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Supplementary Material

Synthesis, Structure, and Biological Assays of Novel Trifluoromethyldiazepine-Metal Complexes

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Figure S1: IR spectra of HDZP and $[Cu(DZP)_2]\cdot 2H_2O$

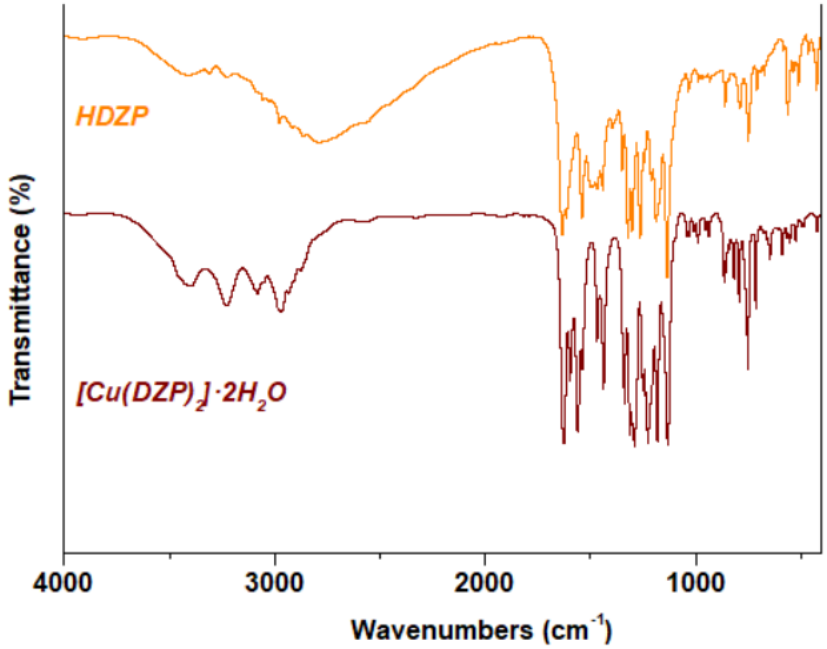


Figure S2: IR spectra of HDZP and $[Ni(DZP)_2]$.

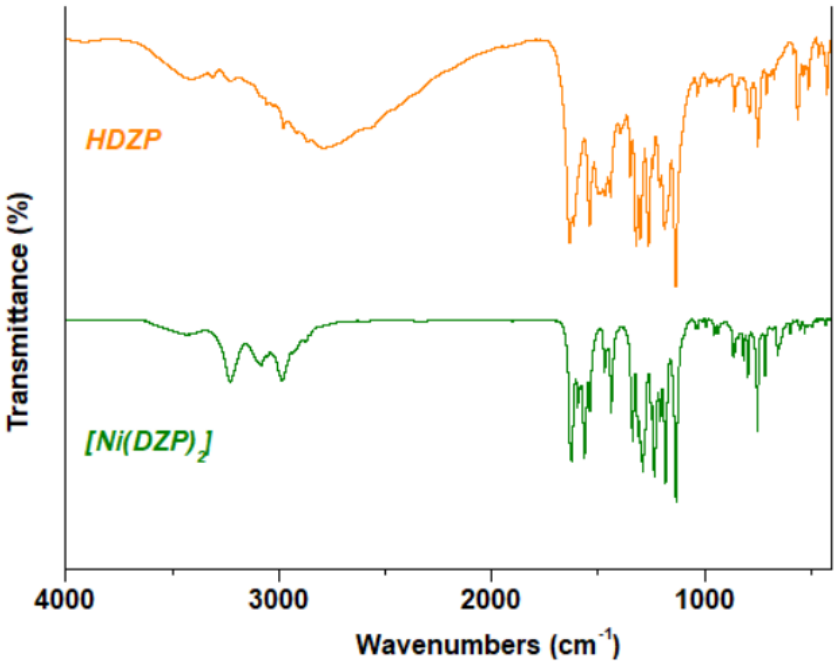


Figure S3: IR spectra of HDZP and $[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$.

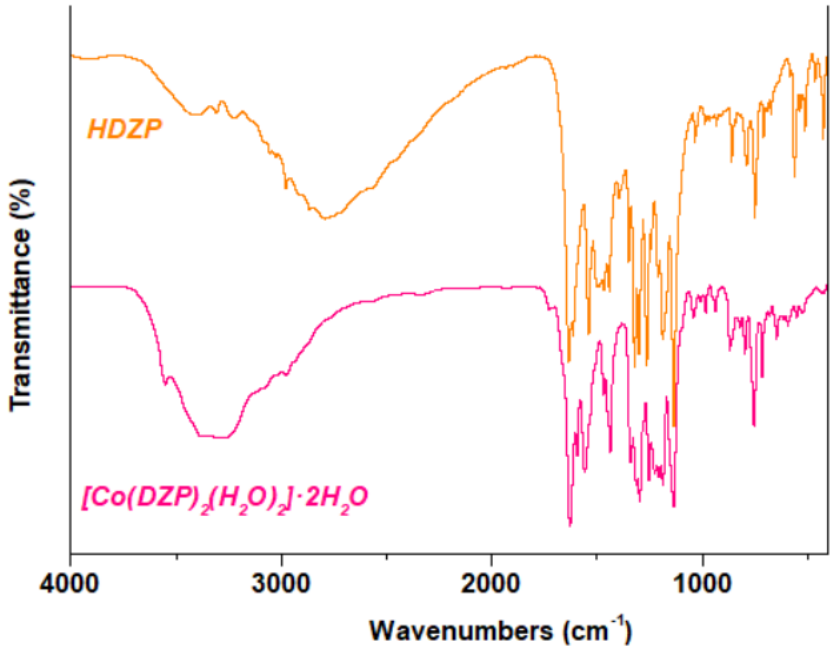


Figure S4: IR spectra of HDZP and $[Mn(DZP)_3]\cdot 2H_2O$.

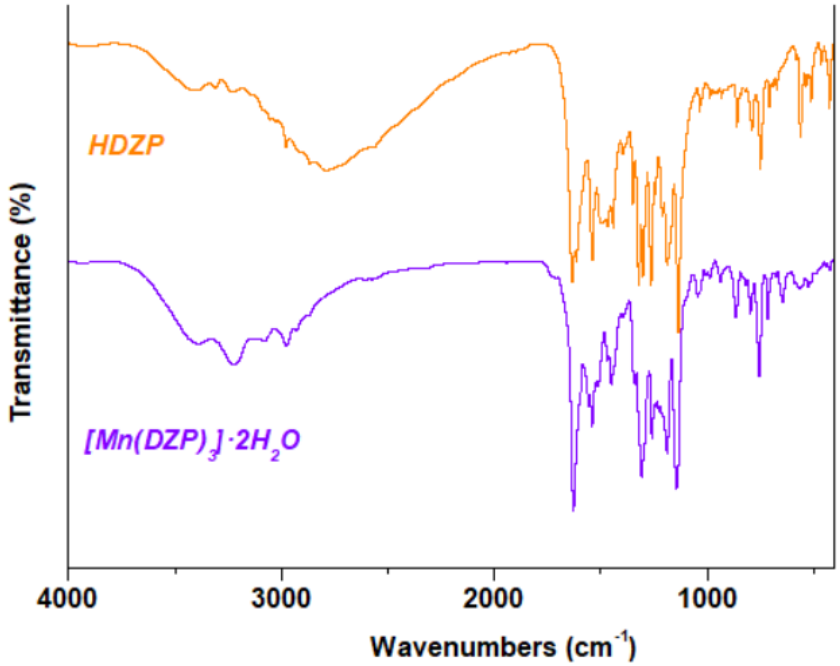


Figure S5: Electronic spectra (in solid state) of HDZP ligand and Cu-DZP, Ni-DZP, Co-DZP and Mn-DZP complexes.

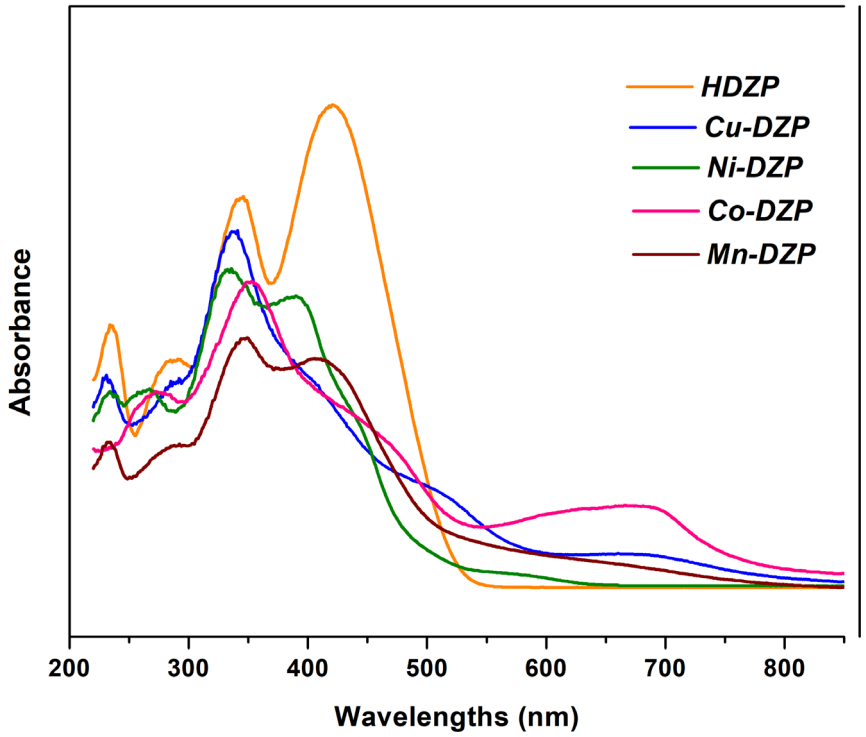


Figure S6: Crystal packing of [Cu(DZP)$_2$] showing C-H···π interactions.

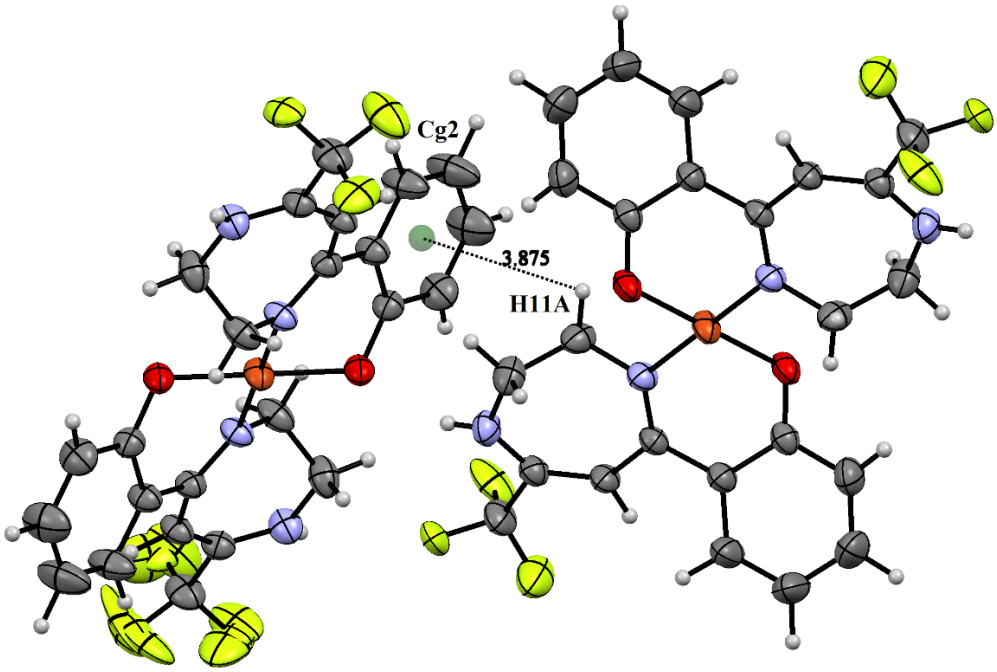


Figure S7: Hirshfeld surface mapped over shape index for [Cu(DZP)$_2$].

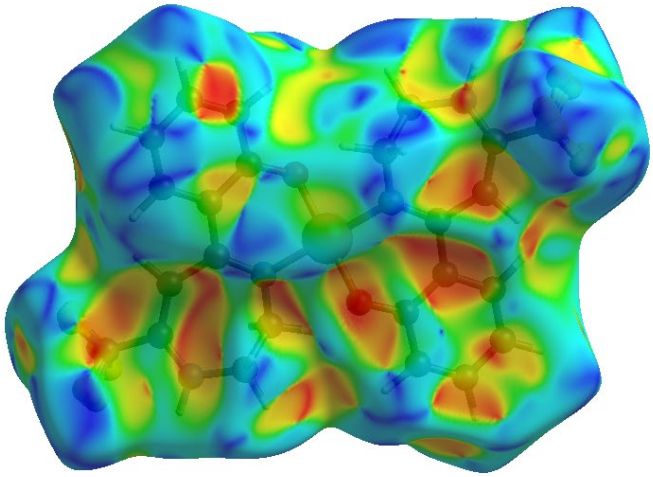


Figure S8: Hirshfeld surface mapped over curvedness for [Cu(DZP)$_2$].

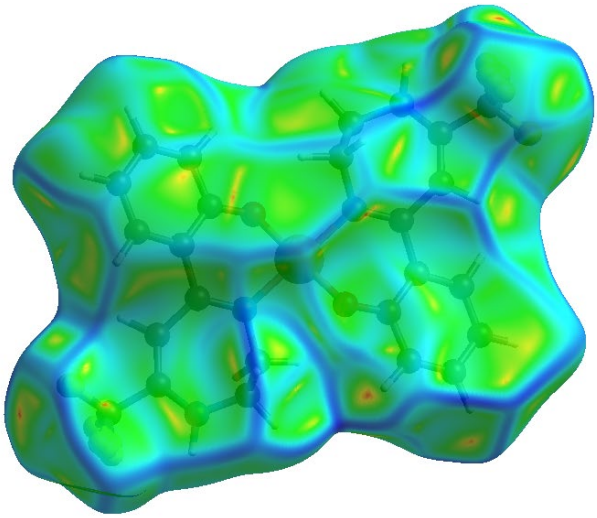


Figure S9: Crystal packing of [Cu(DZP)$_2$] showing C-H···F interactions.

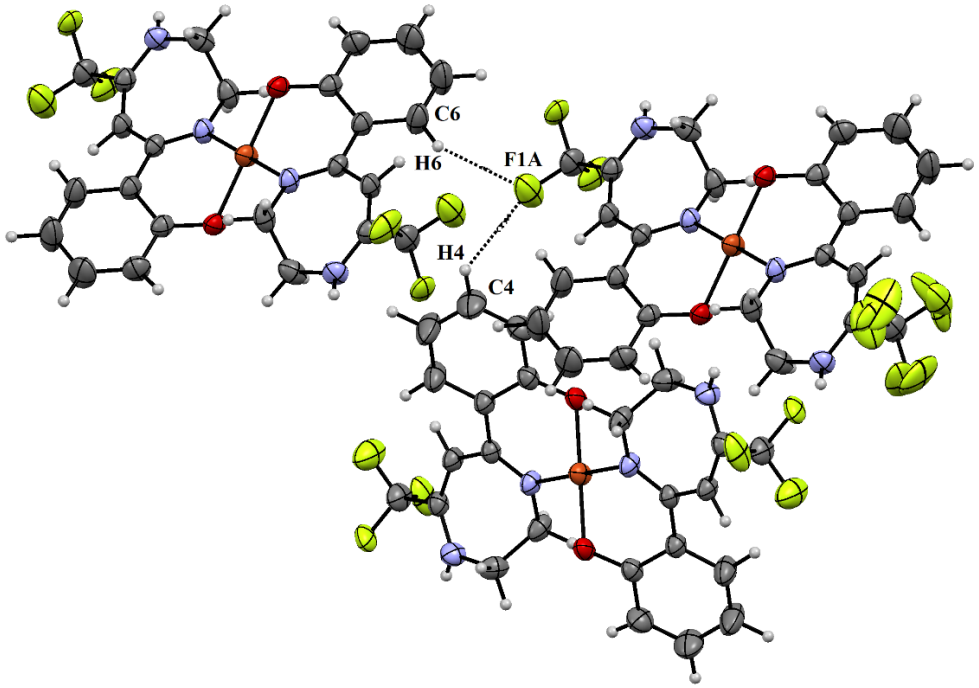


Figure S10: Crystal packing of [Cu(DZP)$_2$] showing non-classical C-H···F intermolecular interactions.

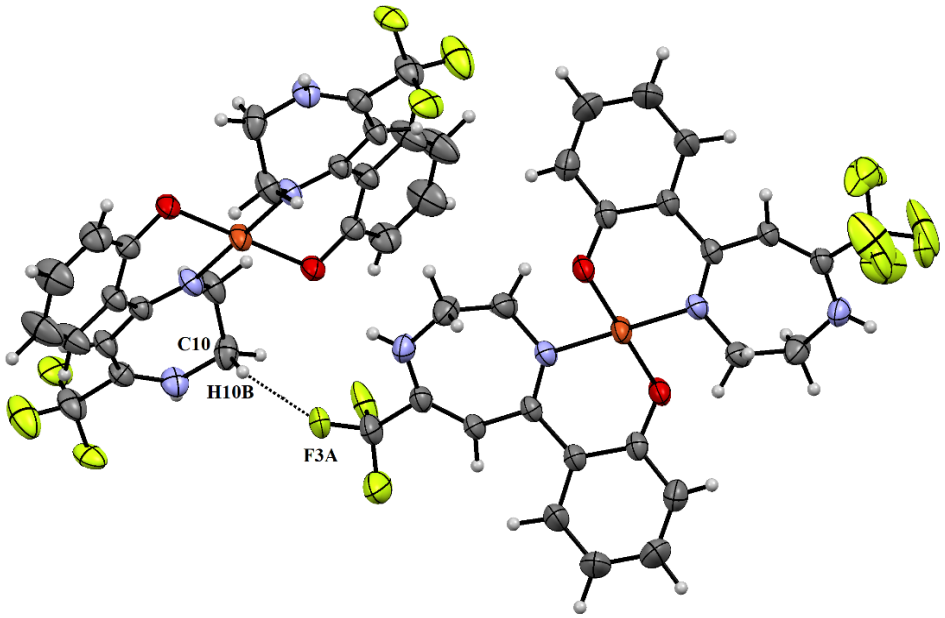


Figure S11: TGA Curve for the thermal decomposition of $[Cu(DZP)_2]\cdot 2H_2O$.

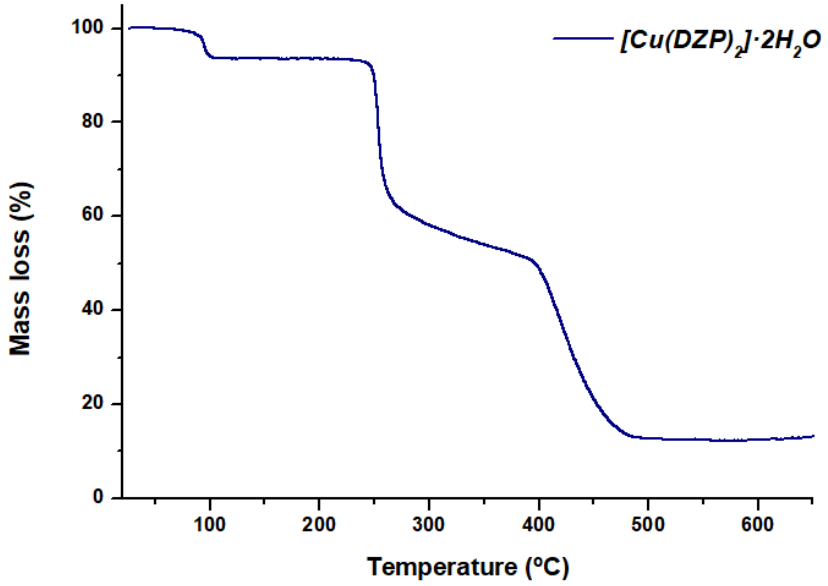


Figure S12: TGA curve for the thermal decomposition of $[Ni(DZP)_2]$.

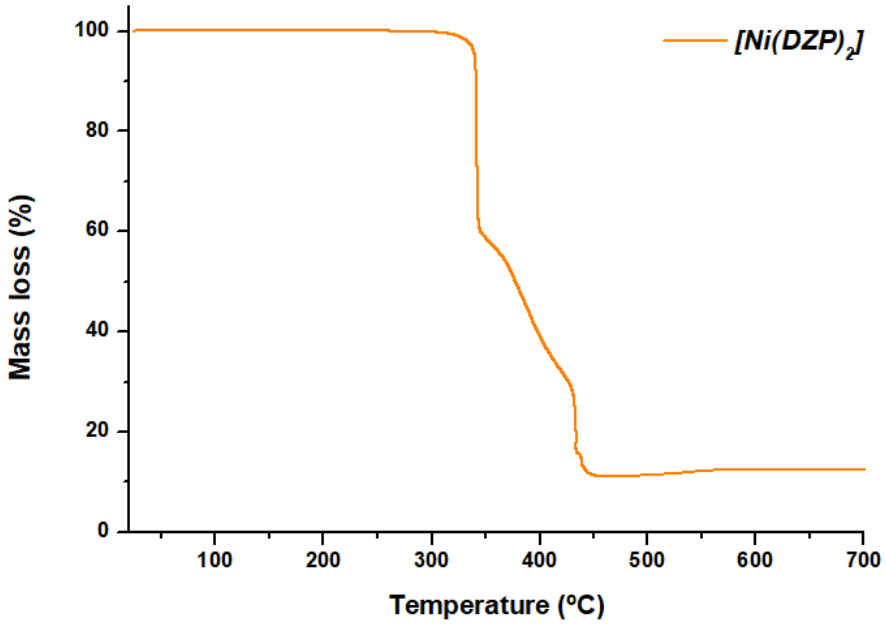


Figure 13: TGA curve for the thermal decomposition of $[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$.

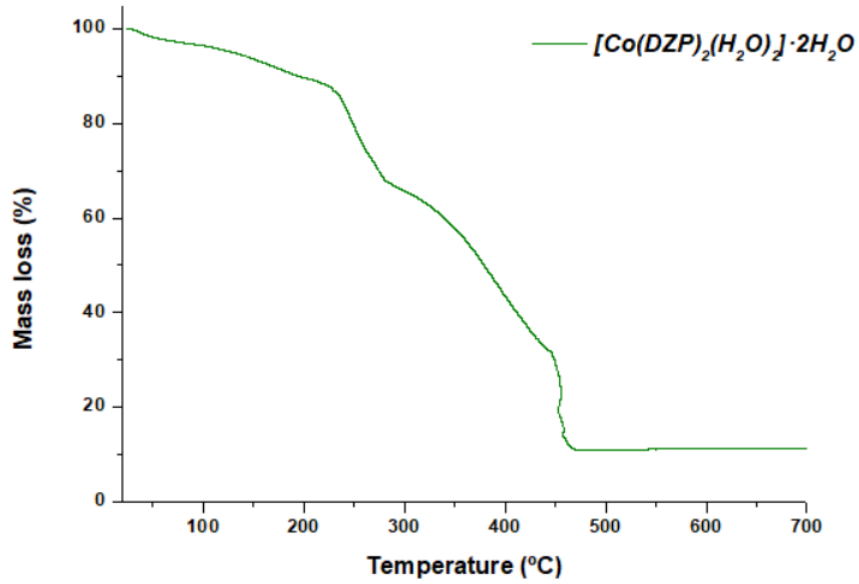


Figure 14: TGA curve for the thermal decomposition of $[Mn(DZP)_3]\cdot 2H_2O$.

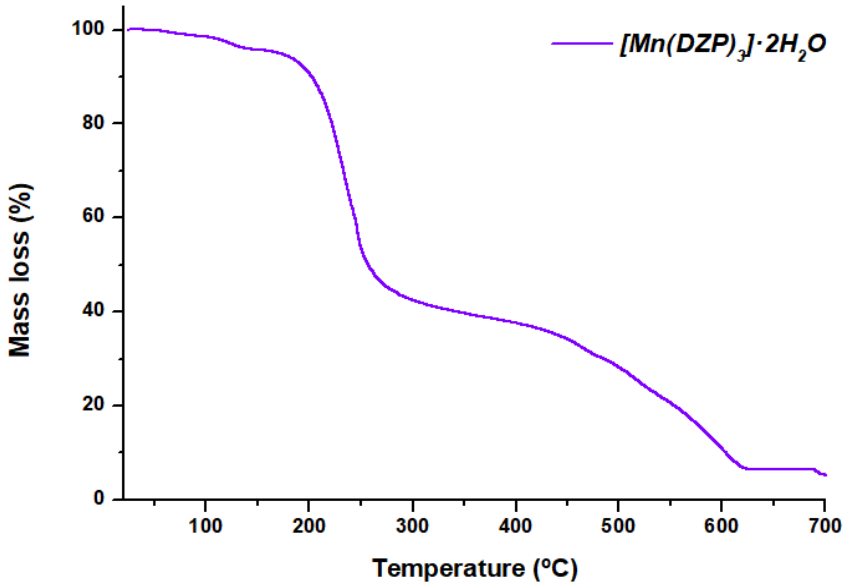
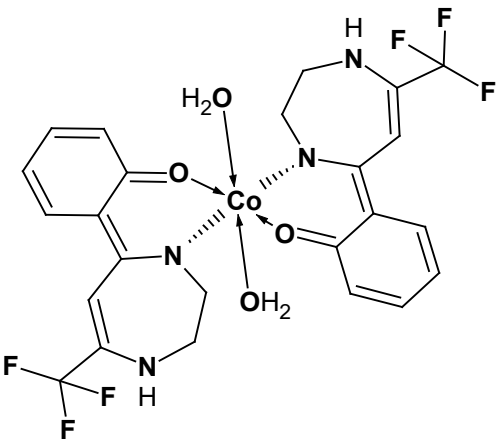


Figure S15: Proposed molecular structures of $[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$ and $[Mn(DZP)_3]\cdot 2H_2O$ complexes.

$[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$



$[Mn(DZP)_3]\cdot 2H_2O$

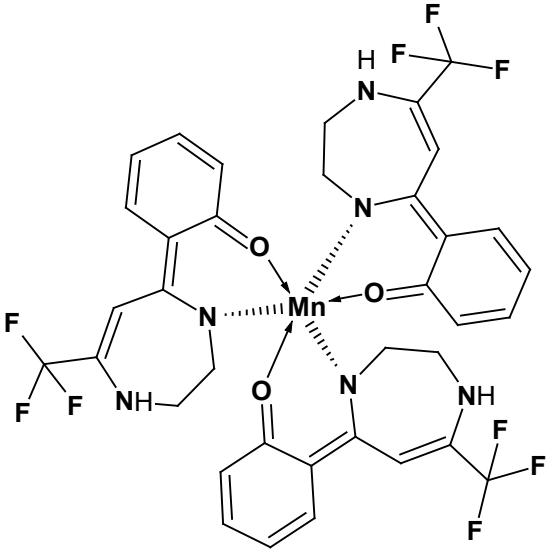


Figure S16: Distribution of bond and ring (red and yellow spheres) critical points in a dimer of $[Cu(DZP)_2]$ complex.

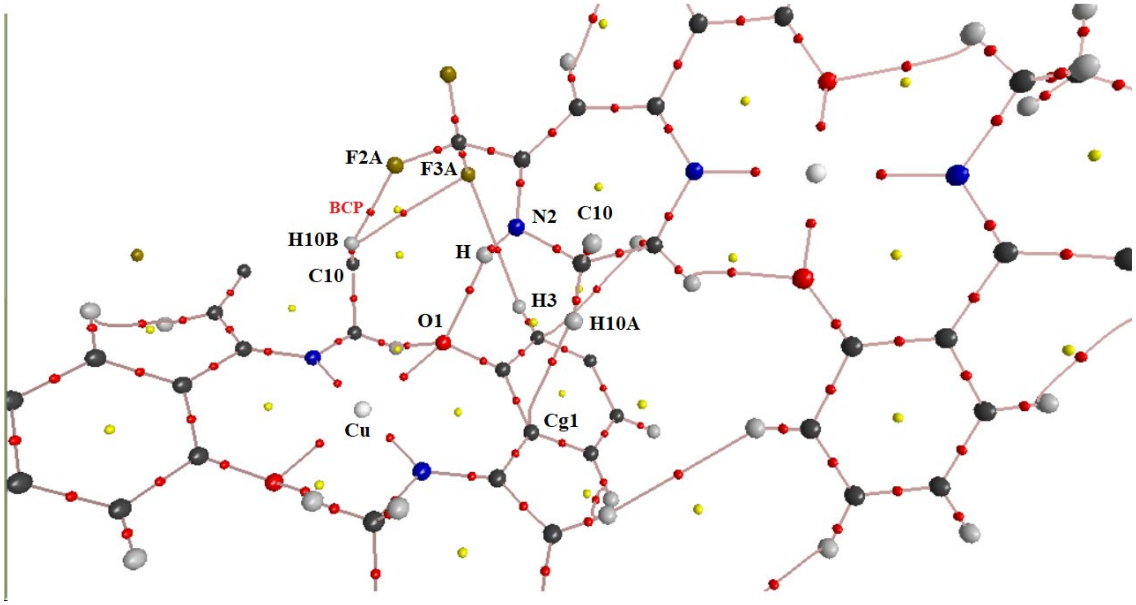


Table S1: Main FTIR bands (in cm^{-1}) and tentative assignment free ligand HDZP and its complexes $[Cu(DZP)_2]\cdot 2H_2O$ (Cu-DZP), $[Ni(DZP)_2]$ (Ni-DZP), $[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$ (Co-DZP) and $[Mn(DZP)_3]\cdot 2H_2O$ (Mn-DZP).

HDZP	***Cu-DZP***	***Ni-DZP***	***Co-DZP***	***Mn-DZP***	***Assignments*** [a]
3242	3229	3226	-	3221	ν N2-H
3054	3052	3051	3076	3080	ν C-H
2978	2971	2985	2978	2978	ν_a CH_2
2921	2935	2936	-	2930	ν_a CH_2
2866	2865	2870	-	2878	ν_s CH_2
2768	-	-	-	-	ν N1-H
1635	1624	1624	1628	1628	ν C=O + ν C10-C11
1615	1596	1596	1594	1598	ν C=C (R1)
1540	1562	1565	1557	1558	ν C-N
1526	1539	1539	1537	1541	δ N2-H
1464	1469	1470	1469	1469	δ CH_2
1442	1438	1439	1437	1448	δ CH_2
1322	1312	1313	1313	1307	ω CH_2
1302	1300	1301	1297	1295	ω CH_2
1263	1291	1290	1254	1259	ν C-C (R1)
1243	1238	1236	-	1241	ν C10-C12
1211	1227	1208	1206	1227	τω CH_2
1189	1183	1183	1186	1188	ν_a CF_3
1136	1132	1134	1136	1145	ν_a CF_3
1036	1039	1040	1042	1044	ν_s CF_3
1028	1031	1030	1033	1034	ρ CH_2
987	-	-	-	-	γ N1-H
934	937	937	937	938	γ N2-H
861	865	865	870	866	δ CCC (R2) + δ CCN (R2)
788	793	796	798	797	δ CCN (R2)
750	752	751	754	755	δ C=O
708	714	715	716	715	δ_s CF_3
673	681	-	681	674	γ NCC (R2)
563	564	-	579	565	δ_a CF_3
536	552	552	552	552	δ CCO (R1)
-	590	597	594	591	ν M-N
-	487	451	489	487	ν M-O

[a] ν: stretching, δ: bending, ω: wagging, τω: twisting, γ: out-of-plane bending modes; a: antisymmetric, s: symmetric.

Table S2: Electronic spectral data of $[Cu(DZP)_2]\cdot 2H_2O$, $[Ni(DZP)_2]$, $[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$ and $[Mn(DZP)_3]\cdot 2H_2O$ complexes.

Complex	***UV-Vis bands (nm)***	***Assignment***
$[Cu(DZP)_2]\cdot 2H_2O$	231	$\pi \rightarrow \pi^*$
	290	$\pi \rightarrow \pi^*$
	337	$n \rightarrow \pi^*$
	387	Charge transfer
	492	$^2B_{1g} \rightarrow {}^2B_{2g}$
	674	$^2B_{1g} \rightarrow {}^2A_{1g}$
$[Ni(DZP)_2]$	234	$\pi \rightarrow \pi^*$
	268	$\pi \rightarrow \pi^*$
	334	$n \rightarrow \pi^*$
	389	Charge transfer
	563	$^1A_{1g} \rightarrow {}^1B_{1g}$
$[Co(DZP)_2(H_2O)_2]\cdot 2H_2O$	273	$\pi \rightarrow \pi^*$
	354	$n \rightarrow \pi^*$
	418	$^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$
	629	$^4T_{1g}(F) \rightarrow {}^4A_{2g}(F)$
$[Mn(DZP)_3]\cdot 2H_2O$	232	$\pi \rightarrow \pi^*$
	290	$\pi \rightarrow \pi^*$
	408	$^6A_{1g} \rightarrow {}^4E_g, {}^4A_{1g}\ (^4G)$

Table S3: Hydrogen bonds for $[Cu(DZP)_2]\cdot 2H_2O$ [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(11)-H(11A)···O#1	0.97	2.47	2.984(3)	113
N(2)-H(2N)···O#2	0.86	2.17	2.871(3)	139

Symmetry transformations used to generate equivalent atoms: (#1) -x+1, -y+1, -z+2; (#2) -x+1, y-1/2, -z+3/2.