Electronic Supplementary Material (ESI) for Dalton Transactions.

Cooperative Influence of Pseudohalides and Ligand Backbone of Schiff-bases on Nuclearity and Stereochemistry of Cobalt(III) Complexes: Experimental and Theoretical Investigation

Arnab Mandal, [a] Sanchari Dasgupta, [a] Sumi Ganguly, [a] Antonio Bauzá, [b] Antonio Frontera,*, [b] and Debasis Das*, [a]

[a] Department of Chemistry, University of Calcutta, 92, A. P. C. Road, Kolkata – 700009, India.

[b] Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122, Palma (Baleares), Spain

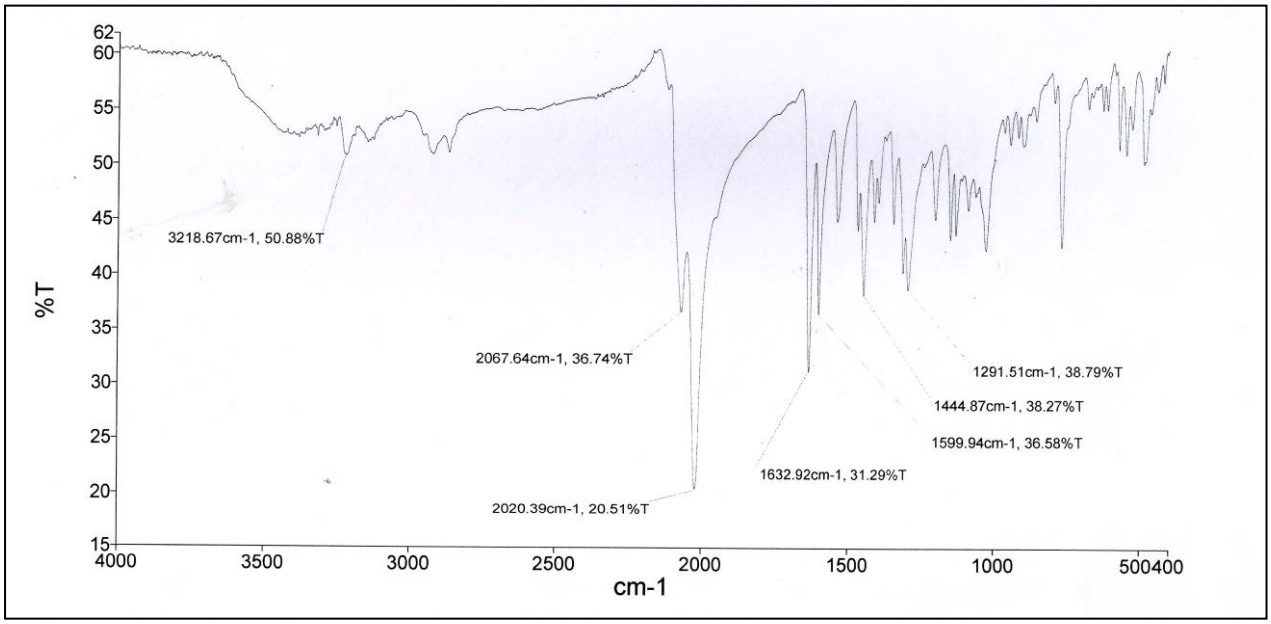


Fig. S1 FT-IR spectrum of complex **2**.

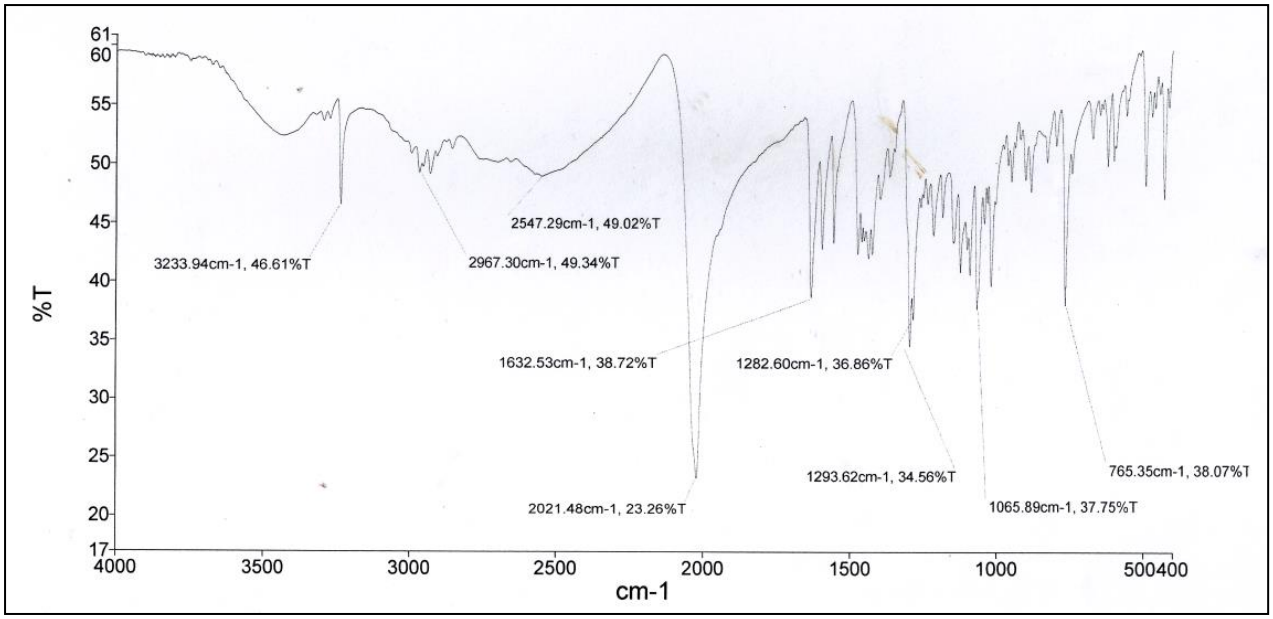
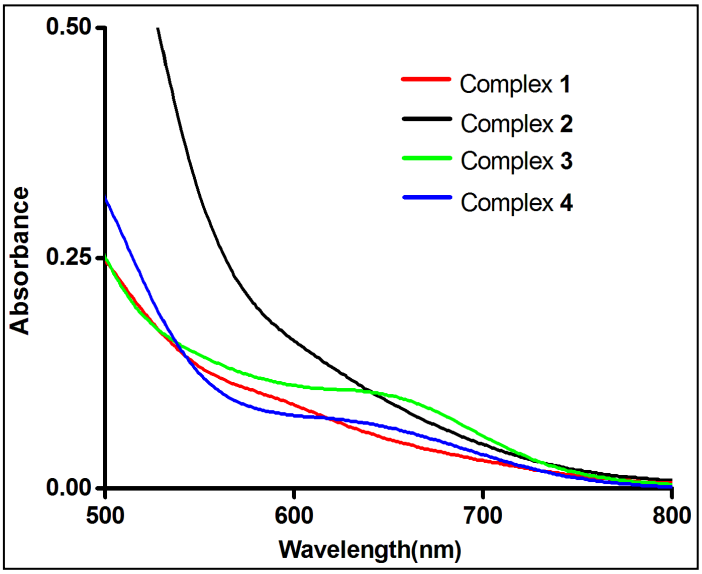
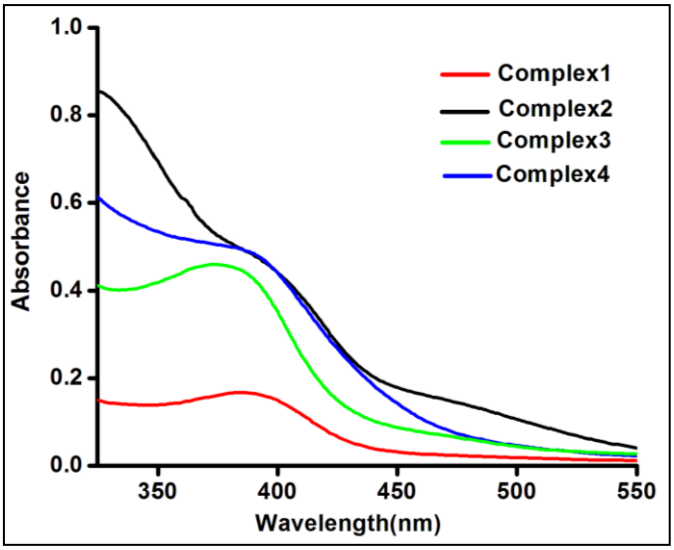


Fig. S2 FT-IR spectrum of complex **4**.



(a)



(b)

Fig. S3 (a) d-d transition and (b) charge transfer spectra of complexes **1-4**.

Table S1 Selected Bond Lengths (A°) and angles (deg) for Complex **1** and **2**

Complex **1**		Complex **2**	
Co1-O1	1.891(2)	Co1-O1	1.882(7)
Co1-O2	1.974(3)	Co1-O2	1.950(7)
Co1-N1	1.867(3)	Co1-N1	1.859(8)
Co1-N2	1.940(3)	Co1-N2	1.924(8)
Co1-N3	1.889(4)	Co1-N3	1.918(8)
Co1-N4	1.895(3)	Co1-Co1	2.981(10)
O1-Co1-O2	91.44(11)	O1-Co1-O2	91.4(3)
O1-Co1-N1	96.88(12)	O1-Co1-N1	94.8(3)
O1-Co1-N2	177.00(12)	O1-Co1-N2	177.6(3)
O1-Co1-N3	90.49(14)	O1-Co1-N3	89.3(3)
O1-Co1-N4	89.85(12)	O2-Co1-N1	172.0(3)
O2-Co1-N1	171.63(11)	O2-Co1-N2	86.3(3)
O2-Co1-N2	85.69(12)	O2-Co1-N3	92.0(3)
O2-Co1-N3	89.48(13)	N1-Co1-N2	87.5(4)
O2-Co1-N4	90.83(12)	N1-Co1-N3	93.0(3)
N1-Co1-N2	86.01(12)	N2-Co1-N3	91.5(3)
N1-Co1-N3	91.37(14)		
N1-Co1-N4	88.28(13)		
N2-Co1-N3	88.63(15)		
N2-Co1-N4	91.04(12)		
N3-Co1-N4	179.54(13)		

Table S2 Selected Bond Lengths (A°) and angles (deg) for Complex **3** and **4**

Complex **3**		Complex **4**	
Co1-O1	1.846(2)	Co1-O1	1.877(3)
Co1-O2	1.934(2)	Co1-O2	1.936(3)
Co1-N1	1.871(2)	Co1-N1	1.888(4)
Co1-N2	1.928(3)	Co1-N2	1.964(5)
Co1-N3	1.895(3)	Co1-N3	1.940(4)
Co1-N4	1.899(3)	Co1-N6	1.941(4)
O1-Co1-O2	86.08(9)	O1-Co1-O2	86.43(14)
O1-Co1-N1	91.47(10)	O1-Co1-N1	92.55(16)
O1-Co1-N2	88.12(9)	O1-Co1-N2	171.44(17)
O1-Co1-N3	91.86(9)	O1-Co1-N3	92.07(17)
O1-Co1-N4	174.70(9)	O1-Co1-N6	92.28(16)
O2-Co1-N1	176.41(11)	O2-Co1-N1	178.98(17)
O2-Co1-N2	85.90(10)	O2-Co1-N2	85.38(16)
O2-Co1-N3	89.90(10)	O2-Co1-N3	89.26(16)
O2-Co1-N4	88.62(10)	O2-Co1-N6	89.05(15)
N1-Co1-N2	91.40(13)	N1-Co1-N2	95.64(19)
N1-Co1-N3	92.81(10)	N1-Co1-N3	90.83(18)
N1-Co1-N4	93.82(10)	N1-Co1-N6	90.93(17)
N2-Co1-N3	175.79(9)	N2-Co1-N3	85.34(19)
N2-Co1-N4	91.32(11)	N2-Co1-N6	90.08(18)
N3-Co1-N4	88.32(11)	N3-Co1-N6	175.23(19)

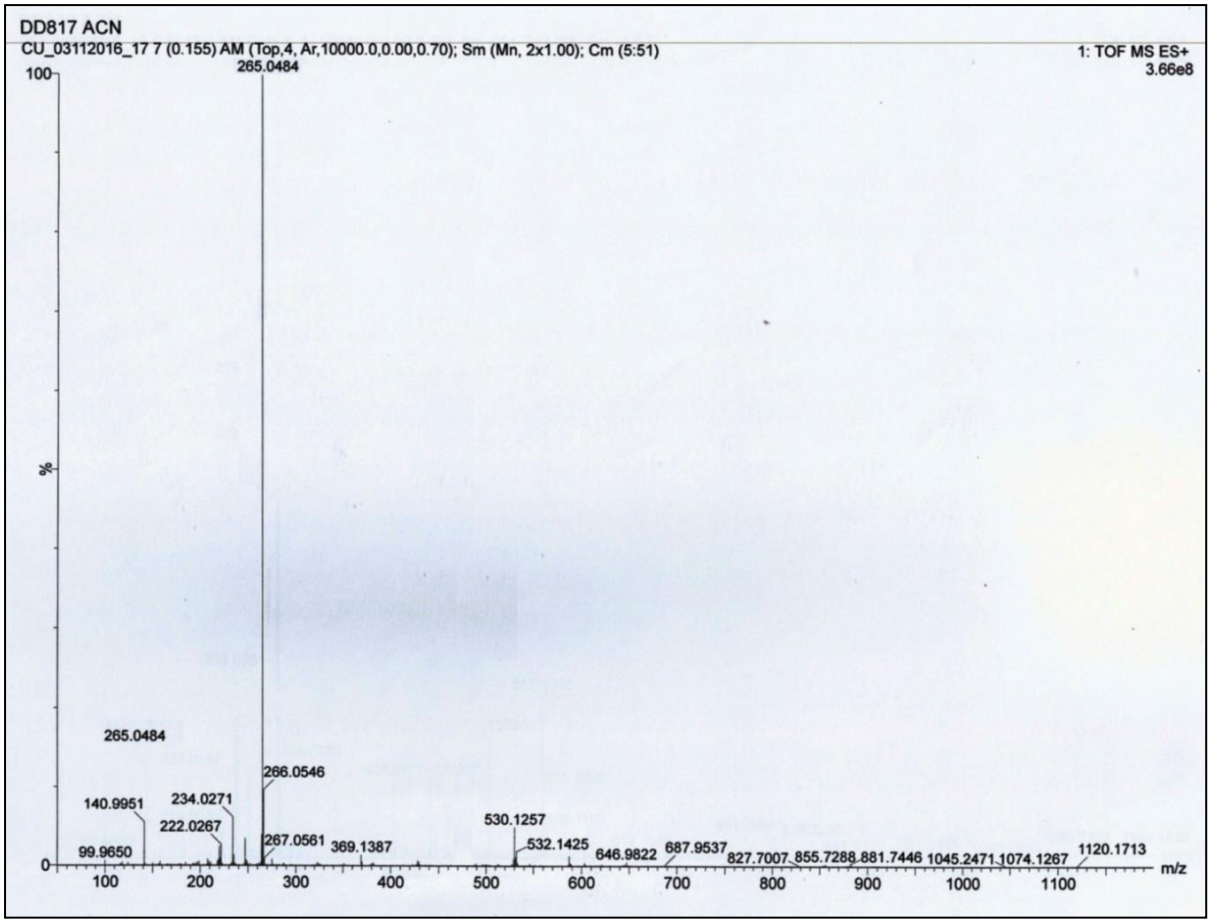


Fig. S4 ESI-MS spectrum of complex **1**.

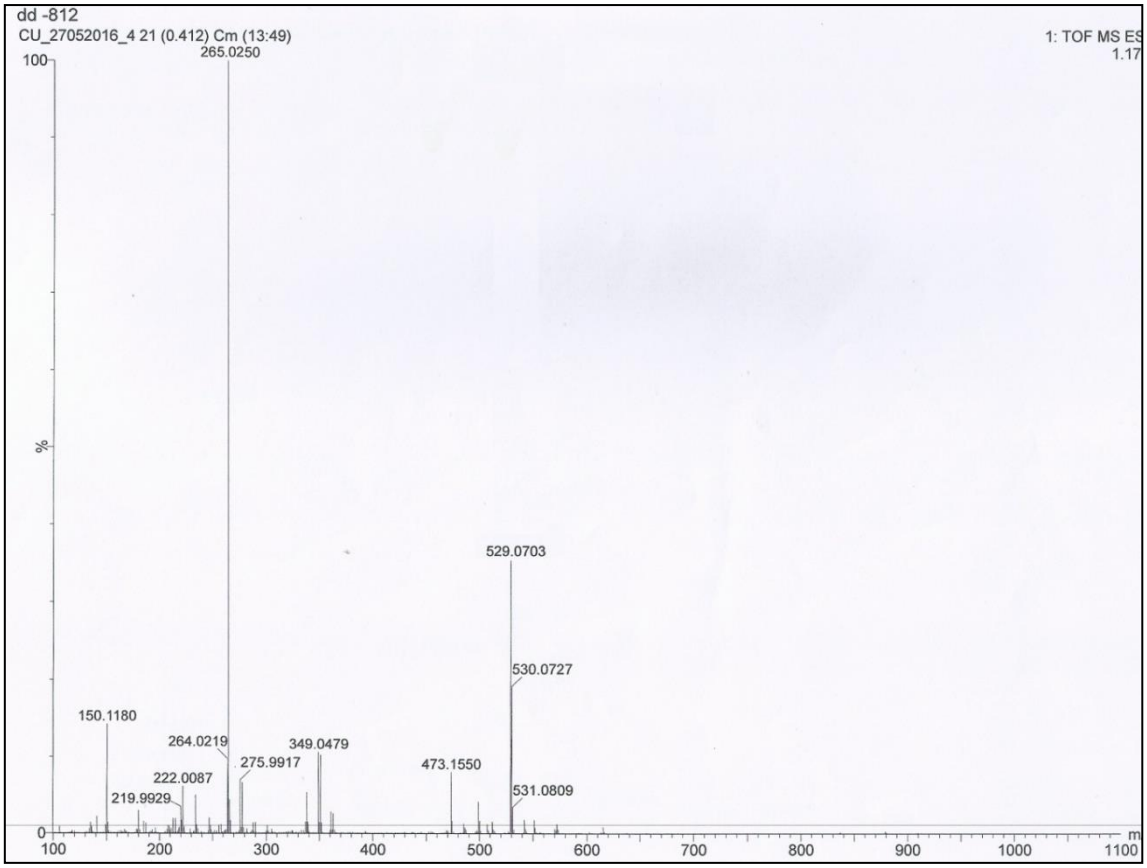


Fig. S5 ESI-MS spectrum of complex **2**.

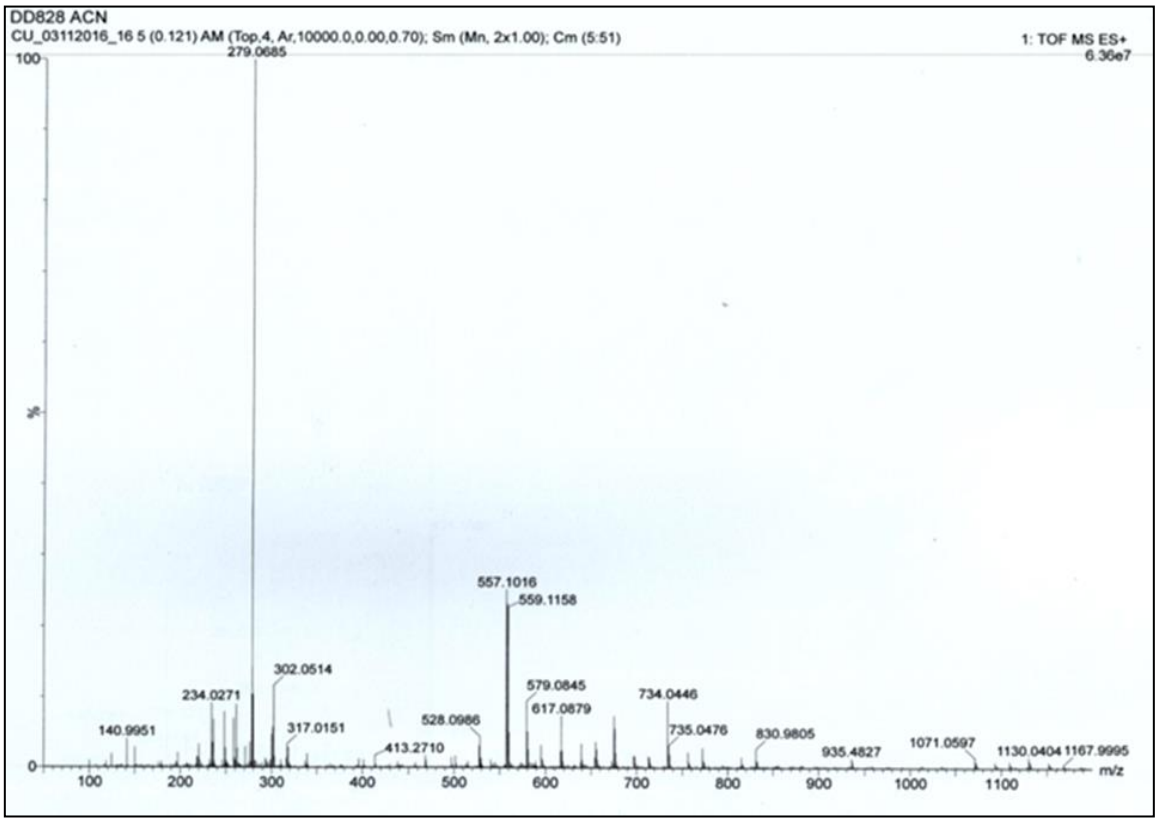


Fig. S6 ESI-MS spectrum of complex **3**.

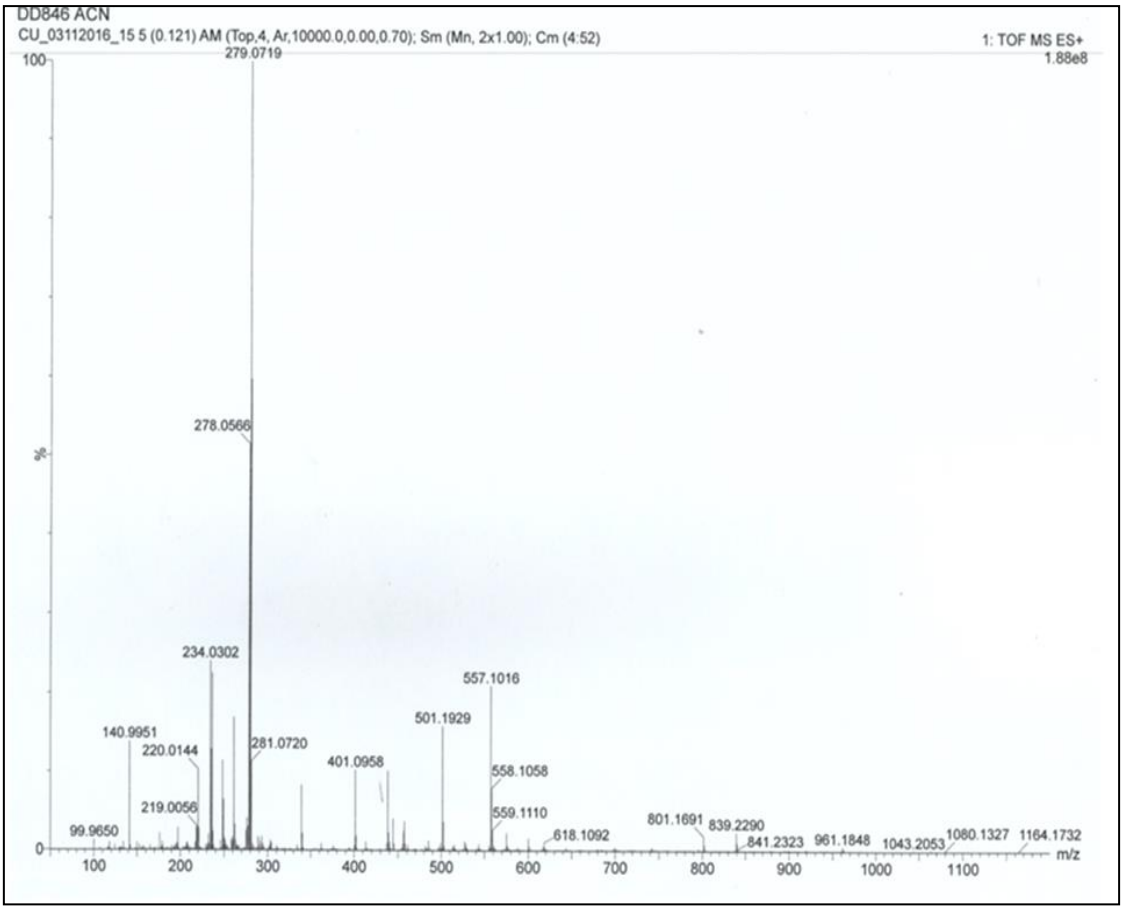
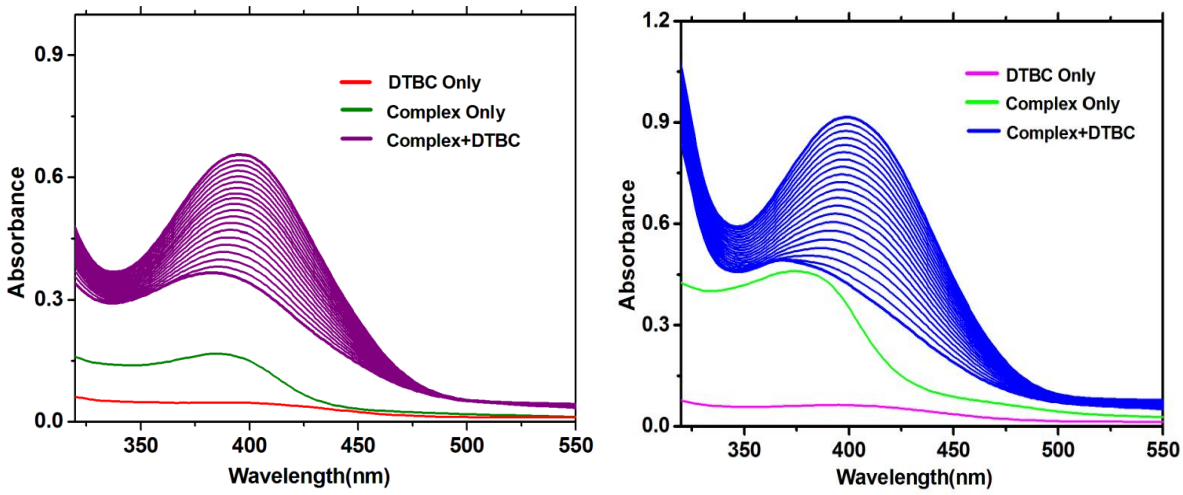


Fig. S7 ESI-MS spectrum of complex **4**.



(a) (b)

Fig. S8 Oxidation of 3,5-DTBC by (a) complex **1** and (b) complex **3** observed in UV-Vis spectroscopy with time.

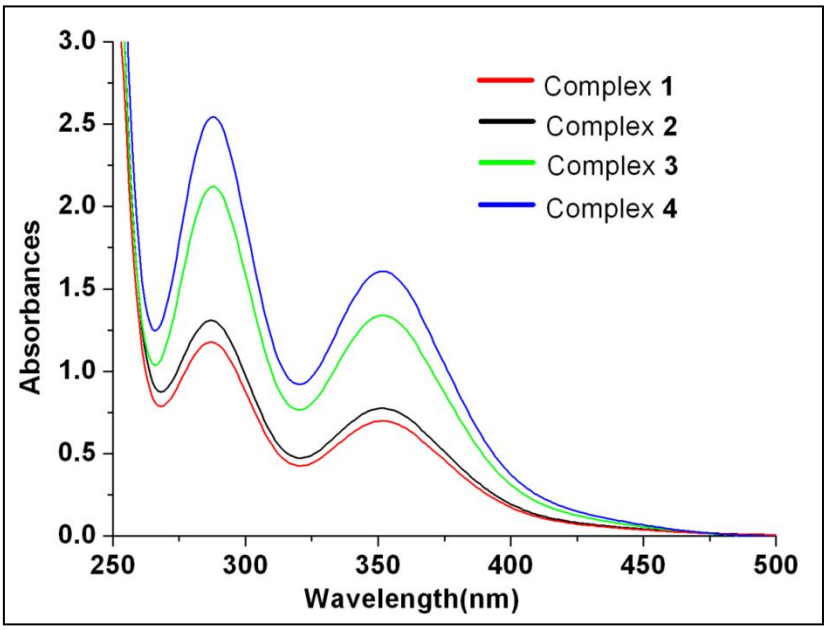
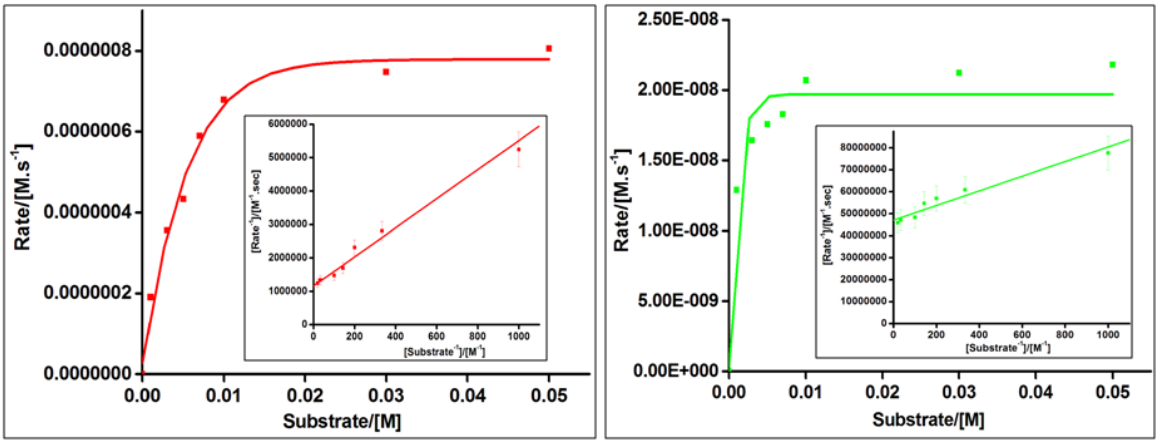


Fig. S9 Detection of H_2O_2 formation during oxidation of 3,5-DTBC observed spectrophotometrically.



(a) (b)

Fig. S10 Dependence of rate of reaction on substrate concentration (inset Lineweaver Burk plot) for (a) complex **1** and (b) complex **3**.