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Electronic Supplementary Information (ESI)

Discrete mononuclear and dinuclear compounds containing the MoO_2^{2+} core and 4-aminobenzhydrazone ligands: synthesis, structure and organic-solvent-free epoxidation activity

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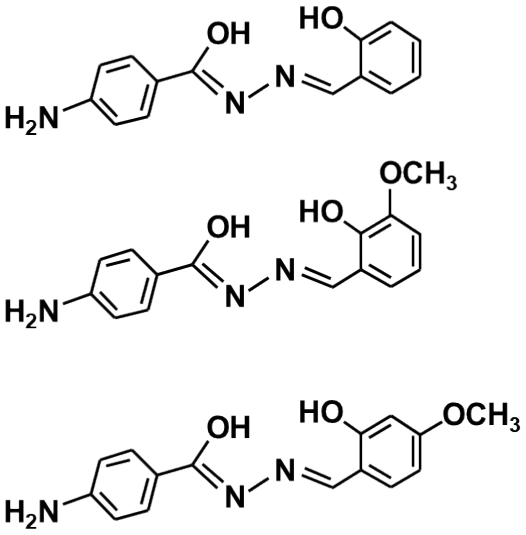
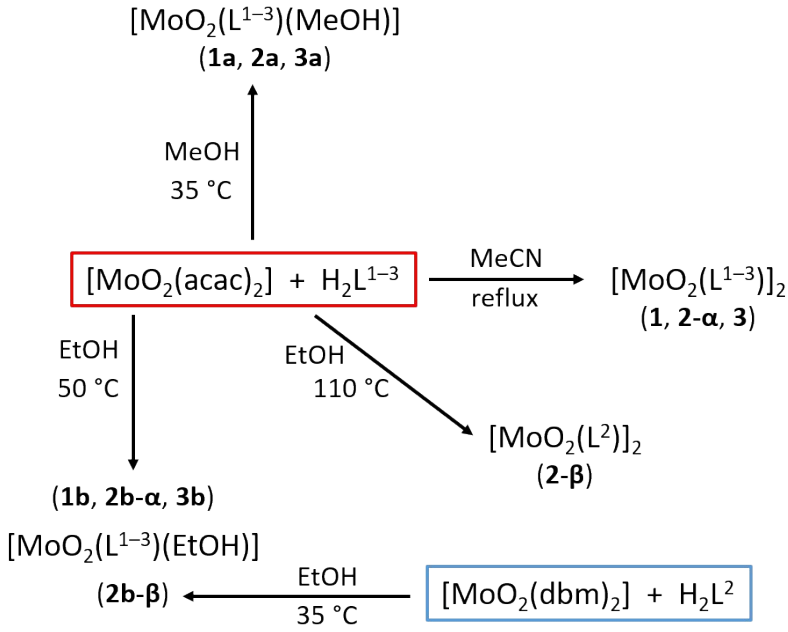
Contents

1. Schemes



Scheme S1 The 4-aminobenzhydrazone–related ligands



Scheme S2 Reaction pathways for the molybdenum(VI) compounds

2. Crystallization of compounds 1c, 2c and 3c·dmf

Compounds **1**–**3** were dissolved in a minimum volume of dmf. The solutions were allowed to stand at room temperature until dark red crystals formed within 5-6 days, which were filtered and dried.

$[MoO_2(L^1)(dmf)]$ (**1c**). Anal. Calcd. for $C_{17}H_{18}MoN_4O_5$ (454.288): C, 44.95; H, 3.99; N, 12.33. Found: C, 44.71; H, 3.73; N, 12.48%. TG: calc. for MoO_3, 31.68%, found 31.42%; calcd. for dmf, 16.09 %, found 16.25%. Selected IR data (cm^{-1}): 1655 $C{=}O_{dmf,}$ 1607 (C=N), 1599 (C=C), 1332 (C−O), 1266 ($C{-}O_{phenolate}$), 930, 916 (MoO_2^{2+}), 908, 887 ($O{=}Mo{-}O_{dmf}$).

$[MoO_2(L^2)(dmf)]$ (**2c**). Anal. Calcd. for $C_{18}H_{20}MoN_4O_6$ (484.31): C, 44.64; H, 4.16; N, 11.57. Found: C, 44.35; H, 3.91; N, 11.40%. TG: calc. for MoO_3, 29.72%, found; 29.63%; calcd. for dmf, 15.09%, found 15.23%. Selected IR data (cm^{-1}): 1650 $C{=}O_{dmf,}$ 1603 (C=N, C=C), 1345 (C−O), 1247 ($C{-}O_{phenolate}$), 943, 922 (MoO_2^{2+}), 894 ($O{=}Mo{-}O_{dmf}$).

$[MoO_2(L^3)(H_2O)]$·dmf (**3c·dmf**). Anal. Calcd. for $C_{18}H_{22}MoN_4O_7$ (502.33): C, 43.04; H, 4.41; N, 11.15. Found: 44.23; H, 4.64; N, 11.29%. TG: calc. for MoO_3, 28.65%, found 28.46%; calcd. for dmf, 14.55%, calcd. for dmf, 3.58%, found (dmf+H_2O) 18.23%. Selected IR data (cm^{-1}): 1649 $C{=}O_{dmf,}$ 1603 (C=N, C=C), 1345 (C−O), 1248 ($C{-}O_{phenolate}$), 943, 922 (MoO_2^{2+}), 894 ($O{=}Mo{-}O_{H2O}$).

3. X-Ray diffraction

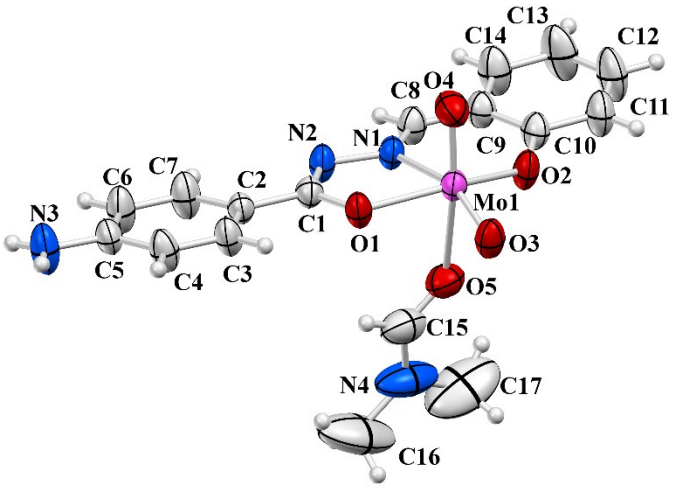


Fig S1 Mercury rendered ORTEP view of the representative mononuclear complex **1c** with atom-labeling scheme. The displacement ellipsoids are drawn at the 50 % probability level at 296(2) K.

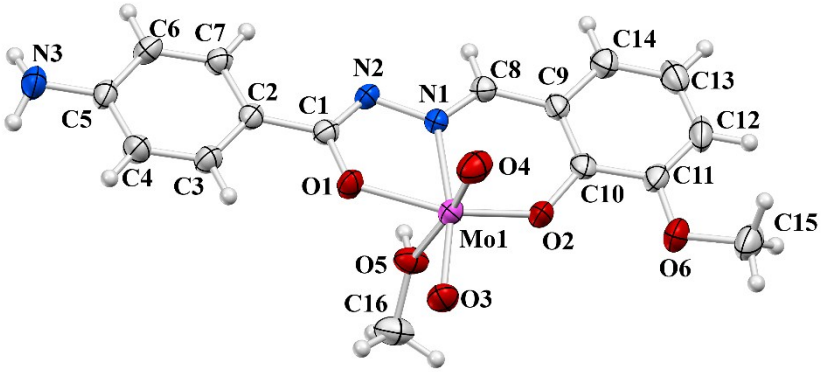


Fig S2 Mercury rendered ORTEP view of the representative mononuclear complex **2a** with atom-labeling scheme. The displacement ellipsoids are drawn at the 50 % probability level at 296(2) K.

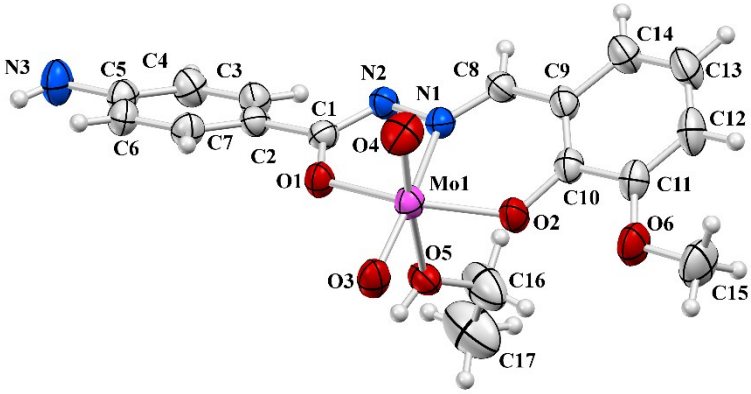


Fig S3 Mercury rendered ORTEP view of the representative mononuclear complexes **2b-α** with atom-labeling scheme. The displacement ellipsoids are drawn at the 50 % probability level at 296(2) K.

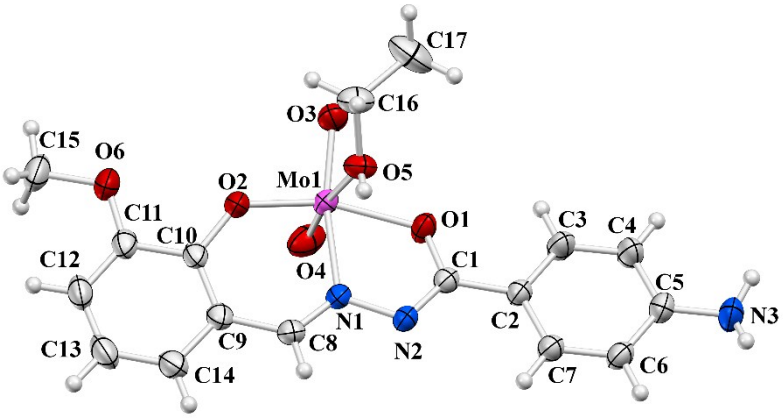


Fig. S4 Mercury rendered ORTEP view of the representative mononuclear **2b-β** with atom-labeling scheme. The displacement ellipsoids are drawn at the 50 % probability level at 296(2) K.

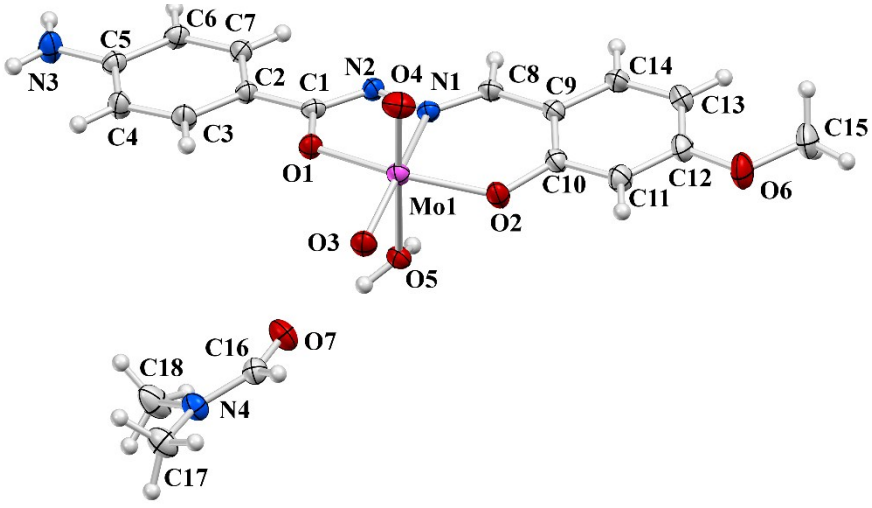
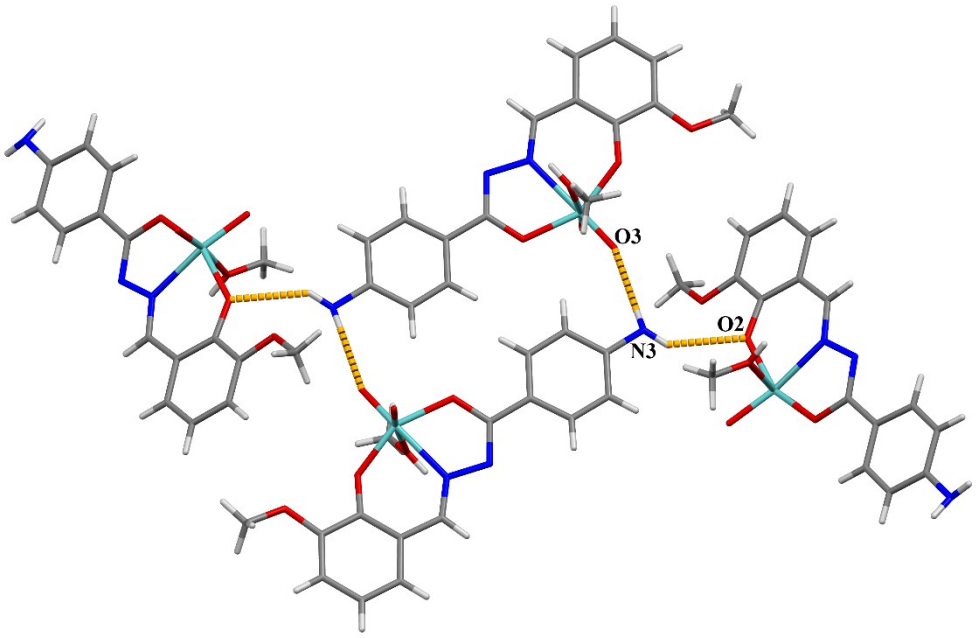
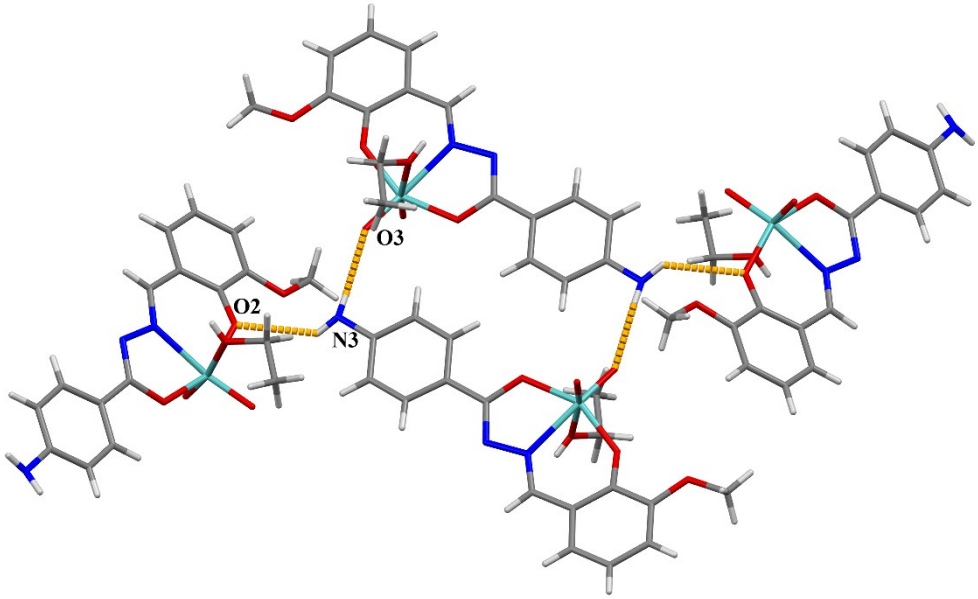


Fig. S5 Mercury rendered ORTEP view of the representative mononuclear complex **3c** with atom-labeling scheme. The displacement ellipsoids are drawn at the 50 % probability level at 150(2) K.

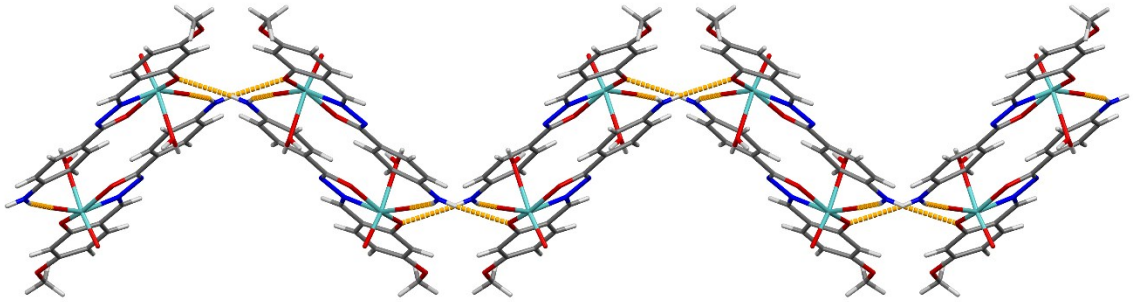


2a

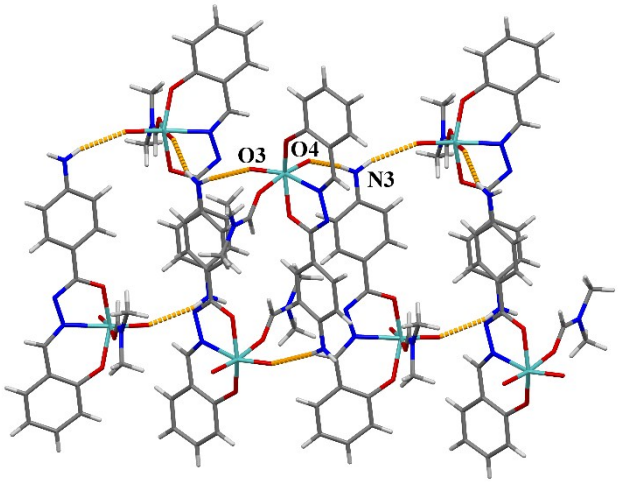


2b-β

Fig. S6 Partial crystal structure in **2a** and **2b-β** showing assembling of molecules via N–H···O intermolecular hydrogen bonds.

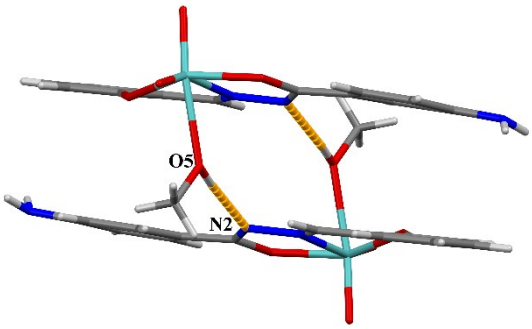


(a)

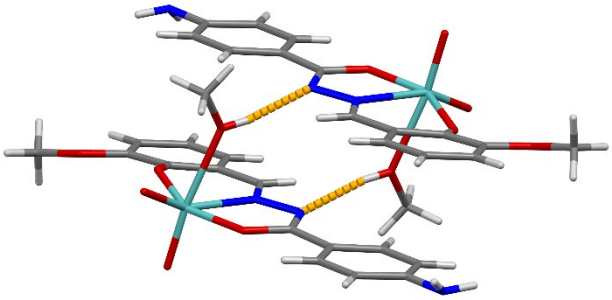


(b)

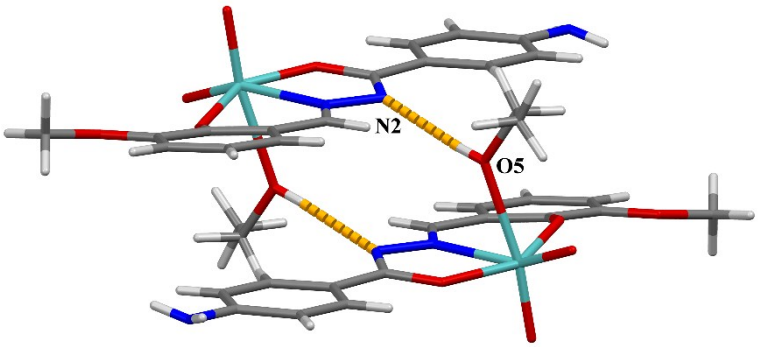
Fig. S7 (a) The amino group in **3c** links complex molecules *via* N3–H13N···O3 and N3–H23N···O2 intermolecular hydrogen bonds into a *zigzag* supramolecular infinite motif in *ab* plane. (b)Supramolecular assembly in the crystal structure of **1c** formed *via* N3–H13N···O4 and N3–H23N···O3 intermolecular hydrogen bonds between the amino group and the oxido oxygen atoms O3 and O4 as proton acceptors.



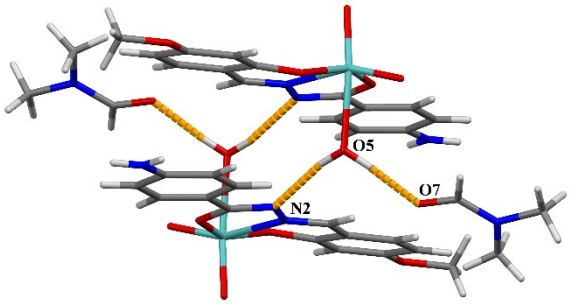
1a



2a



2b-β



3c

Fig. S8 Supramolecular assembly in **1a**, **2a, 2b-β** and **3c** exhibiting participation of the oxygen O5 atom of the coordinated solvent molecule in intermolecular hydrogen bond formation with non-coordinating nitrogen N2 atom as well as hydrogen bond formation with dmf molecule of crystallization with a water molecule in **3c**.

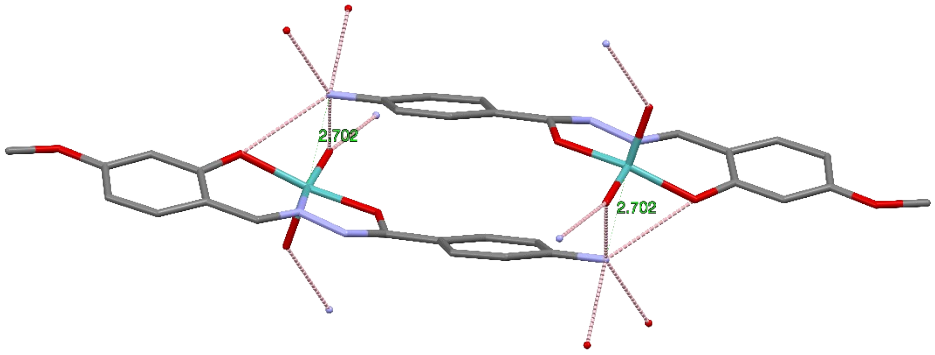


Fig. S9 Molecular structure of the compound **2-α** and its interactions**.** Carbon (grey), oxygen (red), molybdenum (turquoise), nitrogen (blue). Hydrogen bonds (pink). The distance between the nitrogen and Mo atoms of two neighbouring molecules (green) is 2.702 Å. Hydrogen atoms are omitted for clarity.

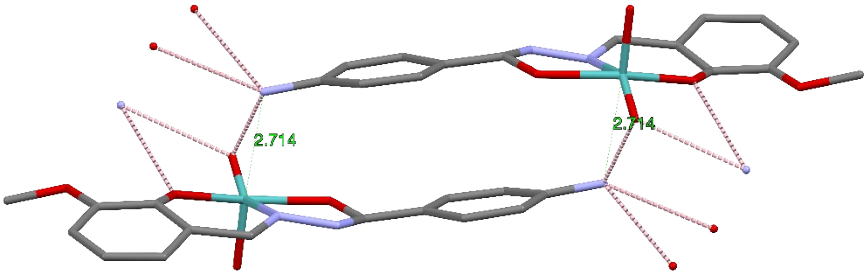


Fig S10 Molecular structure of compound **3** and its interactions**.** Carbon (grey), oxygen (red), molybdenum (turquoise), nitrogen (blue). Hydrogen bonds (pink). The distance between the nitrogen and Mo atoms of two neighbouring molecules (green) is 2.714 Å. Hydrogen atoms are omitted for clarity.

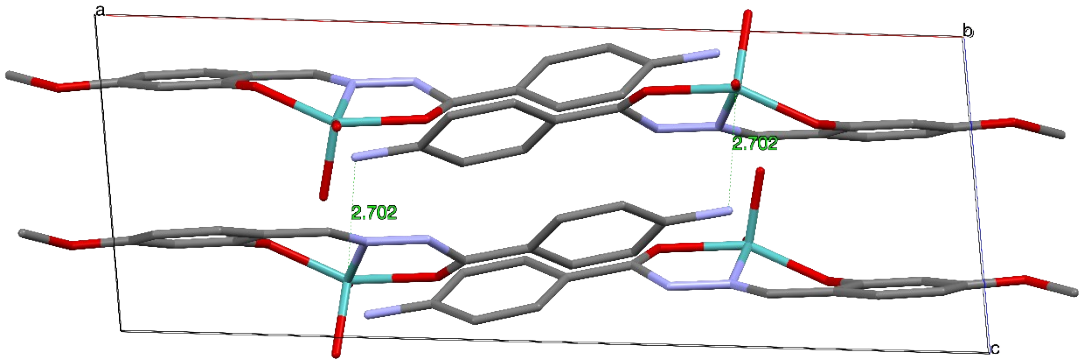


Fig S11 Crystal structure of the compound **2-α** viewed along *b* axis reveals molecular layers, connected with H-bonds and Mo-N interactions. Carbon (grey), oxygen (red), molybdenum (turquoise), nitrogen (blue). Hydrogen bonds (pink). The distance between the nitrogen and Mo atoms of two neighboring molecules (green). Hydrogen atoms are omitted for clarity.

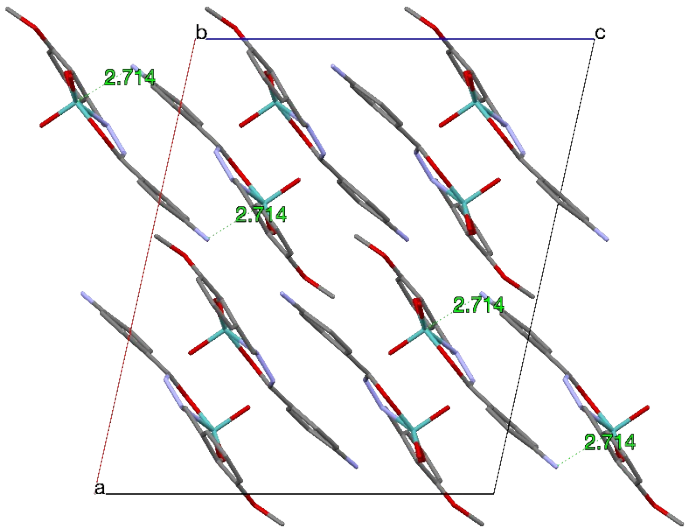


Fig S12 Crystal structure of the compound **3** viewed along *c* axis reveals molecular layers, connected with H-bonds and Mo-N interactions. Carbon (grey), oxygen (red), molybdenum (turquoise), nitrogen (blue). Hydrogen bonds (pink). The distance between the nitrogen and Mo atoms of two neighboring molecules (green). Hydrogen atoms are omitted for clarity.

Table S1. Selected bond distances (Å) and angles (°) within molybdenum atoms primary coordination sphere.

	1a	**1c**	**2-β**	**2a**	**2b-α**	**2b-β**	**3c**
Mo1=O_t[1]	1.6857(14)	1.684(2)	1.682(3)	1.689(3)	1.688(2)	1.6830(16)	1.6891(15)
	1.7198(12)	1.705(2)	1.709(2)	1.704(2)	1.707(2)	1.7057(15)	1.7188(13)
Mo1–N1	2.2308(14)	2.231(2)	2.244(3)	2.235(3)	2.232(3)	2.2418(15)	2.2303(15)
Mo1–O1[2]	2.0133(12)	1.9851(19)	1.969(2)	1.990(2)	2.009(2)	1.9882(13)	1.9989(13)
Mo1–O2[3]	1.9196(12)	1.9089 (19)	1.923(2)	1.916(2)	1.917(2)	1.9214(14)	1.9351(13)
Mo1–O5(or N3)[4]	2.3592(13)	2.313(2)	2.567(4)	2.381(3)	2.318(2)	2.3646(15)	2.3266(14)
O3–Mo1–O4	106.08(7)	105.29(11)	106.17(13)	106.04(13)	106.27(13)	106.10(8)	105.43(7)
O3–Mo1–O1	97.19(5)	97.14(9)	99.78(11)	99.42(11)	95.30(10)	99.80(7)	97.57(6)
O3–Mo1–O2	103.01(6)	102.27(9)	100.03(11)	100.67(11)	105.57(10)	100.60(7)	102.48(6)
O3–Mo1–N1	156.20(6)	158.35(10)	156.42(12)	154.40(11)	160.14(11)	155.64(6)	157.23(7)
O3–Mo1–O5	81.92(6)	84.87(9)		81.11(11)	84.49(11)	82.75(6)	81.99(6)
O4–Mo1–O1	96.32(6)	96.65(9)	97.19(12)	96.27(12)	98.09(11)	96.21(8)	96.19(7)
O2–Mo1–O1	149.98(6)	150.37(9)	148.09(10)	151.07(10)	148.22(10)	150.58(6)	150.63(6)
O4–Mo1–O2	99.09(6)	99.53(10)	100.99(12)	97.93(13)	98.70(12)	98.23(8)	98.86(7)
O4 –Mo1–N1	96.17(6)	94.57(10)	96.67(12)	98.86(12)	90.66(11)	97.52(7)	95.77(6)
O2–Mo1–N1	81.25(5)	82.43(8)	80.89(10)	81.39(10)	81.41(9)	81.48(6)	81.94(6)
O1–Mo1–N1	71.58(5)	71.63(8)	71.07(9)	71.57(9)	71.60(9)	71.29(5)	71.54(5)
O4 –Mo1–O5	170.94(6)	169.71(10)		172.12(10)	168.96(11)	170.36(7)	172.10(6)
O2–Mo1–O5	82.89(5)	79.47(10)		83.74(10)	80.35(9)	83.59(6)	81.87(6)
O1–Mo1–O5	78.18(5)	80.20(9)		79.04(9)	78.06(9)	78.21(6)	79.91(5)
N1–Mo1–O5	75.33(5)	75.14(8)		73.72(9)	78.32(9)	73.32(5)	76.50(5)

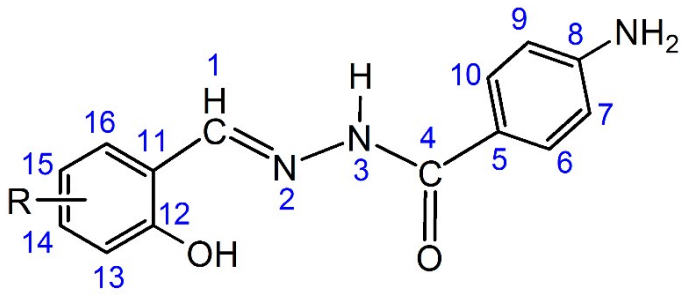
[1] O_t - terminal oxido oxygen atoms O3 and O4; [2] O1 – the oxygen atom from hydrazone part of the ligand;
[3]O2 – the phenolate oxygen atom from aldiminato part of the ligand; [4] O5 – donor atom of the coordinated solvent molecule (MeOH in **1a** and **2a,** dmf in **1c**, EtOH in both forms of **2b** and H_2O in **3c**) or N3 in **2-β**

Table S2. Hydrogen bonds geometry (Å,°)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)	Symmetry code
1a					
O5–H1*O5*···N2	0.81(2)	1.92(2)	2.724(2)	170(2)	–x+1, –y+1, –z+1
N3–H1*N3*···O3	0.85(2)	2.25(2)	3.077(2)	165(2)	x, y, z+1
N3–H2*N3*···O3	0.85(2)	2.15(2)	2.991(2)	176(2)	–x+1, –y+2, –z+1
C6–H6···O4	0.95	2.63	3.259(2)	124	–x+2, –y+1, –z+1
C15–H15···O4	0.98	2.68	3.614(3)	159	x–1,+y,+z
1c					
C8–H8···O3	0.93	2.62	3.487(4)	156	x, –y+3/2, z+1/2
C15–H15···O1	0.93	2.52	3.009(4)	113	
N3–H13*N*···O4	0.84(2)	2.30(2)	3.076(4)	155(3)	–x+1, y–1/2, –z+1/2
N3–H23*N*···O3	0.84(3)	2.25(3)	3.047(4)	159(3)	–x+1, –y+2, –z
C13–H13···O4	0.93	2.69	3.485(5)	159	–x,+y–1/2, –z+1/2
2-β					
N3–H13*N*···O5	0.83(3)	2.35(3)	3.166(4)	172(2)	x–1/2, –y+1/2,+z–1/2
N3–H23*N*···O3	0.83(3)	2.28(3)	3.092(4)	173(1)	x–1/2, –y+1/2,+z–1/2
C8–H8···O4	0.93	2.71	3.395(4)	130	–x+1/2,+y+1/2, –z+3/2
C13–H13···O3	0.93	2.51	3.437(4)	173	x,+y+1,+z
2a					
N3–H13*N*···O3	0.86(4)	2.21(4)	3.019(5)	158(5)	–x+1, –y+1, –z
N3–H23*N*···O2	0.85(3)	2.52(3)	3.243(4)	144(3)	–x+1,+y+1/2, –z+1/2
O5–H1*O5*···N2	0.80(4)	1.99(4)	2.772(3)	167(4)	–x+1, –y+1, –z+1
C7–H7···O5	0.93	2.61	3.422(4)	147	–x+1, –y+1, –z+1
C14–H14···O4	0.93	2.56	3.225(4)	129	–x, –y+1, –z+1
2b-α					
N3–H13*N*···O4	0.86(5)	2.16(5)	2.951(5)	152(4)	x+1,+y,+z
N3–H23*N*···O3	0.85(4)	2.17(4)	3.011(4)	174(4)	–x+2, –y+1, –z+1
C3–H3···O3	0.93	2.50	3.415(4)	168	–x+1/2+1,+y–1/2, –z+1/2
O5–H1*O5*···N2	0.79(3)	1.98(3)	2.745(3)	163(3)	–x+3/2,+y+1/2, –z+1/2
2b-β					
N3–H13*N*···O2	0.83(4)	2.56(4)	3.206(3)	136(3)	–x+1,+y–1/2, –z+1/2+1
N3–H23*N*···O3	0.85(4)	2.26(4)	3.081(3)	163(3)	–x+1, –y+1, –z+1
O5–H15*O*···N2	0.72(4)	2.06(4)	2.771(2)	171(4)	–x+1, –y+1, –z+2
C17–H17*A*···O4	0.96	2.66	3.414(4)	136	x+1, y, z
C14–H14···O4	0.93	2.54	3.330(3)	143	–x, –y+1, –z+2
3c					
O5–H15*O*···O7	0.85(3)	1.86(3)	2.690(3)	170(3)	-
O5–H25*O*···N2	0.82(2)	2.04(2)	2.845(2)	169(2)	–x+1, –y+1, –z+1
N3–H13*N*···O3	0.85(3)	2.15(3)	2.979(3)	168(2)	–x+1, –y+1, –z
N3–H23*N*···O2	0.85(2)	2.45(2)	3.211(2)	149(2)	–x+1,+y+1/2, –z+1/2

C17–H17*B*···O6	0.98	2.46	3.258(3)	138	x+1, –y+1/2, z–1/2
C6–H6···O3	0.95	2.50	3.418(2)	162	–x+1,+y+1/2, –z+1/2
C7–H7···O5	0.95	2.64	3.477(3)	147	–x+1, –y+1, –z+1
C8–H8···O7	0.95	2.47	3.415(2)	172	–x+1, –y+1, –z+1
C13–H13···O4	0.95	2.50	3.173(3)	128	–x, –y+1, –z+1

4. NMR spectroscopy



Scheme S3 The NMR numbering scheme.

Table S3 ^{1}H and ^{13}C chemical shifts (ppm) of $H_2L^{1–3}$ and their $[MoO_2(L^{1-3})]_2$ complexes **1**–**3**. In dmso-d_6 solution, polymorphs **2-α** and **2-β** are presented as the same species **2.**

Atom	H_2L^1		**1**		H_2L^2		**2**		H_2L^3		**3**	
	δ / ppm (^{1}H)	δ / ppm (^{13}C)	δ / ppm (^{1}H)	δ / ppm (^{13}C)	δ / ppm (^{1}H)	δ / ppm (^{13}C)	δ / ppm (^{1}H)	δ / ppm (^{13}C)	δ / ppm (^{1}H)	δ / ppm (^{13}C)	δ / ppm (^{1}H)	δ / ppm (^{13}C)
1	8.56	147.37	8.79	153.59	8.56	147.32	8.76	153.50	8.48	147.84	8.69	153.42
4	–	163.13	–	169.93	–	163.09	–	169.96	–	162.94	–	168.78
5	–	119.23	–	116.12	–	119.42	–	116.17	–	119.35	–	116.36
6	7.70	129.89	7.69	130.37	7.69	129.88	7.69	130.36	7.67	129.77	7.66	130.11
7	6.62	113.13	6.61	113.59	6.61	113.12	6.60	113.59	6.61	113.12	6.59	113.59
8	–	153.03	–	153.17	–	153.01	–	153.16	–	152.92	–	152.87
9	6.62	113.13	6.61	113.59	6.61	113.12	6.60	113.59	6.61	113.12	6.59	113.59
10	7.70	129.89	7.69	130.37	7.69	129.88	6.69	130.36	7.67	129.77	7.66	130.11
11	–	119.19	–	121.10	–	119.23	–	121.35	–	112.40	–	114.39
12	–	157.88	–	159.53	–	147.60	–	148.89	–	159.83	–	161.36
13	6.93	116.85	6.93	118.89	–	148.38	–	149.33	6.50	101.67	6.53	103.46
14	7.29	131.38	7.48	134.57	7.00	114.04	7.19	116.76	–	162.18	–	165.05
15	6.91	119.71	7.05	121.84	6.85	119.37	6.99	121.68	6.52	106.76	6.66	109.52
16	7.47	130.14	7.68	134.15	7.02	121.59	7.25	125.25	7.36	131.61	7.58	135.22
OH	11.56	–	–	–	11.33	–	–	–	11.88	–	–	–
NH	11.76	–	–	–	11.71	–	–	–	11.62	–	–	–
NH_2	5.84	–	5.94	–	5.83	–	5.94	–	5.81	–	5.88	–
OMe	–	–	–	–	3.81	56.28	3.80	56.27	3.78	55.76	3.81	56.21

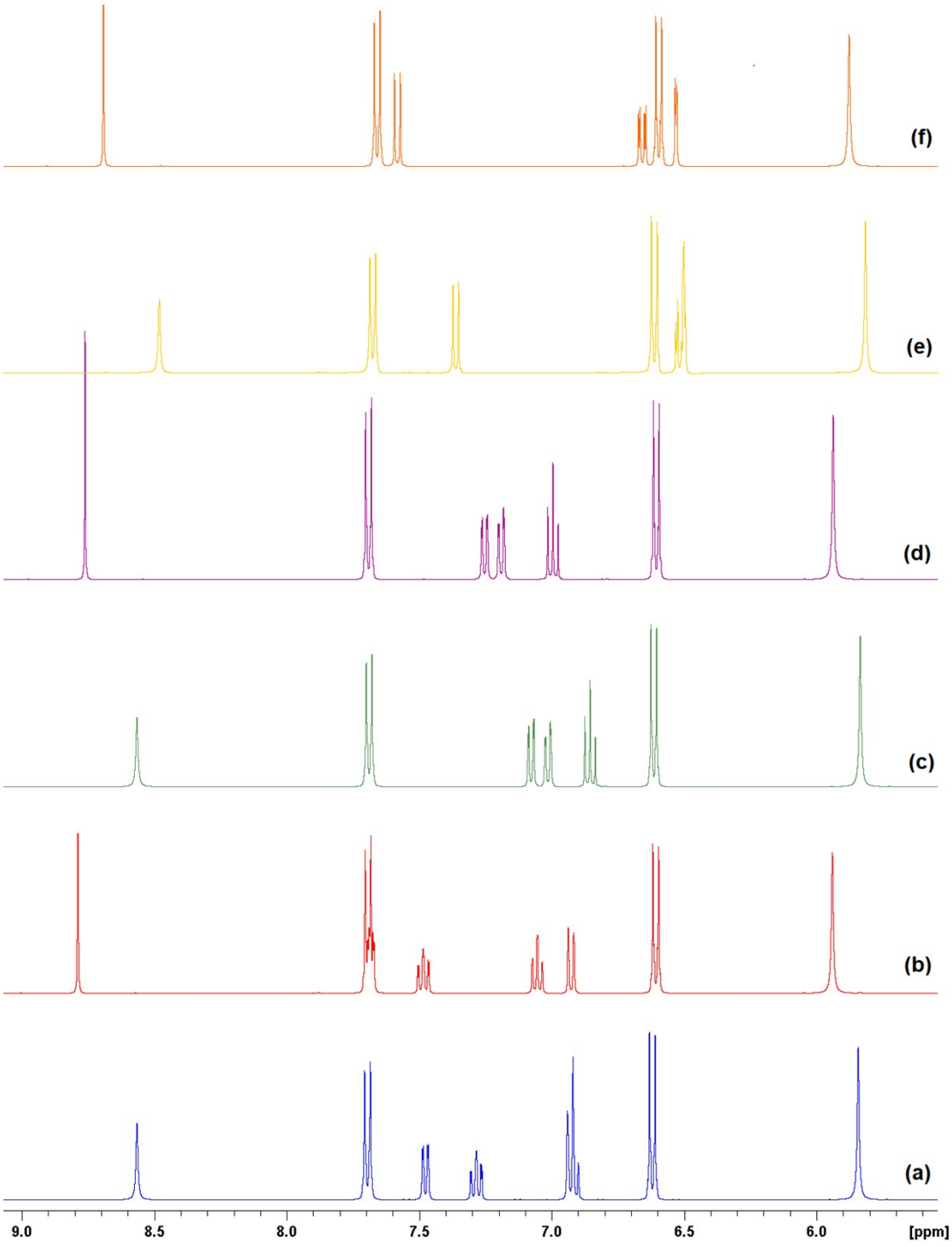


Fig S13 A portion of the ^{1}H NMR spectra in dmso-d_6 of: (a) H_2L^1, (b) $[MoO_2(L^1)]_2$ (**1**); (c) H_2L^2, (d) $[MoO_2(L^2)]_2$ (**2**), (a) H_2L^3, (e) $[MoO_2(L^3)]_2$ (**3**)

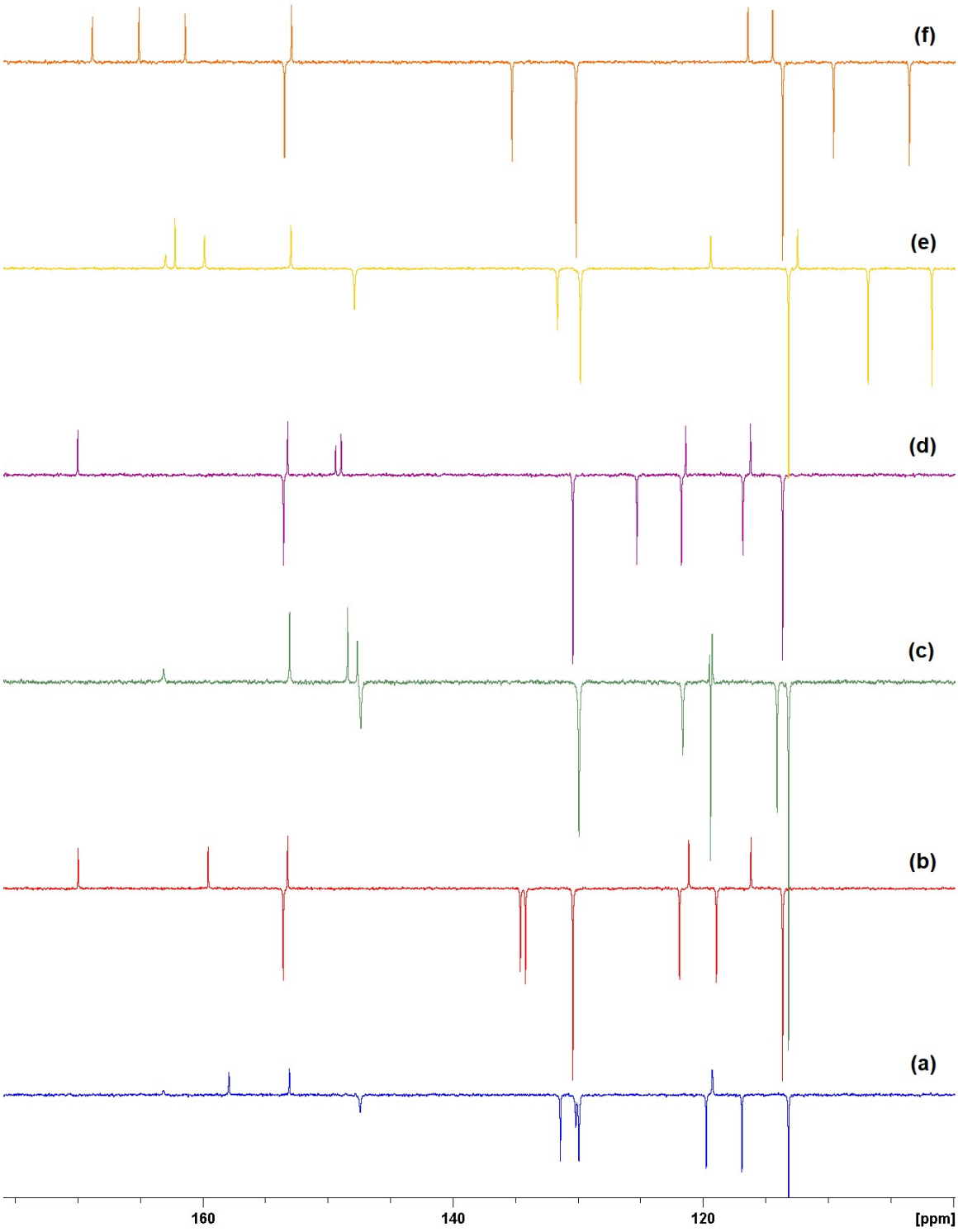


Fig. S14 A portion of the ^{13}C NMR spectra in dmso-d_6 of: (a) H_2L^1, (b) $[MoO_2(L^1)]_2$ (**1**); (c) H_2L^2, (d) $[MoO_2(L^2)]_2$ (**2**), (e) H_2L^3, (f) $[MoO_2(L^3)]_2$ (**3**)

5. Thermogravimetric analysis

Table S4 Thermoanalytical data

Formula	Complex	Loss of solvent	Decomposition of ligand
		Temperature range (°C)	Temperature range (°C)
$[MoO_2(C_{14}H_{11}N_3O_2)]_2$	**1**	–	319–547
$[MoO_2(C_{14}H_{11}N_3O_2)(CH_3OH)]$	**1a**	66–137 [a)]	320–540
$[MoO_2(C_{14}H_{11}N_3O_2)(C_2H_5OH)]$	**1b**	53–150 [b)]	322–536
$[MoO_2(C_{14}H_{11}N_3O_2)(C_3H_7NO)]$	**1c**	114–141 [c)]	303–560
$[MoO_2(C_{15}H_{13}N_3O_3)]_2$	**2-α**	–	275 – 512
$[MoO_2(C_{15}H_{13}N_3O_3)]_2$	**2-β**	–	247 – 497
$[MoO_2(C_{15}H_{13}N_3O_3)(CH_3OH)]$	**2a**	131–170 [a)]	293–507
$[MoO_2(C_{15}H_{13}N_3O_3)(C_2H_5OH)]$	**2b-α**	107–136 [b)]	286–507
$[MoO_2(C_{15}H_{13}N_3O_3)(C_2H_5OH)]$	**2b-β**	113–133 [b)]	281–536
$[MoO_2(C_{15}H_{13}N_3O_3)(C_3H_7NO)]$	**2c**	117–158 [c)]	275–512
$[MoO_2(C_{15}H_{13}N_3O_3)]_2$	**3**	–	288–510
$[MoO_2(C_{15}H_{13}N_3O_3)(CH_3OH)]$	**3a**	130–184 [a)]	278–506
$[MoO_2(C_{15}H_{13}N_3O_3)(C_2H_5OH)]$	**3b**	110–141 [b)]	287–544
$[MoO_2(C_{15}H_{13}N_3O_3)(H_2O)]\cdot C_3H_7NO$	**3c**	97–146 [d)]	281–545

[a)] Corresponding to the loss of MeOH molecule.
[b)] Corresponding to the loss of EtOH molecule.
[c)] Corresponding to the loss of dmf molecule.
[d)] Corresponding to the loss of dmf and water molecules.

6. Catalytic studies

Cyclohexene epoxidation for the complexes 1-3

Additionally, to the cyclooctene, cyclohexene was also tested as a model substrate.

The experimental procedure is mostly the same as reported in the main text for the cyclooctene epoxidation, but with the use of cyclohexene, as a substrate. The reaction temperature was 60 °C.

The kinetic profiles are presented in Fig. S18. As it can be seen, all catalysts show moderate activity, cyclohexene conversions varying from 34 to 77 %. The selectivity towards the corresponding epoxide was very low, 18 % for the complex **1**, 10 % for **2**, 6 % for **3**, implying fast ring opening which resulted with the cyclohexanediol formation. The diol was observed by the GC in the organic phase, but it was not quantified since it is mainly present in the aqueous phase. TOF_{20min} is 95, 132, 451 h^{-1} for the complexes **1**, **2**, **3** respectively, while TON values are 242, 134, 280, respectively.

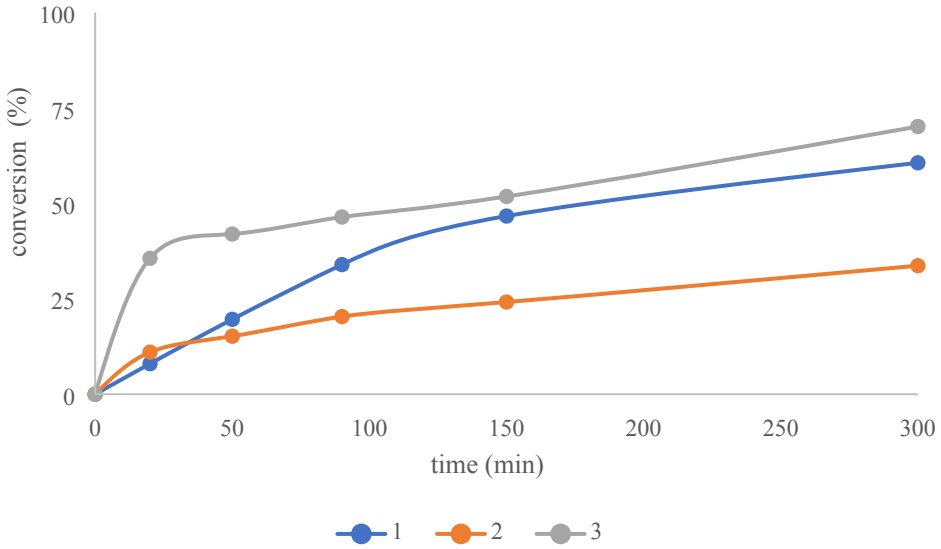


Fig. S15 Converted cyclohexene vs. time with dinuclear non-grinded dioxomolybdenum(VI) complexes. Reaction conditions: catalyst/cyclooctene/TBHP molar ratio: 0.25/100/200, T = 333 K.

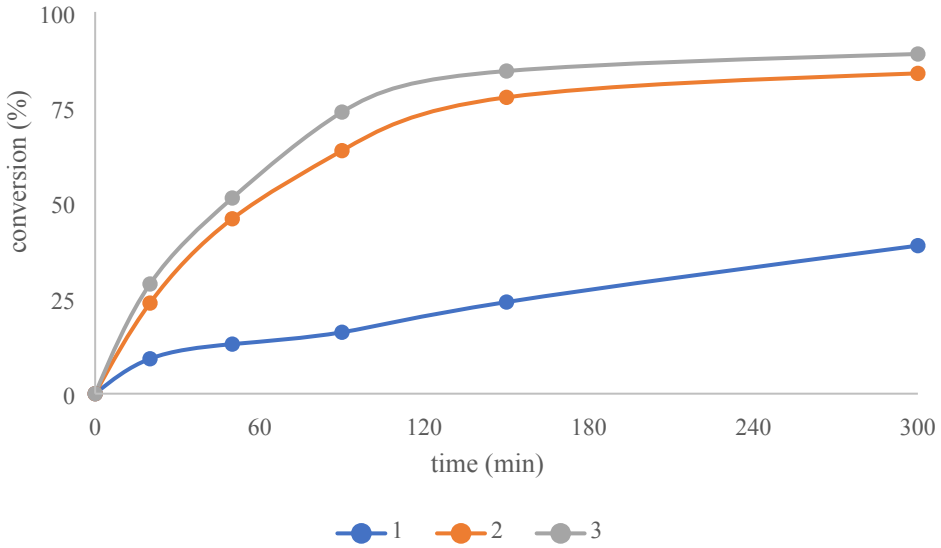


Fig. S16 Converted cyclooctene vs. time with dinuclear dioxomolybdenum(VI) complexes. Reaction conditions: catalyst/cyclooctene/TBHP molar ratio: 0.25/100/200, T = 353 K.

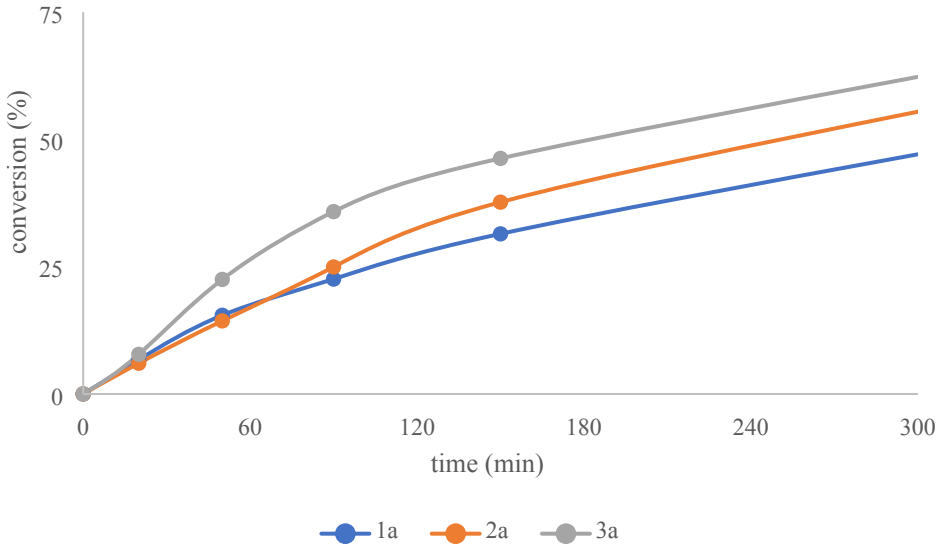


Fig. S17 Converted cyclooctene vs. time with dioxomolybdenum(VI) complexes coordinated with methanol. Reaction conditions: catalyst/cyclooctene/TBHP molar ratio: 0.25/100/200, T = 353 K.

*Additional catalytic testing of dinuclear complexes **1** and **2**.*

Dinuclear complexes tested for the catalytic reactions were used as synthesized. Since complex **1** was the less active one, we tried to improve its performance. For that reason, complexes **1** and **2** were grinded and afterward used for the epoxidation reaction (experimental protocol was the same as stated in the main text). Complex **2** was chosen as representative of very active catalysts. As it is shown from the kinetic profiles, the activity of the grinded complexes **1** is a bit better than non-grinded ones, while for the complex **2** the difference is not so obvious. This effect might be explained by the smaller size of particles and the bigger active surface of the catalyst enabling faster conversion into active species. By grinding, complex **1** becomes more selective towards epoxide (93% of selectivity), while the grinded complex **2** showed selectivity of 93 %.

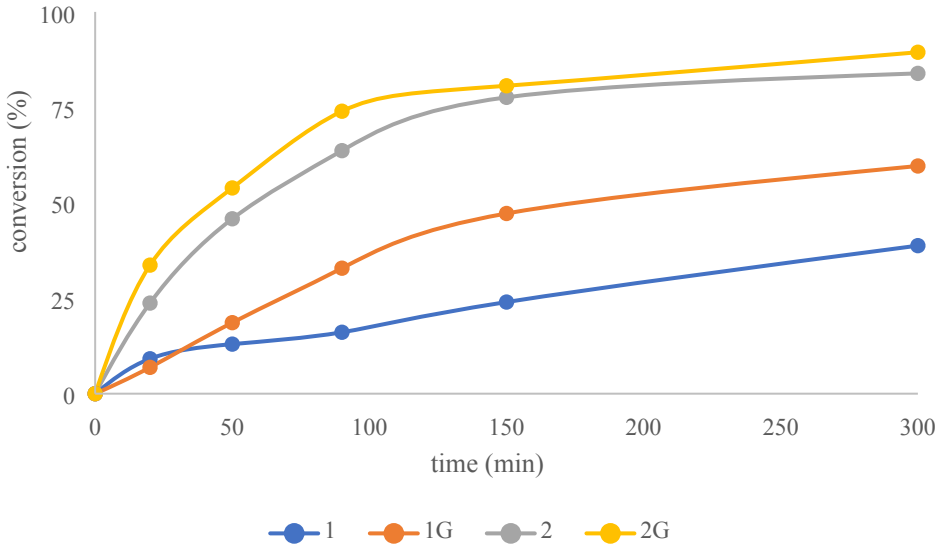


Fig. S18 Converted cyclooctene vs. time with dinuclear grinded and non-grinded dioxomolybdenum(VI) complexes. Reaction conditions: catalyst/cyclooctene/TBHP molar ratio: 0.25/100/200, T = 353 K.

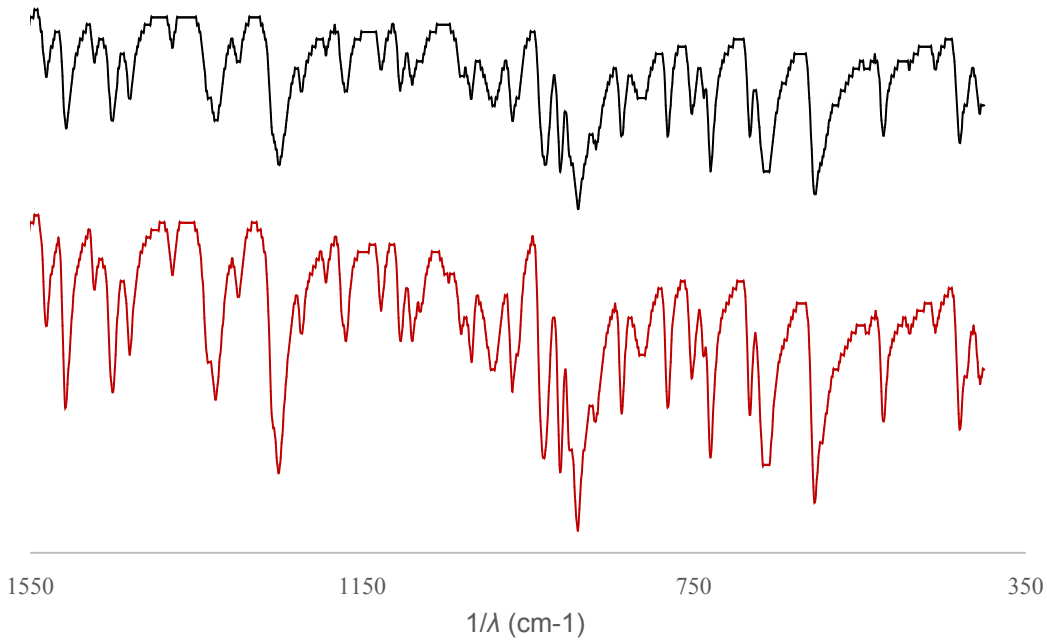
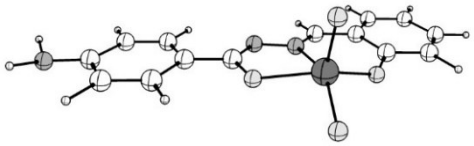


Fig. S19 Comparison of IR spectra of the starting catalyst **2b-α** (red) and recovered one **2b*** (black) in the area 1650 – 400 cm^{-1}.

7. DFT calculations

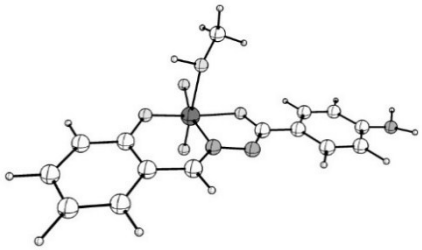
Table S5 Cartesian coordinates of optimized structures

$[MoO_2L^1]$



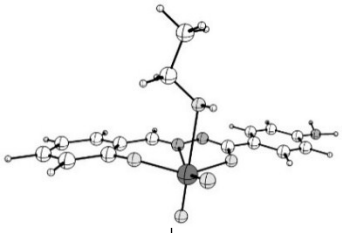
Mo	0.876212	-1.436658	0.078209	H	-5.355913	2.830891	0.130319	H	1.144912	2.766502	0.019674
N	0.584410	0.807363	-0.053652	C	-3.553441	1.671953	0.028116	C	2.914498	1.498960	-0.035011
N	-0.721673	1.244596	-0.062725	H	-2.900956	2.536206	0.090112	C	3.453921	0.200305	-0.222641
O	-1.060216	-1.025230	-0.177678	C	-2.980676	0.389760	-0.074292	C	4.845181	0.021795	-0.247357
O	2.669682	-0.863636	-0.425172	C	-3.834237	-0.724974	-0.150834	H	5.232427	-0.980387	-0.398366
O	0.822934	-2.861778	-0.844492	H	-3.402802	-1.717037	-0.228443	C	5.690222	1.113685	-0.087025
C	-5.784718	0.715306	-0.021419	C	-5.211256	-0.567707	-0.124321	H	6.765819	0.961217	-0.106368
C	-1.530957	0.216714	-0.096729	H	-5.858105	-1.439460	-0.187159	C	5.171479	2.405936	0.094329
C	-4.927734	1.834169	0.053925	C	1.499417	1.736310	-0.023506	H	5.839732	3.252398	0.216795
								C	3.798993	2.590567	0.114499
								H	3.380257	3.584518	0.251984
								O	0.987583	-1.801895	1.731289
								N	-7.158926	0.880567	-0.044720
								H	-7.519328	1.746081	0.334073
								H	-7.717627	0.074660	0.202309

$[MoO_2L^1(MeOH)]$



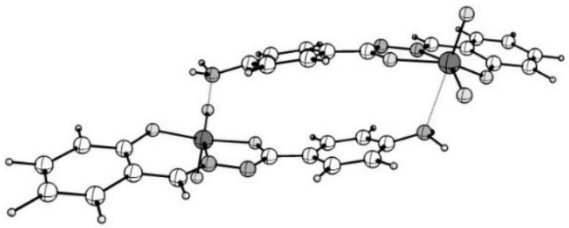
Mo	0.860871	-1.210347	-0.568924	O	0.658802	-1.279668	1.932128	H	-5.406718	2.906	0.428198	
N	0.542767	0.971563	0.045896	H	1.597541	-1.417213	2.142720	C	-3.596987	1.774640	0.204776	
N	-0.767918	1.369770	0.150791	C	-1.561580	0.353517	-0.077915	H	-2.949030	2.622730	0.397670	
N	-7.199676	0.998597	-0.058046	C	-3.015891	0.520527	-0.061086	C	5.653541	1.244651	0.052628	
H	-7.569105	1.799499	0.436754	C	-3.863682	-0.572374	-0.310518	H	6.728467	1.091803	0.008973	
H	-7.757513	0.164589	0.068585	H	-3.426263	-1.542569	-0.519922	C	5.133075	2.544370	0.122989	
O	-1.095461	-0.869865	-0.317436	C	-5.242598	-0.422354	-0.292962	H	5.797342	3.402907	0.133180	
O	2.644619	-0.787754	0.145258	H	-5.884047	-1.277223	-0.494101	C	3.758906	2.722937	0.177060	
O	0.811389	-2.906544	-0.380441	C	-5.823596	0.832206	-0.024773	H	3.340213	3.725156	0.229245	
O	1.071607	-0.876225	-2.217589	C	-4.972966	1.929526	0.224985	C	-0.125837	-2.319361	2.539575	
								H	-1.156775	-2.137182	2.235166	
								H	-0.051268	-2.260412	3.631227	
								H	0.184697	-3.306204	2.183114	
								C	1.452822	1.880238	0.214299	
								H	1.115605	2.901261	0.399560	
								C	2.872493	1.625092	0.153590	
								C	3.414980	0.313434	0.094479	
								C	4.805965	0.141781	0.041567	
								H	5.194546	-0.870596	-0.003614	

$[MoO_2L^1(EtOH)]$



Mo	-0.753637	-1.018985	-1.002920	C	3.710811	1.664893	0.493512	C	-2.751176	1.675313	0.193660	
N	-0.429039	0.984210	0.032450	H	3.065330	2.469336	0.829029	C	-3.316959	0.425696	-0.174907	
N	0.881659	1.327480	0.266515	C	5.086490	1.785189	0.597851	C	-4.709739	0.306190	-0.296759	
N	7.311831	0.885154	0.219600	H	5.522821	2.691702	1.011117	C	-5.533369	1.400760	-0.056583	
O	1.202334	-0.756732	-0.668162	C	5.933571	0.743767	0.164467	H	-6.609598	1.290240	-0.158186	
O	-2.568141	-0.668548	-0.363647	C	5.349609	-0.418980	-0.374626	C	-4.989249	2.638253	0.316745	
O	-0.719915	-2.730453	-1.021365	H	5.988924	-1.228813	-0.718370	H	-5.636494	3.489305	0.504192	
O	-0.870129	-0.469503	-2.601712	C	3.971185	-0.534913	-0.475563	C	-3.614134	2.764340	0.441992	
O	-0.477964	-1.663258	1.462143	H	3.531	-1.434784	-0.891242	H	-3.176338	3.717552	0.728886	
C	1.673317	0.369481	-0.148822	C	-1.330286	1.865557	0.347637	H	-5.117489	-0.659238	-0.578543	
C	3.126960	0.502040	-0.042829	H	-0.974771	2.817067	0.745670	C	-1.502547	-1.555450	2.467481	
								H	-2.447193	-1.956772	2.080253	
								H	-1.633649	-0.482076	2.624209	
								C	-1.092154	-2.248251	3.759407	
								H	-0.956737	-3.325984	3.604539	
								H	-1.866596	-2.117030	4.524216	
								H	-0.152564	-1.834857	4.139888	
								H	7.852854	0.030951	0.196119	
								H	7.669305	1.560180	0.882467	
								H	-0.360677	-2.602664	1.234392	

$[MoO_2L^1]_2$



Mo	4,517127	-1,428592	0,569302	C	6,472306	1,487864	0,031595	O	-4,214122	2,967861	0,106636
N	4,236757	0,834693	0,704699	C	6,868630	0,214188	-0,457181	C	1,972128	-0,723920	-1,939546
N	2,996465	1,259741	1,125153	C	8,174783	0,032552	-0,934351	C	-2,220467	-0,224770	-1,326088
O	2,641535	-1,019429	1,137387	H	8,452958	-0,948959	-1,304380	C	1,138533	-1,849780	-1,829979
O	6,017173	-0,820819	-0,532004	C	9,078365	1,090199	-0,929964	H	1,579720	-2,841926	-1,793451
O	4,214383	-2,968013	-0,106259	H	10,087261	0,930195	-1,300264	C	-0,232874	-1,689999	-1,700602
C	-1,972021	0,723453	1,940245	C	8,698997	2,354742	-0,457455	H	-0,873153	-2,555755	-1,572816
C	2,220572	0,224536	1,326545	H	9,407784	3,176775	-0,457312	C	-0,806373	-0,405610	-1,675477
C	-1,138445	1,849361	1,830937	C	7,407962	2,544419	0,011233	C	0,023870	0,710583	-1,858879
H	-1,579649	2,841507	1,794620	H	7,098147	3,518849	0,381234	H	-0,412358	1,702939	-1,853555
C	0,232965	1,689641	1,701525	O	5,274308	-1,644304	2,070083	C	1,397858	0,553561	-1,999006
H	0,873201	2,555452	1,573888	N	-3,377416	0,875221	1,883955	H	2,034911	1,428205	-2,103181
C	0,806519	0,405282	1,676100	H	-3,705018	1,763198	2,255456	C	-5,139984	-1,749235	-0,516979
C	-0,023695	-0,710977	1,859306	H	-3,889775	0,109593	2,312502	H	-4,863273	-2,779020	-0,748162
H	0,412580	-1,703310	1,853811	Mo	-4,516953	1,428622	-0,569271	C	-6,472709	-1,487524	-0,032398
C	-1,397670	-0,554026	1,999491	N	-4,236894	-0,834684	-0,704819	C	-6,868802	-0,213889	0,456663
H	-2,034698	-1,428709	2,103527	N	-2,996552	-1,259879	-1,125015	C	-8,174987	-0,032073	0,933684
C	5,139620	1,749378	0,516409	O	-2,641290	1,019231	-1,136815	H	-8,452976	0,949399	1,303953
H	4,862756	2,779157	0,747444	O	-6,017122	0,820921	0,531935	C	-9,078828	-1,089493	0,928848
								H	-10,087742	-0,929348	1,299036
								C	-8,699694	-2,353995	0,456032
								H	-9,408683	-3,175853	0,455532
								C	-7,408631	-2,543858	-0,012490
								H	-7,098991	-3,518259	-0,382711
								O	-5,273917	1,644613	-2,070118
								N	3,377611	-0,875807	-1,883279
								H	3,704819	-1,763985	-2,254732
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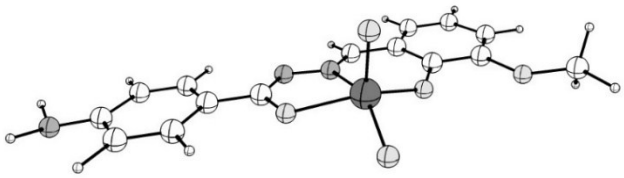
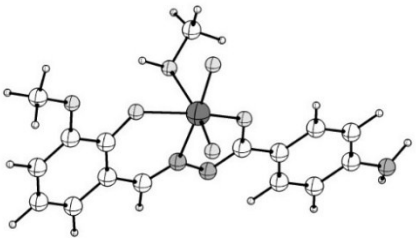
$[MoO_2L^2]$



Mo	0.478306	-1.293780	0.144921	C	-4.262202	-0.857961	-0.161772	H	0.510338	2.917268	-0.002908
N	0.058203	0.929043	-0.039736	H	-3.772889	-1.824488	-0.213474	C	2.347948	1.749703	-0.003248
N	-1.269897	1.290030	-0.076254	C	-5.646421	-0.780545	-0.154611	C	2.945097	0.481056	-0.164947
O	-1.476301	-0.998119	-0.152858	H	-6.240885	-1.689551	-0.206744	C	4.360413	0.363186	-0.156744
O	2.226479	-0.623114	-0.376077	C	-6.294238	0.468671	-0.085500	C	5.139609	1.507258	0.006574
O	0.511358	-2.754415	-0.721593	C	-5.504437	1.636493	-0.023736	H	6.220797	1.429880	0.015405
O	0.591168	-1.587822	1.812434	H	-5.990576	2.608017	0.026788	C	4.540146	2.770088	0.158518
O	4.835592	-0.896408	-0.317294	C	-4.122636	1.553965	-0.029925	H	5.169996	3.645424	0.283309
C	-2.017433	0.215656	-0.100444	H	-3.522081	2.455741	0.021660	C	3.165166	2.895542	0.150357
C	-3.475493	0.305492	-0.098620	C	0.920150	1.907133	-0.018880	H	2.694022	3.867144	0.269123
								C	6.241427	-1.089377	-0.309662
								H	6.727067	-0.543901	-1.129740
								H	6.393444	-2.160701	-0.447586
								H	6.684300	-0.778440	0.645784
								N	-7.675928	0.553504	-0.128648
								H	-8.089155	1.403438	0.231204
								H	-8.188795	-0.278250	0.131902

$[MoO_2L^2(MeOH)]$



Mo	-0.490828	-1.088367	-0.565273	C	3.477400	0.432172	-0.061822	H	-0.520089	3.027780	0.413795
N	-0.050917	1.071201	0.056691	C	4.267394	-0.700454	-0.322520	C	-2.344063	1.851634	0.164694
N	1.279021	1.397780	0.161605	H	3.780275	-1.645479	-0.537401	C	-2.941341	0.571984	0.113558
N	7.680816	0.696689	-0.071480	C	5.652426	-0.620834	-0.309352	C	-4.355573	0.462114	0.060831
O	1.485309	-0.854208	-0.318479	H	6.248795	-1.505767	-0.519246	C	-5.139178	1.615422	0.062003
O	-2.233347	-0.565741	0.169535	C	6.297555	0.600254	-0.034140	H	-6.219647	1.538971	0.019441
O	-0.524777	-2.786588	-0.393240	C	5.504892	1.737423	0.226925	C	-4.540878	2.884228	0.121892
O	-0.691431	-0.728323	-2.210022	H	5.988411	2.689051	0.435762	H	-5.168615	3.770081	0.122285
O	-0.286638	-1.193801	1.936822	C	4.122647	1.652853	0.210874	C	-3.165076	3.002960	0.178807
O	-4.834489	-0.809572	0.022917	H	3.519198	2.531217	0.412463	H	-2.695212	3.981620	0.222650
C	2.015727	0.340776	-0.074670	C	-0.911129	2.026577	0.226981	C	-6.237351	-0.993138	-0.071343
								H	-6.758642	-0.581305	0.803559
								H	-6.393471	-2.072338	-0.116
								H	-6.643277	-0.534555	-0.982763
								C	0.435934	-2.284502	2.530688
								H	0.068461	-3.247245	2.162668
								H	0.365423	-2.234982	3.623178
								H	1.475723	-2.159246	2.227428
								H	8.194396	-0.166088	0.050413
								H	-1.233523	-1.283735	2.137781
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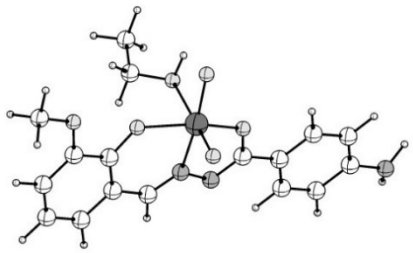
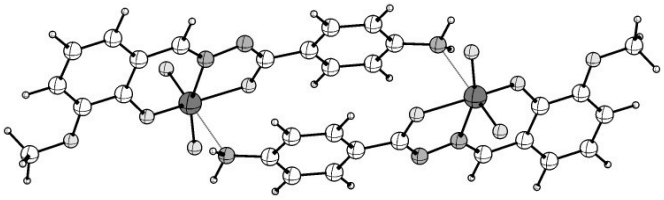
$[MoO_2L^2(EtOH)]$



Mo	-0.406650	-0.964393	-0.895531	C	4.209734	1.581520	0.368950	C	-2.866196	0.626711	-0.060780
N	0.034457	1.063285	0.047716	H	3.608109	2.425278	0.689093	C	-4.281409	0.551667	-0.151845
N	1.364373	1.357362	0.234380	C	5.591824	1.647549	0.429330	C	-5.047638	1.698375	0.051814
N	7.766437	0.640340	0.025192	H	6.077291	2.550563	0.792506	H	-6.128276	1.649478	-0.018684
O	1.569990	-0.775704	-0.620458	C	6.381908	0.554924	0.015277	C	-4.432785	2.925039	0.352555
O	-2.173349	-0.505488	-0.211032	C	5.734765	-0.602538	-0.458741	H	-5.048395	3.805787	0.507529
O	-0.439757	-2.675516	-0.853828	H	6.329627	-1.451779	-0.786972	C	-3.056742	3.008892	0.447913
O	-0.545427	-0.465144	-2.509286	C	4.350189	-0.664057	-0.515610	H	-2.573618	3.954745	0.677116
O	-0.091191	-1.536559	1.585936	H	3.860844	-1.560253	-0.881242	C	-6.179068	-0.821682	-0.584347
O	-4.776087	-0.682136	-0.433221	C	-0.820016	1.994930	0.347292	H	-6.712597	-0.572411	0.343031
C	2.101808	0.349120	-0.162351	H	-0.414589	2.945559	0.696283	H	-6.348357	-1.871813	-0.827266
C	3.562722	0.424051	-0.102303	C	-2.252911	1.864683	0.234200	H	-6.560337	-0.193641	-1.400480
								C	-1.099531	-1.355183	2.597367
								H	-2.065010	-1.723477	2.229673
								H	-1.180457	-0.273020	2.725402
								C	-0.706581	-2.029953	3.904291
								H	-0.621730	-3.116617	3.778489
								H	-1.465810	-1.842561	4.672739
								H	0.254893	-1.649528	4.264071
								H	8.269862	-0.236935	0.024614
								H	8.169577	1.324238	0.651868
								H	-0.022483	-2.485945	1.380525

$[MoO_2L^2]_2$



Mo	0.978134	1.731699	4.341458	C	2.109215	4.517510	4.730844	C	1.569932	0.627658	-1.056132
N	0.198195	3.303184	2.873507	C	2.943058	5.213026	5.644952	H	1.210324	1.121283	-1.951820
N	-0.614964	2.833032	1.867888	C	2.878895	6.604468	5.714665	C	2.086202	1.377521	-0.005520
O	-0.134328	0.842042	2.930847	H	3.510013	7.142530	6.412668	H	2.129709	2.460941	-0.083550
O	2.241974	3.186684	4.656957	C	2.003275	7.323101	4.884726	C	2.488768	0.747684	1.180391
O	1.904541	0.366134	4.783195	H	1.969814	8.405833	4.955961	C	2.451446	-0.654565	1.262840
O	-0.172415	2.010271	5.554970	C	1.191349	6.656617	3.986514	H	2.770121	-1.146067	2.177887
O	3.762486	4.427922	6.390955	H	0.509872	7.205156	3.342241	C	1.945479	-1.400144	0.208779
C	-0.734373	1.532655	1.970613	C	4.593129	5.053404	7.356348	H	1.874341	-2.479230	0.288069
C	-1.463589	0.767480	0.951630	H	5.308533	5.742607	6.887752	C	-0.369417	-4.588446	-2.943319
C	-1.569932	-0.627658	1.056132	H	5.137972	4.245210	7.846487	H	0.178893	-5.205869	-2.230325
H	-1.210324	-1.121283	1.951820	H	4.001093	5.598358	8.103280	C	-1.224862	-5.245298	-3.903049
C	-2.086202	-1.377521	0.005520	Mo	-0.978134	-1.731699	-4.341458	C	-2.109215	-4.517510	-4.730844
H	-2.129709	-2.460941	0.083550	N	-0.198195	-3.303184	-2.873507	C	-2.943058	-5.213026	-5.644952
C	-2.488768	-0.747684	-1.180391	N	0.614964	-2.833032	-1.867888	C	-2.878895	-6.604468	-5.714665
C	-2.451446	0.654565	-1.262840	O	0.134328	-0.842042	-2.930847	H	-3.510013	-7.142530	-6.412668
H	-2.770121	1.146067	-2.177887	O	-2.241974	-3.186684	-4.656957	C	-2.003275	-7.323101	-4.884726
C	-1.945479	1.400144	-0.208779	O	-1.904541	-0.366134	-4.783195	H	-1.969814	-8.405833	-4.955961
H	-1.874341	2.479230	-0.288069	O	0.172415	-2.010271	-5.554970	C	-1.191349	-6.656617	-3.986514
C	0.369417	4.588446	2.943319	O	-3.762486	-4.427922	-6.390955	H	-0.509872	-7.205156	-3.342241
H	-0.178893	5.205869	2.230325	C	0.734373	-1.532655	-1.970613	C	-4.593129	-5.053404	-7.356348
C	1.224862	5.245298	3.903049	C	1.463589	-0.767480	-0.951630	H	-5.308533	-5.742607	-6.887752
								H	-5.137972	-4.245210	-7.846487
								H	-4.001093	-5.598358	-8.103280
								N	-2.827601	-1.513543	-2.320111
								H	-3.480377	-1.046746	-2.944563
								H	-3.162574	-2.448171	-2.104485
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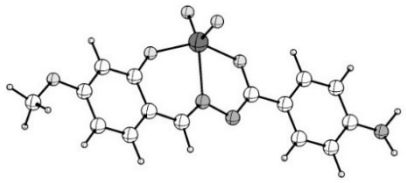
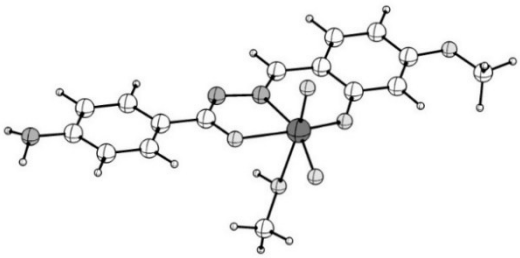
[MoO_2L^3]



Mo	-0.184926	1.565403	0.074256	C	4.473222	0.554517	-0.138181	H	-0.718349	-2.603673	0.013633
O	1.723839	1.034360	-0.163051	H	4.106456	1.572818	-0.208157	C	-2.403824	-1.234441	-0.036387
O	-2.025193	1.114051	-0.395233	C	5.837812	0.308750	-0.112362	C	-2.872899	0.099742	-0.204304
O	-0.261955	1.977025	1.718867	H	6.539185	1.137903	-0.168101	C	-4.241040	0.362560	-0.219497
O	-0.043197	2.960634	-0.884935	C	6.327746	-1.008552	-0.019103	H	-4.593350	1.378631	-0.354208
O	-6.465617	-0.312621	-0.096639	C	5.400689	-2.070122	0.046513	C	-5.162597	-0.680417	-0.069341
N	-0.038005	-0.683049	-0.057698	H	5.763682	-3.093029	0.114962	C	-4.718152	-2.009668	0.091474
N	1.238871	-1.207704	-0.066302	C	4.039210	-1.819712	0.021144	H	-5.420128	-2.825879	0.207150
C	2.112916	-0.236900	-0.092373	H	3.332635	-2.640922	0.075647	C	-3.357351	-2.263959	0.100926
C	3.549897	-0.503174	-0.070948	C	-1.011394	-1.554204	-0.028227	H	-3.005973	-3.285412	0.223917
								C	-7.467518	-1.312069	0.048327
								H	-7.387144	-1.822247	1.016197
								H	-8.420520	-0.783801	-0.004319
								H	-7.416064	-2.051352	-0.760638
								N	7.690150	-1.261777	-0.043059
								H	7.990715	-2.149126	0.337891
								H	8.295304	-0.494795	0.218645

[MoO_2L^3(MeOH)]



Mo	-0.324944	-1.285736	-0.524901	C	4.402339	-0.528604	-0.324613	C	-2.384768	1.549705	0.116875
N	-0.048571	0.904595	0.036028	H	3.986998	-1.512224	-0.515589	C	-2.921844	0.235384	0.037693
N	1.260919	1.337483	0.142085	C	5.777484	-0.344411	-0.319046	C	-4.311373	0.043136	0.007520
N	7.701014	1.128067	-0.122575	H	6.438302	-1.186528	-0.511185	C	-5.172105	1.141047	0.053549
O	1.641889	-0.892942	-0.316914	C	6.329300	0.928014	-0.075629	C	-4.654547	2.452270	0.140789
O	-2.150163	-0.851639	0.032049	C	5.453399	2.007797	0.162055	H	-5.347119	3.285792	0.177048
O	-0.235203	-2.956268	-0.193651	H	5.864016	2.998321	0.344431	C	-3.289754	2.636909	0.174553
O	-0.466433	-1.095628	-2.204092	C	4.081209	1.818755	0.153483	H	-2.885681	3.644216	0.239727
O	-0.035399	-1.194848	1.987646	H	3.414355	2.655004	0.333935	C	0.777720	-2.188750	2.632458
C	2.078118	0.340135	-0.091885	C	-0.976308	1.809944	0.166297	H	0.381436	-3.153245	2.318643
C	3.529463	0.546768	-0.087160	H	-0.644583	2.838780	0.316870	H	0.702885	-2.089965	3.721453
								H	1.823761	-2.109961	2.316040
								H	8.279779	0.310011	0.014248
								H	0.304806	-0.314390	2.212578
								H	8.053615	1.944928	0.358315
								O	-6.523844	1.051272	0.024991
								C	-7.120578	-0.236698	-0.074204
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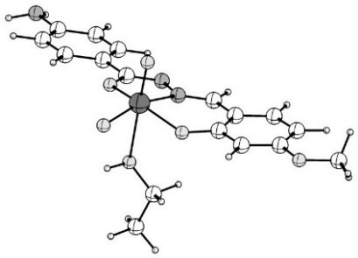
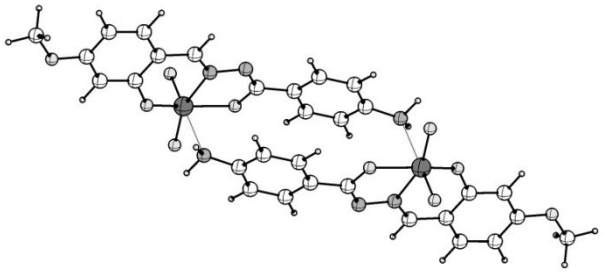
								H	-6.865671	-0.862292	0.790191
								H	-8.197615	-0.063474	-0.092924
								H	-4.673161	-0.975589	-0.047731

[MoO_2L^3(EtOH)]



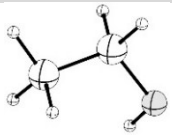
Mo	-0.151912	-1.151493	-1.002901	H	3.388450	2.606094	0.847835	C	-4.194444	-0.144154	-0.286157
N	0.018290	0.855397	0.044038	C	5.456944	2.087786	0.602076	C	-5.110251	0.884444	-0.035314
N	1.300127	1.300890	0.278279	H	5.821363	3.022911	1.021423	C	-4.658231	2.160949	0.351398
N	7.746362	1.373717	0.205099	C	6.382356	1.121634	0.155789	H	-5.352417	2.967794	0.550798
O	1.778804	-0.744239	-0.672332	C	5.890589	-0.079291	-0.390382	C	-3.294185	2.377686	0.472952
O	-1.992932	-0.948500	-0.367104	H	6.590749	-0.832692	-0.743936	H	-2.937036	3.361189	0.768750
O	0.013937	-2.856035	-1.021014	C	4.524871	-0.304432	-0.486453	H	-4.553779	-1.125451	-0.574364
O	-0.311897	-0.613078	-2.601919	H	4.155806	-1.233082	-0.908068	C	-0.855192	-1.763796	2.470890
O	0.172157	-1.789903	1.463828	C	-0.948609	1.664673	0.364486	H	-1.770372	-2.226849	2.081604
C	2.162607	0.412473	-0.144605	H	-0.664014	2.639163	0.764290	H	-1.061247	-0.703841	2.638483
C	3.602774	0.657778	-0.041471	C	-2.346204	1.368911	0.215249	C	-0.394565	-2.437631	3.756185
C	4.094543	1.858643	0.502649	C	-2.823815	0.080888	-0.166026	H	-0.183842	-3.501698	3.591378
								H	-1.174453	-2.367930	4.523620
								H	0.514630	-1.962479	4.138423
								H	8.351761	0.563826	0.177776
								H	8.049210	2.066051	0.877472
								H	0.349609	-2.716086	1.220876
								O	-6.416676	0.550200	-0.186020
								C	-7.407259	1.544965	0.036206
								H	-7.382832	1.912549	1.069991
								H	-7.288712	2.389978	-0.653582
								H	-8.364767	1.056528	-0.151182

$[MoO_2L^3]_2$



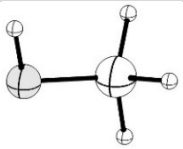
Mo	4.083415	-0.682002	2.370569
O	2.126172	-0.318288	2.174997
O	5.863743	-0.302489	1.640283
O	4.322251	-0.334358	4.012554
O	4.008974	-2.379411	2.186923
O	10.216038	1.401363	1.638055
N	3.777178	1.458704	1.652271
N	2.466963	1.861949	1.506785
C	1.666704	0.868814	1.795575
C	0.215416	0.994661	1.609557
C	-0.630778	-0.086664	1.897265
H	-0.218636	-0.972734	2.366611
C	-1.974866	-0.045899	1.543577
H	-2.612238	-0.904546	1.739222
C	-2.495871	1.071483	0.877158
C	-1.670592	2.186175	0.652375
H	-2.073732	3.056844	0.142692
C	-0.332775	2.145767	1.015376
H	0.316091	2.987979	0.802118
C	4.695176	2.358421	1.453484
H	4.358380	3.373100	1.234862
C	6.107459	2.101628	1.510793
C	6.647278	0.786291	1.623708
C	8.027826	0.603244	1.660547
H	8.434707	-0.398045	1.744069
C	8.895060	1.700820	1.588586
C	8.381254	3.006304	1.466123
H	9.036546	3.866150	1.405860
C	7.006765	3.181883	1.424640
H	6.602445	4.186938	1.332145
C	11.162881	2.461103	1.584874
H	11.036831	3.153747	2.426319
H	12.142553	1.985623	1.651169
H	11.091229	3.016152	0.641046
Mo	-4.083415	0.682002	-2.370569
O	-2.126172	0.318288	-2.174997
O	-5.863743	0.302489	-1.640283
O	-4.322251	0.334358	-4.012554
O	-4.008974	2.379411	-2.186923
O	-10.216038	-1.401363	-1.638055
N	-3.777178	-1.458704	-1.652271
N	-2.466963	-1.861949	-1.506785
C	-1.666704	-0.868814	-1.795575
C	-0.215416	-0.994661	-1.609557
C	0.630778	0.086664	-1.897265
H	0.218636	0.972734	-2.366611
C	1.974866	0.045899	-1.543577
H	2.612238	0.904546	-1.739222
C	2.495871	-1.071483	-0.877158
C	1.670592	-2.186175	-0.652375
H	2.073732	-3.056844	-0.142692
C	0.332775	-2.145767	-1.015376
H	-0.316091	-2.987979	-0.802118
C	-4.695176	-2.358421	-1.453484
H	-4.358380	-3.373100	-1.234862
C	-6.107459	-2.101628	-1.510793
C	-6.647278	-0.786291	-1.623708
C	-8.027826	-0.603244	-1.660547
H	-8.434707	0.398045	-1.744069
C	-8.895060	-1.700820	-1.588586
C	-8.381254	-3.006304	-1.466123
H	-9.036546	-3.866150	-1.405860
C	-7.006765	-3.181883	-1.424640
H	-6.602445	-4.186938	-1.332145
C	-11.162881	-2.461103	-1.584874
H	-11.036831	-3.153747	-2.426319
H	-12.142553	-1.985623	-1.651169
H	-11.091229	-3.016152	-0.641046
N	3.805386	-1.042081	-0.340877
H	4.426456	-0.390374	-0.811839
H	4.241611	-1.958902	-0.285587
N	-3.805386	1.042081	0.340877
H	-4.241611	1.958902	0.285587
H	-4.426456	0.390374	0.811839

EtOH



O	-1.240557	-0.259959	-0.109124
C	-0.085247	0.555965	0.047284
H	-0.129572	1.129988	0.987693
H	-0.130958	1.279814	-0.773099
C	1.216430	-0.239094	-0.022023
H	1.282029	-0.959762	0.803985
H	2.087068	0.424305	0.047211
H	1.275330	-0.795300	-0.963520
H	-1.246538	-0.900601	0.619152

MeOH



O	-0.748606	-0.122482	0.001
C	0.661940	0.019648	0.035
H	1.036807	0.543842	0.893075
H	1.036822	0.543722	-0.893232
H	1.079608	-0.990888	-0.013
H	-1.136031	0.765290	-0.051

Complex 1

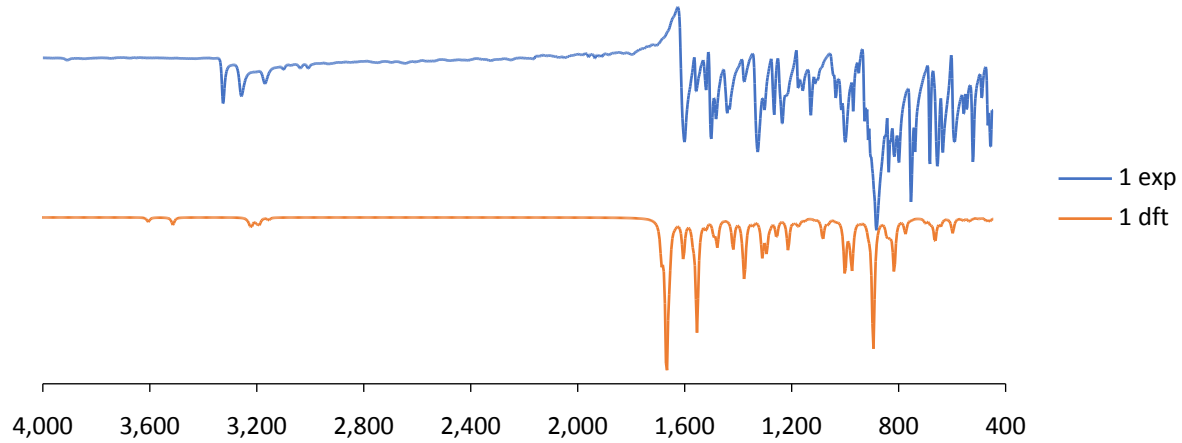


Fig. S20 Infrared spectra (experimental and theoretical) of **1** (x-axis is in cm^{-1}).

Complex 1a

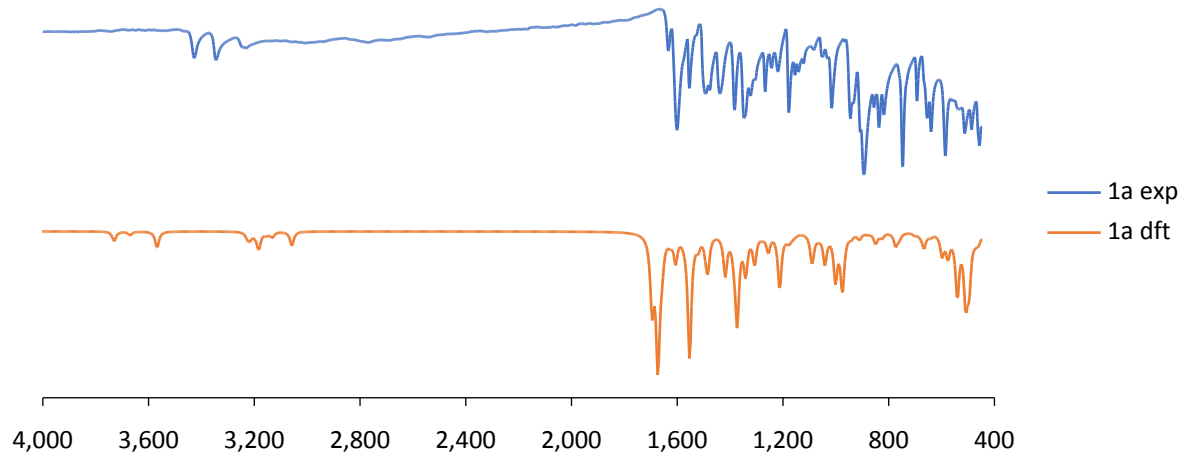


Fig. S21 Infrared spectra (experimental and theoretical) of **1a** (x-axis is in cm^{-1}).

Complex 1b

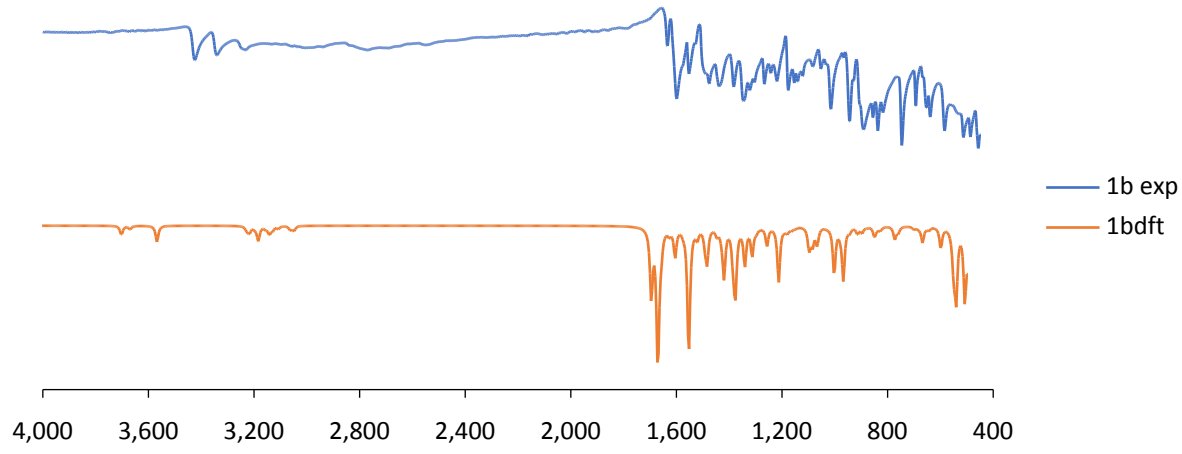


Fig. S22 Infrared spectra (experimental and theoretical) of **1b** (x-axis is in cm^{-1}).

Complex 2

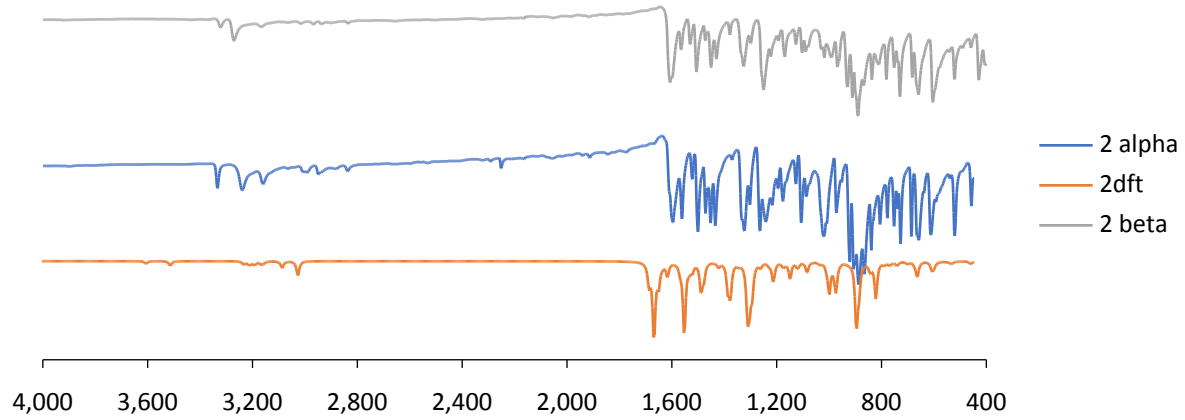


Fig. S23 Infrared spectra (experimental and theoretical) of **2** (x-axis is in cm^{-1}).

Complex 2a

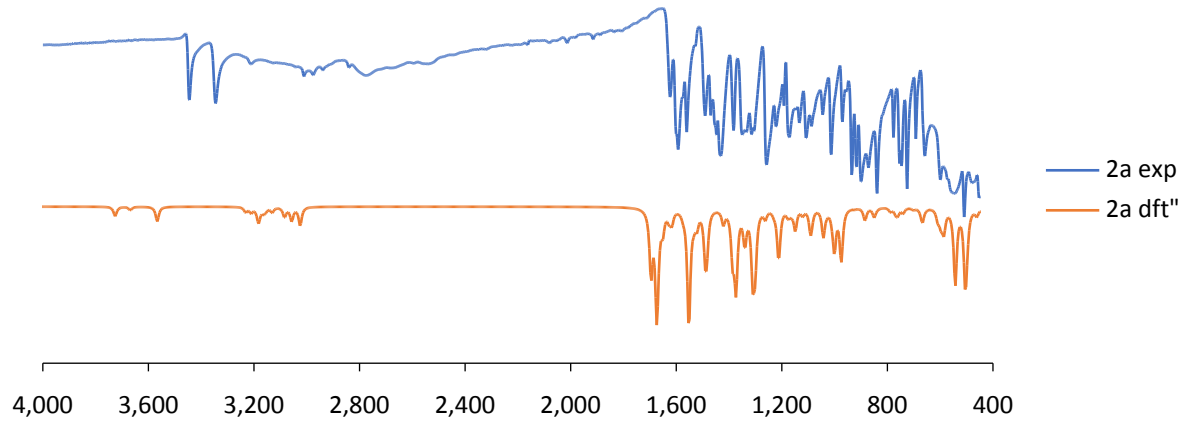


Fig. S24 Infrared spectra (experimental and theoretical) of **2a** (x-axis is in cm^{-1}).

Complex 2b

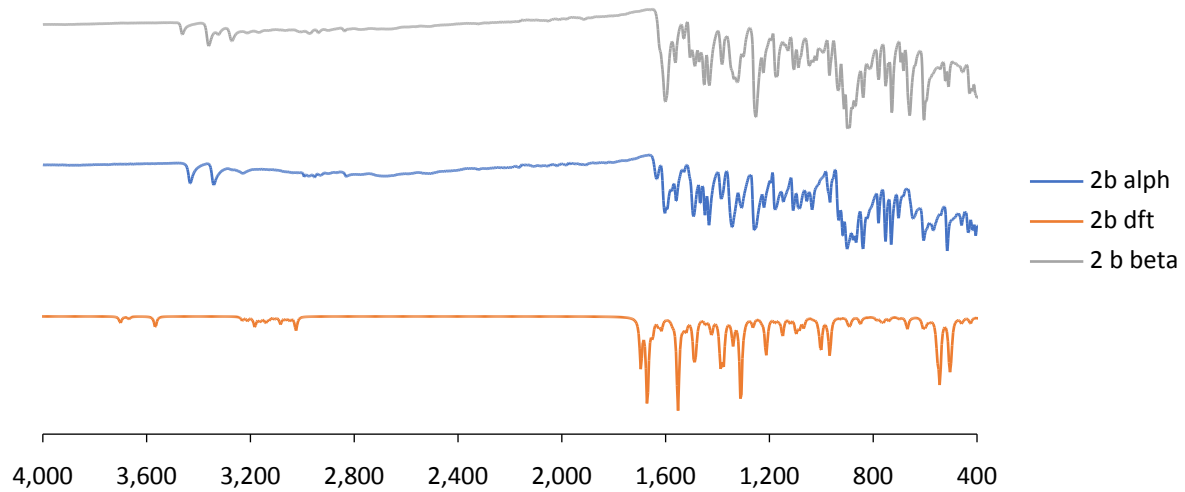


Fig. S25 Infrared spectra (experimental and theoretical) of **2b** (x-axis is in cm^{-1}).

Complex 3

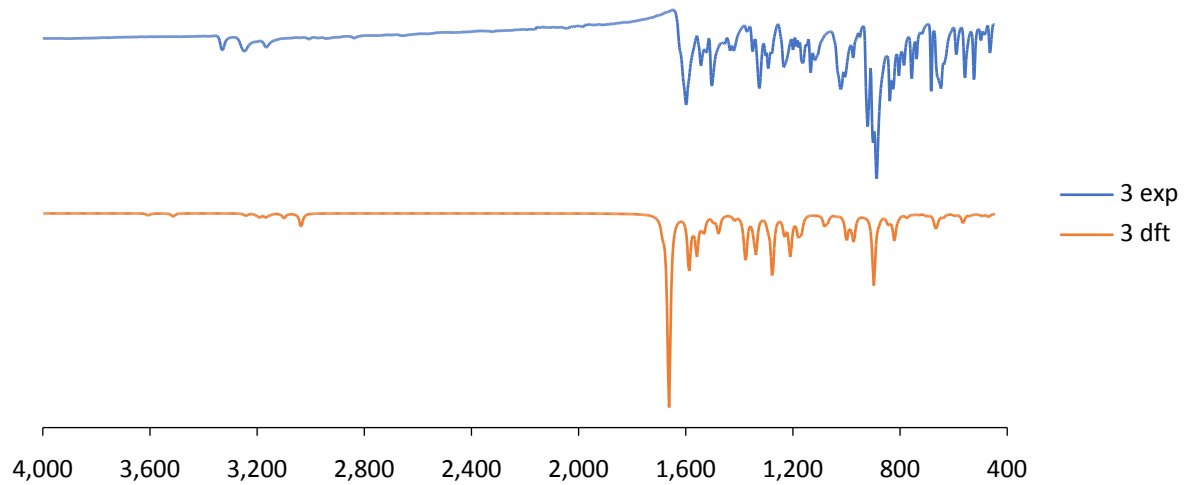


Fig. S26 Infrared spectra (experimental and theoretical) of **3** (x-axis is in cm^{-1}).

Complex 3a

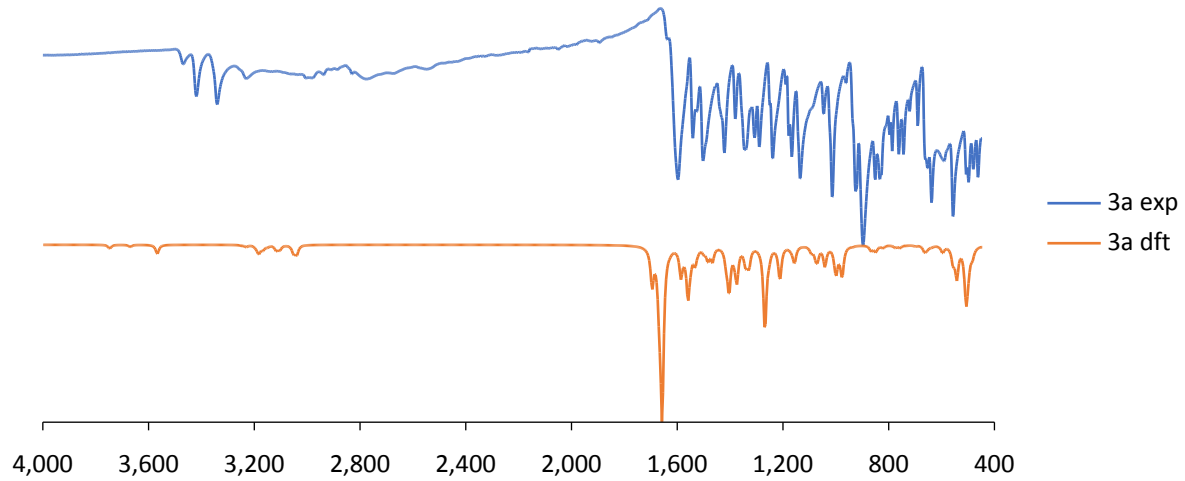


Fig. S27 Infrared spectra (experimental and theoretical) of **3a** (x-axis is in cm^{-1}).

Complex 3b

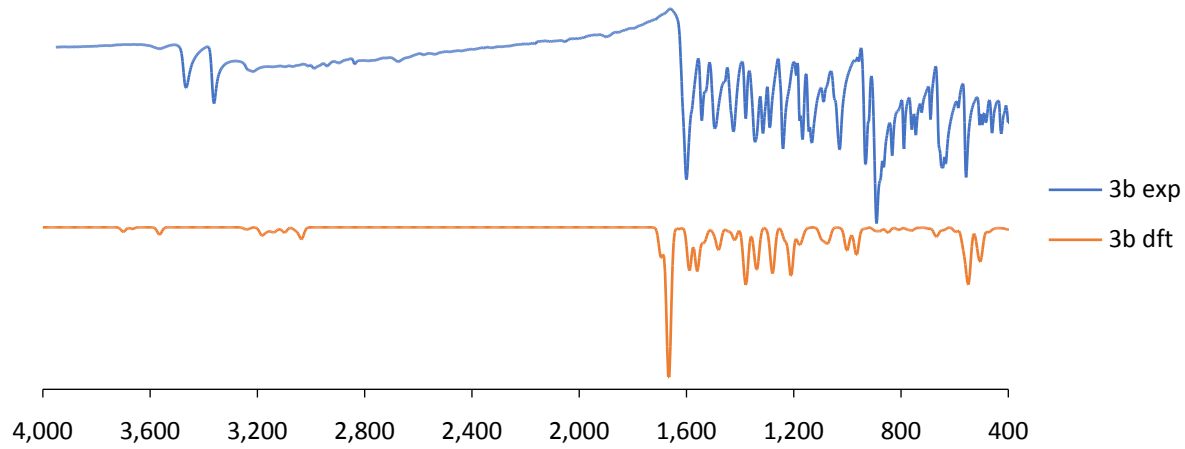


Fig. S28 - Infrared spectra (experimental and theoretical) of 3**b** (x axis is in cm^{-1}).

7. PXRD studies

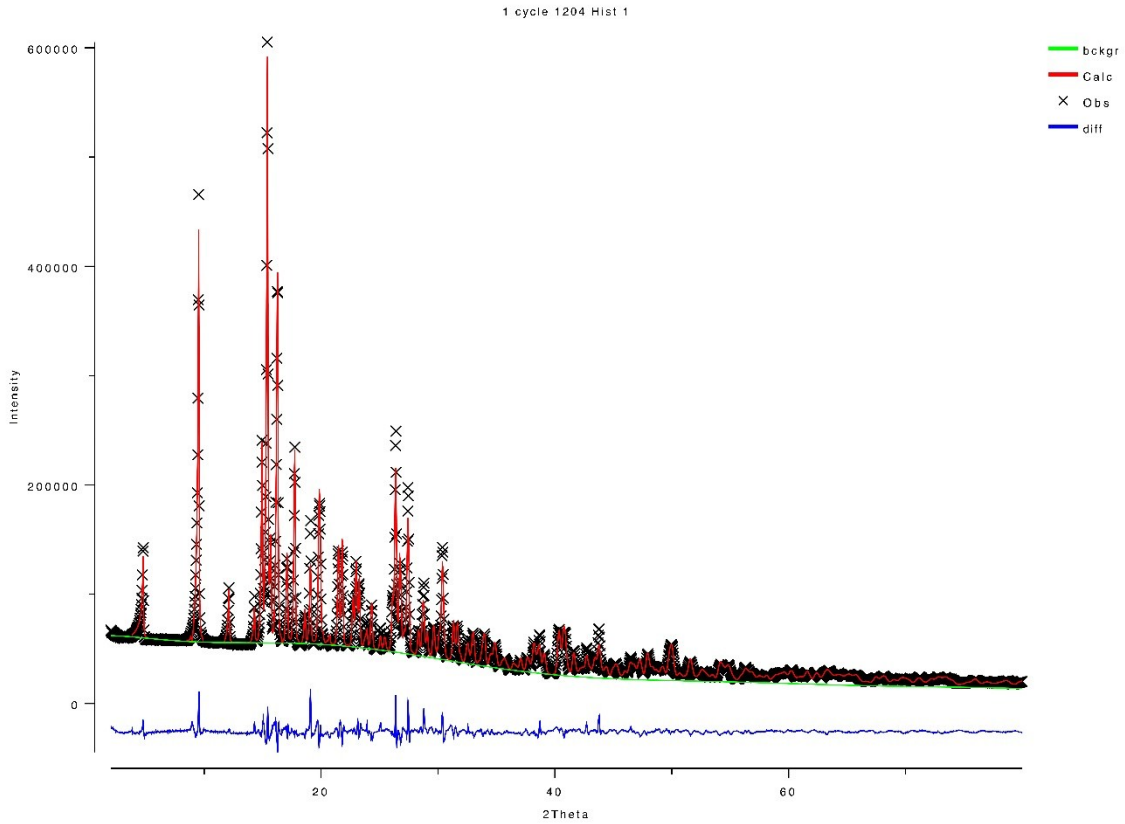


Fig. S29 Rietveld refinement of the structure **2-α**. Observed intensities (black), calculated intensities (red), difference curve (blue), background (green).

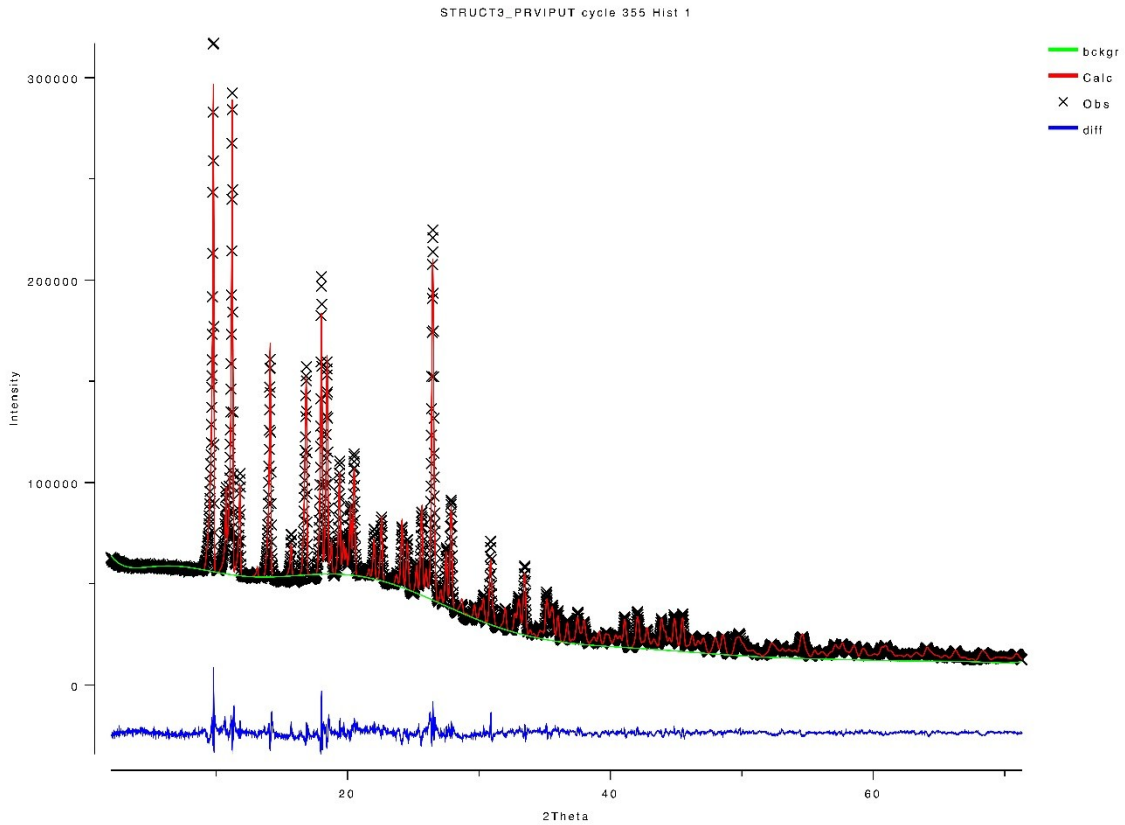


Fig. S30 Rietveld refinement of the structure **3**. Observed intensities (black), calculated intensities (red), difference curve (blue), background (green).