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SUPPLEMENTARY MATERIAL TO

Zn(II) complex with pyridine based 1,3-selenazolyl-hydrazone: Synthesis, structural characterization and DFT study

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ANALYTICAL AND SPECTRAL DATA

The ligand based on (1,3-selenazol-2-yl)hydrazone. Anal. Calcd. for $C_{32}H_{28}Cl_4N_8O_2Se_2Zn_2$ (Fw = 987.08) (%): C, 38.93; H, 2.86; N, 11.35. Found: C, 39.21; H, 3.09; N, 11.16. Λ_M (1×10^{-3} M, MeOH) = 108.2 Ω^{-1} cm^2 mol^{-1}. IR (ATR, νmax/cm^{-1}): 3099 (m), 2924 (s), 2872 (ms), 2836 (ms), 1621 (ms), 1610 (ms), 1600 (ms), 1546 (m), 1532 (ms), 1499 (s), 1469 (s), 1415 (m), 1355 (ms), 1275 (ms), 1229 (s), 1136 (ms), 1022 (ms), 944 (m), 882 (m), 708 (m), 597 (w), 514 (vw). ^{1}H NMR (DMSO-d_6;400 MHz) δ_H (ppm): 3.75 (s, 3H); 6.93 (d, 2H); 7.33 (dd, 1H); 7.54 (s, 1H); 7.75 (d, 2H), 7.80-7.83 (m, 2H); 8.06 (s, 1H); 8.54 (d, 1H); 12.54 (s, 1H). ^{13}C{1H} NMR (DMSO-d_6;126 MHz) δ_C (ppm): 55.55, 106.26, 114.37, 119.64, 124.13, 127.51, 128.56, 137.24, 142.72, 149.90, 153.58, 159.09, 171.30.

Abbreviations used for IR spectra: s, strong; ms, medium-strong; m, medium; w, weak; vw, very weak.

Table S-I. Crystal data and structure refinement for **2-Cl-Se**

Empirical formula	$C_{32}H_{28}Cl_4N_8O_2Se_2Zn_2$
Formula weight	987.08
Temperature/K	298(2)
Crystal system	monoclinic
Space group	*C2/c*
a/Å	14.4341(3)
b/Å	18.6583(4)
c/Å	14.7422(7)
α/°	90
β/°	114.347(4)

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γ/°	90
Volume/Å^3	3617.2(2)
Z	4
ρ_{calc}g/cm^3	1.813
μ/mm^{-1}	7.014
F(000)	1952.0
Crystal size/mm^3	0.2 × 0.12 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.226 to 151.928
Index ranges	-18 ≤ h ≤ 17, -18 ≤ k ≤ 23, -18 ≤ l ≤ 15
Reflections collected	9475
Independent reflections	3728 [R_{int} = 0.0253, R_{sigma} = 0.0354]
Data/restraints/parameters	3728/0/236
Goodness-of-fit on F^2	1.029
Final R indexes *[I>=2σ (I)]*	R_1 = 0.0318, wR_2 = 0.0837
Final R indexes [all data]	R_1 = 0.0345, wR_2 = 0.0866
Largest diff. peak/hole / e Å^{-3}	0.51/-0.65

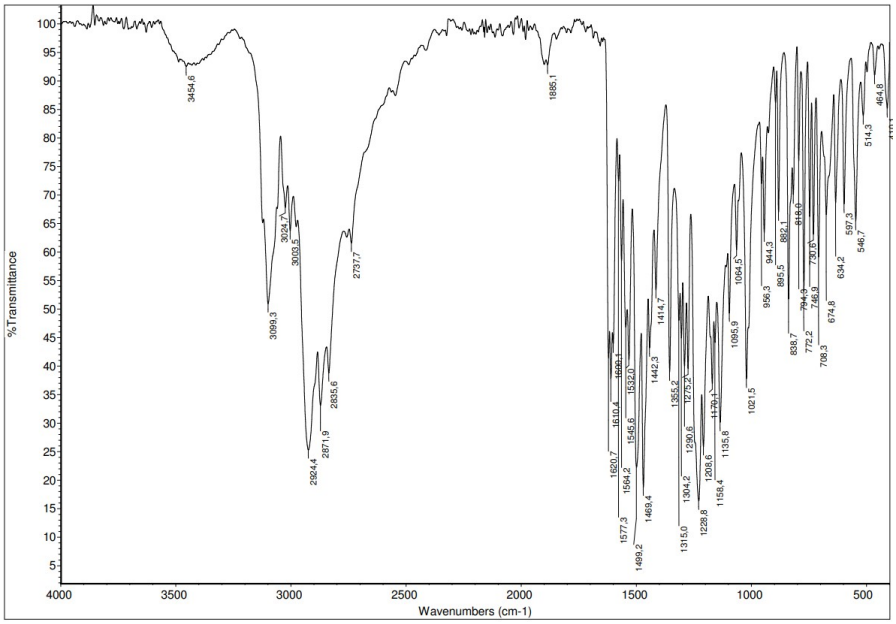

Figure S-1. IR spectrum of **2-Cl-Se**.

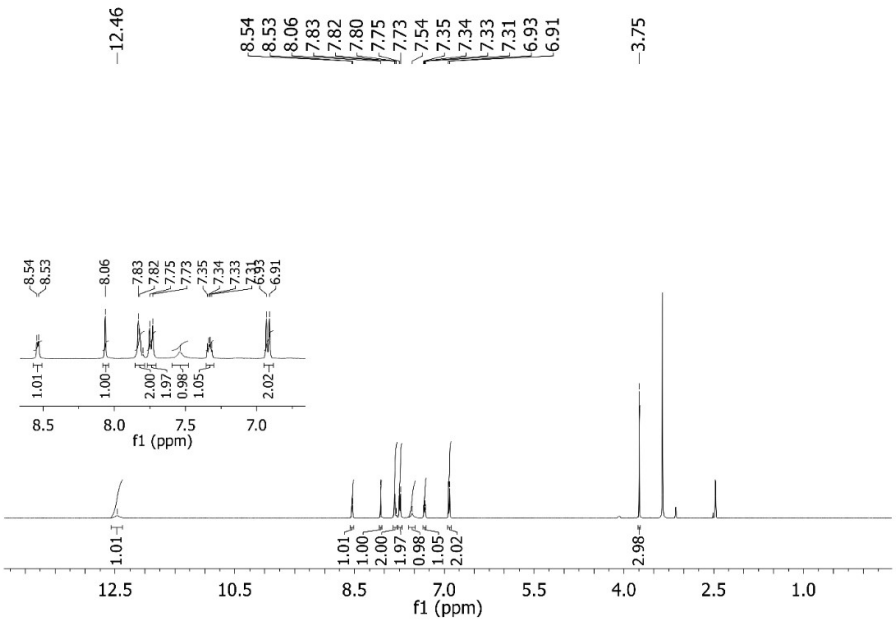

Figure S-2. ^{1}H NMR spectrum of **2-Cl-Se** in DMSO-d_6.

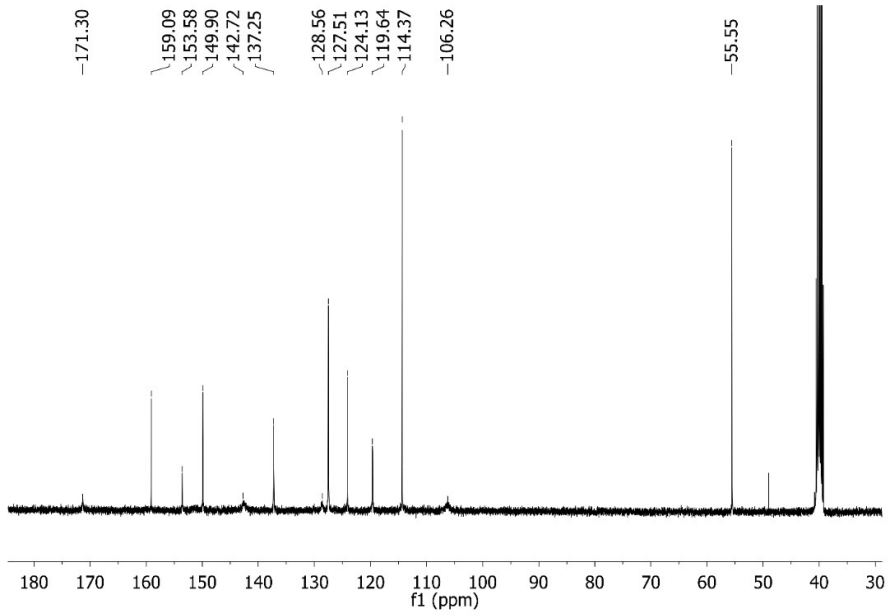

Figure S-3. ^{13}C NMR spectrum of **2-Cl-Se** in DMSO-d_6.

Table S-II. Bond angles for **2-Cl-Se**.

Angle label	Angle / °	Angle label	Angle / °
N1–C1–N2	121.5(2)	C11–N3–N2	123.0(2)
N1–C1–Se1	116.0(2)	C11–N3–Zn1	121.0(2)
N2–C1–Se1	123.0(2)	N2–N3–Zn1	116.0 (1)
C3–C2–Se1	111.80(2)	C12–N4–Zn1	114.0(2)
C2–C3–C4	124.10(2)	C16–N4–C12	117.40(2)
C2–C3–N1	116.50(2)	C16–N4–Zn1	128.0(2)
N1–C3–C4	119.40(2)	C7–O1–C10	116.80(3)
C5–C4–C3	120.40(2)	N1–Zn1–N1^{1}	91.80(1)
C5–C4–C9	118.30(2)	N1^{1}–Zn1–N4^{1}	146.66(7)
C9–C4–C3	121.30(2)	N1–Zn1–N4^{1}	99.39(7)
C6–C5–C4	120.50(3)	N1^{1}–Zn1–N4	99.39(7)
C5–C6–C7	120.70(2)	N1–Zn1–N4	146.66(7)
C6–C7–C8	119.40(2)	N3–Zn1–N1^{1}	122.17(7)
O1–C7–C6	115.80(3)	N3^{1}–Zn1–N1	122.17(7)
O1–C7–C8	124.80(3)	N3–Zn1–N1	74.73(7)
C9–C8–C7	119.50(2)	N3^{1}–Zn1–N1^{1}	74.73(7)
C8–C9–C4	121.50(2)	N3^{1}–Zn1–N3	157.7 (1)
N3–C11–C12	115.80(2)	N3^{1}–Zn1–N4	91.13(7)
C13–C12–C11	121.60(2)	N3^{1}–Zn1–N4^{1}	72.74(7)
N4–C12–C11	115.50(2)	N3–Zn1–N4	72.73(7)
N4–C12–C13	122.90(2)	N3–Zn1–N4^{1}	91.13(7)
C12–C13–C14	118.70(3)	N4^{1}–Zn1–N4	88.4(1)
C15–C14–C13	118.70(3)	Cl1^{2}–Zn2–Cl1	113.66(4)
C14–C15–C16	119.40(3)	Cl1^{2}–Zn2–Cl2	110.57(2)
N4–C16–C15	122.90(3)	Cl1–Zn2–Cl2^{2}	110.56(2)
C1–N1–C3	112.0(2)	Cl1–Zn2–Cl2	106.22(2)
C1–N1–Zn1	113.0(2)	Cl1^{2}–Zn2–Cl2^{2}	106.22(2)
C3–N1–Zn1	133.0(2)	Cl2–Zn2–Cl2^{2}	109.62(4)
N3–N2–C1	114.0(2)	C2–Se1–C1	84.0(2)

Symmetry code: ^{1}-x,+y, ½-z; ^{2}1-x,+y, ½-z

Table S-III. Bond lengths for **2-Cl-Se**.

Bond type	Length / Å	Bond type	Length / Å
C1–N1	1.307(3)	C12–C13	1.382(3)
C1–N2	1.367(3)	C12–N4	1.355(3)
C1–Se1	1.873(2)	C13–C14	1.384(4)
C2–C3	1.349(4)	C14–C15	1.374(5)
C2–Se1	1.867(3)	C15–C16	1.388(4)
C3–C4	1.478(3)	C16–N4	1.329(3)
C3–N1	1.394(3)	N1–Zn1	2.16(2)
C4–C5	1.390(3)	N2–N3	1.355(3)
C4–C9	1.394(3)	N3–Zn1	2.14(2)
C5–C6	1.383(4)	N4–Zn1	2.250(2)
C6–C7	1.387(4)	Cl1–Zn2	2.275(6)
C7–C8	1.389(4)	Cl2–Zn2	2.303(7)
C7–O1	1.363(3)	Zn1–N1^{1}	2.16(2)

C8–C9	1.385(3)	Zn1–N3[1]	2.14(2)
C10–O1	1.432(5)	Zn1–N4[1]	2.250(2)
C11–C12	1.461(4)	Zn2–Cl1[2]	2.275(6)
C11–N3	1.275(3)	Zn2–Cl2[2]	2.303(7)

Symmetry code: [1]-x,+y,½-z; [2]1-x,+y,½-z

Table S-IV. Interaction pair energies in the crystal structure of **2-Cl** based on the B3LYP/ DGDZVP energy model*

R (Å)	Interaction energy, kJ mol^{-1}				
	*E*_ele	*E*_pol	*E*_dis	*E*_rep	*E*_tot
11,25	574,4	–58,5	–18,0	4,0	550,9
7,34	548,4	–76,5	–123,8	127,8	494,3
11,73	481,2	–43,1	–32,5	24,5	463,7
8,27	–618,0	–72,6	–10,0	13,1	–707,7
7,36	–667,3	–132,3	–27,1	35,4	–805,2
7,45	–862,4	–163,1	–30,7	103,5	–995,2
9,60	–648,4	–70,3	–12,6	22,0	–734,8
14,41	408,1	–21,4	–12,5	11,9	412,0

*E_tot represents the sum of individual components with scaling factors (*k*_ele = 1.057; *k*_pol = 0.740; *k*_dis = 0.871; *k*_rep = 0.618), while the individual components are not scaled.