Supporting information

Fluorescent Zinc(II) Thione and Selone Complexes for Light-Emitting Applications

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[#]Equal contribution

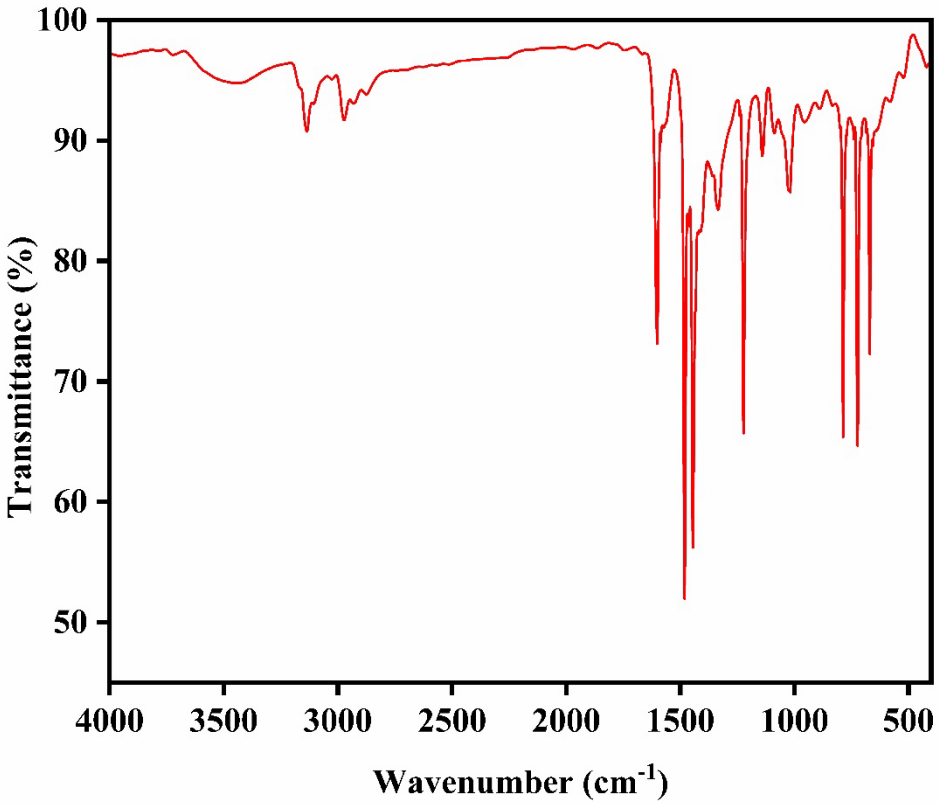


Figure S1: FT-IR spectrum of **1** at RT (KBr).

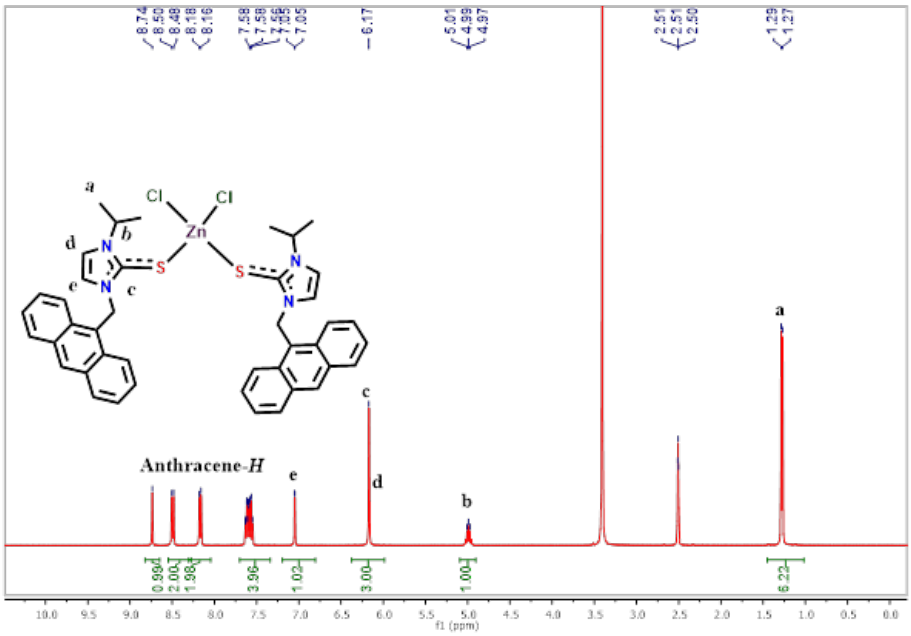


Figure S2: ^{1}H NMR spectrum of **1** in DMSO-d_6 at RT.

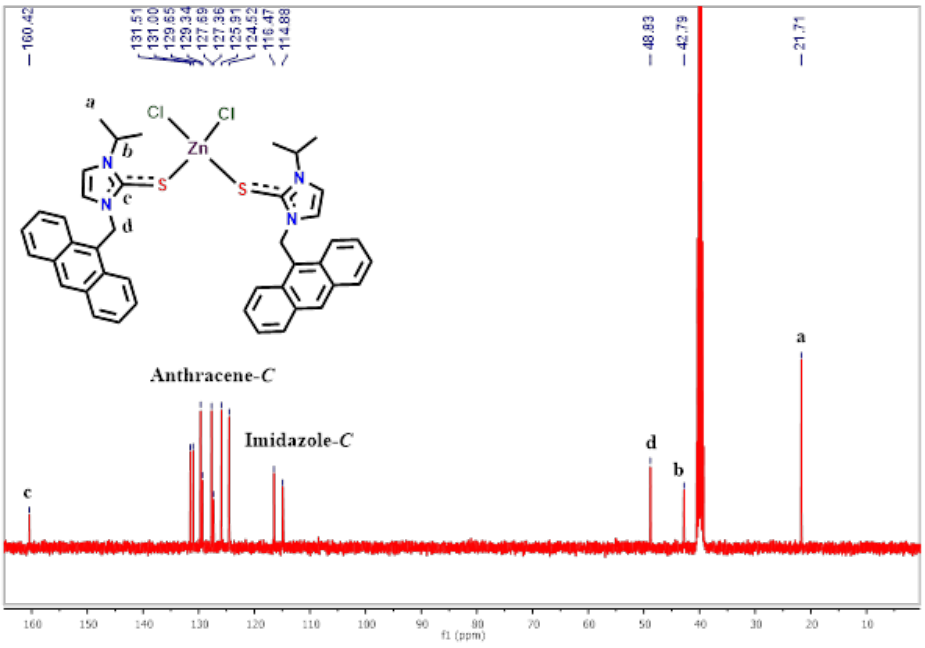


Figure S3: ^{13}C NMR spectrum of **1** in DMSO-d_6 at RT.

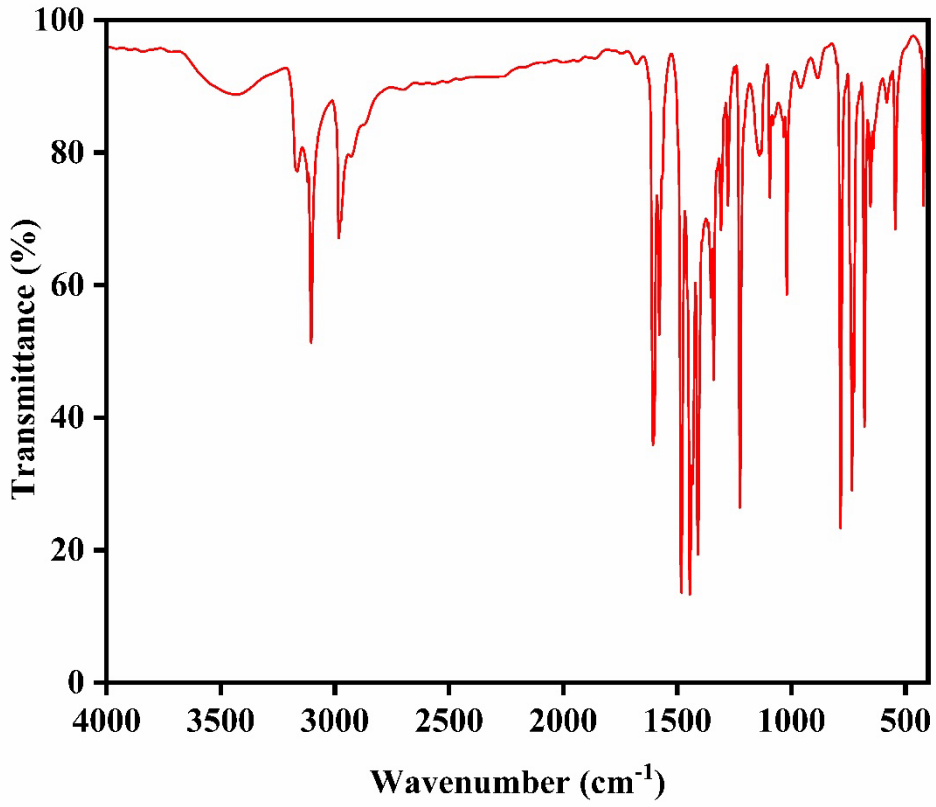


Figure S4: FT-IR spectrum of **2** at RT (KBr).

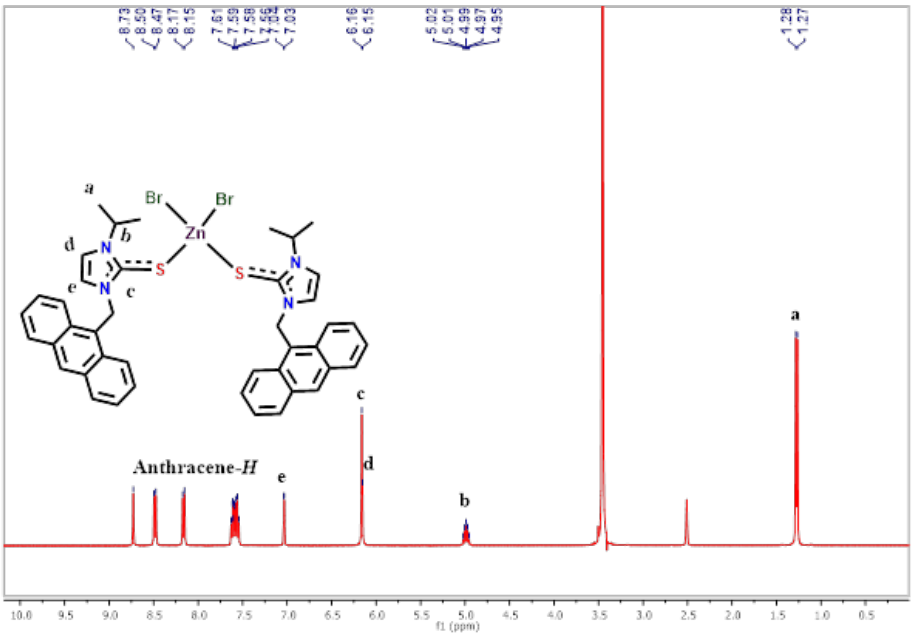


Figure S5: ^{1}H NMR spectrum of **2** in DMSO-d_6 at RT.

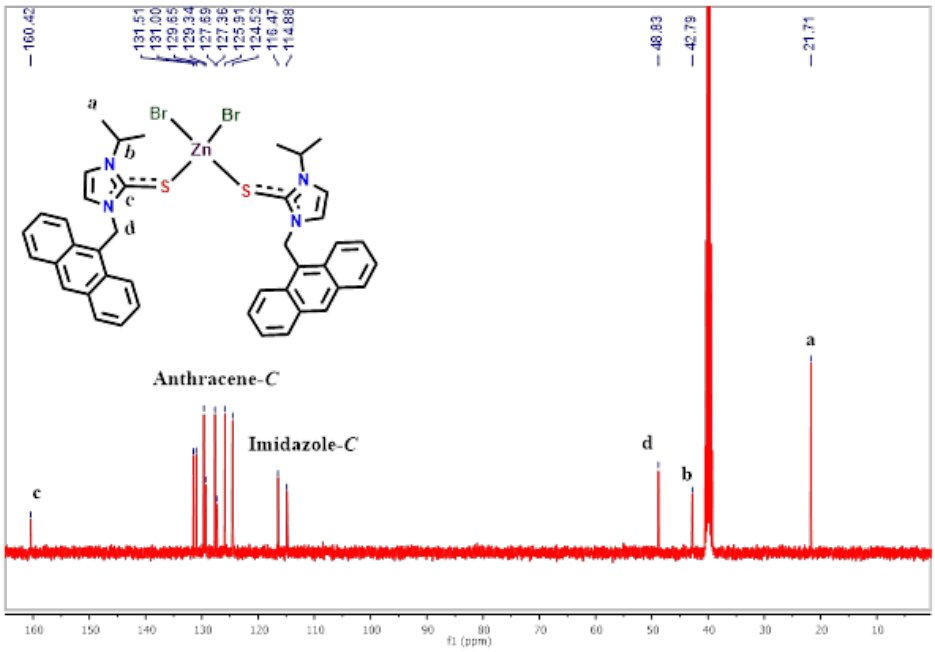


Figure S6: ^{13}C NMR spectrum of **2** in DMSO-d_6 at RT.

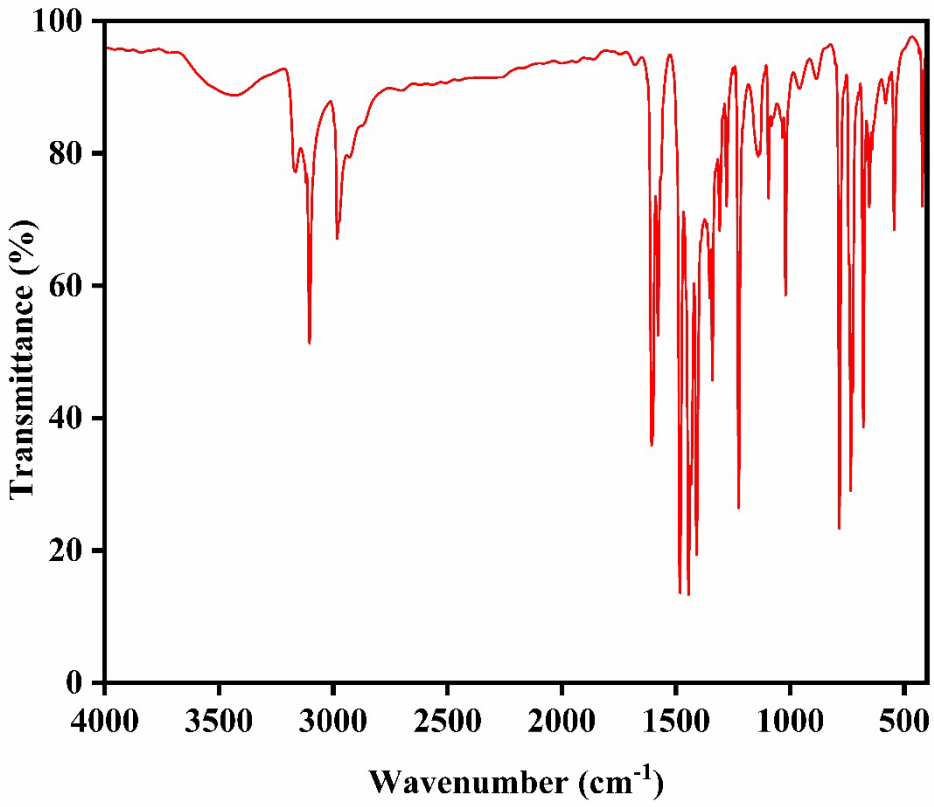


Figure S7: FT-IR spectrum of **3** at RT (KBr).

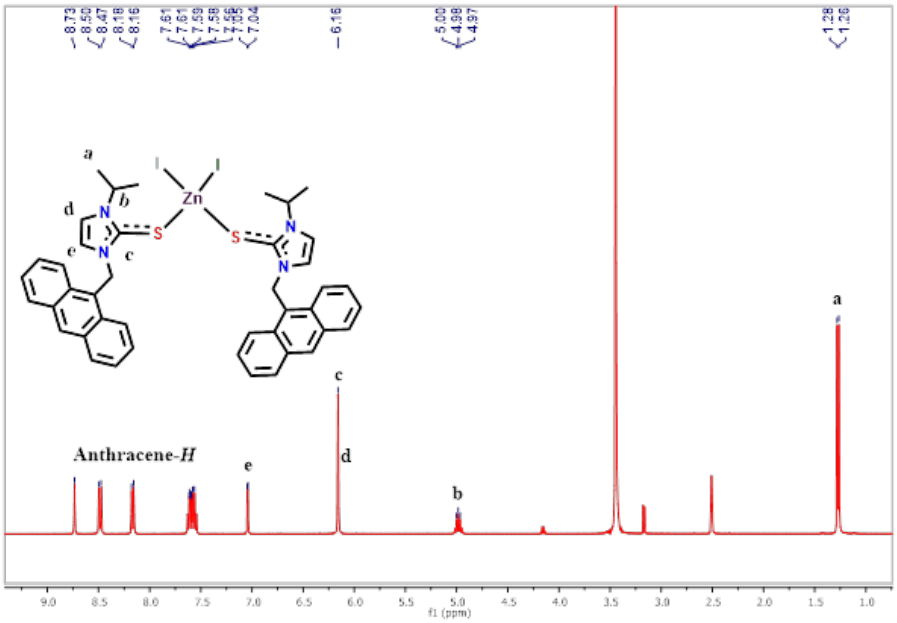


Figure S8: ^{1}H NMR spectrum of **3** in DMSO-d_6 at RT.

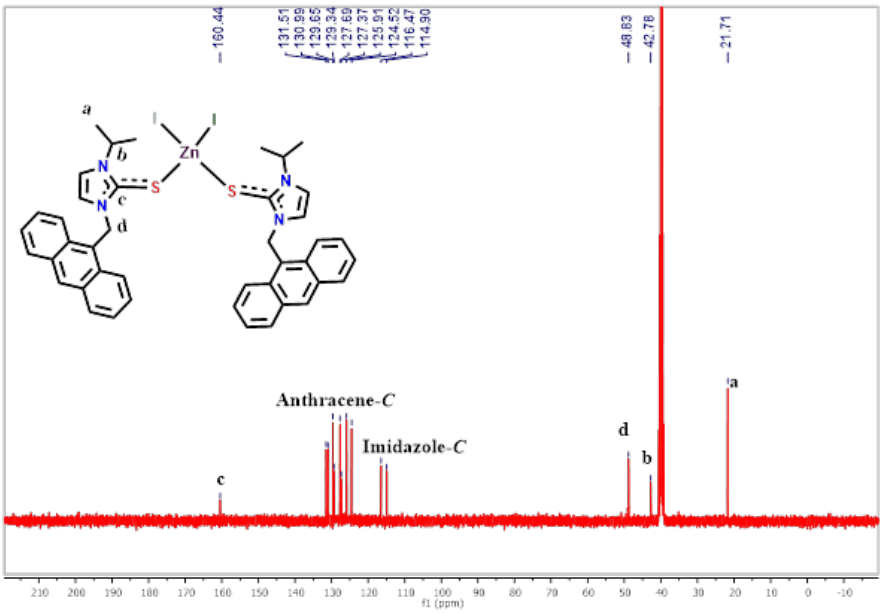


Figure S9: ^{13}C NMR of **3** in DMSO-d_6 at RT.

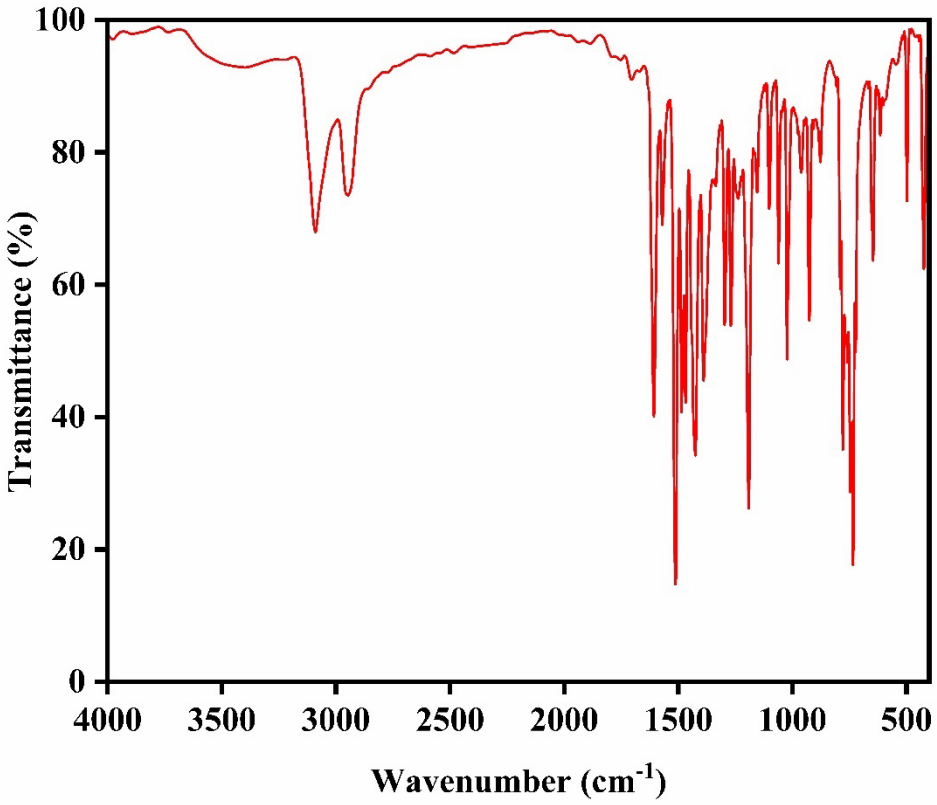


Figure S10: FT-IR spectrum of **4** at RT (KBr).

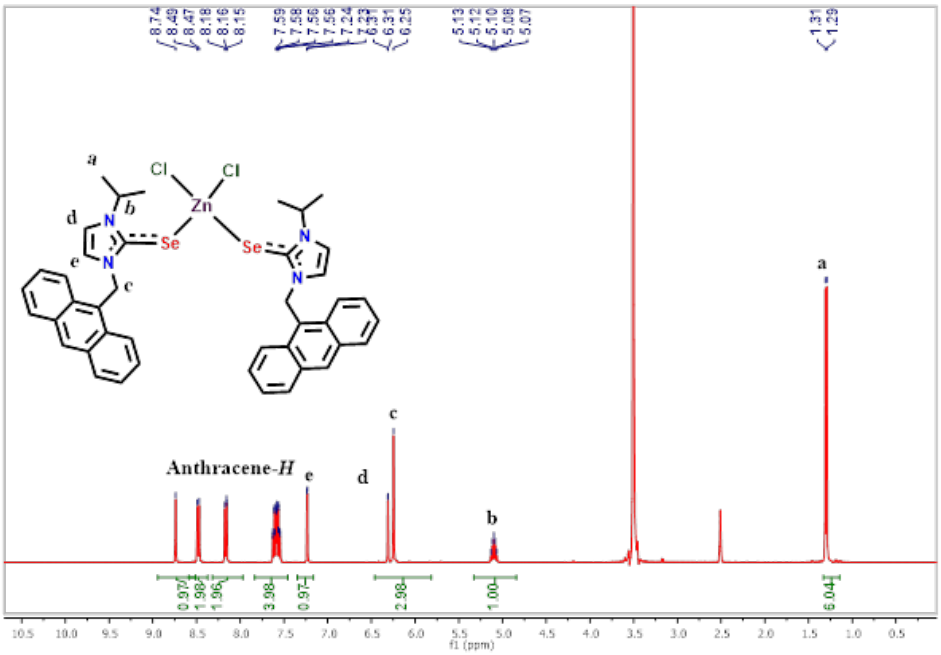


Figure S11: ^{1}H NMR spectrum of **4** in DMSO-d_6 at RT.

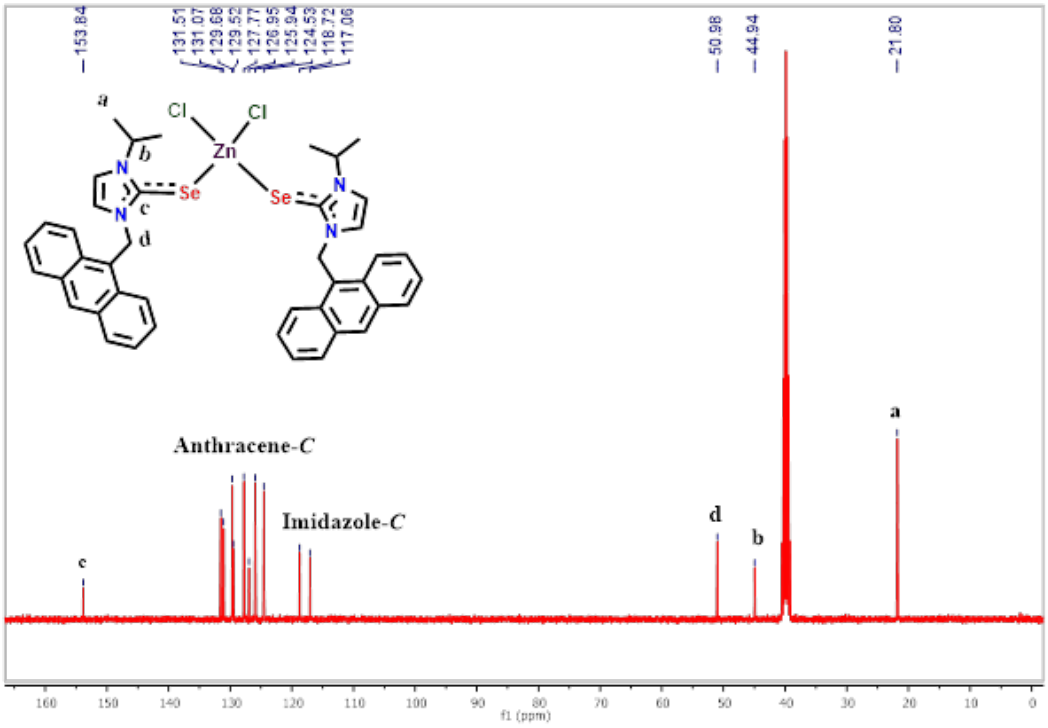


Figure S12: ^{13}C NMR spectrum of **4** in DMSO-d_6 at RT.

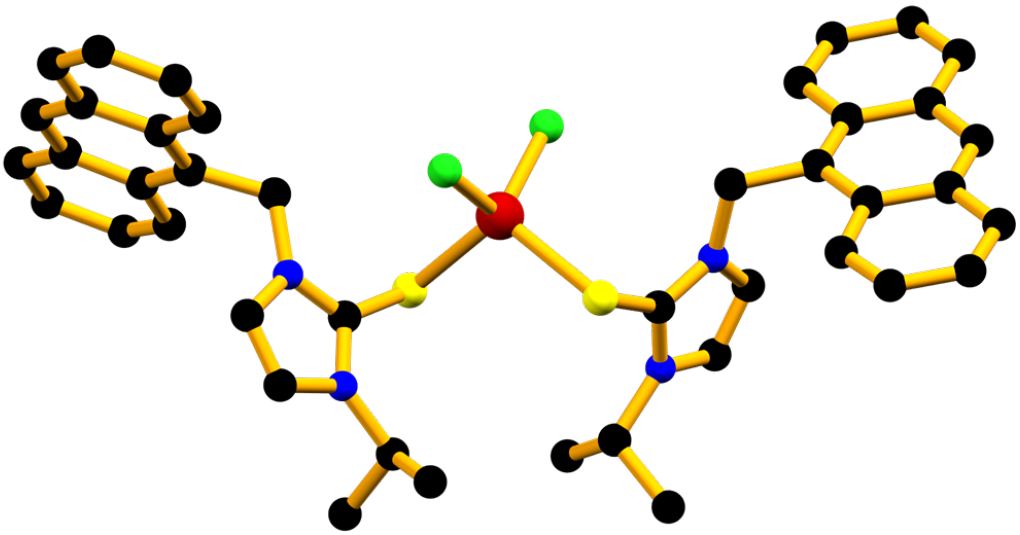


Figure S13: Crystal structure of **1** (Hydrogen atoms are omitted for clarity).

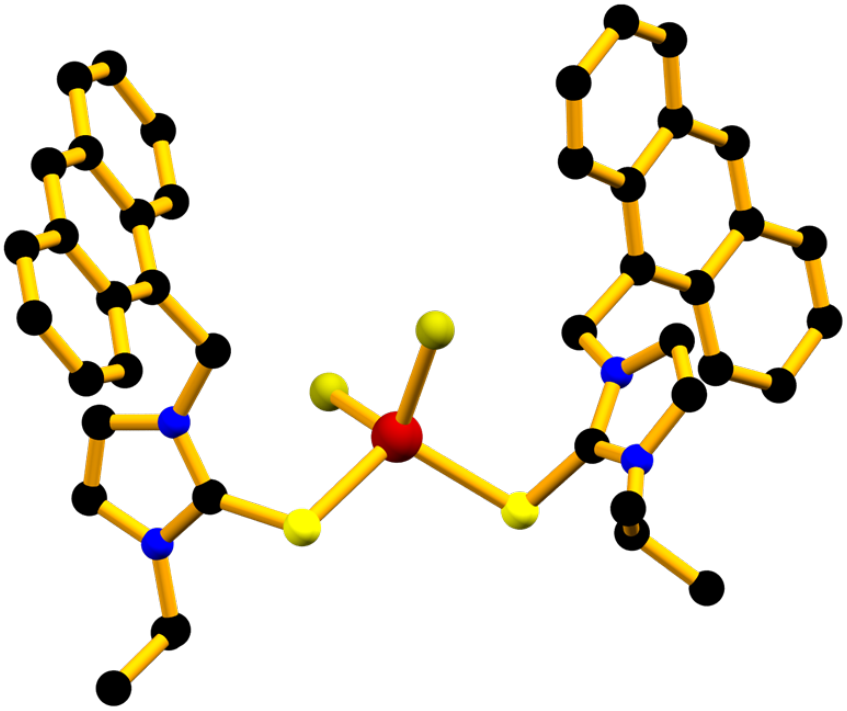


Figure S14: Crystal structure of **2** (Hydrogen atoms are omitted for clarity).

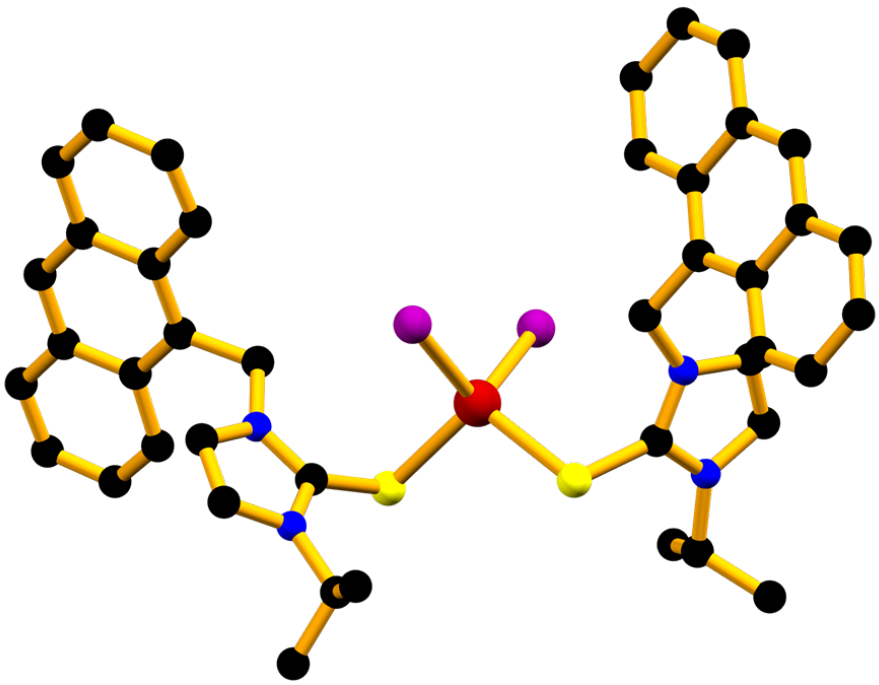


Figure S15: Crystal structure of **3** (Hydrogen atoms are omitted for clarity).

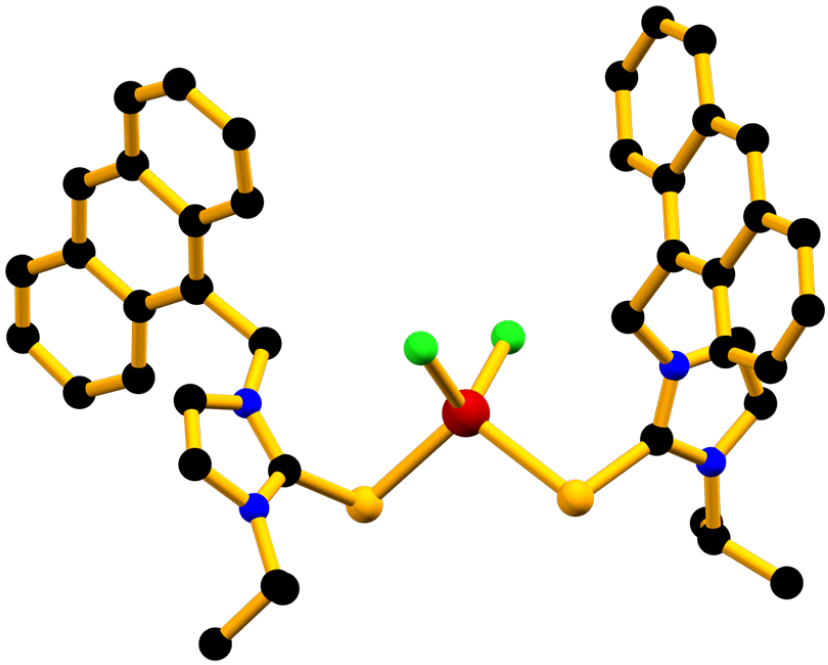


Figure S16: Crystal structure of **4** (Hydrogen atoms are omitted for clarity).

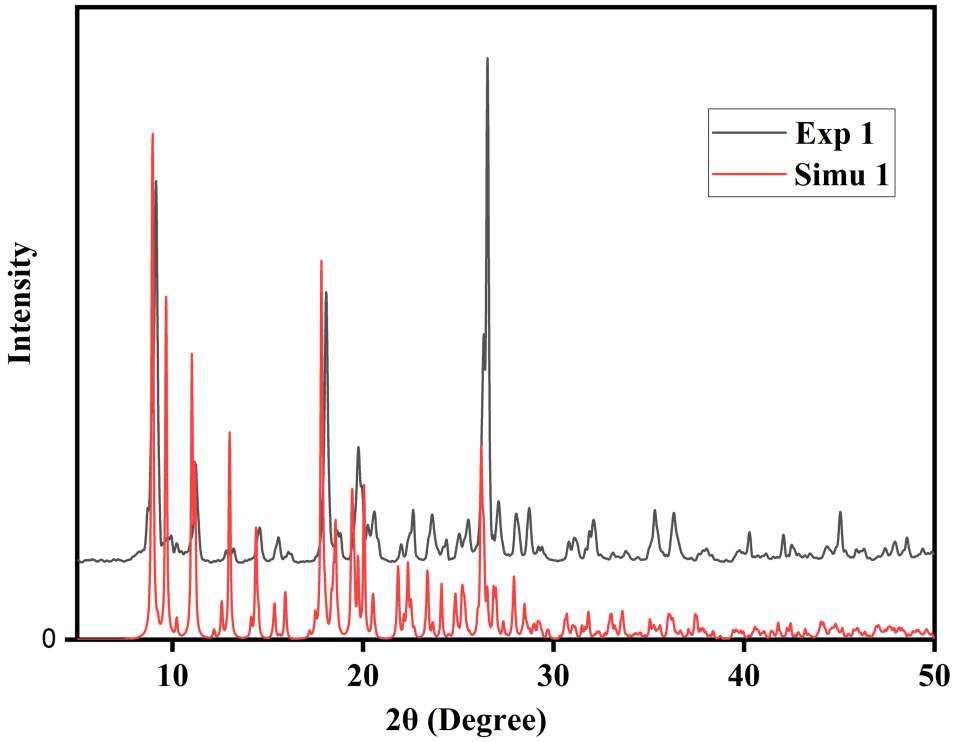


Figure S17: PXRD pattern of **1** at RT (Experimental vs simulated).

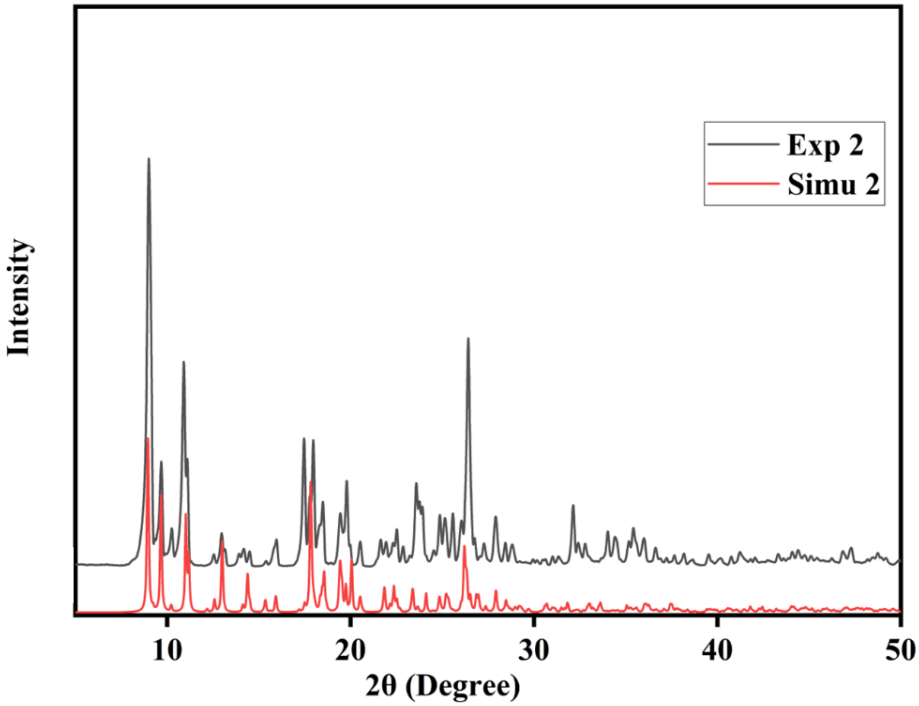


Figure S18: PXRD pattern of **2** at RT (Experimental vs simulated).

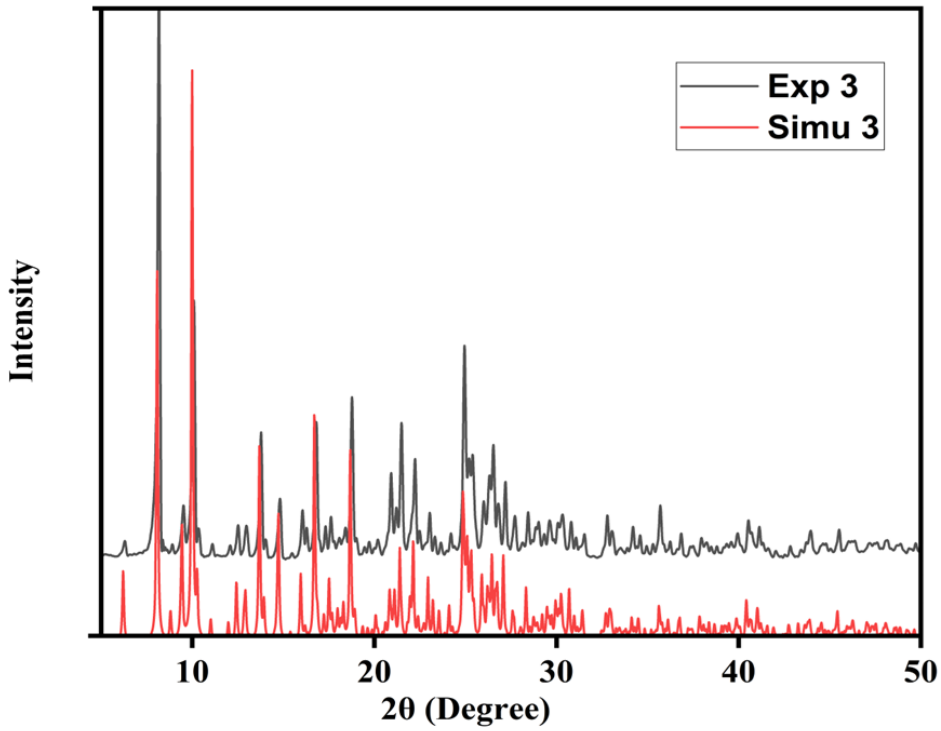


Figure S19: PXRD pattern of **3** at RT (Experimental vs simulated).

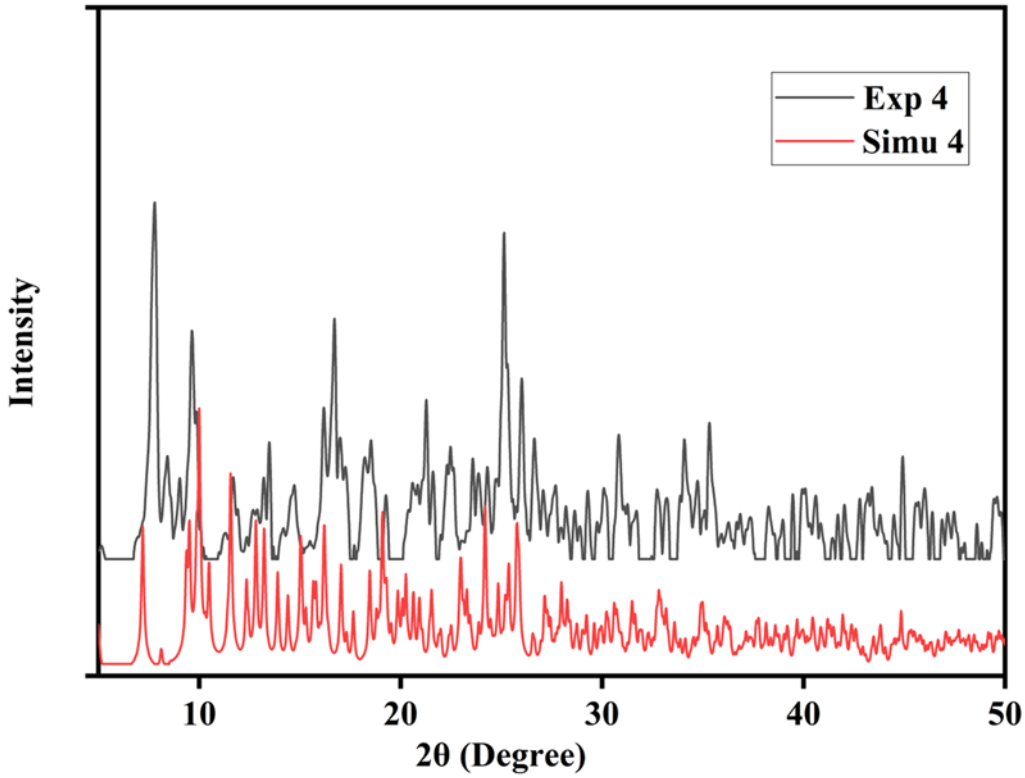


Figure S20: PXRD pattern of **4** at RT (Experimental vs simulated).

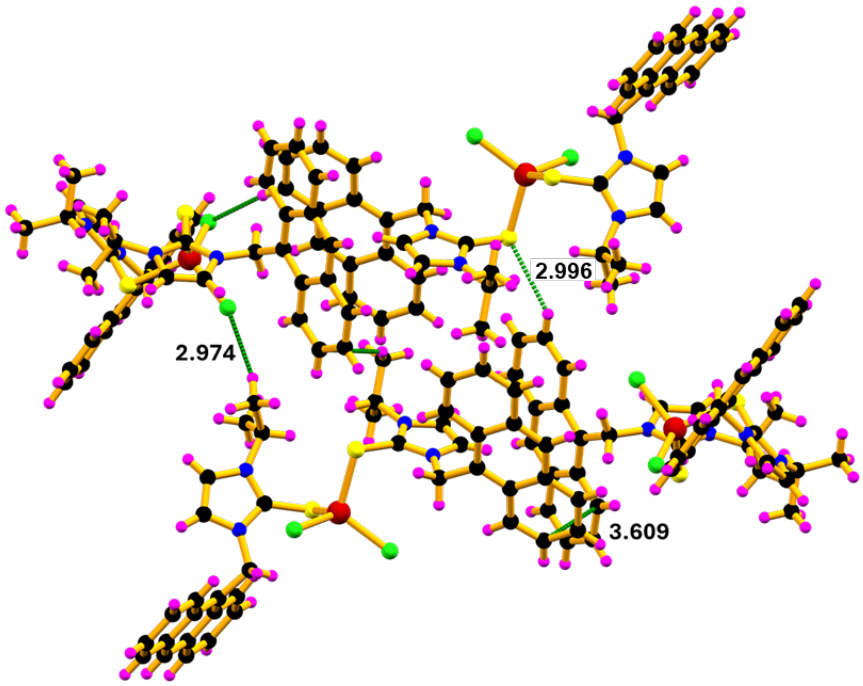


Figure S21: Packing diagram of **1** showing intermolecular interactions.

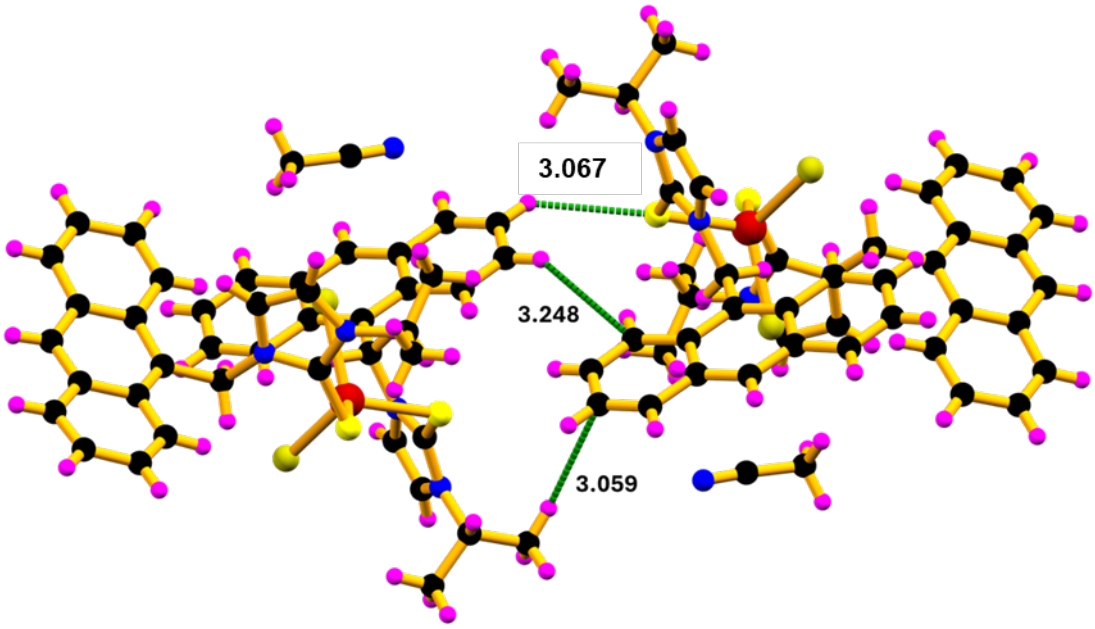


Figure S22: Packing diagram of **2** showing intermolecular interactions.

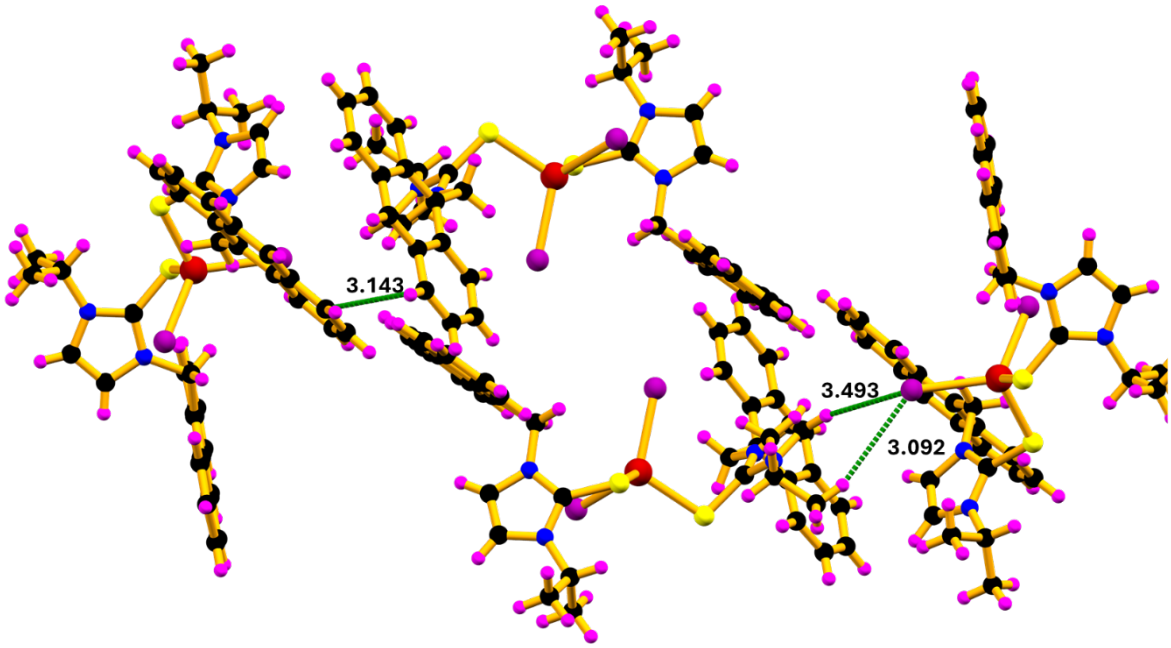


Figure S23: Packing diagram of **3** showing intermolecular interactions.

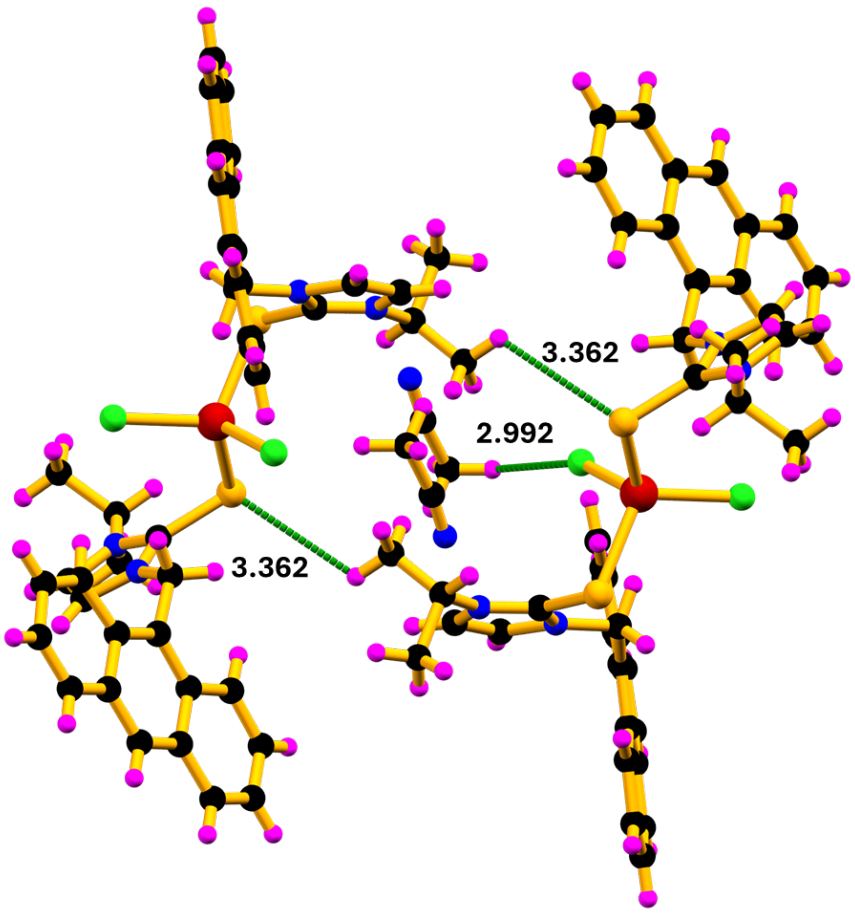


Figure S24: Packing diagram of **4** showing intermolecular interactions.

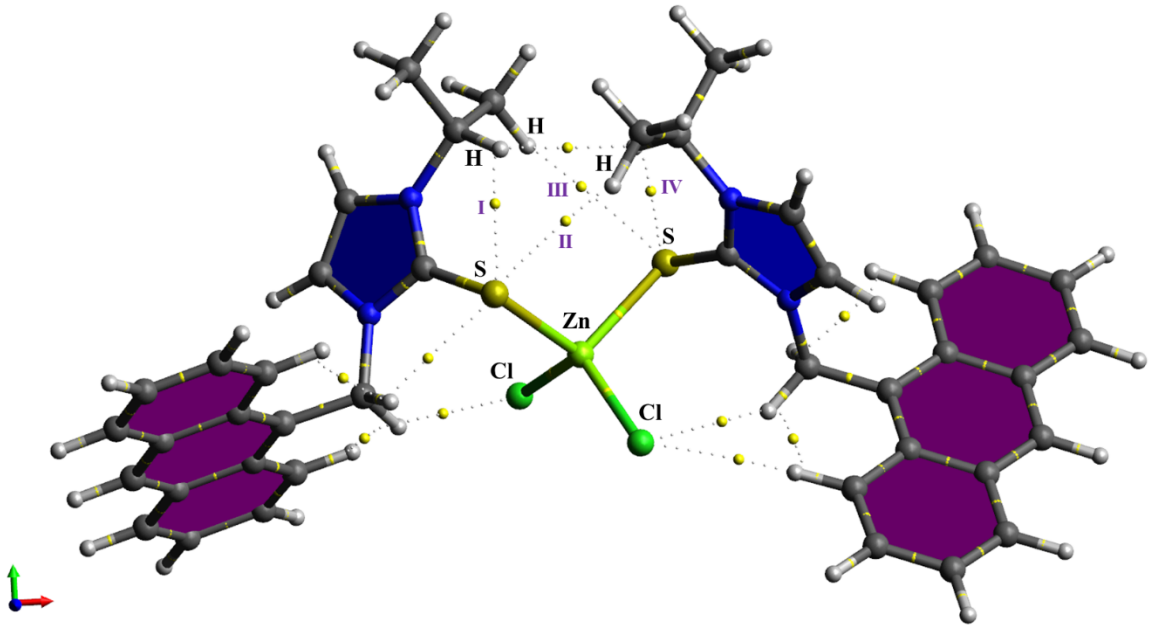


Figure S25: Topological analysis of intramolecular S···H interactions in **1.** (I) $\rho(r) = 0.0145$, $\nabla^2\rho(r) = 0.048$; (II) $\rho(r) = 0.004$, $\nabla^2\rho(r) = 0.0122$; (III) $\rho(r) = 0.0038$, $\nabla^2\rho(r) = 0.0114$; (IV) $\rho(r) = 0.0136$, $\nabla^2\rho(r) = 0.0455$.

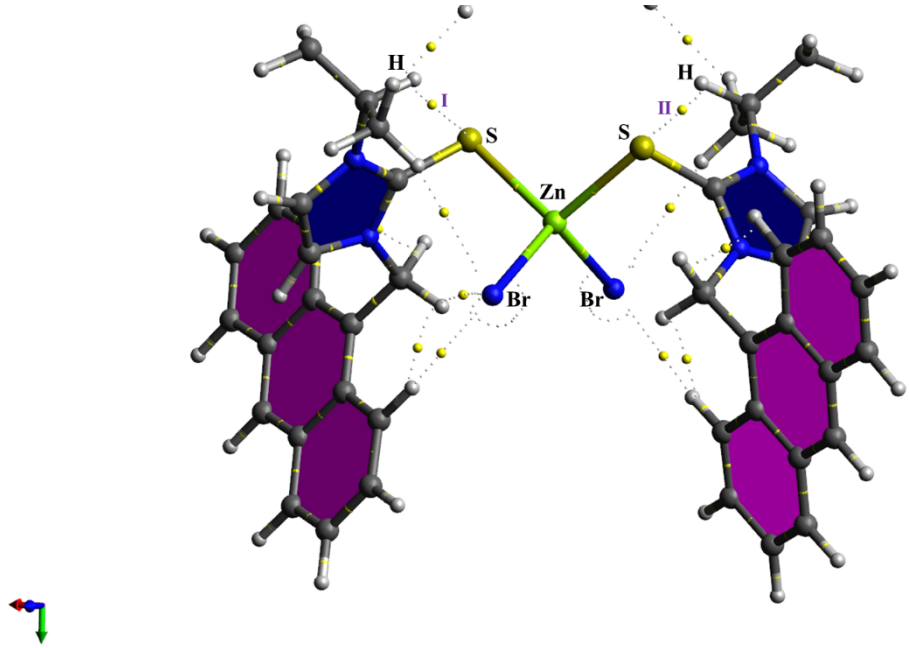


Figure S26: Topological analysis of intramolecular S···H interactions in **2.** (I) ρ(r) = 0.0146, $\nabla^2\rho$(r) = 0.0481; (II) ρ(r) = 0.0146, $\nabla^2\rho$(r) = 0.0481.

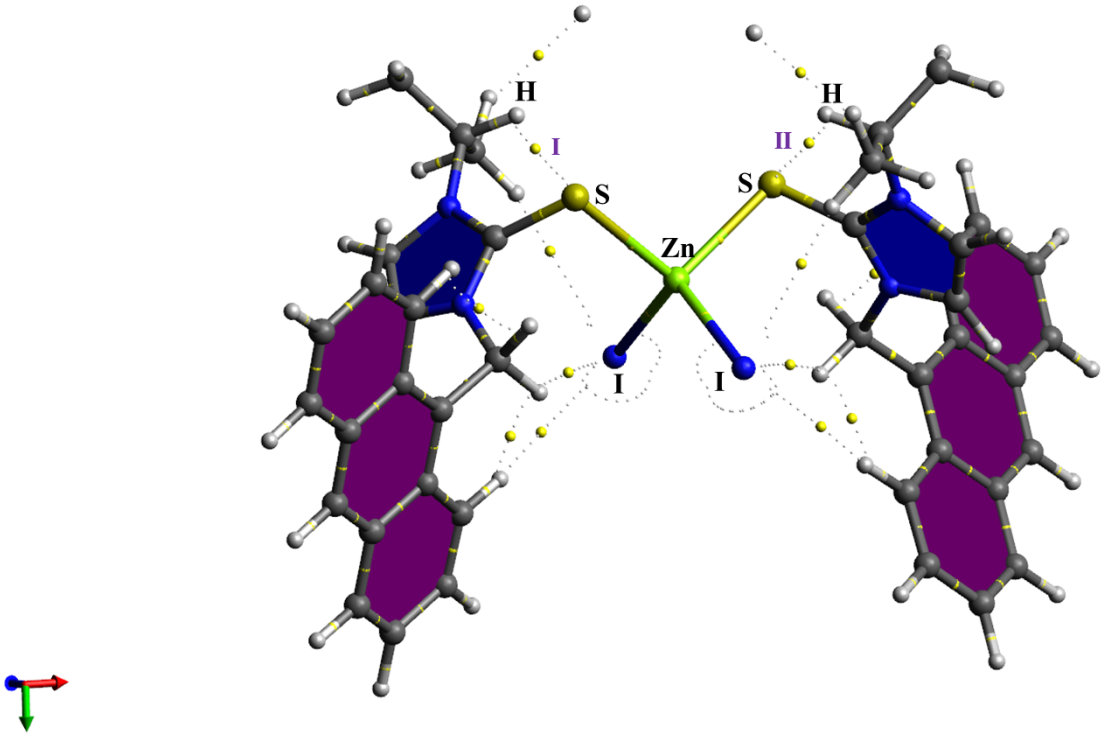


Figure S27: Topological analysis of intramolecular S···H interactions in **3.** (I) $\rho(r) = 0.0146$, $\nabla^2\rho(r) = 0.0483$; (II) $\rho(r) = 0.0146$, $\nabla^2\rho(r) = 0.0482$.

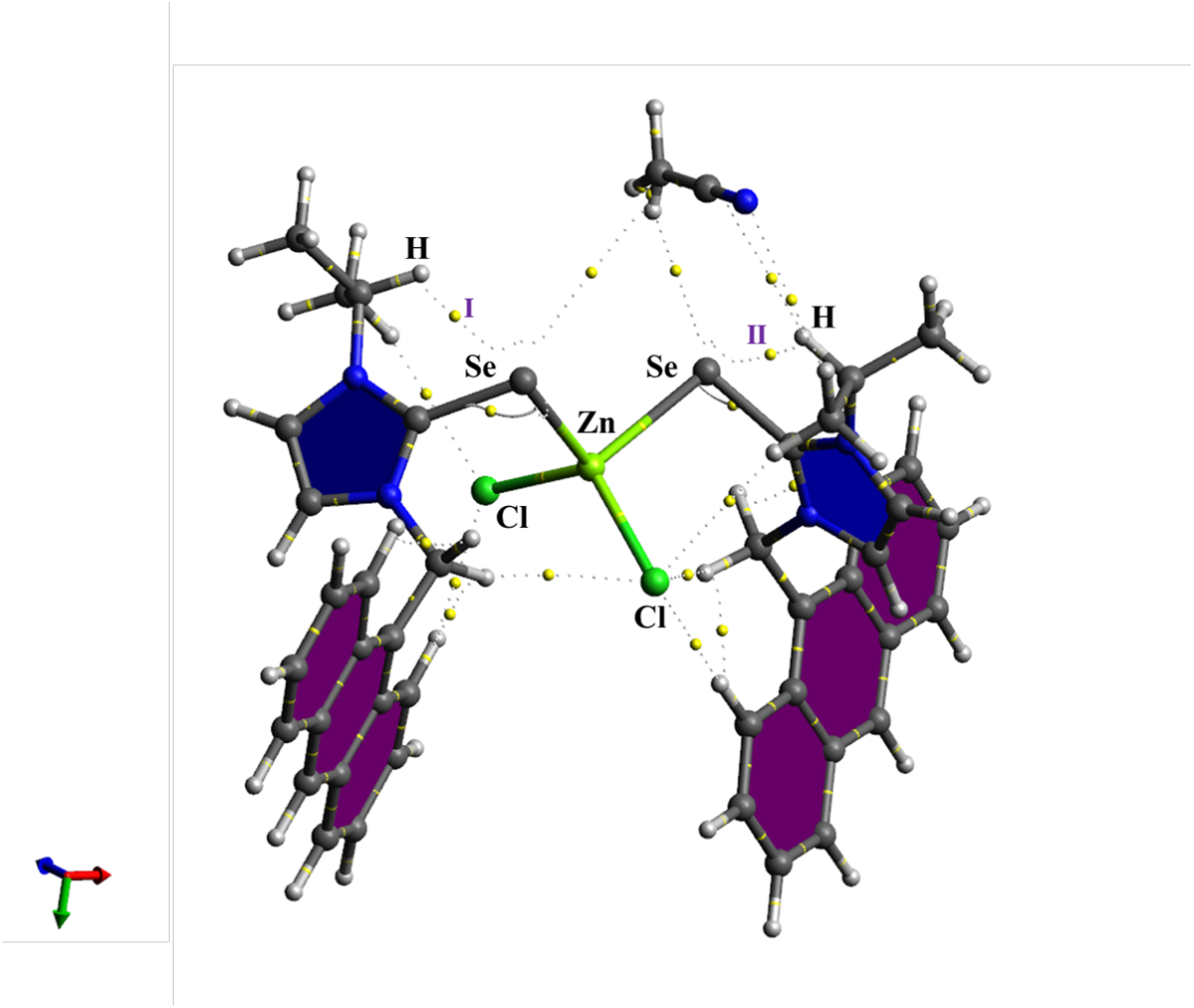


Figure S28: Topological analysis of intramolecular Se···H interactions in **4.** (I) ρ(r) = 0.0135, $\nabla^2\rho$(r) = 0.0404; (II) ρ(r) = 0.0139, $\nabla^2\rho$(r) = 0.0405.

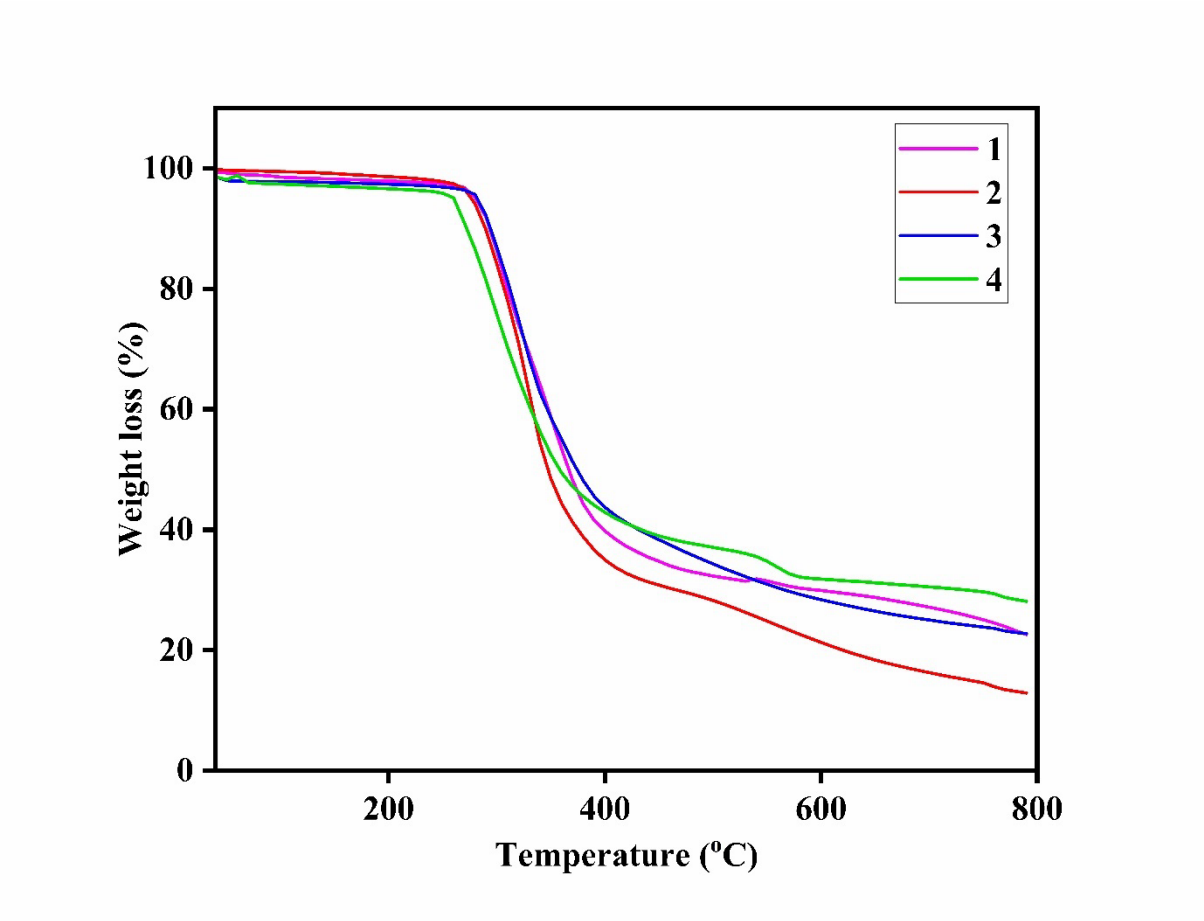


Figure S29: Thermogravimetric analysis of complexes **1-4** from 40-790 °C at a heating range of 10 °C/min under an inert environment.

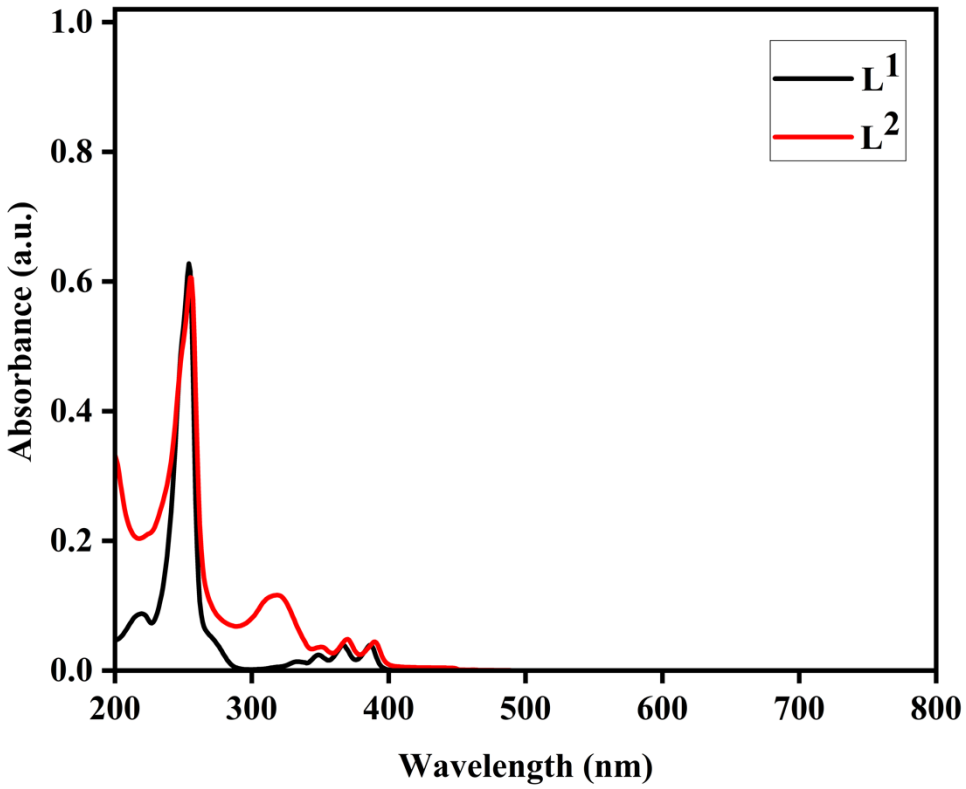


Figure S30: UV-Vis absorption spectra of $\mathbf{L^1}$ and $\mathbf{L^2}$ in acetonitrile at RT (C = 1 x 10^{-5} M).

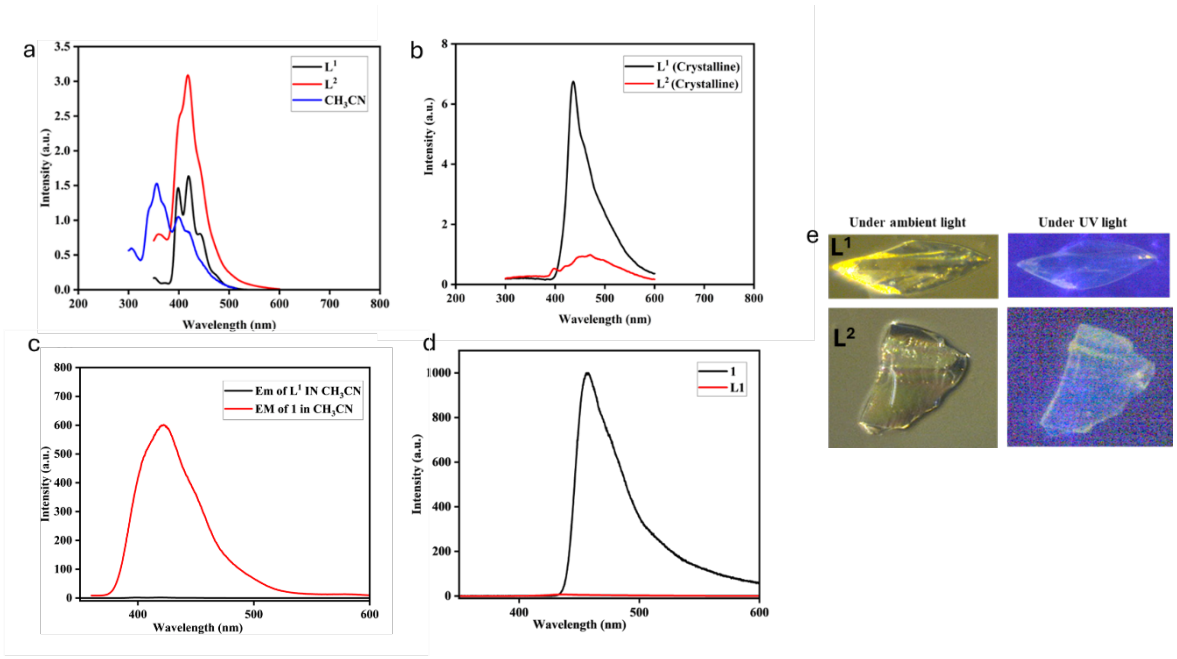


Figure S31: (a) Emission spectra of **L¹** and **L²** at RT in solution state using acetonitrile (C = 1 x 10^{-5} M), (b) Emission spectra of **L¹** and **L²** in the crystalline state at RT, (c) Emission spectra of **L¹** vs **1** in acetonitrile using the same concentration at RT, (d) Emission spectra of **L¹** vs **1** in the crystalline state at RT, (e) Crystal images of **L¹** and **L²** under ambient light vs under UV light.

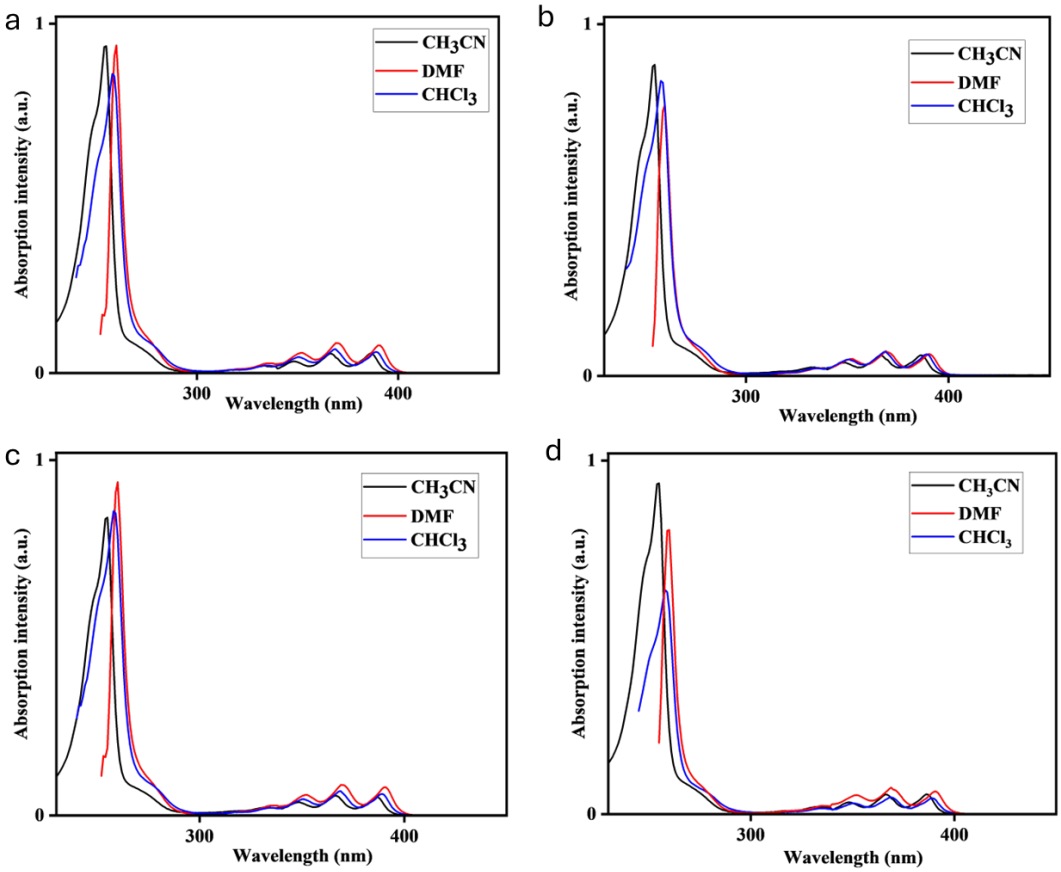


Figure S32: UV-Vis absorption spectra of **1**(a), **2**(b), **3**(c), and **4**(d) in acetonitrile (black solid line), DMF (red solid line), and $CHCl_3$ (blue solid line) (C = 1 x 10^{-5} M).

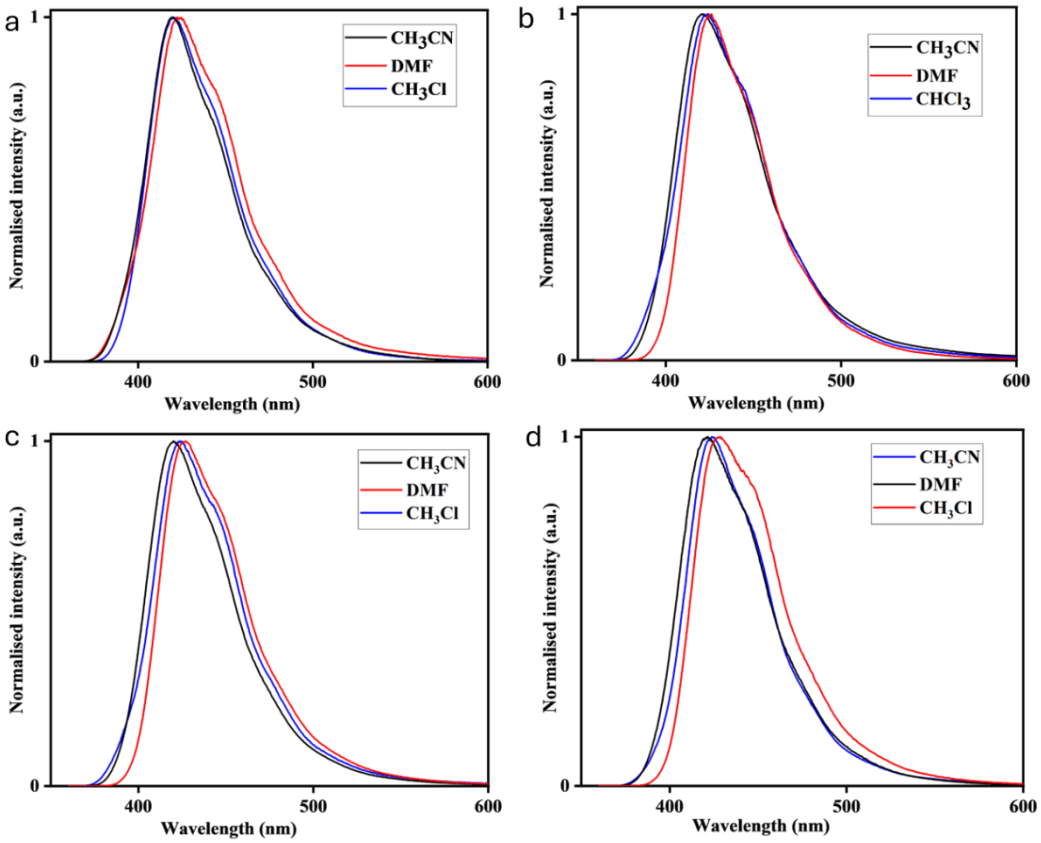


Figure S33: Emission spectra of **1** (a), **2**(b), **3**(c), and **4**(d) in acetonitrile (black solid line), DMF (red solid line), and $CHCl_3$ (blue solid line).

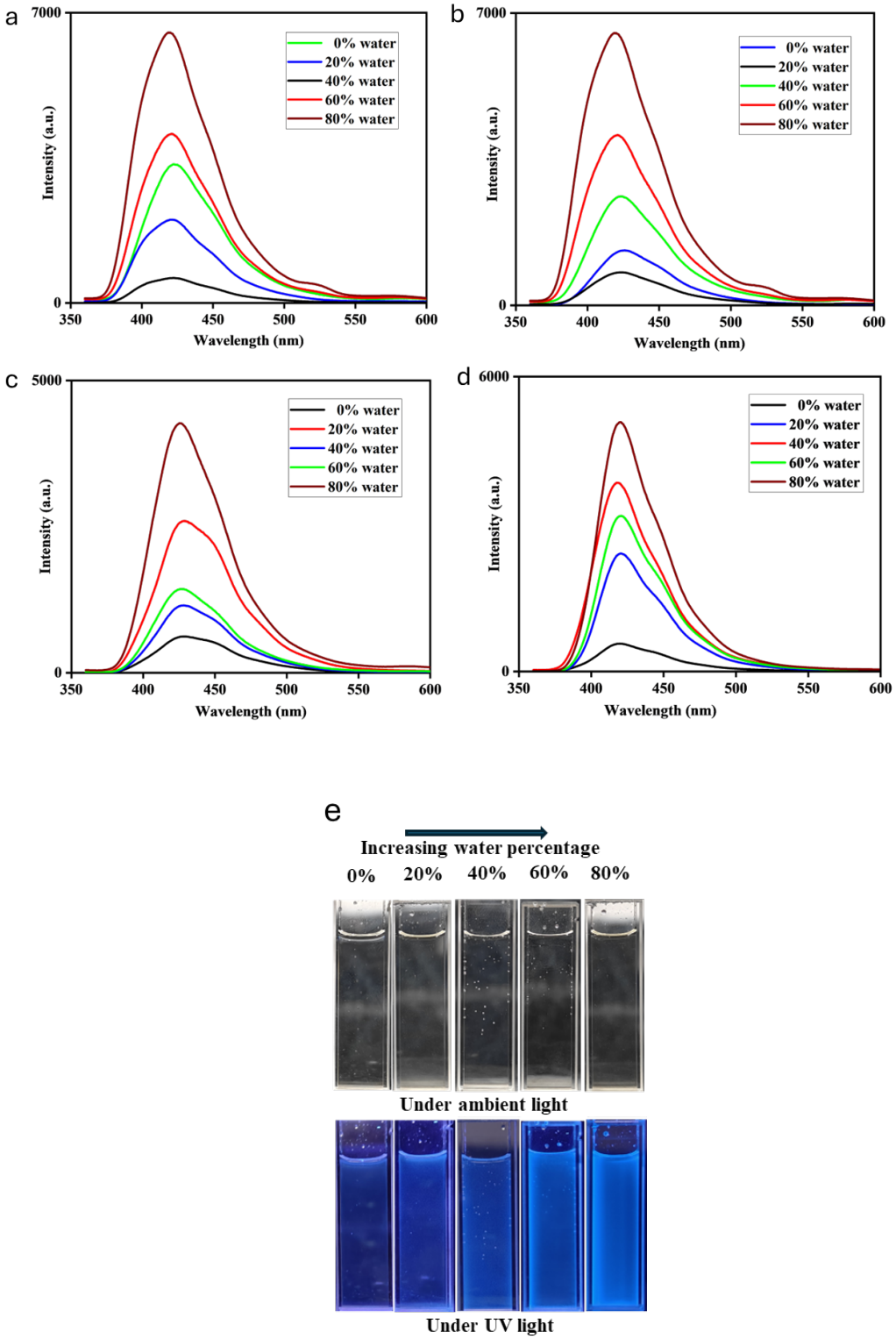


Figure S34: Emission spectra of **1**(a), **2**(b), **3**(c), and **4**(d) in DMF (C = 10^{-5} M) with increasing water concentration from 20% to 80% showing an increase in emission intensity upon aggregation, (e) images of solution of **1** in DMF under ambient light and under UV light with increasing water percentage from 0% to 80%.

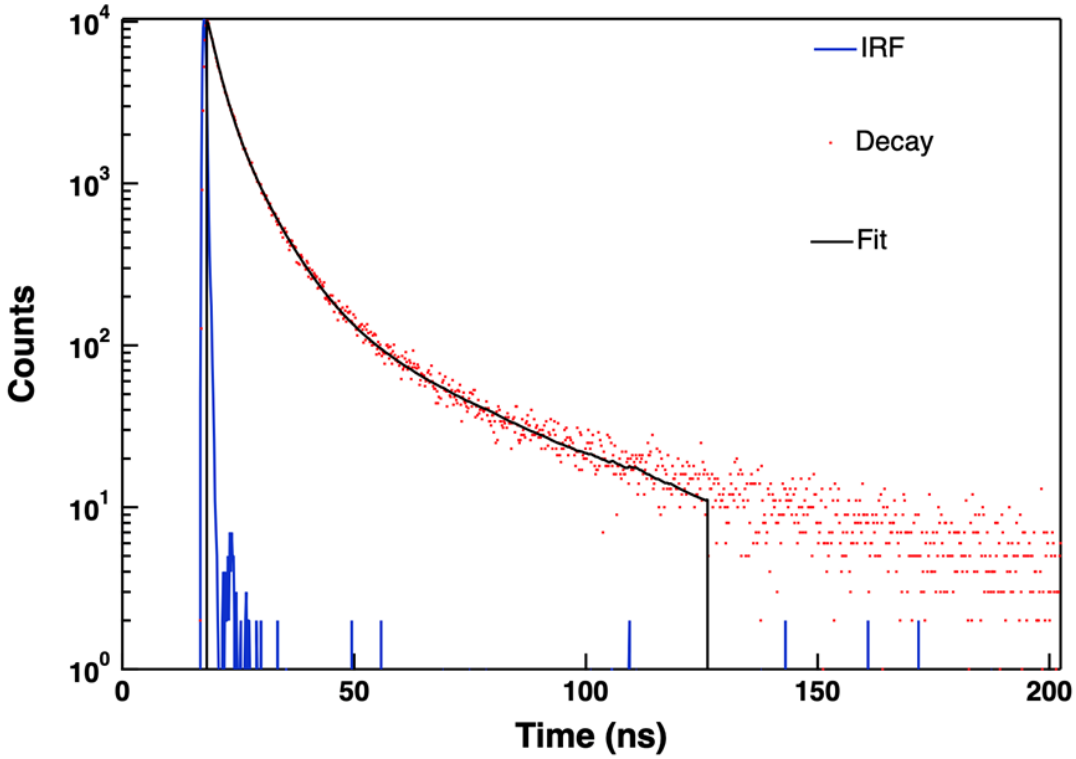


Figure S35: Photoluminescence decay profiles of **1** in crystalline state.

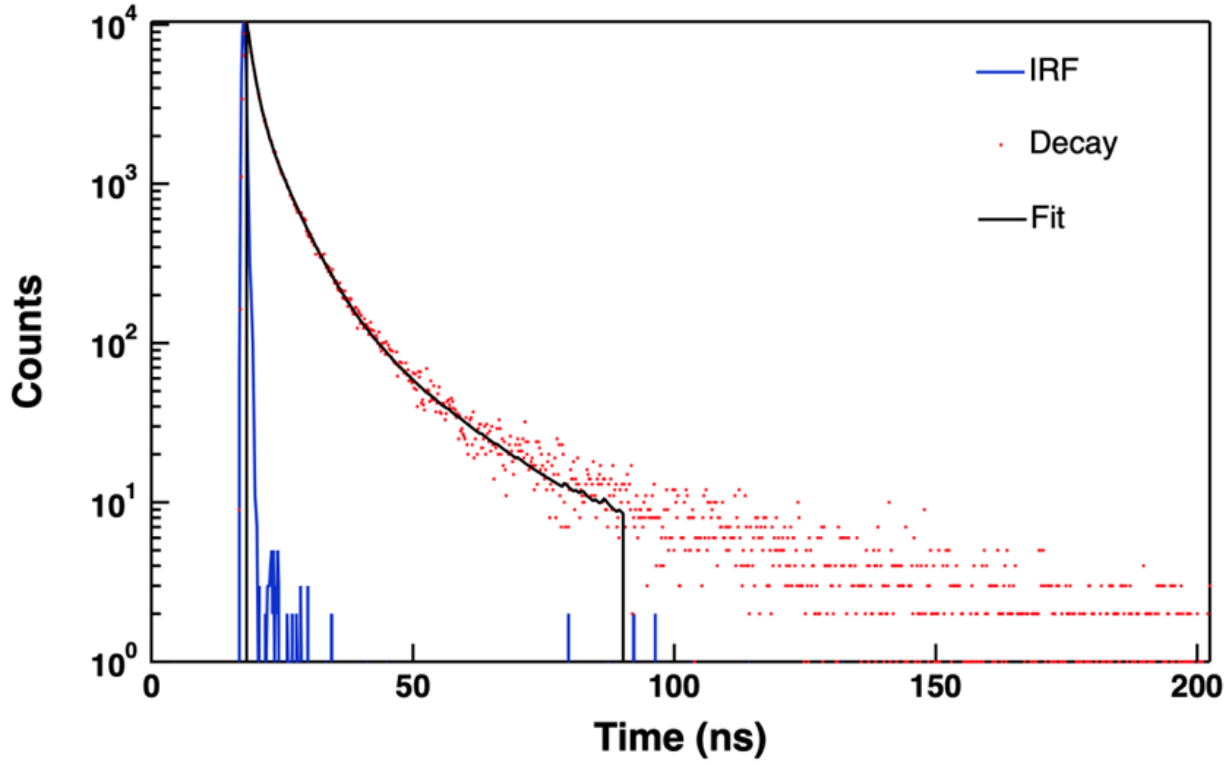


Figure S36: Photoluminescence decay profiles of **2** in crystalline state.

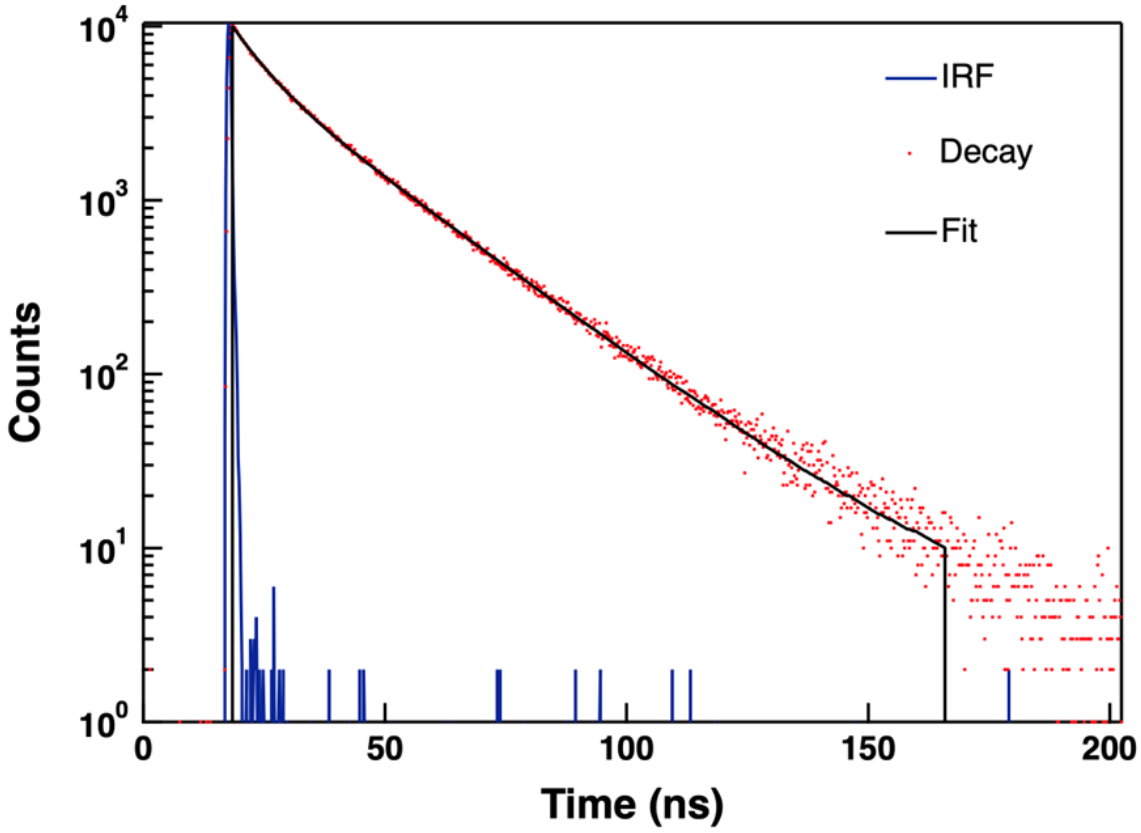


Figure S37: Photoluminescence decay profiles of **3** in crystalline state.

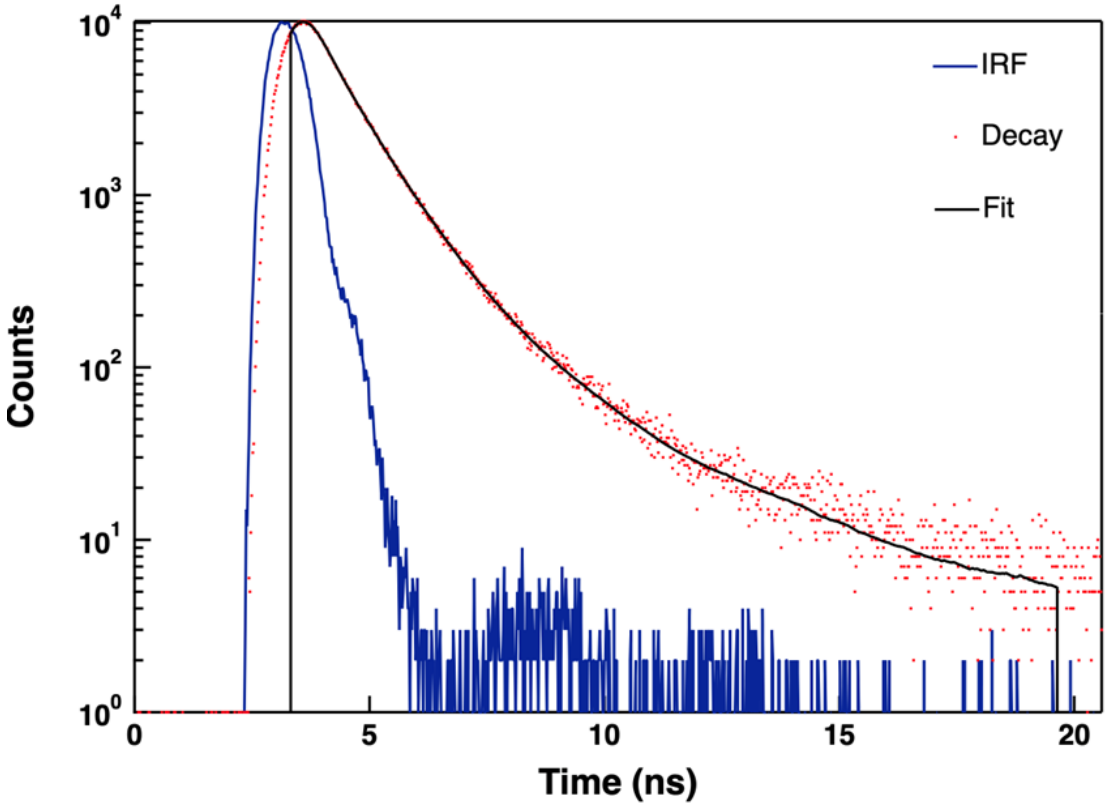


Figure S38: Photoluminescence decay profiles of **4** in crystalline state.

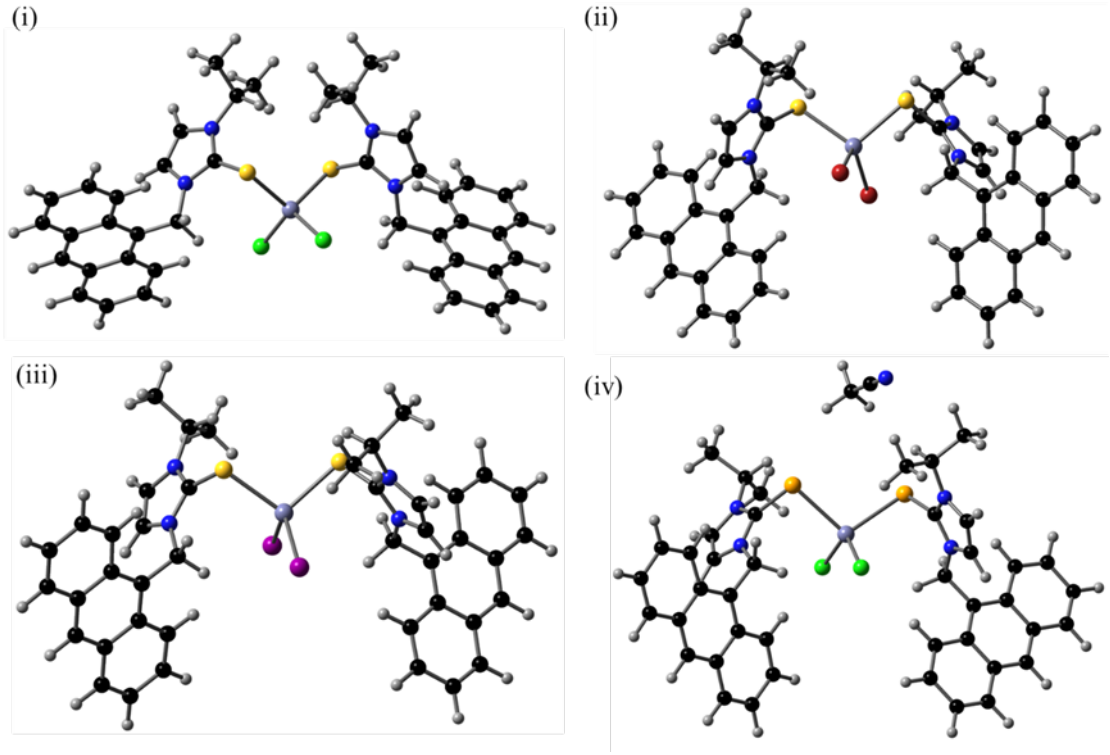


Figure S39: DFT Optimized structures of (i) **1**, (ii) **2**, (iii) **3**, and (iv) **4**.

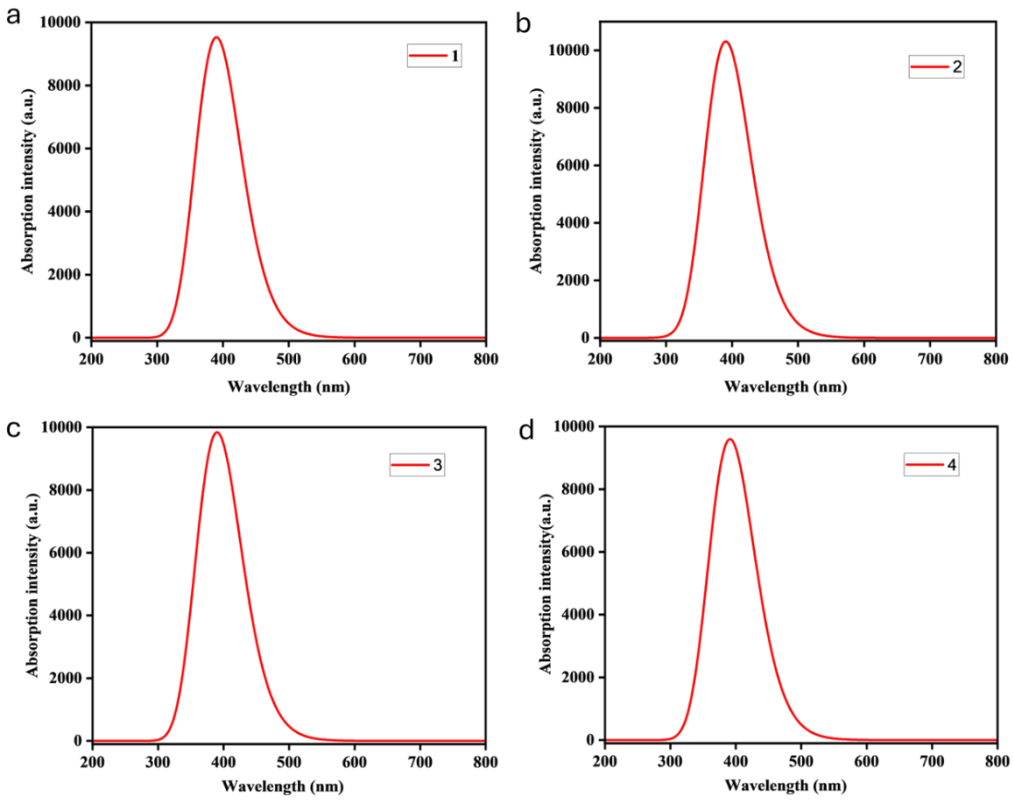


Figure S40: DFT calculated UV-Vis spectra (gas phase) of **1**(a), **2**(b), **3**(c), and **4**(d).

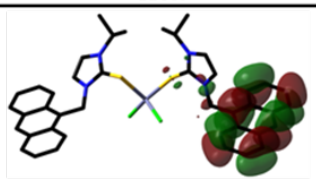
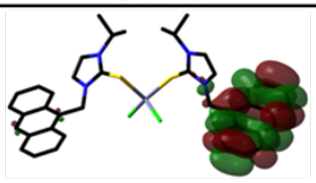
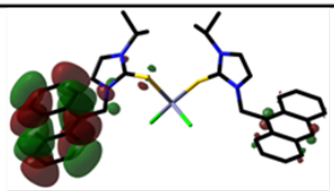
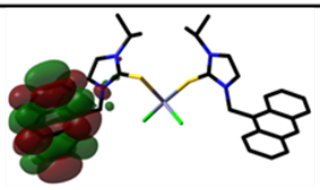
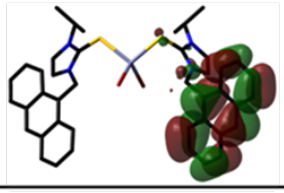
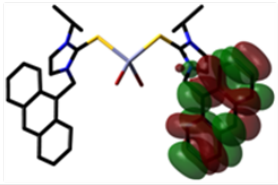
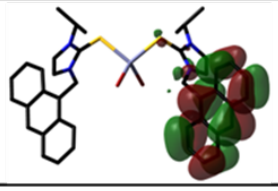
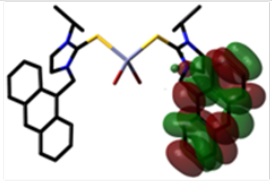
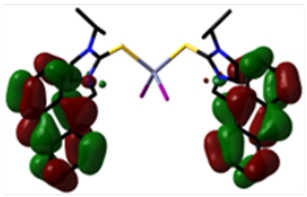
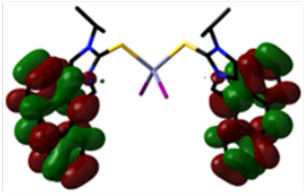
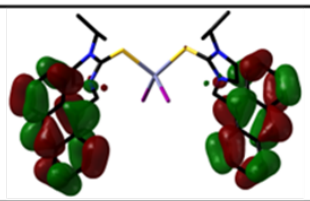
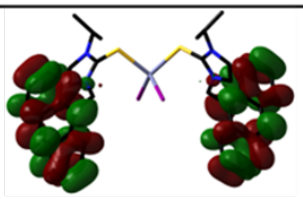
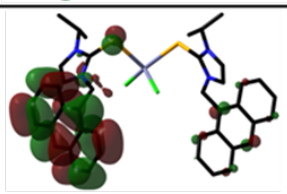
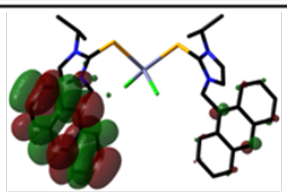
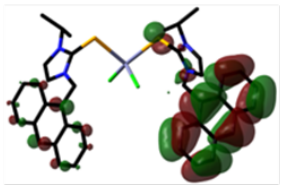
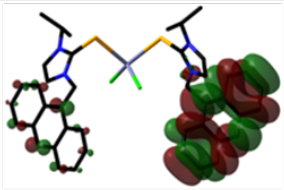
Complex	$\lambda_{calc.}$ (nm)	Hole	Electron
1	S_1 w = 0.73 3.1724 (0.2061) 390.82 nm		
	S_2 w = 0.75 3.1881 (0.064) 388.89 nm		
2	S_1 w =0.52 3.1737 (0.1483) 390.67 nm		
	S_2 w = 0.52 3.1869 (0.0868) 389.04 nm		
3	S_1 w = 0.51 3.1755 (0.1772) 390.43 nm		
	S_2 w =0.51 3.1881 (0.064) 388.89 nm		
4	S_1 w =0.64 3.1605 (0.1086) 392.29 nm		
	S_2 w =0.64 3.1754 (0.126) 390.45 nm		

Figure S41: Natural transition orbitals (NTOs) of complexes **1-4** illustrate the active singlet excited states in the absorption bands. NTO pairs that contribute more than 50% to each excited state.

Table S1: Change in the chemical shift values of the *C*=S and *C*=Se Carbon atom in complexes **1**-**4** compared to that of ligands $\mathbf{L^1}$ and $\mathbf{L^2}$ in DMSO-d_6.

Ligand	*C*=S Carbon (δ_c ppm)	Complex	*C*=S Carbon (δ_c ppm)	Shift in δ_c (ppm)
$\mathbf{L^1}$	167.37 ppm	**1**	160.42 ppm	6.95 ppm
	167.37 ppm	**2**	160.42 ppm	6.95 ppm
	167.37 ppm	**3**	160.44 ppm	6.93 ppm
$\mathbf{L^2}$	160.76 ppm	**4**	154.84 ppm	6.92 ppm

Table S2. Fitting parameters of fluorescence decay of **1**-**4**. (RAx = Relative amplitude of x-th component)

Compound	τ, ns	τ1, ns	τ2, ns	RA1	RA2	decay	Emission nm
1	4.581	1.32	5.11	4330.37	1001.38	bi-exponential	455
2	8.502	2.47	7.03	1893.38	854.30	bi-exponential	475
3	18.08	6.55	21.37	1283	1379.3	bi-exponential	535
4	0.95	0.37	0.99	289.62	246.45	bi-exponential	425

Table S3. The structural parameters of complexes **1**-**4**.

Identification code	**1**	**2**	**3**	**4**
Empirical formula	$C_{42}H_{40}Cl_2N_4S_2Zn$	$C_{42}H_{40}Br_2N_4S_2Zn$	$C_{42}H_{40}I_2N_4S_2Zn$	$C_{43.5}H_{41.5}Cl_2N_5Se_2Zn$
Formula weight	801.17	890.09	984.07	928.567
Temperature/K	273.15	273.15	273.15	298.15
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	C2/c	P-1	$P2_1/c$	P-1
a/Å	39.7664(15)	9.7737(15)	10.1471(17)	9.833(4)
b/Å	10.2851(4)	12.6125(19)	18.739(3)	12.903(5)
c/Å	20.4074(8)	18.399(3)	22.137(4)	18.383(8)
α/°	90	78.893(5)	90	78.137(14)
β/°	105.501(2)	77.020(5)	98.777(6)	76.450(14)
γ/°	90	74.820(5)	90	74.168(14)
Volume/$Å^3$	8043.1(5)	2111.3(6)	4160.0(12)	2156.3(15)
Z	8	2	4	2
$\rho_{calc}g/cm^3$	1.323	1.400	1.571	1.430
μ/mm^{-1}	0.882	2.606	2.209	2.417
F(000)	3328.0	904.0	1952.0	940.6
Crystal size/mm^3	0.27 × 0.21 × 0.17	0.28 × 0.18 × 0.17	0.2 × 0.17 × 0.16	0.28 × 0.17 × 0.17
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.1 to 54.302	3.806 to 54.382	3.724 to 54.702	4.32 to 53.1
Index ranges	-48 ≤ h ≤ 50, -13 ≤ k ≤ 13, -26 ≤ l ≤ 26	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23	-13 ≤ h ≤ 12, -23 ≤ k ≤ 24, -28 ≤ l ≤ 28	-12 ≤ h ≤ 11, -16 ≤ k ≤ 16, -23 ≤ l ≤ 22
Reflections collected	90769	42432	148885	41203
Independent reflections	8911 [R_{int} = 0.0736, R_{sigma} = 0.0366]	9377 [R_{int} = 0.0894, R_{sigma} = 0.0787]	9316 [R_{int} = 0.1543, R_{sigma} = 0.0629]	8945 [R_{int} = 0.0518, R_{sigma} = 0.0437]
Data/restraints/parameters	8911/0/464	9377/0/464	9316/0/464	8945/0/492
Goodness-of-fit on F^2	1.030	1.036	1.016	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.0907	R_1 = 0.0555, wR_2 = 0.1249	R_1 = 0.0471, wR_2 = 0.0908	R_1 = 0.0375, wR_2 = 0.0857
Final R indexes [all data]	R_1 = 0.0648, wR_2 = 0.1028	R_1 = 0.1152, wR_2 = 0.1476	R_1 = 0.0995, wR_2 = 0.1076	R_1 = 0.0626, wR_2 = 0.0959
Largest diff. peak/hole / e $Å^{-3}$	1.02/-0.36	1.06/-1.18	0.88/-0.95	0.69/-0.46

Table S4. Selected bond lengths and angles of complexes **1-4.**

	1	**2**	**3**	**4**
Bond Length [Å]				
M1-E1	2.3882(6)	2.3687(13)	2.3857(13)	2.4854(10)
M1-E2	2.3808(7)	2.3794(13)	2.3725(13)	2.5049(8)
M1-X1	2.2354(7)	2.3862(9)	2.5613(7)	2.2567(13)
M1-X2	2.2433(7)	2.3869(8)	2.6113(7)	2.2541(12)
Bond Angle [˚]				
E1-M1-E2	109.86(2)	108.64(5)	106.49(5)	104.26(17)
X1-M1-X2	115.84(3)	115.32(3)	117.24(2)	114.21(5)
E1-M1-X1	111.94(3)	105.70(4)	108.75(4)	107.99(3)
E2-M1-X2	110.48(3)	105.38(4)	104.89(4)	107.40(3)

Here, M = Zn(II)

E = S/Se

X = Cl / Br / I

Table S5: Key parameters (HOMO/LUMO, band gap, energy level location) from DFT calculations of **1**-**4**.

Compound	HOMO (eV)	LUMO (eV)	HOMO-1 (eV)	LUMO+1 (eV)	Band gap (eV)	Singlet (eV)	Triplet (eV)
1	-5.317	-1.817	-5.324	-1.816	3.50	2.5661	2.4770
2	-5.322	-1.840	-5.345	-1.818	3.48	2.2487	2.1343
3	-5.350	-1.846	-5.352	-1.846	3.50	2.4147	2.3659
4	-5.338	-1.846	-5.343	-1.843	3.49	2.4507	2.3763

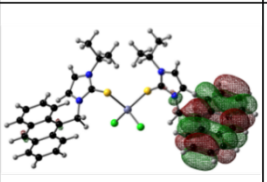
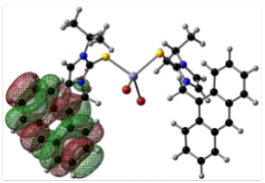
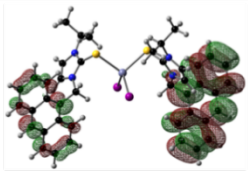
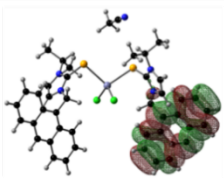
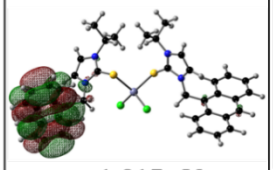
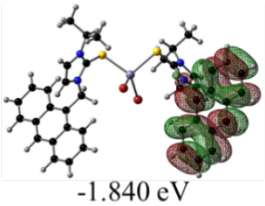
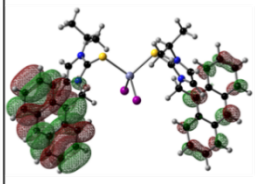
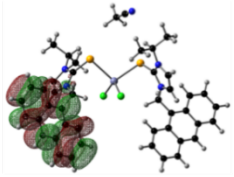
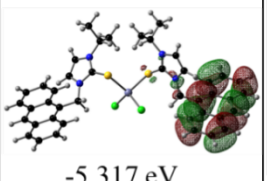
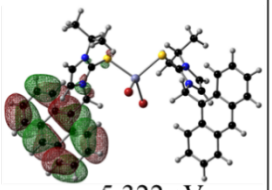
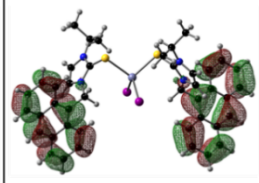
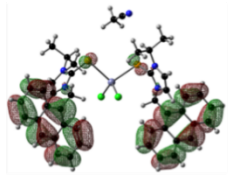
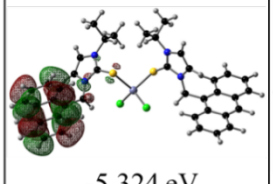
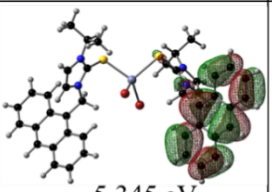
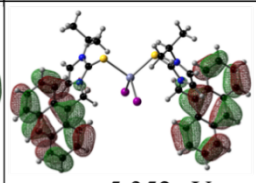
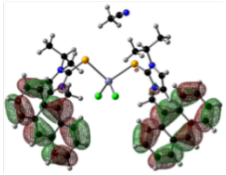
MOs	**1**	**2**	**3**	**4**
LUMO+1	 -1.816 eV	 -1.818 eV	 -1.846 eV	 -1.843 eV
LUMO	 -1.817 eV	 -1.840 eV	 -1.846 eV	 -1.846 eV
HOMO	 -5.317 eV	 -5.322 eV	 -5.350 eV	 -5.338 eV
HOMO-1	 -5.324 eV	 -5.345 eV	 -5.352 eV	 -5.343 eV

Table S6: Excitation energies and oscillator strengths of **1.**

No.	Energy (eV)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	1.7510	708.09	0.0	Triplet-A	HOMO->L+1 (95%)
2	1.7565	705.87	0.0	Triplet-A	H-1->LUMO (95%)
3	3.1724	390.82	0.2061	Singlet-A	H-1->LUMO (24%), HOMO->L+1 (74%)
4	3.1873	388.99	0.0482	Singlet-A	H-1->LUMO (72%), HOMO->L+1 (22%)
5	3.2571	380.66	0.0	Triplet-A	H-12->L+1 (54%), HOMO->L+7 (31%)
6	3.2613	380.16	0.0	Triplet-A	H-13->LUMO (54%), H-1->L+6 (32%)
7	3.2839	377.56	0.0	Triplet-A	HOMO->LUMO (97%)
8	3.2839	377.55	0.0	Singlet-A	HOMO->LUMO (97%)
9	3.2935	376.45	0.0	Triplet-A	H-1->L+1 (97%)
10	3.2936	376.45	0.0	Singlet-A	H-1->L+1 (98%)
11	3.4449	359.91	0.0	Triplet-A	H-8->L+1 (80%)
12	3.4518	359.19	0.0	Triplet-A	H-9->LUMO (78%)
13	3.5308	351.15	0.0002	Singlet-A	H-2->L+1 (90%)
14	3.5395	350.28	0.0003	Singlet-A	H-2->LUMO (89%)
15	3.7990	326.36	0.001	Singlet-A	H-3->L+1 (84%)
16	3.8239	324.23	0.0005	Singlet-A	H-4->LUMO (15%), H-3->LUMO (74%)

Table S7: Excitation energies and oscillator strengths of **2.**

No.	Energy (eV)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	1.7512	708.00	0.0	Triplet-A	H-1->LUMO (97%)
2	1.7512	707.98	0.0	Triplet-A	HOMO->L+1 (97%)
3	3.1737	390.67	0.1483	Singlet-A	H-1->LUMO (45%), HOMO->L+1 (53%)
4	3.1869	389.04	0.0868	Singlet-A	H-1->LUMO (53%), HOMO->L+1 (45%)
5	3.2306	383.78	0.0	Triplet-A	HOMO->LUMO (100%)
6	3.2307	383.77	0.0001	Singlet-A	HOMO->LUMO (100%)
7	3.2547	380.93	0.0	Triplet-A	H-14->LUMO (56%), H-1->L+6 (23%)
8	3.2554	380.86	0.0	Triplet-A	H-13->L+1 (56%), HOMO->L+7 (21%)
9	3.2752	378.55	0.0	Triplet-A	H-1->L+1 (100%)
10	3.2753	378.55	0.0	Singlet-A	H-1->L+1 (100%)
11	3.4422	360.19	0.0	Triplet-A	H-11->LUMO (83%)
12	3.4425	360.16	0.0	Triplet-A	H-10->L+1 (83%)
13	3.4796	356.32	0.0001	Singlet-A	H-2->LUMO (92%)
14	3.4941	354.84	0.0001	Singlet-A	H-2->L+1 (93%)
15	3.5934	345.03	0.0	Singlet-A	H-3->LUMO (99%)
16	3.6117	343.28	0.0	Singlet-A	H-3->L+1 (100%)

Table S8: Excitation energies and oscillator strengths of **3.**

No.	Energy (eV)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	1.7519	707.72	0.0	Triplet-A	H-1->L+1 (38%), HOMO->L+1 (47%)
2	1.7519	707.71	0.0	Triplet-A	H-1->LUMO (47%), HOMO->LUMO (37%)
3	3.1755	390.43	0.1772	Singlet-A	H-1->LUMO (10%), H-1->L+1 (37%), HOMO->LUMO (40%), HOMO->L+1 (11%)
4	3.1881	388.89	0.064	Singlet-A	H-1->LUMO (41%), HOMO->L+1 (44%)
5	3.2166	385.45	0.0	Triplet-A	H-2->LUMO (90%)
6	3.2169	385.41	0.0	Triplet-A	H-2->L+1 (90%)
7	3.2177	385.32	0.0008	Singlet-A	H-2->LUMO (85%), H-2->L+1 (14%)
8	3.2177	385.32	0.0009	Singlet-A	H-2->LUMO (14%), H-2->L+1 (85%)
9	3.2576	380.60	0.0	Triplet-A	H-13->L+1 (47%)
10	3.2576	380.60	0.0	Triplet-A	H-14->LUMO (46%)
11	3.2665	379.57	0.0	Triplet-A	H-1->LUMO (36%), HOMO->LUMO (48%)
12	3.2668	379.57	0.0	Singlet-A	H-1->LUMO (40%), HOMO->LUMO (46%)
13	3.2668	379.53	0.0	Triplet-A	H-1->L+1 (46%), HOMO->L+1 (39%)
14	3.2668	379.52	0.0	Singlet-A	H-1->L+1 (50%), HOMO->L+1 (36%)
15	3.3598	369.03	0.0	Singlet-A	H-3->LUMO (86%), H-3->L+1 (14%)
16	3.3605	368.95	0.0001	Singlet-A	H-3->LUMO (14%), H-3->L+1 (86%)

Table S9: Excitation energies and oscillator strengths of **4.**

No.	Energy (eV)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributors
1	1.7496	708.66	0.0	Triplet-A	H-1->LUMO (46%), HOMO->LUMO (50%)
2	1.7507	708.21	0.0	Triplet-A	H-1->L+1 (50%), HOMO->L+1 (45%)
3	3.1605	392.29	0.1086	Singlet-A	H-1->LUMO (24%), H-1->L+1 (18%), HOMO->LUMO (40%), HOMO->L+1 (16%)
4	3.1754	390.45	0.126	Singlet-A	H-1->LUMO (16%), H-1->L+1 (26%), HOMO->LUMO (19%), HOMO->L+1 (37%)
5	3.2224	384.75	0.0	Triplet-A	H-1->LUMO (50%), HOMO->LUMO (49%)
6	3.2231	384.67	0.0008	Singlet-A	H-1->LUMO (60%), HOMO->LUMO (39%)
7	3.2248	384.47	0.0	Triplet-A	H-1->L+1 (46%), HOMO->L+1 (53%)
8	3.2253	384.41	0.0006	Singlet-A	H-1->L+1 (55%), HOMO->L+1 (45%)
9	3.2508	381.40	0.0	Triplet-A	H-12->LUMO (54%)
10	3.2541	381.01	0.0	Triplet-A	H-13->L+1 (55%)
11	3.3448	370.68	0.0	Triplet-A	H-2->LUMO (93%)
12	3.3567	369.37	0.0005	Singlet-A	H-2->LUMO (95%)
13	3.3597	369.04	0.0	Triplet-A	H-2->L+1 (92%)
14	3.3736	367.52	0.0004	Singlet-A	H-2->L+1 (95%)
15	3.6494	339.74	0.0004	Singlet-A	H-4->LUMO (17%), H-3->LUMO (77%)
16	3.6518	339.52	0.0006	Singlet-A	H-4->L+1 (85%), H-3->L+1 (11%)

Cartesian coordinates of **1**

Symmetry C1

Zn	-0.006293957	-0.235042060	-0.267425038
Cl	0.966302110	-1.745140168	1.063704057
Cl	-1.105304035	-1.057232118	-2.037518166
S	-1.484881066	1.022315030	1.125684064
S	1.586547160	1.226813043	-1.271872110
N	-3.710574222	0.649850003	-0.411194049
N	-2.871479163	2.644831150	-0.600730062
N	3.717918313	0.601585001	0.322100004
N	2.774929245	2.473572136	0.916623045
C	-5.888233356	-1.884179178	-0.988306088
C	-2.702731153	1.448119064	0.008346981
C	-4.507905279	1.336070057	-1.307196115
C	-3.987401245	2.583455146	-1.426416124
C	-2.010513102	3.832059232	-0.435916051
C	-2.811555158	4.990641319	0.168278993
C	-1.334183048	4.192500261	-1.762471147
C	-3.889004239	-0.748075096	0.046068984
C	-5.337692322	-1.159871126	0.092312987
C	-6.130259397	-0.826337098	1.217838070
C	-5.631197361	-0.073016046	2.330183146
C	-6.430664431	0.226849976	3.403413224
C	-7.787450503	-0.201194055	3.446722228
C	-8.307813564	-0.921632105	2.405572156
C	-7.509576513	-1.253820133	1.266992074
C	-8.037988519	-1.985204184	0.198626995
C	-7.271844481	-2.308545205	-0.924100087
C	-7.833490511	-3.047296261	-2.012471164
C	-7.087451451	-3.351004282	-3.118278245
C	-5.729937391	-2.928090254	-3.194870249
C	-5.149069330	-2.222997199	-2.172602173
C	2.701555237	1.446232060	0.020955982
C	4.000796330	-0.664590093	-0.403410048
C	5.419129420	-1.146540130	-0.201377034
C	6.458996528	-0.607322092	-0.998853094
C	7.809095599	-1.096542124	-0.835578078
C	8.067387649	-2.089114196	0.114480989
C	7.057091547	-2.619032235	0.921228046
C	5.699076461	-2.139736202	0.770116037
C	4.698775380	-2.701513241	1.632860096
C	5.019996405	-3.661193306	2.557965165
C	6.355938518	-4.134196342	2.694663174
C	7.343772581	-3.624889307	1.896752117
C	8.855887680	-0.556643088	-1.646200136
C	8.601899640	0.421104983	-2.569721203
C	7.276287559	0.913604020	-2.731665216
C	6.244352499	0.419768984	-1.975529163
C	4.419872363	1.083526031	1.412032081
C	3.837553319	2.252296119	1.780134110
C	1.898449183	3.660662219	0.928108049
C	1.248153137	3.839720231	2.302829149
C	2.676411237	4.897555310	0.464014014
H	-5.365253355	0.878110022	-1.770692148
H	-4.309270264	3.420905205	-2.022389163
H	-1.251485043	3.510937210	0.280747001
H	-3.600702214	5.333864360	-0.509154056
H	-2.146930108	5.838978385	0.357763006

H	-3.273435190	4.697353295	1.115064064
H	-0.744759007	3.353145196	-2.139604172
H	-0.663539004	5.044595321	-1.613329138
H	-2.067431106	4.478512282	-2.524055201
H	-3.422759204	-0.801983102	1.029714055
H	-3.289445193	-1.380517142	-0.607875061
H	-4.602863289	0.271129978	2.330317150
H	-6.023666377	0.796614017	4.233792284
H	-8.402580584	0.044881963	4.307226291
H	-9.341743621	-1.256551132	2.424310153
H	-9.075815596	-2.308416208	0.241291998
H	-8.871813586	-3.360410281	-1.939080159
H	-7.523583517	-3.912710321	-3.939080303
H	-5.143110329	-3.170342270	-4.075902314
H	-4.112522253	-1.920221181	-2.275092181
H	3.789493315	-0.466934078	-1.454739124
H	3.259986277	-1.393744144	-0.075137025
H	9.084593694	-2.456467222	0.231799997
H	3.667522308	-2.372424218	1.563408091
H	4.239870345	-4.068796337	3.193922212
H	6.583992534	-4.898238399	3.432101230
H	8.369090649	-3.973834331	1.988927126
H	9.862638770	-0.943194114	-1.509936127
H	9.404565745	0.823525013	-3.180536250
H	7.080979560	1.690000074	-3.465768270
H	5.248585419	0.822696015	-2.122305172
H	5.262699423	0.553748997	1.821887110
H	4.083699339	2.934299165	2.576691166
H	1.126754124	3.426542202	0.191217995
H	0.683230091	2.948495170	2.586360165
H	0.556895088	4.687545292	2.271252142
H	1.990169190	4.052077246	3.079949202
H	3.486370294	5.145327327	1.158451063
H	2.005706189	5.760735348	0.411967010
H	3.108406269	4.737896295	-0.527678057

Cartesian coordinates of **2**

Symmetry C1

Br	0.573248000	-0.154711000	-2.279053000
Br	0.619886000	0.468473000	1.920045000
Zn	0.689445000	-1.204220000	0.019074000
S	-1.149907000	-2.886911000	0.131970000
S	2.755457000	-2.572328000	0.365833000
N	4.205194000	-0.379399000	1.214807000
N	-2.907045000	-1.229351000	-1.210224000
N	3.757920000	-1.782739000	2.822648000
N	-2.258886000	-2.935127000	-2.404298000
N	-10.940994000	2.277763000	1.309453000
C	-5.401441000	0.159430000	0.450492000
C	-2.113030000	-2.332991000	-1.192501000
C	-6.577039000	1.000536000	0.453619000
C	3.577271000	-1.553457000	1.493581000
C	-4.183448000	1.883618000	-0.813873000
C	-4.214289000	0.623096000	-0.167508000
C	-6.524181000	2.254862000	-0.162021000
C	-5.368004000	2.715422000	-0.798358000
C	4.758450000	0.136150000	2.372577000
C	4.485345000	-0.739786000	3.372155000
C	4.984520000	2.685116000	-0.003308000
C	6.530627000	0.918459000	-0.740274000
C	-7.776254000	0.540614000	1.083393000
C	-1.525597000	-4.137294000	-2.856537000
C	-5.507468000	-1.123403000	1.080805000
C	4.163591000	0.289218000	-0.106749000
C	-2.967754000	-0.229086000	-0.117473000
C	-3.031642000	2.386235000	-1.507462000
C	5.253268000	1.321800000	-0.280587000
C	-5.338177000	3.993235000	-1.440112000
C	-3.534487000	-1.130572000	-2.438548000
C	-3.135160000	-2.194604000	-3.180441000
C	-7.825400000	-0.692187000	1.676859000
C	7.552720000	1.915257000	-0.965749000
C	3.731152000	3.150748000	0.518483000
C	6.017543000	3.671519000	-0.238102000
C	-6.675983000	-1.531708000	1.671244000
C	6.875608000	-0.449213000	-0.995316000
C	-0.634600000	-3.790956000	-4.054193000
C	3.182600000	-2.915296000	3.580917000

C	-4.212859000	4.434927000	-2.081332000
C	-2.500409000	-5.286079000	-3.133884000
C	-3.049908000	3.614260000	-2.117142000
C	5.746821000	5.050241000	0.028601000
C	8.839088000	1.508232000	-1.439112000
C	7.264462000	3.260290000	-0.716642000
C	9.121005000	0.189699000	-1.673810000
C	4.531964000	5.448625000	0.516023000
C	3.517479000	4.481981000	0.767808000
C	8.122867000	-0.798859000	-1.444678000
C	4.295819000	-3.761847000	4.205371000
C	2.162448000	-2.401629000	4.602314000
C	-11.930337000	1.959746000	1.825260000
C	-13.177159000	1.562129000	2.475089000
H	-7.411270000	2.884006000	-0.149637000
H	5.291086000	1.071603000	2.377978000
H	4.739715000	-0.705580000	4.418265000
H	-8.647095000	1.191011000	1.077091000
H	-0.893703000	-4.400810000	-2.005220000
H	-4.654922000	-1.793395000	1.087212000
H	3.173654000	0.732396000	-0.223948000
H	4.229420000	-0.498072000	-0.857563000
H	-2.064584000	0.380315000	-0.174541000
H	-2.895176000	-0.784578000	0.817272000
H	-2.127544000	1.790144000	-1.571960000
H	-6.236768000	4.604000000	-1.408489000
H	-4.201570000	-0.317974000	-2.668914000
H	-3.393576000	-2.480355000	-4.186621000
H	-8.739892000	-1.034906000	2.152689000
H	2.933764000	2.449366000	0.739564000
H	-6.725675000	-2.510048000	2.141229000
H	6.143274000	-1.229843000	-0.823160000
H	-1.229067000	-3.542423000	-4.940441000
H	-0.009862000	-4.653857000	-4.304414000
H	0.012586000	-2.941276000	-3.820652000
H	2.663359000	-3.507256000	2.823900000
H	-4.201511000	5.406236000	-2.566975000
H	-3.104271000	-5.512706000	-2.250423000
H	-1.939546000	-6.185125000	-3.406168000
H	-3.175613000	-5.051376000	-3.964126000
H	-2.162489000	3.964426000	-2.635921000
H	6.534141000	5.774657000	-0.163139000
H	9.590947000	2.274972000	-1.607251000

H	8.034823000	4.007458000	-0.894463000
H	10.101309000	-0.108164000	-2.033424000
H	4.336996000	6.498230000	0.716081000
H	2.558737000	4.801562000	1.164817000
H	8.353743000	-1.844012000	-1.629218000
H	4.860091000	-3.198367000	4.956457000
H	4.994800000	-4.118892000	3.443796000
H	3.857786000	-4.631579000	4.703897000
H	1.662724000	-3.251547000	5.077014000
H	1.410228000	-1.775515000	4.116045000
H	2.644100000	-1.814201000	5.391471000
H	-13.030048000	1.478485000	3.555975000
H	-13.510866000	0.594264000	2.090911000
H	-13.957501000	2.304570000	2.283196000

Cartesian coordinates of **3**

Symmetry C1

I	-0.177334000	0.494377000	2.301611000
I	0.178317000	0.492117000	-2.301760000
Zn	0.000121000	-0.969987000	0.000632000
S	1.949324000	-2.547733000	0.059335000
S	-1.949681000	-2.546919000	-0.056924000
N	3.721961000	-0.692717000	-0.972238000
N	3.291266000	-2.327503000	-2.349874000
N	-3.291194000	-2.324773000	2.352337000
N	-3.721173000	-0.690392000	0.974007000
C	5.962321000	0.446850000	1.129102000
C	-2.994422000	-1.831541000	1.118576000
C	2.994605000	-1.833541000	-1.116378000
C	4.457485000	-0.464016000	-2.120816000
C	4.194903000	-1.484480000	-2.975586000
C	2.693549000	-3.538450000	-2.954201000
C	3.767468000	-4.606773000	-3.181076000
C	1.923413000	-3.169679000	-4.225899000
C	3.626473000	0.220769000	0.189944000
C	4.887911000	1.024562000	0.409194000
C	4.983609000	2.347106000	-0.089739000
C	6.180098000	3.118064000	0.175037000
C	7.222838000	2.540366000	0.903873000
C	7.151485000	1.228320000	1.381227000
C	5.936961000	-0.896611000	1.628120000
C	6.997112000	-1.418531000	2.323842000
C	8.162398000	-0.640310000	2.573952000
C	8.232874000	0.646716000	2.113730000
C	6.278304000	4.456833000	-0.318502000
C	5.264983000	5.016518000	-1.047767000
C	4.091416000	4.260030000	-1.325849000
C	3.952788000	2.976010000	-0.865786000
C	-4.194259000	-1.480942000	2.977802000
C	-4.456403000	-0.460745000	2.122589000
C	-3.625430000	0.222694000	-0.188447000
C	-4.887777000	1.024538000	-0.409685000
C	-4.985820000	2.347463000	0.087771000
C	-3.956539000	2.978787000	0.863912000
C	-4.097448000	4.263081000	1.322514000
C	-5.271961000	5.017485000	1.042776000
C	-6.283875000	4.455481000	0.313344000
C	-6.183268000	3.116349000	-0.178722000
C	-7.224587000	2.536331000	-0.907745000
C	-7.150873000	1.223921000	-1.383737000
C	-8.230794000	0.639955000	-2.116527000
C	-8.157958000	-0.647393000	-2.575478000
C	-6.991655000	-1.423567000	-2.323748000
C	-5.932861000	-0.899370000	-1.627670000

C	-5.960725000	0.444511000	-1.129910000
C	-2.693892000	-3.535606000	2.957309000
C	-1.922612000	-3.166259000	4.228161000
C	-3.768393000	-4.602970000	3.185892000
H	5.094678000	0.397833000	-2.222681000
H	4.565701000	-1.675570000	-3.968665000
H	1.988373000	-3.893715000	-2.199348000
H	4.514801000	-4.279032000	-3.911996000
H	3.301980000	-5.518431000	-3.567032000
H	4.281162000	-4.852677000	-2.247506000
H	1.193157000	-2.382259000	-4.021485000
H	1.394409000	-4.051784000	-4.598870000
H	2.594601000	-2.824014000	-5.019801000
H	3.388599000	-0.400389000	1.053454000
H	2.759495000	0.864114000	0.034380000
H	8.117670000	3.126624000	1.101031000
H	5.068470000	-1.521267000	1.451825000
H	6.947902000	-2.439606000	2.690823000
H	8.989554000	-1.072296000	3.129390000
H	9.115736000	1.254005000	2.295993000
H	7.182958000	5.018860000	-0.101274000
H	5.350342000	6.033766000	-1.418245000
H	3.292529000	4.705916000	-1.910728000
H	3.044983000	2.435037000	-1.109293000
H	-4.565033000	-1.671393000	3.971013000
H	-5.093205000	0.401442000	2.224083000
H	-3.385572000	-0.398545000	-1.051345000
H	-2.759550000	0.867292000	-0.031997000
H	-3.048074000	2.439463000	1.108608000
H	-3.299665000	4.710823000	1.907483000
H	-5.359150000	6.034988000	1.412126000
H	-7.189222000	5.015902000	0.094852000
H	-8.120156000	3.121033000	-1.106166000
H	-9.114449000	1.245706000	-2.300059000
H	-8.984005000	-1.081180000	-3.131165000
H	-6.940558000	-2.444891000	-2.689775000
H	-5.063513000	-1.522498000	-1.450186000
H	-1.989492000	-3.892032000	2.202282000
H	-1.192096000	-2.379372000	4.022623000
H	-1.393788000	-4.048357000	4.601403000
H	-2.593048000	-2.819642000	5.022282000
H	-4.514997000	-4.274064000	3.917033000
H	-3.303271000	-5.514598000	3.572365000
H	-4.282910000	-4.849376000	2.252908000

Cartesian coordinates of **4**

Symmetry C1

Se	-2.127354095	-2.446806208	-0.063762918
Se	2.087287207	-2.368187148	0.541069127
Zn	-0.060016967	-0.798683063	0.460583120
Cl	-0.616422019	0.168288998	2.484033266
Cl	0.271206039	0.661356047	-1.314567009
N	3.645793296	-0.285409982	-0.787562969
N	-3.883053249	-0.276097074	0.782315145
N	3.178407280	-1.915885103	-2.154065068
N	-3.825358223	-1.868757186	2.266672251
N	0.871869165	-6.172255433	-2.543933099
C	3.008641260	-1.479391074	-0.882214977
C	-3.335805195	-1.485741153	1.060764165
C	-5.631540374	1.663804043	-1.319895009
C	-4.431711312	1.753136063	-0.572440955
C	-4.034642301	2.983015159	0.009649087
C	-6.428261491	2.852372118	-1.528332021
C	4.198989329	0.039266048	-2.012109059
C	-3.550580233	0.535799987	-0.416284943
C	-4.842809373	4.163070232	-0.208979929
C	-6.116099408	0.439638950	-1.887398047
C	-6.007042433	4.065448211	-0.976086984
C	-7.633681543	2.766208097	-2.292793080
C	3.912366319	-0.979630026	-2.862058120
C	-2.865782215	3.121569183	0.829893148
C	3.602528277	0.596423083	0.403389115
C	-7.281098521	0.397819932	-2.609134102
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