Supporting Information

Structures and Single Crystal to Single Crystal Transformations of Cadmium Frameworks Using a Flexible Tripodal Ligand

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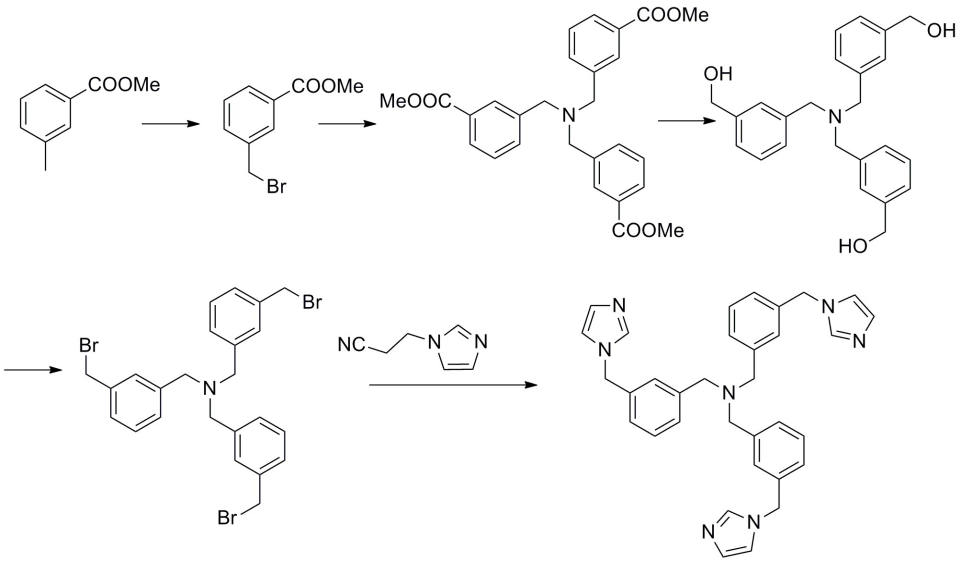
Table S1. Crystal data and structure refinement parameters for **L** and complexes **1-4**.

Complex	**L**	**1**	**2**	**3**	**4**
formula	$C_{33}H_{34.5}Cl_{1.5}N_7O_6$	$C_{66}H_{66}CdCl_2N_{14}O_8$	$C_{66}H_{66}Cd_2Cl_4N_{14}$	$C_{74}H_{78}Cd_2N_{14}O_8$	$C_{66}H_{66}CdCl_2N_{14}$
fw (g mol^{-1})	678.35	1366.63	1421.92	1516.30	1238.62
T (K)	150(2)	150(2)	150(2)	150(2)	150(2)
crystal system	Triclinic	Trigonal	Monoclinic	Triclinic	Trigonal
space group	$P\bar{1}$	$R\bar{3}$	$P2_1/n$	$P\bar{1}$	$R\bar{3}$
a (Å)	9.7961(10)	12.1835(13)	14.010(6)	14.180(9)	13.094(3)
b (Å)	11.3348(16)	12.1835(13)	23.380(9)	15.386(8)	13.094(3)
c (Å)	15.5663(15)	38.086(5)	21.272(9)	18.466(12)	37.435(10)
α (°)	85.817(4)	90	90	101.133(19)°	90
β (°)	84.393(4)	90	96.13(4)	92.04(3)°.	90
γ (°)	76.837(4)	120	90	92.143(19)°	120
Volume ($Å^3$)	1672.7(3)	4896.0(10)	6928(5)	3946(4)	5559(3)
Z	2	3	4	2	3
μ (mm^{-1})	0.209	0.482	0.817	0.598	0.411
F(000)	710	2118	2896	1560	1926
θ range	2.212 to 26.344°	2.207 to 25.991°	2.274 to 26.719°	2.250 to 26.394°	2.822 to 26.457°
reflections collected	36986	29258	51946	36826	10167
independent reflections	11816 [R(int)= 0.0330]	2132 [R(int)=0.0452]	14432 [R(int) = 0.2096]	16017 [R(int)=0.1417]	2559 [R(int)=0.0674]
Goof	1.071	1.107	1.012	0.995	1.054
final R indices [R > 2σ (I)]	$R1^a$ = 0.0566 wR_2^b = 0.1134	$R1^a$ = 0.0934 wR_2^b = 0.2668	$R1^a$ = 0.1173 wR_2^b = 0.3208	$R1^a$ = 0.0708 wR_2^b = 0.1388	$R1^a$ = 0.0506 wR_2^b = 0.1351
R indices (all data)	$R1^a$ = 0.0788 wR_2^b = 0.1270	$R1^a$ = 0.1003 wR_2^b = 0.2781	$R1^a$ = 0.2261 wR_2^b = 0.3844	$R1^a$ = 0.1613 wR_2^b = 0.1684	$R1^a$ = 0.0631 wR_2^b = 0.1418

$^a R_1 = \Sigma||F_o| - |F_c|| / |F_o|$, $^b wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{0.5}$



Scheme S1. Synthetic route of ligand **L**.

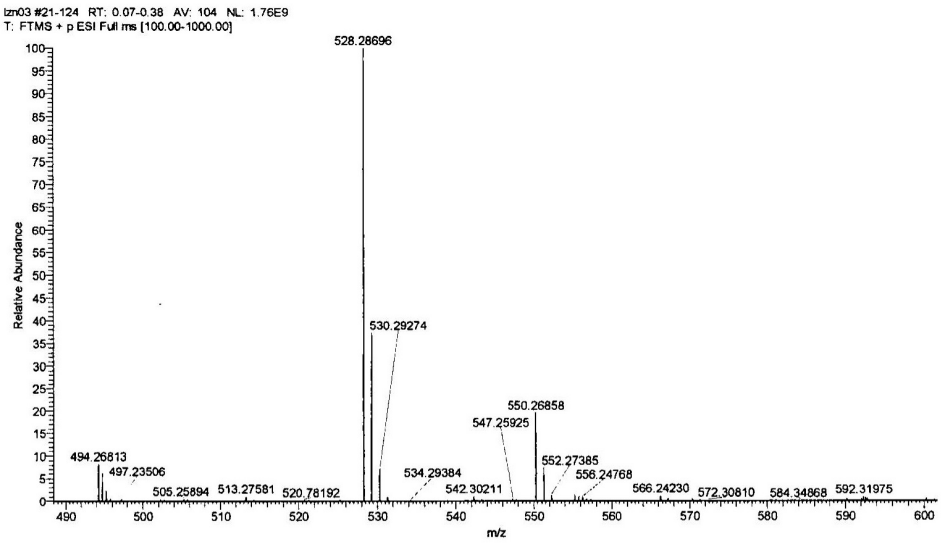


Figure S1. High-resolution mass spectrum of **L**.

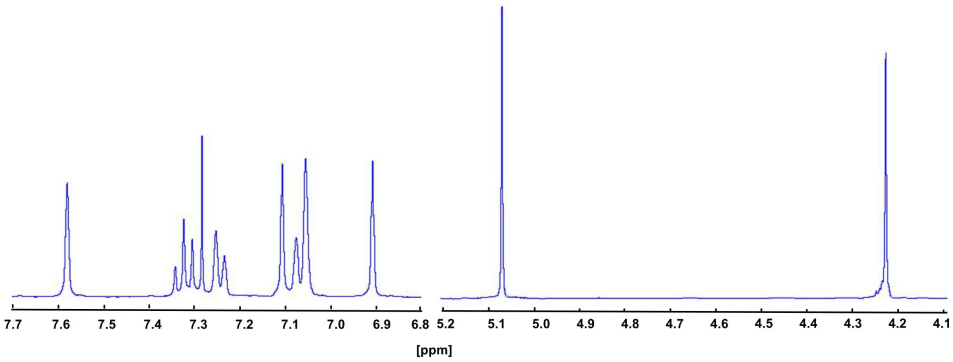


Figure S2. ^{1}H NMR spectrum of **L** in $CDCl_3$.

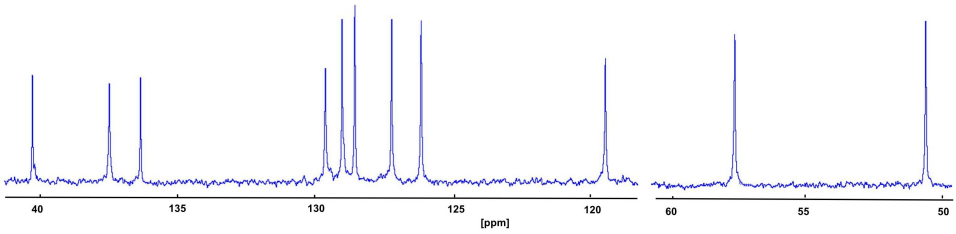


Figure S3. ^{13}C NMR spectrum of **L** in $CDCl_3$.

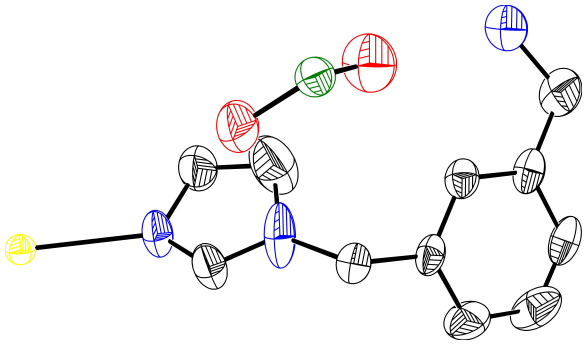


Figure S4. Thermal ellipsoid plot (50% probability) of the X-ray structure of complex **1**. All hydrogen atoms are omitted for clarity.

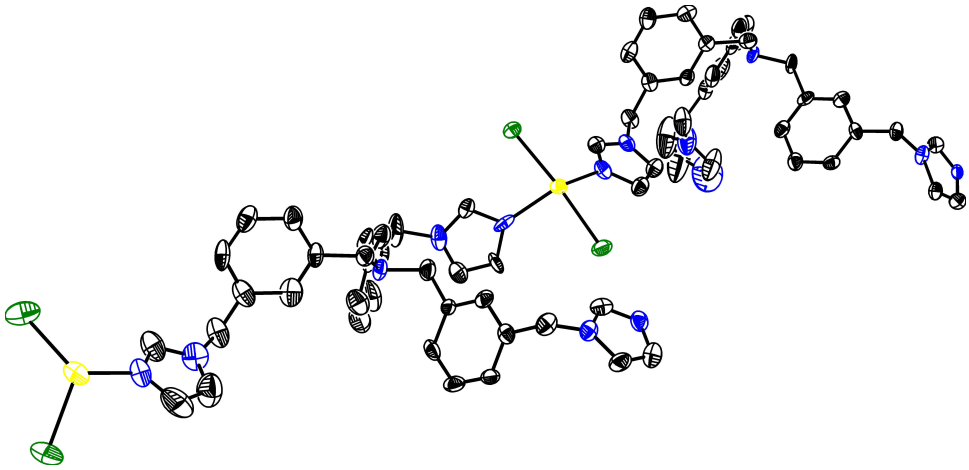


Figure S5. Thermal ellipsoid plot (50% probability) of the X-ray structure of complex **2**. All hydrogen atoms are omitted for clarity.

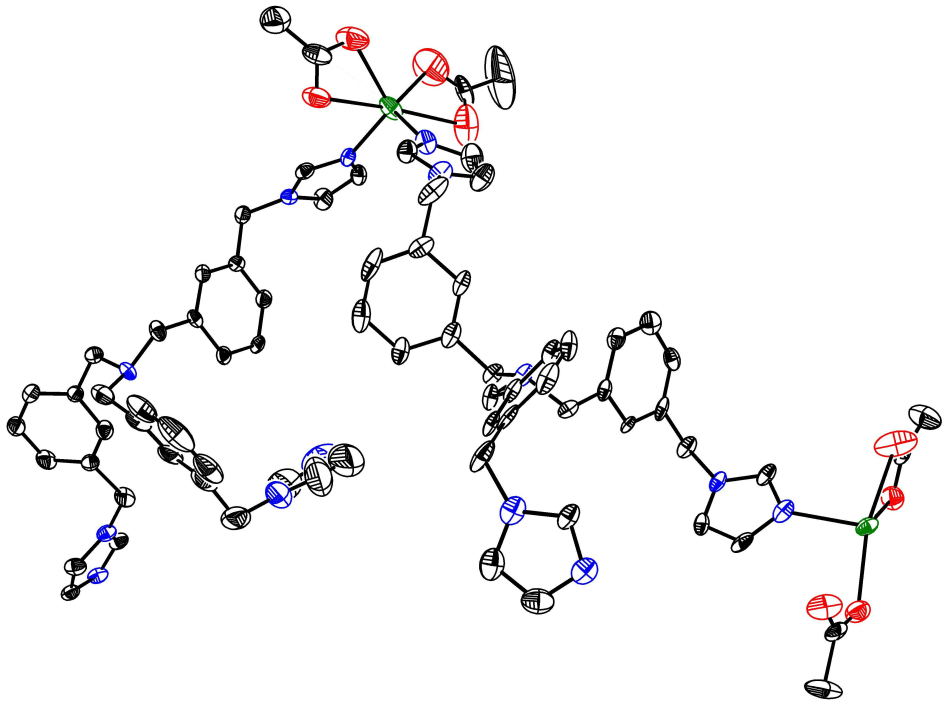


Figure S6. Thermal ellipsoid plot (50% probability) of the X-ray structure of complex **3**. All hydrogen atoms are omitted for clarity.

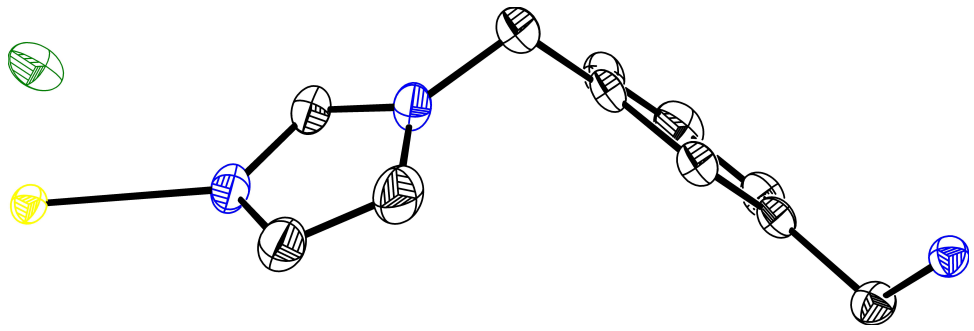


Figure S7. Thermal ellipsoid plot (50% probability) of the X-ray structure of complex **4**. All hydrogen atoms are omitted for clarity.

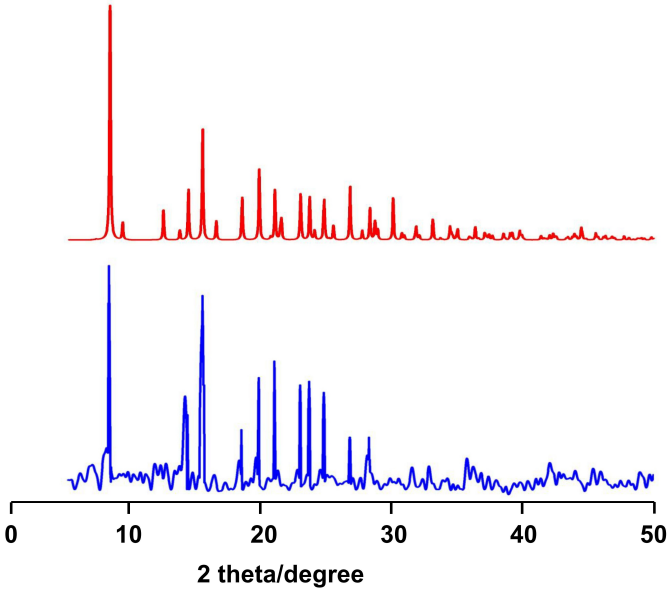


Figure S8. PXRD pattern of complex **4**. Top: calculated; bottom: experimental.

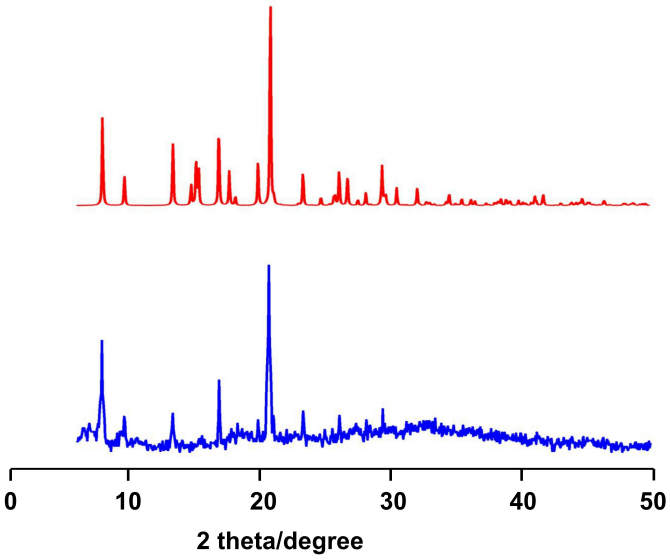


Figure S9. PXRD pattern of complex **1**. Top: calculated; bottom: experimental.

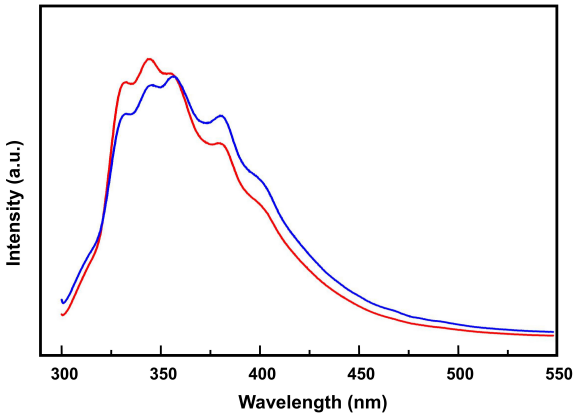


Figure S10. Solid-state emission spectra of complex **1** (red) and **4** (blue).

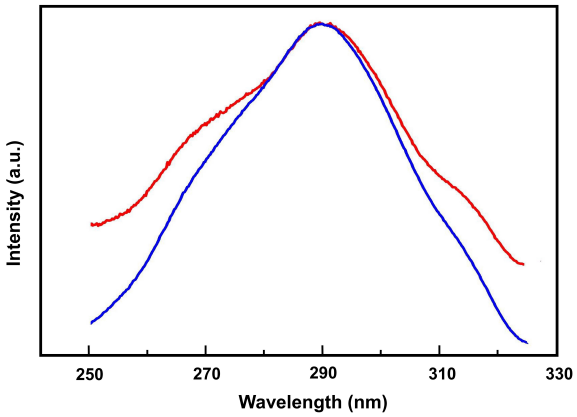


Figure S11. Solid-state excitation spectra of complex **1** (red) and **4** (blue).

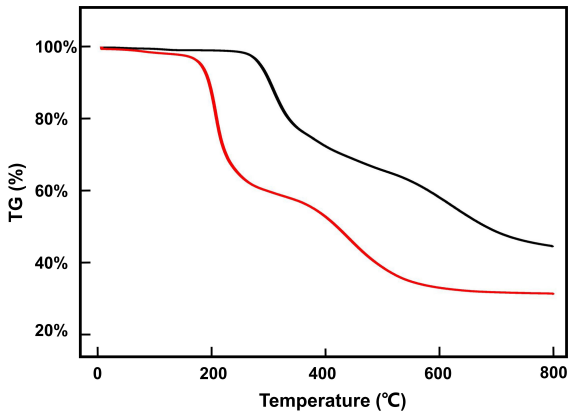


Figure S12. TGA analysis of complex **1** (black) and **4** (red).

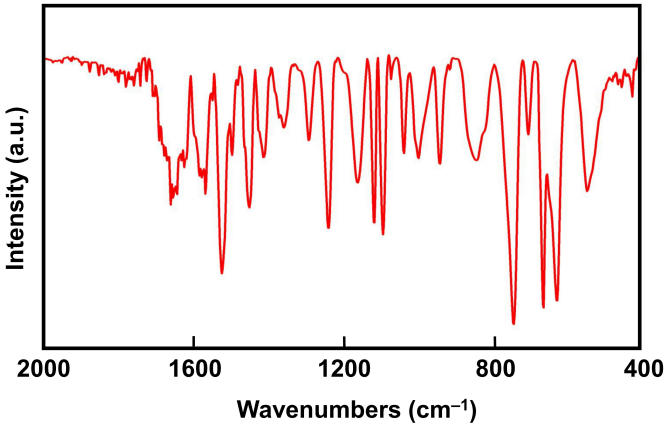


Figure S13. FTIR spectrum of complex **2**.

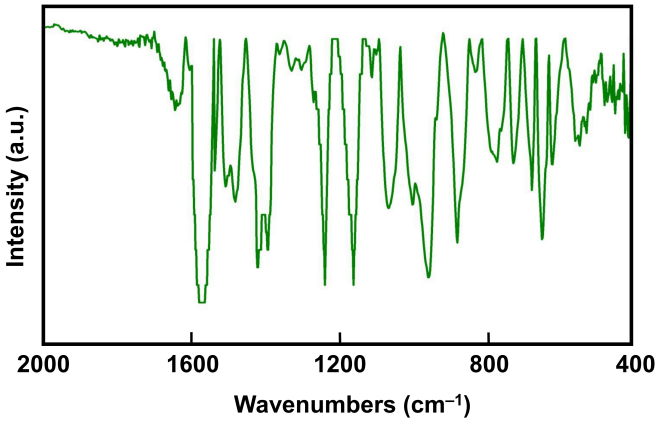


Figure S14. FTIR spectrum of complex **3**.