Electronic Supplementary Information (ESI)

Synthesis, structural investigations and corrosion inhibition studies on Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) complexes with 2-amino-benzoic acid (phenyl-pyridin-2-yl-methylene)-hydrazide

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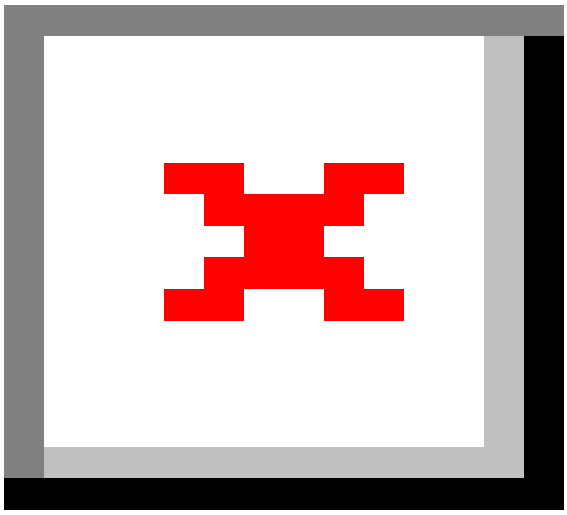


Fig. S1 ^{1}H NMR spectra of Habph in DMSO-d_6.

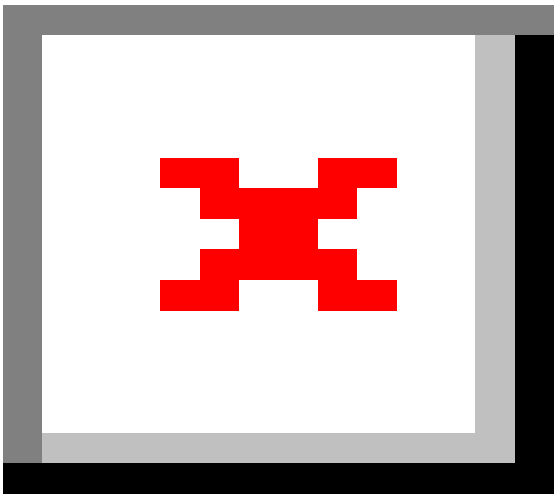


Fig. S2 ^{1}H NMR spectra of [Zn(abph)$_2$] in DMSO-d$_6$.

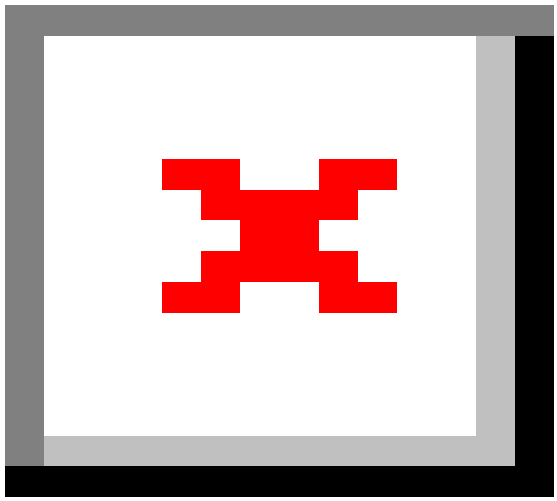


Fig. S3 ^{13}C NMR spectra of Habph in DMSO-d_6.

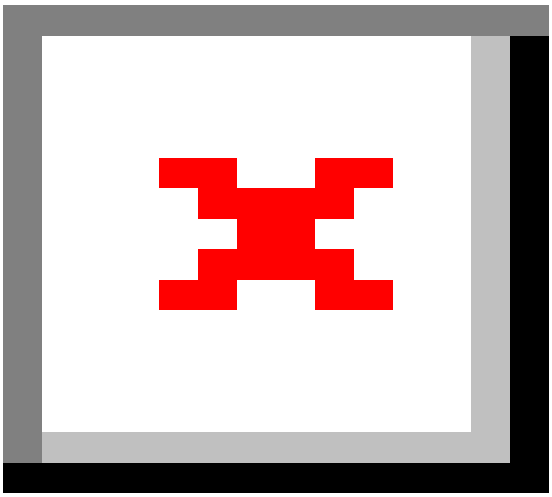


Fig. S4 ^{13}C NMR spectra of $[Zn(abph)_2]$ in DMSO-d_6.

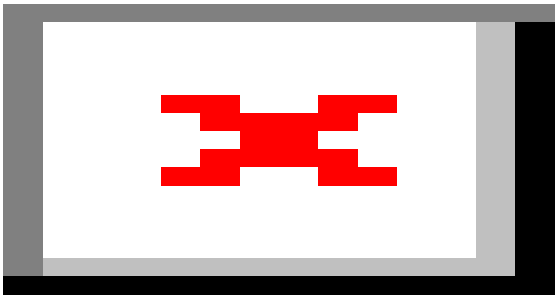


Fig. S5 Various types of C-H···π interactions in Habph.

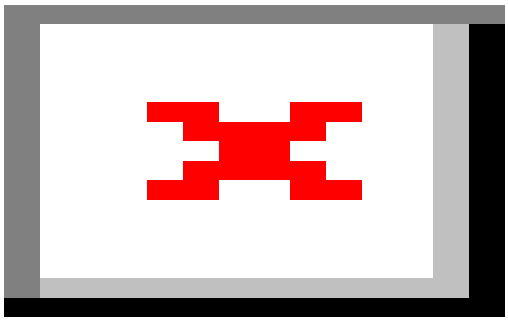


Fig. S6 Various types of π···π and C-H···π interactions in $[Mn(abph)_2]$.

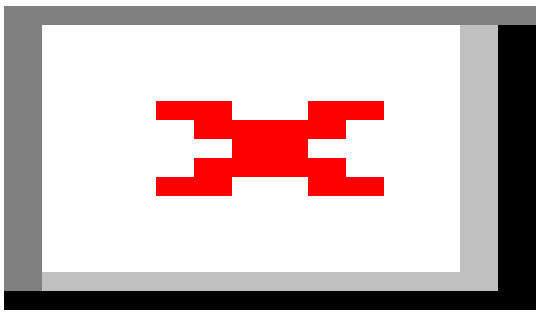


Fig. S7 Various types of π···π and C-H···π interactions in [Ni(abph)$_2$].

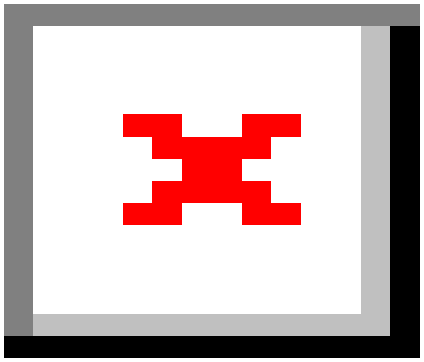


Fig. S8 Various types of π···π and C-H···π interactions in [Cu(abph)$_2$].

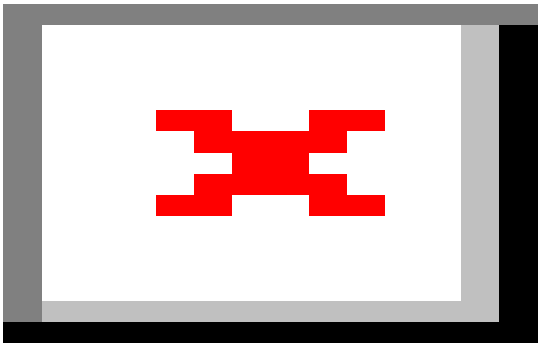
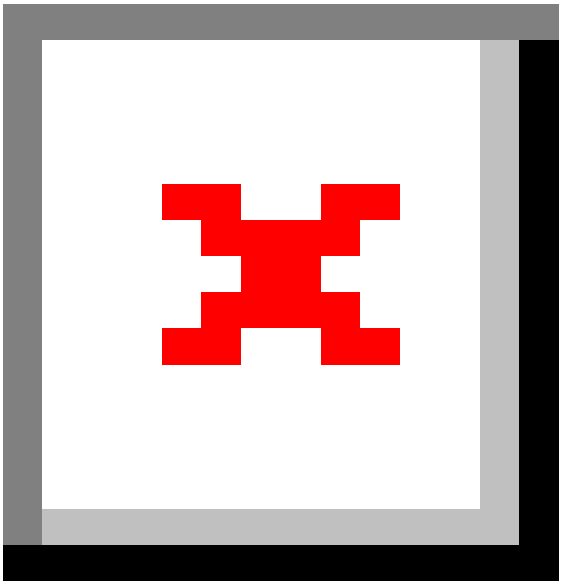


Fig. S9 Various types of π···π and C-H···π interactions in [Zn(abph)$_2$]. 2H$_2$O.



Bond length (Å)		**Bond angles (°)**	
Co–N(1)	2.199	O(2)–Co–N(6)	74.6
Co–N(2)	2.097	N(6)–Co–N(5)	74.9
Co–O(1)	2.084	N(5)–Co-O(1)	89.2
Co–N(5)	2.193	N(2)–Co–O(1)	74.5
Co–N(6)	2.097	O(2)–Co–O(1)	107.2
Co–O(2)	2.088	N(2)–Co–N(1)	89.5
N(2)–C(6)	1.364	N(5)–Co–N(5)	75.0
N(3)–C(13)	1.308		
C(25)–N(6)	1.364		
C(32)–N(7)	1.308		
C(13)–O(1)	1,274		

Fig. S10. Orbital diagram showing electronic transitions in Co(II) complex.

Table S1 Selected bond lengths and angles calculated by UB3LYP method for Co(II) complex.

C(32)–O(2)	1.274

Table S2 Comparison of experimental and theoretical vibrational frequencies of Co(II) complex.

Table S3 TDDFT calculations for UV-Vis transitions and their assignments.

S.N.	UV (Exp.) λ_{max} (nm)	UV (Calc.) λ_{max} (nm)	Transition	Assignments
1	-	1304	HOMO-1→ LUMO+1 (β) 0.28	d_{xy}, d_{yz}, d_{xz} to $d_{x^2-y^2}$, d_{z^2}
2	659	663	HOMO(α)→LUMO+2 (β) 0.51	π (Ligand), d_{xy}, d_{yz}, d_{xz} to $d_{x^2-y^2}$, π of C=N, π (Ligand)
3	492	492	HOMO-1 → LUMO (α) 0.54 HOMO → LUMO+1 (α) 0.74	π (Ligand) to $d_{x^2-y^2}$ π (Ligand), d_{xy}, d_{yz}, d_{xz} to $d_{x^2-y^2}$, π(Ligand)

Experimental values (cm^{-1})		Calculated values (cm^{-1})		Intensity (calculated)	Band assignments
3449s, 3386s		3433, 3372			ν(NH_2)
4	1581m	1567	HOMO-2 → LUMO+1 (β) 0.37	64.247	π (Ligand) to d_{z^2}, $d_{x^2-y^2}$ ν(C=N)
5	1609m	1616	HOMO-4→ LUMO+1 (β)	215.642	ν(N=C–O) π (Ligand) to, π (Ligand)
	1337m	1315	0.85	400.636	ν(C–O)
6	1028w	1013	HOMO-4 → LUMO+2 (β)	80.150	ν(N–N)
	469m	460	0.87	61.883	ν(M-O) π (Ligand) to $d_{x^2-y^2}$, π of C=N, π (Ligand)