NMR experiments

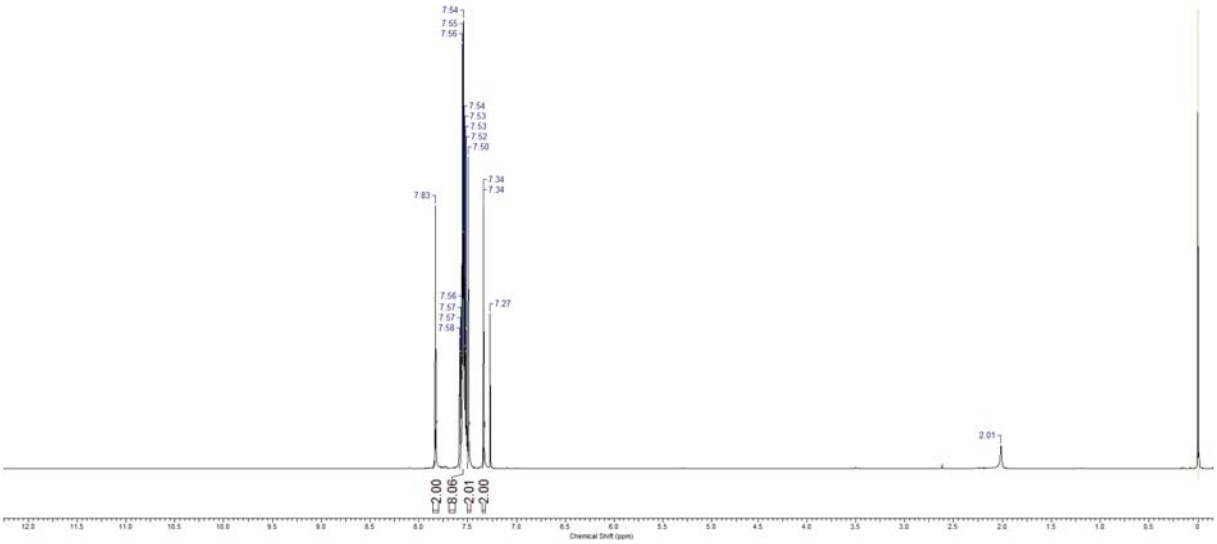


*Figure S1. ^{1}H-NMR spectrum recorded in $CDCl_3$ of **L**.*

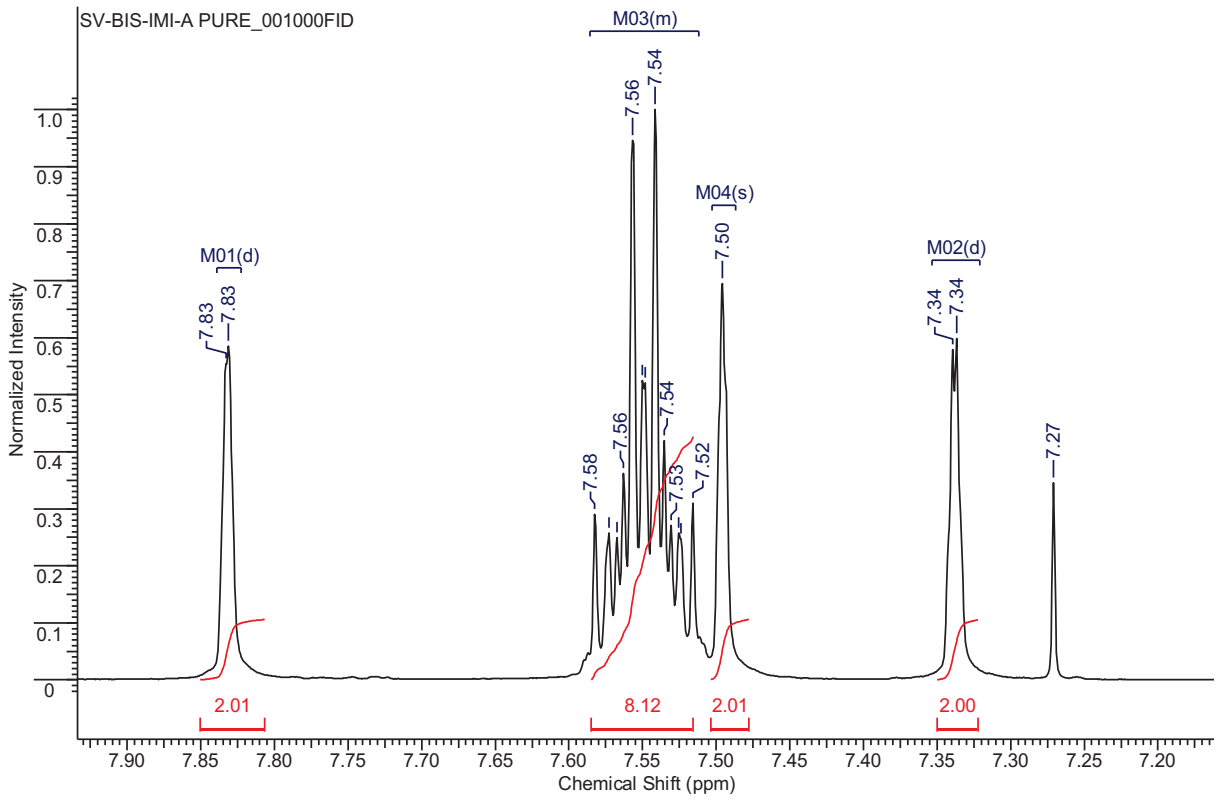


*Figure S2. ^{1}H-NMR spectrum of **L** in $CDCl_3$ (zoomed aromatic region).*

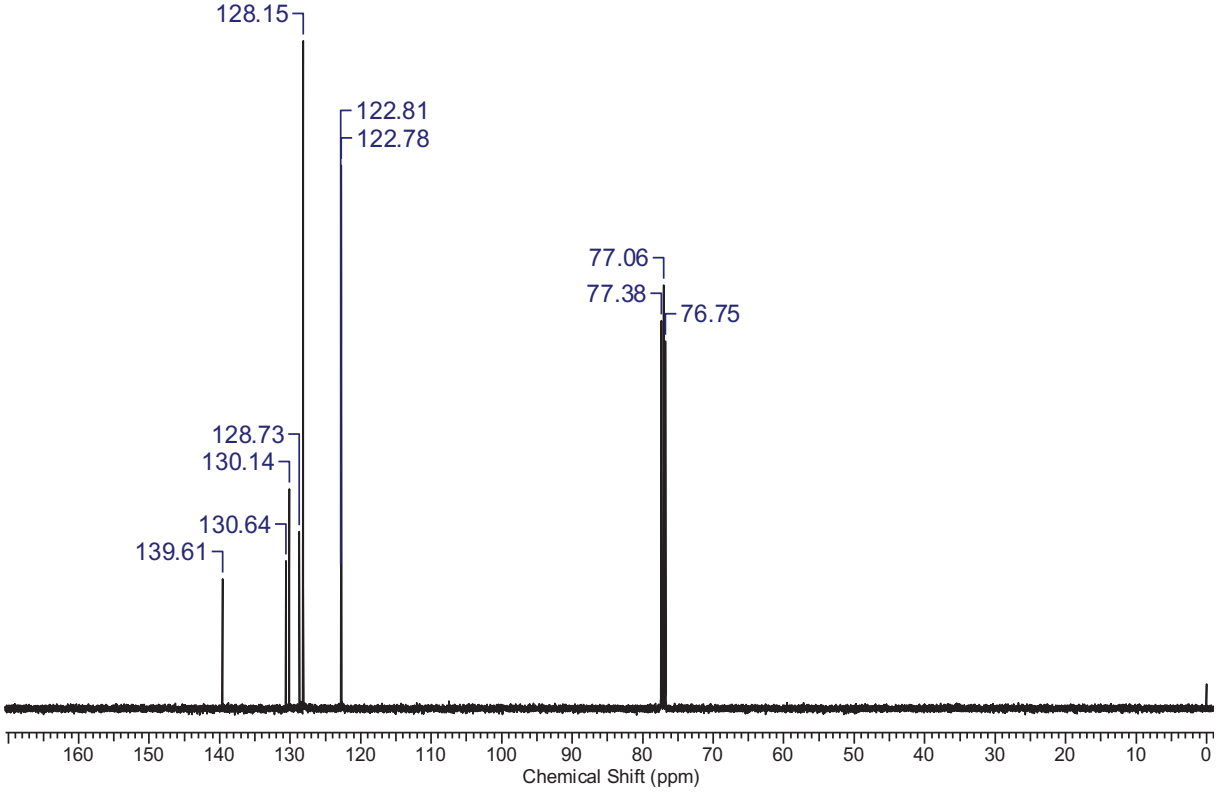


*Figure S3. ^{13}C-NMR for ligand **L** in $CDCl_3$*

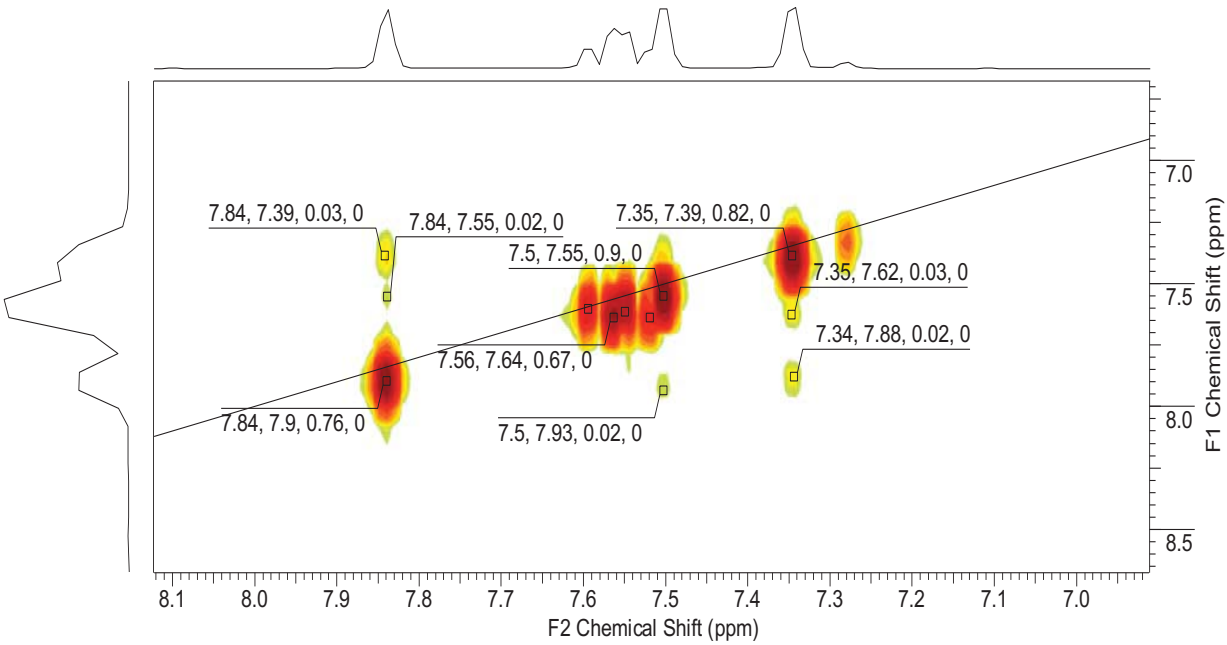


*Figure S4. 2D-COSY-NMR experiment for **L** in $CDCl_3$*

HR-MS

Ion mass = 311.1288330

Charge = +1

*** Mass Analysis for mass 311.1288330

#	C	H	N	mass	DBE	error
1	**20**	**15**	**4**	**311.1291229**	15.5	2.899e-04
2	19	13	5	311.1165469	16.0	1.229e-02
3	21	17	3	311.1416990	15.0	1.287e-02
4	13	15	10	311.1475670	11.5	1.873e-02
5	18	11	6	311.1039708	16.5	2.486e-02
6	22	19	2	311.1542750	14.5	2.544e-02
7	14	17	9	311.1601430	11.0	3.131e-02
8	17	9	7	311.0913947	17.0	3.744e-02
9	23	21	1	311.1668511	14.0	3.802e-02
10	15	19	8	311.1727191	10.5	4.389e-02

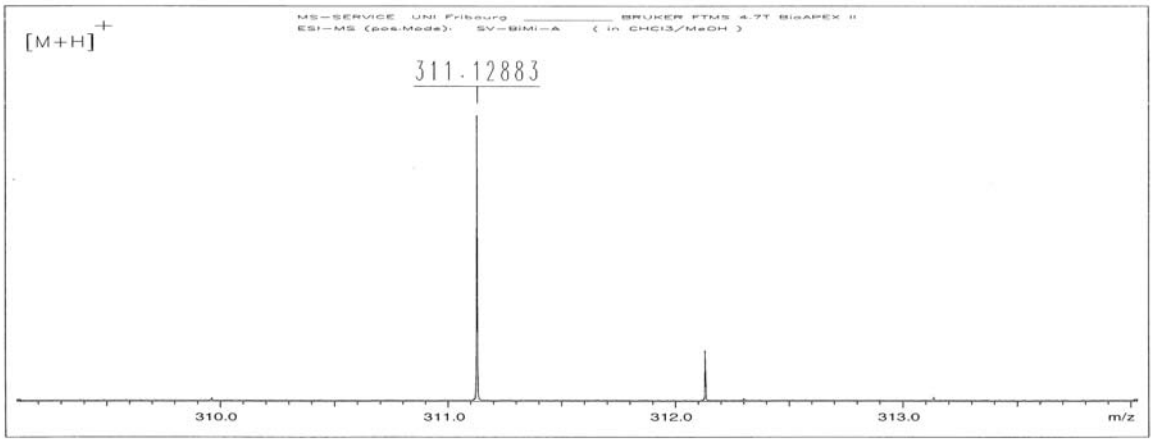


*Figure S5. HR-MS of the **L** (9,10-di(1-H-imidazol-1-yl)-anthracene)*

$\{[Zn(\mu_2\text{-}L)_2](ClO_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (1)

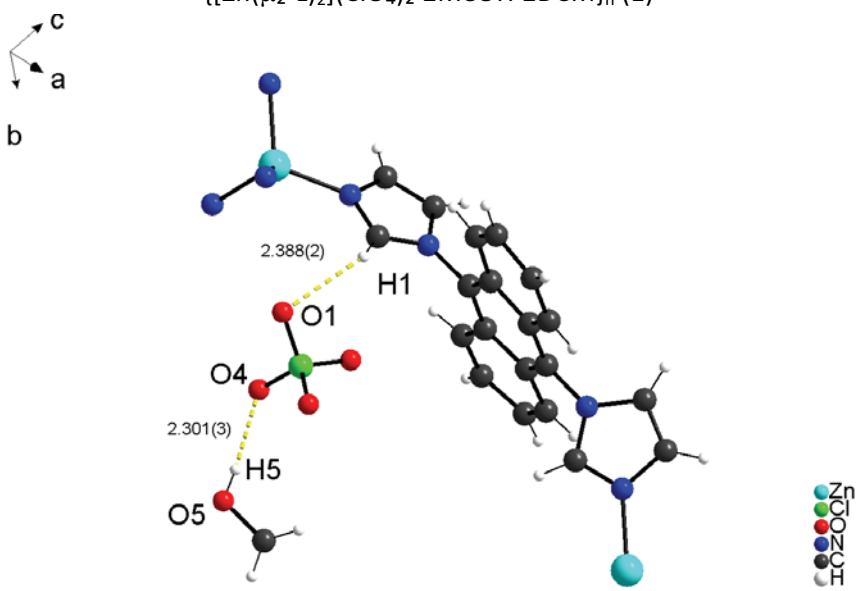


Figure S6. Asymmetric unit of $\{[Zn(\mu_2\text{-}L)_2](ClO_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (1)

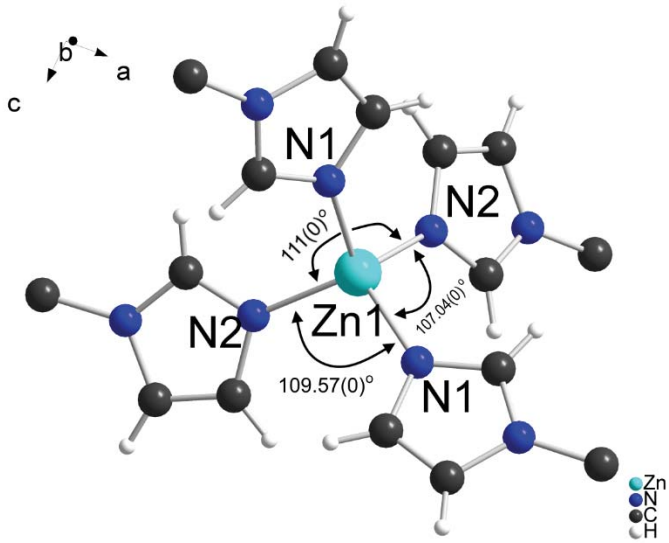


Figure S7. Coordination environment of Zn^{II} in $\{[Zn(\mu_2\text{-}L)_2](ClO_4)_2\cdot 2MeOH\cdot 2DCM\}_n$, distorted tetrahedral geometry of Zn^{II} with following bond angles 109.57^0 and 107.04^0 respectively.

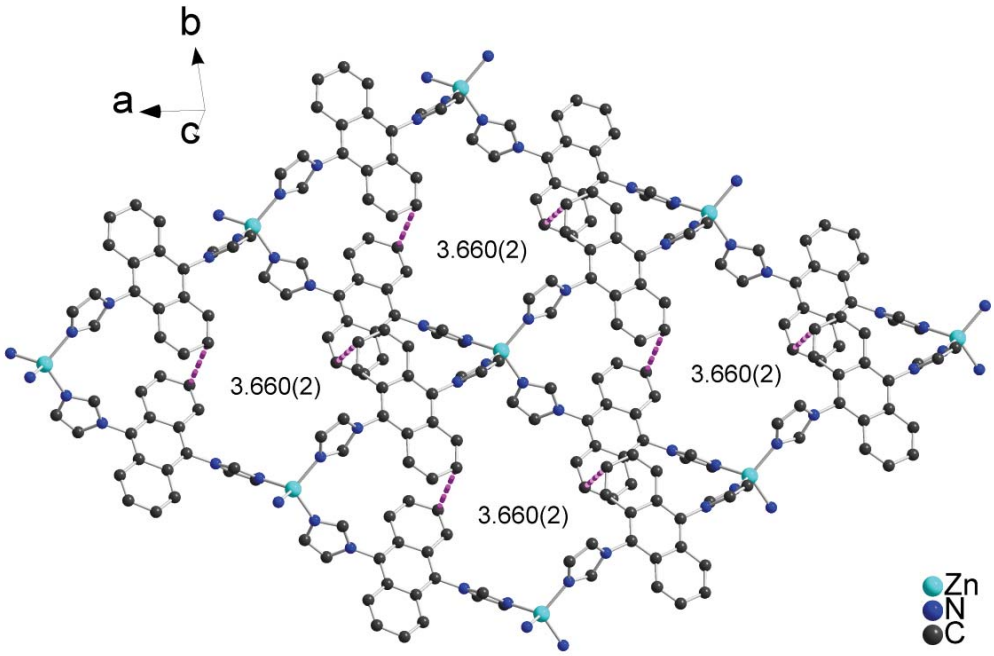


Figure S8. Formation of 2D net with topology 4,4 of $\{[Zn(\mu_2\text{-}L)_2](ClO_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (1). Formation of $\pi-\pi$ interaction in distance 3.660(2) Å (magenta dash-line)

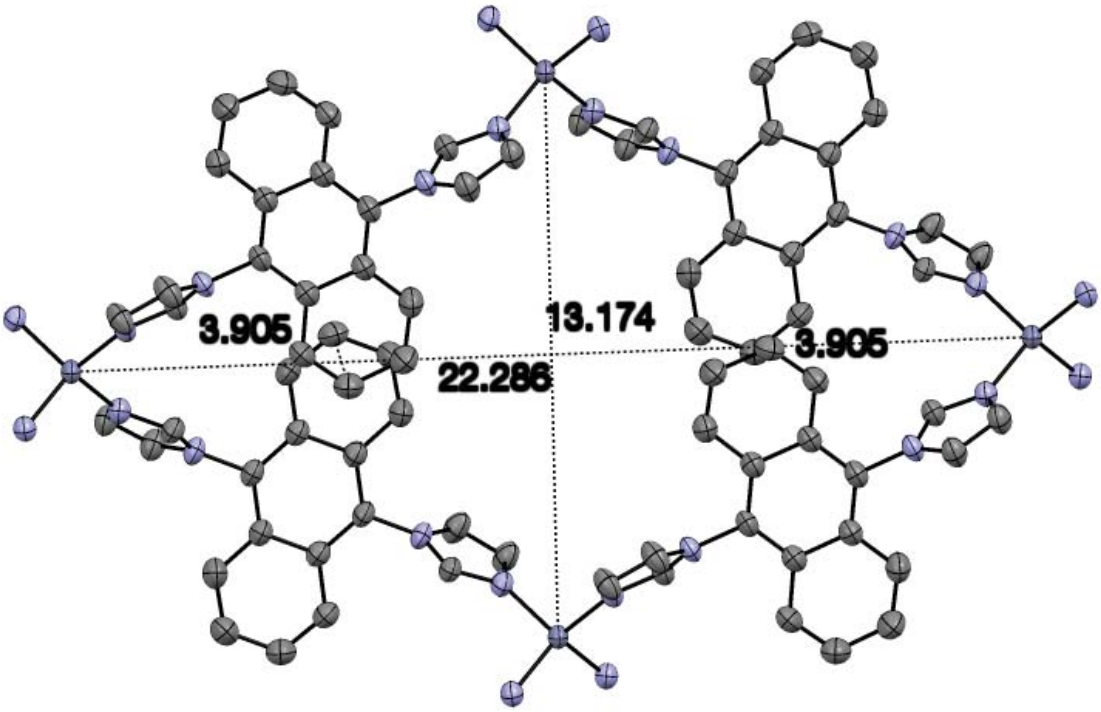


Figure S9. Formation of rhombohedral grid of Zn^{II} diagonal distances between Zn^{II} 22.286 and 13.174 Å

Figure S10. Ligand demonstrates in the structure (1) cis-conformation of the imidazole groups while coordinates to the Zn^{II}: with following torsion angles.

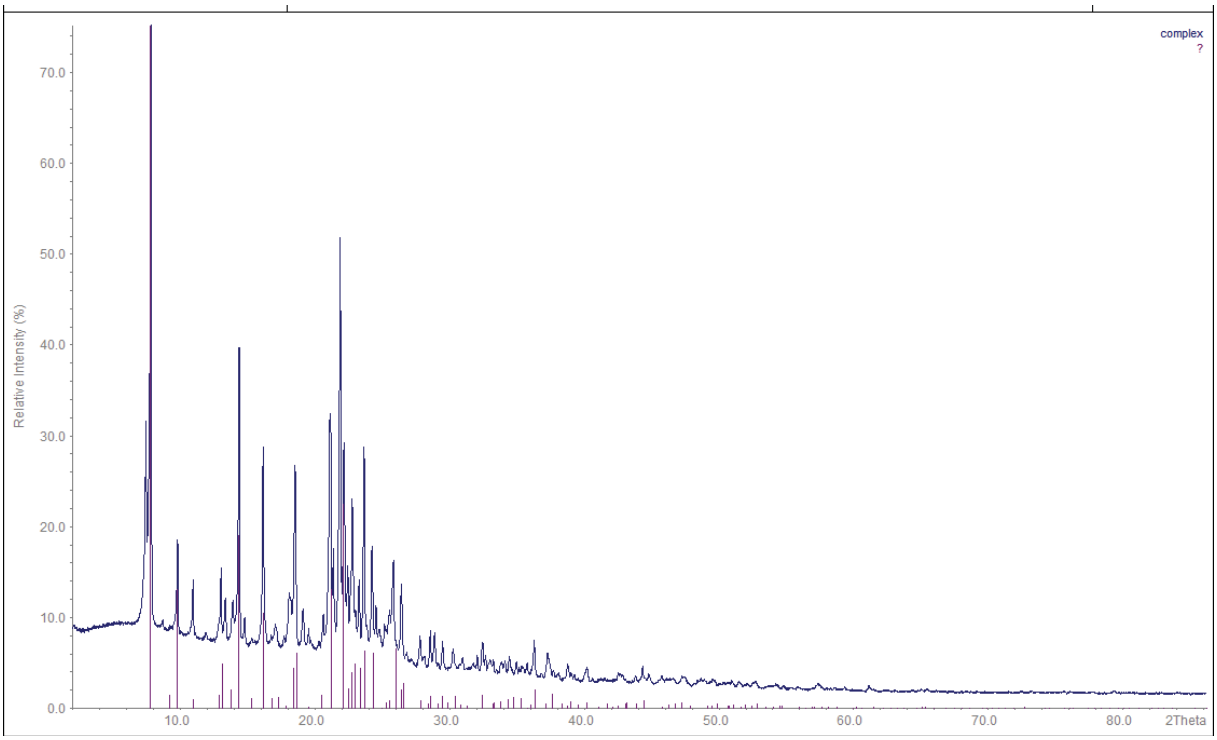


Figure S11. Powder X-Ray Diffraction of complex {[Zn(μ_2-L)$_2$](ClO$_4$)$_2$·2MeOH·2DCM}$_n$ (1). Fitting calculated – magenta, experimental – blue.

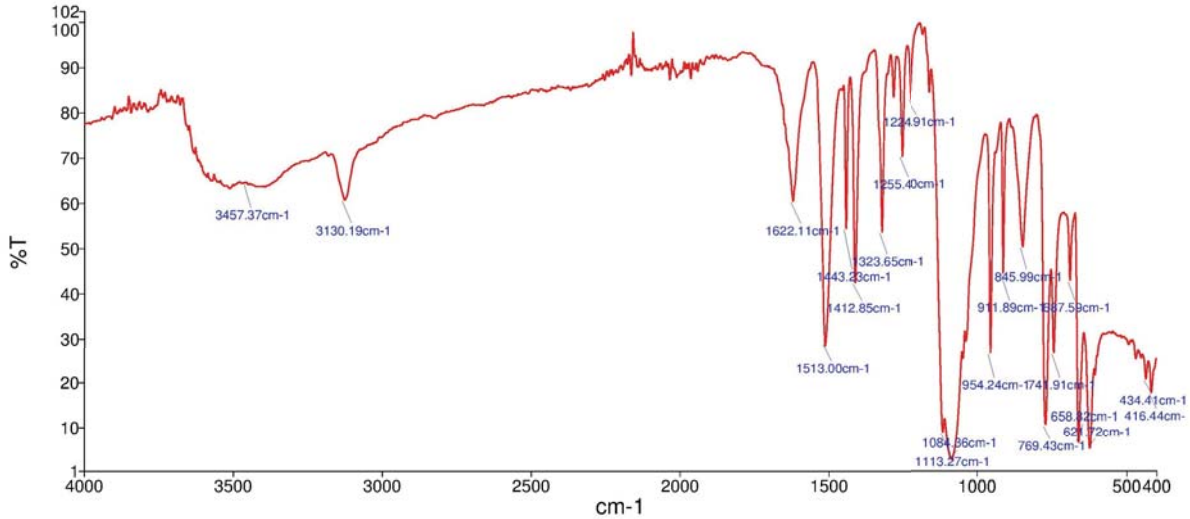


Figure 12. IR spectrum of the complex {[Zn(μ_2-L)$_2$](ClO$_4$)$_2$·2MeOH·2DCM}$_n$ (1)

$\{[Zn(\mu_2\text{-}L)_4](BF_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (2).

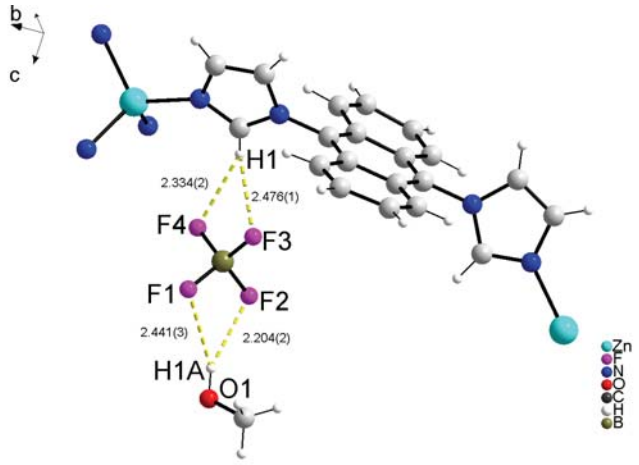


*Figure S13. Asymmetric unit of the complex $\{[Zn(\mu_2\text{-}L)_2](BF_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (**2**).*

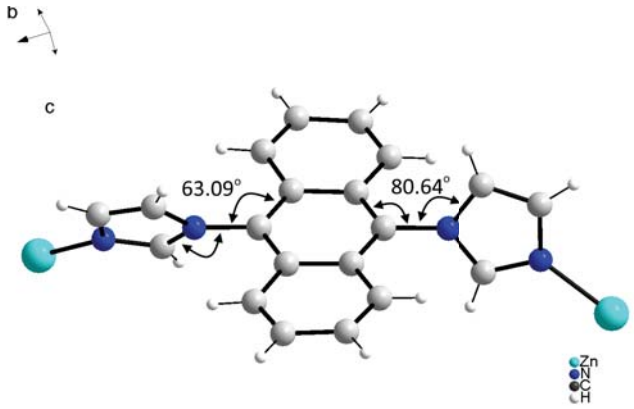


*Figure S14. Torsion angles between imidazole groups and anthracene plane in compound $\{[Zn(\mu_2\text{-}L)_2](BF_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (**2**).*

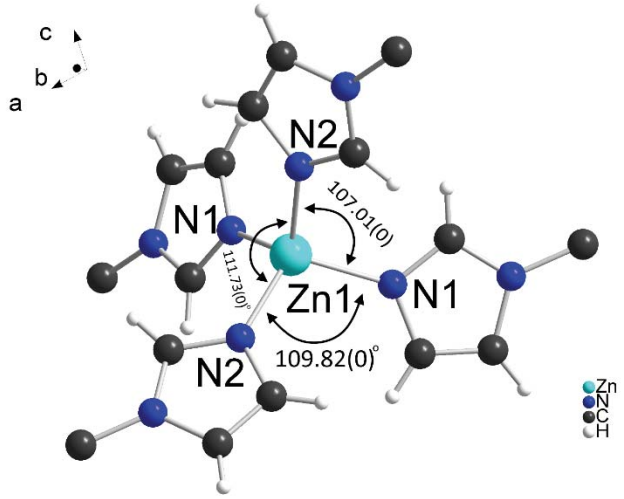


*Figure S15. Representing of coordination environment of Zn^{II} in $\{[Zn(\mu_2\text{-}L)_2](BF_4)_2\cdot 2MeOH\cdot 2DCM\}_n$ (**2**) distorted tetrahedral geometry of Zn^{II} with following bond angles 109.82^0 and 107.01^0 respectively.*

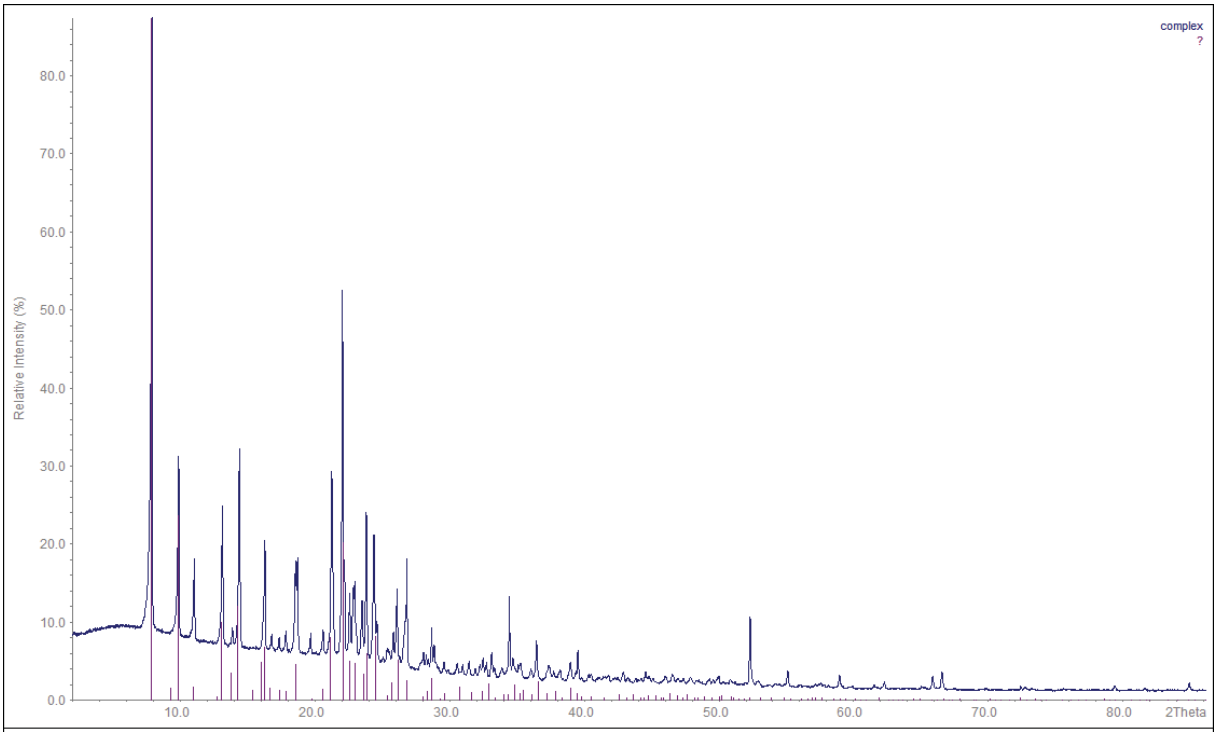


*Figure S16. Powder X-Ray Diffraction of complex {[Zn(μ_2-L)$_2$](BF$_4$)$_2$·2MeOH·2DCM }$_n$ (**2**). Fitting calculated – magenta, experimental – blue.*

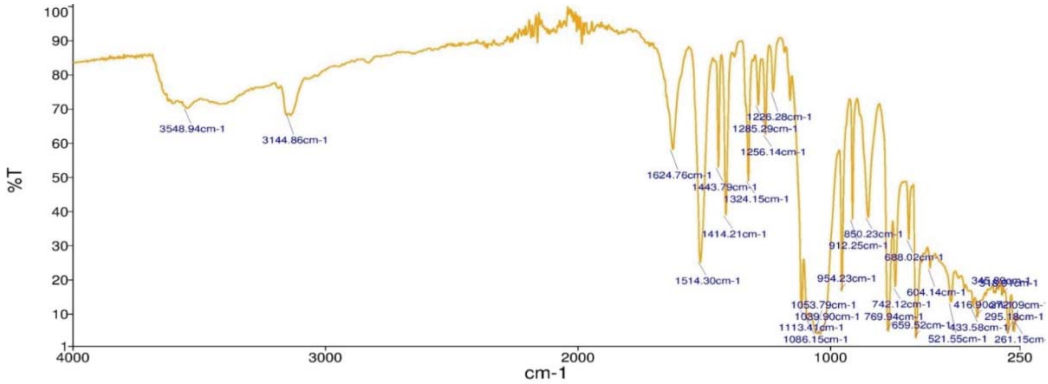


Figure S17. IR spectrum of the complex {[Zn(μ_2-L)$_2$](BF$_4$)$_2$·2MeOH·2DCM }$_n$ (2)

{[Zn(μ_2–**L**)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**)

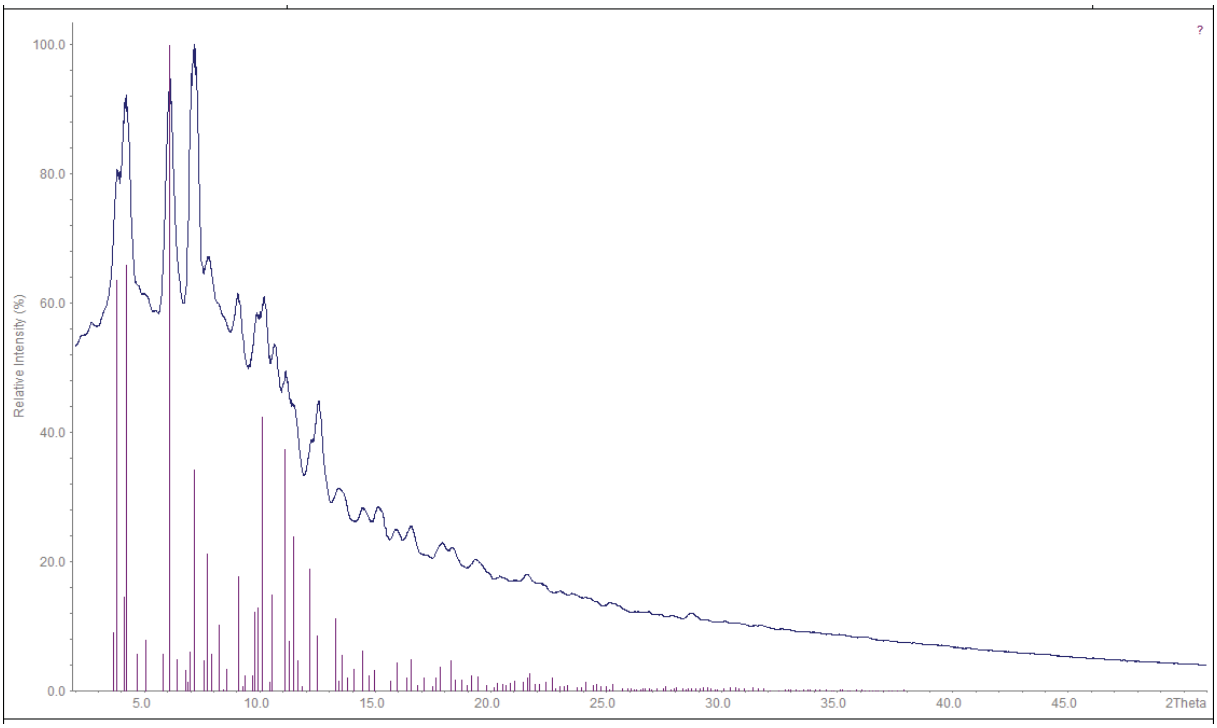


*Figure S18. PXRD for complex {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**) presence of an amorphous phase is observed. Fitting calculated – magenta, experimental – blue. (it always decomposes giving an amorphous phase at rt)*

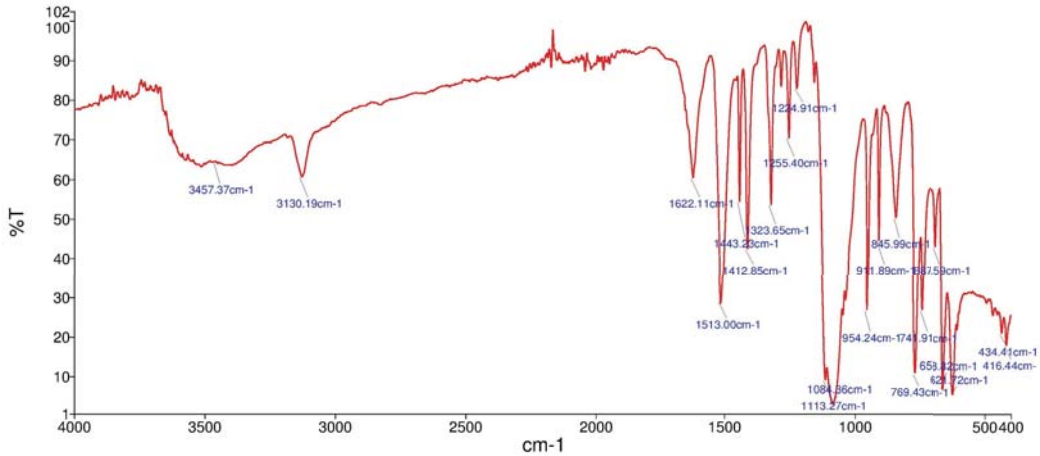


*Figure S19. IR spectrum of the complex {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**).*

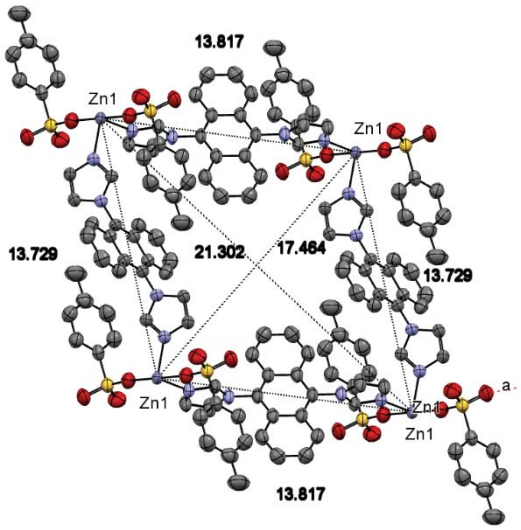


*Figure S20. Formation of tetranuclear grid of Zn(II) in compound {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**) in ab-plane.*

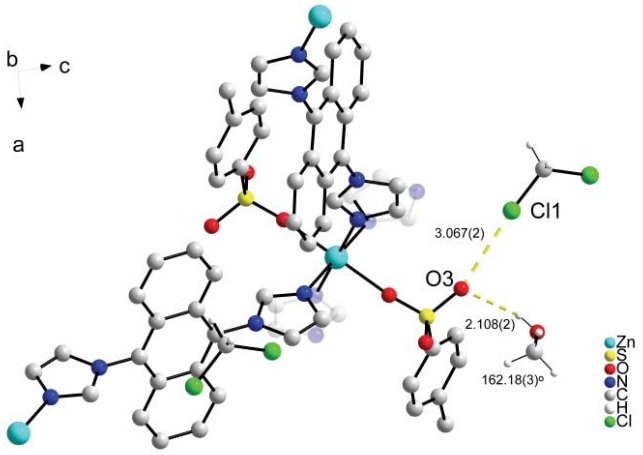


*Figure S21. Short contact between Cl1...O3$_{(tosylate)}$ 3.067(2) Å and hydrogen bonding between methanol molecules and tosylate H-O…O3 = 2.108(2) Å with angle 162.18(3)^o in compound {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**).*

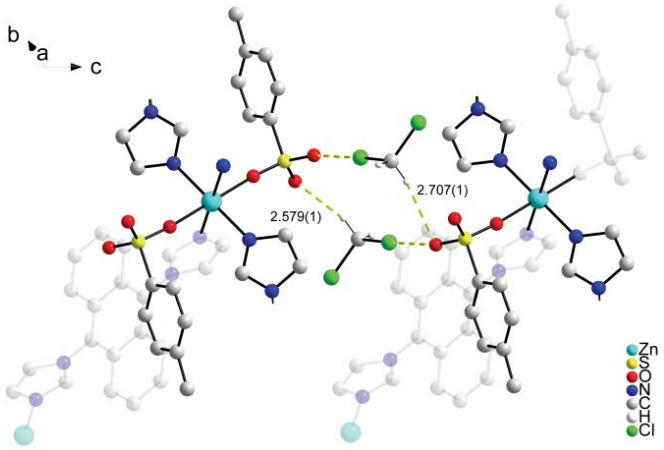


*Figure S22. Short contact H $_{(dcm)}$ to O $_{(Tosylate)}$ in distances: 2.579(1) and 2.707(1) Å in compound {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**).*

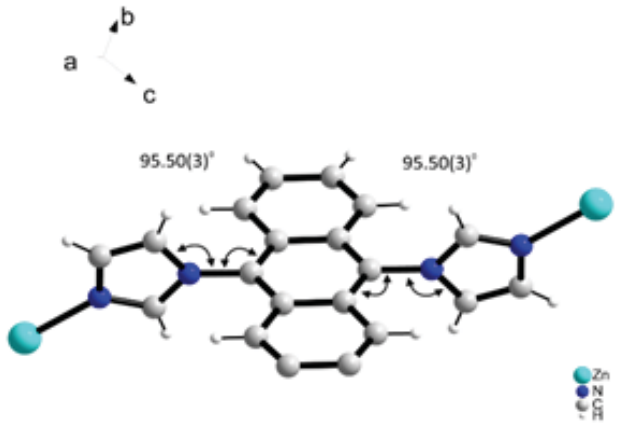


*Figure S23. Revealing trans-conformation of functional groups of **L** with torsion 95.50^{o} {[Zn(μ_2–L)$_2$(p-Tos)$_2$]·2DCM·2MeOH}$_n$ (**3**).*

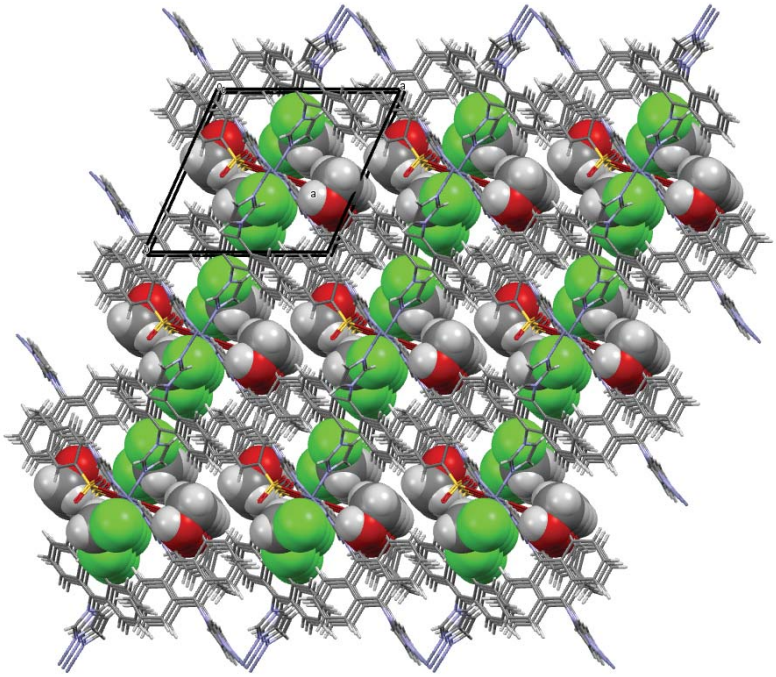


*Figure S24. Formation of 3D structure of the coordination polymer (**3**). Guest molecules illustrated in Van der Waals shapes which are trapped between the lattices of 2-D network.*

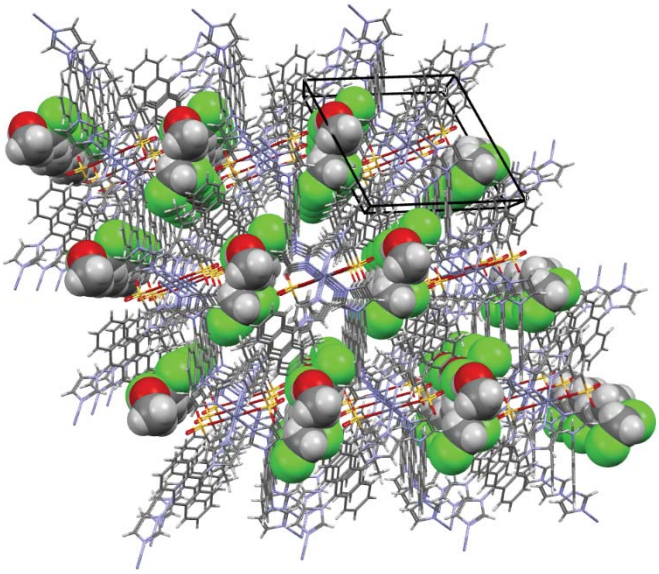


*Figure S25. c-direction view for compound (**3**), demonstrated a formation of channels for solvent molecules in the compound.*

{[Cd(μ_2−*trans*-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (**4**)

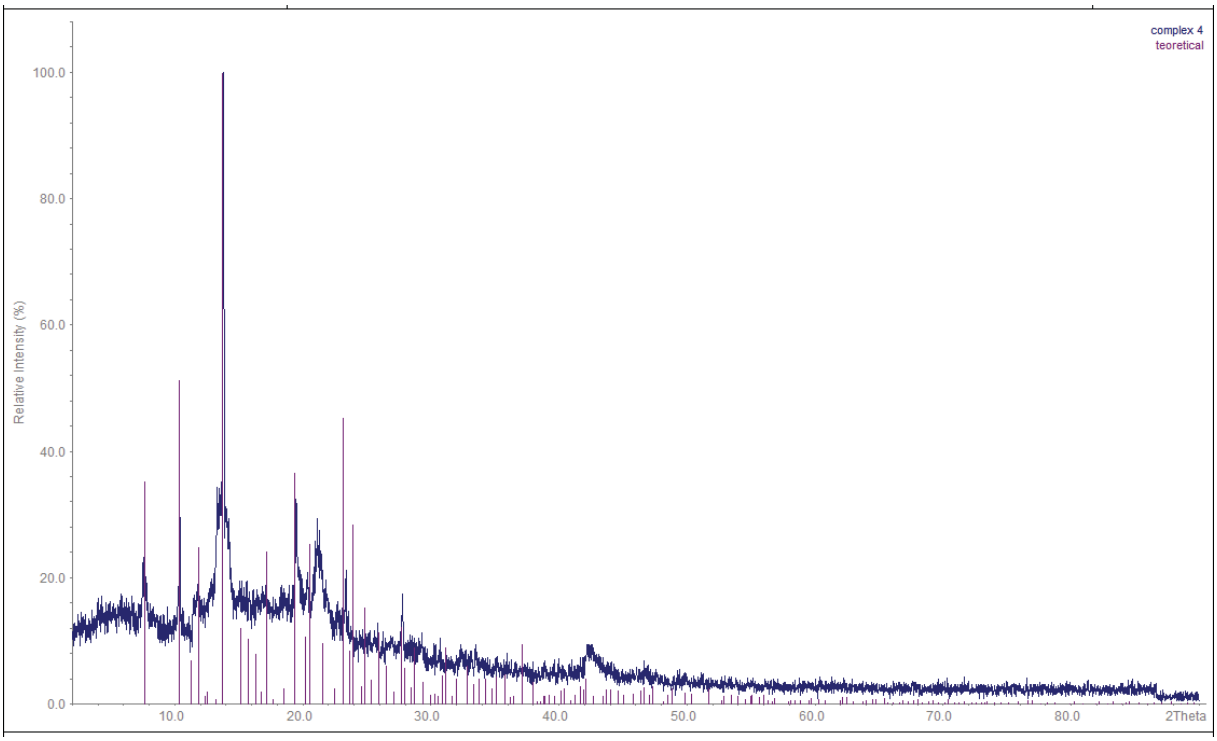


*Figure S26. Powder X-Ray Diffraction of complex {[Cd(μ_2−trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (**4**). Fitting calculated – magenta, experimental – blue. (Decomposes when exposed to air at rt, therefore X-ray powder diffraction was collected at quick run)*

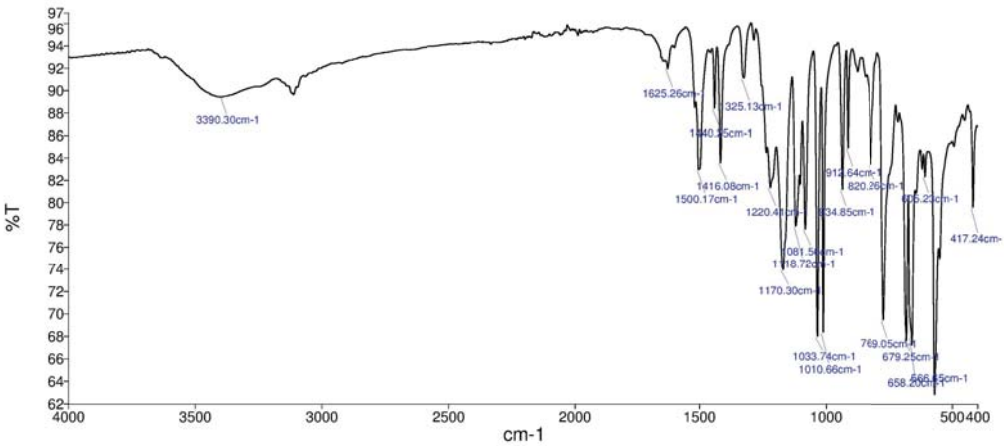


*Figure S27. IR spectrum of complex {[Cd(μ_2−trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (**4**).*

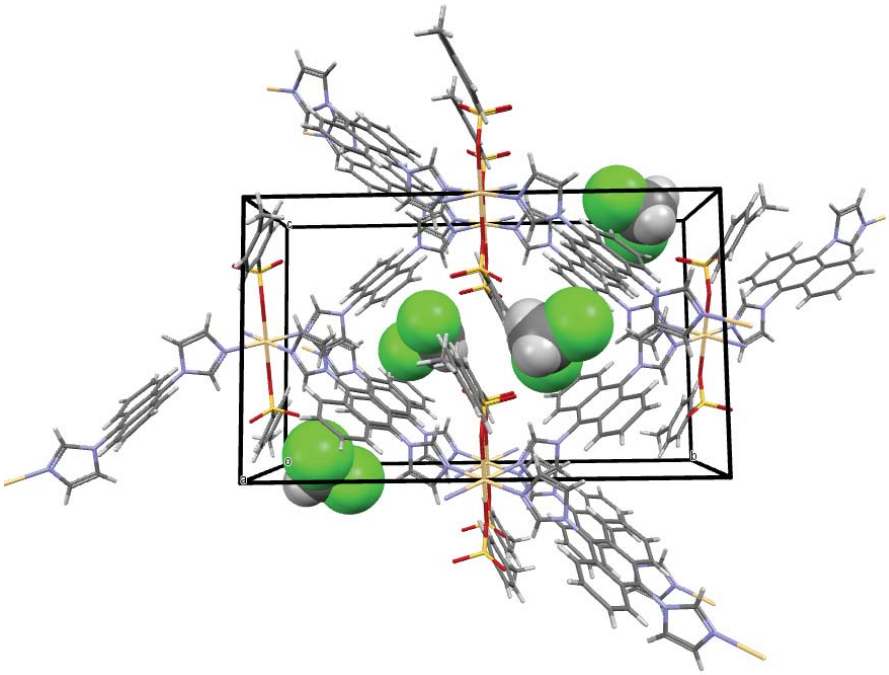


*Figure S28. Crystal packing of the compound {[Cd(μ_2−trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (**4**).*

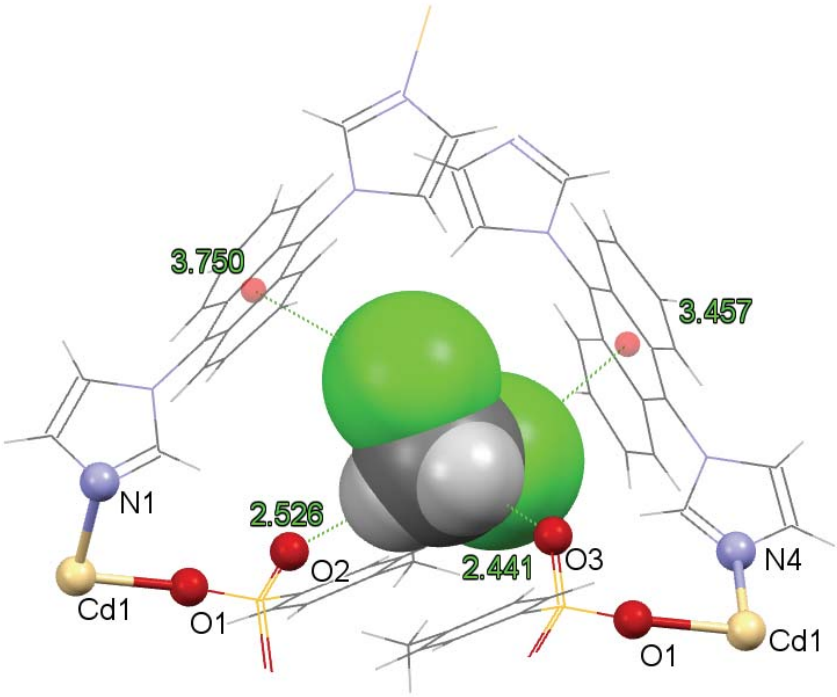


Figure S29. Weak interaction of DCM in {[Cd(μ_2−trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ with anthracene linkers from ligand L through π-Cl interaction in distances = 3.457 Å and 3.750 Å, and at the same time formation of weak contacts by protons from DCM with O atoms from tosylate anion O2…H (DCM) = 2.526 Å and O3…H (DCM) = 2.441 Å.

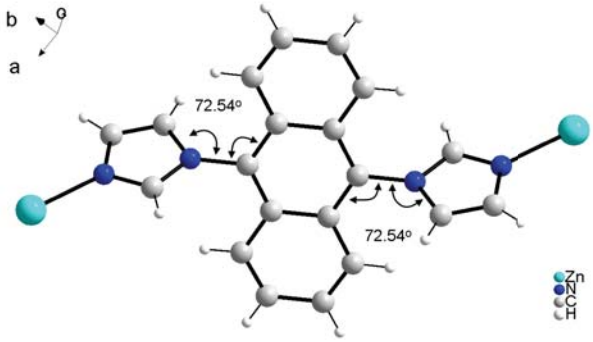


*Figure S30. Ligand conformation of the imidazole groups in trans-mode with following torsions 72.54° in {[Cd(μ_2–trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$.(**4**)*

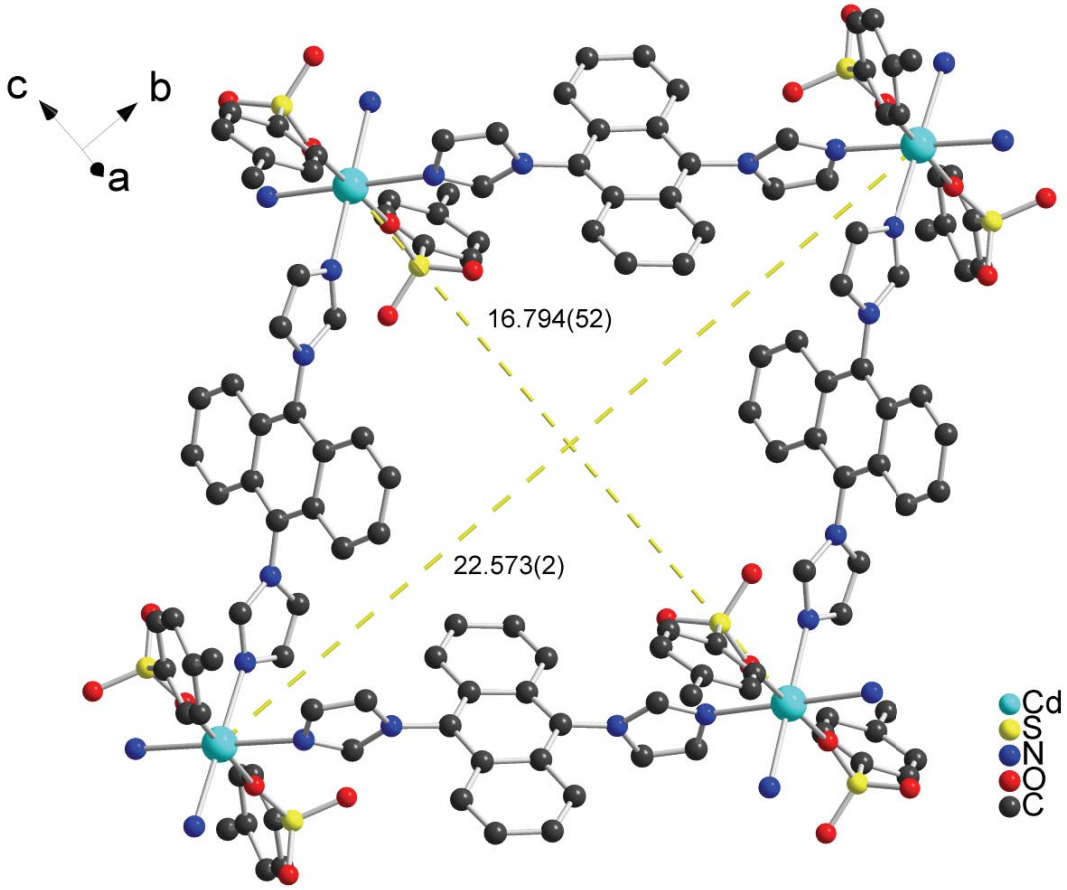


*Figure S31. Rhombohedral grid of Cd^{II} connected by trans-**L** in distances 16.794(52) Å and 22.573(2) Å of compound {[Cd(μ_2–trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (**4**).*

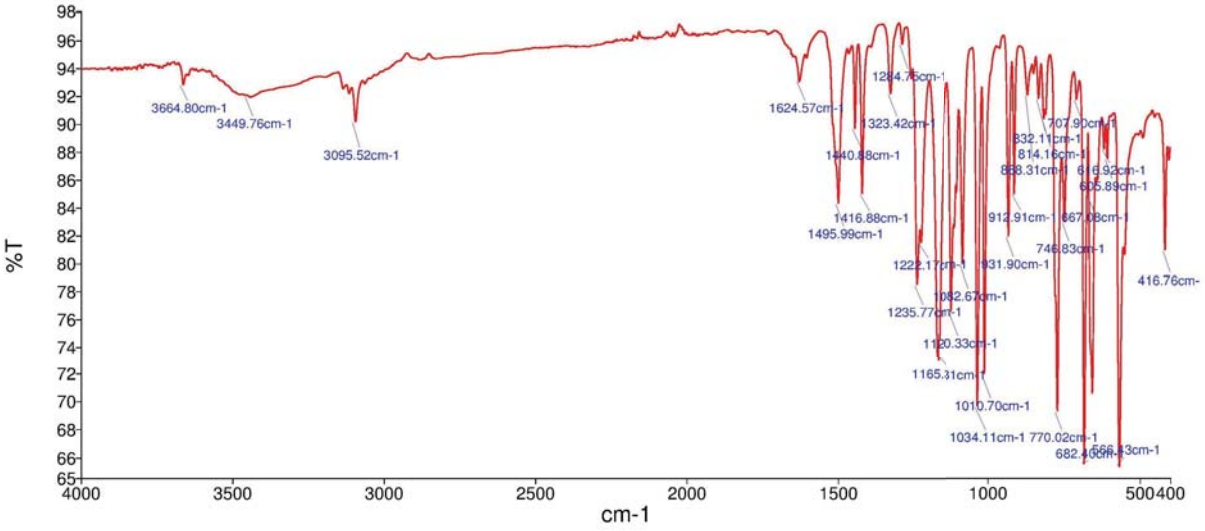


Figure S32. IR spectrum of complex {[Cd(μ_2–trans-L)$_2$(p-Tos)$_2$]·2DCM}$_n$ (4).

Complex $\{[Cd(\mu_2\text{-}cis\text{-}L)_2(p\text{-}Tos)_2]\cdot 2MeOH\cdot 2Dioxane\}_n$ (**5**)

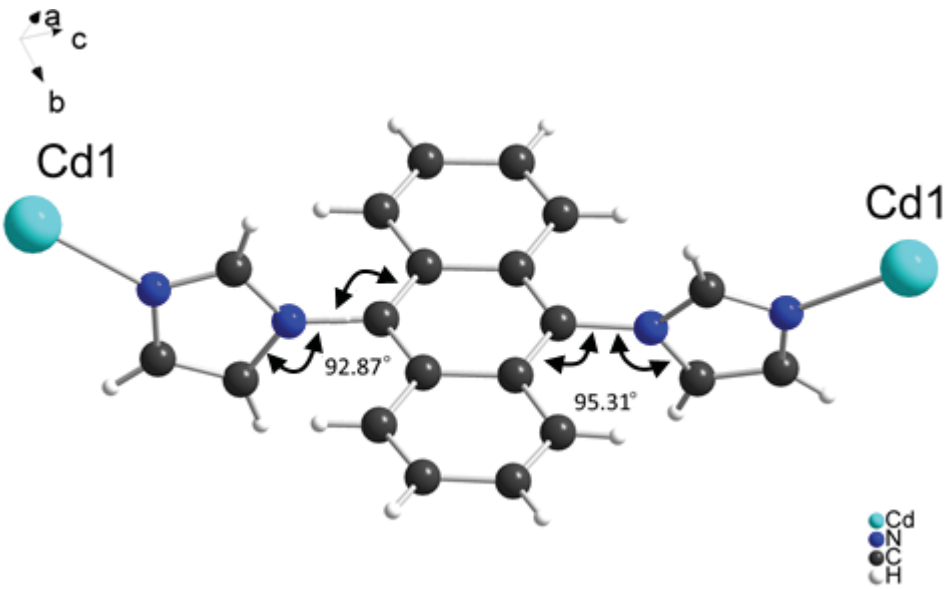


*Figure S33. Torsions between imidazole-groups and anthracene plane moiety in crystal structure of complex $\{[Cd(\mu_2\text{-cis-}L)_2(p\text{-}Tos)_2]\cdot 2MeOH\cdot 2Dioxane\}_n$ (**5**).*

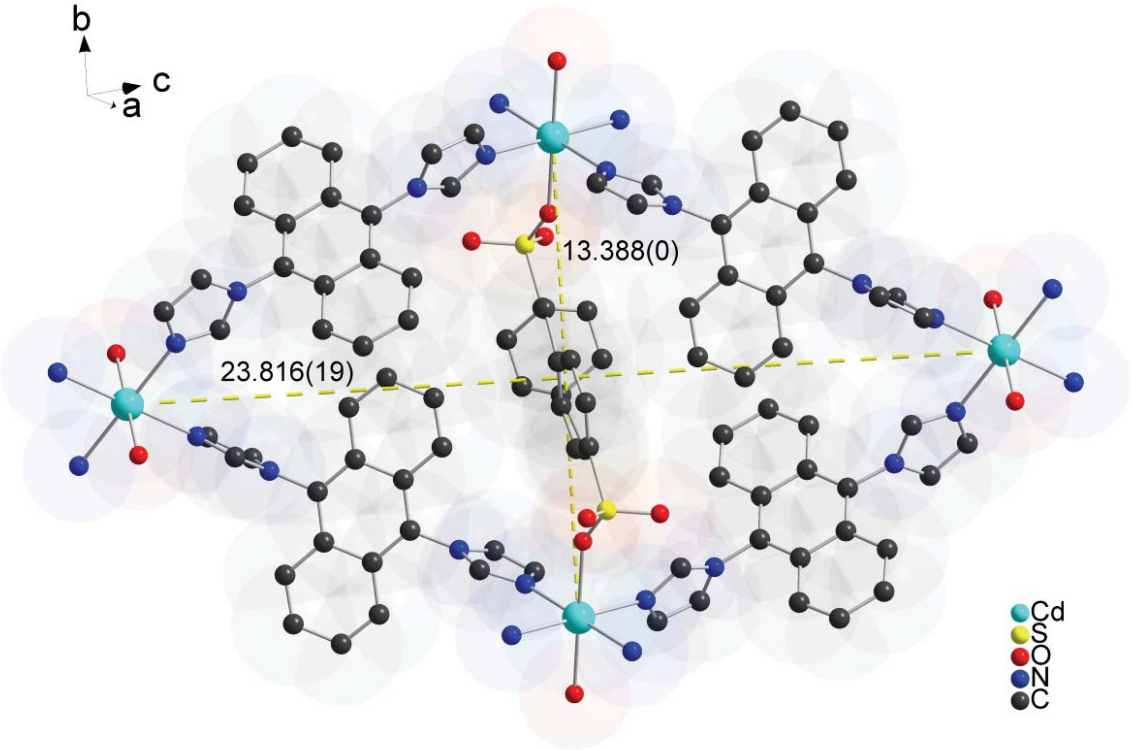


*Figure S34. Formation of rhombohedral grid of Cd^{II} in compound $\{[Cd(\mu_2\text{-cis-}L)_2(p\text{-}Tos)_2]\cdot 2MeOH\cdot 2Dioxane\}_n$ (**5**) by cis-**L**.*

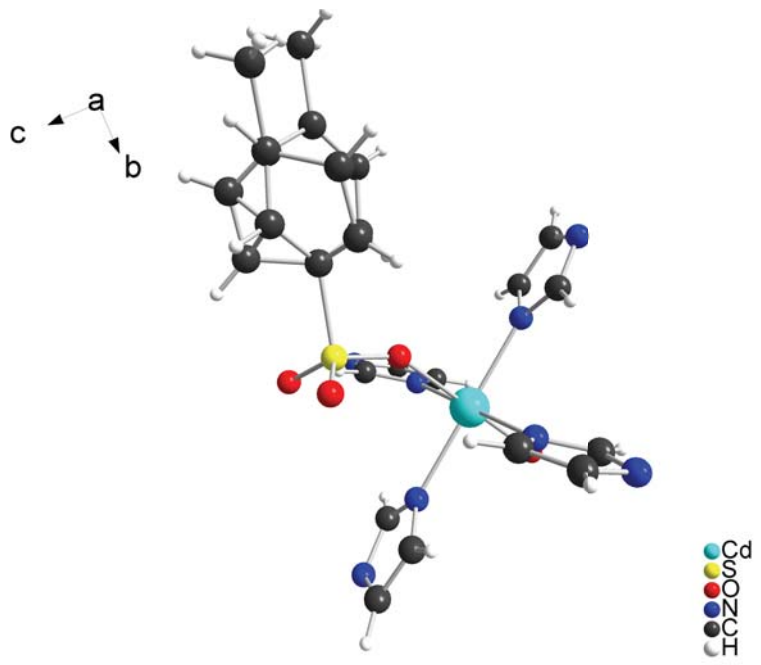


Figure S35. Positional disorder of tolyl-fragment of tosylate anion in crystal structure of complex {[Cd(μ_2-cis-L)$_2$(p-Tos)$_2$]·2MeOH·2Dioxane}$_n$ ***5****.*

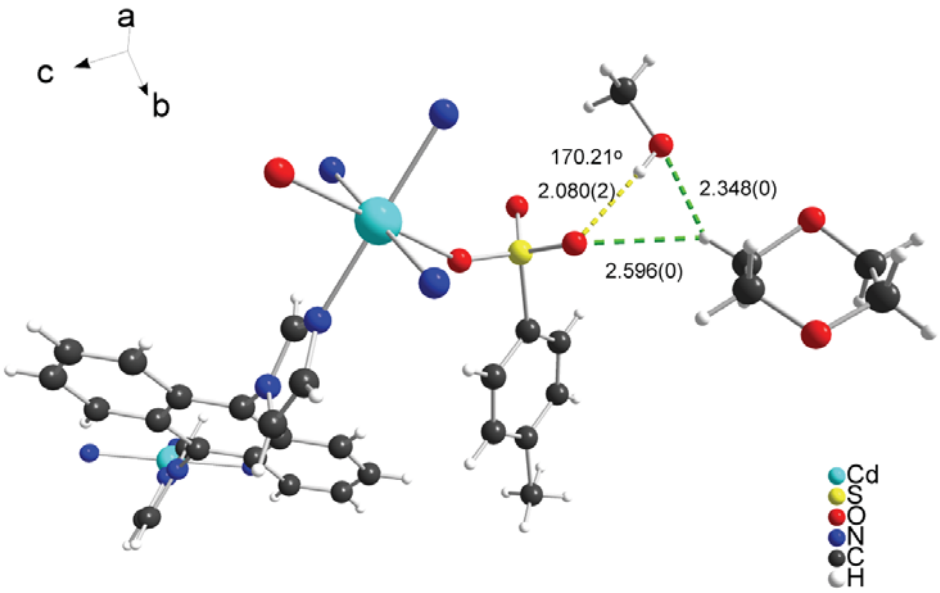


*Figure S36. Asymmetric unit of compound {[Cd(μ_2-cis-L)$_2$(p-Tos)$_2$]·2MeOH·2Dioxane}$_n$ (**5**), presence of hydrogen bond between methanol molecule to tosylate anion in distance 2.080(2) Å and short-contact between dioxane molecule and tosylate oxygen in distance 2.596 Å.*

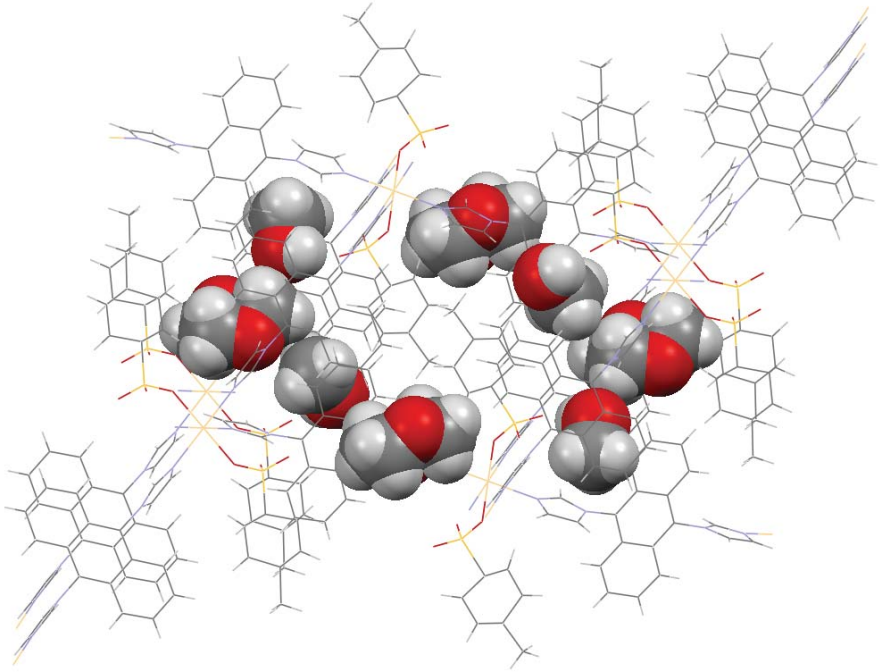


*Figure S37. Crystal packing of compound {[Cd(μ_2-cis-L)$_2$(p-Tos)$_2$]·2MeOH·2Dioxane}$_n$ (**5**), illustrated solvent molecules which are trapped between lattices of 4,4-topological nets.*

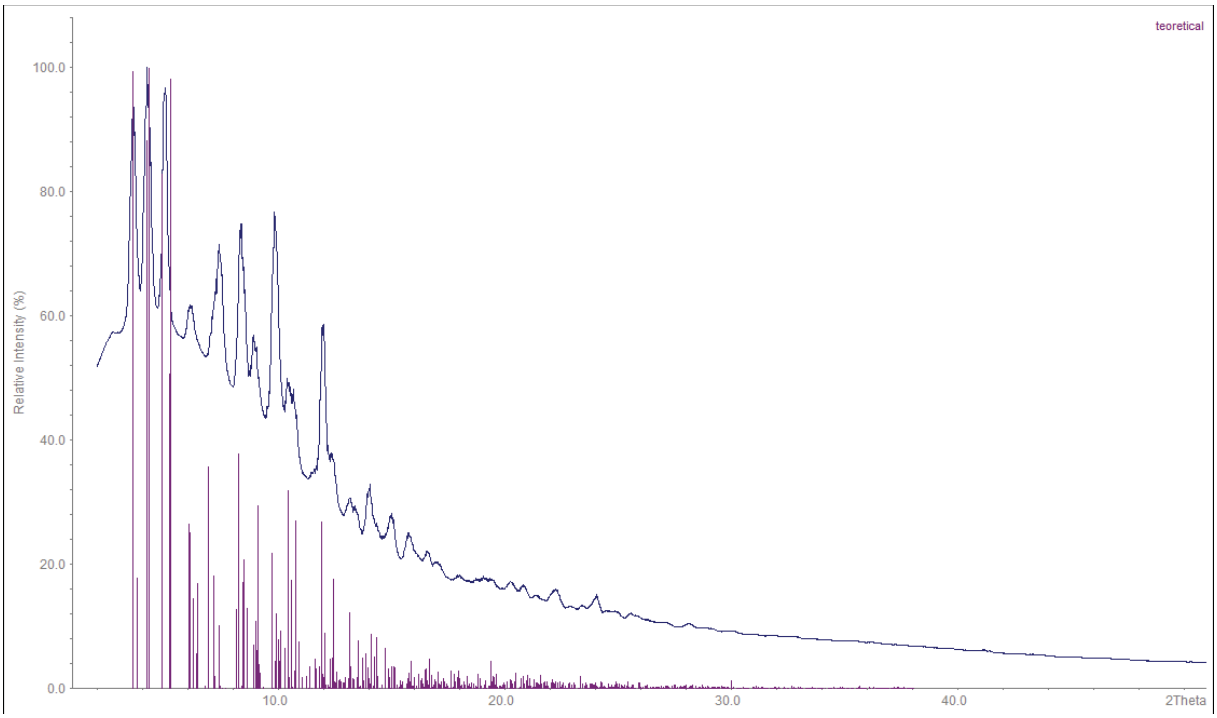


Figure S38. PXRD of complex {[Cd(μ_2-cis-L)$_2$(p-Tos)$_2$]·2MeOH·2Dioxane}$_n$ (5). magenta - theoretical pattern; blue – obtained. (Compound 5 is very unstable and decomposes when exposed to the air at room temperature, leading to amorphous phase)

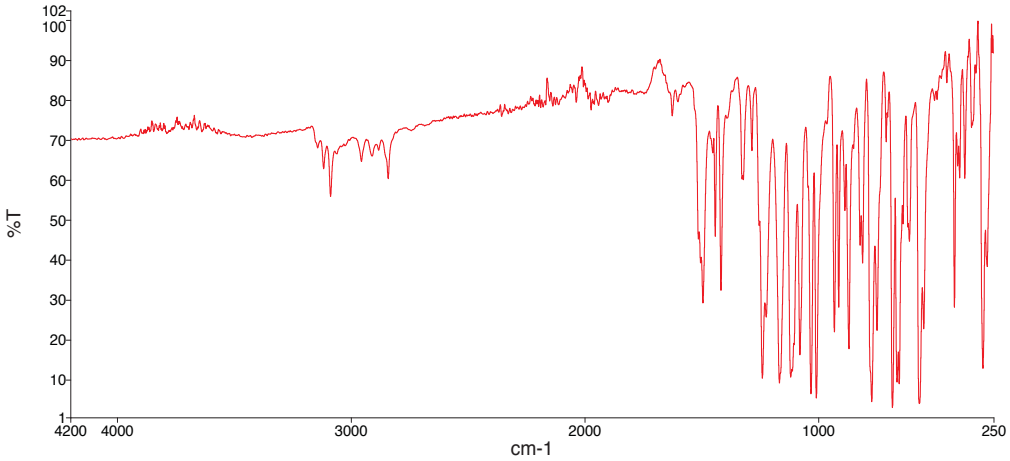


*Figure 39. IR spectrum of complex {[Cd(μ_2-cis-L)$_2$(p-Tos)$_2$]·2MeOH·2Dioxane}$_n$ (**5**)*

Complex {[Zn(μ_2-L)$_2$(CF_3CO_2)$_2$]·2Dioxane}$_n$ (**6**).

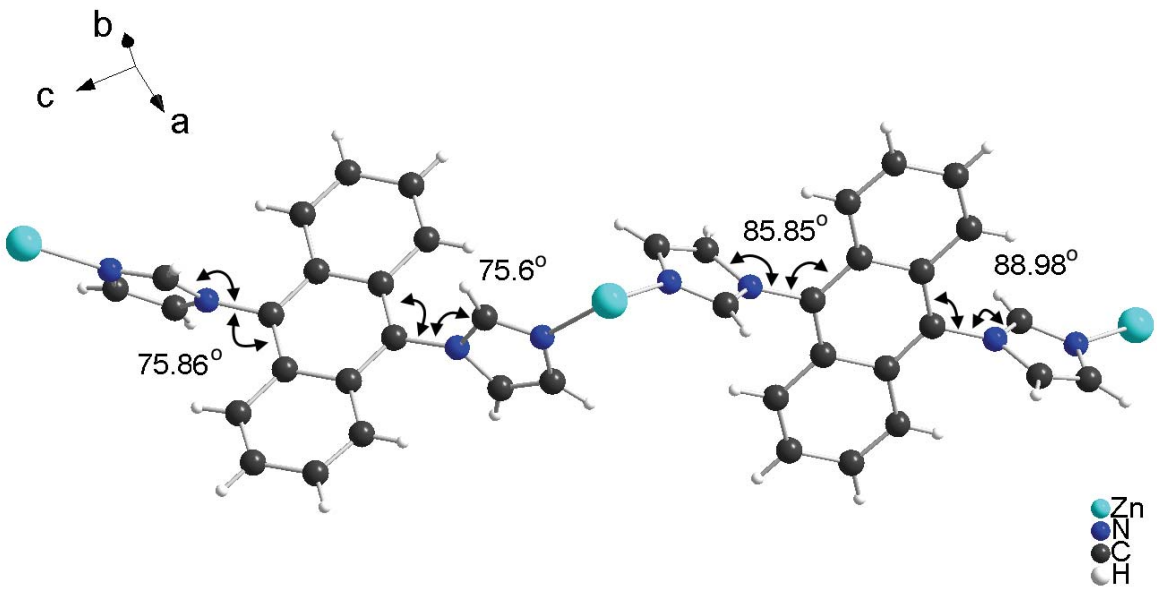


*Figure S40. Cis and trans-configuration of L with different torsion illustrated {[Zn(μ_2-L)$_2$(CF_3CO_2)$_2$]·2Dioxane}$_n$ (**6**).*

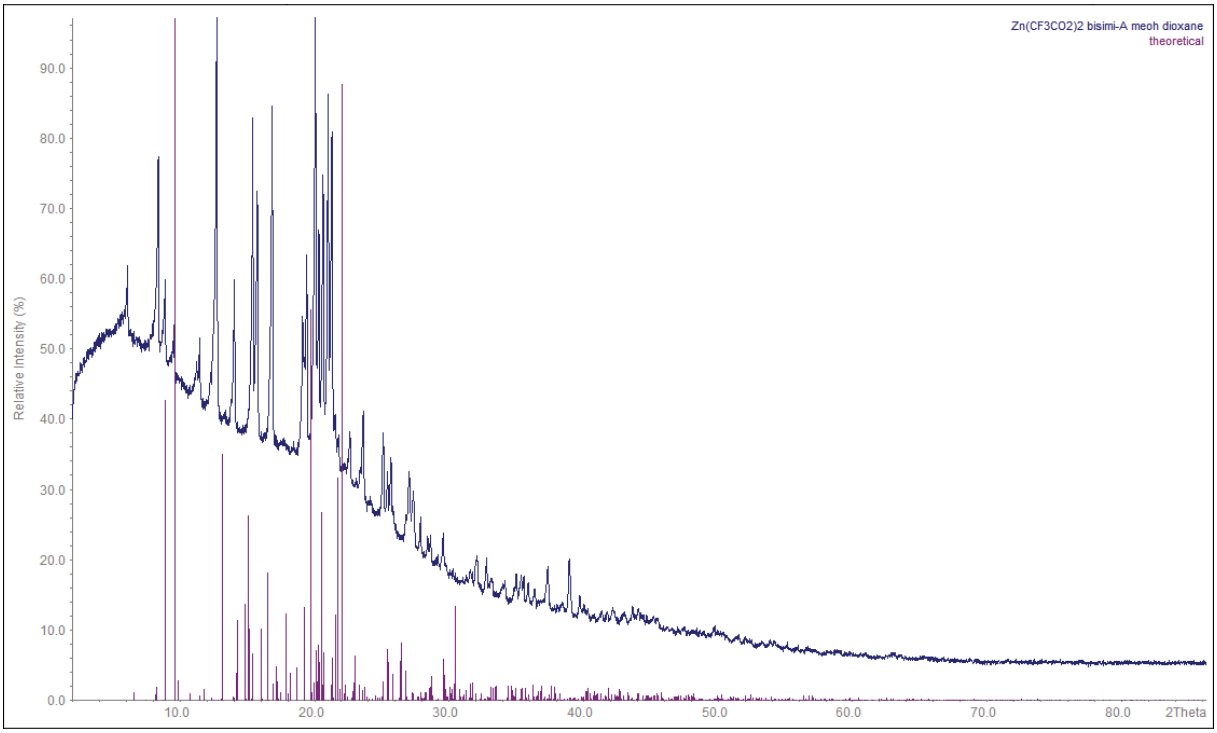


*Figure S41. PXRD of complex {[Zn(μ_2-L)$_2$(CF$_3$CO$_2$)$_2$]·2Dioxane}$_n$ (**6**). Magenta – calculated; blue – obtained. (Compound 6, as was found unstable when exposed to the air at room temperature*

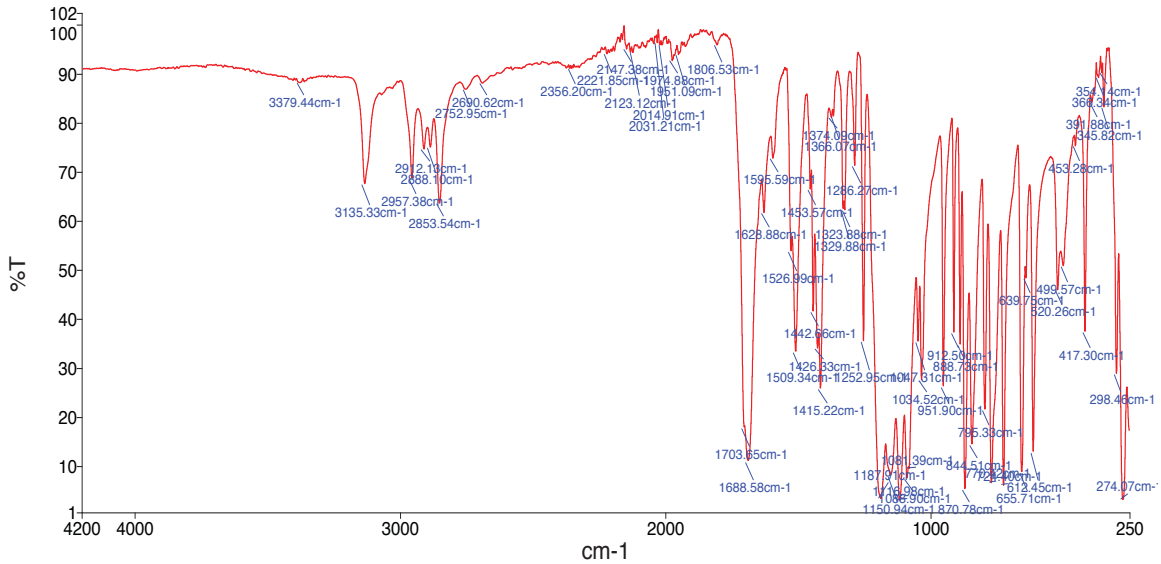


*Figure S42. IR spectrum of complex {[Zn(μ_2-L)$_2$(CF$_3$CO$_2$)$_2$]·2Dioxane}$_n$ (**6**).*

TGA of the complexes (1)-(6)

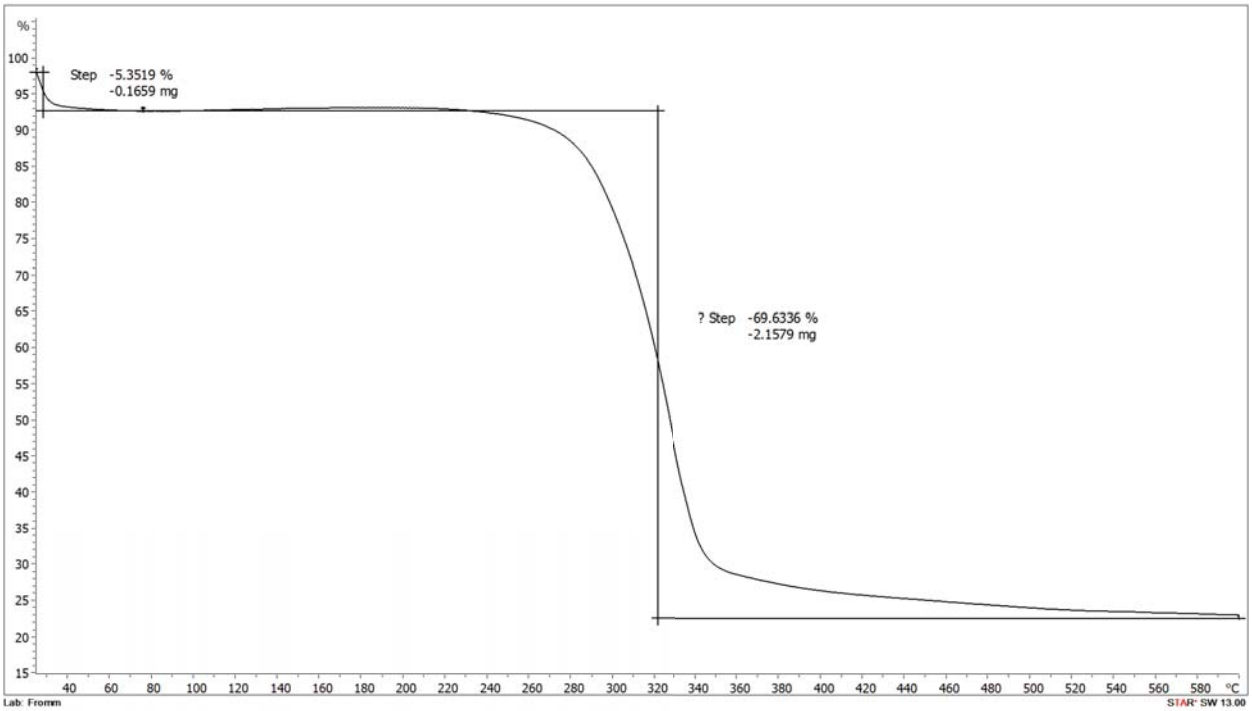


Figure S43. TGA for complex (1).

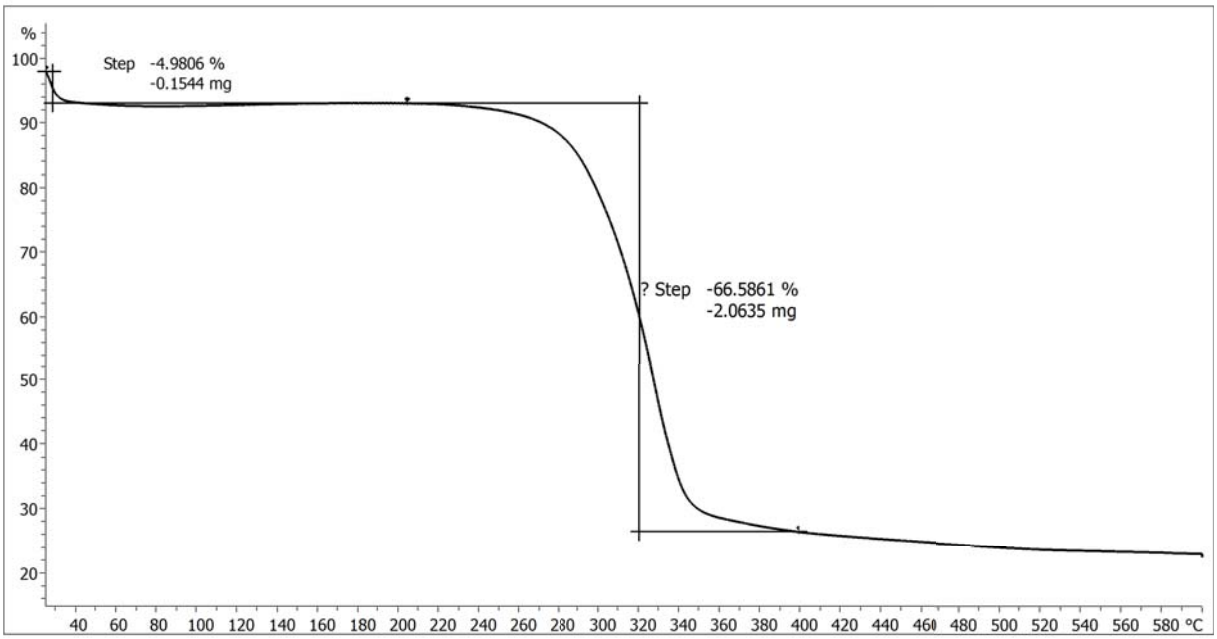


Figure S44. TGA for complex (2).

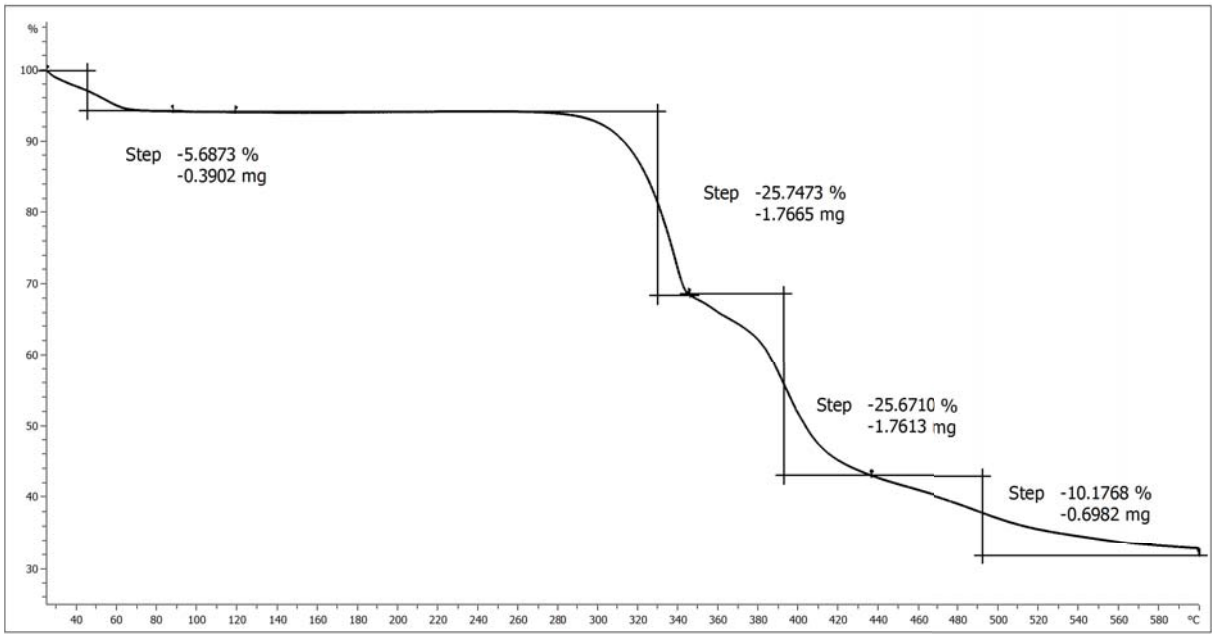


Figure S45. TGA for complex (3).

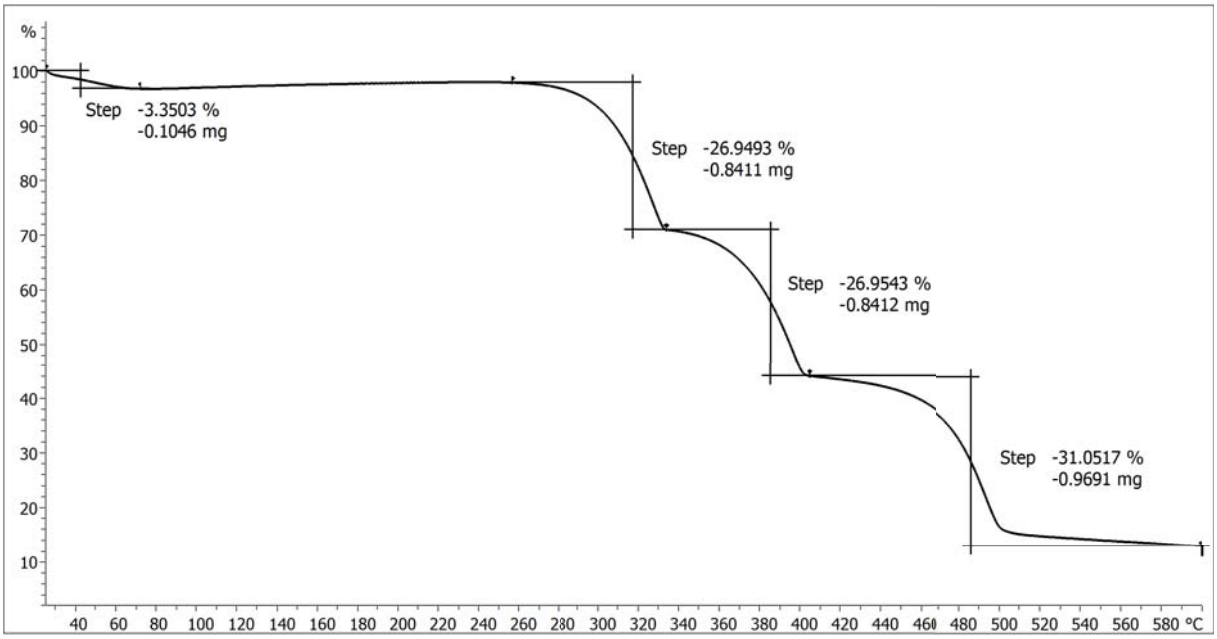


Figure S46. TGA for complex (4).

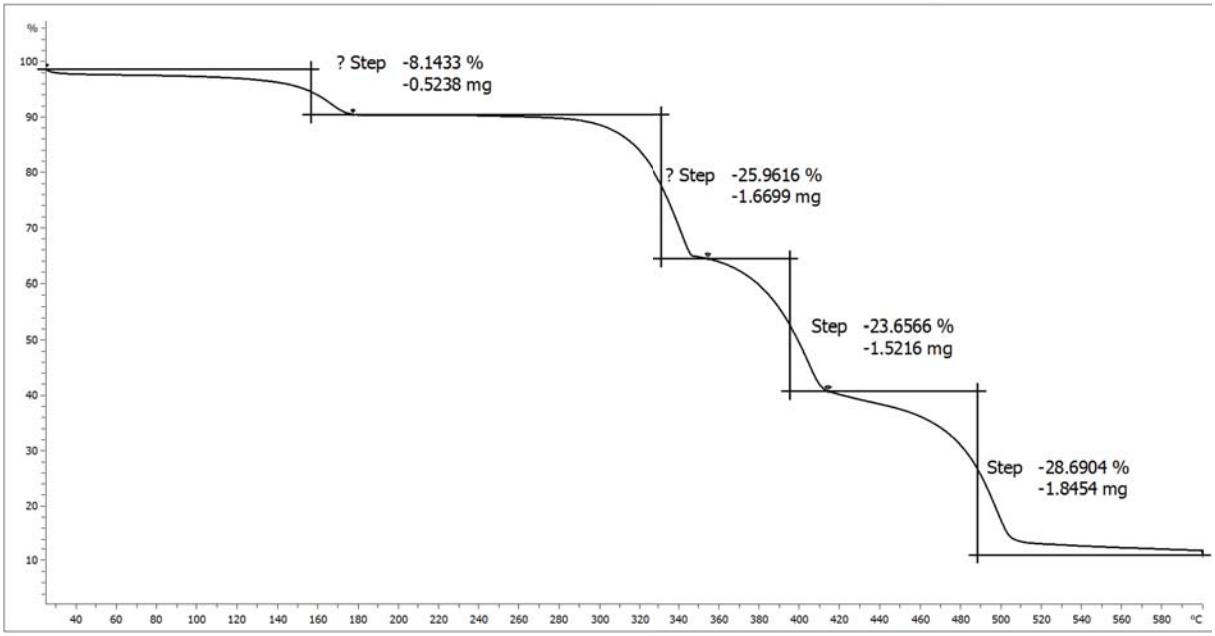


Figure S47. TGA of complex 5

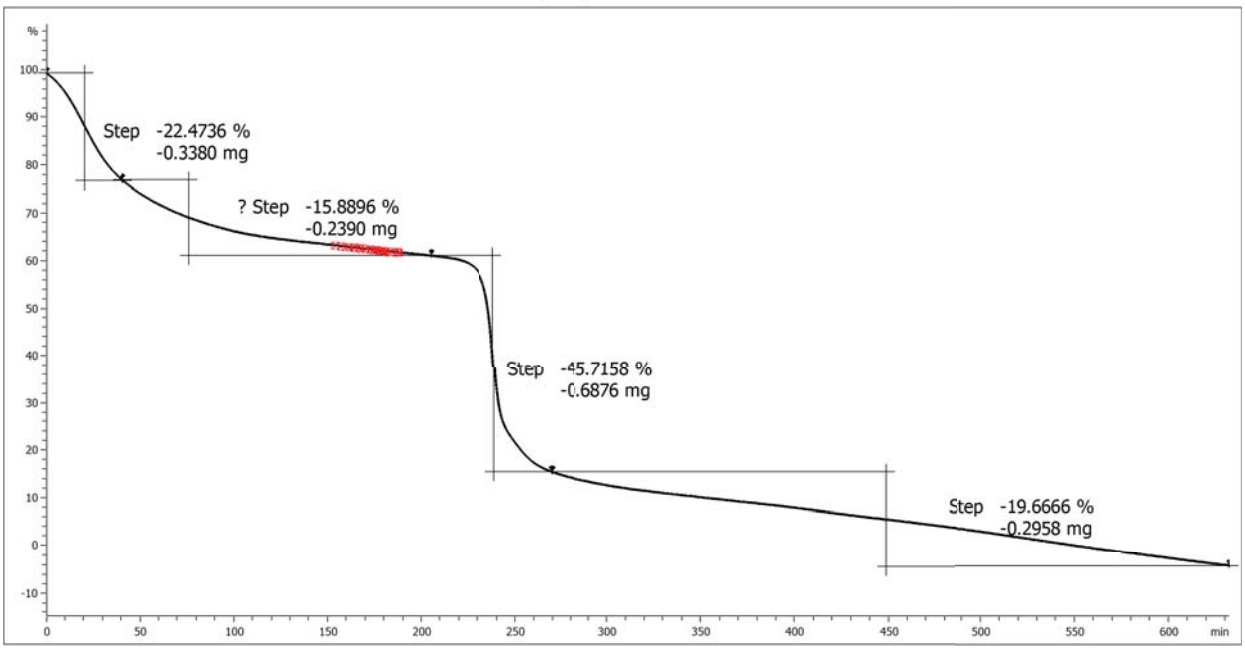


Figure S48. TGA of complex (6)

Optical properties: Fluorescence and UV-Vis

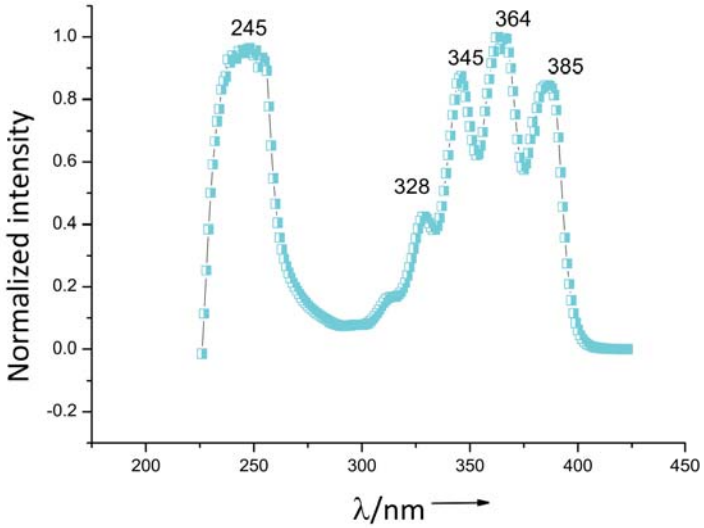


*Figure S49. UV-Vis spectrum of **L** in $CHCl_3$ (5mM). 245 nm absorption band could be assigned to imidazole group, absorptions from 328nm to 385 nm with well-defined vibrational structure corresponding to anthracene moiety.*

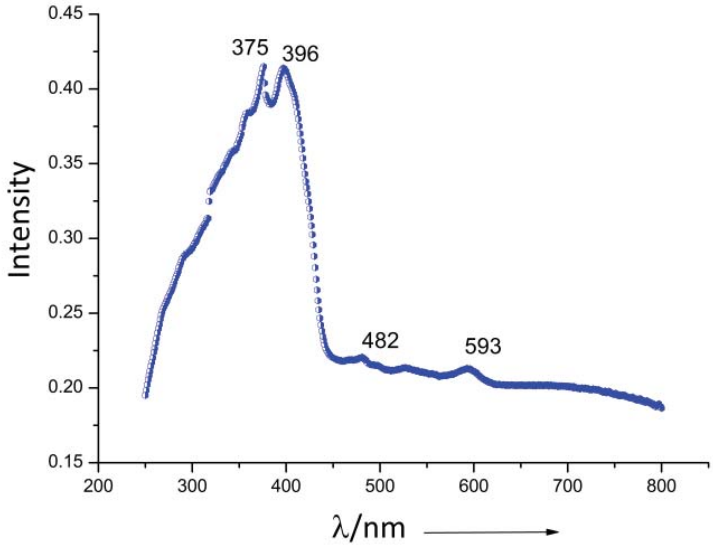


*Figure S50. Solid state UV-Vis spectrum of **L*** measured using integrating sphere.

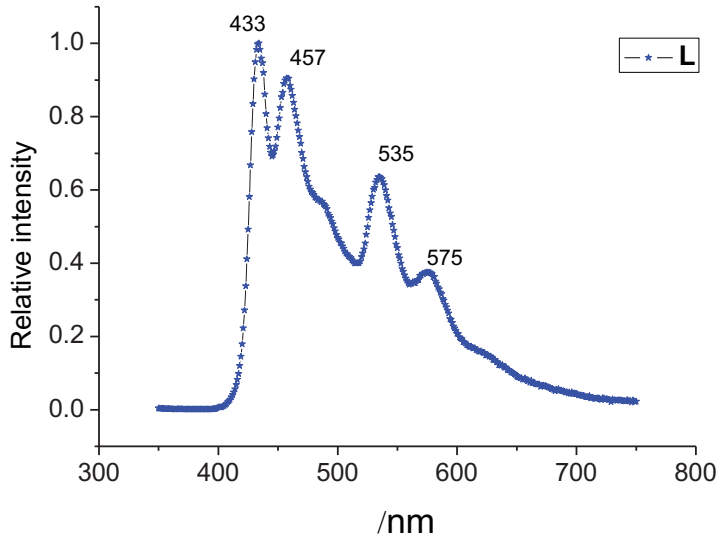
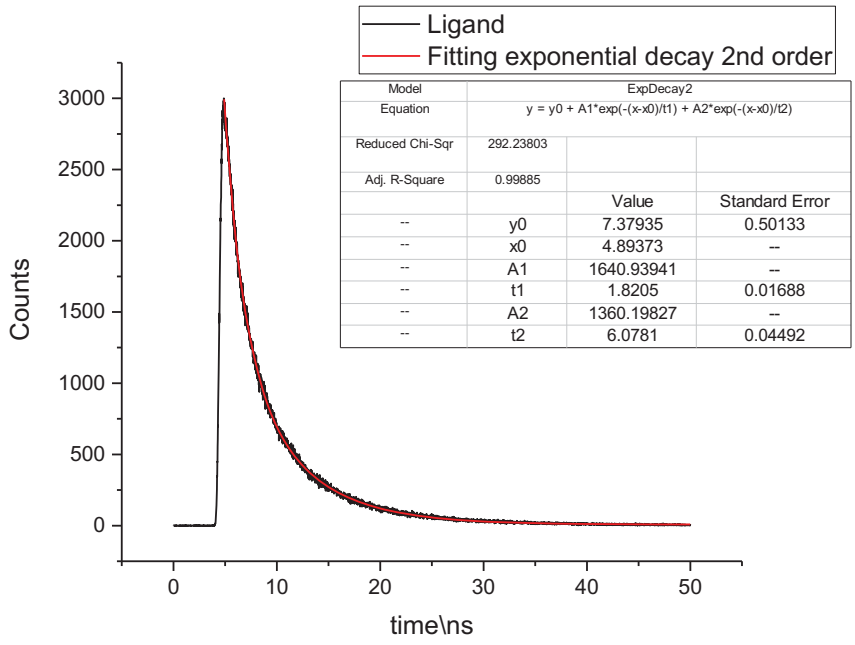


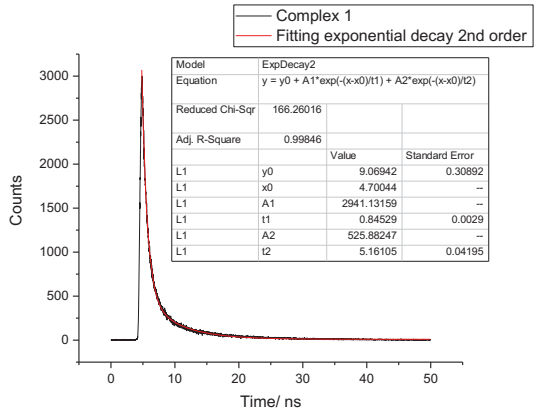
*Figure S51. Solid-state emission spectrum of **L** at rt.*



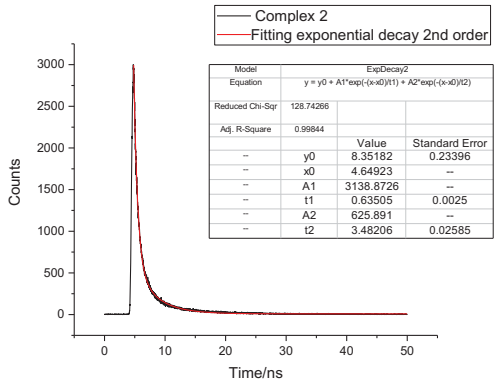
Model	ExpDecay2		
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)		
Reduced Chi-Sqr	292.23803		
Adj. R-Square	0.99885		
		Value	Standard Error
--	y0	7.37935	0.50133
--	x0	4.89373	--
--	A1	1640.93941	--
--	t1	1.8205	0.01688
--	A2	1360.19827	--
--	t2	6.0781	0.04492

Figure S52. Lifetime measurements of luminescence of L.

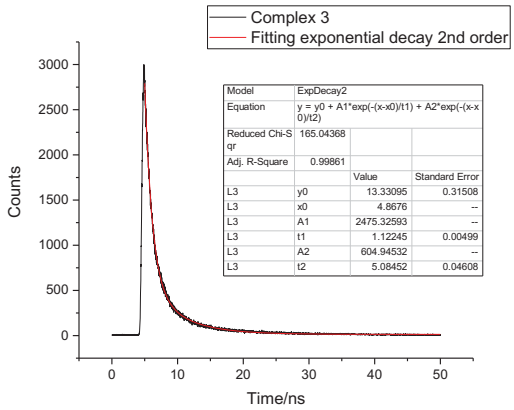
Lifetime measurements of luminescence.



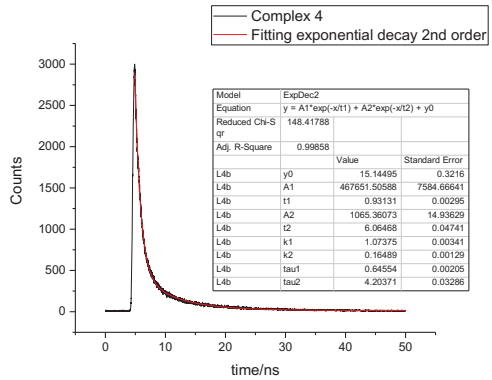
Model	ExpDecay2		
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)		
Reduced Chi-Sqr	166.26016		
Adj. R-Square	0.99846		
		Value	Standard Error
L1	y0	9.06942	0.30892
L1	x0	4.70044	--
L1	A1	2941.13159	--
L1	t1	0.84529	0.0029
L1	A2	525.88247	--
L1	t2	5.16105	0.04195



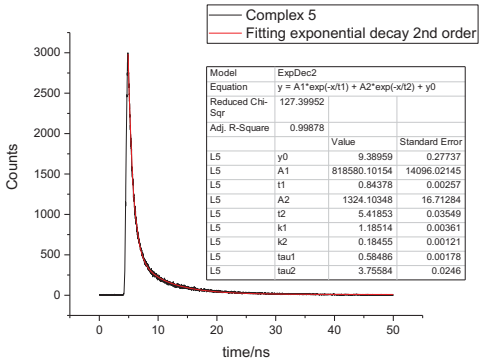
Model	ExpDecay2		
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)		
Reduced Chi-Sqr	128.74266		
Adj. R-Square	0.99844		
		Value	Standard Error
--	y0	8.35182	0.23396
--	x0	4.64923	--
--	A1	3138.8726	--
--	t1	0.63505	0.0025
--	A2	625.891	--
--	t2	3.48206	0.02585



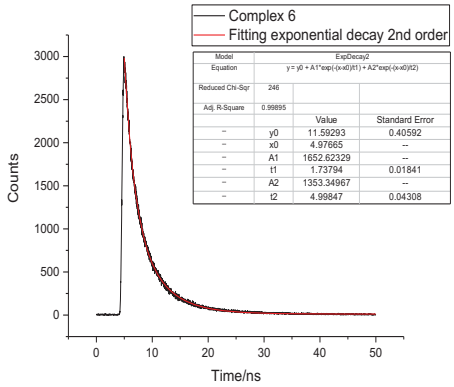
Model	ExpDecay2		
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)		
Reduced Chi-Sqr	165.04368		
Adj. R-Square	0.99861		
		Value	Standard Error
L3	y0	13.33095	0.31508
L3	x0	4.8676	--
L3	A1	2475.32593	--
L3	t1	1.12245	0.00499
L3	A2	604.94532	--
L3	t2	5.08452	0.04608



Model	ExpDec2		
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0		
Reduced Chi-Sqr	148.41788		
Adj. R-Square	0.99858		
		Value	Standard Error
L4b	y0	15.14495	0.3216
L4b	A1	467651.50588	7584.66641
L4b	t1	0.93131	0.00295
L4b	A2	1065.36073	14.93629
L4b	t2	6.06468	0.04741
L4b	k1	1.07375	0.00341
L4b	k2	0.16489	0.00129
L4b	tau1	0.64554	0.00205
L4b	tau2	4.20371	0.03286



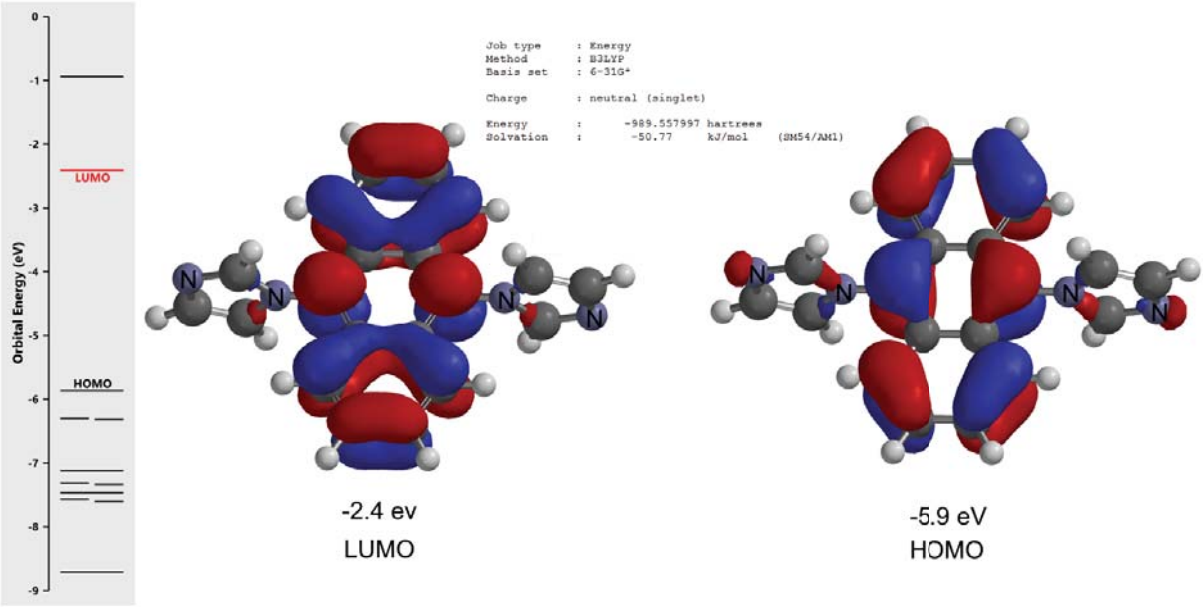
Model	ExpDec2		
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0		
Reduced Chi-Sqr	127.39952		
Adj. R-Square	0.99878		
		Value	Standard Error
L5	y0	9.38959	0.27737
L5	A1	818580.10154	14096.02145
L5	t1	0.84378	0.00257
L5	A2	1324.10348	16.71284
L5	t2	5.41853	0.03549
L5	k1	1.18514	0.00361
L5	k2	0.18455	0.00121
L5	tau1	0.58486	0.00178
L5	tau2	3.75584	0.0246



Model	ExpDecay2		
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)		
Reduced Chi-Sqr	246		
Adj. R-Square	0.99895		
		Value	Standard Error
--	y0	11.59293	0.40592
--	x0	4.97665	--
--	A1	1652.62329	--
--	t1	1.73794	0.01841
--	A2	1353.34967	--
--	t2	4.99847	0.04308

*Figure S53. Lifetime measurements of fluorescence of complexes **1** – **6***

DFT calculations



*FigureS54. DFT calculation B3LYP 6-31G*basis set reveals for trans-configuration ground state energy of -989.557997 hartrees, solvation energy -50.77 kJ/mol.*

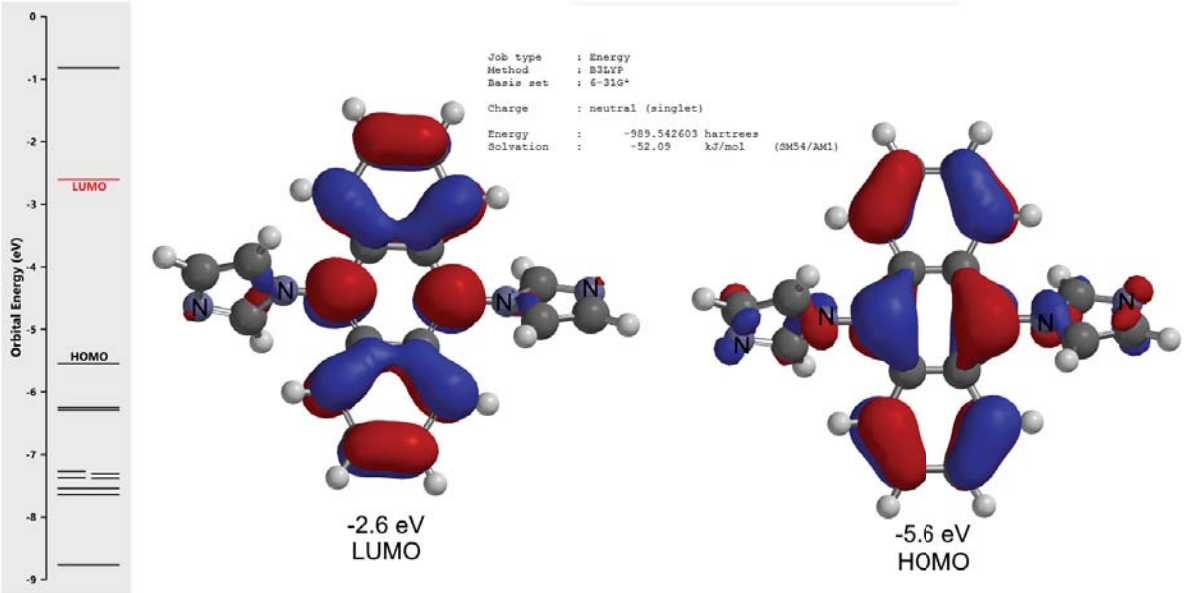


*Figure S55. DFT calculation B3LYP 6-31G*basic set reveals for cis-configuration ground state energy of -989.542603 hartrees, solvation energy -52.09 kJ/mol.*

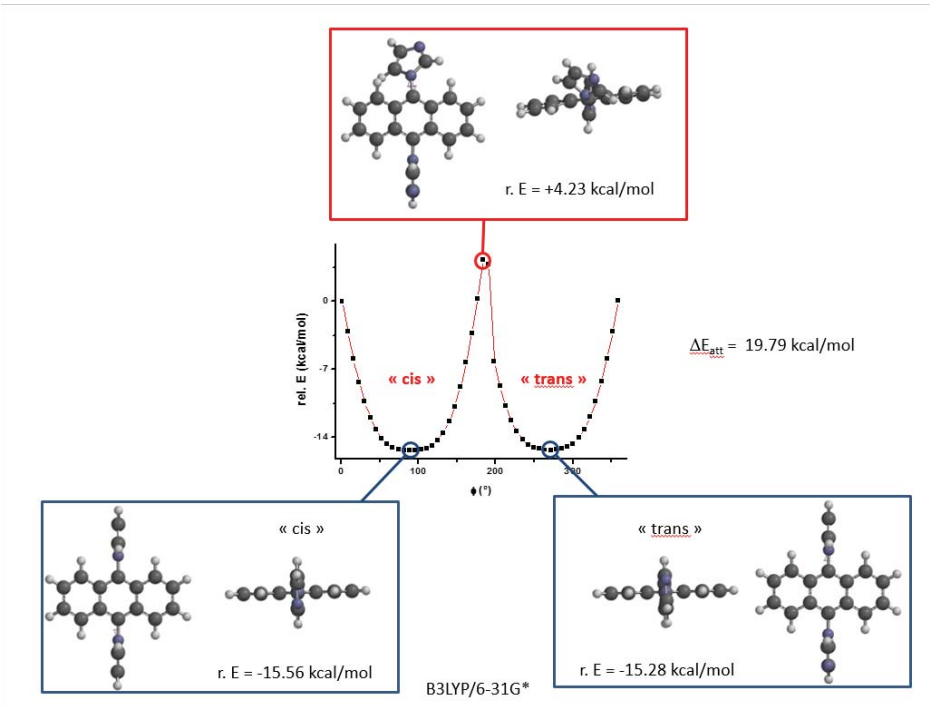


Figure S56. DFT calculation using B3LYP/6-3G rotational profile, transformation trans-**L** to cis-**L**.*

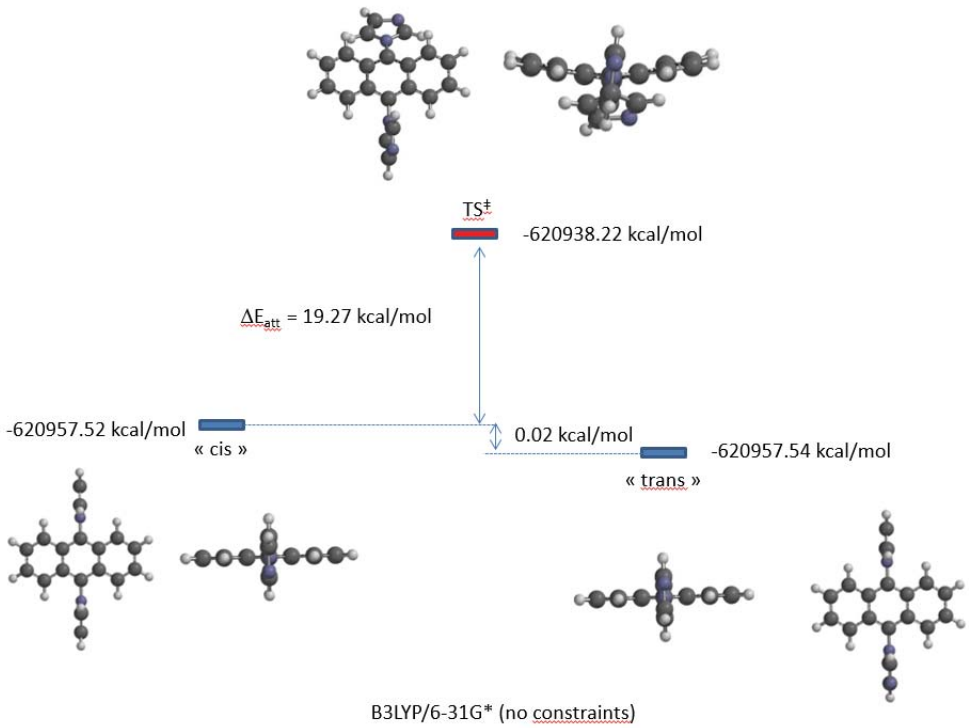


Figure S57. DFT calculation using B3LYP/6-3G: energy barrier, transition trans-**L** to cis-**L**.*

Luminescent sensing of nitro explosives

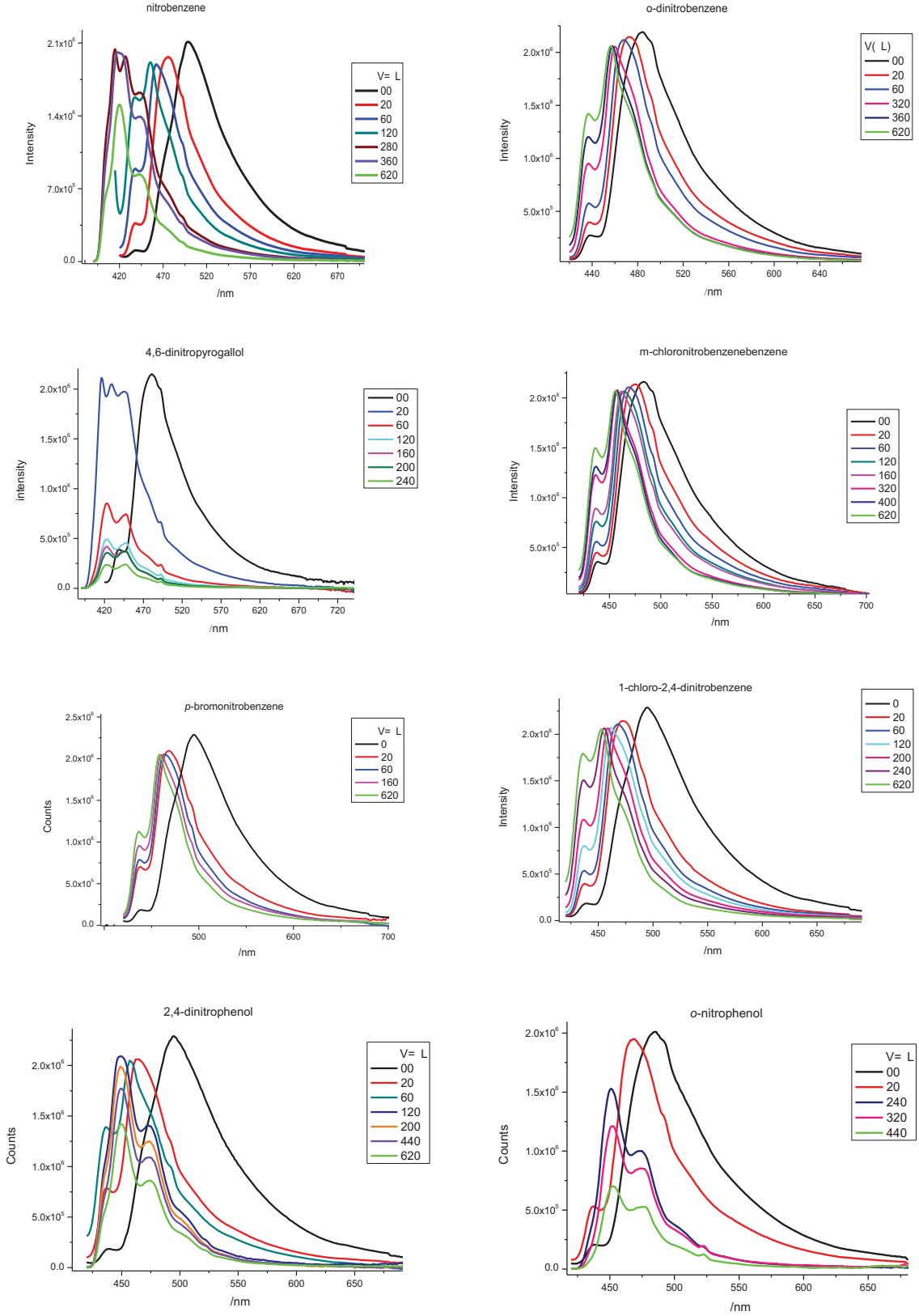


Figure S58. Luminescent sensing of nitro compounds with complex 6.

Crystallography data

1

Crystal Data. $C_{42}H_{36}C_{12}N_8O_{10}Zn$, M_r = 949.08, monoclinic, *C2/c* (No. 15), a = 22.1784(12) Å, b = 13.3509(7) Å, c = 16.1723(9) Å, b = 96.174(4)°, a = g = 90°, V = 4760.9(4) Å^3, T = 200(2) K, Z = 4, Z' = 1, m(MoKa) = 0.689, 30110 reflections measured, 4245 unique (R_{int} = 0.0990) which were used in all calculations. The final wR_2 was 0.1435 (all data) and R_1 was 0.0581 (I > 2(I)).

Compound	**1**
Formula	$C_{42}H_{36}C_{12}N_8O_{10}Zn$
$D_{calc.}$/ g cm^{-3}	1.324
m/mm^{-1}	0.689
Formula Weight	949.08
Color	colorless
Shape	prism
Size/mm^3	0.130× 0.105 × 0.084
T/K	200(2)
Crystal System	monoclinic
Space Group	*C2/c*
a/Å	22.1784(12)
b/Å	13.3509(7)
c/Å	16.1723(9)
a/°	90
b/°	96.174(4)
g/°	90
V/Å^3	4760.9(4)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	*MoKa*
Q_{min}/°	1.783
Q_{max}/°	25.119
Measured Refl.	30110
Independent Refl.	4245
Reflections Used	2910
R_{int}	0.0990
Parameters	288
Restraints	0
Largest Peak	0.395
Deepest Hole	-0.504
GooF	1.042
wR_2 (all data)	0.1435
wR_2	0.1313
R_1 (all data)	0.0883
R_1	0.0581

Table 2: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	**y**	**z**	U_{eq}

Zn15000	6038.3(5)	2500	45.6(2)
Cl13772.6(6)	3808.0(9)	4027.7(8)	77.2(4)
N14412.1(13)	5214(2)	1782(2)	48.2(8)
N33578.8(13)	4392(2)	1352(2)	48.2(8)
N2477.8(13)	1884(2)	1791(2)	49.2(8)
O44003.9(15)	4796(2)	3932(2)	71.0(9)
N41235.9(13)	2742(2)	1370(2)	52.0(8)
C181035.3(17)	2236(3)	1997(3)	51.9(10)
C42980.0(16)	3970(3)	1345(3)	49.2(9)
C122312.4(17)	2521(3)	1256(3)	51.0(9)
C13872.0(17)	4910(3)	1977(3)	52(1)
C52495.2(17)	4617(3)	1423(3)	50.8(10)
C172914.3(17)	2931(3)	1272(3)	50.4(9)
O54221(2)	3205(3)	4447(3)	117.1(15)
C111832.4(16)	3173(3)	1362(3)	51.1(10)
O13713(2)	2527(4)	6065(3)	112.3(14)
C101902.4(17)	4193(3)	1456(3)	54.3(10)
C132234(2)	1469(3)	1126(3)	61.4(11)
C20324.8(18)	2192(3)	982(3)	58.1(11)
C163403.8(18)	2258(3)	1218(3)	60.7(11)
C19787.0(17)	2720(3)	711(3)	58.4(11)
C24456.1(19)	4861(3)	998(3)	63.5(12)
C62555(2)	5679(3)	1462(3)	63.9(12)
C33952(2)	4358(3)	719(3)	61.4(11)
C91415(2)	4852(4)	1589(3)	69.3(13)
C142713(2)	863(3)	1044(3)	69.9(13)
O33587(4)	3393(4)	3248(3)	179(3)
C153309(2)	1268(3)	1101(4)	72.7(14)
C72081(2)	6274(3)	1578(4)	74.2(14)
O23279(2)	3837(4)	4539(4)	145(2)
C81503(2)	5847(4)	1650(4)	80.0(15)
C213305(5)	1770(6)	5870(5)	153(4)

Table 3: Anisotropic Displacement Parameters ($\times 10^4$) **1**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn132.0(3)	42.4(4)	62.7(4)	0	6.2(3)	0
Cl182.5(8)	62.0(8)	83.2(9)	12.9(6)	-8.3(7)	-9.3(6)
N141.8(17)	45.2(18)	59(2)	3.3(16)	9.5(15)	-4.3(13)
N338.8(16)	46.8(17)	59(2)	-2.9(15)	5.5(15)	-9.5(13)
N235.8(16)	48.5(18)	62(2)	-3.4(16)	0.5(15)	0.3(13)
O480(2)	57.6(18)	75(2)	-0.3(16)	6.3(17)	-17.6(16)
N436.9(16)	54(2)	65(2)	1.7(17)	5.7(16)	-11.6(14)
C1840(2)	53(2)	62(3)	1(2)	2.4(19)	-5.5(17)
C437.9(18)	46(2)	63(2)	3(2)	4.9(17)	-9.0(17)
C1244(2)	50(2)	59(3)	-1.9(19)	5.0(18)	-8.8(17)
C142(2)	50(2)	64(3)	-2(2)	7.6(19)	-7.2(17)
C545(2)	44(2)	63(3)	1.6(19)	5.0(19)	-7.9(16)
C1742(2)	49(2)	60(3)	4.3(19)	4.0(18)	-4.2(16)
O5119(3)	83(3)	143(4)	30(3)	-15(3)	26(2)
C1138(2)	49(2)	67(3)	0.4(19)	6.0(18)	-12.2(16)
O1118(3)	129(4)	89(3)	13(3)	6(3)	-27(3)
C1042(2)	49(2)	72(3)	2(2)	6.1(19)	-1.7(16)
C1352(2)	52(2)	81(3)	-4(2)	9(2)	-8.5(19)

C2044(2)	62(3)	67(3)	-1(2)	1(2)	-6.4(19)
C1644(2)	54(3)	84(3)	4(2)	9(2)	-2.4(18)
C1944(2)	67(3)	63(3)	6(2)	0(2)	-11.5(19)
C252(2)	71(3)	70(3)	-9(2)	19(2)	-16(2)
C653(2)	49(2)	88(3)	2(2)	3(2)	-5.8(19)
C360(3)	67(3)	60(3)	-12(2)	18(2)	-18(2)
C946(2)	59(3)	103(4)	-9(3)	11(2)	0(2)
C1468(3)	43(2)	101(4)	-4(2)	17(3)	-6(2)
O3315(8)	114(4)	90(3)	30(3)	-68(4)	-124(5)
C1551(2)	51(3)	119(4)	-1(3)	19(3)	0.8(19)
C763(3)	40(2)	117(4)	-3(2)	0(3)	-1(2)
O298(3)	132(4)	217(6)	51(4)	65(4)	-11(3)
C853(3)	59(3)	128(5)	-7(3)	10(3)	6(2)
C21221(10)	111(6)	125(6)	-13(5)	15(6)	-76(6)

Table 3: Bond Lengths in Å for **1**.

AtomAtom	**Length/Å**
Zn1N1	1.983(3)
Zn1N1[1]	1.983(3)
Zn1N2[2]	1.993(3)
Zn1N2[3]	1.993(3)
Cl1O4	1.430(3)
Cl1O5	1.397(4)
Cl1O3	1.398(5)
Cl1O2	1.441(5)
N1C1	1.335(5)
N1C2	1.366(5)
N3C4	1.442(4)
N3C1	1.334(5)
N3C3	1.385(5)
N2Zn1[4]	1.993(3)
N2C18	1.332(5)
N2C20	1.378(5)
N4C18	1.335(5)
N4C11	1.444(4)
N4C19	1.378(5)
C4C5	1.395(5)
C4C17	1.399(5)
C12C17	1.440(5)
C12C11	1.400(5)
C12C13	1.428(6)
C5C10	1.438(5)
C5C6	1.426(6)
C17C16	1.419(6)
C11C10	1.378(6)
O1C21	1.371(8)
C10C9	1.427(6)
C13C14	1.353(6)
C20C19	1.355(6)
C16C15	1.348(6)
C2C3	1.340(6)
C6C7	1.347(6)
C9C8	1.344(7)
C14C15	1.423(6)

C7C8	1.418(7)

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[1]1-X,+Y,1/2-Z; [2]1/2+X,1/2+Y,+Z; [3]1/2-X,1/2+Y,1/2-Z; [4]-1/2+X,-1/2+Y,+Z

Table 4: Bond Angles in ° for **1**.

AtomAtom	**Atom**	**Angle/°**
N1Zn1	N1[1]	112.62(18)
N1[1]Zn1	N2[2]	107.11(12)
N1Zn1	N2[2]	109.50(13)
N1Zn1	N2[3]	107.11(12)
N1[1]Zn1	N2[3]	109.50(13)
N2[3]Zn1	N2[2]	111.04(18)
O4Cl1	O2	109.9(3)
O5Cl1	O4	109.9(3)
O5Cl1	O3	109.5(4)
O5Cl1	O2	106.3(3)
O3Cl1	O4	110.0(2)
O3Cl1	O2	111.1(4)
C1N1	Zn1	125.5(3)
C1N1	C2	105.6(3)
C2N1	Zn1	128.8(3)
C1N3	C4	125.6(3)
C1N3	C3	107.2(3)
C3N3	C4	127.2(3)
C18N2	Zn1[4]	126.4(3)
C18N2	C20	105.0(3)
C20N2	Zn1[4]	128.6(3)
C18N4	C11	126.1(3)
C18N4	C19	107.8(3)
C19N4	C11	126.0(3)
N2C18	N4	111.4(4)
C5C4	N3	118.4(3)
C5C4	C17	123.2(3)
C17C4	N3	118.4(3)
C11C12	C17	118.5(4)
C11C12	C13	123.1(3)
C13C12	C17	118.3(4)
N3C1	N1	110.9(4)
C4C5	C10	118.5(3)
C4C5	C6	123.4(4)
C6C5	C10	118.1(4)
C4C17	C12	117.8(3)
C4C17	C16	124.0(3)
C16C17	C12	118.2(4)
C12C11	N4	117.6(3)
C10C11	N4	119.0(3)
C10C11	C12	123.4(3)
C11C10	C5	118.5(3)
C11C10	C9	123.3(4)
C9C10	C5	118.2(4)
C14C13	C12	121.1(4)
C19C20	N2	110.2(4)
C15C16	C17	121.4(4)
C20C19	N4	105.7(4)

C3C2	N1	110.2(4)
C7C6	C5	121.4(4)
C2C3	N3	106.1(4)
C8C9	C10	120.9(4)
C13C14	C15	120.1(4)
C16C15	C14	120.7(4)
C6C7	C8	120.0(4)
C9C8	C7	121.1(4)

---
[1]1-X,+Y,1/2-Z; [2]1/2+X,1/2+Y,+Z; [3]1/2-X,1/2+Y,1/2-Z; [4]-1/2+X,-1/2+Y,+Z

Table 5: Torsion Angles in ° for **1**.

AtomAtom	**Atom**	**Atom**	**Angle/°**
Zn1N1	C1	N3	178.3(3)
Zn1N1	C2	C3	-178.1(3)
Zn1[1]N2	C18	N4	177.4(3)
Zn1[1]N2	C20	C19	-177.2(3)
N1C2	C3	N3	-0.4(5)
N3C4	C5	C10	-177.0(4)
N3C4	C5	C6	3.7(7)
N3C4	C17	C12	-179.3(4)
N3C4	C17	C16	1.0(6)
N2C20	C19	N4	-0.2(5)
N4C11	C10	C5	-178.2(4)
N4C11	C10	C9	2.0(7)
C18N2	C20	C19	0.1(5)
C18N4	C11	C12	75.9(5)
C18N4	C11	C10	-104.2(5)
C18N4	C19	C20	0.2(5)
C4N3	C1	N1	-178.7(3)
C4N3	C3	C2	179.0(4)
C4C5	C10	C11	-3.7(6)
C4C5	C10	C9	176.1(4)
C4C5	C6	C7	-176.7(5)
C4C17	C16	C15	-176.2(5)
C12C17	C16	C15	4.2(7)
C12C11	C10	C5	1.8(7)
C12C11	C10	C9	-178.0(5)
C12C13	C14	C15	1.0(8)
C1N1	C2	C3	0.4(5)
C1N3	C4	C5	60.9(6)
C1N3	C4	C17	-118.2(4)
C1N3	C3	C2	0.1(5)
C5C4	C17	C12	1.6(6)
C5C4	C17	C16	-178.0(4)
C5C10	C9	C8	2.4(8)
C5C6	C7	C8	-1.0(8)
C17C4	C5	C10	2.0(7)
C17C4	C5	C6	-177.3(4)
C17C12	C11	N4	-178.1(4)
C17C12	C11	C10	1.9(7)
C17C12	C13	C14	2.1(7)
C17C16	C15	C14	-1.2(8)
C11N4	C18	N2	-176.1(4)

C11N4	C19	C20	176.2(4)
C11C12	C17	C4	-3.6(6)
C11C12	C17	C16	176.1(4)
C11C12	C13	C14	-178.6(5)
C11C10	C9	C8	-177.8(5)
C10C5	C6	C7	4.0(7)
C10C9	C8	C7	0.5(9)
C13C12	C17	C4	175.8(4)
C13C12	C17	C16	-4.5(6)
C13C12	C11	N4	2.6(6)
C13C12	C11	C10	-177.4(4)
C13C14	C15	C16	-1.5(8)
C20N2	C18	N4	0.0(4)
C19N4	C18	N2	-0.1(5)
C19N4	C11	C12	-99.4(5)
C19N4	C11	C10	80.6(6)
C2N1	C1	N3	-0.4(5)
C6C5	C10	C11	175.6(4)
C6C5	C10	C9	-4.6(7)
C6C7	C8	C9	-1.3(9)
C3N3	C4	C5	-117.8(5)
C3N3	C4	C17	63.1(6)
C3N3	C1	N1	0.2(5)

[1]-1/2+X,-1/2+Y,+Z

Table 6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **sv-2-23**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	y	z	U_{eq}
H181256.63	2142.45	2513.4	62
H13720.47	5040.59	2479.92	62
H1A3789.09	2808.03	5637.81	168
H131846.18	1195.52	1095.92	74
H20-42.37	2057.05	667.94	70
H163798.05	2505.03	1263.82	73
H19798.64	3008.39	189.53	70
H24788.02	4955.64	700.65	76
H62930.49	5968.56	1406.44	77
H33869.02	4049.38	203.76	74
H91031.79	4590.11	1633.38	83
H142652.27	181.61	951.28	84
H153637.66	845.19	1057.54	87
H72132.25	6964.5	1610.44	89
H81180.4	6261.72	1741.17	96
H21A2954.05	2033.94	5542.71	229
H21B3186.38	1483.5	6372.47	229
H21C3488.51	1263.36	5558.58	229

2

Crystal Data. $C_{42}H_{36}B_2F_8N_8O_2Zn$, M_r = 923.80, monoclinic, *C2/c* (No. 15), a = 22.2863(8) Å, b = 13.1735(6) Å, c = 16.2124(6) Å, b = 97.265(3)°, a = g = 90°, V = 4721.6(3) Å^3, T = 293(2) K, Z = 4, Z' = 1, m(MoKa) = 0.594, 30675 reflections measured, 4199 unique (R_{int} = 0.0734) which were used in all

calculations. The final wR_2 was 0.1164 (all data) and R_1 was 0.0463 (I > 2(I)).

Compound	**2**
Formula	$C_{42}H_{36}B_2F_8N_8O_2Zn$
$D_{calc.}$/ g cm^{-3}	1.300
m/mm^{-1}	0.594
Formula Weight	923.80
Colour	yellow
Shape	block
Size/mm^3	0.210 × 0.157 × 0.110
T/K	200(2)
Crystal System	monoclinic
Space Group	*C2/c*
a/Å	22.2863(8)
b/Å	13.1735(6)
c/Å	16.2124(6)
a/°	90
b/°	97.265(3)
g/°	90
V/Å^3	4721.6(3)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoKa
Q_{min}/°	1.799
Q_{max}/°	25.082
Measured Refl.	30675
Independent Refl.	4199
Reflections Used	3361
R_{int}	0.0734
Parameters	287
Restraints	0
Largest Peak	0.554
Deepest Hole	-0.444
GooF	1.046
wR_2 (all data)	0.1164
wR_2	0.1111
R_1 (all data)	0.0602
R_1	0.0463

Table 9: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	**y**	**z**	U_{eq}
Zn15000	3936.5(3)	7500	33.54(15)
F15989.6(9)	5202.8(14)	6075.0(12)	60.9(5)
N15591.9(9)	4786.4(17)	8216.5(15)	37.1(5)
N29527.5(9)	8085.0(18)	8209.0(15)	37.7(5)
N38768.3(10)	7253.0(18)	8626.7(15)	38.8(5)
N46431.0(9)	5606.5(18)	8650.3(15)	36.6(5)
O16308.9(13)	7360(2)	3956.1(16)	68.0(7)
F25753.0(14)	6764(2)	5570.9(19)	104.8(9)
F36373.4(18)	6599(2)	6747.2(16)	123.4(13)

F46665.1(13)	6177(2)	5499(2)	112.1(10)
C36121.8(11)	5103(2)	8015.1(18)	36.6(6)
C188969.9(12)	7748(2)	7991.3(19)	39.5(6)
C57100.5(12)	7079(2)	8732.6(18)	38.8(6)
C107698.2(12)	7494(2)	8733.5(18)	38.8(6)
C47027.0(11)	6026(2)	8650.5(18)	37.9(6)
C118171.9(12)	6828(2)	8630.6(18)	39.2(6)
C128098.3(12)	5784(2)	8540.7(19)	40.8(7)
C177505.6(12)	5365(2)	8575.0(18)	39.6(6)
C209687.9(13)	7784(2)	9024.0(19)	45.9(7)
C199217.1(13)	7273(2)	9289(2)	46.6(7)
C66617.4(13)	7765(2)	8806(2)	48.2(7)
C97779.1(14)	8560(2)	8856(2)	47.4(7)
C15569.4(14)	5108(2)	9019(2)	49.4(8)
C167438.5(14)	4286(2)	8538(2)	48.9(8)
C26082.8(14)	5608(3)	9297(2)	50.1(8)
C76716.7(15)	8770(2)	8920(3)	60.1(9)
C138579.5(14)	5114(3)	8428(2)	55.7(9)
C157912.3(15)	3679(3)	8440(3)	60.2(9)
C87307.8(15)	9173(2)	8954(2)	58.0(9)
C148492.2(16)	4097(3)	8374(3)	64.1(10)
B16199(2)	6188(3)	5994(3)	58.6(10)
C216606(4)	8259(4)	4150(4)	158(3)

Table 10: Anisotropic Displacement Parameters ($\times 10^4$) **2**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn122.3(2)	30.9(2)	47.9(3)	0	6.03(17)	0
F177.6(13)	48.4(11)	56.8(12)	-2.0(9)	8.7(10)	-10.8(10)
N128.0(11)	38.6(13)	45.4(14)	3.2(10)	8.2(10)	-3.0(9)
N228.3(11)	36.9(12)	47.7(14)	-1.7(10)	3.9(10)	-1.0(9)
N327.8(11)	41.8(13)	47.2(14)	0.1(10)	6.4(10)	-9.9(10)
N427.7(11)	37.8(12)	44.8(13)	-0.1(10)	6.1(10)	-9.9(9)
O184.8(18)	60.7(16)	58.7(15)	3.9(12)	10.7(14)	1.0(14)
F2116(2)	79.1(18)	111(2)	18.1(15)	-18.1(17)	26.1(16)
F3212(3)	78.9(18)	67.6(16)	14.7(13)	-28.4(19)	-71(2)
F483.4(18)	111(2)	149(3)	25(2)	43.5(18)	-13.3(16)
C328.4(13)	36.3(15)	45.8(16)	1.6(12)	6.9(12)	-4.1(11)
C1831.1(13)	39.8(16)	47.6(17)	1.1(12)	4.8(12)	-6.6(11)
C532.6(13)	39.8(16)	44.2(16)	1.4(12)	5.7(12)	-4.9(11)
C1032.4(13)	38.8(15)	45.7(16)	0.8(12)	6.5(12)	-5.6(11)
C428.0(12)	39.0(15)	46.7(16)	1.0(13)	5.1(11)	-9.0(12)
C1130.3(13)	40.6(15)	46.9(16)	-0.1(12)	5.4(12)	-8.1(12)
C1231.7(13)	38.0(16)	53.3(18)	0.1(12)	7.2(12)	-4.7(11)
C1734.0(14)	37.9(15)	46.8(17)	1.1(12)	5.0(12)	-5.8(12)
C2031.2(14)	55.6(19)	49.6(18)	1.7(14)	0.7(12)	-6.9(13)
C1936.7(15)	55.7(19)	46.6(17)	5.8(14)	2.4(13)	-8.9(13)
C634.2(14)	44.4(17)	67(2)	0.2(14)	10.3(14)	-2.3(13)
C937.8(15)	42.1(16)	63(2)	-3.4(14)	9.0(14)	-9.6(13)
C141.8(16)	58(2)	52.1(19)	-9.8(15)	19.3(14)	-15.8(14)
C1638.5(15)	37.9(16)	69(2)	0.5(14)	3.1(14)	-8.2(13)
C245.6(17)	59(2)	48.0(18)	-9.9(15)	15.7(14)	-17.6(15)
C744.6(17)	41.4(19)	97(3)	-3.6(17)	19.0(17)	2.9(14)
C1334.6(15)	53(2)	80(2)	-5.1(17)	10.9(15)	-0.9(14)

C1551.0(19)	37.2(18)	92(3)	-1.8(16)	6.5(18)	-0.7(14)
C854.9(19)	35.2(18)	86(3)	-5.1(16)	15.5(18)	-6.0(14)
C1445.8(18)	46(2)	102(3)	-6.4(18)	15.0(18)	5.3(14)
B165(2)	50(2)	58(2)	12.7(19)	-2.4(19)	-9.7(19)
C21292(10)	79(4)	106(5)	-21(3)	35(5)	-71(5)

Table 11: Bond Lengths in Å for **2**.

AtomAtom	**Length/Å**
Zn1N1[1]	1.989(2)
Zn1N1	1.989(2)
Zn1N2[2]	1.999(2)
Zn1N2[3]	1.999(2)
F1B1	1.391(4)
N1C3	1.331(3)
N1C1	1.375(4)
N2Zn1[4]	1.999(2)
N2C18	1.325(3)
N2C20	1.382(4)
N3C18	1.343(4)
N3C11	1.443(3)
N3C19	1.372(4)
N4C3	1.340(4)
N4C4	1.439(3)
N4C2	1.381(4)
O1C21	1.374(6)
F2B1	1.365(5)
F3B1	1.347(5)
F4B1	1.390(5)
C5C10	1.440(4)
C5C4	1.400(4)
C5C6	1.423(4)
C10C11	1.400(4)
C10C9	1.426(4)
C4C17	1.395(4)
C11C12	1.390(4)
C12C17	1.440(4)
C12C13	1.419(4)
C17C16	1.429(4)
C20C19	1.361(4)
C6C7	1.350(4)
C9C8	1.350(5)
C1C2	1.348(4)
C16C15	1.350(5)
C7C8	1.415(5)
C13C14	1.355(5)
C15C14	1.421(5)

[1]1-X,+Y,3/2-Z; [2]3/2-X,-1/2+Y,3/2-Z; [3]-1/2+X,-1/2+Y,+Z; [4]1/2+X,1/2+Y,+Z

Table 12: Bond Angles in ° for **2**.

AtomAtom	**Atom**	**Angle/°**
N1[1]Zn1	N1	111.49(13)
N1[1]Zn1	N2[2]	107.04(9)
N1[1]Zn1	N2[3]	109.80(9)

N1Zn1	N2[3]	107.04(9)
N1Zn1	N2[2]	109.80(9)
N2[3]Zn1	N2[2]	111.72(13)
C3N1	Zn1	125.20(19)
C3N1	C1	106.0(2)
C1N1	Zn1	128.69(17)
C18N2	Zn1[4]	125.4(2)
C18N2	C20	106.2(2)
C20N2	Zn1[4]	128.26(18)
C18N3	C11	126.1(2)
C18N3	C19	108.0(2)
C19N3	C11	125.8(2)
C3N4	C4	125.1(2)
C3N4	C2	107.5(2)
C2N4	C4	127.4(2)
N1C3	N4	110.6(2)
N2C18	N3	110.6(3)
C4C5	C10	118.3(2)
C4C5	C6	123.8(2)
C6C5	C10	117.9(3)
C11C10	C5	118.2(3)
C11C10	C9	123.4(2)
C9C10	C5	118.4(3)
C5C4	N4	118.5(2)
C17C4	N4	118.4(2)
C17C4	C5	123.1(2)
C10C11	N3	117.8(2)
C12C11	N3	118.7(2)
C12C11	C10	123.5(2)
C11C12	C17	118.2(3)
C11C12	C13	123.2(3)
C13C12	C17	118.6(3)
C4C17	C12	118.6(3)
C4C17	C16	123.2(3)
C16C17	C12	118.2(3)
C19C20	N2	109.1(3)
C20C19	N3	106.1(3)
C7C6	C5	121.5(3)
C8C9	C10	121.2(3)
C2C1	N1	109.7(2)
C15C16	C17	121.0(3)
C1C2	N4	106.2(3)
C6C7	C8	120.6(3)
C14C13	C12	121.3(3)
C16C15	C14	120.8(3)
C9C8	C7	120.4(3)
C13C14	C15	120.1(3)
F2B1	F1	109.5(3)
F2B1	F4	105.4(3)
F3B1	F1	110.6(3)
F3B1	F2	109.9(4)
F3B1	F4	112.1(4)
F4B1	F1	109.2(4)

[1]1-X,+Y,3/2-Z; [2]-1/2+X,-1/2+Y,+Z; [3]3/2-X,-1/2+Y,3/2-Z; [4]1/2+X,1/2+Y,+Z

Table 13: Torsion Angles in ° for **2**.

AtomAtom	Atom	Atom	Angle/°
Zn1N1	C3	N4	-176.11(18)
Zn1N1	C1	C2	175.6(2)
Zn1^{1}N2	C18	N3	-176.05(18)
Zn1^{1}N2	C20	C19	175.6(2)
N1C1	C2	N4	0.6(4)
N2C20	C19	N3	0.6(4)
N3C11	C12	C17	177.8(3)
N3C11	C12	C13	-1.3(5)
N4C4	C17	C12	177.5(3)
N4C4	C17	C16	-3.1(4)
C3N1	C1	C2	-0.3(4)
C3N4	C4	C5	117.4(3)
C3N4	C4	C17	-63.1(4)
C3N4	C2	C1	-0.6(4)
C18N2	C20	C19	-0.5(3)
C18N3	C11	C10	-77.3(4)
C18N3	C11	C12	103.3(3)
C18N3	C19	C20	-0.5(3)
C5C10	C11	N3	179.6(3)
C5C10	C11	C12	-1.1(5)
C5C10	C9	C8	-1.2(5)
C5C4	C17	C12	-3.0(5)
C5C4	C17	C16	176.4(3)
C5C6	C7	C8	1.2(6)
C10C5	C4	N4	179.9(3)
C10C5	C4	C17	0.4(4)
C10C5	C6	C7	-3.6(5)
C10C11	C12	C17	-1.5(5)
C10C11	C12	C13	179.4(3)
C10C9	C8	C7	-1.3(6)
C4N4	C3	N1	178.2(2)
C4N4	C2	C1	-178.3(3)
C4C5	C10	C11	1.6(4)
C4C5	C10	C9	-177.1(3)
C4C5	C6	C7	177.1(3)
C4C17	C16	C15	178.0(3)
C11N3	C18	N2	176.7(3)
C11N3	C19	C20	-177.1(3)
C11C10	C9	C8	-179.9(3)
C11C12	C17	C4	3.5(4)
C11C12	C17	C16	-175.9(3)
C11C12	C13	C14	177.5(3)
C12C17	C16	C15	-2.6(5)
C12C13	C14	C15	-0.9(6)
C17C12	C13	C14	-1.6(5)
C17C16	C15	C14	0.2(6)
C20N2	C18	N3	0.3(3)
C19N3	C18	N2	0.1(3)
C19N3	C11	C10	98.7(4)
C19N3	C11	C12	-80.7(4)
C6C5	C10	C11	-177.7(3)
C6C5	C10	C9	3.5(4)

C6C5	C4	N4	-0.8(4)
C6C5	C4	C17	179.7(3)
C6C7	C8	C9	1.4(6)
C9C10	C11	N3	-1.7(4)
C9C10	C11	C12	177.7(3)
C1N1	C3	N4	0.0(3)
C16C15	C14	C13	1.6(6)
C2N4	C3	N1	0.4(3)
C2N4	C4	C5	-65.2(4)
C2N4	C4	C17	114.3(3)
C13C12	C17	C4	-177.4(3)
C13C12	C17	C16	3.3(5)

[1]1/2+X,1/2+Y,+Z

Table 14: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	y	z	U_{eq}
H1A6320.69	7007.6	4375.03	102
H36258.44	4990.63	7504.04	44
H188748.71	7840.16	7470.72	47
H2010058.08	7911.19	9340.51	55
H199202.69	6994.1	9812.91	56
H66224.57	7517.12	8775.33	58
H98163.72	8838.07	8867.91	57
H15248.62	4997.2	9323.03	59
H167062.88	3998.23	8582.11	59
H26182.61	5896.36	9820.09	60
H76393.74	9200.51	8975.75	72
H138962.3	5377.2	8391.52	67
H157858.64	2979	8416.58	72
H87371.96	9863.51	9044.01	70
H148812.4	3670.89	8292.4	77
H21A6639.34	8631.42	3649.35	237
H21B7003.49	8119.61	4430.63	237
H21C6384.03	8652.7	4506.92	237

3

Crystal Data. $C_{58}H_{54}Cl_4N_8O_8S_2Zn$, M_r = 1262.38, triclinic, *P-1* (No. 2), a = 11.7749(19) Å, b = 12.2678(19) Å, c = 12.1740(19) Å, a = 111.157(12)°, b = 93.629(13)°, g = 110.389(12)°, V = 1500.9(4) Å^3, T = 298(2) K, Z = 1, Z' = 0.5, m(MoK_α) = 0.716, 19284 reflections measured, 5343 unique (R_{int} = 0.1103) which were used in all calculations. The final wR_2 was 0.1386 (all data) and R_1 was 0.0518 (I > 2(I)).

Compound	**3**
Formula	$C_{58}H_{54}Cl_4N_8O_8S_2Zn$
$D_{calc.}$/ g cm^{-3}	1.397
m/mm^{-1}	0.716
Formula Weight	1262.38
Colour	colorless
Shape	block
Size/mm^3	0.38×0.29×0.24
T/K	200(2)

Crystal System	triclinic
Space Group	*P-1*
a/Å	11.7749(19)
b/Å	12.2678(19)
c/Å	12.1740(19)
a/°	111.157(12)
b/°	93.629(13)
g/°	110.389(12)
V/Å^3	1500.9(4)
Z	1
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK_α
Q_{min}/°	1.837
Q_{max}/°	25.172
Measured Refl.	19284
Independent Refl.	5343
Reflections Used	4448
R_{int}	0.1103
Parameters	370
Restraints	0
Largest Peak	0.348
Deepest Hole	-0.596
GooF	1.035
wR_2 (all data)	0.1386
wR_2	0.1312
R_1 (all data)	0.0622
R_1	0.0518

Table 16: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **shelx**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	**y**	**z**	U_{eq}
Zn15000	5000	5000	44.55(16)
S17328.4(7)	5742.6(7)	7508.9(6)	53.7(2)
O16458(2)	5469(2)	6449.8(19)	67.2(6)
O27706(3)	4718(2)	7384(3)	79.8(7)
O36873(2)	6173(2)	8597.8(19)	72.1(7)
N13691(2)	3885(2)	5707(2)	51.3(6)
N22086(2)	2327(2)	5767(2)	50.2(6)
N35296(2)	3345(2)	3929(2)	52.0(6)
N45352(3)	1741(2)	2392(2)	55.8(6)
C13685(3)	4065(3)	6894(3)	57.2(8)
C22707(3)	3113(3)	6948(3)	56.8(8)
C32719(3)	2833(3)	5063(3)	51.4(7)
C44983(3)	2719(3)	2741(2)	53.0(7)
C55891(4)	2743(3)	4351(3)	64.4(9)
C65932(4)	1757(3)	3421(3)	71.5(10)
C76134(3)	1090(3)	560(3)	54.5(7)
C85162(3)	856(3)	1162(2)	53.7(7)
C94040(3)	-188(3)	655(3)	54.2(7)
C103053(3)	-438(3)	1272(3)	66.2(9)
C111976(4)	-1469(4)	741(3)	73.7(10)
C121802(4)	-2350(4)	-459(3)	74.1(10)

C132709(3)	-2169(3)	-1085(3)	65.6(8)
C141176(3)	12(3)	4801(2)	48.2(6)
C151017(3)	1141(3)	5366(2)	47.7(6)
C16-122(3)	1178(3)	5577(2)	48.4(6)
C17-294(3)	2328(3)	6127(3)	60.9(8)
C18-1423(4)	2318(3)	6292(3)	71.1(9)
C19-2463(3)	1151(4)	5905(3)	69.7(9)
C20-2357(3)	26(3)	5379(3)	59.1(8)
C2111854(4)	10218(5)	7838(5)	111.8(17)
C2210699(3)	9104(4)	7701(4)	75.6(10)
C239837(4)	9289(4)	8384(4)	77.3(10)
C248820(3)	8270(3)	8349(3)	65.8(8)
C258644(3)	7050(3)	7603(2)	54.4(7)
C269485(3)	6852(4)	6876(3)	69.6(9)
C2710494(4)	7881(4)	6936(4)	78.7(10)
O48680(3)	6870(3)	10726(3)	105.5(10)
C288841(5)	5753(5)	10566(4)	110.8(16)
Cl15160.5(13)	6768.0(13)	10311.3(11)	107.8(4)
Cl25076.7(11)	8284.8(12)	12729.3(11)	101.7(4)
C294245(4)	6990(4)	11368(4)	94.2(13)

Table 17: Anisotropic Displacement Parameters ($\times 10^4$) **3**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn152.1(3)	34.5(2)	36.1(2)	7.89(18)	13.04(18)	11.28(19)
S160.5(5)	52.2(4)	42.1(4)	13.4(3)	9.0(3)	22.0(4)
O162.7(13)	67.5(14)	52.6(12)	19.0(11)	-2(1)	13.1(11)
O297.9(19)	67.6(15)	93.7(18)	39.9(14)	34.1(15)	45.9(14)
O376.3(15)	79.0(15)	47.0(12)	14.1(11)	22.0(11)	25.9(13)
N156.0(14)	45.3(12)	41.1(12)	13.6(10)	13(1)	10.9(11)
N249.9(13)	45.0(12)	45.5(12)	16.8(10)	11.4(10)	8.9(10)
N366.4(15)	42.7(12)	37.9(11)	9.5(10)	13.5(11)	18.7(11)
N480.0(17)	46.7(13)	35.6(12)	6.3(10)	11.3(11)	30.7(13)
C162.5(18)	49.7(16)	41.1(15)	10.9(13)	12.9(13)	9.5(14)
C262.3(18)	55.4(17)	38.6(14)	15.9(13)	12.2(13)	10.9(14)
C355.0(16)	46.0(15)	44.3(14)	17.7(12)	11.9(12)	10.8(13)
C471.0(19)	42.4(14)	39.4(14)	8.5(12)	13.8(13)	23.9(14)
C598(3)	56.3(18)	38.0(15)	12.3(13)	12.4(15)	37.1(18)
C6108(3)	66(2)	46.8(17)	12.9(15)	8.2(17)	53(2)
C770.5(19)	48.0(15)	42.7(15)	11.9(12)	10.3(13)	28.2(14)
C876(2)	45.7(15)	35.8(13)	6.5(12)	11.0(13)	30.4(15)
C972.1(19)	50.2(16)	42.1(14)	13.2(13)	13.2(13)	32.2(15)
C1083(2)	66(2)	49.9(17)	17.5(15)	21.5(16)	35.2(19)
C1176(2)	82(2)	67(2)	31.2(19)	25.0(18)	33(2)
C1272(2)	67(2)	70(2)	24.3(18)	7.9(18)	18.5(18)
C1377(2)	55.3(18)	52.1(17)	12.7(15)	6.5(16)	23.4(16)
C1449.3(15)	49.2(15)	43.6(14)	17.7(12)	11.8(12)	17.8(13)
C1547.7(15)	43.5(14)	44.2(14)	16.5(12)	9.8(12)	11.2(12)
C1653.5(16)	45.2(14)	45.2(14)	18.2(12)	12.0(12)	18.1(12)
C1769(2)	48.3(16)	61.3(18)	16.8(14)	15.2(15)	24.3(15)
C1880(2)	66(2)	72(2)	20.3(17)	21.6(18)	42.5(19)
C1962(2)	83(2)	73(2)	29.4(19)	22.6(17)	40.9(19)
C2051.8(17)	64.3(19)	58.7(18)	23.0(15)	17.1(14)	21.8(15)
C2187(3)	115(4)	118(4)	69(3)	12(3)	3(3)

C2263(2)	85(3)	74(2)	42(2)	6.4(18)	16.6(19)
C2379(2)	61(2)	73(2)	18.5(18)	7.2(19)	17.0(18)
C2467(2)	59.9(19)	60.0(19)	16.4(15)	11.5(16)	22.6(16)
C2556.7(17)	61.2(18)	38.8(14)	14.8(13)	4.8(12)	23.3(14)
C2665(2)	74(2)	60.1(19)	18.1(17)	11.8(16)	27.4(18)
C2764(2)	97(3)	70(2)	31(2)	17.5(18)	29(2)
O4115(3)	114(2)	65.9(18)	28.7(17)	6.7(16)	33(2)
C28123(4)	116(4)	81(3)	21(3)	9(3)	56(3)
Cl1124.3(10)	122(1)	76.6(7)	33.8(7)	34.2(7)	53.5(8)
Cl291.7(8)	102.6(8)	91.5(7)	16.7(6)	27.3(6)	39.8(6)
C2990(3)	95(3)	83(3)	34(2)	22(2)	22(2)

Table 18: Bond Lengths in Å for **3**.

AtomAtom	**Length/Å**
Zn1N1	2.129(2)
Zn1N1^{1}	2.129(2)
Zn1N3^{1}	2.141(2)
Zn1N3	2.141(2)
Zn1O1	2.142(2)
Zn1O1^{1}	2.142(2)
S1O2	1.435(3)
S1O3	1.451(2)
S1O1	1.451(2)
S1C25	1.760(3)
N1C3	1.311(3)
N1C1	1.382(4)
N2C3	1.347(3)
N2C2	1.381(4)
N2C15	1.440(3)
N3C4	1.324(3)
N3C5	1.374(4)
N4C4	1.350(4)
N4C6	1.378(4)
N4C8	1.445(3)
C1C2	1.349(4)
C5C6	1.344(4)
C7C8	1.400(4)
C7C13^{2}	1.428(4)
C7C9^{2}	1.441(4)
C8C9	1.383(4)
C9C10	1.427(4)
C9C7^{2}	1.441(4)
C10C11	1.347(5)
C11C12	1.419(5)
C12C13	1.353(5)
C13C7^{2}	1.428(4)
C14C15	1.391(4)
C14C20^{3}	1.435(4)
C14C16^{3}	1.437(4)
C15C16	1.394(4)
C16C17	1.419(4)
C16C14^{3}	1.437(4)
C17C18	1.353(5)

C18C19	1.411(5)
C19C20	1.350(5)
C20C14[3]	1.435(4)
C21C22	1.502(5)
C22C27	1.375(6)
C22C23	1.380(5)
C23C24	1.381(5)
C24C25	1.374(4)
C25C26	1.395(5)
C26C27	1.374(5)
O4C28	1.395(6)
Cl1C29	1.737(4)
Cl2C29	1.744(5)

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[1]1-X,1-Y,1-Z; [2]1-X,-Y,-Z; [3]-X,-Y,1-Z

Table 19: Bond Angles in ° for **3**.

AtomAtom	**Atom**	**Angle/°**
N1Zn1	N1[1]	180.00(10)
N1Zn1	N3[1]	90.42(9)
N1[1]Zn1	N3[1]	89.58(9)
N1Zn1	N3	89.58(9)
N1[1]Zn1	N3	90.42(9)
N3[1]Zn1	N3	180.0
N1Zn1	O1	90.20(9)
N1[1]Zn1	O1	89.80(9)
N3[1]Zn1	O1	89.26(10)
N3Zn1	O1	90.74(10)
N1Zn1	O1[1]	89.80(9)
N1[1]Zn1	O1[1]	90.20(9)
N3[1]Zn1	O1[1]	90.74(10)
N3Zn1	O1[1]	89.26(10)
O1Zn1	O1[1]	180.0
O2S1	O3	113.55(16)
O2S1	O1	112.92(16)
O3S1	O1	111.22(15)
O2S1	C25	107.55(16)
O3S1	C25	106.69(14)
O1S1	C25	104.18(14)
S1O1	Zn1	173.07(15)
C3N1	C1	105.5(2)
C3N1	Zn1	125.43(19)
C1N1	Zn1	129.08(19)
C3N2	C2	107.2(2)
C3N2	C15	126.7(2)
C2N2	C15	126.0(2)
C4N3	C5	106.2(2)
C4N3	Zn1	127.6(2)
C5N3	Zn1	126.14(19)
C4N4	C6	107.3(2)
C4N4	C8	125.5(3)
C6N4	C8	127.2(3)
C2C1	N1	110.1(3)
C1C2	N2	105.7(3)

N1C3	N2	111.6(2)
N3C4	N4	110.4(3)
C6C5	N3	109.7(3)
C5C6	N4	106.4(3)
C8C7	C13[2]	123.7(3)
C8C7	C9[2]	118.2(3)
C13[2]C7	C9[2]	118.2(3)
C9C8	C7	123.8(3)
C9C8	N4	118.1(3)
C7C8	N4	118.1(3)
C8C9	C10	123.9(3)
C8C9	C7[2]	118.1(3)
C10C9	C7[2]	118.0(3)
C11C10	C9	121.8(3)
C10C11	C12	120.1(3)
C13C12	C11	120.7(3)
C12C13	C7[2]	121.2(3)
C15C14	C20[3]	123.2(3)
C15C14	C16[3]	118.8(3)
C20[3]C14	C16[3]	118.0(3)
C14C15	C16	123.2(2)
C14C15	N2	118.3(3)
C16C15	N2	118.5(2)
C15C16	C17	123.4(3)
C15C16	C14[3]	118.0(3)
C17C16	C14[3]	118.6(3)
C18C17	C16	121.4(3)
C17C18	C19	120.2(3)
C20C19	C18	121.2(3)
C19C20	C14[3]	120.7(3)
C27C22	C23	118.4(3)
C27C22	C21	121.4(4)
C23C22	C21	120.2(4)
C22C23	C24	121.2(4)
C25C24	C23	119.7(3)
C24C25	C26	119.7(3)
C24C25	S1	120.4(3)
C26C25	S1	119.9(2)
C27C26	C25	119.4(3)
C26C27	C22	121.5(4)
Cl1C29	Cl2	112.2(2)

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[1]1-X,1-Y,1-Z; [2]1-X,-Y,-Z; [3]-X,-Y,1-Z

Table 20: Torsion Angles in ° for **3**.

AtomAtom	**Atom**	**Atom**	**Angle/°**
C3N1	C1	C2	0.1(4)
Zn1N1	C1	C2	-178.0(2)
N1C1	C2	N2	-0.3(4)
C3N2	C2	C1	0.4(4)
C15N2	C2	C1	176.2(3)
C1N1	C3	N2	0.2(4)
Zn1N1	C3	N2	178.3(2)
C2N2	C3	N1	-0.3(4)

C15N2	C3	N1	-176.2(3)
C5N3	C4	N4	0.2(3)
Zn1N3	C4	N4	178.48(19)
C6N4	C4	N3	-0.2(4)
C8N4	C4	N3	179.9(3)
C4N3	C5	C6	-0.1(4)
Zn1N3	C5	C6	-178.5(2)
N3C5	C6	N4	0.0(4)
C4N4	C6	C5	0.1(4)
C8N4	C6	C5	-180.0(3)
C13^{1}C7	C8	C9	180.0(3)
C9^{1}C7	C8	C9	-0.5(5)
C13^{1}C7	C8	N4	-1.3(5)
C9^{1}C7	C8	N4	178.3(3)
C4N4	C8	C9	-84.6(4)
C6N4	C8	C9	95.5(4)
C4N4	C8	C7	96.6(4)
C6N4	C8	C7	-83.3(4)
C7C8	C9	C10	179.3(3)
N4C8	C9	C10	0.6(5)
C7C8	C9	C7^{1}	0.5(5)
N4C8	C9	C7^{1}	-178.3(3)
C8C9	C10	C11	-179.9(3)
C7^{1}C9	C10	C11	-1.1(5)
C9C10	C11	C12	0.6(6)
C10C11	C12	C13	-0.1(6)
C11C12	C13	C7^{1}	0.1(6)
C20^{2}C14	C15	C16	-177.8(3)
C16^{2}C14	C15	C16	-0.6(5)
C20^{2}C14	C15	N2	1.3(4)
C16^{2}C14	C15	N2	178.5(2)
C3N2	C15	C14	68.5(4)
C2N2	C15	C14	-106.6(4)
C3N2	C15	C16	-112.4(3)
C2N2	C15	C16	72.5(4)
C14C15	C16	C17	-178.4(3)
N2C15	C16	C17	2.5(4)
C14C15	C16	C14^{2}	0.6(5)
N2C15	C16	C14^{2}	-178.5(2)
C15C16	C17	C18	178.7(3)
C14^{2}C16	C17	C18	-0.3(5)
C16C17	C18	C19	-0.6(6)
C17C18	C19	C20	0.8(6)
C18C19	C20	C14^{2}	0.0(5)
C27C22	C23	C24	3.1(6)
C21C22	C23	C24	-174.5(4)
C22C23	C24	C25	-1.4(6)
C23C24	C25	C26	-0.9(5)
C23C24	C25	S1	-178.0(3)
O2S1	C25	C24	-143.1(3)
O3S1	C25	C24	-21.0(3)
O1S1	C25	C24	96.8(3)
O2S1	C25	C26	39.8(3)
O3S1	C25	C26	161.9(3)
O1S1	C25	C26	-80.3(3)

C24C25	C26	C27	1.4(5)
S1C25	C26	C27	178.5(3)
C25C26	C27	C22	0.3(6)
C23C22	C27	C26	-2.5(6)
C21C22	C27	C26	175.0(4)

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[1]1-X,-Y,-Z; [2]-X,-Y,1-Z

Table 21: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	y	z	U_{eq}
H14270	4742	7559	69
H22495	3009	7637	68
H32493	2479	4226	62
H44568	2923	2219	64
H56216	2981	5158	77
H66283	1197	3462	86
H103156	127	2062	79
H111346	-1603	1162	88
H121057	-3061	-819	89
H132576	-2757	-1871	79
H17382	3104	6378	73
H18-1513	3083	6661	85
H19-3236	1157	6015	84
H20-3055	-731	5131	71
H21A11665	10952	7983	168
H21B12166	10018	7113	168
H21C12471	10396	8506	168
H239942	10114	8877	93
H248257	8410	8828	79
H269364	6030	6355	83
H2711051	7746	6447	94
H4A8070	6704	10233	158
H28A8894	5341	9746	166
H28B8148	5193	10742	166
H28C9591	5956	11099	166
H29A3905	6225	11514	113
H29B3556	7126	11044	113

4

Crystal Data. $C_{56}H_{46}CdCl_4N_8O_6S_2$, M_r = 1245.34, monoclinic, $P2_1/n$ (No. 14), a = 9.2922(9) Å, b = 22.5731(13) Å, c = 13.4673(12) Å, b = 93.281(7)°, a = g = 90°, V = 2820.2(4) Å^3, T = 298(2) K, Z = 2, Z' = 0.5, m(MoK_α) = 0.708, 35509 reflections measured, 5004 unique (R_{int} = 0.1080) which were used in all calculations. The final wR_2 was 0.1355 (all data) and R_1 was 0.0495 (I > 2(I)).

Compound	**4**
Formula	$C_{56}H_{46}CdCl_4N_8O_6S_2$
$D_{calc.}$/ g cm^{-3}	1.467
m/mm^{-1}	0.708
Formula Weight	1245.34
Colour	colorless

Shape	plate
Size/mm^3	0.20×0.17×0.10
T/K	250(2)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	9.2922(9)
b/Å	22.5731(13)
c/Å	13.4673(12)
a/°	90
b/°	93.281(7)
g/°	90
V/Å^3	2820.2(4)
Z	2
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK_α
Q_{min}/°	1.763
Q_{max}/°	25.192
Measured Refl.	35509
Independent Refl.	5004
Reflections Used	2106
R_{int}	0.1080
Parameters	351
Restraints	42
Largest Peak	0.732
Deepest Hole	-0.634
GooF	0.804
wR_2 (all data)	0.1355
wR_2	0.1171
R_1 (all data)	0.1248
R_1	0.0495

Table 23: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	y	z	U_{eq}
Cd110000	5000	10000	40.2(2)
S18654.7(16)	4970.7(13)	7402.9(10)	56.1(4)
N212182(7)	6590(3)	8884(5)	46.2(16)
O18747(5)	5031(3)	8468(3)	67.7(11)
N111474(6)	5776(3)	9610(5)	48.0(17)
N413421(6)	9261(3)	5459(5)	52.0(17)
N312686(7)	8438(3)	6128(5)	52.8(18)
O38888(7)	4358(3)	7140(5)	107(2)
C1112562(9)	7956(4)	6842(6)	52(2)
C311438(9)	6088(3)	8790(6)	53(2)
C513531(8)	7104(3)	7680(6)	43.8(19)
C212689(8)	6607(3)	9854(7)	55(2)
C412304(8)	7041(3)	8171(6)	46(2)
C1813503(7)	8942(3)	6278(6)	47(2)
C1013683(9)	7574(4)	6982(6)	53(2)
C112268(8)	6112(3)	10299(6)	53(2)
C1211244(8)	7934(4)	7340(6)	52(2)
C1711142(9)	7440(3)	8031(6)	50(2)

C2012522(9)	8967(4)	4792(6)	63(2)
C1912033(9)	8456(4)	5173(6)	65(2)
O29501(8)	5382(4)	6939(5)	142(3)
C914969(9)	7613(4)	6479(6)	66(3)
C256880(8)	5127(4)	7019(5)	75(3)
C614703(9)	6716(3)	7839(6)	57(2)
C169846(9)	7409(4)	8562(6)	67(3)
C816058(10)	7234(4)	6644(7)	78(3)
C1310102(9)	8357(4)	7233(7)	67(3)
C148989(10)	8309(4)	7788(8)	83(3)
C715965(10)	6769(4)	7380(7)	77(3)
C245748(8)	5011(5)	7573(6)	85(2)
C158810(10)	7826(5)	8432(8)	88(3)
C266620(10)	5413(5)	6102(7)	119(4)
C234336(11)	5133(5)	7235(10)	120(4)
C275252(13)	5576(7)	5773(9)	147(5)
C224112(12)	5433(6)	6332(10)	128(4)
C212586(12)	5641(8)	5942(11)	208(8)
Cl110209(6)	6924.3(17)	5301(5)	240(3)
Cl28021(4)	6366(2)	4220(3)	196(2)
C289725(12)	6270(5)	4836(9)	130(4)

Table 24: Anisotropic Displacement Parameters ($\times 10^4$) **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cd156.9(3)	25.0(3)	39.6(3)	-0.7(5)	10.0(2)	-1.4(5)	
S169.2(9)	57.5(9)	41.2(7)	3.1(14)	0.5(6)	-10.1(15)	
N266(4)	34(4)	37(4)	12(3)	-6(3)	-11(3)	
O195(3)	69(3)	38(2)	-7(4)	-4.6(18)	12(4)	
N168(4)	34(4)	42(4)	7(3)	6(3)	-5(3)	
N460(4)	38(4)	58(5)	7(4)	3(3)	-14(3)	
N363(4)	47(4)	48(5)	13(3)	-3(3)	-14(3)	
O3117(5)	89(5)	112(5)	-53(4)	-28(4)	38(4)	
C1163(5)	44(5)	47(6)	16(4)	-9(4)	-17(4)	
C389(6)	35(5)	33(5)	2(4)	-2(4)	-7(4)	
C555(5)	28(4)	48(5)	7(3)	0(4)	0(3)	
C263(5)	39(4)	62(6)	7(4)	-3(4)	-13(4)	
C461(5)	31(5)	46(6)	10(4)	4(4)	-11(4)	
C1848(4)	39(5)	56(6)	10(4)	5(4)	-20(4)	
C1055(5)	55(6)	49(6)	3(4)	7(4)	-15(4)	
C171(5)	40(4)	47(5)	5(4)	-6(4)	-13(4)	
C1256(5)	46(5)	53(6)	15(4)	-1(4)	-11(4)	
C1763(5)	42(5)	43(5)	15(4)	-2(4)	-9(4)	
C2079(6)	63(6)	45(5)	19(4)	-14(4)	-21(4)	
C1985(6)	64(6)	44(5)	19(4)	-24(4)	-26(5)	
O2139(6)	194(8)	89(5)	72(5)	-15(4)	-99(5)	
C979(6)	49(5)	71(7)	18(4)	11(5)	5(5)	
C2576(4)	90(8)	59(4)	-3(4)	-4(3)	-5(4)	
C668(5)	46(5)	56(5)	15(4)	8(4)	-4(4)	
C1661(6)	75(7)	66(6)	27(5)	18(5)	-17(5)	
C886(7)	68(6)	85(7)	32(5)	38(5)	4(5)	
C1363(5)	54(5)	85(7)	27(4)	11(5)	8(4)	
C1474(6)	82(7)	94(7)	36(6)	21(5)	20(5)	
C783(6)	69(6)	80(7)	15(5)	8(5)	7(5)	

C2484(5)	60(4)	113(6)	-6(7)	12(4)	-12(7)
C1559(6)	106(9)	100(8)	29(7)	11(5)	15(6)
C2688(6)	186(11)	84(7)	26(7)	-4(5)	25(7)
C2393(7)	127(11)	141(9)	-11(8)	11(6)	12(7)
C27112(8)	225(14)	100(8)	11(9)	-14(7)	52(9)
C2283(7)	180(11)	120(9)	-39(9)	-11(7)	28(7)
C21108(9)	330(20)	180(14)	-69(14)	-34(9)	71(12)
Cl1256(5)	101(2)	369(9)	-47(4)	88(5)	-35(3)
Cl2158(3)	266(5)	164(3)	112(3)	-3(2)	64(3)
C28144(10)	96(7)	148(11)	-11(8)	-2(8)	25(8)

Table 25: Bond Lengths in Å for **4**.

AtomAtom	**Length/Å**
Cd1O1[1]	2.312(4)
Cd1O1	2.312(4)
Cd1N1	2.303(6)
Cd1N1[1]	2.303(6)
Cd1N4[2]	2.328(6)
Cd1N4[3]	2.328(6)
S1O1	1.438(4)
S1O3	1.447(6)
S1O2	1.389(6)
S1C25	1.736(8)
N2C3	1.330(8)
N2C2	1.363(9)
N2C4	1.410(8)
N1C3	1.307(9)
N1C1	1.379(8)
N4Cd1[4]	2.328(6)
N4C18	1.316(9)
N4C20	1.363(9)
N3C11	1.461(9)
N3C18	1.375(8)
N3C19	1.392(9)
C11C10	1.358(10)
C11C12	1.430(10)
C5C4	1.357(9)
C5C10	1.430(10)
C5C6	1.405(9)
C2C1	1.337(9)
C4C17	1.410(10)
C10C9	1.409(10)
C12C17	1.459(9)
C12C13	1.429(10)
C17C16	1.437(10)
C20C19	1.350(10)
C9C8	1.334(11)
C25C24	1.350(10)
C25C26	1.401(11)
C6C7	1.362(11)
C16C15	1.351(11)
C8C7	1.449(11)
C13C14	1.315(11)
C14C15	1.408(12)

C24C23	1.391(12)
C26C27	1.373(13)
C23C22	1.398(15)
C27C22	1.373(16)
C22C21	1.556(14)
Cl1C28	1.657(11)
Cl2C28	1.759(11)

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[1]2-X,1-Y,2-Z; [2]-1/2+X,3/2-Y,1/2+Z; [3]5/2-X,-1/2+Y,3/2-Z; [4]5/2-X,1/2+Y,3/2-Z

Table 26: Bond Angles in ° for **4**.

AtomAtom	**Atom**	**Angle/°**
O1Cd1	O1[1]	180.0(2)
O1Cd1	N4[2]	85.5(2)
O1[1]Cd1	N4[2]	94.5(2)
O1Cd1	N4[3]	94.5(2)
O1[1]Cd1	N4[3]	85.5(2)
N1[1]Cd1	O1	87.2(2)
N1[1]Cd1	O1[1]	92.8(2)
N1Cd1	O1[1]	87.2(2)
N1Cd1	O1	92.8(2)
N1[1]Cd1	N1	180.0(3)
N1Cd1	N4[3]	95.34(16)
N1Cd1	N4[2]	84.66(16)
N1[1]Cd1	N4[3]	84.67(16)
N1[1]Cd1	N4[2]	95.33(16)
N4[2]Cd1	N4[3]	180.0
O1S1	O3	109.5(4)
O1S1	C25	106.2(3)
O3S1	C25	105.9(4)
O2S1	O1	112.5(4)
O2S1	O3	115.6(5)
O2S1	C25	106.4(4)
C3N2	C2	105.3(6)
C3N2	C4	127.8(7)
C2N2	C4	126.6(6)
S1O1	Cd1	152.3(3)
C3N1	Cd1	127.9(6)
C3N1	C1	105.1(7)
C1N1	Cd1	124.5(5)
C18N4	Cd1[4]	127.5(5)
C18N4	C20	106.8(7)
C20N4	Cd1[4]	123.1(6)
C18N3	C11	125.7(7)
C18N3	C19	108.6(6)
C19N3	C11	125.7(7)
C10C11	N3	118.4(8)
C10C11	C12	125.8(8)
C12C11	N3	115.9(7)
N1C3	N2	112.9(7)
C4C5	C10	121.0(8)
C4C5	C6	121.7(7)
C6C5	C10	117.3(8)
C1C2	N2	108.2(7)

C5C4	N2	120.7(7)
C5C4	C17	121.7(7)
C17C4	N2	117.5(7)
N4C18	N3	109.0(7)
C11C10	C5	117.3(8)
C11C10	C9	124.0(8)
C9C10	C5	118.8(8)
C2C1	N1	108.4(7)
C11C12	C17	114.5(8)
C13C12	C11	125.5(8)
C13C12	C17	120.0(8)
C4C17	C12	119.7(8)
C4C17	C16	124.0(7)
C16C17	C12	116.2(8)
C19C20	N4	111.9(8)
C20C19	N3	103.7(7)
C8C9	C10	122.4(8)
C24C25	S1	123.6(6)
C24C25	C26	118.4(8)
C26C25	S1	118.0(6)
C7C6	C5	123.7(8)
C15C16	C17	120.9(9)
C9C8	C7	120.3(8)
C14C13	C12	119.5(8)
C13C14	C15	122.6(9)
C6C7	C8	117.5(8)
C25C24	C23	122.1(9)
C16C15	C14	120.7(9)
C27C26	C25	121.2(10)
C24C23	C22	118.1(10)
C26C27	C22	119.3(12)
C23C22	C21	121.9(12)
C27C22	C23	120.7(10)
C27C22	C21	117.4(13)
Cl1C28	Cl2	106.6(6)

[1]2-X,1-Y,2-Z; [2]-1/2+X,3/2-Y,1/2+Z; [3]5/2-X,-1/2+Y,3/2-Z; [4]5/2-X,1/2+Y,3/2-Z

Table 27: Torsion Angles in ° for **4**.

AtomAtom	**Atom**	**Atom**	**Angle/°**
Cd1N1	C3	N2	164.5(5)
Cd1N1	C1	C2	-164.2(5)
Cd1[1]N4	C18	N3	-160.2(5)
Cd1[1]N4	C20	C19	162.1(6)
S1C25	C24	C23	-178.9(8)
S1C25	C26	C27	-176.8(11)
N2C2	C1	N1	-0.5(9)
N2C4	C17	C12	176.8(7)
N2C4	C17	C16	-0.6(11)
O1S1	C25	C24	-31.4(9)
O1S1	C25	C26	145.8(8)
N4C20	C19	N3	-0.5(10)
N3C11	C10	C5	-179.6(7)
N3C11	C10	C9	0.0(12)
N3C11	C12	C17	178.7(7)

N3C11	C12	C13	-3.5(12)
O3S1	O1	Cd1	65.6(10)
O3S1	C25	C24	85.0(9)
O3S1	C25	C26	-97.8(8)
C11N3	C18	N4	176.5(7)
C11N3	C19	C20	-176.9(8)
C11C10	C9	C8	179.2(9)
C11C12	C17	C4	1.2(10)
C11C12	C17	C16	178.8(7)
C11C12	C13	C14	-175.1(9)
C3N2	C2	C1	1.6(9)
C3N2	C4	C5	-105.0(10)
C3N2	C4	C17	78.4(10)
C3N1	C1	C2	-0.8(9)
C5C4	C17	C12	0.2(11)
C5C4	C17	C16	-177.2(8)
C5C10	C9	C8	-1.1(13)
C5C6	C7	C8	-3.7(14)
C2N2	C3	N1	-2.2(9)
C2N2	C4	C5	82.2(10)
C2N2	C4	C17	-94.4(10)
C4N2	C3	N1	-176.2(7)
C4N2	C2	C1	175.7(7)
C4C5	C10	C11	0.8(11)
C4C5	C10	C9	-178.9(8)
C4C5	C6	C7	-178.5(8)
C4C17	C16	C15	176.2(9)
C18N4	C20	C19	-0.6(10)
C18N3	C11	C10	-75.0(10)
C18N3	C11	C12	104.7(9)
C18N3	C19	C20	1.3(9)
C10C11	C12	C17	-1.7(12)
C10C11	C12	C13	176.2(8)
C10C5	C4	N2	-177.7(7)
C10C5	C4	C17	-1.2(11)
C10C5	C6	C7	0.9(12)
C10C9	C8	C7	-1.7(15)
C1N1	C3	N2	1.9(9)
C12C11	C10	C5	0.7(12)
C12C11	C10	C9	-179.6(8)
C12C17	C16	C15	-1.3(13)
C12C13	C14	C15	-5.5(16)
C17C12	C13	C14	2.6(13)
C17C16	C15	C14	-1.4(15)
C20N4	C18	N3	1.4(9)
C19N3	C11	C10	103.0(10)
C19N3	C11	C12	-77.4(11)
C19N3	C18	N4	-1.8(9)
O2S1	O1	Cd1	-64.4(11)
O2S1	C25	C24	-151.5(8)
O2S1	C25	C26	25.7(9)
C9C8	C7	C6	4.1(15)
C25S1	O1	Cd1	179.6(8)
C25C24	C23	C22	-5.8(17)
C25C26	C27	C22	-3(2)

C6C5	C4	N2	1.8(12)
C6C5	C4	C17	178.3(7)
C6C5	C10	C11	-178.7(7)
C6C5	C10	C9	1.6(11)
C13C12	C17	C4	-176.8(7)
C13C12	C17	C16	0.8(11)
C13C14	C15	C16	5.1(17)
C24C25	C26	C27	0.5(17)
C24C23	C22	C27	3.2(19)
C24C23	C22	C21	-174.2(11)
C26C25	C24	C23	3.9(15)
C26C27	C22	C23	1(2)
C26C27	C22	C21	178.5(13)

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[1]5/2-X,1/2+Y,3/2-Z

Table 28: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atomx	y	z	U_{eq}
H310944.61	5970.16	8203	63
H213233.17	6910.06	10153.84	66
H1814027.15	9040.65	6863.36	57
H112476.09	6010.68	10961.47	64
H2012275.97	9101.38	4152.42	76
H1911406.08	8181.74	4867.98	78
H915061.97	7914.76	6016.22	79
H614612.43	6404.91	8284	68
H169719.53	7098.31	9000.73	80
H816879.12	7267.82	6284.43	94
H1310144.45	8663.7	6774.21	81
H148292.31	8605.19	7754.06	99
H716737.87	6517.31	7532.73	93
H245916.83	4843.82	8200.05	103
H157969.27	7794.21	8770.89	106
H267388.71	5493.36	5710.17	143
H233563.76	5018.05	7600.5	144
H275099.07	5781.39	5177.23	176
H21A1866.95	5429.58	6283.87	312
H21B2461.26	5563.84	5241.14	312
H21C2487.58	6058.24	6059.49	312
H28A9673.95	5979.59	5364.44	156
H28B10417.4	6133.77	4374.14	156

5

Crystal Data for $C_{64}H_{66}CdN_8O_{12}S_2$ (M =1315.76 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 10.6432(3) Å, b = 13.3880(4) Å, c = 21.5624(6) Å, β = 91.374(2)°, V = 3071.57(15) Å^3, Z = 2, T = 200 K, μ(MoKα) = 0.493 mm^{-1}, *Dcalc* = 1.423 g/cm^3, 37774 reflections measured (3.582° ≤ 2Θ ≤ 50.336°), 5455 unique (R_{int} = 0.0342, R_{sigma} = 0.0173) which were used in all calculations. The final R_1 was 0.0583 (I > 2σ(I)) and wR_2 was 0.1533 (all data).

Identification code	sv-2-33
Empirical formula	$C_{64}H_{66}CdN_8O_{12}S_2$
Formula weight	1315.76
Temperature/K	200
Crystal system	monoclinic

Space group	$P2_1/n$
a/Å	10.6432(3)
b/Å	13.3880(4)
c/Å	21.5624(6)
α/°	90
β/°	91.374(2)
γ/°	90
Volume/Å^3	3071.57(15)
Z	2
ϱ_{calc}g/cm^3	1.423
μ/mm^{-1}	0.493
F(000)	1364.0
Crystal size/mm^3	0.53 × 0.3 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.582 to 50.336
Index ranges	$-12 \le h \le 12$, $-15 \le k \le 15$, $-25 \le l \le 25$
Reflections collected	37774
Independent reflections	5455 [R_{int} = 0.0342, R_{sigma} = 0.0173]
Data/restraints/parameters	5455/1/354
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0583, wR_2 = 0.1458
Final R indexes [all data]	R_1 = 0.0692, wR_2 = 0.1533
Largest diff. peak/hole / e Å^{-3}	1.91/-1.42

Table30. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cd1	5000	0	5000	30.87(15)
S1	6713.7(15)	1738.0(14)	4080.2(7)	68.7(4)
O1	6083(4)	1323(3)	4605.0(17)	62.6(10)
O2	7983(4)	1373(7)	4045(3)	136(3)
O3	5984(4)	1625(4)	3509(2)	82.5(14)
N1	4562(3)	991(3)	5849.6(16)	35.8(8)
N2	8135(3)	4484(3)	9505.4(15)	35.1(8)
N3	4827(3)	1884(3)	6696.9(16)	35.9(8)
N4	6839(3)	3784(3)	8830.6(16)	34.7(8)
C1	5367(4)	1277(3)	6284(2)	39.4(10)
C2	3442(4)	1442(4)	5992(2)	43.7(11)
C3	3599(4)	2000(4)	6509(2)	47.9(12)
C4	5410(4)	2341(3)	7233.7(19)	33.7(9)
C5	5861(4)	3317(3)	7175.2(19)	33.6(9)
C6	5839(4)	3844(4)	6606(2)	42.4(11)
C7	6270(5)	4795(4)	6574(2)	48.6(12)
C8	6734(5)	5283(4)	7113(2)	47.3(12)
C9	6772(4)	4812(3)	7665(2)	40.6(10)
C10	6357(4)	3805(3)	7721.1(19)	34.1(9)
C11	6375(4)	3279(3)	8278.9(19)	33.6(9)
C12	5950(4)	2303(3)	8335(2)	35.4(9)
C13	5993(5)	1761(4)	8903(2)	45.9(11)
C14	5563(5)	812(4)	8932(3)	54.8(13)
C15	5049(5)	334(4)	8396(3)	50.6(12)
C16	4989(4)	816(3)	7848(2)	43.3(11)
C17	5442(4)	1817(3)	7790(2)	35.4(9)
C18	8052(4)	3935(3)	9000.4(19)	34.9(9)
C19	6107(4)	4267(4)	9253.6(19)	38.7(10)
C20	6918(4)	4696(4)	9667(2)	38.4(10)
C24A	7058(11)	4578(11)	3844(5)	68.7(4)
C25A	6845(11)	3600(11)	3716(6)	68.7(4)
C26A	7334(11)	3206(11)	4760(5)	68.7(4)

C27A	7594(11)	4197(11)	4872(6)	68.7(4)
C28A	7710(12)	5973(10)	4532(5)	68.7(4)
C24B	7472(4)	3872(4)	4106(2)	68.7(4)
C23	7330(5)	4840(3)	4326(2)	68.7(4)
C27B	6388(6)	5056(4)	4742(3)	68.7(4)
C26B	5589(5)	4303(5)	4936(3)	68.7(4)
C25B	5731(5)	3335(4)	4716(3)	68.7(4)
C22	6672(5)	3120(3)	4300(2)	68.7(4)
C28B	6236(11)	6230(10)	4933(5)	68.7(4)
O4	7541(9)	1056(5)	2487(4)	147(3)
C21	8236(9)	204(7)	2681(7)	142(5)
O5A	5413(9)	2097(7)	957(5)	77.0(15)
O6A	3175(10)	2959(8)	1370(6)	77.0(15)
C29A	4586(12)	2578(11)	559(7)	77.0(15)
C30A	3280(13)	2524(12)	766(7)	77.0(15)
C31A	4017(14)	2462(12)	1797(7)	77.0(15)
C32A	5426(16)	2511(15)	1573(9)	77.0(15)
O5B	5702(11)	2351(9)	1419(7)	82.8(18)
O6B	3259(10)	2984(8)	1767(6)	82.8(18)
C29B	4979(13)	3017(11)	1071(8)	82.8(18)
C30B	3582(16)	2879(13)	1178(10)	82.8(18)
C31B	3984(14)	2359(12)	2164(9)	82.8(18)
C32B	5330(13)	2558(11)	2069(8)	82.8(18)

Table 31 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for sv-2-33. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cd1	33.6(2)	37.4(3)	21.2(2)	-2.55(17)	-8.35(15)	1.67(18)
S1	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
O1	85(3)	50(2)	54(2)	7.7(17)	17(2)	-16(2)
O2	44(3)	270(9)	93(4)	20(5)	4(3)	7(4)
O3	79(3)	112(4)	55(2)	19(2)	-20(2)	-18(3)
N1	36.9(19)	41(2)	28.8(18)	-6.5(15)	-5.8(15)	-1.1(16)
N2	35.4(19)	43(2)	26.7(17)	-1.2(15)	-9.0(14)	-1.3(16)
N3	32.1(18)	43(2)	32.6(18)	-9.6(15)	-4.0(15)	-0.2(16)
N4	34.1(18)	41(2)	28.1(17)	-7.5(15)	-5.7(14)	0.7(15)
C1	38(2)	46(3)	35(2)	-10.8(19)	-5.7(18)	5(2)
C2	32(2)	55(3)	44(3)	-15(2)	-7.2(19)	0(2)
C3	29(2)	60(3)	55(3)	-22(2)	-2(2)	3(2)
C4	30(2)	41(2)	31(2)	-10.4(18)	-3.9(16)	1.0(17)
C5	29(2)	42(2)	30(2)	-6.3(18)	-1.3(16)	2.2(18)
C6	43(2)	53(3)	31(2)	-4(2)	-5.9(19)	-5(2)
C7	54(3)	54(3)	38(2)	7(2)	-5(2)	-8(2)
C8	48(3)	43(3)	51(3)	2(2)	-2(2)	-10(2)
C9	39(2)	44(3)	39(2)	-5.6(19)	-5.9(19)	-5.8(19)
C10	31(2)	39(2)	32(2)	-6.6(18)	-3.7(17)	0.0(17)
C11	31(2)	40(2)	29(2)	-8.8(18)	-5.5(16)	-0.2(18)
C12	33(2)	40(2)	33(2)	-2.8(18)	-1.1(17)	2.9(18)
C13	53(3)	51(3)	34(2)	-1(2)	-3(2)	3(2)
C14	68(3)	50(3)	47(3)	8(2)	4(2)	1(3)
C15	57(3)	37(2)	58(3)	0(2)	9(2)	-4(2)
C16	43(3)	40(2)	47(3)	-9(2)	3(2)	-1(2)
C17	31(2)	38(2)	37(2)	-6.4(18)	-0.5(17)	1.3(18)
C18	34(2)	43(2)	28(2)	-3.2(18)	-5.4(17)	1.8(18)
C19	34(2)	51(3)	32(2)	-6.9(19)	-2.9(17)	4.7(19)

C20	40(2)	49(3)	26(2)	-5.0(18)	-4.0(18)	4(2)
C24A	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C25A	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C26A	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C27A	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C28A	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C24B	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C23	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C27B	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C26B	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C25B	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C22	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
C28B	58.1(8)	96.6(10)	50.8(7)	25.9(7)	-6.6(6)	-21.0(7)
O4	206(8)	101(5)	139(6)	0(4)	87(6)	17(5)
C21	76(6)	76(6)	278(16)	-25(7)	56(8)	-5(4)
O5A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
O6A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
C29A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
C30A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
C31A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
C32A	69(3)	82(3)	80(4)	10(3)	5(3)	16(3)
O5B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)
O6B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)
C29B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)
C30B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)
C31B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)
C32B	66(3)	71(3)	111(5)	2(3)	18(3)	-1(2)

Table 32 Bond Lengths for 5.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Cd1	O1[1]	2.289(3)		C13	C14	1.352(7)
Cd1	O1	2.289(3)		C14	C15	1.419(8)
Cd1	N1	2.318(3)		C15	C16	1.346(7)
Cd1	N1[1]	2.318(3)		C16	C17	1.430(6)
Cd1	N2[2]	2.335(3)		C19	C20	1.355(6)
Cd1	N2[3]	2.335(3)		C24A	C25A	1.356(19)
S1	O1	1.441(4)		C24A	C23	1.128(13)
S1	O2	1.440(6)		C25A	C22	1.430(12)
S1	O3	1.447(4)		C26A	C27A	1.376(19)
S1	C22	1.911(5)		C26A	C22	1.207(12)
N1	C1	1.312(5)		C27A	C23	1.479(12)
N1	C2	1.378(6)		C28A	C23	1.628(14)
N2	C18	1.315(5)		C24B	C23	1.3900
N2	C20	1.379(6)		C24B	C22	1.3900
N3	C1	1.345(6)		C23	C27B	1.3900
N3	C3	1.367(6)		C27B	C26B	1.3900
N3	C4	1.437(5)		C27B	C28B	1.634(15)
N4	C11	1.445(5)		C26B	C25B	1.3900
N4	C18	1.348(5)		C25B	C22	1.3900
N4	C19	1.375(5)		O4	C21	1.417(12)
C2	C3	1.349(6)		O5A	C29A	1.375(16)
C4	C5	1.399(6)		O5A	C32A	1.44(2)
C4	C17	1.389(6)		O6A	C30A	1.435(19)
C5	C6	1.416(6)		O6A	C31A	1.432(18)
C5	C10	1.436(6)		C29A	C30A	1.472(18)

C6	C7	1.356(7)		C31A	C32A	1.59(2)
C7	C8	1.410(7)		O5B	C29B	1.39(2)
C8	C9	1.347(7)		O5B	C32B	1.49(2)
C9	C10	1.424(6)		O6B	C30B	1.33(2)
C10	C11	1.394(6)		O6B	C31B	1.414(19)
C11	C12	1.389(6)		C29B	C30B	1.52(2)
C12	C13	1.423(6)		C31B	C32B	1.476(19)
C12	C17	1.439(6)				

[1]1-X,-Y,1-Z; [2]-1/2+X,1/2-Y,-1/2+Z; [3]3/2-X,-1/2+Y,3/2-Z

Table 33 Bond Angles for 5.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1[1]	Cd1	O1	180.0		C11	C10	C9	123.7(4)
O1[1]	Cd1	N1[1]	87.93(13)		C10	C11	N4	118.1(4)
O1[1]	Cd1	N1	92.07(13)		C12	C11	N4	118.3(4)
O1	Cd1	N1[1]	92.06(13)		C12	C11	C10	123.6(4)
O1	Cd1	N1	87.94(13)		C11	C12	C13	123.4(4)
O1	Cd1	N2[2]	91.78(14)		C11	C12	C17	118.1(4)
O1	Cd1	N2[3]	88.22(14)		C13	C12	C17	118.5(4)
O1[1]	Cd1	N2[3]	91.78(14)		C14	C13	C12	120.9(5)
O1[1]	Cd1	N2[2]	88.22(14)		C13	C14	C15	120.7(5)
N1	Cd1	N1[1]	180.0		C16	C15	C14	120.5(5)
N1[1]	Cd1	N2[2]	89.60(12)		C15	C16	C17	121.2(5)
N1	Cd1	N2[2]	90.40(12)		C4	C17	C12	118.5(4)
N1[1]	Cd1	N2[3]	90.40(12)		C4	C17	C16	123.3(4)
N1	Cd1	N2[3]	89.60(12)		C16	C17	C12	118.2(4)
N2[2]	Cd1	N2[3]	180.00(15)		N2	C18	N4	110.8(4)
O1	S1	O3	112.1(3)		C20	C19	N4	105.9(4)
O1	S1	C22	99.4(2)		C19	C20	N2	109.5(4)
O2	S1	O1	111.5(3)		C23	C24A	C25A	121.7(11)
O2	S1	O3	113.8(4)		C24A	C25A	C22	106.3(11)
O2	S1	C22	111.7(4)		C22	C26A	C27A	110.3(11)
O3	S1	C22	107.3(3)		C26A	C27A	C23	112.9(10)
S1	O1	Cd1	147.0(3)		C23	C24B	C22	120.0
C1	N1	Cd1	126.2(3)		C24A	C23	C27A	126.3(10)
C1	N1	C2	105.4(4)		C24A	C23	C28A	126.6(9)
C2	N1	Cd1	128.3(3)		C27A	C23	C28A	106.5(7)
C18	N2	Cd1[4]	125.7(3)		C27B	C23	C24B	120.0
C18	N2	C20	106.2(3)		C23	C27B	C26B	120.0
C20	N2	Cd1[4]	128.1(3)		C23	C27B	C28B	116.1(5)
C1	N3	C3	107.1(4)		C26B	C27B	C28B	123.8(5)
C1	N3	C4	127.4(4)		C25B	C26B	C27B	120.0
C3	N3	C4	125.5(4)		C26B	C25B	C22	120.0
C18	N4	C11	126.9(4)		C25A	C22	S1	102.3(7)
C18	N4	C19	107.7(3)		C26A	C22	S1	106.3(8)
C19	N4	C11	125.3(4)		C26A	C22	C25A	126.5(8)
N1	C1	N3	111.5(4)		C24B	C22	S1	127.5(3)
C3	C2	N1	109.7(4)		C25B	C22	S1	112.5(3)
C2	C3	N3	106.3(4)		C25B	C22	C24B	120.0
C5	C4	N3	117.9(4)		C29A	O5A	C32A	112.8(11)
C17	C4	N3	118.7(4)		C31A	O6A	C30A	109.5(11)
C17	C4	C5	123.3(4)		O5A	C29A	C30A	112.5(12)
C4	C5	C6	123.0(4)		O6A	C30A	C29A	110.5(14)
C4	C5	C10	118.1(4)		O6A	C31A	C32A	111.5(13)

C6	C5	C10	118.8(4)		O5A	C32A	C31A	106.0(15)
C7	C6	C5	120.9(4)		C29B	O5B	C32B	103.3(11)
C6	C7	C8	120.4(5)		C30B	O6B	C31B	111.4(12)
C9	C8	C7	120.9(5)		O5B	C29B	C30B	111.9(13)
C8	C9	C10	121.0(4)		O6B	C30B	C29B	114.1(16)
C9	C10	C5	118.0(4)		O6B	C31B	C32B	109.0(13)
C11	C10	C5	118.3(4)		C31B	C32B	O5B	112.2(14)

[1]1-X,-Y,1-Z; [2]-1/2+X,1/2-Y,-1/2+Z; [3]3/2-X,-1/2+Y,3/2-Z; [4]3/2-X,1/2+Y,3/2-Z

Table 34 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.

Atom	*x*	*y*	*z*	U(eq)
H1	6206.93	1084.54	6303.79	47
H2	2691.63	1373.2	5766.55	52
H3	2993.67	2385.55	6700.4	58
H6	5524.64	3533.94	6248.59	51
H7	6259.78	5128.33	6195.69	58
H8	7016.37	5938.31	7085.79	57
H9	7074.94	5149.46	8014.7	49
H13	6321.31	2063.71	9259.99	55
H14	5605.78	468.27	9306.28	66
H15	4750.63	-316.73	8423.02	61
H16	4647.73	492.66	7501.41	52
H18	8735.4	3685.36	8789.22	42
H19	5233.49	4292.61	9255.46	46
H20	6690.1	5075.86	10007.53	46
H24A	6977.25	5045.14	3526.31	82
H25A	6816.46	3301.78	3326.91	82
H26A	7625.18	2677.57	5003.71	82
H27A	7904.56	4437.3	5249.85	82
H28A	7709.51	6395.31	4171.94	103
H28B	8533.66	5970.95	4723.7	103
H28C	7112.69	6220.32	4820.65	103
H24B	8101.29	3727.91	3827.75	82
H23	7864.48	5343.57	4196	82
H26B	4959.32	4447.48	5214.36	82
H25B	5196.11	2831.81	4846.12	82
H28D	6783.18	6377.9	5280.64	103
H28E	5380.95	6357.38	5041.23	103
H28F	6452.57	6643.92	4587.75	103
H4	7026.11	1196.41	2749.77	221
H21A	8777.88	-2.67	2355.61	214
H21B	7667.99	-328.89	2775.61	214
H21C	8733.86	365.9	3044.84	214
H29A	4635.66	2280.74	150.14	92
H29B	4831.1	3273.84	525.6	92
H30A	2733.95	2876.85	473.34	92
H30B	3012.93	1831.81	777.51	92
H31A	3765.32	1768.54	1835.79	92
H31B	3964.22	2771.25	2201.97	92
H32A	5720.75	3196.8	1568.14	92
H32B	5974.1	2125.66	1847.8	92
H29C	5141.92	2921.4	634.49	99
H29D	5219.29	3694.19	1180.94	99
H30C	3118.14	3362.12	927.38	99

H30D	3335.42	2218.22	1037	99
H31C	3797.97	1664.12	2073.26	99
H31D	3780.75	2488.45	2592.43	99
H32C	5828.61	2145.67	2350.38	99
H32D	5508.08	3251.76	2166.74	99

Table 35 Atomic Occupancy for 5.

Atom	*Occupancy*		Atom	*Occupancy*		Atom	*Occupancy*
C24A	0.500(4)		H24A	0.500(4)		C25A	0.500(4)
H25A	0.500(4)		C26A	0.500(4)		H26A	0.500(4)
C27A	0.500(4)		H27A	0.500(4)		C28A	0.500(4)
H28A	0.500(4)		H28B	0.500(4)		H28C	0.500(4)
C24B	0.500(4)		H24B	0.500(4)		H23	0.500(4)
C27B	0.500(4)		C26B	0.500(4)		H26B	0.500(4)
C25B	0.500(4)		H25B	0.500(4)		C28B	0.500(4)
H28D	0.500(4)		H28E	0.500(4)		H28F	0.500(4)
O5A	0.500(4)		O6A	0.500(4)		C29A	0.500(4)
H29A	0.500(4)		H29B	0.500(4)		C30A	0.500(4)
H30A	0.500(4)		H30B	0.500(4)		C31A	0.500(4)
H31A	0.500(4)		H31B	0.500(4)		C32A	0.500(4)
H32A	0.500(4)		H32B	0.500(4)		O5B	0.500(4)
O6B	0.500(4)		C29B	0.500(4)		H29C	0.500(4)
H29D	0.500(4)		C30B	0.500(4)		H30C	0.500(4)
H30D	0.500(4)		C31B	0.500(4)		H31C	0.500(4)
H31D	0.500(4)		C32B	0.500(4)		H32C	0.500(4)
H32D	0.500(4)						

6

Crystal Data for $C_{52}H_{44}F_6N_8O_8Zn$ (M =1088.32 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 13.6068(5) Å, b = 18.0054(5) Å, c = 20.3919(7) Å, β = 96.256(3)°, V = 4966.2(3) Å^3, Z = 4, T = 200(2) K, μ(MoKα) = 0.581 mm^{-1}, *Dcalc* = 1.456 g/cm^3, 8867 reflections measured (3.026° ≤ 2Θ ≤ 50.688°), 8867 unique (R_{sigma} = 0.0658) which were used in all calculations. The final R_1 was 0.0838 (I > 2σ(I)) and wR_2 was 0.1664 (all data).

Table 36 Crystal data and structure refinement for 6.

Identification code	6
Empirical formula	$C_{52}H_{44}F_6N_8O_8Zn$
Formula weight	1088.32
Temperature/K	200(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.6068(5)
b/Å	18.0054(5)
c/Å	20.3919(7)
α/°	90
β/°	96.256(3)
γ/°	90
Volume/Å^3	4966.2(3)
Z	4
ϱ_{calc}g/cm^3	1.456
μ/mm^{-1}	0.581
F(000)	2240.0
Crystal size/mm^3	0.52 × 0.253 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.026 to 50.688
Index ranges	-16 ≤ h ≤ 16, -21 ≤ k ≤ 21, -3 ≤ l ≤ 24

Reflections collected	8867
Independent reflections	8867 [R_{int} = ?, R_{sigma} = 0.0658]
Data/restraints/parameters	8867/105/714
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0838, wR_2 = 0.1493
Final R indexes [all data]	R_1 = 0.1085, wR_2 = 0.1664
Largest diff. peak/hole / e $Å^{-3}$	0.82/-0.92

Table 37 Fractional Atomic Coordinates ($\times10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2\times10^3$) for 6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Zn1	4941.3(4)	2366.8(3)	2597.7(2)	31.69(15)
F1	7702(4)	597(3)	3182(2)	105.4(17)
F2	8477(3)	861(3)	2373(3)	100.1(15)
F3	7020(4)	463(2)	2209(2)	94.8(15)
O1	6302(3)	1744(2)	2597.2(18)	47.1(9)
O2	3555(3)	2989(2)	2625.4(19)	50.6(9)
O3	7827(4)	2197(3)	2676(4)	121(3)
N1	4385(3)	1608(2)	1860.2(19)	35.4(9)
N2	4444(3)	1623(2)	3321.3(19)	37.4(9)
N3	5538(3)	3118(2)	3326.2(19)	35.2(9)
N4	338(3)	1838(2)	6874.5(19)	35.9(9)
N5	4343(3)	792(2)	1059(2)	38.8(10)
N6	3609(3)	1158(2)	4090(2)	39.6(10)
N7	5638(3)	3997(2)	4075(2)	39(1)
N8	1084(3)	1287(2)	6104(2)	39.8(10)
C1	4901(4)	1269(3)	1441(2)	37.8(11)
C2	3410(4)	826(4)	1256(3)	62.9(19)
C3	3443(4)	1334(3)	1744(3)	53.7(16)
C4	4666(4)	378(3)	519(2)	38.5(11)
C5	4553(4)	712(3)	-104(2)	38.1(11)
C6	4122(4)	1428(3)	-224(3)	49.0(14)
C7	4036(5)	1724(3)	-833(3)	58.6(16)
C8	4363(5)	1333(4)	-1371(3)	61.7(16)
C9	4783(5)	651(3)	-1279(3)	52.0(14)
C10	4902(4)	314(3)	-648(2)	39.0(11)
C11	3814(4)	1771(3)	3749(2)	42.7(13)
C12	4643(4)	877(3)	3388(3)	41.7(12)
C13	4129(4)	586(3)	3860(3)	46.5(13)
C14	2960(4)	1137(3)	4603(2)	37.7(11)
C15	1946(4)	1160(3)	4422(2)	40.8(12)
C16	1508(5)	1171(4)	3756(3)	55.3(15)
C17	518(5)	1246(4)	3601(3)	63.2(18)
C18	-114(5)	1300(4)	4107(3)	58.3(16)
C19	264(4)	1273(3)	4751(3)	51.7(14)
C20	1294(4)	1198(3)	4935(2)	43.3(12)
C21	1720(4)	1193(3)	5592(3)	40.9(12)
C22	2735(4)	1151(3)	5770(2)	42.5(13)
C23	3169(5)	1154(3)	6439(3)	50.1(14)
C24	4158(5)	1173(4)	6588(3)	66.8(18)
C25	4804(5)	1185(4)	6082(3)	59.3(16)
C26	4426(4)	1154(3)	5442(3)	51.6(14)
C27	3386(4)	1134(3)	5257(3)	41.9(12)

C28	955(4)	1929(3)	6427(2)	37.6(11)
C29	64(4)	1103(3)	6839(3)	43.7(13)
C30	525(4)	756(3)	6372(3)	47.1(13)
C31	5032(4)	3519(3)	3719(2)	34.9(11)
C32	6501(4)	3351(3)	3442(3)	44.4(13)
C33	6569(4)	3895(3)	3898(3)	54.2(15)
C34	4864(4)	5170(3)	4316(2)	37.1(11)
C35	5321(4)	4513(3)	4549(2)	36.9(11)
C36	5474(4)	4324(3)	5212(2)	39.3(11)
C37	5911(5)	3638(3)	5447(3)	50.8(14)
C38	6015(5)	3469(3)	6099(3)	57.4(16)
C39	5705(5)	3985(3)	6567(3)	54.1(14)
C40	5292(4)	4632(3)	6367(3)	47.9(13)
C41	2661(4)	3062(4)	2510(3)	63.6(17)
C42	2242(6)	3769(6)	2713(4)	95(2)
C43	7206(4)	1694(3)	2630(3)	52.2(14)
C44	7592(5)	907(4)	2590(3)	59.5(16)
F4A	2818(8)	4386(5)	2568(8)	159(5)
F5A	1400(20)	4066(14)	2435(11)	107(7)
F6A	2000(20)	3480(20)	3351(10)	180(9)
O4B	2075(6)	2493(8)	2396(9)	140(7)
F4B	2496(11)	4008(7)	3280(6)	136(5)
F5B	1920(20)	4025(18)	2152(11)	177(8)
F6B	1314(11)	3762(13)	2685(11)	188(7)
O4A	2149(18)	2897(10)	1963(9)	95(7)
O5	1896(3)	4319(2)	317(2)	61.8(11)
O6	2884(4)	3044(3)	-52(3)	81.4(15)
C49	2837(6)	3224(4)	612(4)	79(2)
C50	2745(5)	4043(4)	701(3)	65.7(18)
C51	1959(6)	4138(4)	-353(3)	63.8(17)
C52	2027(6)	3323(4)	-446(4)	74(2)
O7	3269(4)	3580(4)	4808(3)	108(2)
O8	2237(4)	3487(3)	5921(3)	98.5(19)
C45	3152(6)	3140(4)	5901(4)	82(2)
C46	3292(7)	2956(5)	5199(4)	92(3)
C47	2382(8)	3976(6)	4849(5)	128(5)
C48	2288(8)	4154(5)	5569(5)	119(4)

Table 38 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for sv-2-rem_tw. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Zn1	34.6(3)	31.7(3)	30.3(3)	-6.3(2)	10.0(2)	-5.2(2)
F1	135(5)	105(4)	75(3)	21(2)	4(3)	45(3)
F2	68(3)	106(4)	132(4)	-17(3)	33(3)	34(3)
F3	96(3)	59(2)	121(4)	-36(2)	-30(3)	15(2)
O1	34(2)	55(2)	51(2)	-11.3(18)	4.4(17)	9.0(17)
O2	36(2)	57(2)	61(2)	-6.9(19)	11.5(18)	6.2(17)
O3	53(3)	87(4)	231(8)	-78(5)	47(4)	-28(3)
N1	36(2)	38(2)	34(2)	-9.9(17)	11.2(17)	-3.1(18)
N2	44(3)	33(2)	38(2)	-4.3(17)	16.4(19)	-6.5(19)
N3	37(2)	33(2)	37(2)	-6.5(17)	9.1(17)	-0.6(18)
N4	35(2)	38(2)	37(2)	2.2(17)	11.8(18)	3.7(18)
N5	32(2)	43(2)	42(2)	-24.3(19)	7.8(18)	-1.6(19)
N6	42(2)	39(2)	41(2)	0.6(18)	20(2)	-1(2)
N7	37(2)	35(2)	44(2)	-18.3(18)	2.9(19)	-0.5(18)

N8	45(3)	36(2)	42(2)	-4.1(18)	22(2)	-0.1(19)
C1	34(3)	44(3)	36(2)	-15(2)	9(2)	-4(2)
C2	38(3)	78(4)	76(4)	-48(4)	20(3)	-15(3)
C3	36(3)	65(4)	63(4)	-33(3)	17(3)	-13(3)
C4	33(3)	41(3)	43(3)	-19(2)	7(2)	0(2)
C5	34(3)	37(3)	44(3)	-16(2)	5(2)	0(2)
C6	49(3)	45(3)	54(3)	-15(3)	8(3)	7(3)
C7	63(4)	41(3)	71(4)	-7(3)	6(3)	8(3)
C8	76(5)	56(4)	55(3)	0(3)	12(3)	11(4)
C9	62(4)	52(3)	43(3)	-13(3)	12(3)	-3(3)
C10	37(3)	37(3)	43(3)	-15(2)	6(2)	-3(2)
C11	58(3)	32(3)	42(3)	1(2)	23(2)	-1(2)
C12	47(3)	34(3)	48(3)	0(2)	22(2)	2(2)
C13	54(3)	33(3)	57(3)	2(2)	27(3)	6(2)
C14	43(3)	31(2)	43(3)	2(2)	23(2)	0(2)
C15	45(3)	41(3)	39(3)	-3(2)	15(2)	-3(2)
C16	50(4)	71(4)	48(3)	-10(3)	15(3)	-13(3)
C17	57(4)	89(5)	44(3)	-8(3)	7(3)	-10(4)
C18	43(3)	71(4)	62(4)	-15(3)	9(3)	-7(3)
C19	47(3)	55(3)	57(3)	-9(3)	20(3)	-7(3)
C20	47(3)	43(3)	43(3)	-4(2)	21(3)	-4(3)
C21	45(3)	34(3)	47(3)	0(2)	21(2)	1(2)
C22	54(3)	37(3)	40(3)	2(2)	20(2)	4(2)
C23	53(4)	59(4)	40(3)	9(2)	16(3)	17(3)
C24	65(5)	90(5)	45(3)	2(3)	4(3)	21(4)
C25	47(4)	75(4)	56(4)	5(3)	6(3)	20(3)
C26	49(3)	56(4)	52(3)	2(3)	18(3)	8(3)
C27	46(3)	36(3)	47(3)	5(2)	19(2)	6(2)
C28	40(3)	36(3)	39(3)	-1(2)	17(2)	-2(2)
C29	51(3)	35(3)	49(3)	2(2)	25(3)	-3(2)
C30	61(4)	34(3)	51(3)	-2(2)	26(3)	-8(3)
C31	36(3)	31(3)	37(2)	-9.1(19)	2(2)	-2(2)
C32	35(3)	46(3)	52(3)	-18(2)	8(2)	-6(2)
C33	39(3)	52(3)	72(4)	-32(3)	8(3)	-7(3)
C34	38(3)	33(3)	39(3)	-10(2)	-1(2)	0(2)
C35	36(3)	33(3)	41(3)	-14(2)	-1(2)	0(2)
C36	40(3)	34(3)	42(3)	-9(2)	-4(2)	4(2)
C37	58(4)	43(3)	51(3)	-9(2)	3(3)	13(3)
C38	64(4)	48(3)	58(4)	0(3)	-5(3)	16(3)
C39	60(4)	59(4)	42(3)	1(3)	1(3)	2(3)
C40	58(4)	46(3)	40(3)	-7(2)	4(2)	2(3)
C41	37(3)	91(4)	61(4)	-32(3)	-7(3)	6(3)
C42	53(4)	150(7)	79(4)	-28(5)	-10(4)	46(4)
C43	44(3)	55(4)	59(3)	-18(3)	14(3)	2(3)
C44	49(4)	72(4)	56(4)	-7(3)	0(3)	14(3)
F4A	120(8)	97(6)	262(14)	-63(8)	38(9)	16(5)
F5A	79(9)	131(14)	102(13)	-40(10)	-32(10)	68(8)
F6A	200(20)	280(30)	67(9)	-9(12)	47(11)	105(17)
O4B	37(4)	153(12)	230(16)	-133(12)	9(7)	-22(6)
F4B	171(10)	123(8)	104(6)	-71(6)	-35(7)	86(7)
F5B	173(17)	227(17)	123(10)	24(12)	-24(11)	114(15)
F6B	71(5)	267(17)	228(14)	-64(12)	19(8)	71(9)
O4A	125(17)	71(12)	77(11)	-26(8)	-46(11)	0(11)
O5	59(3)	56(3)	72(3)	-12(2)	17(2)	15(2)
O6	91(4)	54(3)	103(4)	-16(3)	26(3)	19(3)
C49	80(5)	67(5)	91(5)	10(4)	20(4)	14(4)
C50	64(5)	66(4)	67(4)	-11(3)	7(3)	6(3)
C51	65(4)	58(4)	69(4)	-5(3)	12(4)	9(3)

C52	80(5)	64(4)	80(5)	-22(4)	16(4)	-5(4)
O7	83(4)	123(5)	128(5)	58(4)	54(4)	29(4)
O8	87(4)	77(4)	142(5)	20(3)	59(4)	8(3)
C45	78(6)	80(5)	88(5)	0(4)	14(4)	0(4)
C46	95(7)	72(5)	111(7)	-3(5)	23(5)	9(5)
C47	117(8)	152(10)	127(8)	73(7)	67(7)	77(7)
C48	108(8)	85(6)	175(10)	39(7)	65(8)	40(6)

Table 39 Bond Lengths for sv-2-rem_tw.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Zn1	O1	2.166(3)		C16	C17	1.357(9)
Zn1	O2	2.200(4)		C17	C18	1.416(8)
Zn1	N1	2.110(4)		C18	C19	1.359(8)
Zn1	N2	2.155(4)		C19	C20	1.417(8)
Zn1	N3	2.105(4)		C20	C21	1.401(8)
Zn1	N4[1]	2.165(4)		C21	C22	1.391(8)
F1	C44	1.324(7)		C22	C23	1.428(8)
F2	C44	1.330(7)		C22	C27	1.444(7)
F3	C44	1.310(7)		C23	C24	1.346(9)
O1	C43	1.228(6)		C24	C25	1.427(9)
O2	C41	1.220(7)		C25	C26	1.353(8)
O3	C43	1.234(7)		C26	C27	1.424(8)
N1	C1	1.315(6)		C29	C30	1.351(7)
N1	C3	1.370(7)		C32	C33	1.347(7)
N2	C11	1.315(6)		C34	C35	1.396(7)
N2	C12	1.375(6)		C34	C36[3]	1.437(7)
N3	C31	1.326(6)		C34	C40[3]	1.431(7)
N3	C32	1.372(6)		C35	C36	1.388(7)
N4	C28	1.316(6)		C36	C37	1.431(7)
N4	C29	1.375(6)		C37	C38	1.354(8)
N5	C1	1.338(6)		C38	C39	1.429(8)
N5	C2	1.375(7)		C39	C40	1.337(8)
N5	C4	1.437(6)		C41	C42	1.472(11)
N6	C11	1.350(6)		C41	O4B	1.303(12)
N6	C13	1.362(6)		C41	O4A	1.283(17)
N6	C14	1.440(6)		C42	F4A	1.409(14)
N7	C31	1.348(6)		C42	F5A	1.33(2)
N7	C33	1.368(7)		C42	F6A	1.47(3)
N7	C35	1.439(6)		C42	F4B	1.247(11)
N8	C21	1.437(6)		C42	F5B	1.27(2)
N8	C28	1.350(6)		C42	F6B	1.258(17)
N8	C30	1.373(6)		C43	C44	1.517(8)
C2	C3	1.348(7)		F5B	F6B	1.51(4)
C4	C5	1.399(7)		O5	C50	1.413(8)
C4	C10[2]	1.390(7)		O5	C51	1.416(7)
C5	C6	1.426(7)		O6	C49	1.400(8)
C5	C10	1.444(6)		O6	C52	1.433(9)
C6	C7	1.344(8)		C49	C50	1.493(9)
C7	C8	1.416(8)		C51	C52	1.484(9)
C8	C9	1.358(8)		O7	C46	1.375(9)
C9	C10	1.416(8)		O7	C47	1.411(9)
C12	C13	1.355(7)		O8	C45	1.398(9)
C14	C15	1.390(8)		O8	C48	1.405(9)
C14	C27	1.395(8)		C45	C46	1.501(11)
C15	C16	1.422(8)		C47	C48	1.522(13)

C15	C20	1.445(7)				

[1]1/2+X,1/2-Y,-1/2+Z; [2]1-X,-Y,-Z; [3]1-X,1-Y,1-Z

Table 40. Bond Angles for sv-2-rem_tw.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Zn1	O2	178.45(15)		C20	C21	N8	118.4(5)
N1	Zn1	O1	84.52(15)		C22	C21	N8	118.5(5)
N1	Zn1	O2	96.08(15)		C22	C21	C20	123.0(5)
N1	Zn1	N2	88.33(15)		C21	C22	C23	123.0(5)
N1	Zn1	N4[1]	92.23(15)		C21	C22	C27	118.9(5)
N2	Zn1	O1	90.61(16)		C23	C22	C27	118.0(5)
N2	Zn1	O2	87.98(15)		C24	C23	C22	121.0(5)
N2	Zn1	N4[1]	175.63(16)		C23	C24	C25	121.1(6)
N3	Zn1	O1	93.95(15)		C26	C25	C24	119.9(6)
N3	Zn1	O2	85.46(15)		C25	C26	C27	121.3(5)
N3	Zn1	N1	178.33(16)		C14	C27	C22	117.9(5)
N3	Zn1	N2	92.38(15)		C14	C27	C26	123.4(5)
N3	Zn1	N4[1]	87.17(15)		C26	C27	C22	118.6(5)
N4[1]	Zn1	O1	93.76(15)		N4	C28	N8	111.1(4)
N4[1]	Zn1	O2	87.65(15)		C30	C29	N4	109.8(4)
C43	O1	Zn1	152.8(4)		C29	C30	N8	106.1(4)
C41	O2	Zn1	152.8(4)		N3	C31	N7	110.3(4)
C1	N1	Zn1	126.1(3)		C33	C32	N3	109.5(5)
C1	N1	C3	106.0(4)		C32	C33	N7	106.6(5)
C3	N1	Zn1	127.8(3)		C35	C34	C36[4]	118.2(4)
C11	N2	Zn1	127.2(3)		C35	C34	C40[4]	123.7(4)
C11	N2	C12	105.5(4)		C40[4]	C34	C36[4]	118.0(5)
C12	N2	Zn1	127.0(3)		C34	C35	N7	118.3(4)
C31	N3	Zn1	126.2(3)		C36	C35	N7	118.1(4)
C31	N3	C32	106.2(4)		C36	C35	C34	123.6(4)
C32	N3	Zn1	127.3(3)		C35	C36	C34[4]	118.2(5)
C28	N4	Zn1[2]	128.0(3)		C35	C36	C37	123.5(5)
C28	N4	C29	105.8(4)		C37	C36	C34[4]	118.3(5)
C29	N4	Zn1[2]	125.8(3)		C38	C37	C36	121.2(5)
C1	N5	C2	106.5(4)		C37	C38	C39	120.2(5)
C1	N5	C4	125.3(4)		C40	C39	C38	120.4(5)
C2	N5	C4	128.1(4)		C39	C40	C34[4]	121.8(5)
C11	N6	C13	107.2(4)		O2	C41	C42	116.6(6)
C11	N6	C14	125.0(4)		O2	C41	O4B	121.8(8)
C13	N6	C14	127.8(4)		O2	C41	O4A	125.3(12)
C31	N7	C33	107.5(4)		O4B	C41	C42	118.8(7)
C31	N7	C35	124.3(4)		O4A	C41	C42	104.7(11)
C33	N7	C35	128.2(4)		F4A	C42	C41	112.4(7)
C28	N8	C21	125.2(4)		F4A	C42	F6A	130.4(18)
C28	N8	C30	107.1(4)		F5A	C42	C41	124.7(12)
C30	N8	C21	127.6(4)		F5A	C42	F4A	93.7(17)
N1	C1	N5	111.6(4)		F5A	C42	F6A	104.5(17)
C3	C2	N5	106.8(5)		F6A	C42	C41	94.3(14)
C2	C3	N1	109.1(5)		F4B	C42	C41	118.8(8)
C5	C4	N5	117.4(4)		F4B	C42	F5B	138.2(19)
C10[3]	C4	N5	118.6(5)		F4B	C42	F6B	102.7(13)
C10[3]	C4	C5	124.0(4)		F5B	C42	C41	99.7(14)
C4	C5	C6	123.2(4)		F6B	C42	C41	113.4(14)
C4	C5	C10	118.1(5)		F6B	C42	F5B	73.4(18)

C6	C5	C10	118.7(5)		O1	C43	O3	128.7(6)
C7	C6	C5	120.7(5)		O1	C43	C44	114.5(5)
C6	C7	C8	121.0(6)		O3	C43	C44	116.8(6)
C9	C8	C7	120.4(6)		F1	C44	F2	105.1(6)
C8	C9	C10	121.1(5)		F1	C44	C43	110.5(5)
C4[3]	C10	C5	117.9(5)		F2	C44	C43	114.0(6)
C4[3]	C10	C9	124.0(5)		F3	C44	F1	106.5(6)
C9	C10	C5	118.1(5)		F3	C44	F2	105.4(5)
N2	C11	N6	111.3(4)		F3	C44	C43	114.6(5)
C13	C12	N2	109.7(4)		C42	F5B	F6B	53.0(12)
C12	C13	N6	106.3(4)		C42	F6B	F5B	53.6(12)
C15	C14	N6	118.5(5)		C50	O5	C51	108.8(5)
C15	C14	C27	123.4(4)		C49	O6	C52	109.9(5)
C27	C14	N6	118.0(5)		O6	C49	C50	111.1(6)
C14	C15	C16	123.6(5)		O5	C50	C49	110.7(6)
C14	C15	C20	118.6(5)		O5	C51	C52	111.3(6)
C16	C15	C20	117.7(5)		O6	C52	C51	109.5(6)
C17	C16	C15	121.7(5)		C46	O7	C47	110.1(6)
C16	C17	C18	120.3(6)		C45	O8	C48	105.9(6)
C19	C18	C17	120.4(6)		O8	C45	C46	109.4(7)
C18	C19	C20	121.2(5)		O7	C46	C45	112.1(7)
C19	C20	C15	118.7(5)		O7	C47	C48	109.1(8)
C21	C20	C15	118.0(5)		O8	C48	C47	109.1(8)
C21	C20	C19	123.2(5)					

[1]1/2+X,1/2-Y,-1/2+Z; [2]-1/2+X,1/2-Y,1/2+Z; [3]1-X,-Y,-Z; [4]1-X,1-Y,1-Z

Table 41. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6.

Atom	*x*	*y*	*z*	U(eq)
H1	5569.89	1349.93	1412.7	45
H2	2861.25	551.4	1086.34	75
H3	2911.24	1475.78	1965.69	64
H6	3897.52	1692.44	121.75	59
H7	3757.13	2192.84	-901.54	70
H8	4288.89	1543.45	-1789.6	74
H9	4996.29	401.59	-1636.92	62
H11	3544.69	2237.8	3808.7	51
H12	5066.07	611.4	3145.96	50
H13	4130.06	93.75	3998.15	56
H16	1911.26	1126.33	3417.92	66
H17	253.38	1262.44	3161.35	76
H18	-791.92	1353.51	3997.13	70
H19	-160.87	1305.13	5077.86	62
H23	2763.71	1143.64	6777.77	60
H24	4423.3	1177.34	7028.17	80
H25	5484.64	1214.16	6193.22	71
H26	4853.23	1145.33	5115.25	62
H28	1261.89	2375.27	6344.25	45
H29	-373.61	879.11	7098.67	52
H30	473.64	256.78	6254.95	56
H31	4356.55	3477.15	3744.97	42
H32	7025.85	3163.39	3236.21	53
H33	7138.19	4149.98	4060.96	65
H37	6126.39	3301.4	5147.89	61
H38	6290.43	3016.87	6241.16	69

H39	5790.77	3870.31	7014.45	65
H40	5100.32	4961.8	6680.03	57
H49A	3428.64	3046.99	873.2	94
H49B	2272.29	2977.36	767.63	94
H50A	2702.03	4152.52	1162.87	79
H50B	3328.98	4287.83	571.49	79
H51A	2536.72	4375.2	-498.97	77
H51B	1379.53	4326.21	-620.26	77
H52A	1438.5	3084.13	-317.76	89
H52B	2072.75	3212.75	-907.47	89
H45A	3178.44	2688.54	6162.67	98
H45B	3677.82	3466.42	6086.1	98
H46A	3922.13	2707.08	5188.09	110
H46B	2775.23	2617.5	5023.38	110
H47A	1822.61	3679.66	4667.23	154
H47B	2388.39	4431.99	4596.75	154
H48A	2854.53	4441.92	5753.55	143
H48B	1696.48	4446.19	5602.31	143

Citations

[1]. O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

[2]. Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C27**, 3-8.

[3]. Sheldrick, G.M., ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.*, (2015), **A71**, 3-8.