Electronic Supplemental information

A Hydrogen bonded Co(II) Coordination Complex and a Triply Interpenetrating 3-D Manganese(II) Coordination Polymer from a Diaza Crown Ether with Dibenzoate Sidearms

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Figure S1. Single crystal of **L**H_2 chloride salt. (Black C, Grey H, Red O, Green Cl)

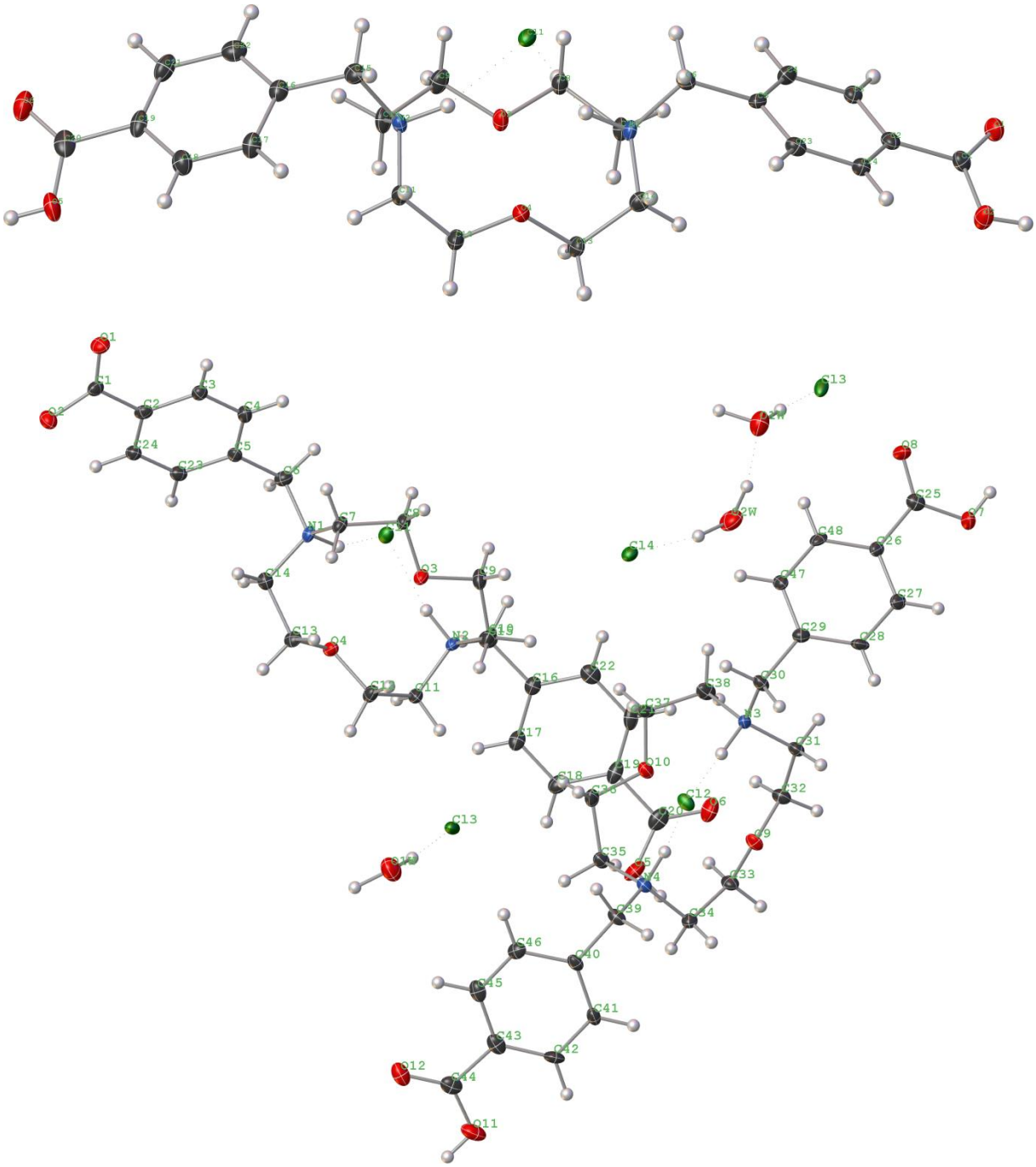


Figure S2a. Powder X-ray and simulated (from single crystal x-ray data) diffraction patterns of **1)**.

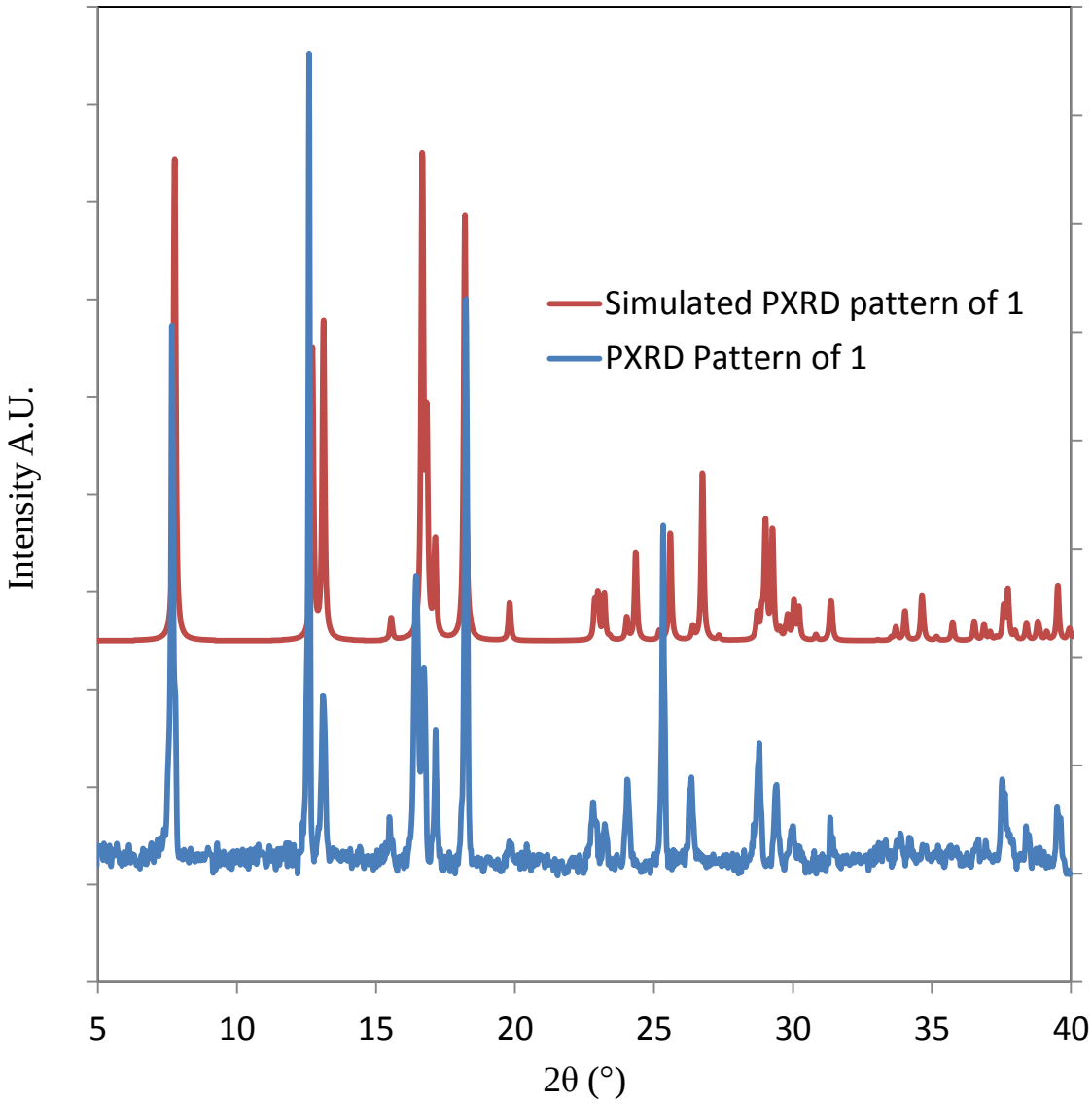


Figure S2b. Powder X-ray and simulated (from single crystal x-ray data) diffraction patterns of **2**.

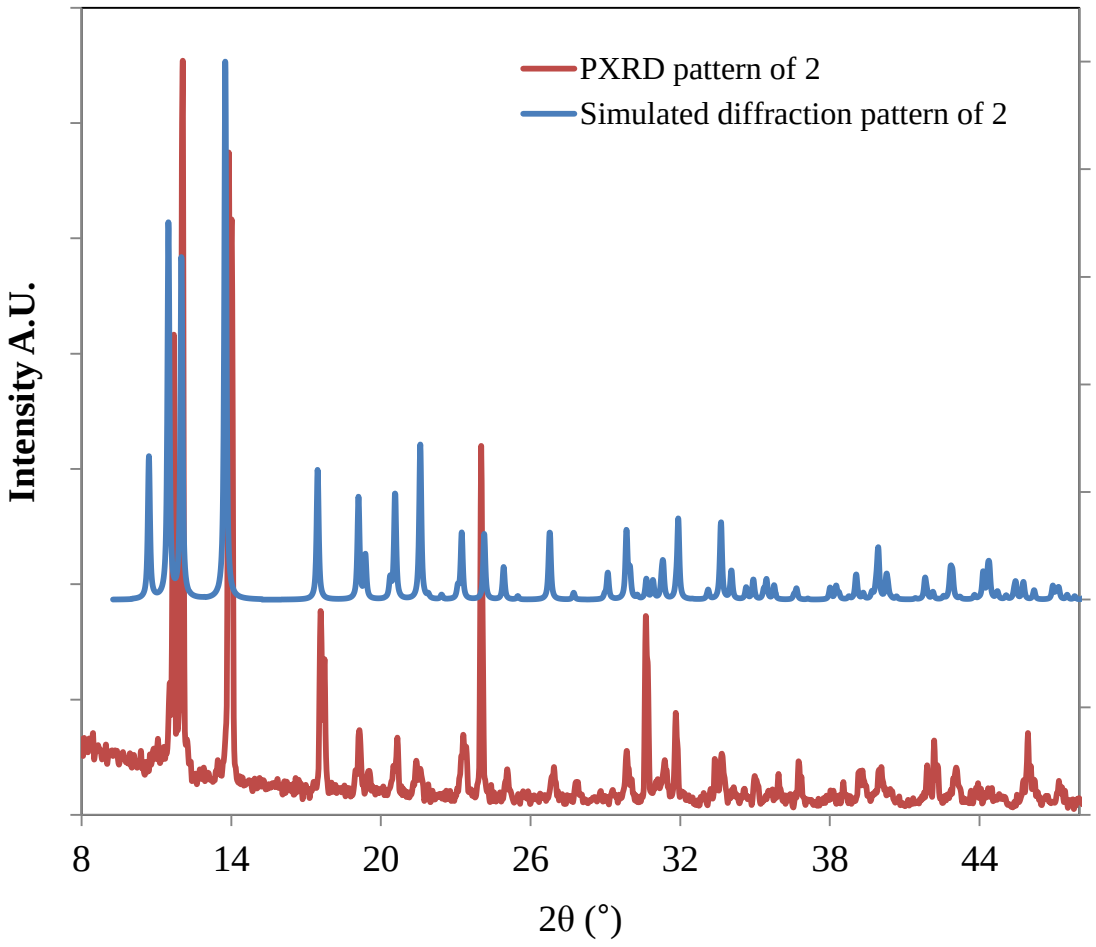
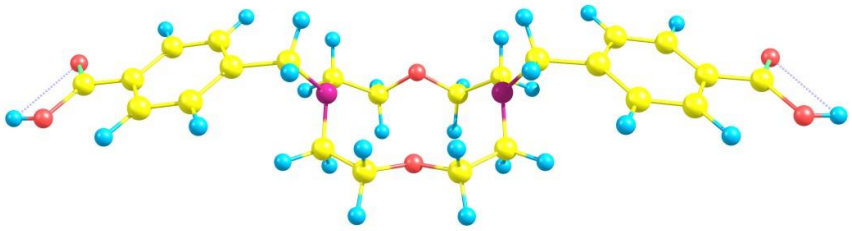
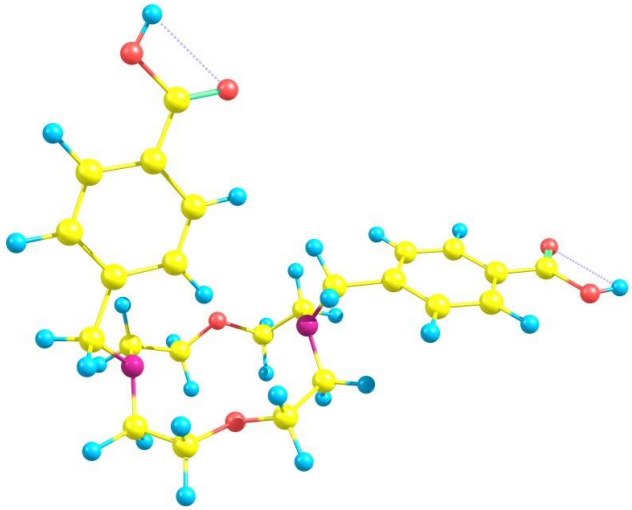


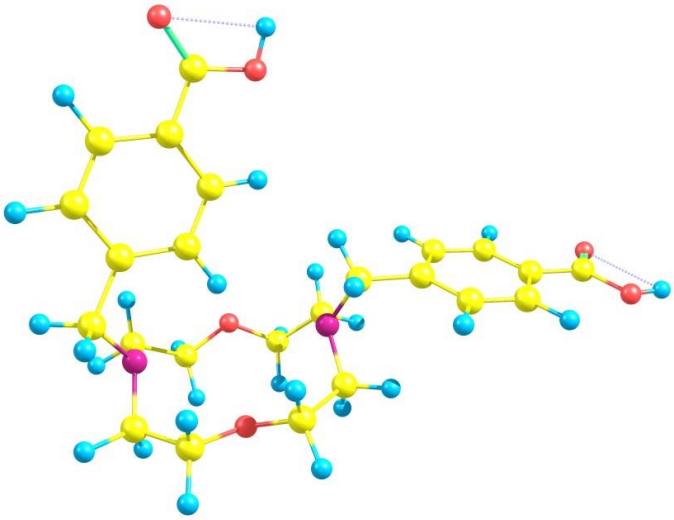
Figure S3: M06-2X/6-311+G(d,p) level optimized conformers of neutral ligand (**LH_2**) structure.



LH_2-Comp

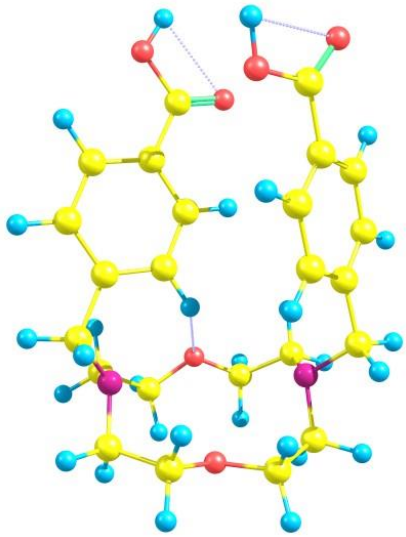


LH_2-C1

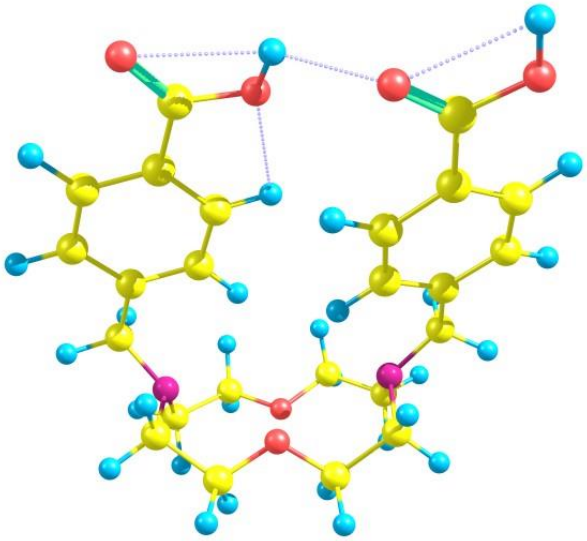


LH_2-C2

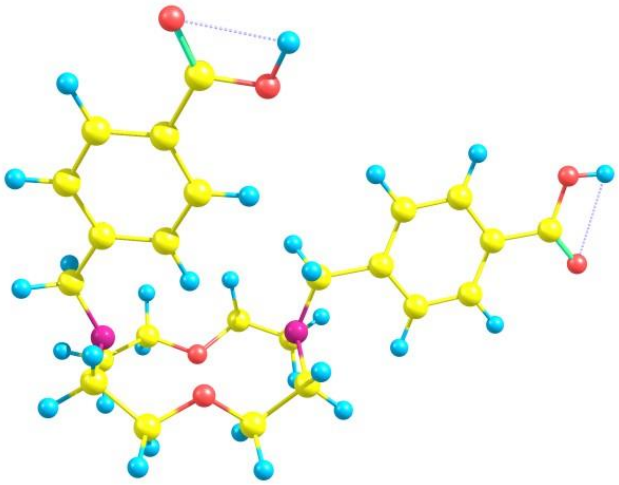
LH_2-C3



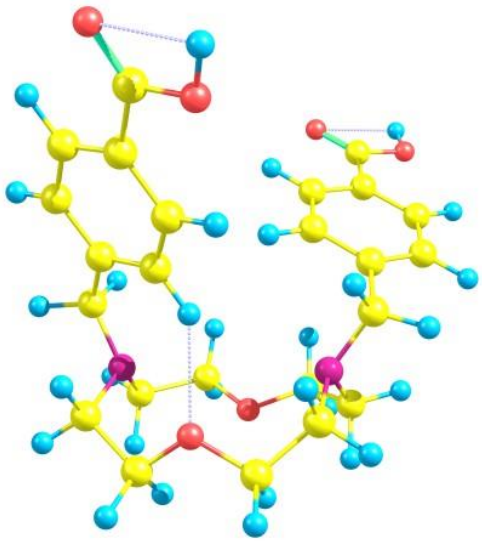
LH_2-C4



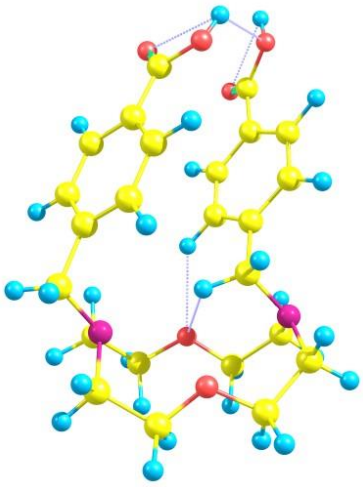
LH_2-C5



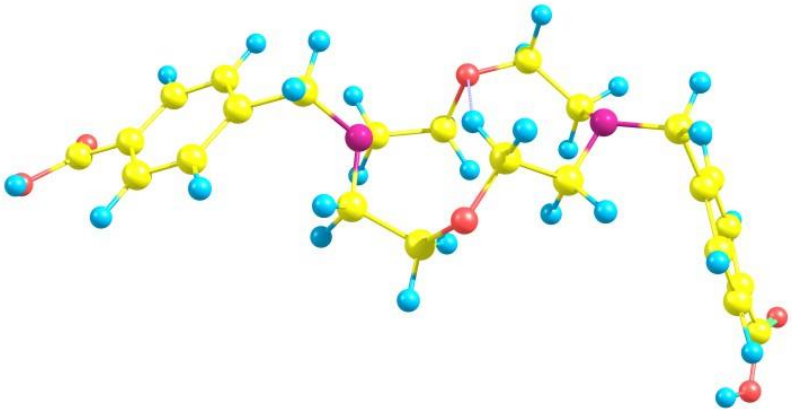
LH_2-C6



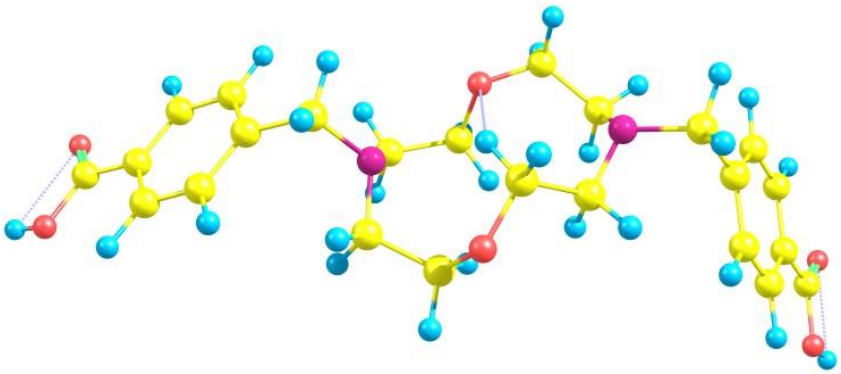
LH_2-C7



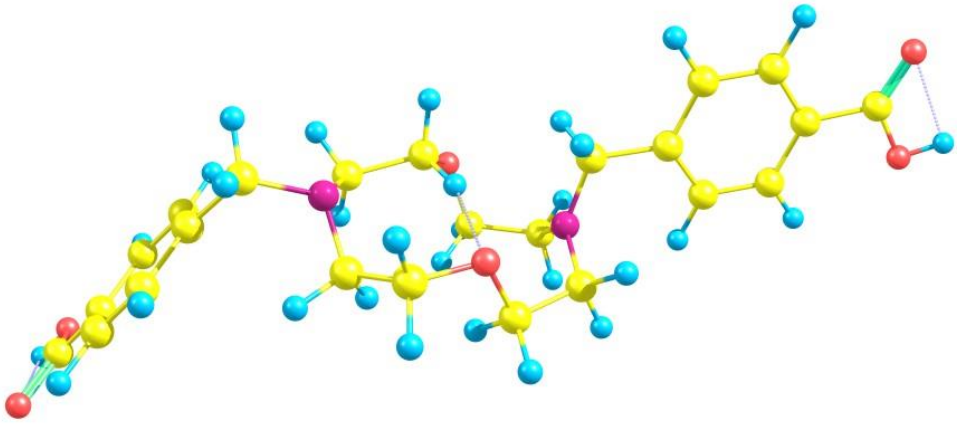
LH_2-C8



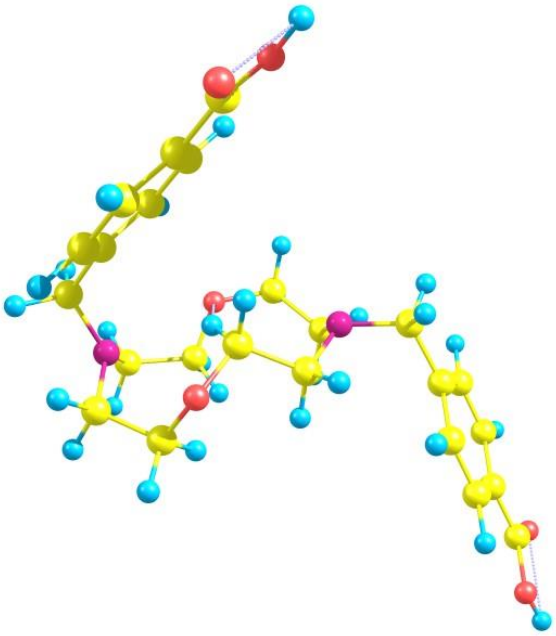
LH_2-C9



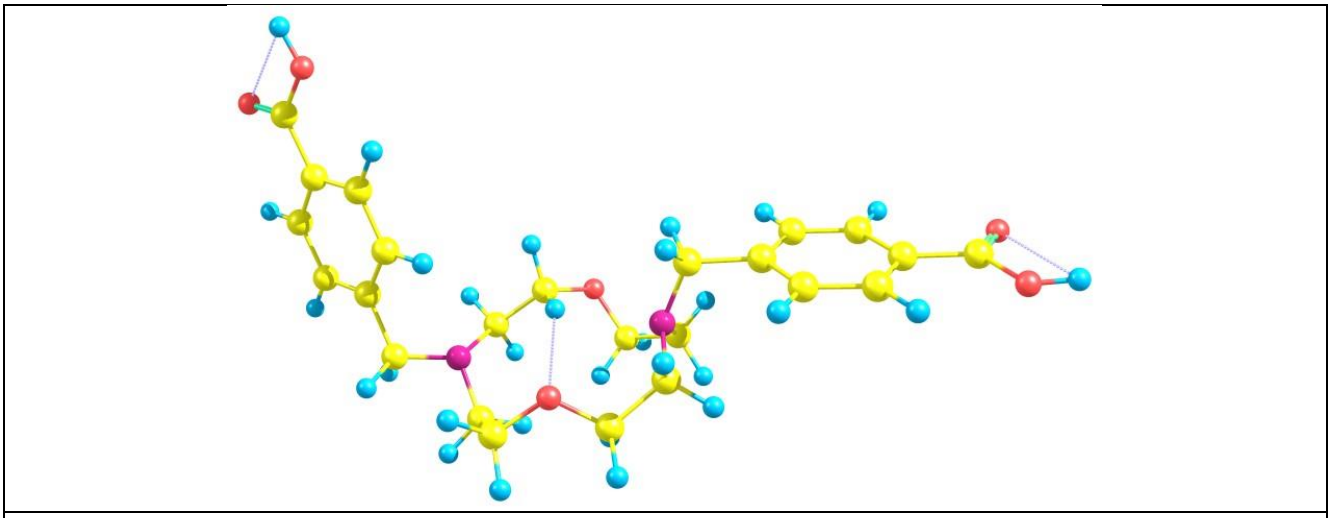
LH_2-C10



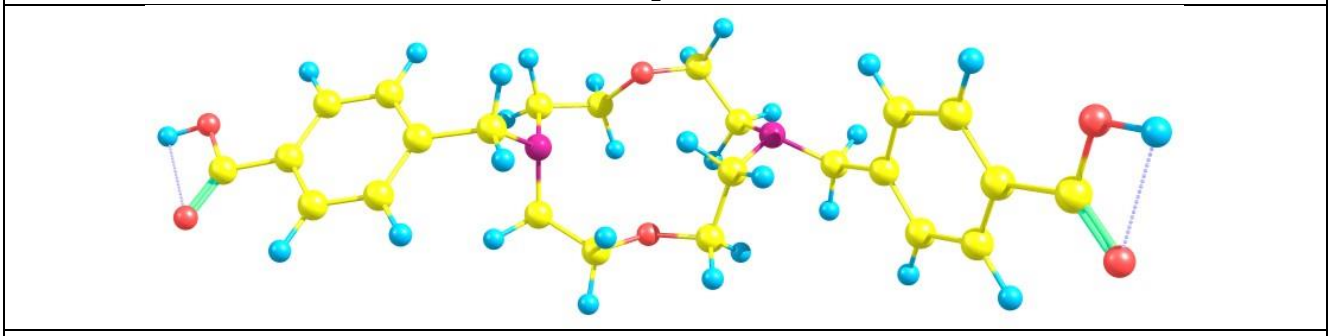
LH_2-C11



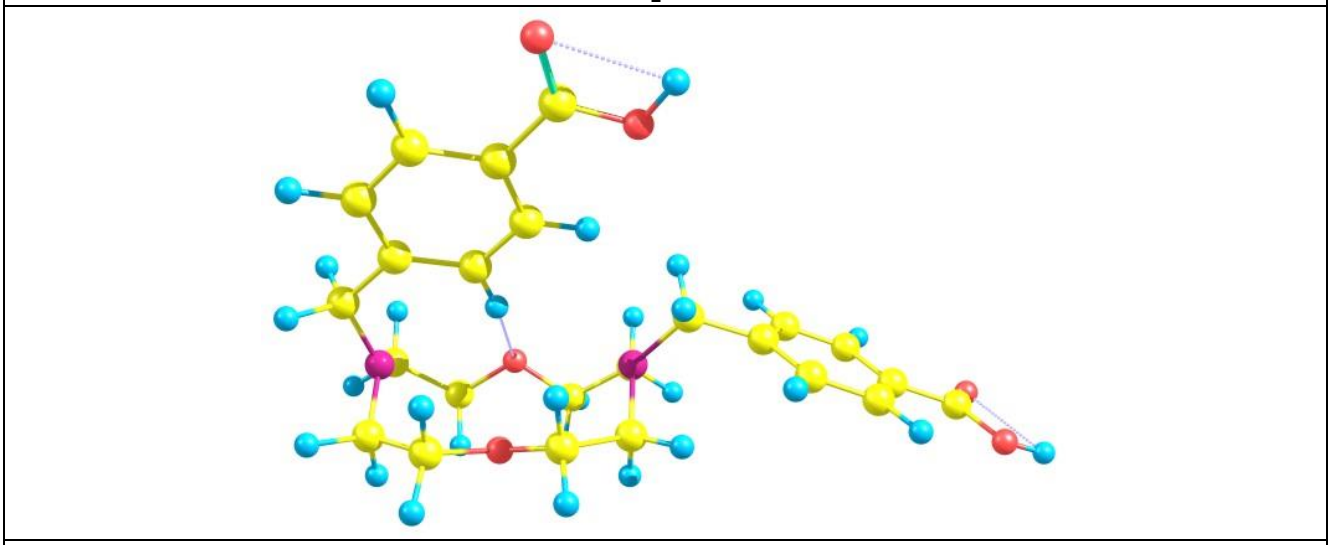
LH_2-C12



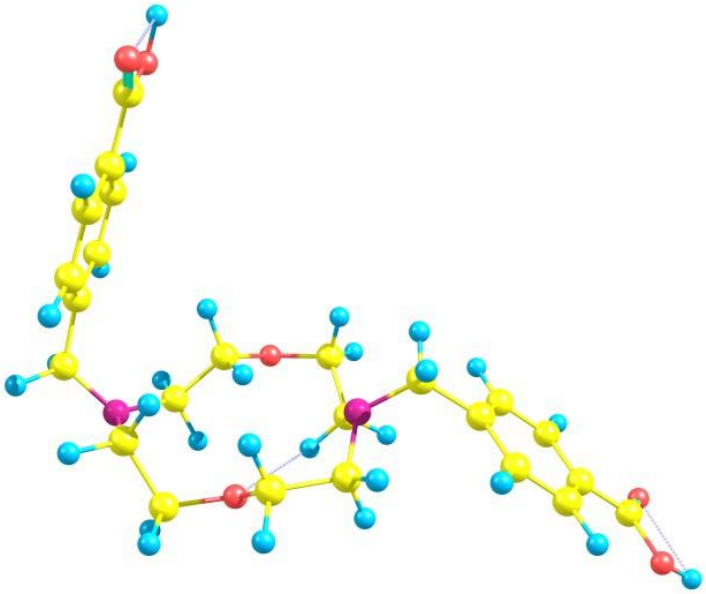
LH_2-C13



LH_2-C14

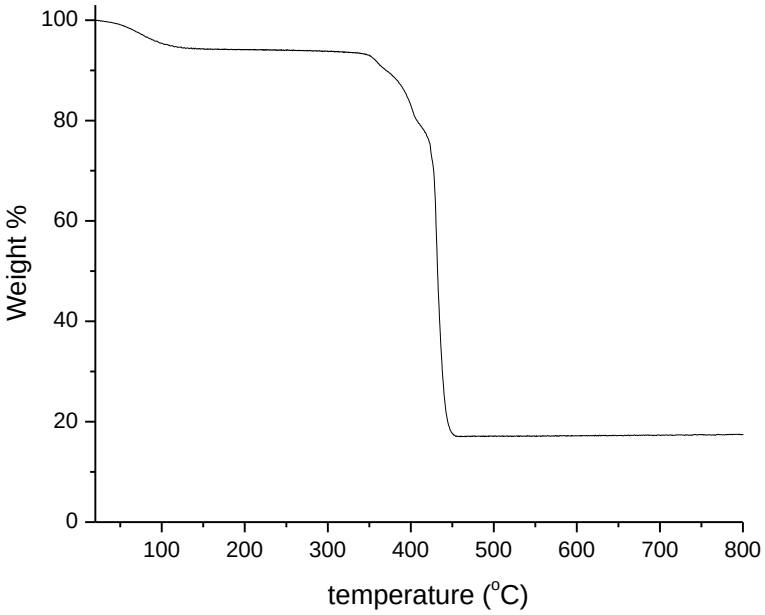


LH_2-C15

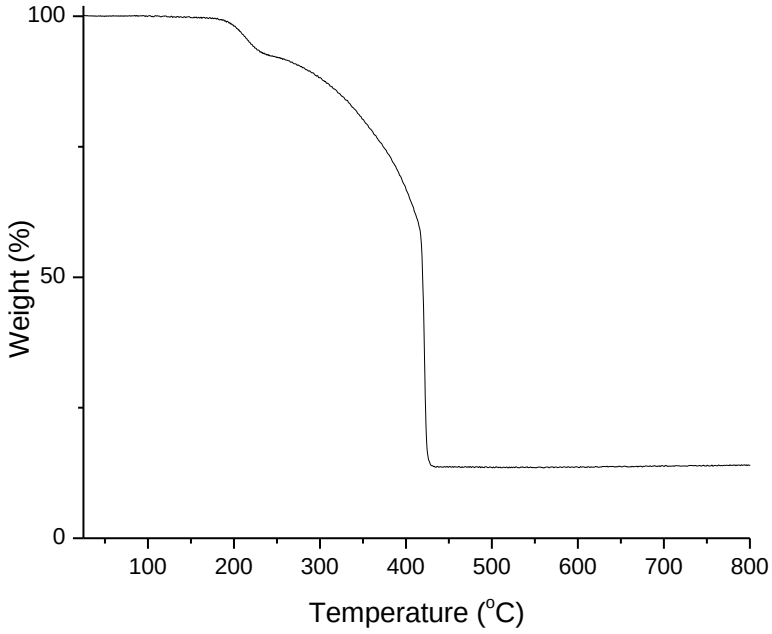


LH_2-C16

Figure S4. Thermogravimetric-analysis curves of **1** and **2**.



1



2

Table S1. Selected Bond Lengths and Bond Angles for **1** and **2**

Bond Length /Å			
	1		**2**
Co-O1	2.114(4)	Mn-O3	2.3203(19)
Co-O6	2.031(4)	Mn-O1	2.1278(18)
Co-O2	2.118(4)	Mn-N1[1]	2.393(2)
Co-O5	2.019(4)		
Co-N1[1]	2.242(3)	*Bond Angles*/°	
		O3-Mn-O3[1]	110.22(12)
Bond Angles/°		O3-Mn1-N1	73.93(7)
O1-Co1-O2	87.10(15)	O3[1]-Mn1-N1	73.32(8)
O1-Co-N1[1]	79.68(8)	O1[1]-Mn1-O3	150.28(7)
O6-Co1-O1	175.8(2)	O1-Mn1-O3	82.52(8)
O6-Co1-O2	88.74(17)	O1[1]-Mn1-O1	99.63(11)
O6-Co1-N1[1]	99.39(8)	O1[1]-Mn1-N1	135.71(8)
O2-Co1-N1[1]	77.19(8)	O1-Mn1-N1	85.43(8)
O5-Co1-O1	87.75(16)	O1-Mn1-N1[1]	135.71(8)
O5-Co1-O6	96.41(17)	N1[1]-Mn-1N1	120.94(11)
O5-Co1-O2	174.85(18)	C1-O1-Mn1	107.43(15)
O5-Co1-N1[1]	101.88(8)	C8[3]-N1-Mn1	108.19(14)
N1-Co1-N1[1]	147.69(16)	C12[1]-N1-Mn1	110.07(16)
C4[1]-O2-Co1	108.6(2)		
[1]+X,-Y,+Z, [1]-1/2-X,-3/2-Y,+Z		-3/4-X,3/4+Y,-1/4+Z;	

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	***x***	***y***	***z***	**U(eq)**
Co1	4800.2(7)	0	7014.0(8)	13.38(16)
O1	7211(5)	0	10858(7)	15.4(8)
O6	2603(6)	0	3259(7)	18.2(9)
O2	6525(6)	0	6183(7)	16.7(8)
O5	3362(5)	0	8136(8)	17.8(9)
O3	6138(4)	4048.4(11)	10446(5)	21.6(6)
C6	4500(5)	2003.5(14)	6829(8)	16.2(8)
N1	5620(4)	945.5(13)	7513(5)	15.3(6)
C12	6193(5)	3817.5(15)	8882(7)	17.7(7)
C9	5529(5)	3189.1(15)	8106(6)	15.4(7)
C5	4008(5)	1356.8(16)	6216(6)	16.8(7)
C7	4685(5)	2359.5(18)	5402(7)	18.1(8)
C3	6615(5)	1026.7(16)	6589(7)	18.8(7)
C10	5261(5)	2843.2(16)	9463(6)	18.0(7)
C11	4766(6)	2259.1(19)	8840(7)	18.7(8)
C2	6910(5)	1026.7(16)	10301(6)	16.9(7)
O4	6742(5)	4057.1(13)	7909(7)	39.6(9)
C1	8279(5)	531.5(15)	11670(7)	18.3(7)
C8	5220(5)	2943.4(17)	6064(7)	18.2(7)

C4	6216(6)	535.7(16)	4859(7)	19.3(7)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Co1	15.1(3)	9.6(3)	16.8(3)	0	11.2(2)	0
O1	16.6(19)	11(2)	17.6(18)	0	10.8(16)	0
O6	21(2)	8(2)	19.6(19)	0	10.8(18)	0
O2	25(2)	10(2)	21.6(18)	0	18.6(17)	0
O5	18(2)	12(2)	27(2)	0	16.7(18)	0
O3	26.6(15)	14.6(14)	21.4(13)	-5.5(10)	15.0(12)	-4.0(11)
C6	15(2)	9.3(15)	21.4(16)	-1.2(15)	10.7(17)	-1.3(12)
N1	17.4(14)	12.4(16)	16.0(13)	0.7(11)	11.0(12)	-0.3(12)
C12	14.8(16)	13.2(17)	20.9(15)	1.0(14)	10.1(13)	2.0(14)
C9	13.8(15)	9.8(17)	18.4(14)	1.4(12)	8.9(13)	2.3(13)
C5	17.7(16)	11.6(18)	21.3(16)	-0.3(13)	12.9(14)	-0.9(14)
C7	19.0(18)	16(2)	16.0(15)	-1.0(14)	10.2(14)	-0.8(15)
C3	22.7(18)	14.7(19)	22.0(16)	3.1(13)	16.1(15)	-0.4(14)
C10	19.6(17)	14.5(19)	21.6(17)	-1.9(13)	14.4(15)	-2.0(14)
C11	21.0(19)	13(2)	25.4(18)	1.6(14)	16.9(16)	-1.2(15)
C2	19.4(18)	12.1(18)	17.4(15)	-2.2(13)	11.4(14)	0.6(14)
O4	68(2)	19.2(17)	69(2)	-16.4(15)	62(2)	-19.8(16)
C1	18.5(17)	15.3(19)	19.9(15)	-1.8(13)	12.2(14)	-3.8(14)
C8	19.9(18)	13.7(18)	21.4(17)	0.8(13)	13.8(15)	-0.5(14)
C4	28.1(19)	14.6(19)	24.0(16)	2.6(14)	21.0(15)	-0.2(15)

Table S4. Torsion Angles for **1**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Co1	O1	C1	C2	37.9(3)	C5	N1	C2	C1	166.4(3)
Co1	O2	C4	C3	57.8(3)	C7	C6	C5	N1	89.9(4)
Co1	N1	C5	C6	170.5(2)	C7	C6	C11	C10	-2.2(6)
Co1	N1	C3	C4	19.5(3)	C3	N1	C5	C6	-67.3(4)
Co1	N1	C2	C1	46.0(3)	C3	N1	C2	C1	-69.5(4)
O3	C12	C9	C10	-13.9(5)	C10	C9	C8	C7	-1.2(5)
O3	C12	C9	C8	167.8(3)	C11	C6	C5	N1	-90.6(4)
C6	C7	C8	C9	-1.9(6)	C11	C6	C7	C8	3.5(6)
N1	C3	C4	O2	-50.4(4)	C2	N1	C5	C6	55.7(4)
N1	C2	C1	O1	-57.2(4)	C2	N1	C3	C4	131.6(3)
C12	C9	C10	C11	-175.9(4)	O4	C12	C9	C10	166.2(4)
C12	C9	C8	C7	177.3(3)	O4	C12	C9	C8	-12.2(5)
C9	C10	C11	C6	-0.9(6)	C11	O1	C1	C2	170.9(2)
C5	C6	C7	C8	-177.0(3)	C8	C9	C10	C11	2.5(5)
C5	C6	C11	C10	178.3(3)	C41	O2	C4	C3	179.8(3)
C5	N1	C3	C4	-105.0(3)					

Table S5 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×10^3) for **1.**

Atom	x	y	z	U(eq)
H5A	3300	1245	6672	20
H5B	3230	1305	4412	20
H7	4448	2205	3997	22
H3A	7921	1042	8018	23
H3B	6253	1398	5699	23
H10	5415	3006	10795	22
H11	4609	2033	9777	22
H2A	6218	1046	10838	20
H2B	7557	1396	10739	20
H1A	9039	520	11240	22
H1B	9063	580	13477	22
H8	5373	3171	5127	22
H4A	4959	556	3278	23
H4B	7025	557	4514	23
H6	2040(70)	356(14)	2180(80)	50(16)
H5	2650(50)	343(3)	7950(120)	75

Table S6. Hydrogen Bonds in **1**.

D-H-A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O6-H6-O3[1]	0.994(6)	1.641(7)	2.635(3)	179(6)
O5-H5-O42	0.993(6)	1.619(8)	2.607(4)	173(4)

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

Table S7 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 of the trace of the orthogonalised U_{IJ} tensor**.**

Atom	*x*	*y*	*z*	U(eq)
Mn1	-2500	-7500	-14884.7(3)	14.48(11)
C11	-2483.8(9)	-4627(4)	-13772(3)	33.8(7)
C5	-3865.5(6)	-2917(2)	-16906.6(15)	18.1(4)
O3	-2784.4(6)	-5667(2)	-14078.3(14)	28.9(4)
C2	-3222.4(6)	-4561(2)	-16250.3(15)	18.0(4)
C8	-4211.6(6)	-2040(2)	-17265.5(15)	20.2(4)
C3	-3181.4(6)	-3039(2)	-16370.5(16)	19.2(4)
C4	-3501.5(6)	-2233(2)	-16697.7(16)	19.6(4)
C1	-2879.4(7)	-5433(2)	-15890.7(17)	21.7(4)
O1	-2952.0(5)	-6789.8(19)	-15718.9(13)	24.9(4)
O2	-2547.8(7)	-4826(3)	-15759.3(19)	31.9(5)
C7	-3583.6(7)	-5259(3)	-16466(2)	24.8(5)
C6	-3900.8(6)	-4445(2)	-16790.5(18)	24.4(5)
N1	-3045.6(6)	-8653(3)	-14168.1(14)	25.5(4)
C12	-2112.1(9)	-5450(4)	-13500(2)	33.8(6)
C10	-3049.8(9)	-6181(4)	-13466(2)	36.4(7)
C9	-3302.7(9)	-7411(3)	-13853(2)	34.1(7)
O1W	-3019.3(10)	-8987(3)	-16929.3(18)	46.

Table S8 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$**.**

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	13.09(14)	16.36(14)	14.0(2)	0	0	-0.96(13)
C11	36.7(14)	29.1(12)	35.5(19)	-11.2(12)	5.1(11)	-11.8(10)
C5	14.8(7)	21.5(7)	18.1(11)	-1.2(7)	-2.7(7)	4.2(6)
O3	30.5(8)	31.0(7)	25.1(10)	-8.6(7)	6.2(8)	-2.7(7)
C2	14.7(7)	21.3(7)	17.9(10)	1.3(7)	-3.4(7)	3.0(6)
C8	17.5(7)	25.8(8)	17.2(11)	-2.1(7)	-3.1(7)	7.7(7)
C3	14.8(7)	19.9(7)	22.7(12)	0.8(7)	-0.4(7)	1.1(6)
C4	16.3(7)	20.9(6)	21.6(11)	1.9(7)	-1.6(8)	2.7(6)
C1	21.5(8)	23.3(8)	20.1(12)	0.1(8)	-4.1(8)	6.0(7)
O1	29.4(8)	22.7(6)	22.5(10)	1.5(6)	-6.8(7)	6.3(6)

O2	19.0(7)	37.5(11)	39.3(16)	-2.5(10)	-10.8(8)	3.8(6)
C7	19.1(8)	21.1(7)	34.4(15)	2.7(9)	-6.6(9)	0.9(7)
C6	16.4(8)	22.9(7)	34.1(14)	-0.4(8)	-8.8(8)	0.5(6)
N1	24.0(8)	35.6(9)	16.8(10)	-1.9(8)	1.8(8)	-13.4(7)
C12	35.6(12)	43.6(14)	22.1(14)	-6.2(12)	1.5(11)	-15.4(12)
C10	33.5(12)	41.0(13)	34.8(18)	-14.3(12)	12.1(12)	-12.9(11)
C9	25.6(11)	40.7(13)	36.0(17)	-13.0(12)	11.8(12)	-9.0(9)
O1W	65.1(17)	39.5(10)	34.3(14)	-12.9(10)	-12.8(12)	-5.3(12

Table S9. Hydrogen Bonds for **2.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O1	0.999(16)	1.87(2)	2.821(3)	158(4)
O1W	H1WB	O2[1]	0.990(18)	2.02(4)	2.893(4)	146(5)

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

Table S10. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×10^3) for **2.**

Atom	**x**	**y**	**z**	**U(eq)**
H11A	-2598	-4063	-13310	41
H11B	-2411	-3914	-14205	41
H8B	-4101	-1356	-17680	24
H8A	-4396	-2735	-17547	24
H12A	-1903	-4737	-13321	41
H12B	-2180	-6097	-13035	41
H9A	-3495	-7805	-13445	41
H9B	-3463	-6992	-14307	41
H1WA	-3059(16)	-8120(50)	-16560(30)	69
H1WB	-2789(13)	-9590(60)	-16730(30)	69
H4	-3455(12)	-1178(15)	-16850(20)	23(5)
H3	-2913(5)	-2570(30)	-16260(30)	23(5)
H6	-4143(7)	-5050(30)	-16930(30)	23(5)
H7	-3615(13)	-6354(10)	-16410(30)	32(10)
H10A	-3241(11)	-5350(40)	-13360(30)	43(8)
H10B	-2883(13)	-6630(50)	-13020(20)	43(8)

Table S11: Total energy (*E*, in Hartrees) and relative energy (Δ*E*, in kcal/mol) for different conformers obtained at the M06-2X/6-31G(d) and M06-2X/6-311+G(d,p) levels.

Sl. No.	Conformer	M06-2X/6-31G(d)		M06-2X/6-311+G(d,p)	
		E (Hartrees)	Δ*E* (kcal/mol)	*E* (Hartrees)	Δ*E* (kcal/mol)
1	**LH_2-Comp**	-1492.83425	8.06	–1493.26942	6.75
2	**LH_2-C1**	-1492.84254	2.86	–1493.27689	2.06
3	**LH_2-C2**	-1492.84243	2.93	–1493.27681	2.12
4	**LH_2-C3**	-1492.83239	9.23	–1493.26804	7.62
5	**LH_2-C4**	-1492.84573	0.86	–1493.28019	–0.01
6	**LH_2-C5**	-1492.84710	0.00	–1493.28018	0.00
7	**LH_2-C6**	-1492.84159	3.46	–1493.27623	2.48
8	**LH_2-C7**	-1492.84499	1.32	–1493.27946	0.46
9	**LH_2-C8**	-1492.84421	1.81	–1493.27733	1.79
10	**LH_2-C9**	-1492.80618	25.68	–1493.24192	24.01
11	**LH_2-C10**	-1492.82961	10.98	–1493.26374	10.32
12	**LH_2-C11**	-1492.83170	9.66	–1493.26570	9.09
13	**LH_2-C12**	-1492.82988	10.81	–1493.26456	9.80
14	**LH_2-C13**	-1492.83242	9.21	–1493.26658	8.53
15	**LH_2-C14**	-1492.83544	7.32	–1493.27034	6.18
16	**LH_2-C15**	-1492.84326	2.41	–1493.27736	1.77
17	**LH_2-C16**	-1492.83434	8.01	–1493.26938	6.78

Table 12: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for ligand**,** **LH_2** chloride salt. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	**x**	**y**	**z**	U_{eq}
O1	-10783(4)	829(2)	11225(2)	20.6(10)
O3	-4327(4)	1848.7(19)	8354(2)	16.2(10)
O4	-2702(4)	950.5(19)	9083(2)	15.6(9)
O2	-9172(4)	420(2)	11743(2)	21.3(10)
O5	3458(4)	1928(2)	6374(2)	25.5(11)
O6	2372(5)	2215(2)	5543(2)	29.7(11)
N1	-5390(5)	949(2)	9155(2)	12.7(11)
N2	-2263(5)	1247(2)	7797(2)	13.3(11)
C3	-9185(6)	928(3)	10190(3)	13.9(13)
C7	-5819(6)	1605(3)	9098(3)	15.7(13)
C23	-7051(6)	192(3)	10204(3)	16.5(14)
C1	-9719(5)	625(3)	11245(3)	15.2(13)
C13	-3291(6)	1168(3)	9617(3)	15.5(13)
C8	-5650(5)	1818(3)	8454(3)	15.5(13)

Atom	x	y	z	U_{eq}
C24	-7804(6)	221(3)	10710(3)	15.6(14)
C2	-8879(6)	587(3)	10707(3)	16.1(13)
C5	-7340(6)	534(3)	9687(3)	13.7(13)
C12	-1721(6)	1354(3)	8886(3)	17.6(14)
C17	411(6)	1041(3)	7101(3)	18.3(14)
C14	-4538(6)	837(3)	9681(3)	16.8(14)
C11	-1280(6)	1163(3)	8273(3)	16.9(14)
C20	2438(7)	1962(3)	6029(3)	21.6(15)
C6	-6494(6)	499(3)	9142(3)	17.2(14)
C18	1464(6)	1296(3)	6820(3)	21.1(15)
C10	-2613(6)	1907(3)	7685(3)	19.0(14)
C16	-797(6)	1173(3)	6894(3)	15.8(13)
C4	-8416(6)	901(3)	9688(3)	18.3(14)
C19	1319(6)	1666(2)	6318(3)	18.6(14)
C15	-1937(6)	913(3)	7215(3)	18.4(14)
C9	-4017(6)	1998(3)	7749(3)	19.1(14)
C21	126(7)	1777(3)	6099(3)	21.2(15)
C22	-930(6)	1533(3)	6382(3)	20.7(15)
O10	470(4)	3214.9(19)	6712(2)	17.2(10)
O9	2212(4)	4024.7(18)	5957(2)	16.6(10)
O7	-3966(4)	4542(2)	3208(2)	23.6(11)
O8	-5666(4)	4204(2)	3708(2)	23.4(11)
O11	7641(4)	2948(2)	9165(2)	30.0(12)
O12	6072(5)	2692(2)	9794(2)	26.2(11)
N4	2663(5)	3773(2)	7185(2)	13.5(11)
N3	-567(5)	4095(2)	5914(2)	12.8(11)
C34	3712(6)	3801(3)	6728(3)	16.9(14)
C40	3907(6)	3863(3)	8155(3)	15.5(13)
C26	-3822(6)	4430(3)	4264(3)	14.0(13)
C47	-3482(6)	4150(3)	5300(3)	15.4(13)
C25	-4589(6)	4375(3)	3709(3)	17.7(14)
C35	2256(6)	3127(3)	7331(3)	17.1(14)
C42	6045(6)	3608(3)	8428(3)	20.3(14)
C27	-2755(6)	4804(3)	4283(3)	15.9(14)
C41	5195(6)	3898(3)	8043(3)	16.4(13)
C36	847(6)	3070(3)	7311(3)	18.9(14)
C39	2960(6)	4153(3)	7742(3)	15.5(13)
C48	-4187(6)	4113(3)	4771(3)	15.5(14)
C29	-2415(6)	4517(3)	5324(3)	15.6(14)
C33	3226(6)	3623(3)	6109(3)	17.1(14)
C28	-2066(6)	4852(3)	4815(3)	17.1(14)
C46	3486(6)	3553(3)	8666(3)	17.0(14)
C43	5607(6)	3286(3)	8921(3)	19.5(15)
C37	-862(6)	3247(3)	6637(3)	17.4(14)
C45	4326(6)	3266(3)	9045(3)	19.5(14)
C30	-1628(6)	4562(3)	5890(3)	16.1(13)
C44	6460(6)	2953(3)	9349(3)	20.3(14)
C31	313(6)	4161(3)	5387(3)	16.1(14)
C32	1510(6)	3794(3)	5456(3)	17.6(14)
C38	-1069(6)	3449(3)	6001(3)	19.5(15)
Cl4	-4088.2(13)	2662.0(7)	6284.2(8)	18.0(3)
Cl2	447.6(14)	4749.0(6)	7042.7(7)	16.6(3)
Cl1	-4510.7(14)	337.2(6)	7958.1(7)	15.9(3)
Cl3	1273.8(14)	2119.2(7)	8523.4(8)	20.5(3)
O1W	1338(5)	2883(2)	9672(3)	32.2(12)
O2W	-4041(5)	2385(2)	4916(3)	31.5(12)

Table S13: Anisotropic Displacement Parameters ($\times 10^4$) for ligand**,** $\mathbf{LH_2}$ chloride salt. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	14(2)	27(2)	21(3)	-1(2)	4(2)	2.4(17)
O3	12(2)	21(2)	16(2)	2.9(19)	4.5(18)	1.5(16)
O4	14(2)	20(2)	12(2)	-0.9(19)	1.1(18)	-4.3(17)
O2	17(2)	29(2)	17(3)	3(2)	3(2)	5.7(19)
O5	20(3)	26(2)	31(3)	1(2)	11(2)	-5.4(18)
O6	34(3)	32(3)	23(3)	3(2)	11(2)	-3(2)
N1	14(3)	13(2)	11(3)	1(2)	5(2)	0.1(19)
N2	10(3)	16(2)	15(3)	1(2)	2(2)	-1.3(19)
C3	15(3)	13(3)	14(3)	-1(3)	0(3)	-2(2)
C7	15(3)	15(3)	17(3)	2(3)	6(3)	1(2)
C23	15(3)	15(3)	20(4)	0(3)	-3(3)	-1(2)
C1	13(3)	14(3)	19(3)	3(3)	0(3)	-2(2)
C13	14(3)	17(3)	15(3)	-4(3)	4(3)	2(2)
C8	15(3)	17(3)	15(3)	4(3)	4(3)	0(2)
C24	14(3)	19(3)	14(4)	0(3)	-1(3)	-1(2)
C2	14(3)	17(3)	18(4)	-4(3)	0(3)	-4(2)
C5	15(3)	15(3)	11(3)	-1(3)	-1(3)	-3(2)
C12	17(3)	21(3)	14(3)	-2(3)	3(3)	-5(2)
C17	21(3)	14(3)	20(4)	2(3)	6(3)	4(2)
C14	19(3)	17(3)	15(3)	1(3)	-1(3)	2(2)
C11	13(3)	24(3)	14(3)	3(3)	2(3)	-1(3)
C20	27(4)	13(3)	24(4)	-7(3)	7(3)	-1(3)
C6	14(3)	20(3)	17(4)	-4(3)	0(3)	-2(2)
C18	19(3)	20(3)	24(4)	-1(3)	5(3)	2(2)
C10	20(3)	16(3)	21(4)	5(3)	8(3)	-1(2)
C16	19(3)	12(3)	16(4)	-2(3)	3(3)	1(2)
C4	19(4)	22(3)	14(4)	3(3)	-1(3)	-2(3)
C19	27(3)	10(3)	19(4)	-2(3)	11(3)	1(2)
C15	18(3)	20(3)	17(4)	-7(3)	2(3)	-1(2)
C9	22(4)	19(3)	16(4)	5(3)	4(3)	5(2)
C21	34(4)	13(3)	16(4)	2(3)	6(3)	3(3)
C22	24(4)	16(3)	22(4)	-5(3)	-3(3)	2(2)
O10	19(2)	18(2)	15(2)	2.9(19)	-4.4(19)	-1.9(17)
O9	20(2)	17(2)	12(2)	-2.9(19)	-6(2)	-0.3(17)
O7	24(3)	33(3)	14(3)	7(2)	-2(2)	-8(2)
O8	16(2)	35(3)	18(3)	2(2)	-3(2)	-9(2)
O11	22(3)	33(3)	36(3)	0(2)	-13(2)	3(2)
O12	35(3)	23(2)	20(3)	2(2)	-6(2)	3(2)
N4	14(3)	14(2)	12(3)	0(2)	-2(2)	1.3(19)
N3	13(3)	13(2)	13(3)	3(2)	-2(2)	-2.1(19)
C34	12(3)	20(3)	19(4)	4(3)	0(3)	1(2)
C40	19(3)	14(3)	13(3)	-2(3)	-4(3)	-1(2)
C26	13(3)	11(3)	17(3)	2(3)	0(3)	1(2)
C47	11(3)	22(3)	13(4)	0(3)	2(3)	2(2)
C25	19(3)	13(3)	20(4)	-2(3)	-2(3)	1(2)
C35	20(3)	14(3)	17(4)	1(3)	-4(3)	-2(2)
C42	12(3)	25(3)	25(4)	-1(3)	-6(3)	-1(2)
C27	15(3)	12(3)	21(4)	3(3)	-1(3)	2(2)
C41	21(3)	15(3)	13(3)	3(3)	-3(3)	-2(2)
C36	22(3)	18(3)	16(4)	5(3)	-1(3)	-6(3)
C39	15(3)	17(3)	14(3)	-5(3)	-2(3)	7(2)
C48	6(3)	17(3)	23(4)	1(3)	2(3)	1(2)
C29	11(3)	16(3)	20(4)	-2(3)	0(3)	2(2)
C33	13(3)	23(3)	16(4)	-1(3)	0(3)	5(2)
C28	12(3)	19(3)	20(4)	2(3)	-5(3)	-3(2)
C46	17(3)	18(3)	16(4)	-4(3)	2(3)	0(2)
C43	29(4)	12(3)	18(4)	-4(3)	-7(3)	1(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C37	13(3)	17(3)	22(4)	2(3)	-6(3)	-3(2)
C45	31(4)	15(3)	13(3)	-4(3)	0(3)	3(3)
C30	16(3)	17(3)	15(3)	0(3)	-4(3)	0(2)
C44	22(4)	13(3)	26(4)	-6(3)	-5(3)	0(2)
C31	15(3)	20(3)	14(4)	1(3)	-3(3)	0(2)
C32	16(3)	19(3)	17(4)	-4(3)	-3(3)	1(2)
C38	21(3)	12(3)	25(4)	0(3)	-5(3)	-3(2)
Cl4	12.2(7)	22.3(7)	19.5(8)	3.9(7)	1.8(6)	-0.5(5)
Cl2	18.6(8)	18.5(7)	12.6(8)	-3.0(6)	-2.9(6)	4.7(5)
Cl1	18.1(7)	18.0(7)	11.6(8)	-2.2(6)	1.0(6)	-3.8(5)
Cl3	13.7(7)	26.8(7)	20.9(8)	11.0(7)	-6.5(7)	-6.8(6)
O1W	35(3)	32(3)	30(3)	6(2)	-5(3)	2(2)
O2W	23(3)	40(3)	32(3)	-2(3)	8(2)	-4(2)

Table S14: Bond Lengths in Å for ligand**, L**H_2 chloride salt

Atom	Atom	Length/Å
O1	C1	1.216(7)
O3	C8	1.423(7)
O3	C9	1.419(8)
O4	C13	1.422(7)
O4	C12	1.433(7)
O2	C1	1.324(8)
O5	C20	1.327(9)
O6	C20	1.214(9)
N1	C7	1.510(7)
N1	C14	1.496(8)
N1	C6	1.529(8)
N2	C11	1.496(8)
N2	C10	1.509(7)
N2	C15	1.523(8)
C3	C2	1.406(9)
C3	C4	1.382(9)
C7	C8	1.512(9)
C23	C24	1.378(9)
C23	C5	1.401(9)
C1	C2	1.492(9)
C13	C14	1.515(9)
C24	C2	1.392(8)
C5	C6	1.508(9)
C5	C4	1.396(9)
C12	C11	1.499(9)
C17	C18	1.397(9)
C17	C16	1.391(9)
C20	C19	1.496(9)
C18	C19	1.385(9)
C10	C9	1.510(9)
C16	C15	1.515(9)
C16	C22	1.390(9)
C19	C21	1.377(10)
C21	C22	1.390(9)
O10	C36	1.424(8)
O10	C37	1.424(7)
O9	C33	1.429(7)
O9	C32	1.430(8)
O7	C25	1.343(8)
O8	C25	1.203(7)
O11	C44	1.318(8)
O12	C44	1.212(8)
N4	C34	1.508(8)
N4	C35	1.511(7)
N4	C39	1.522(8)
N3	C30	1.521(8)
N3	C31	1.502(8)
N3	C38	1.523(7)
C34	C33	1.515(9)
C40	C41	1.391(9)
C40	C39	1.500(9)
C40	C46	1.394(9)
C26	C25	1.481(9)
C26	C27	1.397(8)
C26	C48	1.376(9)
C47	C48	1.394(9)
C47	C29	1.388(9)
C35	C36	1.501(9)
C42	C41	1.395(9)
C42	C43	1.381(10)
C27	C28	1.392(9)
C29	C28	1.395(9)
C29	C30	1.512(9)
C46	C45	1.376(9)
C43	C45	1.387(9)
C43	C44	1.500(9)
C37	C38	1.494(9)
C31	C32	1.510(8)

Table S15: Bond Angles in ° for ligand**, LH_2** chloride salt.

Atom	Atom	Atom	Angle/°
C9	O3	C8	112.8(5)
C13	O4	C12	111.5(5)
C7	N1	C6	112.2(5)
C14	N1	C7	113.8(5)
C14	N1	C6	111.9(5)
C11	N2	C10	114.0(5)
C11	N2	C15	112.4(5)
C10	N2	C15	112.0(5)
C4	C3	C2	120.0(6)
N1	C7	C8	109.6(5)
C24	C23	C5	121.0(6)
O1	C1	O2	124.2(6)
O1	C1	C2	123.0(6)
O2	C1	C2	112.7(5)
O4	C13	C14	107.5(5)
O3	C8	C7	106.3(5)
C23	C24	C2	119.9(6)
C3	C2	C1	119.1(5)
C24	C2	C3	119.8(6)
C24	C2	C1	121.2(6)
C23	C5	C6	119.9(5)
C4	C5	C23	119.0(6)
C4	C5	C6	121.1(6)
O4	C12	C11	109.3(5)
C16	C17	C18	120.4(6)
N1	C14	C13	112.2(5)
N2	C11	C12	112.9(5)
O5	C20	C19	112.2(6)
O6	C20	O5	125.7(6)
O6	C20	C19	122.1(7)
C5	C6	N1	114.2(5)
C19	C18	C17	120.2(6)
N2	C10	C9	110.7(5)
C17	C16	C15	120.2(6)
C22	C16	C17	118.8(6)
C22	C16	C15	121.0(6)
C3	C4	C5	120.5(6)
C18	C19	C20	120.5(6)
C21	C19	C20	120.2(6)
C21	C19	C18	119.2(6)
C16	C15	N2	113.5(5)
O3	C9	C10	106.7(5)
C19	C21	C22	121.0(6)
C16	C22	C21	120.3(6)
C36	O10	C37	113.5(5)
C33	O9	C32	111.0(4)
C34	N4	C35	113.1(5)
C34	N4	C39	111.8(5)
C35	N4	C39	113.3(5)
C30	N3	C38	111.6(5)
C31	N3	C30	111.7(5)
C31	N3	C38	113.9(5)
N4	C34	C33	110.4(5)
C41	C40	C39	121.7(6)
C41	C40	C46	119.1(6)
C46	C40	C39	119.1(6)

Atom	Atom	Atom	Angle/°
C27	C26	C25	121.2(6)
C48	C26	C25	119.0(5)
C48	C26	C27	119.9(6)
C29	C47	C48	120.2(6)
O7	C25	C26	113.4(5)
O8	C25	O7	123.4(6)
O8	C25	C26	123.2(6)
C36	C35	N4	110.8(5)
C43	C42	C41	119.9(6)
C28	C27	C26	119.7(6)
C40	C41	C42	120.1(6)
O10	C36	C35	106.8(5)
C40	C39	N4	113.8(5)
C26	C48	C47	120.5(6)
C47	C29	C28	119.3(6)
C47	C29	C30	121.3(6)
C28	C29	C30	119.4(5)
O9	C33	C34	108.2(5)
C27	C28	C29	120.4(6)
C45	C46	C40	120.7(6)
C42	C43	C45	120.2(6)
C42	C43	C44	123.0(6)
C45	C43	C44	116.8(6)
O10	C37	C38	105.7(5)
C46	C45	C43	119.9(6)
C29	C30	N3	113.2(5)
O11	C44	C43	112.4(6)
O12	C44	O11	124.9(6)
O12	C44	C43	122.6(6)
N3	C31	C32	113.2(5)
O9	C32	C31	109.2(5)
C37	C38	N3	110.0(5)

Table S16: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for ligand**, LH_2** chloride salt. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H2	-9704	408	12023	32
H5	4050	2123	6210	38
H1	-4879	861	8786	15
H2A	-3042	1046	7955	16
H3	-9920	1176	10186	17
H7A	-5320	1867	9372	19
H7B	-6718	1638	9214	19
H23	-6326	-63	10206	20
H13A	-3432	1615	9589	19
H13B	-2750	1086	9971	19
H8A	-6045	1525	8171	19
H8B	-6040	2225	8396	19
H24	-7590	-8	11059	19
H12A	-1009	1340	9175	21
H12B	-2041	1780	8871	21
H17	519	776	7437	22
H14A	-4378	392	9718	20
H14B	-4961	975	10054	20
H11A	-524	1404	8164	20
H11B	-1032	726	8286	20
H6A	-7005	579	8777	21
H6B	-6156	78	9110	21
H18	2284	1216	6973	25
H10A	-2346	2027	7274	23
H10B	-2165	2172	7976	23
H4	-8621	1135	9340	22
H15A	-1777	477	7309	22
H15B	-2671	932	6940	22
H9A	-4245	2428	7661	23
H9B	-4477	1729	7466	23
H21	22	2024	5750	25
H22	-1746	1612	6224	25
H7	-4464	4541	2913	35
H11	8106	2818	9443	45
H4A	1919	3973	6991	16
H3A	-62	4193	6282	15
H34A	4398	3519	6848	20
H34B	4060	4221	6713	20
H47	-3732	3924	5645	19
H35A	2635	2840	7036	21
H35B	2563	3014	7737	21
H42	6925	3633	8352	24
H27	-2501	5025	3935	19
H41	5495	4120	7704	20
H36A	587	2648	7416	23
H36B	454	3356	7602	23
H39A	3283	4557	7612	19
H39B	2170	4223	7969	19
H48	-4925	3867	4760	19
H33A	3909	3659	5808	20

Atom	x	y	z	U_{eq}
H33B	2927	3194	6114	20
H28	-1353	5115	4832	21
H46	2610	3540	8753	20
H37A	-1233	3545	6923	21
H37B	-1252	2842	6708	21
H45	4029	3055	9391	23
H30A	-2181	4504	6245	19
H30B	-1262	4978	5916	19
H31A	534	4599	5339	19
H31B	-127	4028	5016	19
H32A	1302	3358	5523	21
H32B	2021	3826	5084	21
H38A	-1981	3438	5907	23
H38B	-631	3166	5723	23
H1WA	1700(70)	2600(30)	9980(20)	48
H1WB	1340(80)	2630(30)	9290(20)	48
H2WA	-4840(40)	2580(30)	4770(30)	50(30)
H2WB	-3960(80)	2450(50)	5361(15)	90(40)

Table S17: Hydrogen Bond information for ligand**, LH_2** chloride salt.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1W	H1WA	$O6^{1}$	1.01(3)	1.79(3)	2.781(7)	167(7)

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