Electronic Supplementary Information

Three-Dimensional-Coordination Polymer of Zn(II)-Carboxylate: Structural Elucidation, Photoelectrical Conductivity, and Biological Activity

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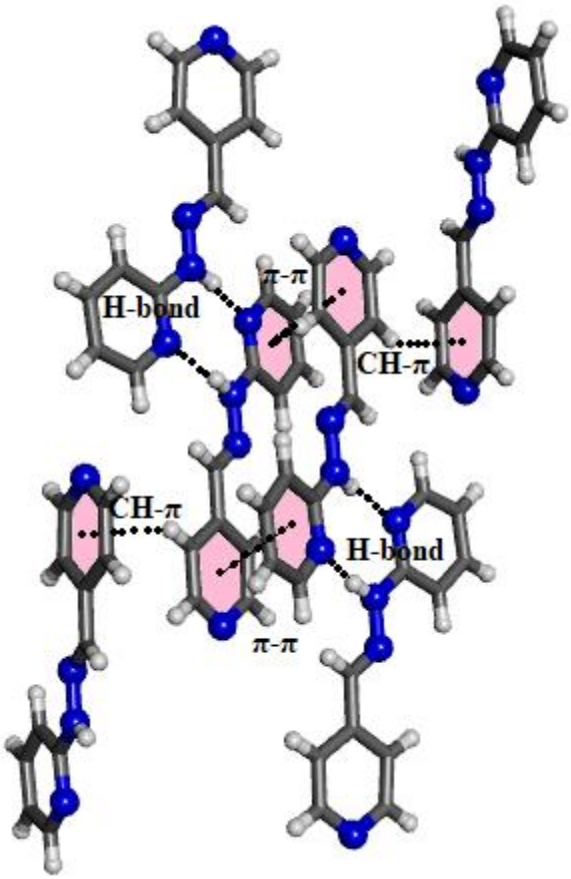


Figure S1. Packing of **ppmh** ligand along crystallographic axis “b”.

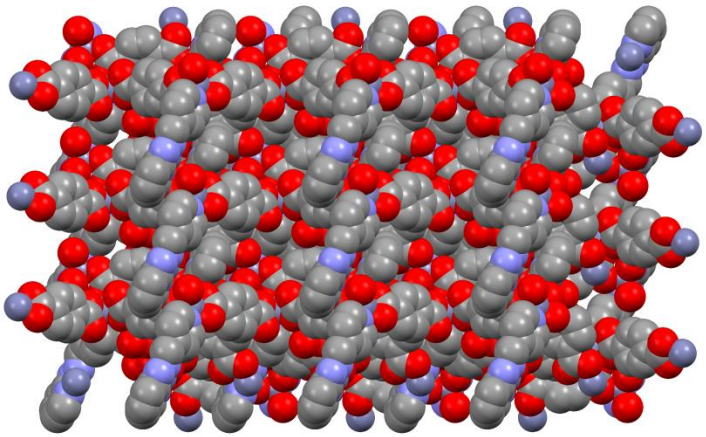
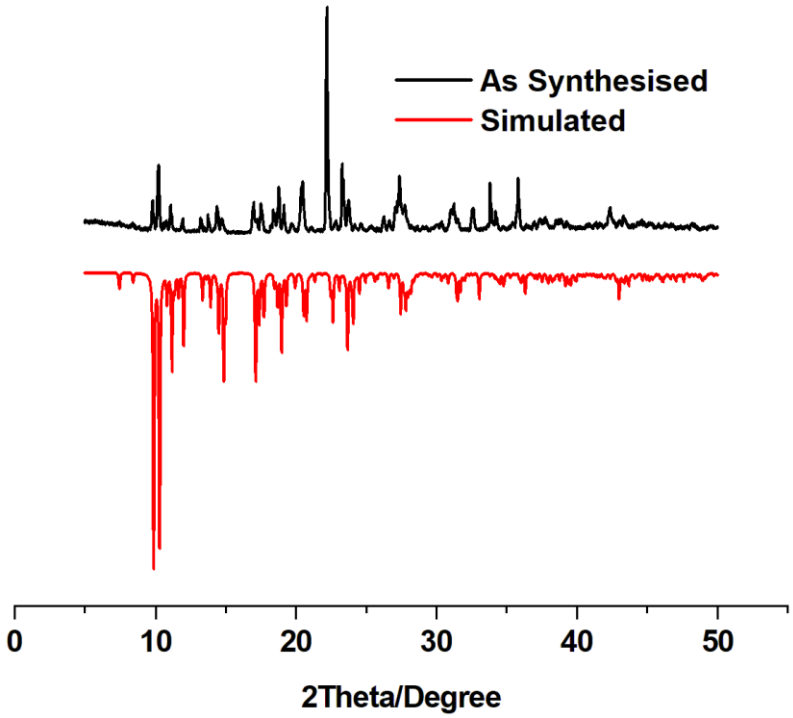
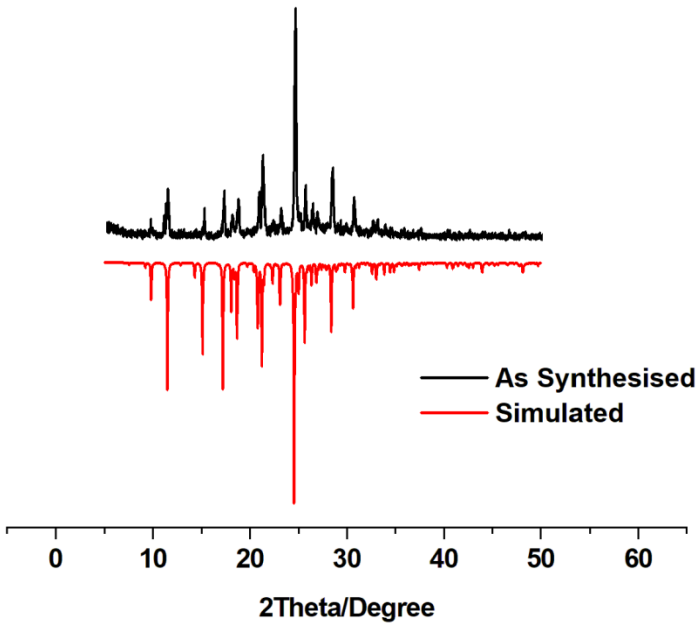


Figure S2. Spacefill view of supramolecular aggregation for the polymeric compound **1** along crystallographic axis "b".



(a)



(b)

Figure S3. Powder X-ray diffraction patterns of **(a)** compound **1 (b) ppmh** [simulated (black) and as-synthesized (red).]

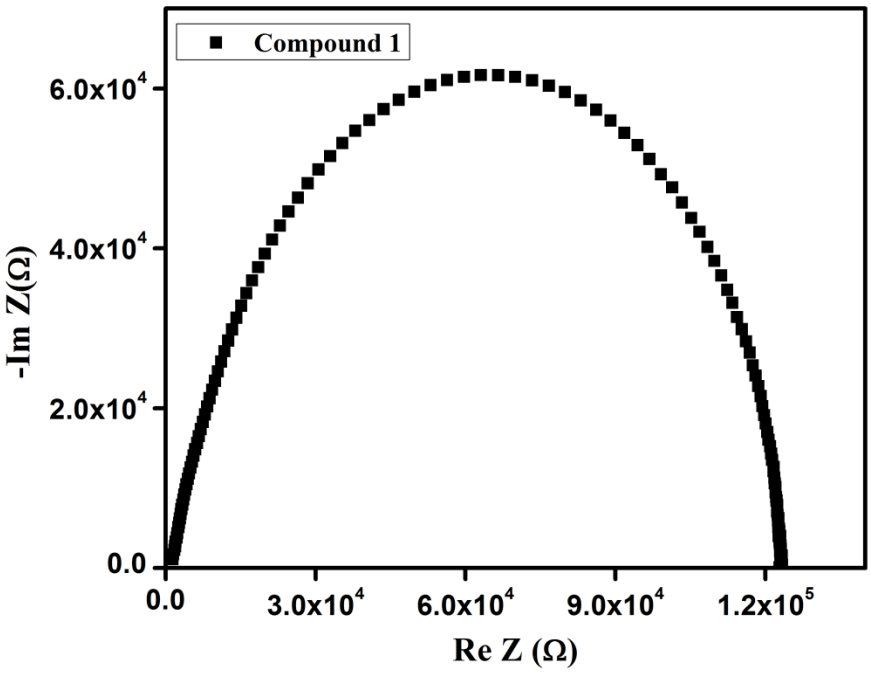
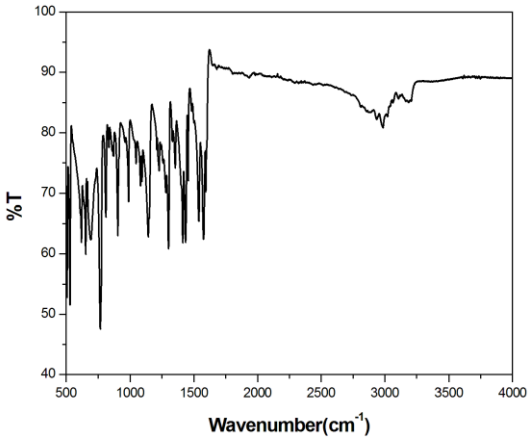
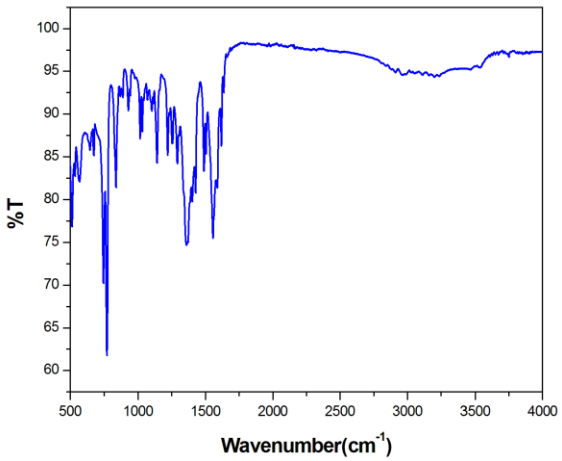


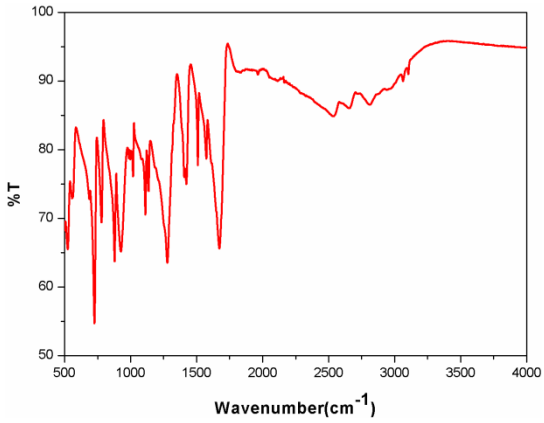
Figure S4. Nyquist Plot of Compound **1**



(a) IR spectrum of **ppmh**

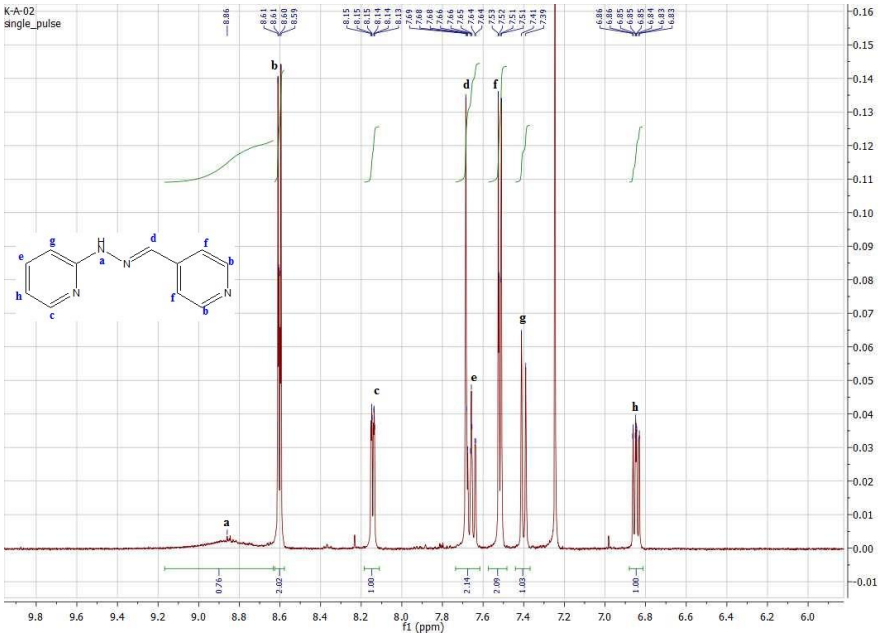


(b) IR spectrum of Compound **1**.

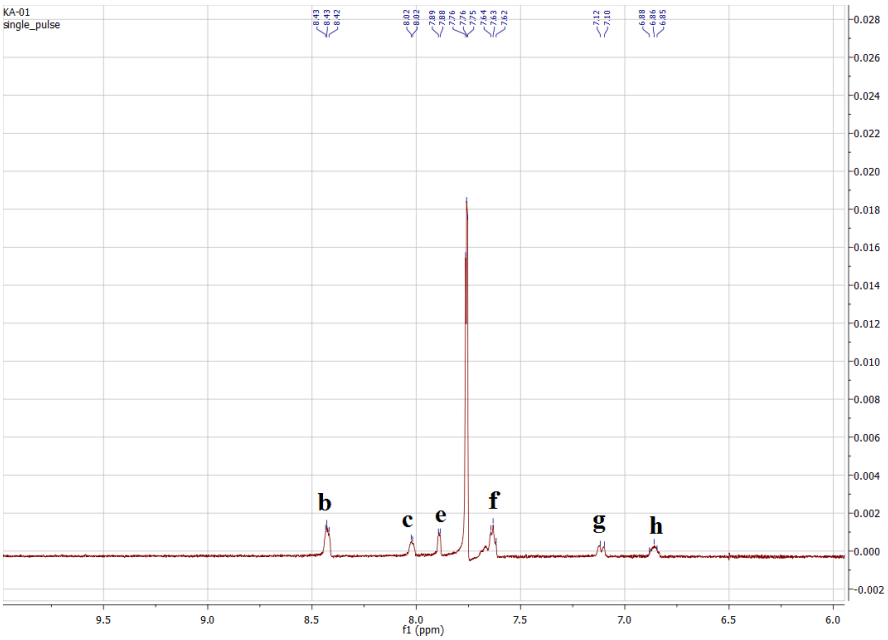


(c) IR spectrum of H_2**bdc**.

Figure S5: (a) IR spectrum of **ppmh, (b)** IR spectrum of Compound **1**. **(c)** IR spectrum of H_2**bdc**.

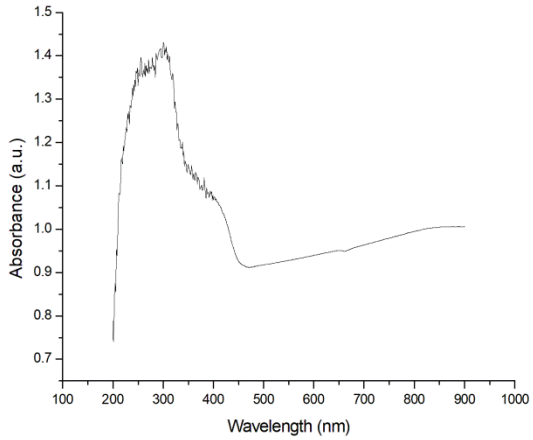


(a) ^{1}H NMR Spectrum of **ppmh** in $CDCl_3$

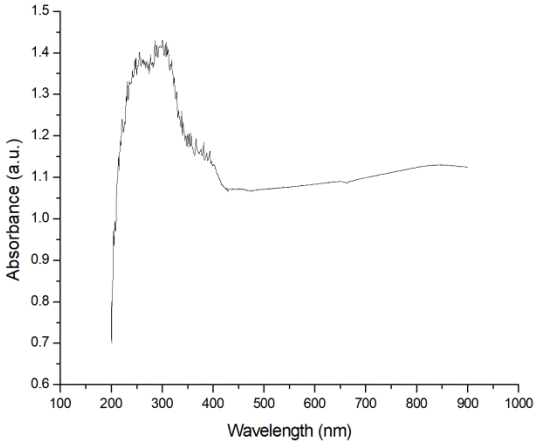


(b) ^{1}H NMR spectrum of the compound **1** after 24 h of solution (DMSO-d_6 and D_2O mixture, 1:10 (v/v))

Figure S6: (a) ^{1}H NMR Spectrum of **ppmh** in $CDCl_3$, (b) ^{1}H NMR spectrum of the compound **1** after 24 h of solution (DMSO-d_6 and D_2O mixture, 1:10 (v/v)).

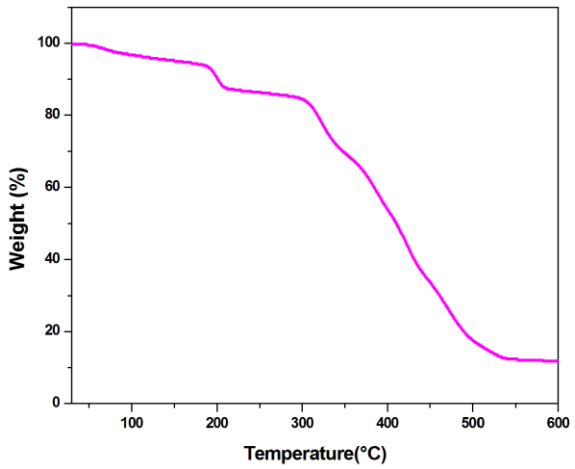


(a)

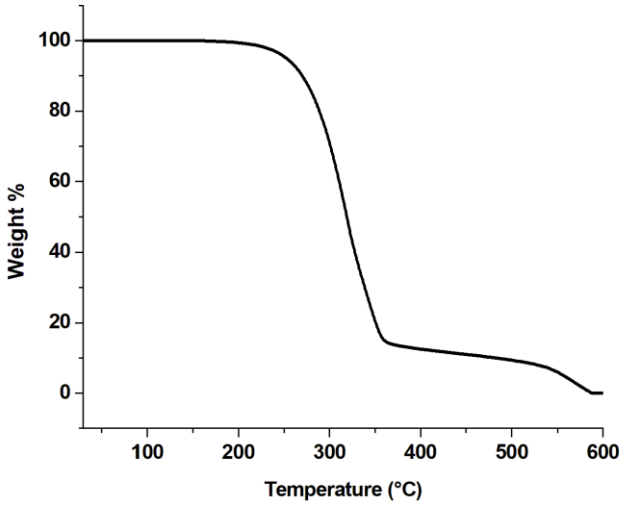


(b)

Figure S7: Solid State UV-vis spectra of (a) **ppmh** at wavelength 378 nm and (b) Compound **1** **at** 396 nm



(a)



(b)

Figure S8. TGA plot of **(a)** compound **1** (pink) and **(b) ppmh** under N_2 atmosphere.

Table S1. Selected bond lengths in **ppmh**

N1- C8	1.375(3)	C8- H8	0.9300
N4- N5	1.3551(19)	C10- C9	1.373(3)
N4- C6	1.371(2)	C3- C4	1.385(3)
N4- H33	0.8600	C3- C2	1.376(3)
N3- C6	1.330(2)	C2- C1	1.375(3)
N3- C11	1.338(2)	C6- C7	1.382(3)
N5- C5	1.273(2)	C5- C3	1.456(2)
N1- C1	1.322(3)	C7- C9	1.362(3)
N7- C19	1.373(2)	C11- C10	1.328(3)
C4- H32	0.9300	C4- C8	1.358(3)

Table S2. Selected bond lengths and bond angles in compound **1**

Zn01-O1	1.997(7)	Zn04-O3	1.986(7)
Zn01-O8	2.533(9)	Zn04-O5	2.058(10)
Zn01-O9	1.975(8)	Zn04-O6	1.973(7)
Zn01-O14	2.729(10)	Zn04-O7	2.689(8)
Zn01-O15	1.984(8)	Zn04-N6_h	2.452(10)
Zn01-N2	2.035(8)	Zn04-N8_h	2.038(10)
Zn02-O2	1.982(7)	O1-Zn01-O9	122.1(3)
Zn02-O18	2.083(8)	O1-Zn01-O14	146.7(3)
Zn02- N3_e	2.441(9)	O1-Zn01-O15	96.0(3)
Zn02-N5_e	2.045(10)	O1-Zn01-N2	95.5(3)
Zn02-O12_f	1.979(7)	O8-Zn01-O9	56.4(3)
Zn02-O13_f	2.692(7)	O8-Zn01-O14	96.5(3)
Zn03- O10	2.622(11)	O8-Zn01-O15	85.5(3)
Zn03- O11	2.000(8)	O8-Zn01-N2	161.6(3)
Zn03-N1	2.033(8)	O9-Zn01-O14	88.4(3)
Zn03- O16_c	2.134(11)	O9-Zn01-O15	123.2(3)
Zn03-O17_c	2.255(10)	O9-Zn01-N2	105.9(3)
Zn03-O4_i	2.014(7)	O14-Zn01-O15	52.7(3)
O1-Zn01-O8	91.1(3)	O14-Zn01-N2	87.4(3)
O15-Zn01-N2	110.7(3)	O2-Zn02-O12_f	101.6(3)
O2-Zn02-O18	99.2(3)	O2-Zn02-O13_f	153.0(2)
O2-Zn02-N3_e	90.9(3)	O18 -Zn02-N3_e	169.3(3)
O2-Zn02-N5_e	116.8(3)	O18- Zn02-N5_e	98.9(3)
O18-Zn02-O12_f	97.6(3)	O18-Zn02-O13_f	94.5(3)
N3_e-Zn02-N5_e	73.3(3)	N3_e-Zn02-O12_f	83.5(3)
N3_e-Zn02-O13_f	77.6(3)	N5_e-Zn02-O12_f	134.7(3)
N5_e-Zn02-O13_f	83.6(3)	O12_f-Zn02-O13_f	53.3(3)
O10-Zn03-O11	53.8(4)	O10-Zn03-N1	88.1(3)
O10-Zn03-O16_c	86.7(4)	O10-Zn03-O17_c	91.2(4)
O10-Zn03-C30_c	87.0(4)	O10-Zn03-O4_i	145.7(3)
O11-Zn03-N1	110.5(3)	O11-Zn03-O16_c	130.7(4)
O11-Zn03-O17_c	89.3(3)	O11-Zn03-C30_c	109.4(4)
O11-Zn03-O4_i	93.4(3)	N1-Zn03-O16_c	94.1(4)
N1-Zn03-O17_c	154.5(3)	N1-Zn03-C30_c	125.7(5)
N1-Zn03-O4_i	96.2(3)	O16_c -Zn03-O17_c	60.3(4)
O16_c-Zn03-C30_c	31.6(5)	O16_c-Zn03-O4_i	126.7(4)
O17_c- Zn03-C30_c	28.8(5)	O17_c-Zn03-O4_i	98.7(4)
C30_c-Zn03-O4_i	116.6(5)	O3-Zn04-O5	98.5(3)
O3-Zn04-O6	100.9(3)	O3-Zn04-O7	152.9(3)
O3-Zn04-N6_h	91.7(3)	O3-Zn04-N8_h	117.8(3)
O5-Zn04-O6	97.7(3)	O5-Zn04-O7	93.9(3)

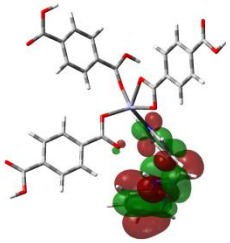
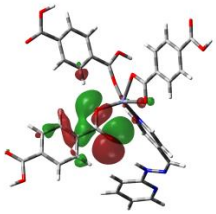
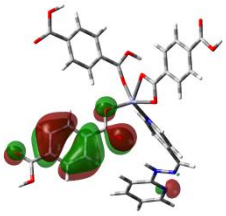
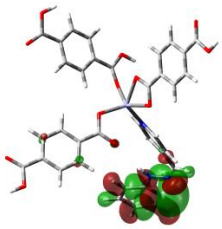
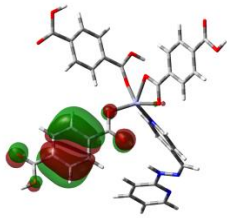
O5-Zn04-N6_h	169.1(3)	O5-Zn04-N8_h	98.4(4)
O6-Zn04-O7	53.4(3)	O6-Zn04-N6_h	84.2(3)
O6-Zn04-N8_h	135.1(3)	O7-Zn04-N6_h	78.5(3)
O7-Zn04-N8_h	83.9(3)	N6_h -Zn04-N8_h	73.2(3)
Zn01-O1-C1	131.6(7)	Zn02-O2-C1	126.9(6)
Zn04-O3-C8	126.9(6)	C8-O4-Zn03_j	131.8(7)
Zn04-O6 -C9	108.4(6)	Zn04-O7-C9	75.7(6)
Zn01-O8-C17	78.3(7)	Zn01-O9-C17	103.5(7)
Zn03-O10-C22	78.1(7)	Zn03-O11 -C22	108.5(8)
C16-O12-Zn02_a	107.5(6)	C16-O13-Zn02_a	75.3(6)
Zn01-O14-C25	74.4(7)	Zn01-O15-C25	108.8(7)
C30-O16-Zn03_d	88.9(9)	C30-O17-Zn03_d	85.9(9)
Zn03-N1- C44	121.0(6)	Zn03-N1-C48	121.8(7)
C44-N1-C48	116.6(9)	Zn01-N2-C33	122.1(7)
Zn01-N2-C37	120.6(6)	C33-N2-C37	116.8(9)
N4-N3-C38	114.9(9)	N4-N3-Zn02_b	105.7(6)
C38-N3-Zn02_b	137.4(7)	N3-N4-C39	119.7(10)
C39-N5-C43	117.3(11)	C39-N5-Zn02_b	121.0(7)
C43-N5-Zn02_b	121.7(9)	N7-N6-C49	114.9(10)
N7-N6-Zn04_g	105.6(6)	C49-N6-Zn04_g	136.1(8)
N6-N7-C50	121.8(9)	C50-N8-C54	115.6(10)
C50-N8-Zn04_g	122.2(7)	C54-N8-Zn04_g	121.8(9)

Symmetry code: a = -1+x,y,-1+z; b = -1+x,y,z; c = x,y,-1+z; d = x,y,1+z; e = 1+x,y,z; f = 1+x,y,1+z; g = 1-x,-1/2+y,1-z; h = 1-x,1/2+y,1-z ; i = 2-x,-1/2+y,1-z; j = 2-x,1/2+y,1-z

Table S3: TDDFT Table of **ppmh** and Compound **1**

Excitation energy (eV)	Wavelength Exp. (nm)	Wavelength Thro. (nm)	Oscillation Frequency (f)	Key Transitions
ppmh				
3.28 eV	378	332.53	f=0.7436	HOMO→LUMO, 49.56%
Compound **1**				
3.13 eV	396	378.00	f=0.4749	HOMO→ LUMO+1, 48.15%

Table S4. DFT table of compound **1**.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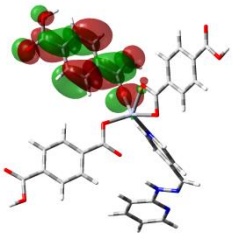	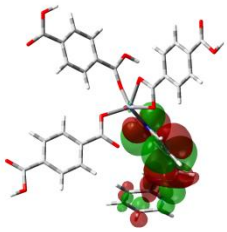			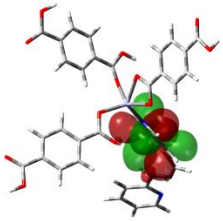
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Table S5. DFT table of **ppmh**.

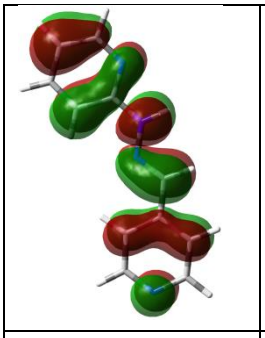
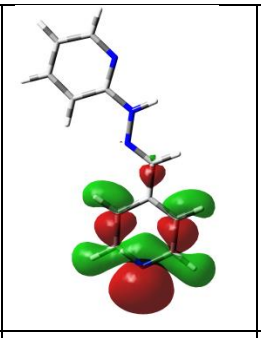
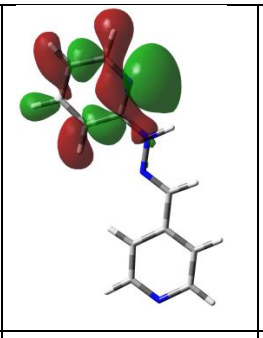
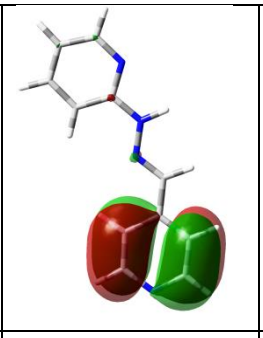
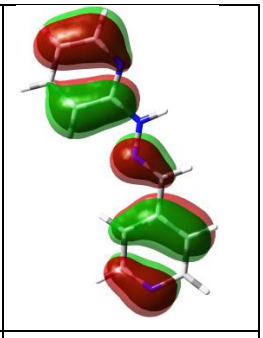
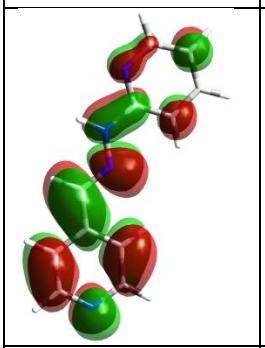
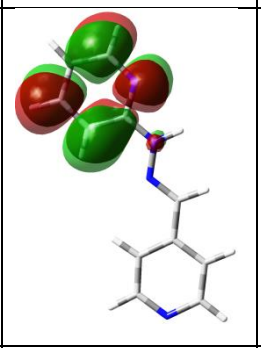
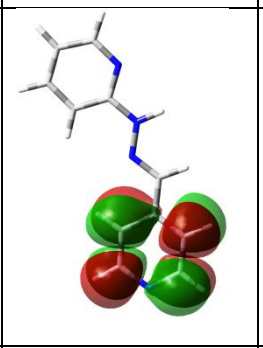
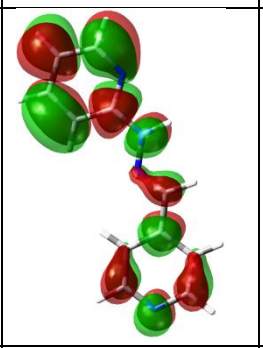
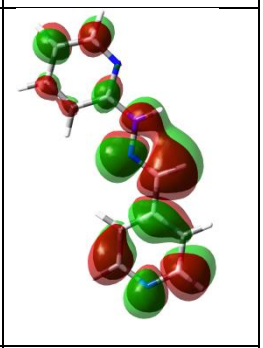
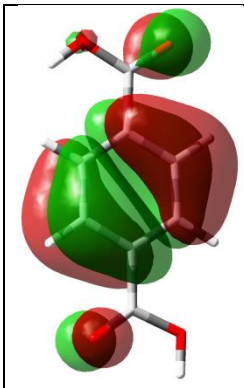
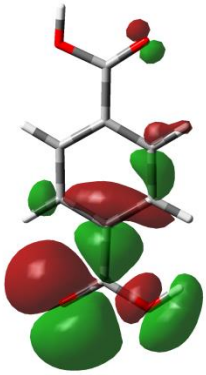
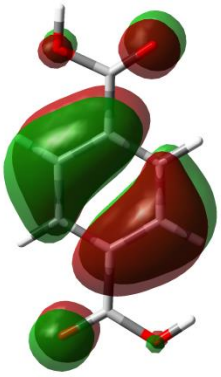
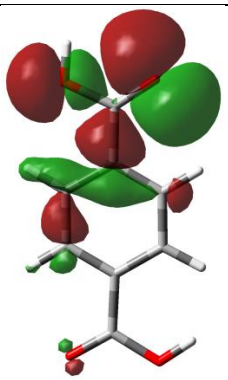
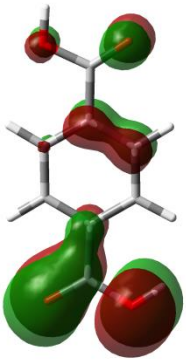
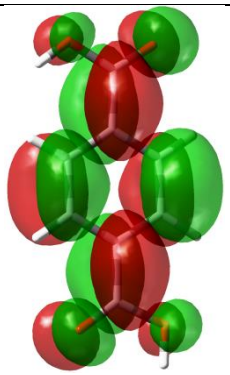
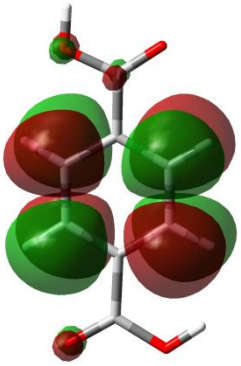
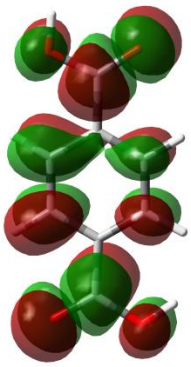
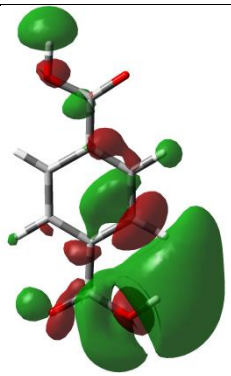
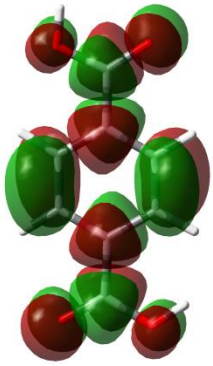
				
HOMO **Energy:** **-6.00 eV**	**HOMO-1** **Energy:** **-6.83 eV**	**HOMO-2** **Energy:** **-7.32 eV**	**HOMO-3** **Energy:** **-7.44 eV**	**HOMO-4** **Energy:** **-7.64 eV**
				
LUMO **Energy:** **-2.03 eV**	**LUMO+1** **Energy:** **-1.02 eV**	**LUMO+2** **Energy:** **-0.67 eV**	**LUMO+3** **Energy:** **-0.28 eV**	**LUMO+4** **Energy:** **0.59 eV**

Table S6. DFT table of H_2**bdc**

				
HOMO **Energy** **-7.58 eV**	**HOMO-1** **Energy** **-7.83eV**	**HOMO-2** **Energy** **-7.89eV**	**HOMO-3** **Energy** **-8.09eV**	**HOMO-4** **Energy** **-8.78 eV**
				
LUMO **Energy** **-2.70 eV**	**LUMO+1** **Energy** **-1.27 eV**	**LUMO+2** **Energy** **-0.82 eV**	**LUMO+3** **Energy** **0.69eV**	**LUMO+4** **Energy** **1.07 eV**