

## Electronic Supplementary Information (ESI)

### Structure and magnetic characterization of bicompartamental [N6O2] divalent metal(II) complexes of bis(phenolato) ligand bearing two pendant bis(pyridyl) amine arms<sup>†</sup>

Franz A. Mautner <sup>\*a</sup>, Roland C. Fischer <sup>b</sup>, Ana Torvisco <sup>b</sup>, Kai Nakashima <sup>c</sup>, Makoto Handa <sup>c</sup>, Masahiro Mikuriya <sup>d</sup>, Nahed M. H. Salem <sup>e</sup>, Gabriel J. Overby <sup>f</sup>, Madison R. Maier <sup>f</sup>, Febee R. Louka <sup>e</sup> and Salah S. Massoud <sup>\*ef</sup>

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<sup>a</sup> *Institut für Physikalische and Theoretische Chemie, Technische Universität Graz, Stremayrgasse 9/II, A-8010, Graz, Austria*

<sup>b</sup> *Institut für Anorganische Chemie, Technische Universität Graz, Stremayrgasse 9, A-8010 Graz, Austria*

<sup>c</sup> *Department of Chemistry, Interdisciplinary Graduate School of Science and Engineering, Shimane University, 1060 Nishikawatsu, Matsue 690-8504 Japan*

<sup>d</sup> *Department of Applied Chemistry for Environment, School of Biological and Environmental Sciences, Kwansai Gakuin University, 1 Gakuen Uegahara, Sanda 669-1330 Japan*

<sup>e</sup> *Department of Chemistry, Faculty of Science, Alexandria University, Moharam Bey, 21511 Alexandria, Egypt*

<sup>f</sup> *Department of Chemistry, University of Louisiana at Lafayette, P.O. Box 43700 Lafayette, LA 70504-4370, USA*

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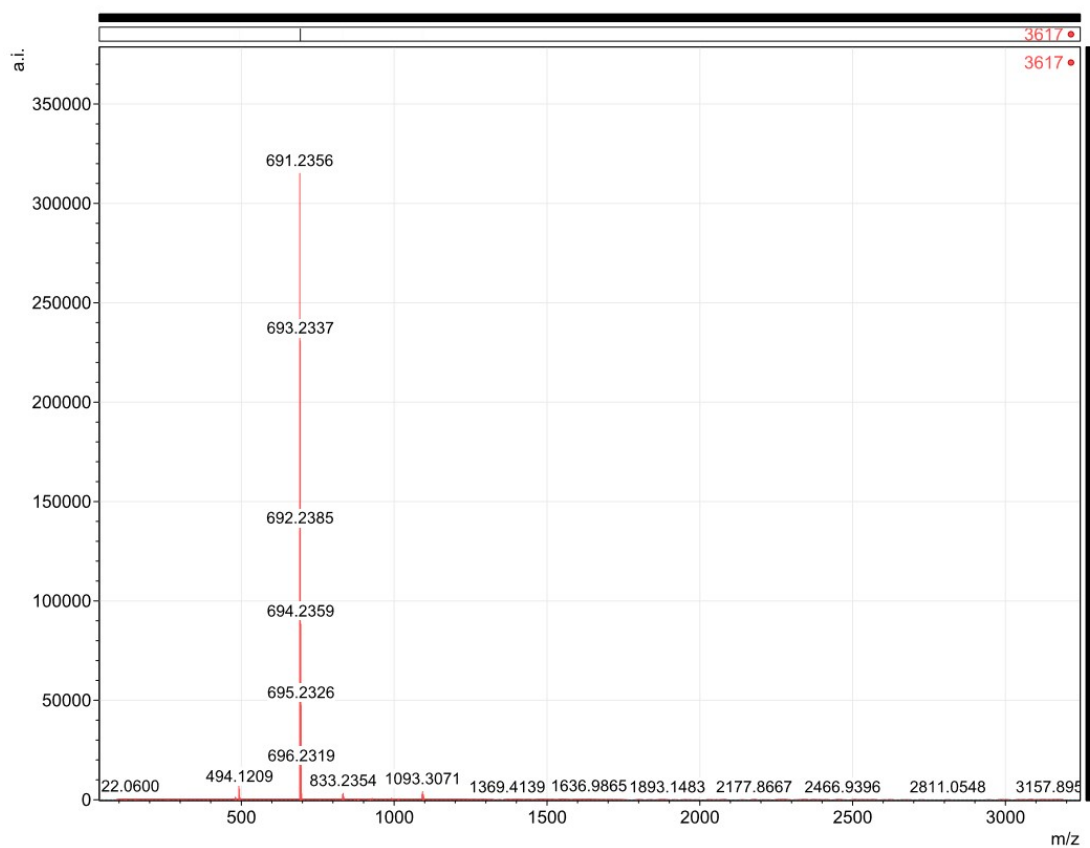
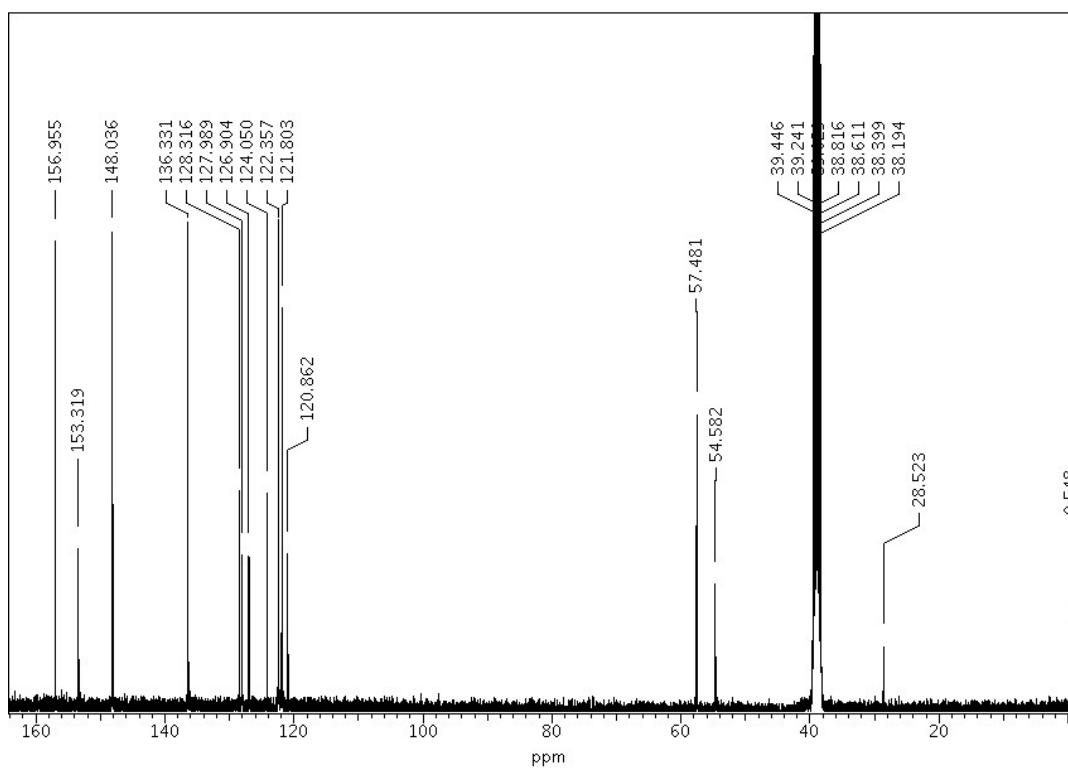
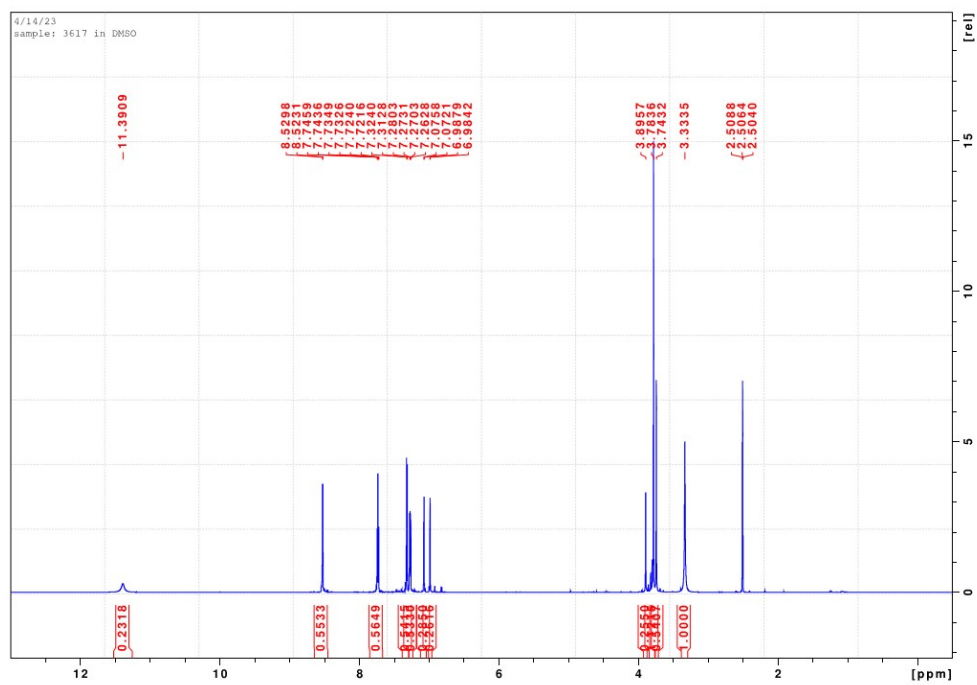


Fig. S1 ESI-MS of H<sub>2</sub>L in methanol



**Fig. S2**  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of  $\text{H}_2\text{L}$  in  $d_6\text{-DMSO}$

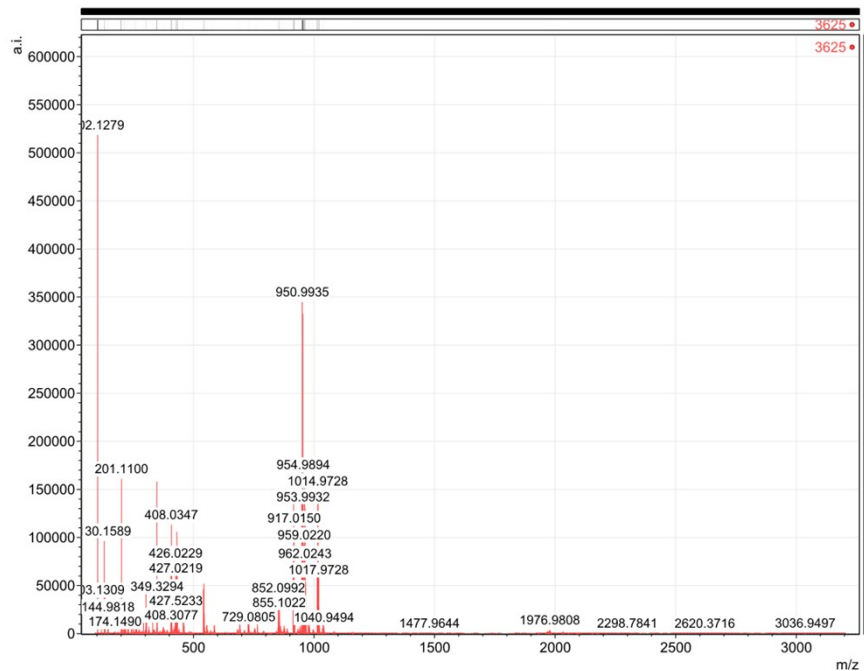


Fig. S3. ESI-MS of 2 in acetonitrile

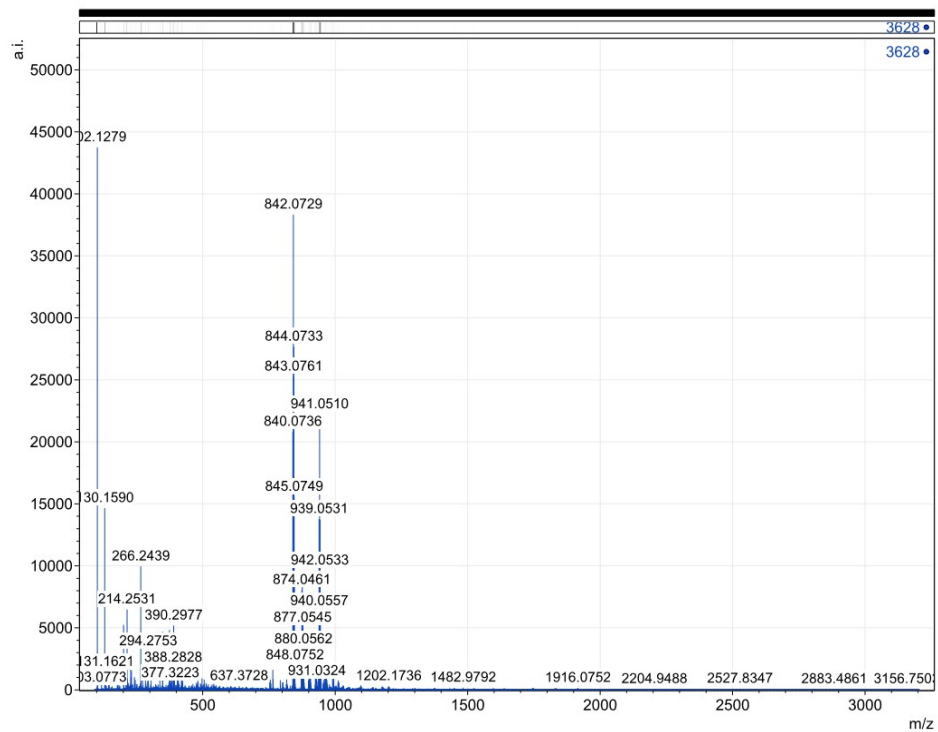


Fig. S4 ESI-MS of 3 in acetonitrile

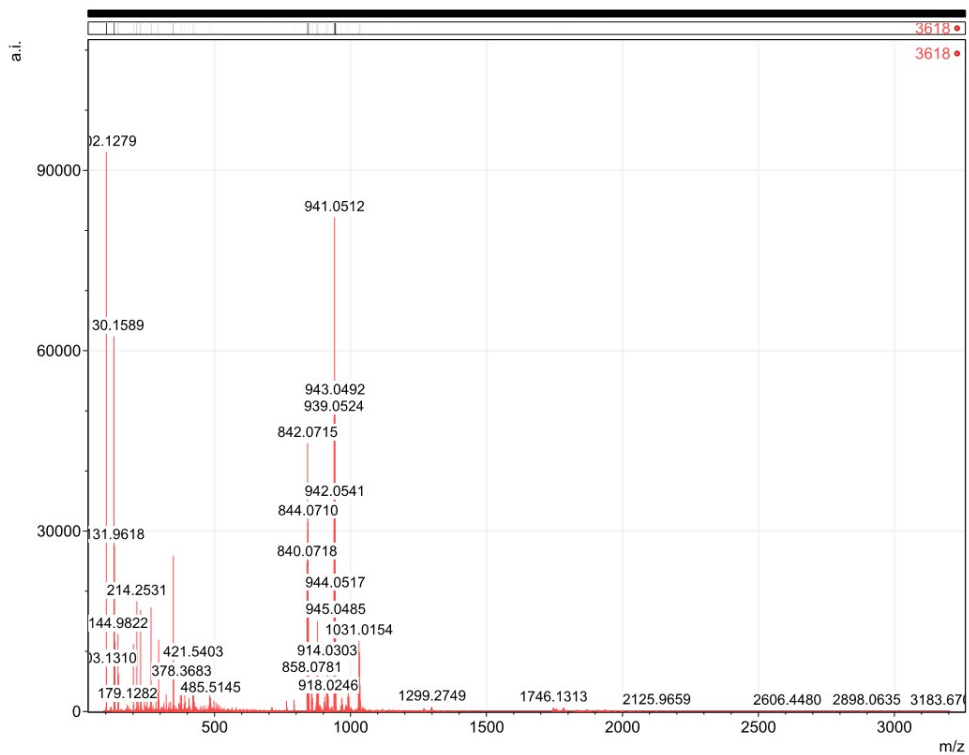


Fig. S5 ESI-MS of 4 in acetonitrile

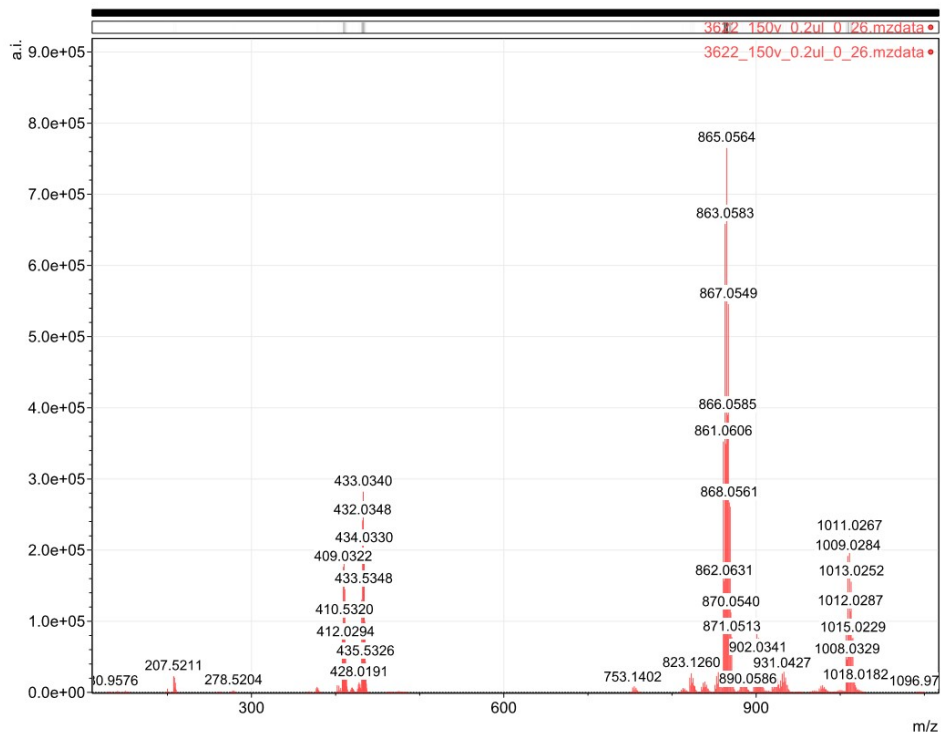


Fig. S6 ESI-MS of 5 in acetonitrile

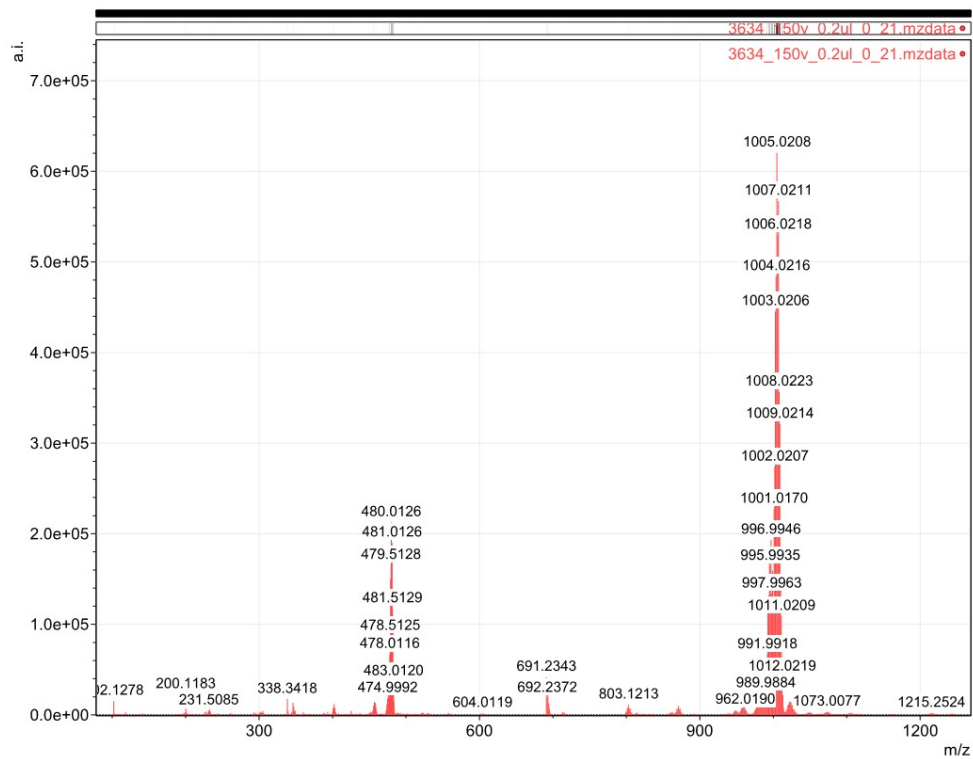


Fig. S7 ESI-MS of 6 in acetonitrile

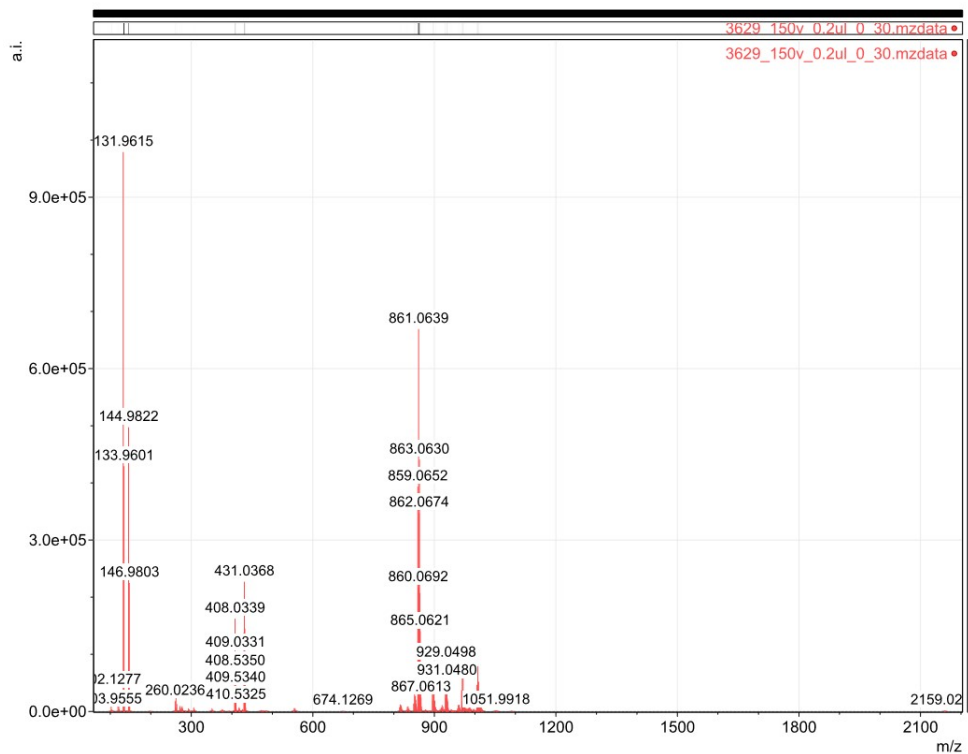
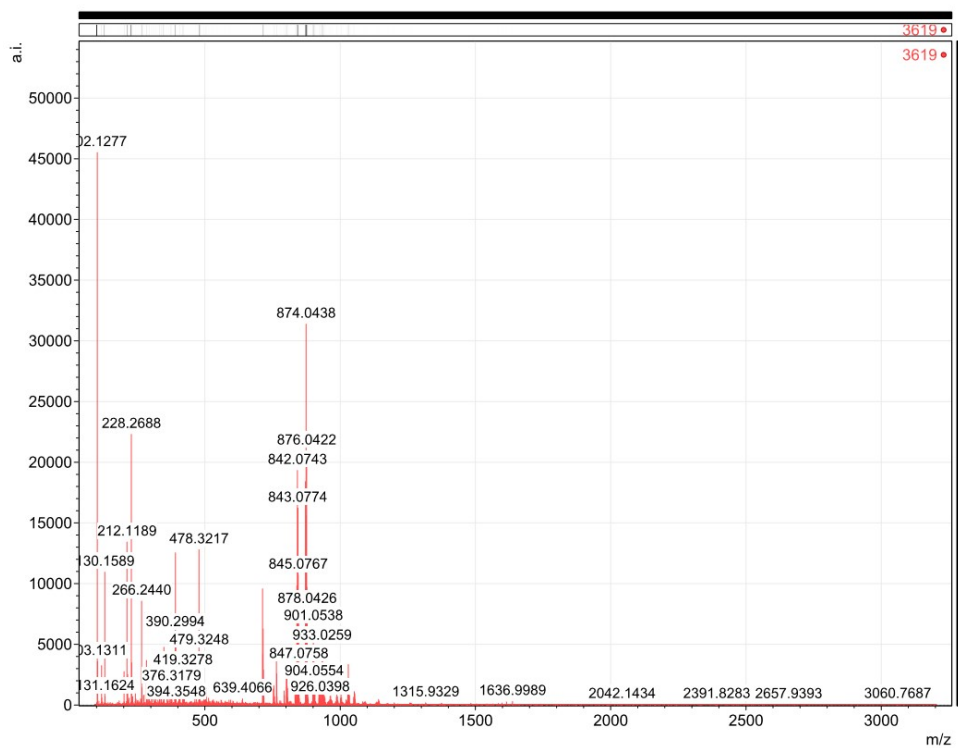


Fig. S8 ESI-MS of 7 in acetonitrile



**Fig. S9** ESI-MS of **8** in acetonitrile

**Table S1** Selected bond distances (Å) and bond angles (°).

Compound 1			
Mn1-O1	2.164(3)	Mn1-N1	2.280(3)
Mn1-O3	2.110(3)	Mn1-N2	2.335(3)
Mn1-O5	2.073(3)	Mn1-N3	2.2933(4)
Mn2-O2	2.141(3)	Mn2-N4	2.277(3)
Mn2-O4	2.115(3)	Mn2-N5	2.361(3)
Mn2-O6	2.091(3)	Mn2-N6	2.284(3)
Mn2-O4-C40	140.2(3)	Mn2-O6-C42	144.6(3)
Mn1-O3-C40	147.9(3)	Mn1-O5-C42	147.0(3)
Compound 4			
Cu1-O1	2.219(5)	Cu1-N1c	2.059(5)
Cu1-N2	1.999(5)	Cu1-N3	2.002(5)
Cu1-N7	1.999(5)	Cu1-N22b	2.650(6)
Cu2-O2	2.538(4)	Cu2-N4	2.033(7)
Cu2-N5	2.006(5)	Cu2-N6	2.008(5)
Cu2-N10	1.957(6)	Cu2-N21	2.527(5)
Cu3-O3	2.658(4)	Cu3-N12	2.584(5)
Cu3-N13	2.016(6)	Cu3-N14	2.003(7)
Cu3-N15	2.004(7)	Cu3-N19	1.942(6)
Cu4-O4	2.214(4)	Cu4-N7a	2.725(6)
Cu4-N16	2.045(5)	Cu4-N17	2.002(5)
Cu4-N18	2.018(5)	Cu4-N22	1.995(5)
N7-N8	1.203(8)	N8-N9	1.164(8)
N10-N11	1.205(8)	N11-N12	1.166(9)
N19-N20	1.187(9)	N20-N21	1.137(7)



N22-N23	1.175(8)	N23-N24	1.165(8)
N10-N11-N12	176.2(7)	N7-N8-N9	176.0(6)
N19-N20-N21	175.3(7)	N22-N23-N24	175.0(6)
<b>Compound 5</b>			
Zn1-O1	2.141(4)	Zn1-N1	2.110(5)
Zn1-O5	2.231(10)	Zn1-N2	2.210(5)
Zn1-O3	2.032(4)	Zn1-N3	2.105(5)
Zn2-O2	1.986(4)	Zn2-N4	2.089(4)
Zn2-O4	2.019(4)	Zn2-N5	2.241(5)
Zn2-N6	2.084(6)	Zn1-O5A	1.94(4)
Zn1-O3-C40	141.0(4)	Zn2-O4-C40	120.6(4)
<b>Compound 6</b>			
Cd1-O1	2.401(2)	Cd1-O3	2.626(2)
Cd1-O4	2.332(2)	Cd1-O5	2.273(2)
Cd1-N2	2.478(2)	Cd1-N3	2.381(3)
Cd1-N4	2.330(3)	Cd2-O2	2.2734(19)
Cd2-O3	2.316(2)	Cd2-O6	2.296(2)
Cd2-O8	2.698(2)	Cd2-N5	2.542(3)
Cd2-N6	2.352(3)	Cd2-N7	2.393(3)
Cd1-O3-C40	86.35(17)	Cd1-O4-C40	100.83(18)
Cd2-O6-42C	103.1(2)	Cd2-O8-C42	83.79(18)
Cd1-O3-Cd2	135.10(9)	O3-Cd1-O4	52.25(7)
O6-Cd2-O8	51.46(7)		

Symmetry codes for 4: (a)  $-1/2+x, 3/2-y, 1/2+z$ ; (b)  $1/2+x, 3/2-y, -1/2+z$ .

**Table S2** Possible hydrogen bonds

D-H...A*	Symmetry of A	D...A (Å)	D-H..A (°)
<b>Compound 1</b>			
O1-H1...O2		2.398(3)	172
<b>Compound 4</b>			
O11-H11A...O11	[-x,1-y,1-z]	2.908(10)	126
O11-H11B...O5		2.974(10)	130
O12-H12A...O6		3.054(12)	149
O12-H12A...O7		3.175(9)	157
O12-H12B...O8		2.871(10)	172
O13-H13A...O9		2.898(9)	148
O13-H13B...O12		3.031(9)	143
O14-H14A...O10		2.776(9)	168
O14-H14B...N9	[1/2-x,-1/2+y,1/2-z]	3.093(10)	154
<b>Compound 5</b>			
O2-H2...O1		2.460(6)	170
O5-H5A...F4	[1-x,1-y,1-z]	2.857(7)	154
O5-H5B..O6		2.700(9)	140
<b>Compound 6</b>			
O1-H2...O2		2.407(3)	172
O5-H5A...O7		2.680(4)	154
O5-H5B...O8		2.757(3)	165
O7-H7C...O8	[1-x,1-y,1-z]	2.802(4)	166
O7-H7D...F3		2.934(4)	164

**Table S3** Non-covalent ring-ring interactions.

	ring(A)	ring(B)	Cg(A)...Cg(B) (Å)
Compound <b>1</b>	Cg(C1-C6)	Cg(C1-C6)[-x,1-y,1-z]	3.690(2)
	Cg(N2,C16-C20)	Cg(N2,C16-C20)[1-x,1-y,2-z]	3.522(2)
Compound <b>5</b>	Cg(N4,C010,C34-C37)	Cg(N6,C28-C32)[-x,1-y,1-z]	3.636(4)
	Cg(C14-C19)	Cg(C14-C19)[1-x,1-y,-z]	3.750(3)

Cg = center of gravity of ring

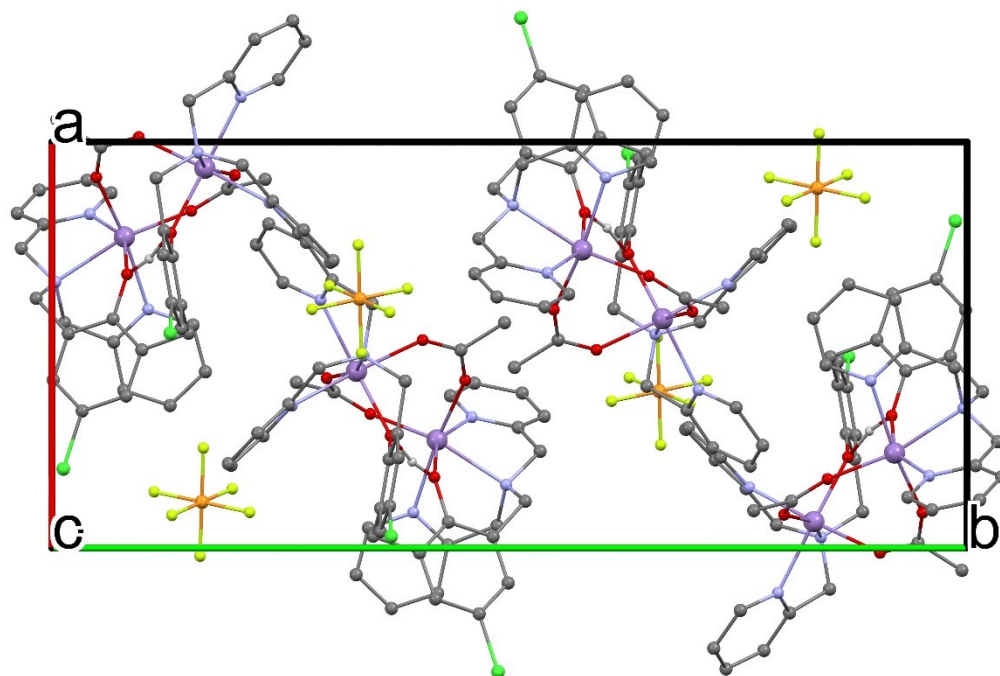


Fig. S10. Packing plot of 1.

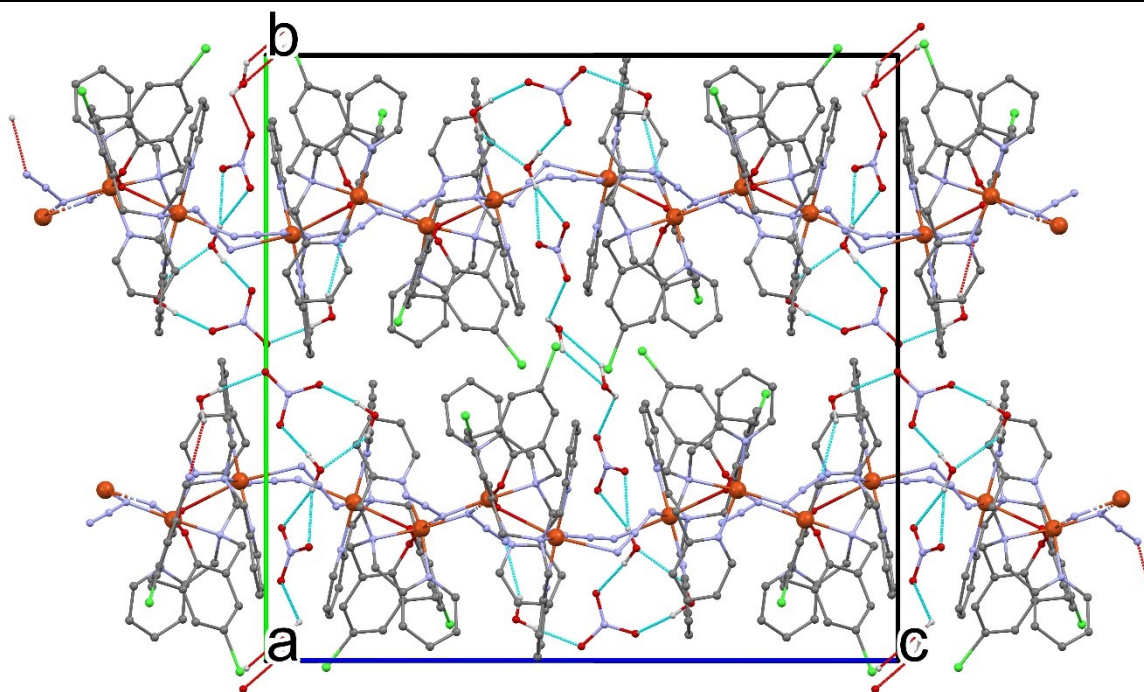
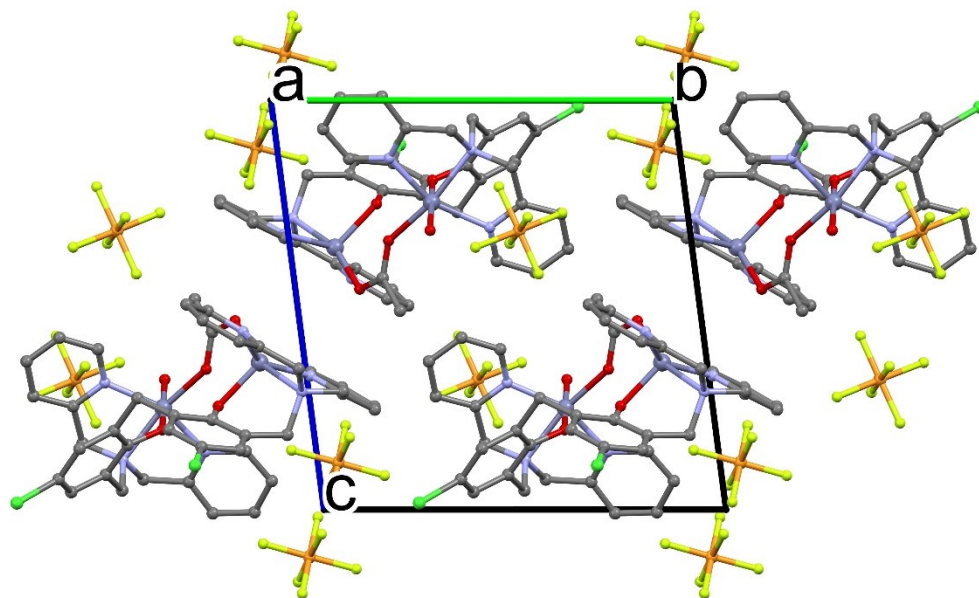
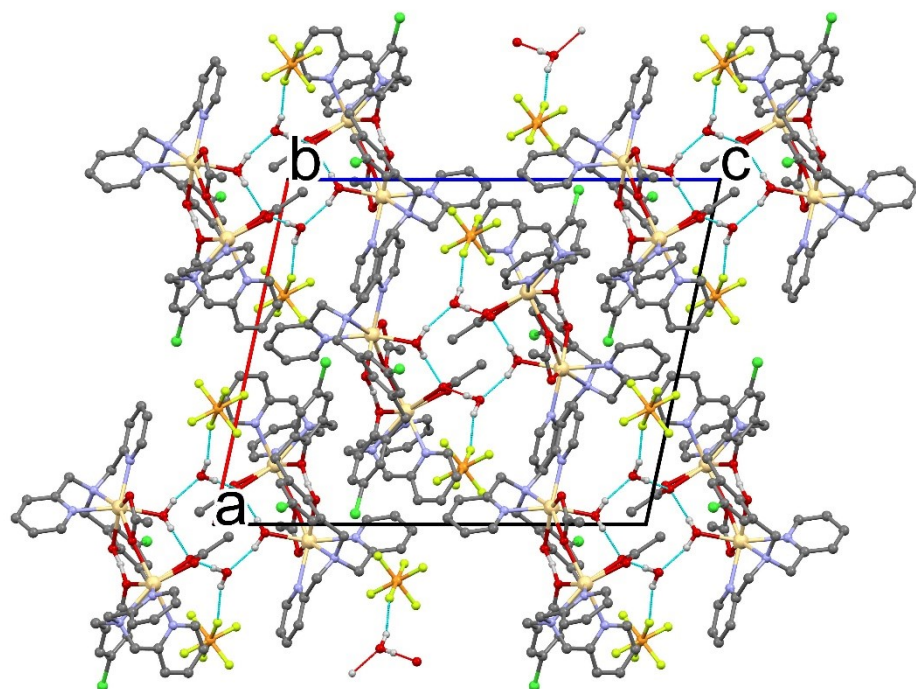


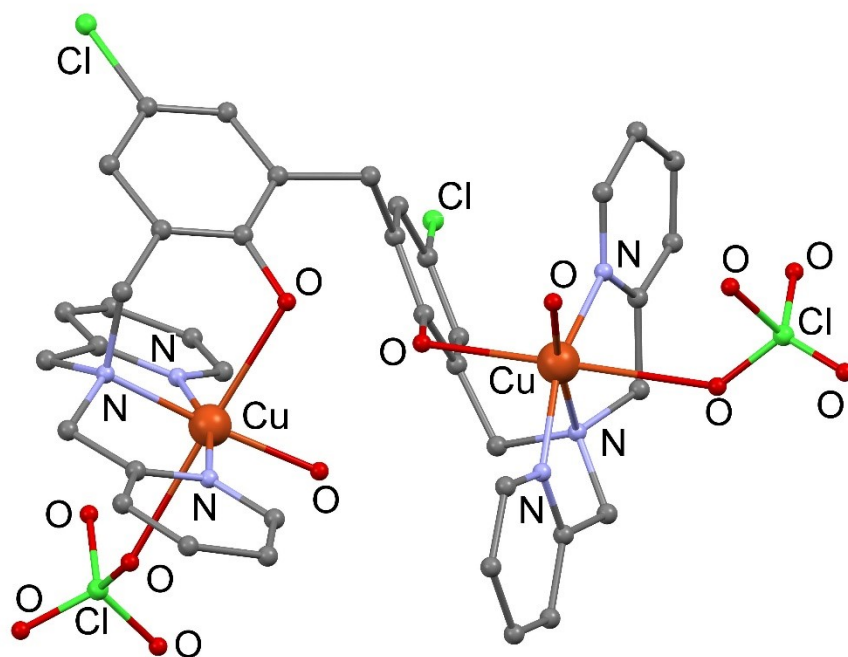
Fig. S11 Packing plot of 4.



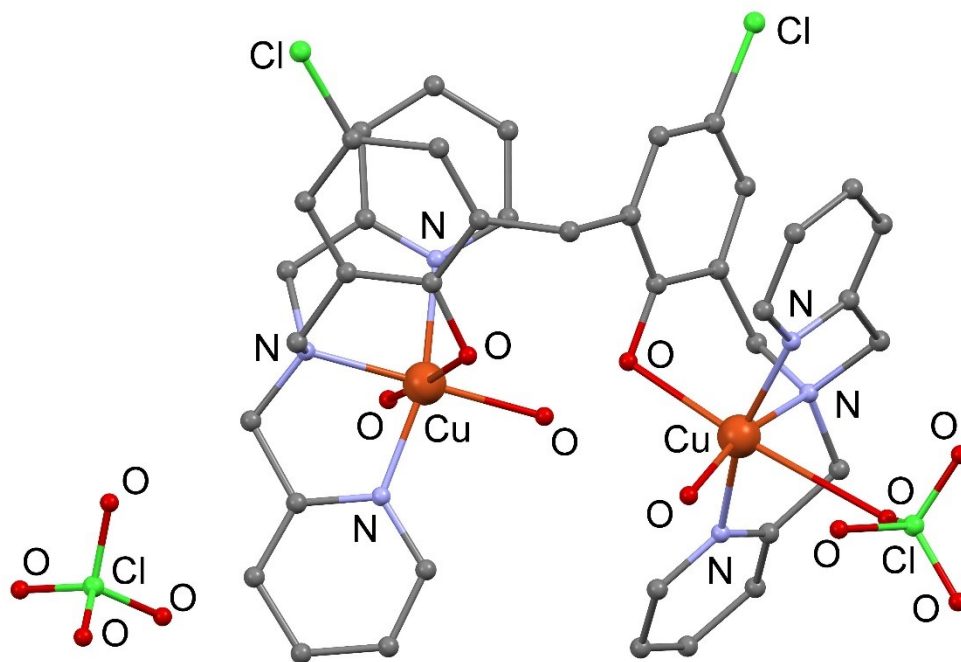
**Fig. S12** Packing plot of **5**. Disordered parts with minor occupancy omitted for clarity.



**Fig. S13** Packing plot of **6**.



**Fig. S14a** Perspective view of Cu1-Cu2 dimeric unit in **2**.



**Fig. S14b** Perspective view of Cu3-Cu4 dimeric unit in **2**.

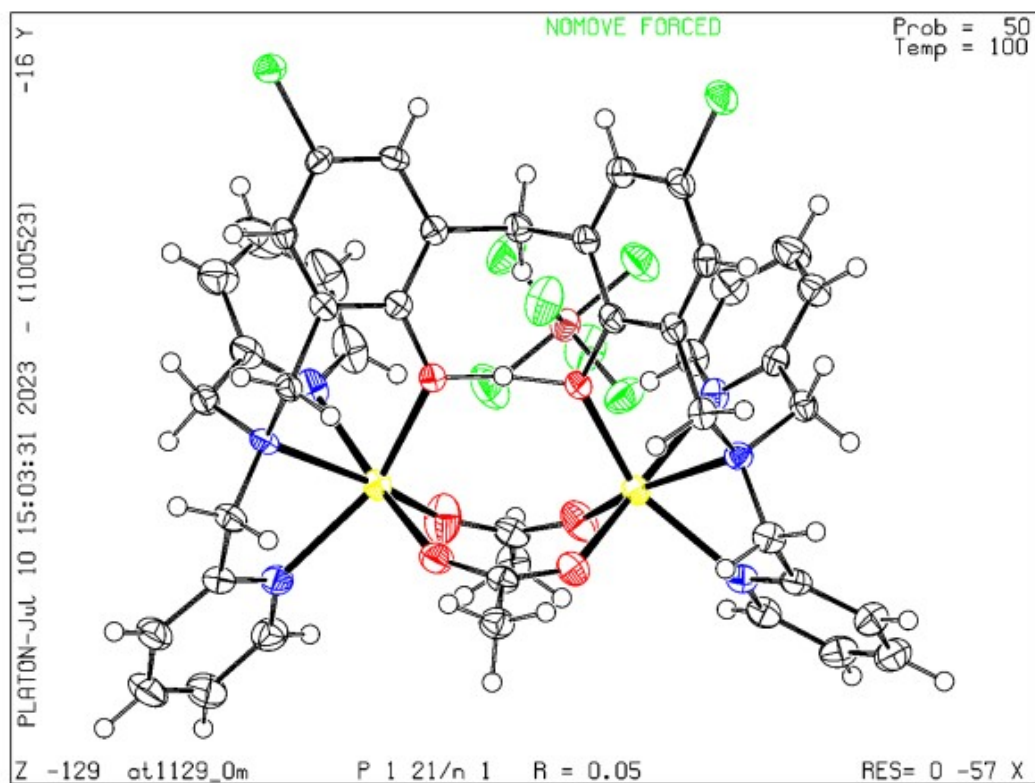


Fig. S15 ORTEP plot of 1.

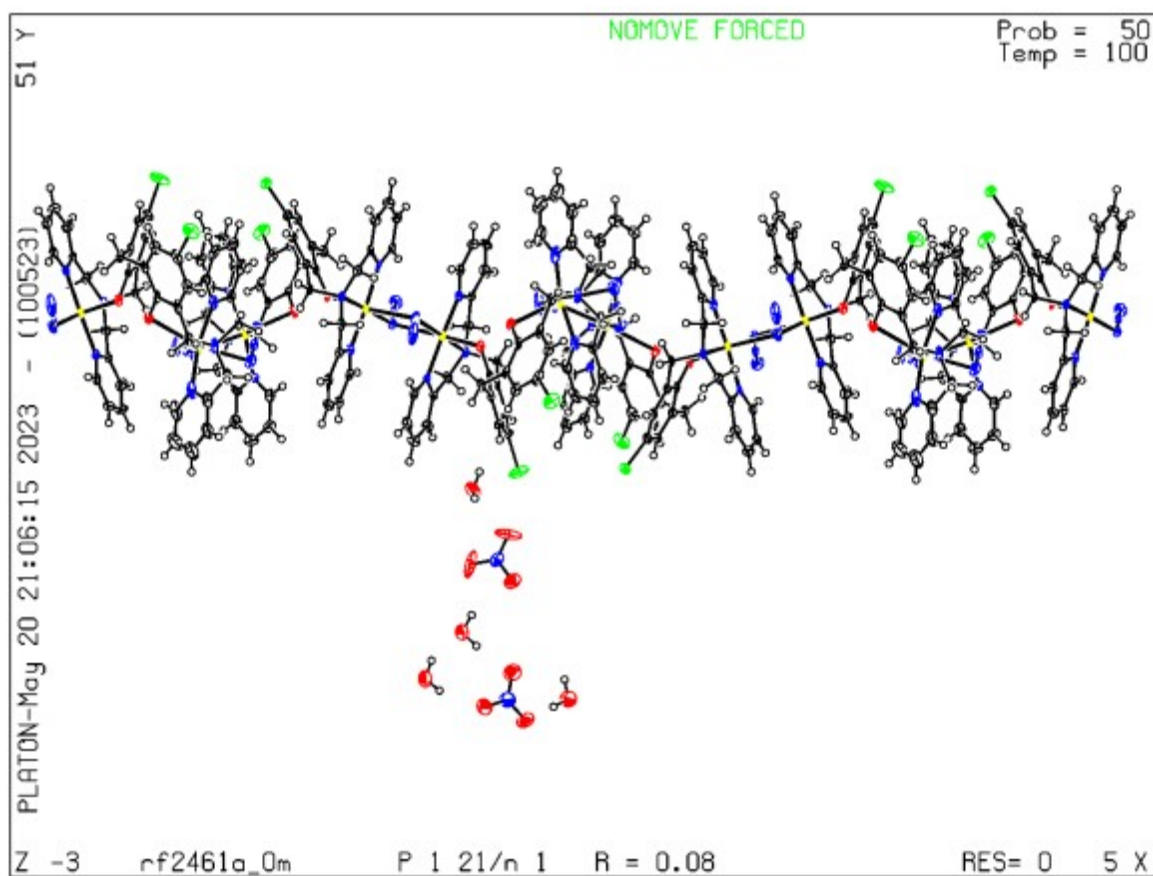


Fig. S16 ORTEP plot of 4.



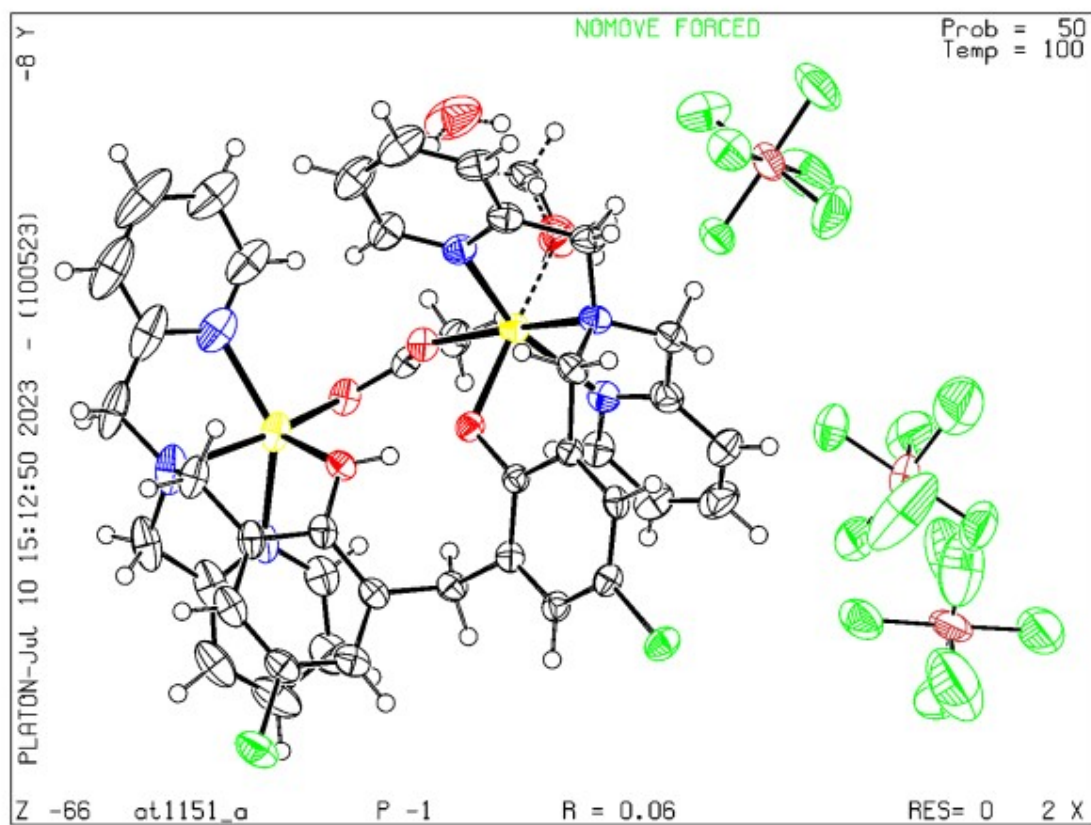


Fig. S17 ORTEP plot of 5.

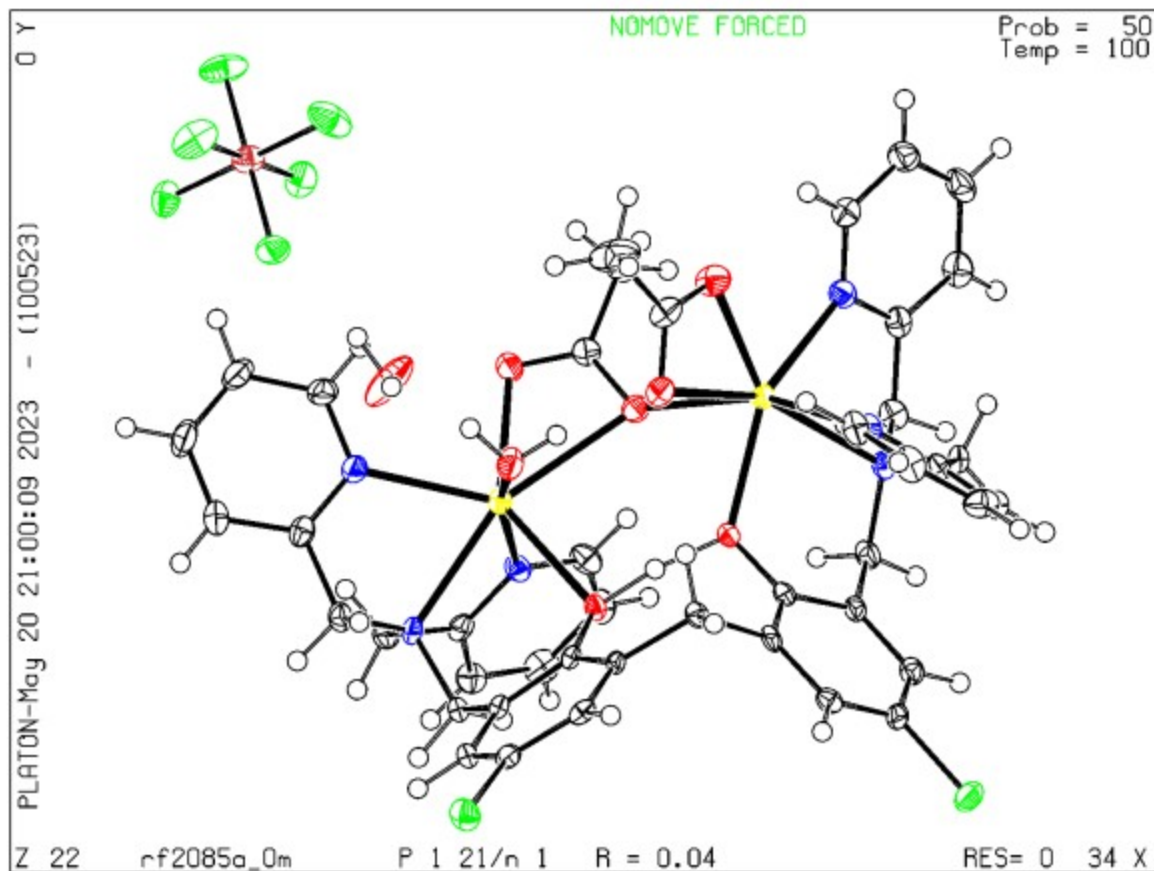


Fig. S18 ORTEP plot of 6.