Electronic Supplementary Information (ESI)

Synthesis, characterization, theoretical studies and catecholase like activities of [MO_6] type complexes

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Table S1. Selected bond lengths (Å) and angles (°) for the complexes

			1			
Atom	Atom	Length	Atom	Atom	Atom	Angle
O1	C1	1.312(3)	Co1	O1	C1	117.34(13)
O1	Co1	2.0008(14)	Co1	O2	C7	110.40(12)
O2	C7	1.382(2)	Co1	O2	C8	129.88(13)
O2	C8	1.432(3)	O1	Co1	O1	157.56(8)
O2	Co1	2.2475(14)	O2	Co1	O1	89.27(6)
O3	C5	1.228(3)	O2	Co1	O1	75.33(5)
Co1	O4	2.0434(15)	O2	Co1	O2	93.71(8)
C2	C1	1.406(3)	O4	Co1	O1	98.14(6)
C3	C4	1.399(3)	O4	Co1	O1	97.52(6)
C1	C7	1.421(3)	O4	Co1	O2	88.05(6)
C7	C6	1.371(3)	O4	Co1	O2	172.59(6)
C5	C4	1.447(3)	O4	Co1	O4	91.12(9)
			2			
Zn1	O1	1.9836(14)	O1	Zn1	O1	156.15(8)
Zn1	O4	2.0217(16)	O1	Zn1	O4	99.53(6)
Zn1	O2	2.3069(14)	O1	Zn1	O4	96.87(6)
O1	C1	1.312(2)	O4	Zn1	O4	92.78(10)
O2	C6	1.379(2)	O1	Zn1	O2	88.77(5)
O2	C7	1.431(2)	O4	Zn1	O2	171.36(6)
O3	C8	1.229(3)	O1	Zn1	O2	74.49(5)
C1	C2	1.402	C1	O1	Zn1	118.85(12)
C1	C6	1.421(3)	C6	O2	Zn1	109.34(11)
C2	C3	1.376(3)	C7	O2	Zn1	130.61(12)
C3	C4	1.392(3)	Zn1	O4	H4A	119(2)
C4	C5	1.406(3)	Zn1	O4	H4A	125(2)
C5	C6	1.373(3)	C6	O2	C7	117.71(16)

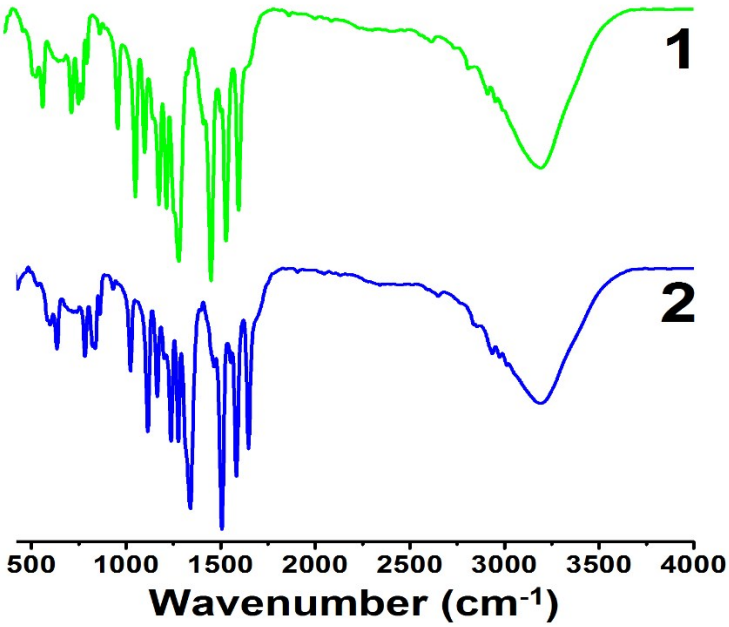

Fig. S1. FTIR spectra of **1** and **2**.

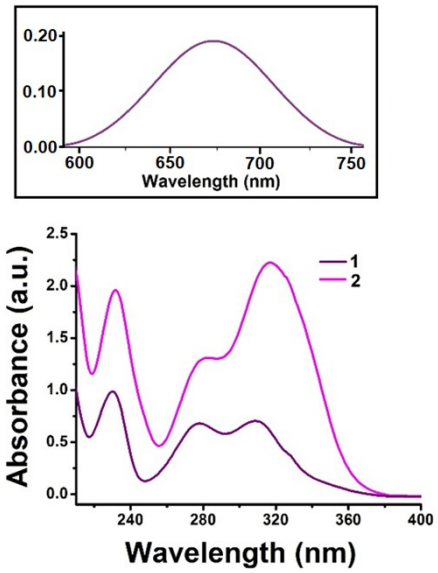

Fig. S2. Electronic spectra of **1** and **2**.

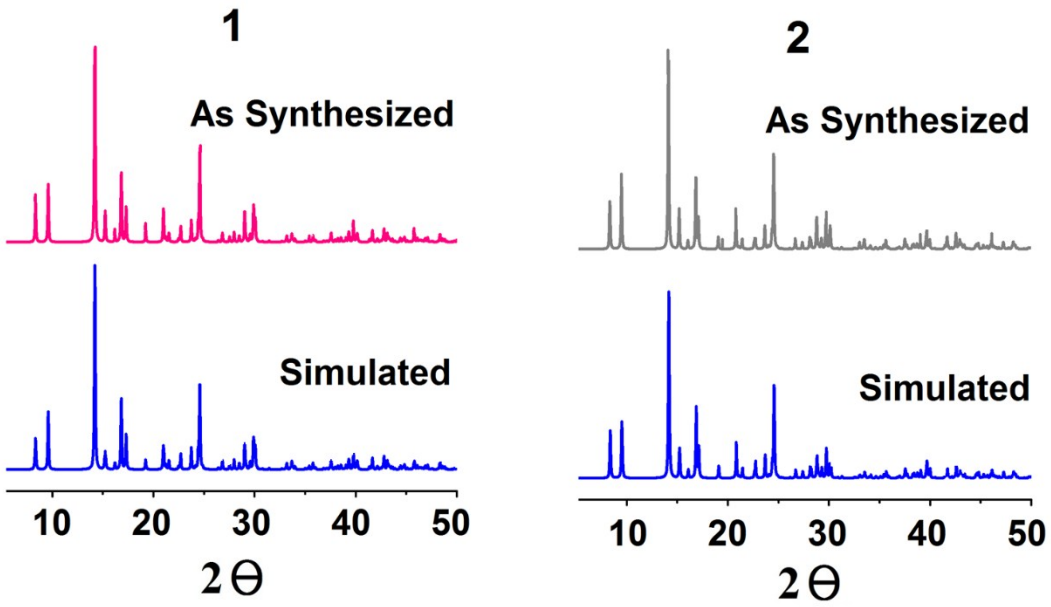

Fig. S3. As-synthesized and simulated PXRD patterns of **1** and **2**.

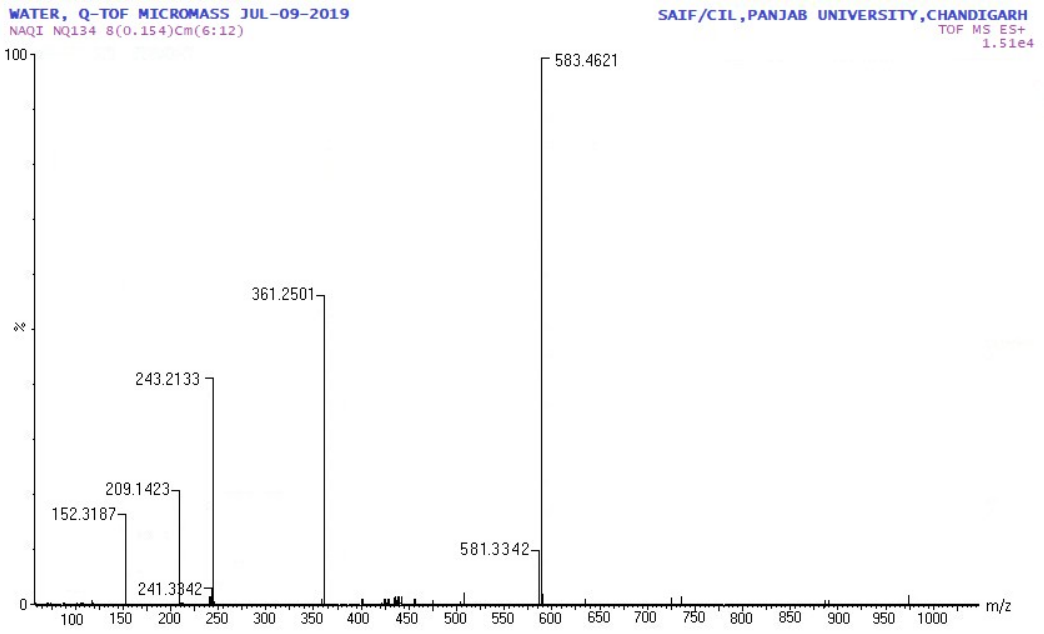

Fig. S4. ESI-MS spectrum (positive mode) of a mixture of **1** and 3,5DTBC recorded in ethanol.

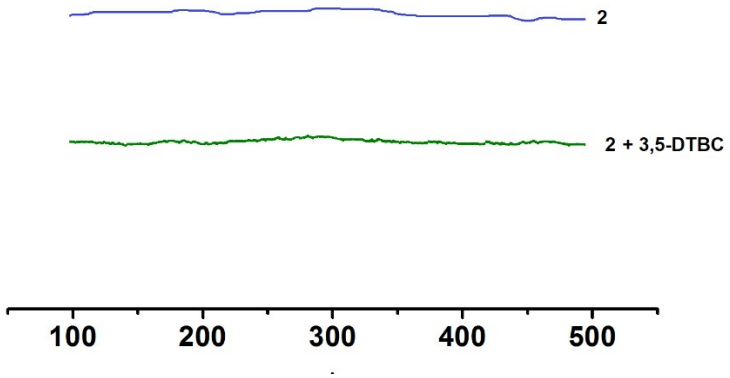

Fig. S5. EPR spectra of **2** before and after addition of 3,5-DTBC.

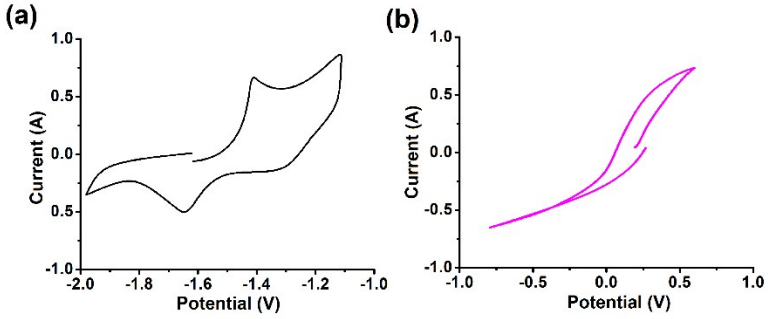

Fig. S6. Cyclic voltammograms of **1** (a) and **2** (b).

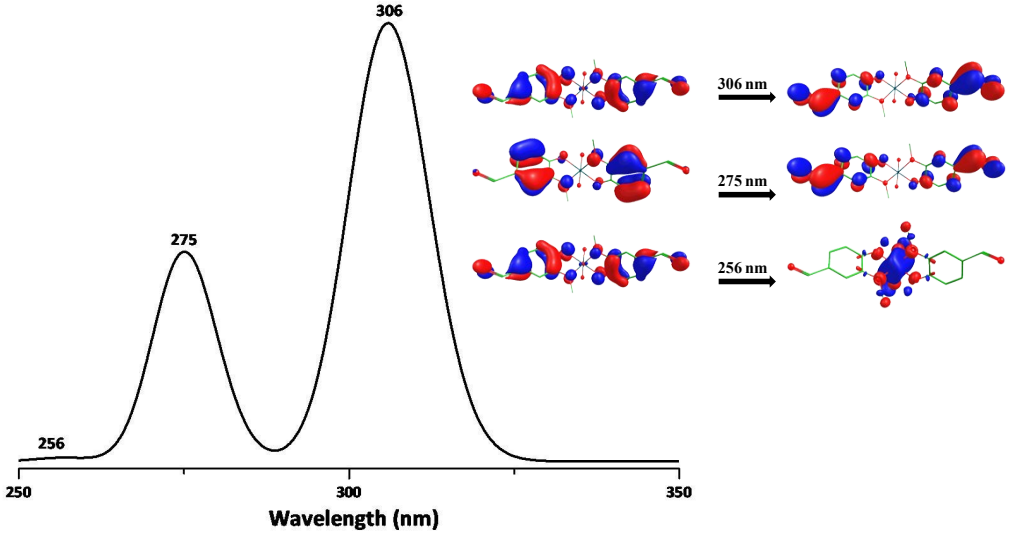

Fig S7. B3LYP TDDFT simulated electronic absorption spectra of the **2** and its corresponding orbitals involved in the transitions.