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Electronic Supporting Infomation

Synthesis, X-ray Characterization, DFT Calculations and Hirshfeld Surface Analysis Studies of carbohydrazone based on Zn(II) complexes

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1. Crystal data.

Table S1. Bond distances (Å) and angles (º) for **1**

Zn1 O1 2.140(2)	O1 Zn1 O1 91.91(11)
Zn1 O1 2.134(2)	O1 Zn1 N6 95.85(9)
Zn1 N2 2.082(3)	O1 Zn1 N6 150.55(9)
Zn1 N5 2.054(3)	N2 Zn1 O1 112.02(9)
Zn1 N6 2.168(3)	N2 Zn1 O1 74.27(9)
Zn1 N3 2.133(3)	N2 Zn1 N6 97.43(10)
	N2 Zn1 N3 75.36(10)
	N5 Zn1 O1 101.50(9)
	N5 Zn1 O1 74.58(9)
	N5 Zn1 N2 171.99(10)
	N5 Zn1 N6 76.04(10)
	N5 Zn1 N3 109.55(10)
	N3 Zn1 O1 92.47(9)
	N3 Zn1 O1 148.69(9)
	N3 Zn1 N6 95.41(10)
	Zn1 O1 Zn1 133.86(10)

Table S2. Bond distances (Å) and angles (º) for **2**

Zn1 N2 2.095(3)	N2 Zn1 O4 112.38(11)	N11 Zn3 N14 178.27(12)
Zn1 O4 2.095(3)	N2 Zn1 N23 172.44(12)	N11 Zn3 O3 107.90(11)
Zn1 N23 2.099(3)	O4 Zn1 N23 74.94(11)	N14 Zn3 O3 73.71(11)
Zn1 N1 2.147(3)	N2 Zn1 N1 74.38(12)	N11 Zn3 N13 104.59(12)
Zn1 O1 2.152(3)	O4 Zn1 N1 93.37(11)	N14 Zn3 N13 73.89(12)
Zn1 N24 2.152(3)	N23 Zn1 N1 107.75(12)	O3 Zn3 N13 146.96(11)
Zn2 N5 2.062(3)	N2 Zn1 O1 74.62(10)	N11 Zn3 N12 75.90(12)
Zn2 N8 2.097(3)	O4 Zn1 O1 91.29(10)	N14 Zn3 N12 103.43(12)
Zn2 O2 2.135(2)	N23 Zn1 O1 103.99(11)	O3 Zn3 N12 95.13(11)
Zn2 O1 2.138(2)	N1 Zn1 O1 148.05(11)	N13 Zn3 N12 98.44(12)
Zn2 N7 2.143(3)	N2 Zn1 N24 97.74(12)	N11 Zn3 O2 73.96(11)
Zn2 N6 2.167(3)	O4 Zn1 N24 149.63(11)	N14 Zn3 O2 106.75(11)
Zn3 N11 2.065(3)	N23 Zn1 N24 74.84(12)	O3 Zn3 O2 92.36(9)
Zn3 N14 2.116(3)	N1 Zn1 N24 98.56(12)	N13 Zn3 O2 90.85(11)
Zn3 O3 2.119(2)	O1 Zn1 N24 93.08(11)	N12 Zn3 O2 149.80(11)
Zn3 N13 2.138(3)	N5 Zn2 N8 173.74(12)	N17 Zn4 N20 174.52(13)
Zn3 N12 2.164(3)	N5 Zn2 O2 106.23(11)	N17 Zn4 O3 74.57(11)
Zn3 O2 2.188(2)	N8 Zn2 O2 74.70(11)	N20 Zn4 O3 110.43(11)
Zn4 N17 2.057(3)	N5 Zn2 O1 75.06(11)	N17 Zn4 N19 106.01(12)
Zn4 N20 2.059(3)	N8 Zn2 O1 111.19(11)	N20 Zn4 N19 76.57(12)
Zn4 O3 2.130(3)	O2 Zn2 O1 90.83(10)	O3 Zn4 N19 90.73(11)
Zn4 N19 2.135(3)	N5 Zn2 N7 105.20(12)	N17 Zn4 N18 76.06(12)
Zn4 N18 2.159(3)	N8 Zn2 N7 74.66(12)	N20 Zn4 N18 98.88(12)
Zn4 O4 2.162(2)	O2 Zn2 N7 148.11(11)	O3 Zn4 N18 150.61(11)
	O1 Zn2 N7 92.04(11)	N19 Zn4 N18 98.40(12)
	N5 Zn2 N6 76.00(12)	N17 Zn4 O4 103.34(11)
	N8 Zn2 N6 97.77(12)	N20 Zn4 O4 74.61(11)
	O2 Zn2 N6 95.73(11)	O3 Zn4 O4 92.47(10)
	O1 Zn2 N6 151.01(11)	N19 Zn4 O4 150.26(11)
	N7 Zn2 N6 96.96(12)	N18 Zn4 O4 93.15(11)

Table S3. Bond distances (Å) and angles (º) for **3**

Zn1 N13 2.134(2)	N2 Zn1 N14 174.54(9)	N17 Zn3 N8 168.42(9)
Zn1 O1 2.159(2)	N2 Zn1 O3 101.21(8)	N17 Zn3 O3 74.77(8)
Zn1 N1 2.170(2)	N14 Zn1 O3 74.65(8)	N8 Zn3 O3 115.66(8)
Zn2 N20 2.065(2)	N2 Zn1 N13 109.42(9)	N17 Zn3 N7 110.85(9)
Zn2 N5 2.078(2)	N14 Zn1 N13 75.13(9)	N8 Zn3 N7 74.72(9)
Zn2 O1 2.1286(19)	O3 Zn1 N13 148.76(8)	O3 Zn3 N7 93.46(8)
Zn2 O4 2.139(2)	N2 Zn1 O1 74.38(8)	N17 Zn3 O2 101.76(9)
Zn2 N19 2.150(2)	N14 Zn1 O1 109.01(8)	N8 Zn3 O2 73.82(8)
Zn2 N6 2.161(2)	O3 Zn1 O1 91.59(8)	O3 Zn3 O2 91.91(8)
Zn3 N17 2.070(2)	N13 Zn1 O1 90.82(8)	N7 Zn3 O2 147.23(9)
Zn3 N8 2.105(2)	N2 Zn1 N1 75.92(9)	N17 Zn3 N18 75.41(10)
Zn3 O3 2.114(2)	N14 Zn1 N1 100.49(9)	N8 Zn3 N18 94.32(10)
Zn3 N7 2.152(2)	O3 Zn1 N1 92.53(8)	O3 Zn3 N18 150.02(9)
Zn3 O2 2.164(2)	N13 Zn1 N1 100.57(9)	N7 Zn3 N18 94.21(9)
Zn3 N18 2.181(2)	O1 Zn1 N1 150.25(8)	O2 Zn3 N18 97.09(9)
Zn4 N11 2.059(2)	N20 Zn2 N5 178.40(10)	N11 Zn4 N23 172.61(10)
Zn4 N23 2.105(3)	N20 Zn2 O1 105.46(8)	N11 Zn4 O4 110.75(9)
Zn4 O4 2.105(2)	N5 Zn2 O1 75.15(8)	N23 Zn4 O4 74.31(9)
Zn4 N24 2.142(2)	N20 Zn2 O4 74.58(8)	N11 Zn4 N24 100.69(10)
Zn4 O2 2.163(2)	N5 Zn2 O4 106.92(8)	N23 Zn4 N24 75.04(10)
Zn4 N12 2.164(2)	O1 Zn2 O4 92.03(8)	O4 Zn4 N24 147.96(9)
	N20 Zn2 N19 76.89(9)	N11 Zn4 O2 74.97(9)
	N5 Zn2 N19 101.61(9)	N23 Zn4 O2 110.74(9)
	O1 Zn2 N19 95.44(8)	O4 Zn4 O2 91.93(8)
	O4 Zn2 N19 151.46(8)	N24 Zn4 O2 90.28(9)
	N20 Zn2 N6 104.47(9)	N11 Zn4 N12 75.61(10)
	N5 Zn2 N6 75.10(9)	N23 Zn4 N12 98.82(10)
	O1 Zn2 N6 149.36(8)	O4 Zn4 N12 95.69(9)
	O4 Zn2 N6 89.66(9)	N24 Zn4 N12 97.99(9)
	N19 Zn2 N6 97.54(9)	O2 Zn4 N12 150.43(9)

Table S4. Hydrogen bonds in compound **4** (Å)

N1 ···O3	2.708
N2 ···O3	2.936
O1 ···O3	2.797
O1 ···O2	2.795
N5 ···O2	2.933
N6 ···O2	2.700

Table S5. Bond distances (Å) and angles (º) for **5**

Zn1 N5 2.078(3)	N5 Zn1 N2 174.49(13)
Zn1 N2 2.083(3)	N5 Zn1 O1 110.23(11)
Zn1 O1 2.137(3)	N2 Zn1 O1 75.03(11)
Zn1 O1 2.149(3)	N5 Zn1 O1 74.47(11)
Zn1 N6 2.150(4)	N2 Zn1 O1 104.08(11)
Zn1 N1 2.189(4)	O1 Zn1 O1 92.52(14)
	N5 Zn1 N6 75.90(13)
	N2 Zn1 N6 105.90(13)
	O1 Zn1 N6 92.78(12)
	O1 Zn1 N6 149.91(12)
	N5 Zn1 N1 99.64(13)
	N2 Zn1 N1 75.03(13)
	O1 Zn1 N1 149.98(11)
	O1 Zn1 N1 92.58(12)
	N6 Zn1 N1 97.44(13)

2. Figures S1 to S4.

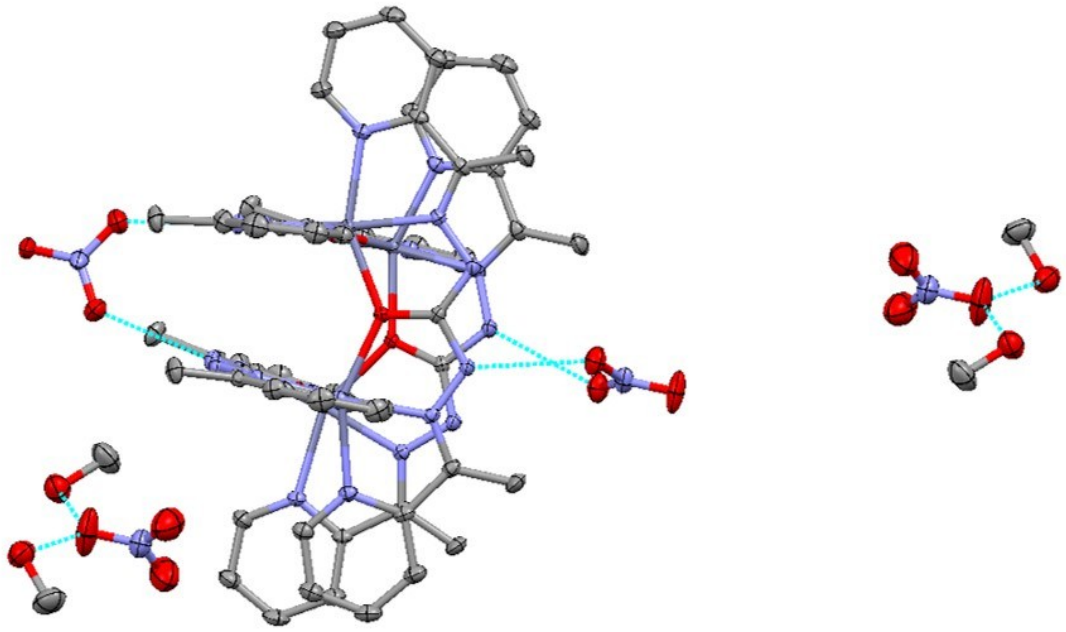

Fig. S1. H-bonds in compound **1** (represented by blue dashed lines)

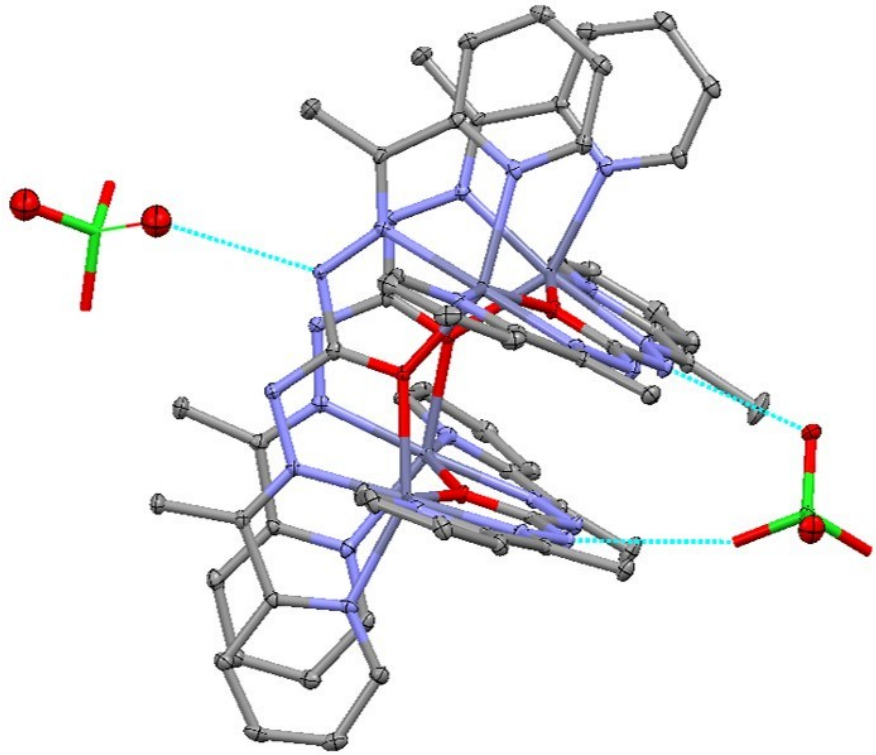

Fig. S2. H-bonds in compound **2** (represented by blue dashed lines)

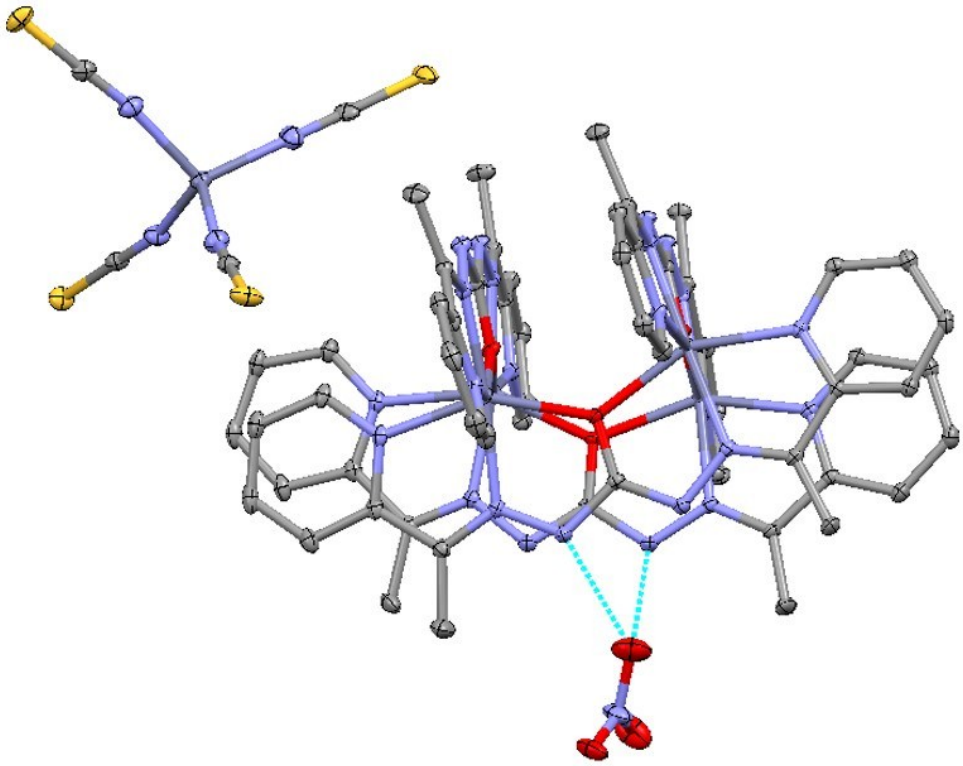

Fig. S3 H-bonds in compound **3** (represented by blue dashed lines)

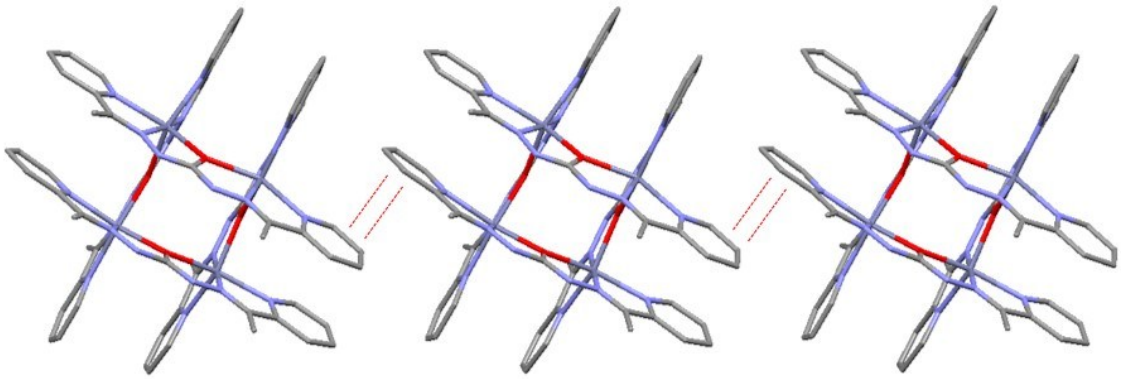

Fig. S4 π-Stacking interactions in compound **3** (represented using red lines)

3. Hirshfeld studies.

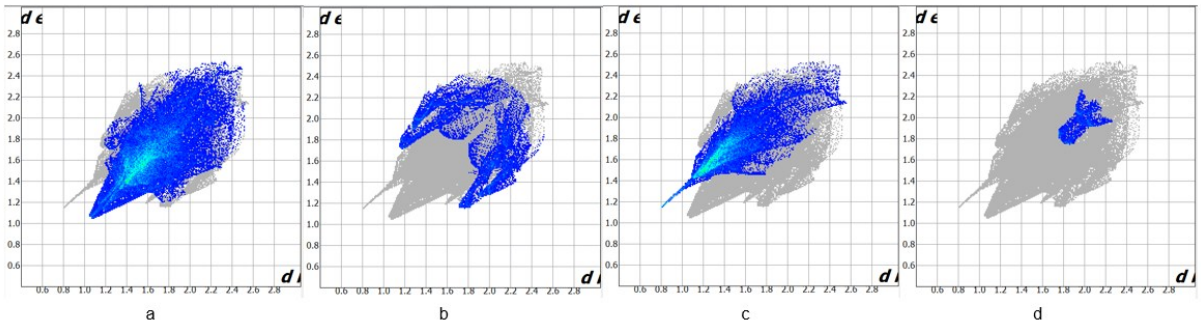

Fig. S5 Decomposed fingerprint plots for 1: a) H···H, b) H···C, c) H···O, d) C···C.

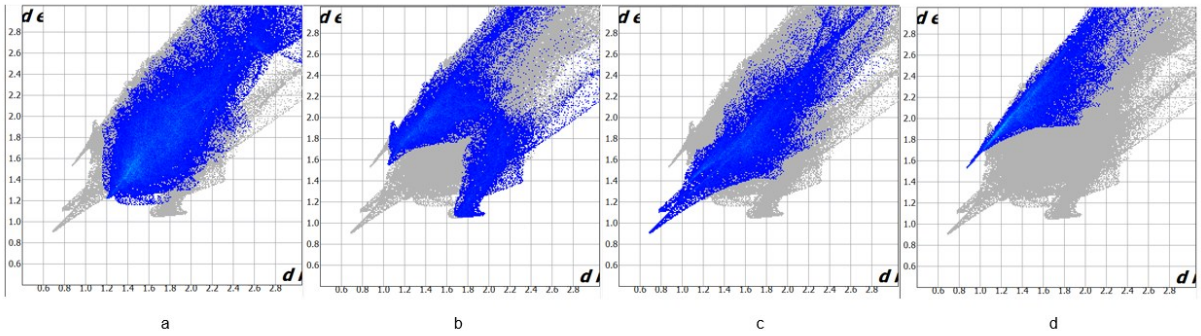

Fig. S6 Decomposed fingerprint plots for 3: a) H···H, b) H···C, c) H···O, d) H···S.

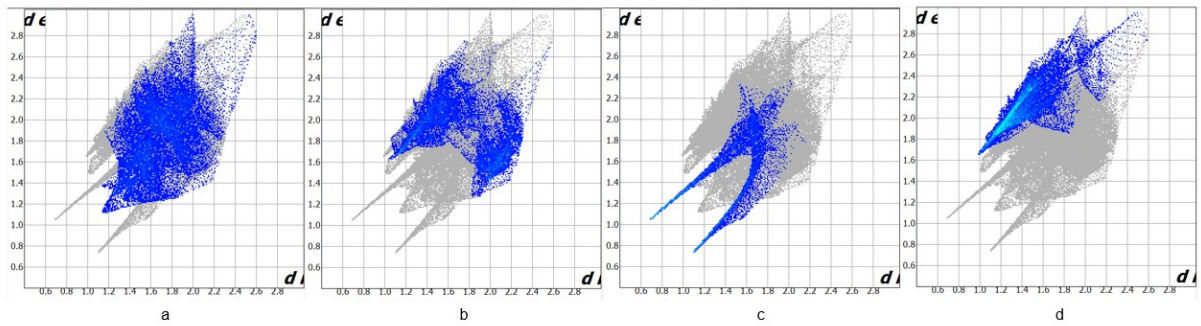

Fig. S7. Decomposed fingerprint plots of 4: a) H···H, b) H···C, c) H···O, d) H···S.

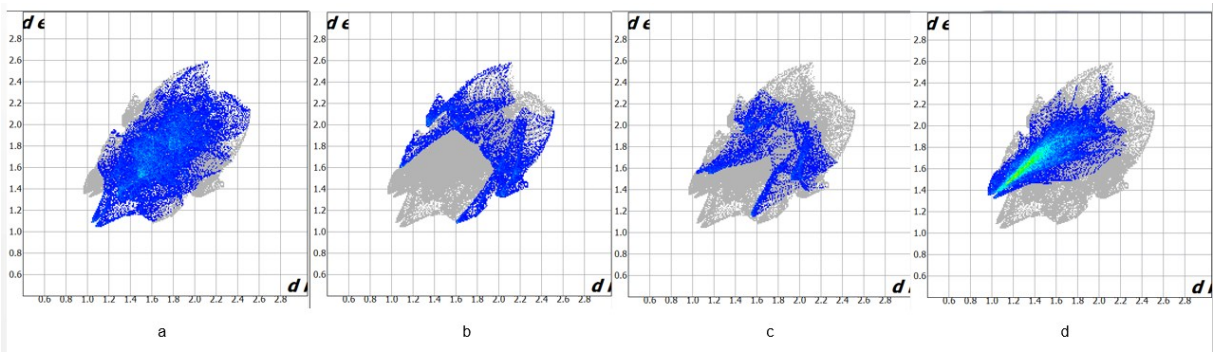

Fig. S8 Decomposed fingerprint plots of 5: a) H···H, b) H···C, c) H···N, d) H···O.