Supplementary Materials

A series of tetrabromocatecholate chelated cobalt(III) complexes with various N-donor ancillary ligands: syntheses, crystal structures, co-crystallization, thermally induced valence tautomerism and electrochemical studies

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Table S1. Crystal data and structure refinements of **1 - 9**

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Empirical formula	$C_{20}H_{33}Br_8Cl_2Co_2N_8O_{12.50}$	$C_{12}H_{20}Br_4ClCoN_4O_6$	$C_{17}H_{32}Br_4CoN_5O_6$	$C_{18}H_{16}Br_4ClCoN_4O_6$	$C_{50}H_{40}Br_8Co_2N_{10}O_{12}$	$C_{61}H_{36}Br_8Cl_2Co_2N_8O_{13}$	$C_{34}H_{26}Br_8CoN_5O_9$	$C_{26}H_{26}Br_8CoN_5O_5$	$C_{39}H_{70}Br_{12}Co_3N_{15}O_{20}$
Formula weight	1413.58	730.34	781.05	798.37	1730.06	1917.02	1346.81	1183.70	2204.72
T/ K	298(2)	100(2)	150(2)	150(2)	150(2)	298(2)	150(2)	298(2)	150(2)
Crystal system	Orthorhombic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_12_12$	$P\bar{1}$	$P2_1/n$	C2/c	C2/c	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P2_1$
a / Å	15.560(6)	8.476(2)	16.136(6)	6.546(2)	30.152(8)	14.845(3)	12.733(3)	10.637(3)	18.519(3)
b / Å	28.240(10)	9.327(3)	8.720(3)	31.167(11)	12.333(3)	15.798(3)	20.347(6)	10.995(4)	14.082(3)
c / Å	8.992(3)	13.954(5)	19.343(6)	11.809(3)	30.405(5)	16.567(3)	15.916(3)	16.387(4)	26.628(4)
α / º	90	85.45(2)	90	90	90	115.922(1)	90	96.351(2)	90
β / °	90	80.36(3)	105.92(2)	104.7(1)	97.4(1)	103.402(1)	100.65(2)	93.693(2)	91.790(3)
γ / º	90	81.06(2)	90	90	90	102.119(1)	90	104.486(2)	90
V / Å^3, *Z*	3951.7(2), 4	1072.8(1), 2	2617.2(2), 2	2330(2), 4	11212(4), 8	3176.7(12), 2	4052.6 (2), 4	1835.7(1), 2	6941(3), 4
D_{calc} / g cm^{-3}	2.376	2.261	1.982	2.276	2.050	2.004	2.208	2.147	2.094
μ / mm^{-1}	9.129	8.410	6.804	7.757	6.365	5.709	8.371	9.215	7.691
θ range / °	2.26 – 27.45	3.55 – 27.44	3.03 – 27.47	2.21 – 27.48	2.77 – 2.77	3.84 – 27.49	3.27 – 27.50	3.86 – 27.51	1.10–27.50
Reflections collected	14873	8000	10876	5192	18530	25468	15593	13511	27800
Unique reflections / R_{int}	8705 / 0.037	4808 / 0.026	5962 / 0.048	2640 / 0.024	12557 / 0.039	14402 / 0.042	9253 / 0.047	8322 / 0.044	31908/0.042
Observed reflections [I>2σ(I)]	7335	4105	4243	2231	8942	10183	6720	5730	21296
Data/Restr./param.	8705/15/464	4808/0/259	5962/0/304	2640/0/173	18530/0/747	14402/0/849	15593/0/520	8322/0/418	27800/1/1604
GOF on F^2	1.093	1.050	0.964	1.119	0.984	1.020	1.020	1.009	1.016
R_1, wR_2 [I>2σ(I)]	0.0652, 0.1518	0.0330 / 0.0869	0.0351 / 0.0571	0.0548 / 0.1402	0.0520 / 0.1254	0.0499, 0.1300	0.0421 / 0.0943	0.0562 / 0.1585	0.0633/0.1375
R_1, wR_2 (all data)	0.0795, 0.1585	0.0401 / 0.0901	0.0658 / 0.0638	0.0653 / 0.1605	0.0815 / 0.1402	0.0756, 0.1476	0.0716/ 0.1044	0.0825 / 0.1721	0.0932/0.1536

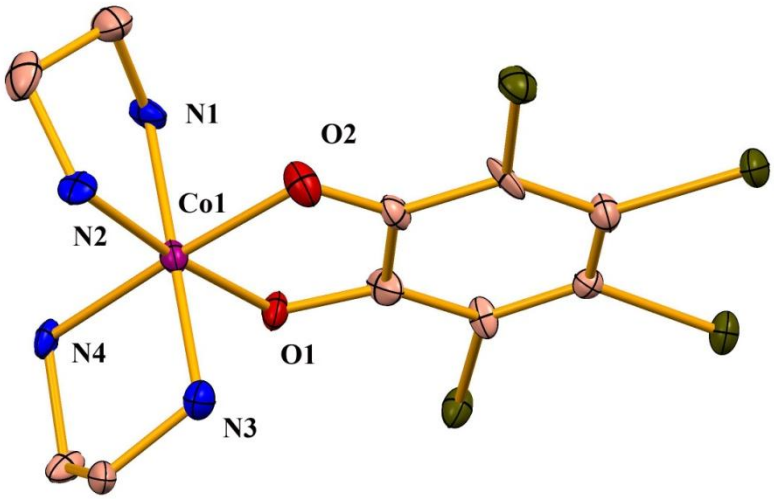

Fig. S1. Perspective view of the representative structure of complex cation of **1**. Ellipsoids are drawn at 50% probability level.

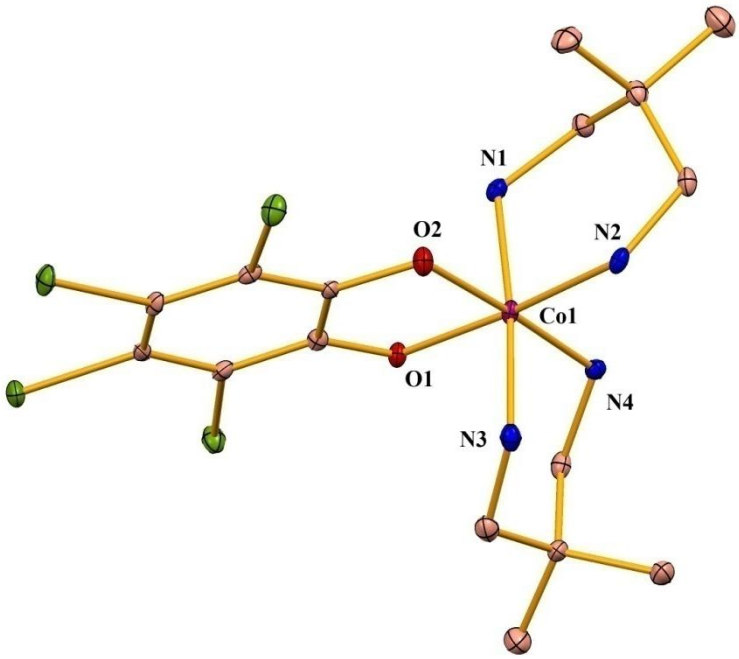

Fig. S2. Structure of complex cation of **3**. Ellipsoids are drawn at 30% probability level.

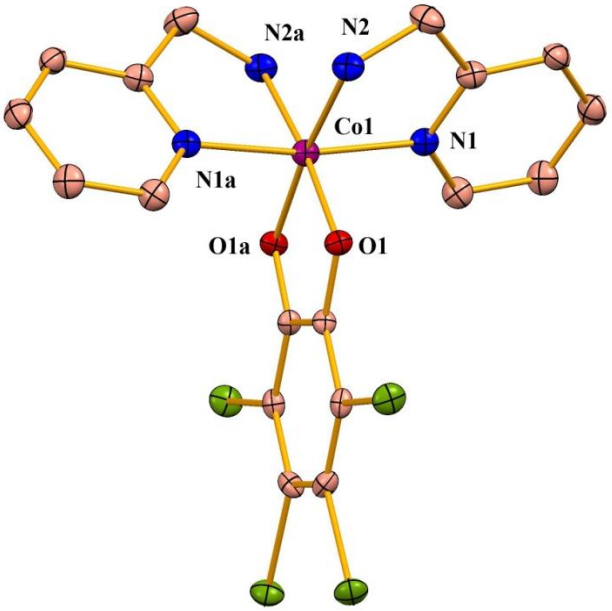

Fig. S3. Structure of complex cation of **4**. Ellipsoids are drawn at 50% probability level. Symmetry code: a = 1–x, y, 3/2–z.

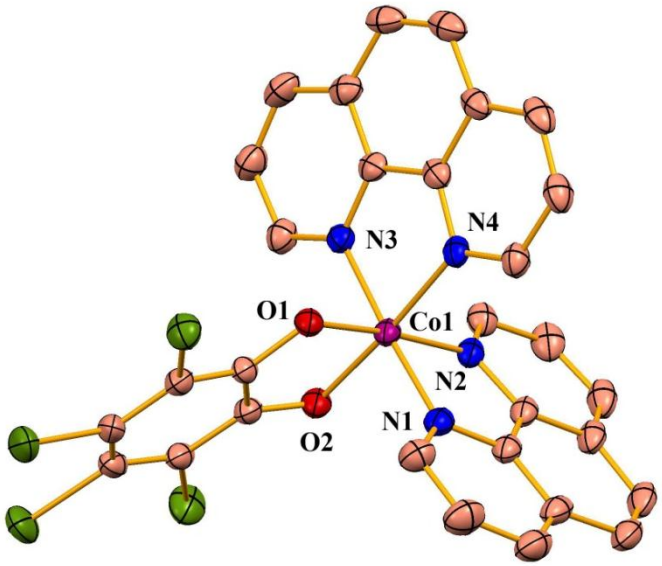

Fig. S4. Structure of complex cation of **6**. Ellipsoids are drawn at 50% probability level.

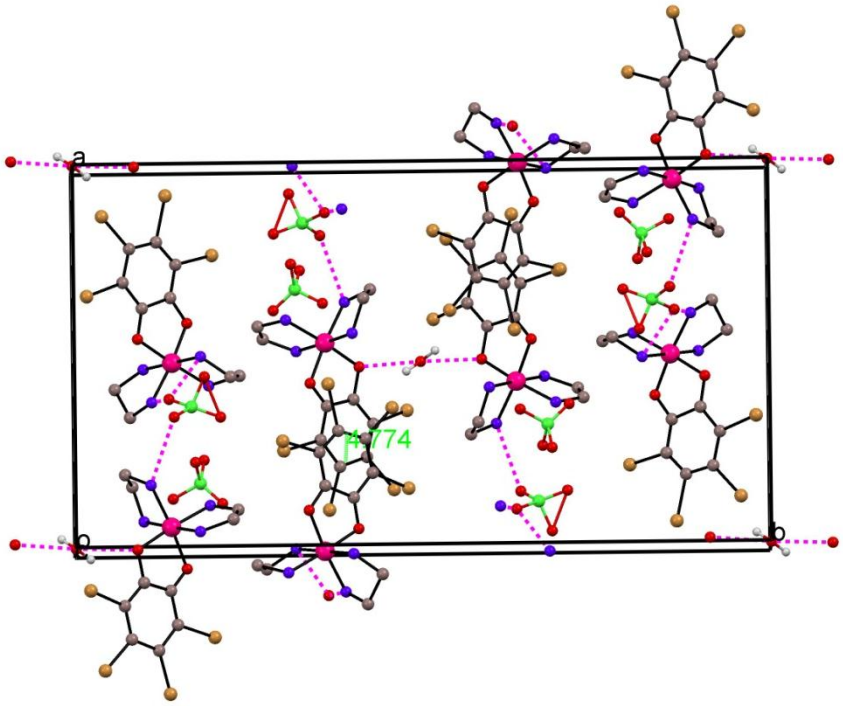

Fig. S5. A part of molecular packing of complex **1** showing π···π stacking interaction and hydrogen bonding schemes.

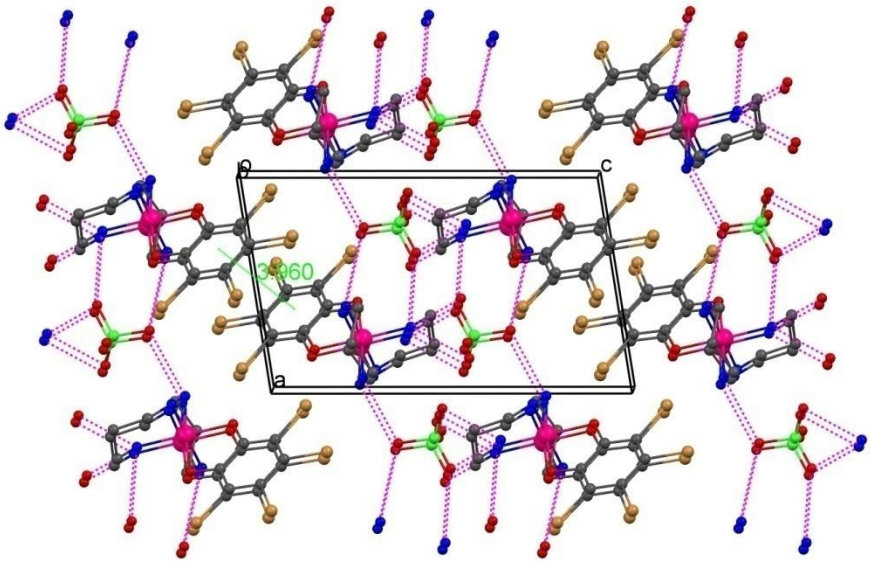

Fig. S6. Molecular packing diagram of **2** showing π···π stacking interaction and hydrogen bonding schemes.

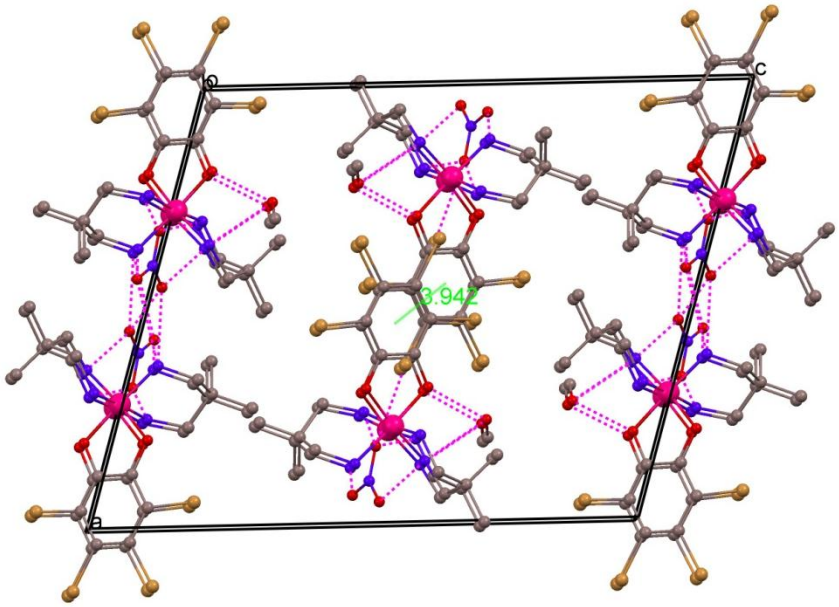

Fig. S7. Molecular packing diagram of **3** showing π···π stacking interaction and hydrogen bonding schemes.

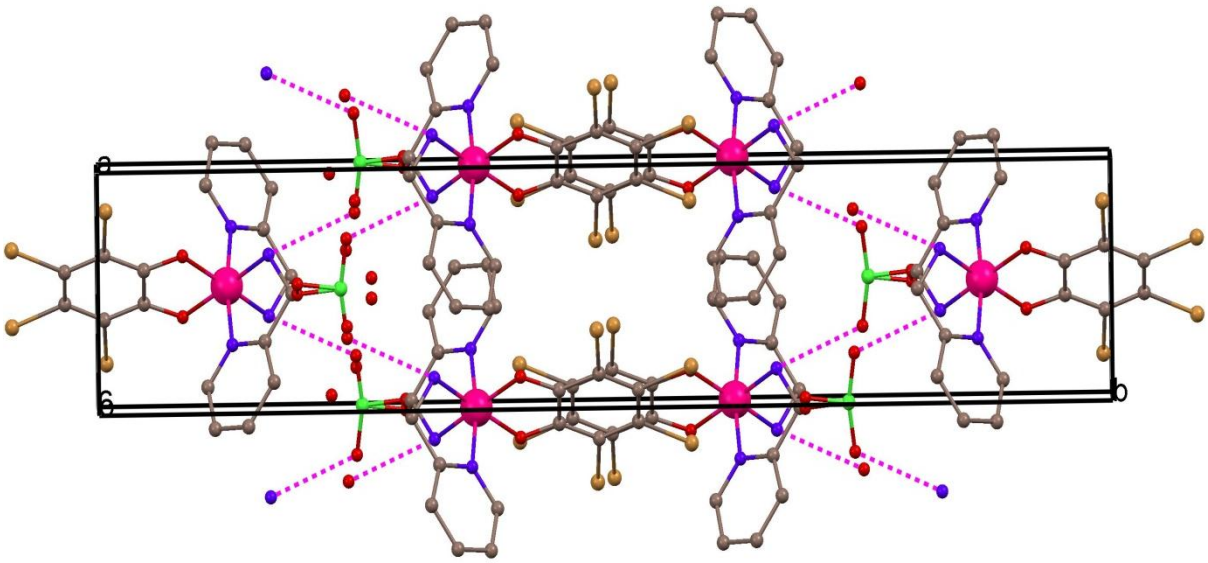

Fig. S8. Molecular packing diagram of **4** showing π···π stacking interaction and hydrogen bonding schemes.

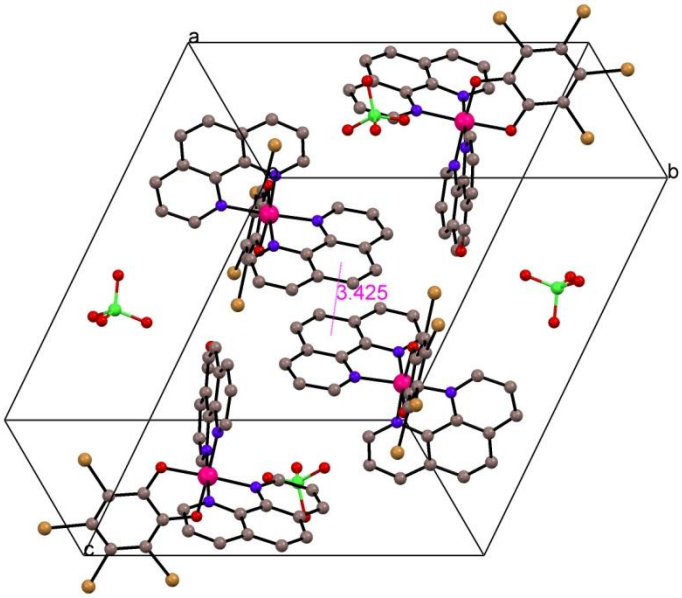

Fig. S9. A part of molecular packing diagram of **6** showing π···π stacking interaction and hydrogen bonding schemes.

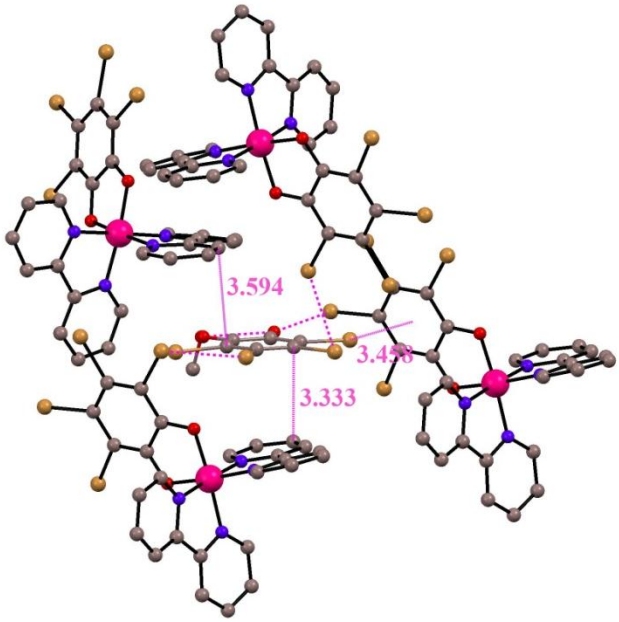

Fig. S10. A part of packing diagram of **7** showing π···π and σ···π interactions and hydrogen bonding schemes.

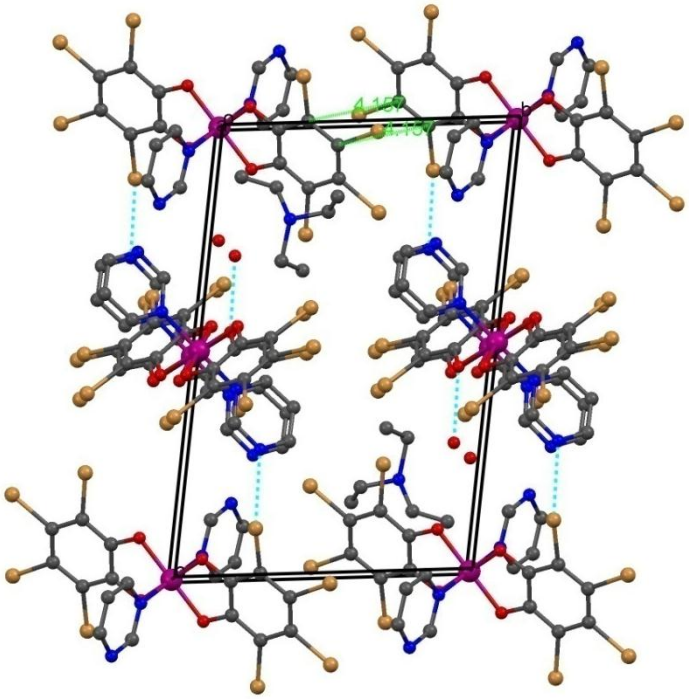

Fig. S11. Molecular packing diagram of **8** showing π···π stacking interaction and hydrogen bonding schemes.

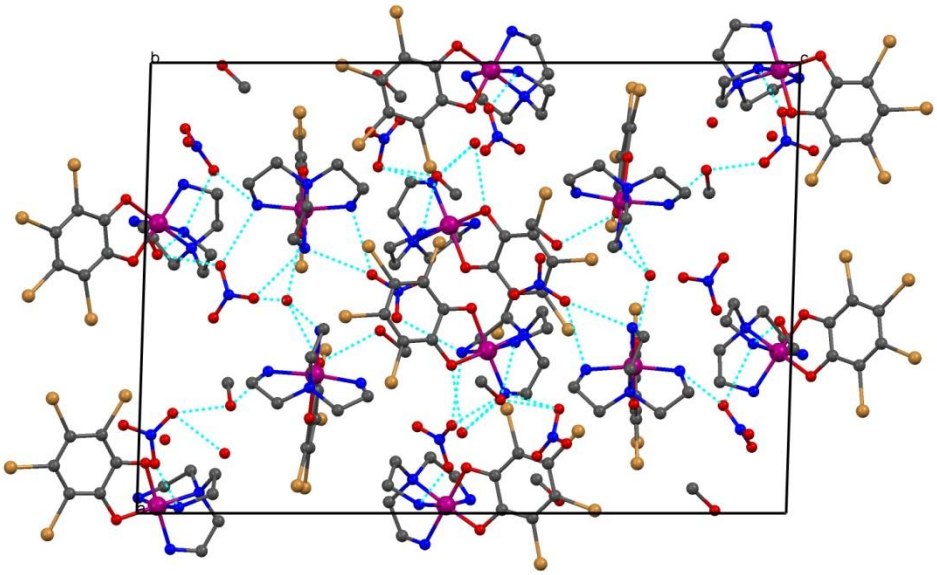

Fig. S12. Molecular packing diagram of **9** showing hydrogen bonding interactions.

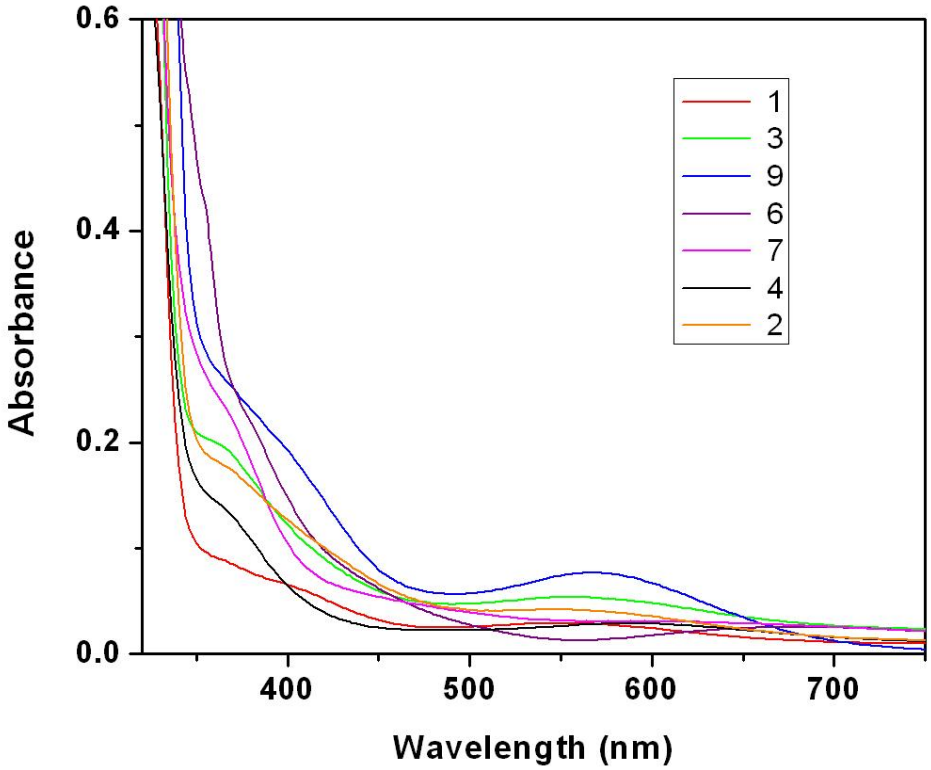

Fig. S13. Absorption spectra of **1**-**4**,**6**,**7** and **9** in methanol.