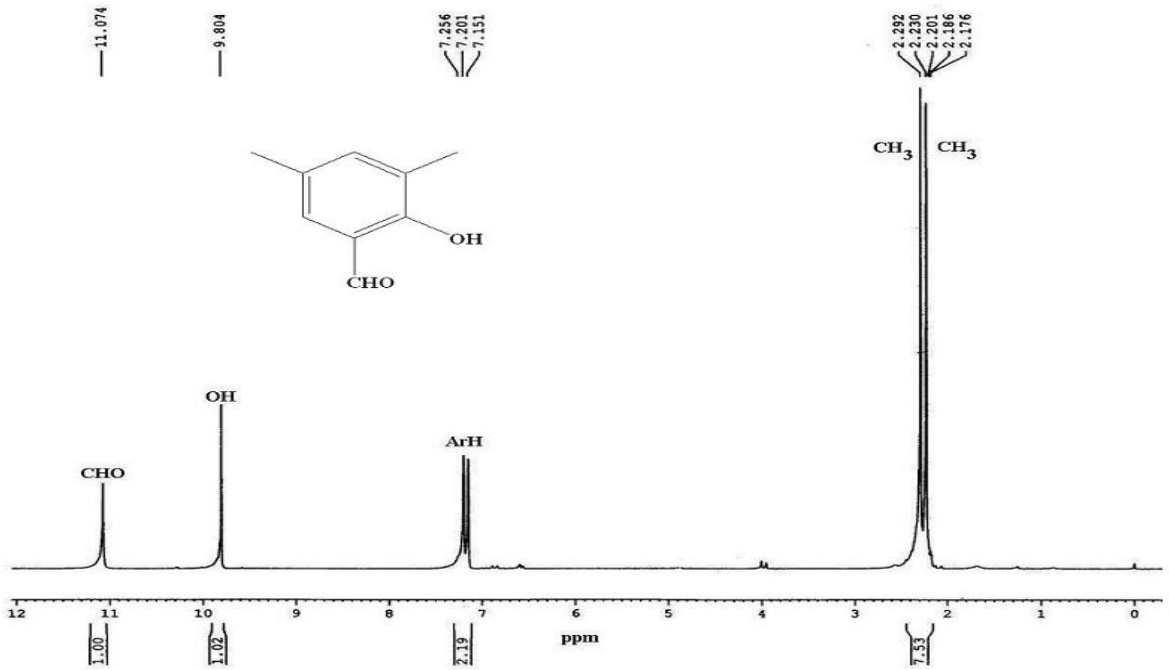


Fig. S5 The ^{1}H NMR spectra of aldehyde (A) in $CDCl_3$.

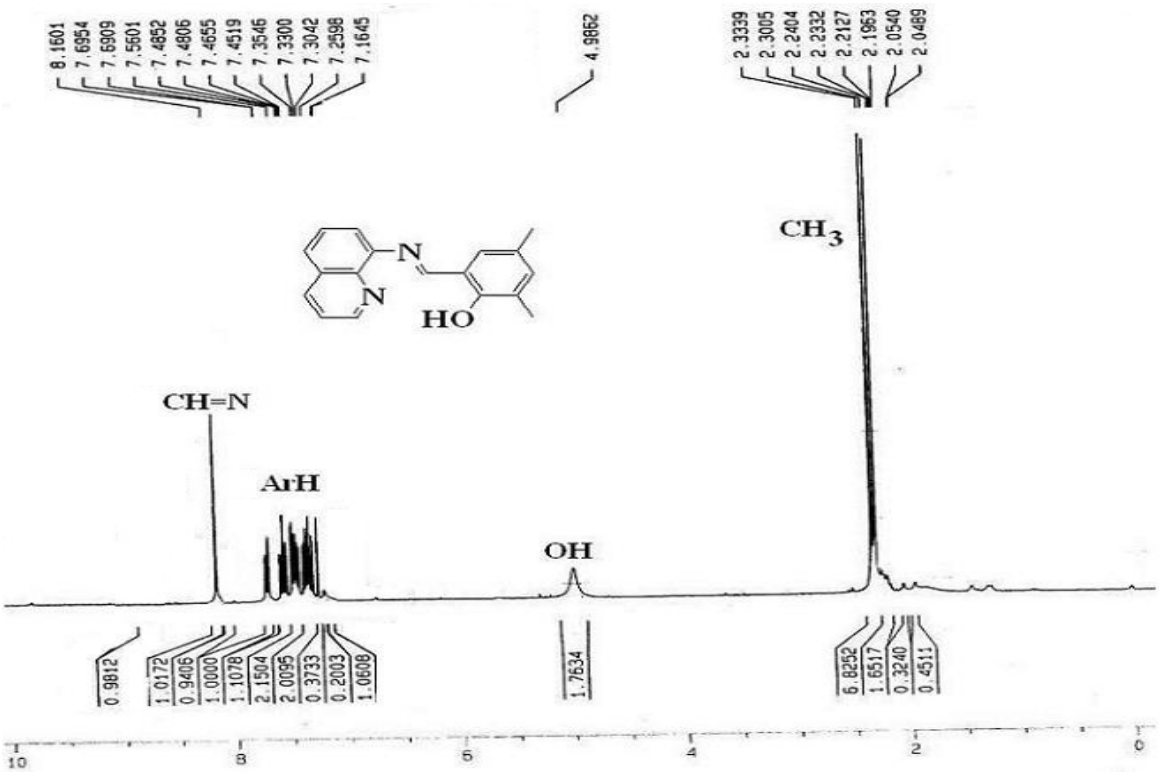


Fig. S6 The ^{1}H NMR spectra of HL in $CDCl_3$.

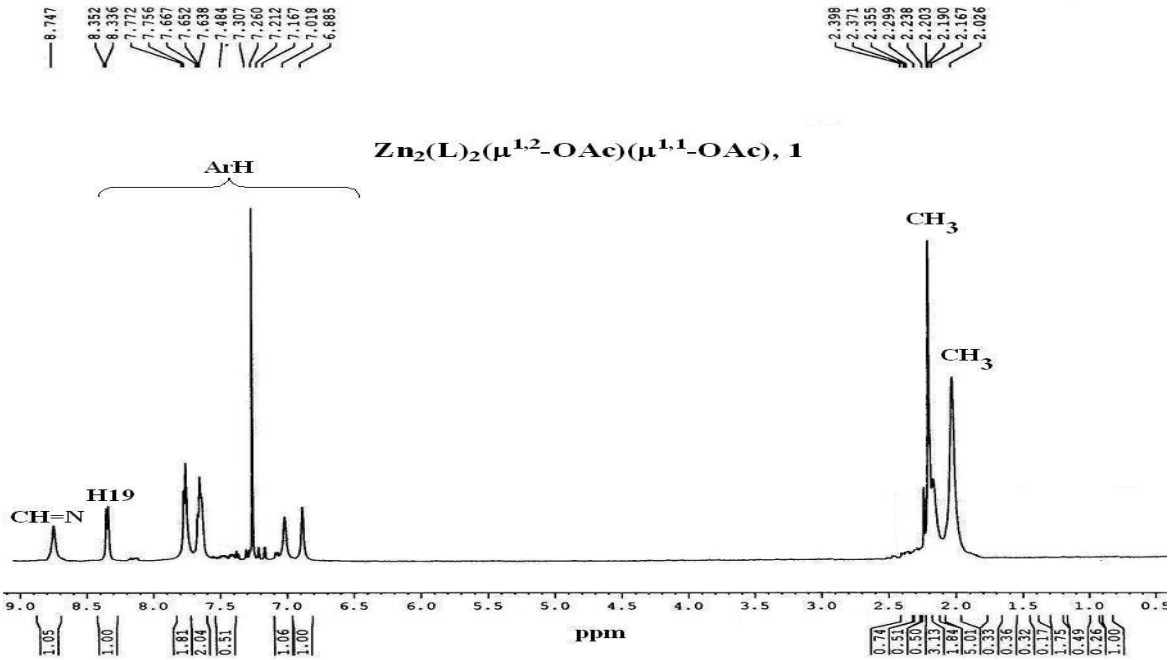


Fig. S7 The ^{1}H NMR spectra of complex **1** in $CDCl_3$.

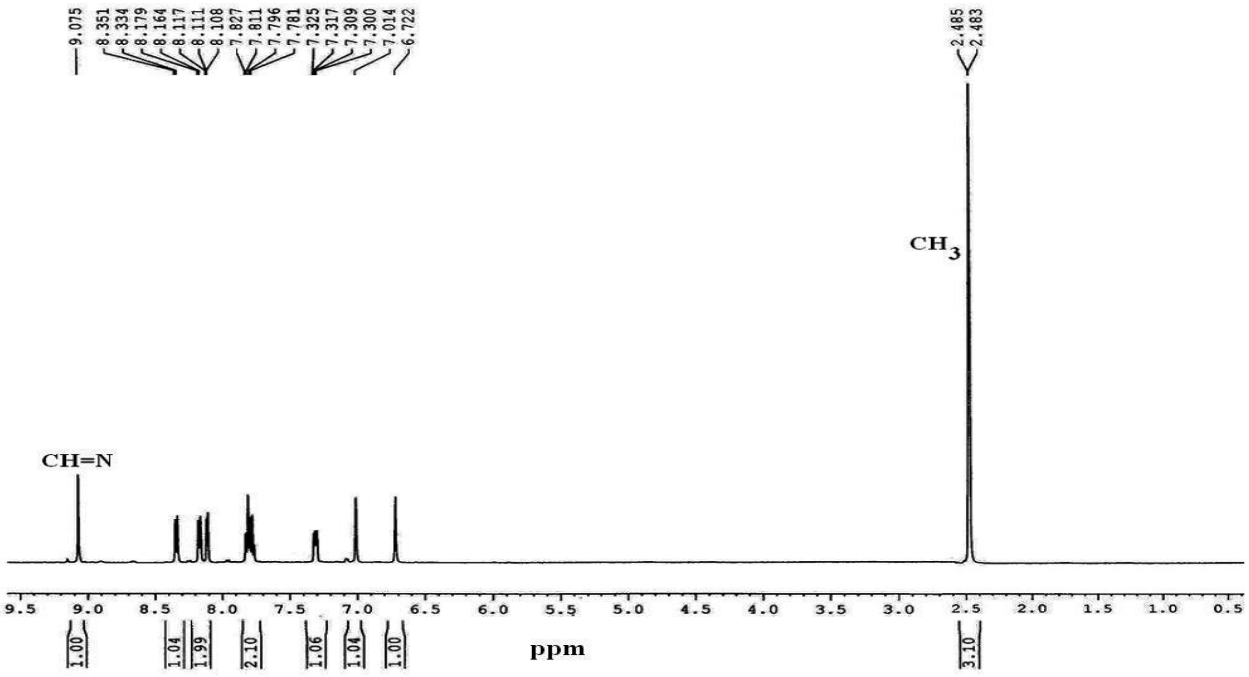


Fig. S8 The ^{1}H NMR spectra of complex **2** in CD_3CN.

IR spectra

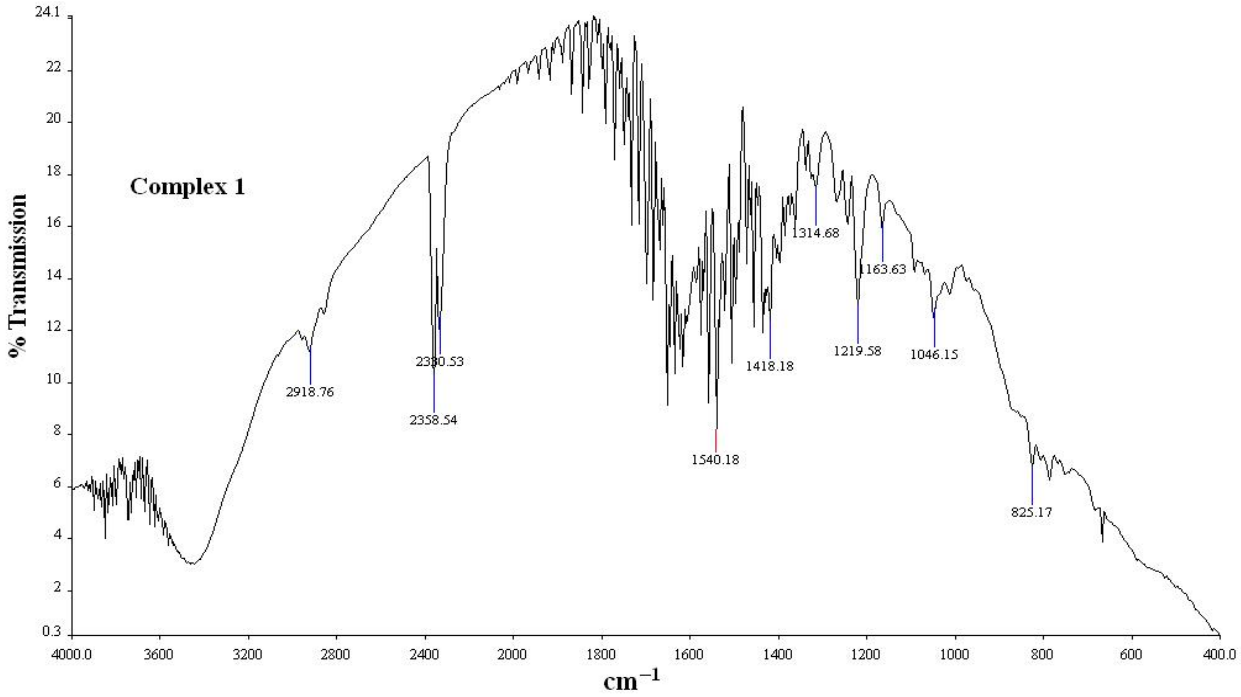


Fig. S9 IR spectra of complex **1** respectively.

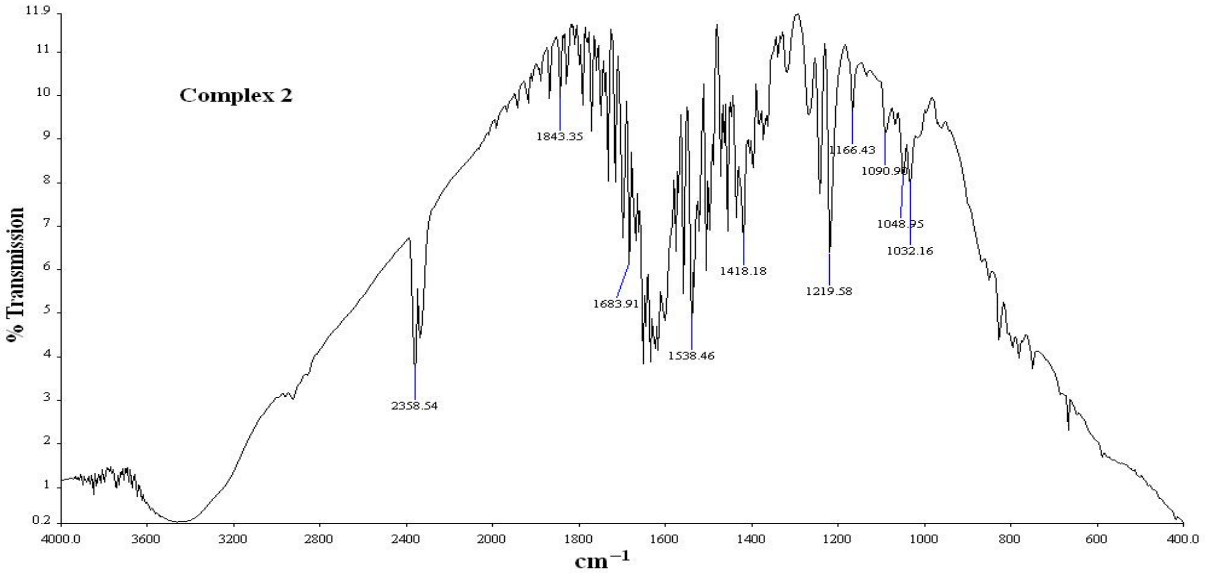
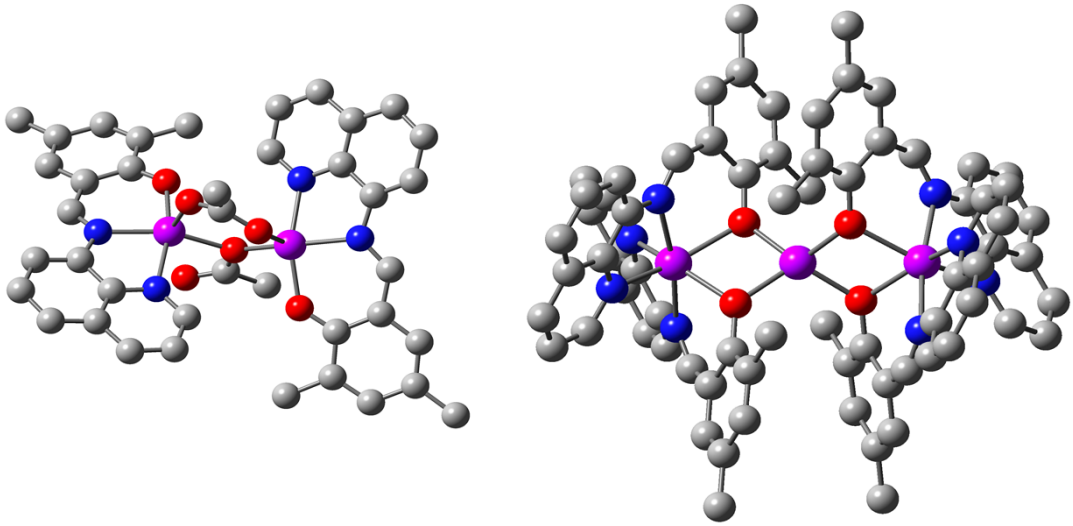


Fig. S10 IR spectra of complexes **2** respectively.

Table S1 Selected Optimized Geometrical Parameters of complex **1** in the Ground (S_0) State at B3LYP Levels and Experimental Bond length (Å) and Angle (°) for complex **1**

Bond length (Å)					
Atoms	Soln. phase	Experimental	Atoms	Soln. phase	Experimental
Zn1-O1	2.009	1.988(2)	Zn2-O3	2.046	2.000(3)
Zn1-O2	2.005	2.098(2)	Zn2-O4	2.082	2.0293(18)
Zn1-O4	2.031	2.0664(19)	Zn2-O6	2.016	1.999(2)
Zn1-N1	2.146	2.148(3)	Zn2-N3	2.166	2.166(3)
Zn1-N2	2.091	2.077(2)	Zn2-N4	2.078	2.086(2)
Bond Angle(°)					
Atoms	Soln. phase	Experimental	Atoms	Soln. phase	Experimental
O1-Zn1-O2	100.75	92.53(9)	O3-Zn2-O4	98.95	103.40(8)
N1-Zn1-N2	78.67	77.94(9)	N3-Zn2-O6	158.08	165.84(10)
N1Zn1-O4	94.69	95.67(9)	N4-Zn2-O4	125.34	127.30(9)
N2-Zn1-O4	136.85	136.82(9)	N3-Zn2-N4	78.67	76.99(10)
O1-Zn1-N1	165.89	165.85(9)	N3-Zn2-O4	93.58	92.57(9)



(1) **(2)**

Fig. S11 Optimized molecular structures of **1** and **2**. (Zn: Pale violet, N: Blue, O: Red, C: Grey. Hydrogen atoms are omitted for clarity).

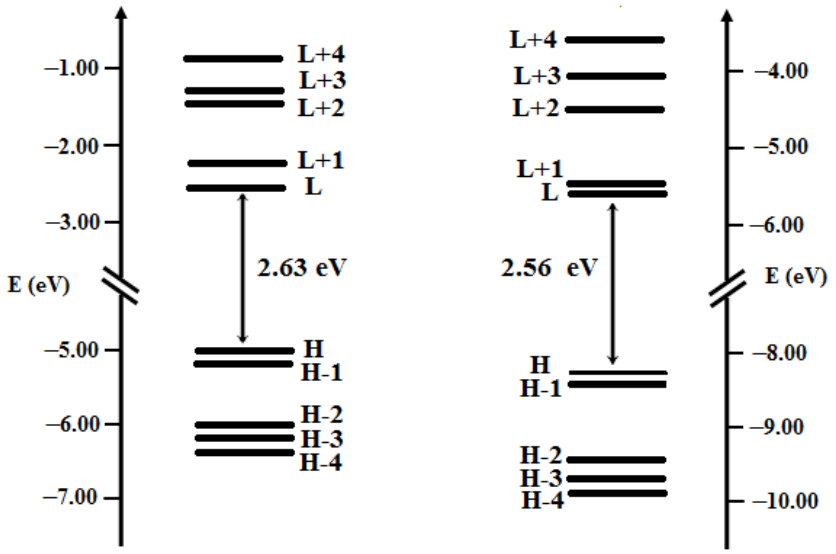


Fig. S12 Partial molecular orbital diagram with some isodensity frontier molecular orbital mainly involved in the electronic transitions for complexes **1**and **2**.

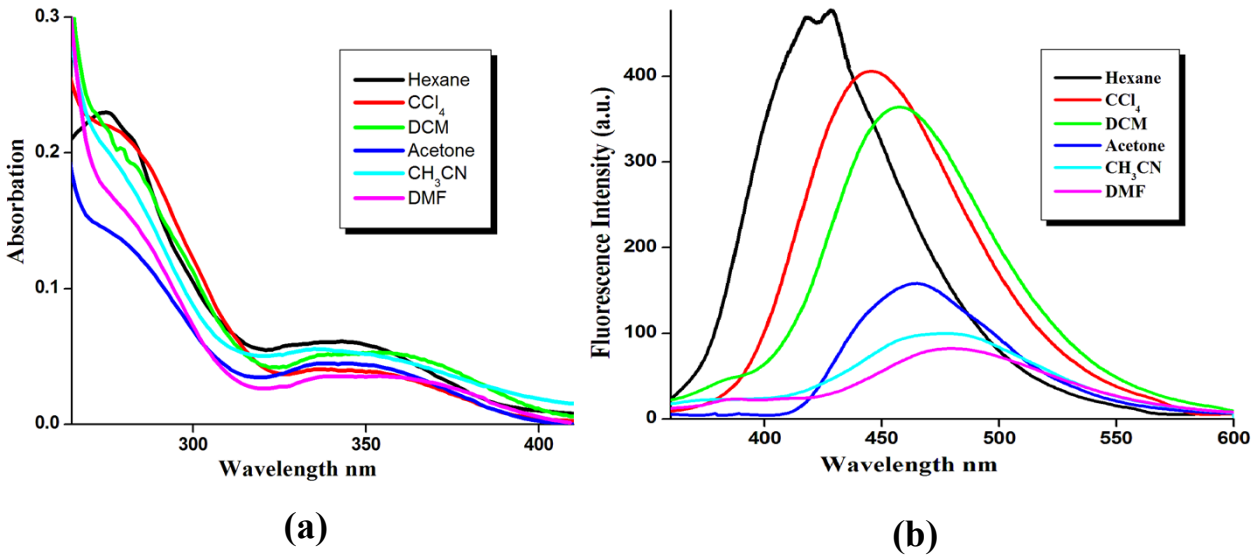


Fig. S13 (a) The absorbance spectra of HL (~1 x 10^{-5} M) in different solvents at room temperature. **(b)** The emission spectra of HL (1 x 10^{-5} M) in different solvents at room temperature (slit width 10/10).

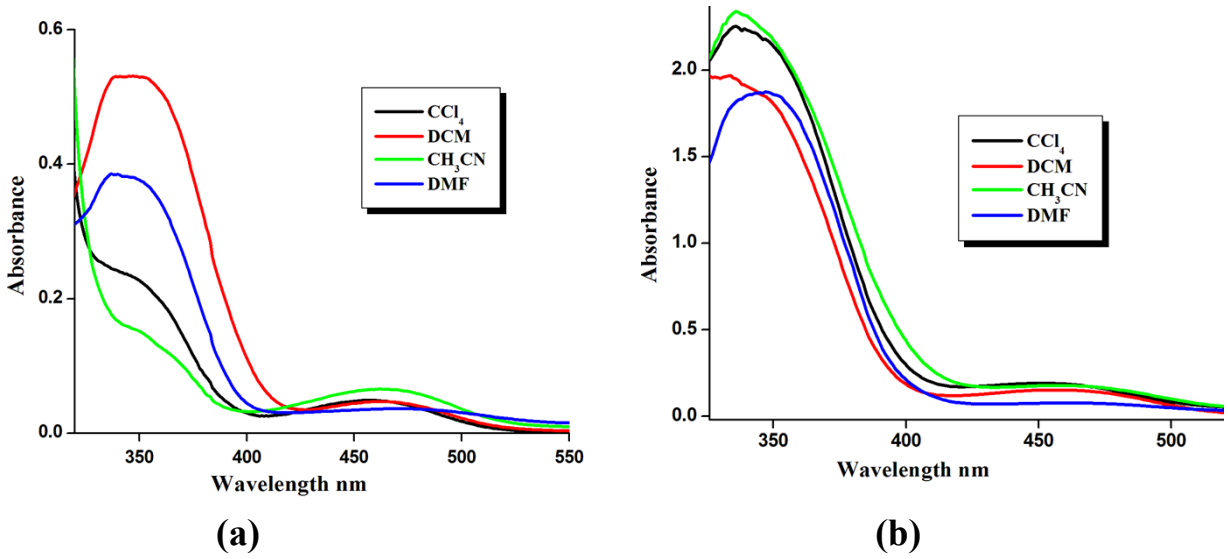


Fig. S14 The absorbance spectra of **2** (a) and **3** (b) (~1 x 10^{-5} M) in different solvents at room temperature.

Table S2 Photophysical parameters of complex **2** in different solvent at room temperature

Solvent	λ_{abs} (nm)	λ_{em}[a] (nm)	Quantum yield(Φ_f)	τ_1 (ns)	τ_2 (ns)	χ^2	k_rx10^8	k_{nr}x10^8
CCl_4	456	588	0.67	0.50	2.01	1.22	3.3	1.64
DCM	462	594	0.50	0.62	2.48	1.24	2.0	2.01
CH_3CN	464	606	0.31	0.81	4.23	1.02	0.7	1.63
DMF	470	619	0.12	1.17	5.29	1.29	0.02	1.57

Table S3 Photophysical parameters of complex **3** in different solvent at room temperature

Solvent	λ_{abs} (nm)	λ_{em}[a] (nm)	Quantum yield(Φ_f)	τ_1 (ns)	τ_2 (ns)	χ^2	k_rx10^8	k_{nr}x10^9
CCl_4	451	578	0.23	0.56	2.54	1.08	0.9	0.3
DCM	456	584	0.18	0.99	4.63	1.01	0.3	1.19
CH_3CN	459	590	0.07	1.17	4.71	1.02	0.1	1.97
DMF	464	597	0.03	2.14	8.57	1.01	0.03	1.13

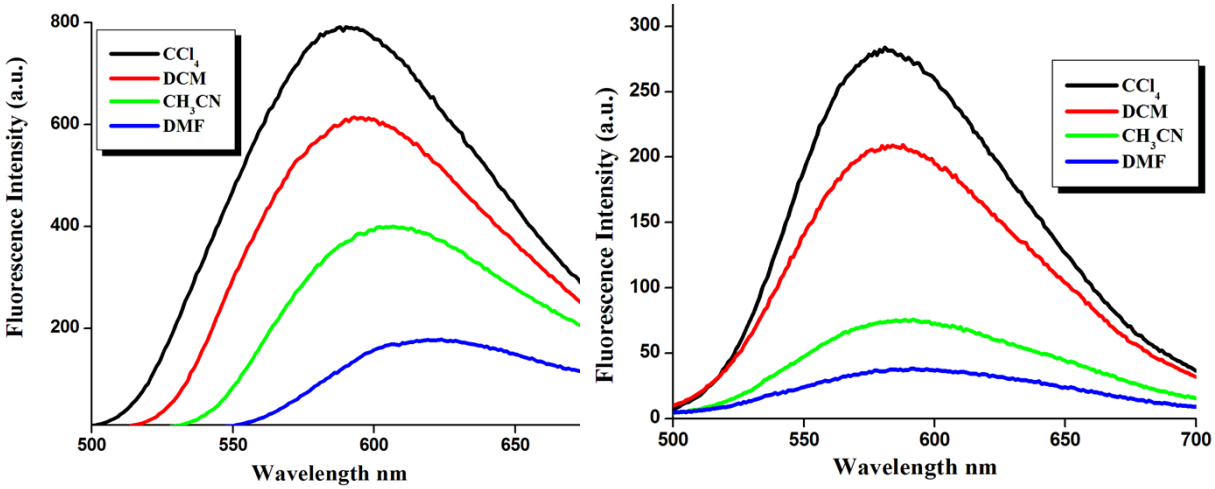


Fig. S15 The emission spectra of **2** (a) and **3** (b) (~1 x 10^{-5} M) in different solvents at room temperature.

Table S4. Hydrogen bonding parameters in **1**

Atoms	D-H(Å)	H···A(Å)	D-H···A(Å)	< D-H···A (º)	Symmetry
N6-H6A···N5	0.8600	2.3100	2.671(7)	105.00	---
C7-H7···O5	0.9300	2.4000	3.325(4)	171.00	1-x,1-y,1-z
C10-H10···O5	0.97(3)	2.42(3)	3.341(4)	161(3)	1-x,1-y,1-z
C18-H18A···O1	0.9600	2.3400	2.795(5)	109.00	---
C36-H36A···O6	0.9600	2.3300	2.794(5)	109.00	---

Table S5. Hydrogen bonding parameters in **2**

Atoms	D-H(Å)	H···A(Å)	D-H···A(Å)	< D-H···A (º)	Symmetry
C18-H18A···O1	0.9600	2.3900	2.843(6)	108.00	---
C25-H25···O5	0.9300	2.5400	3.143(13)	123.00	---
C26-H26A···O2	0.9600	2.3500	2.817(5)	109.00	---
C35-H35···O3	0.9300	2.4400	3.301(11)	153.00	x, -y, -1/2+z

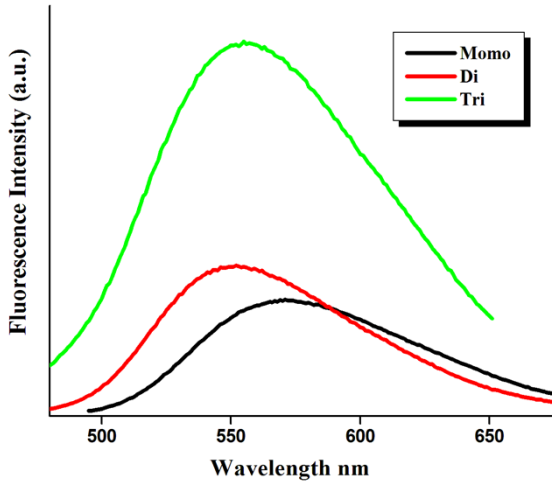


Fig. S16 The emission spectra of the complexes at solid state λ_{ex} around 450 nm at room temperature.

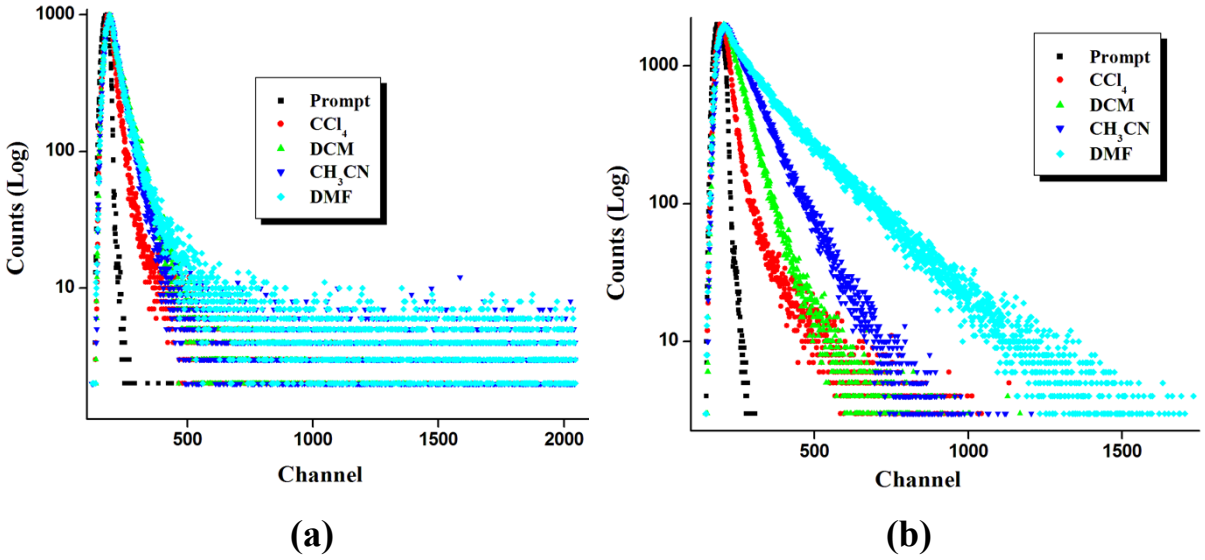


Fig. S17 Changes in the time-resolved photoluminescence decay of **2** and **3** in solvent of different polarity at room temperature obtained with 360 nm excitation