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Discrete and polymeric ensembles based on dinuclear molybdenum(VI) building blocks with adaptive carbohydrazide ligands: from the design to catalytic epoxidation

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Electronic Supplementary Information

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Molecular and crystal structures

Table S1. General and crystal data, summary of intensity data collection and structure refinement for **1a**, **1b·CH_3CN, 5a·CH_3OH, 5a·0.64CH_3OH, 5b·CH_3CN, 6a, 6b·2CH_3CN** and **H_4L^6**

Identification code	**1a**	**1b·CH_3CN**	**5a·CH_3OH**	**5a'·0.64CH_3OH**	**5b·CH_3CN**	**6a**	**6b·2CH_3CN**	**H_4L^6**
Empirical formula	$C_{17}H_{18}Mo_2N_4O_9$	$C_{23}H_{21}Mo_2N_9O_7$	$C_{20}H_{26}Mo_2N_4O_{12}$	$C_{19.64}H_{22}Mo_2N_4O_{11.64}$	$C_{25}H_{25}Mo_2N_9O_9$	$C_{19}H_{22}Mo_2N_4O_{11}$	$C_{27}H_{28}Mo_2N_{10}O_9$	$C_{17}H_{18}N_4O_5$
M_r	614.23	727.37	706.33	692.21	787.42	674.28	828.47	358.35
T/K	295(2)	150(2)	150(2)	150(2)	150(2)	295(2)	150(2)	298(2)
Crystal system	triclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$C2/c$
a/Å	7.2762(3)	8.6920(4)	9.6337(5)	7.4466(4)	8.2715(3)	7.4676(3)	8.6152(4)	9.3305(8)
b/Å	11.2625(3)	26.7430(8)	11.0989(6)	13.8570(9)	12.1751(5)	11.7394(4)	13.1856(7)	10.2881(7)
c/Å	25.8472(7)	11.6059(4)	13.1012(8)	14.0640(8)	15.0901(5)	14.8772(6)	15.5721(8)	18.0461(16)
α/°	88.871(2)	90	112.619(5)	112.516(5)	85.958(3)	105.949(3)	75.325(4)	90
β/°	86.314(3)	96.219(4)	98.807(5)	98.637(4)	87.645(3)	103.394(3)	74.393(4)	104.692(8)
γ/°	89.709(2)	90	94.858(4)	97.085(5)	81.166(3)	96.009(3)	85.158(4)	90
V/Å^3	2113.32(12)	2681.92(17)	1261.91(13)	1299.16(14)	1497.20(10)	1199.98(8)	1647.89(15)	1675.7(2)
Z	4	4	2	2	2	2	2	4
ρ_{calc}/g cm^{-3}	1.931	1.801	1.859	1.774	1.747	1.866	1.67	1.420
μ/mm^{-1}	1.245	0.997	1.064	1.031	0.905	1.111	0.827	0.107
F(000)	1216	1448	708	689.9	788	672	832	752.0
Crystal size/mm^3	0.38 × 0.25 × 0.03	0.30 × 0.03 × 0.01	0.42 × 0.32 × 0.09	0.13 × 0.07 × 0.06	0.4 × 0.3 × 0.1	0.18 × 0.10 × 0.03	0.3 × 0.2 × 0.1	0.2 x 0.2 x 0.05
Radiation	Mo $K\alpha$ (λ = 0.71073 Å)							
2Θ range/°	8.18 to 52.998	8.264 to 57.994	8.342 to 66.08	5.42 to 59	4.2 to 65.71	8.448 to 58	4.724 to 58.998	8.26 to 53.974
Index ranges	$-9 \le h \le 9$ $-14 \le k \le 14$ $-32 \le l \le 29$	$-11 \le h \le 11$ $-36 \le k \le 36$ $-9 \le l \le 15$	$-14 \le h \le 14$ $-16 \le k \le 16$ $-19 \le l \le 20$	$-10 \le h \le 10$ $-17 \le k \le 19$ $-19 \le l \le 19$	$-10 \le h \le 12$ $-18 \le k \le 17$ $-22 \le l \le 22$	$-10 \le h \le 8$ $-16 \le k \le 15$ $-18 \le l \le 20$	$-11 \le h \le 11$ $-18 \le k \le 18$ $-21 \le l \le 20$	$-11 \le h \le 11$ $-13 \le k \le 13$ $-22 \le l \le 22$
Reflections collected	15343	22137	28141	22705	18424	12820	18887	7739
Independent reflections	8699 [R_{int} = 0.0259, R_{sigma} = 0.0456]	6465 [R_{int} = 0.0636, R_{sigma} = 0.0865]	8570 [R_{int} = 0.0378, R_{sigma} = 0.0427]	7244 [R_{int} = 0.0916, R_{sigma} = 0.1160]	9788 [R_{int} = 0.0315, R_{sigma} = 0.0513]	6347 [R_{int} = 0.0399, R_{sigma} = 0.0703]	9170 [R_{int} = 0.0488, R_{sigma} = 0.0770]	1821 [R_{int} = 0.0566, R_{sigma} = 0.0697]

Data/restraints/ parameters	8699/12/593	6465/2/377	8570/3/357	7244/12/356	9788/1/437	6347/2/335	9170/2/443	1821/5/125
g_1, g_2 in w[a]	0.0013, 15.8437	0.0343, 0.3084	0.0401, 1.5379	0.0511, 0.9217	0.0277, 0.6461	0.0343, 0	0.0391, 0	0.0317, 0
Goodness-of-fit on F^2, S[b]	1.194	1.019	1.045	1.054	1.061	1.001	1.021	1.053
Final R and wR[c] values $[I \geq 2\sigma(I)]$	$R_1 = 0.0529$, $wR_2 = 0.1176$	$R_1 = 0.0472$, $wR_2 = 0.0853$	$R_1 = 0.0364$, $wR_2 = 0.0859$	$R_1 = 0.0633$, $wR_2 = 0.1267$	$R_1 = 0.0344$, $wR_2 = 0.0723$	$R_1 = 0.0433$, $wR_2 = 0.0814$	$R_1 = 0.0433$, $wR_2 = 0.0906$	$R_1 = 0.0664$, $wR_2 = 0.1061$
Final R and wR[c] values [all data]	$R_1 = 0.0597$, $wR_2 = 0.1205$	$R_1 = 0.0865$, $wR_2 = 0.0977$	$R_1 = 0.0521$, $wR_2 = 0.0968$	$R_1 = 0.1156$, $wR_2 = 0.1477$	$R_1 = 0.0508$, $wR_2 = 0.0803$	$R_1 = 0.0783$, $wR_2 = 0.0929$	$R_1 = 0.0724$, $wR_2 = 0.1001$	$R_1 = 0.1372$, $wR_2 = 0.1242$
Largest diff. peak/hole / e Å^{-3}	0.90/–0.71	0.76/–0.59	1.56/–0.84	1.26/–1.17	1.29/–0.81	0.73/–0.59	0.80/–0.66	0.14/–0.14

[a] $w = 1/[\sigma^2(F_o^2) + (g_1P)^2 + g_2P]$ where $P = (F_o^2 + 2F_c^2)/3$

[b] $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(N_r - N_p)\}^{1/2}$ where N_r = number of independent reflections, N_p = number of refined parameters.

[c] $R = \Sigma||F_o| - |F_c||/\ \Sigma|F_o|$; $wR = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

Description of molecular and crystal structure of H_4L^6

Molecule of H_4L^6 is almost planar and in the solid state assumes a *syn* conformation. Both hydroxyaryl subunits participate in intramolecular hydrogen bond (O1–H1···N1), as well as intermolecular hydrogen bonding (N2–H2···O1) with adjacent molecules building a supramolecular chain $C_1^1(7)$ motif (Figure S2).

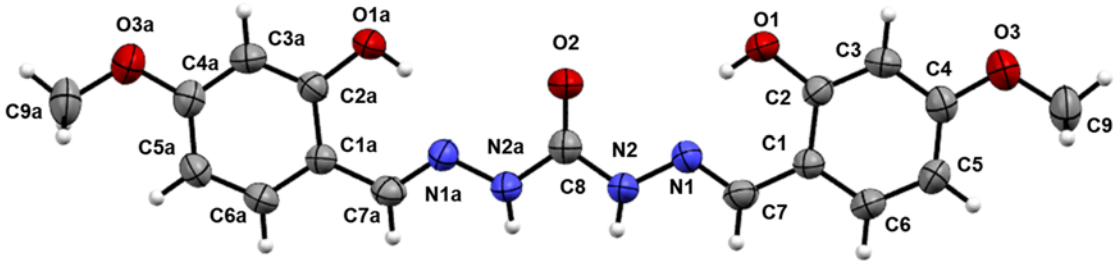


Figure S1. Mercury-ORTEP view of molecular structure of H_4L^6.The displacement ellipsoids are drawn at 50% probability level. Hydrogen atoms are presented as spheres of arbitrary small radii.

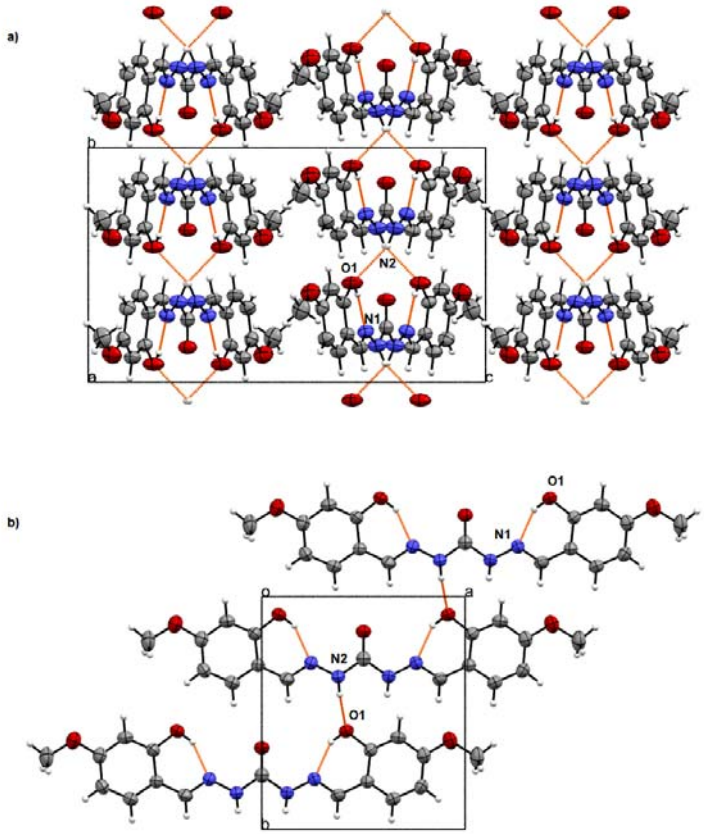


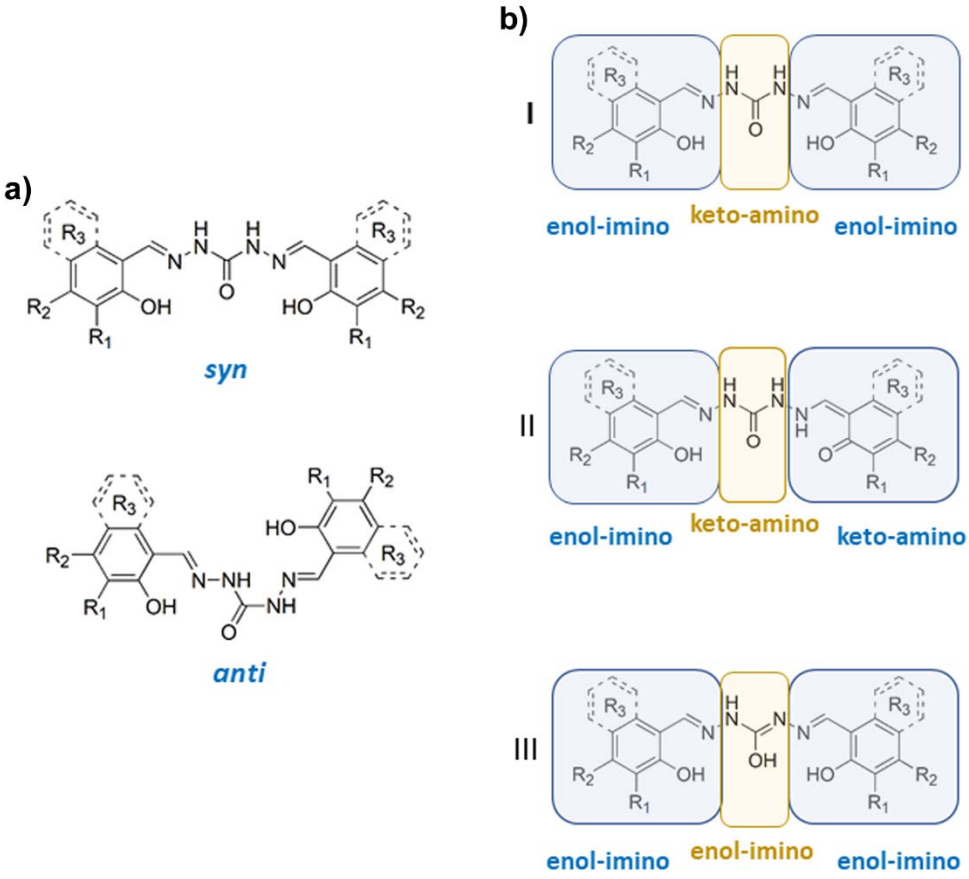
Figure S2. Crystal packing in H_4L^6 shown down the: (a) *a*-axis; and (b) *c*-axis. Hydrogen bonds of the O–H···N type are presented by orange dashed lines. Hydrogen bonds of the N2–H2···O1 type shape supramolecular motifs $C_1^1(7)$ and $R_4^4(32)$.

Table S2. Bond lengths and bond angles for H_4L^6.

Bond	Length / Å	Angle	Angle / °
C1–C6	1.388(4)	C2–C1–C6	117.1(2)
C1–C7	1.443(4)	C2–C1–C7	121.8(2)
C1–C2	1.407(3)	C6–C1–C7	121.09(19)
C2–C3	1.370(4)	O1–C2–C1	121.2(2)
C3–C4	1.386(4)	O1–C2–C3	118.25(19)
C4–C5	1.388(3)	C1–C2–C3	120.6(2)
C5–C6	1.381(4)	C2–C3–C4	121.0(2)
N1–N2	1.368(3)	C3–C4–C5	119.8(2)
N1–C7	1.283(3)	O3–C4–C3	115.23(19)
N2–H2	0.854(18)	O3–C4–C5	125.0(2)
N2–C8	1.372(3)	C4–C5–C6	118.6(2)
O1–C2	1.371(3)	C1–C6–C5	122.9(2)
O1–H1	0.84(2)	N1–C7–C1	120.08(19)
O2–C8	1.214(4)	N2–C8–N2a	110.6(2)
O3–C4	1.363(3)	O2–C8–N2	124.68(13)
O3–C9	1.420(3)	N2–N1–C7	118.64(19)
		N1–N2–H2	122.6(19)
		N1–N2–C8	118.68(19)
		C8–N2–H2	115.4(18)
		C2–O1–H1	106.9(14)
		C4–O3–C9	118.6(2)

Table S3. Geometry of hydrogen bonds (Å, º) for H_4L^6.

D–H···A	D–H	H···A	D···A	∠D–H···A	Symmetry code
H_4L^6					
O1–H1···N1	0.84(2)	1.81(2)	2.571(3)	150(2)	-
N2–H2···O1	0.854(18)	2.246(19)	3.060(3)	159.2(19)	3/2–*x*, ½+*y*, ½–*z*



Scheme S1. Some of the possible: a) conformers and b) tautomers for H_4L^1–H_4L^6.

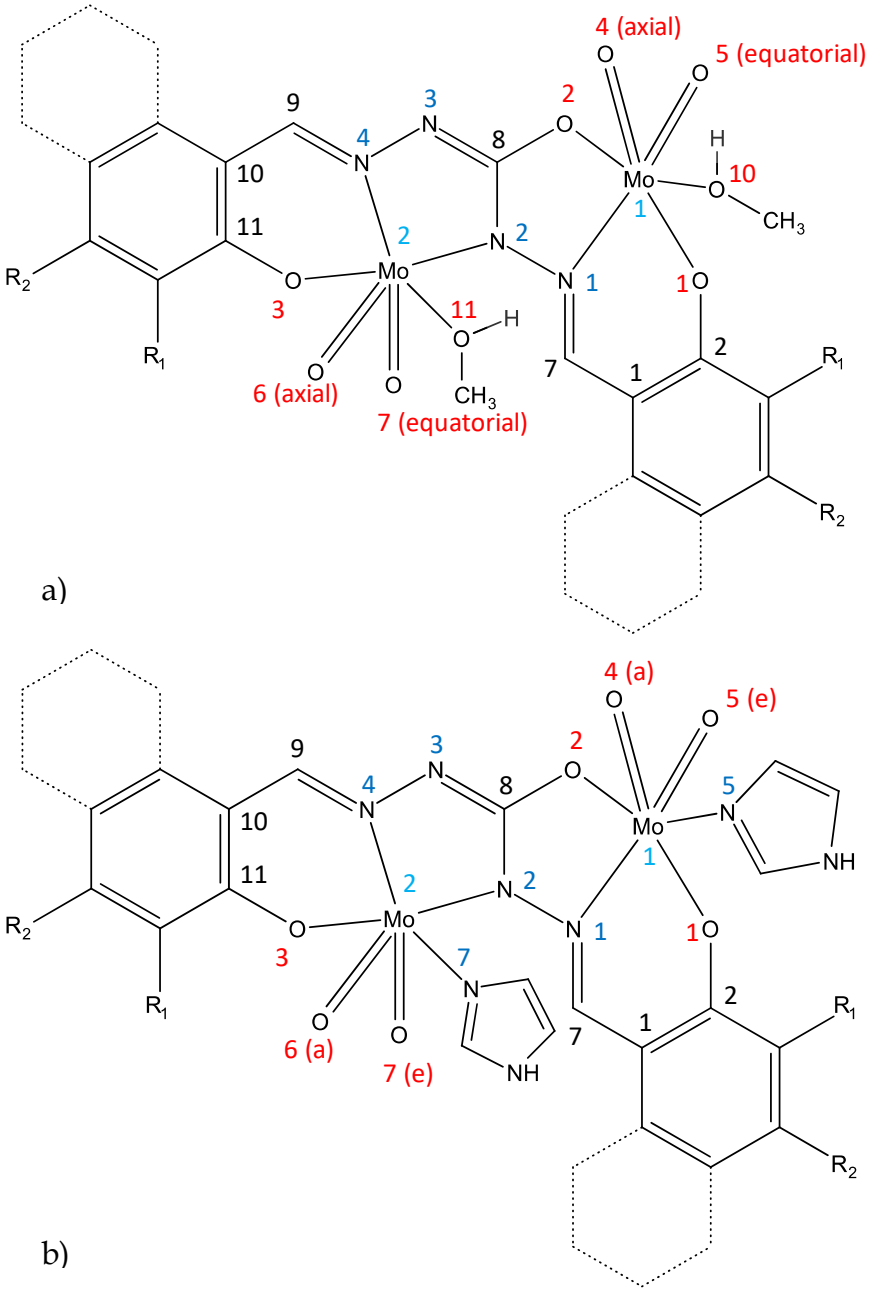


Figure S3. The numbering scheme for relevant atoms used in description of geometric parameters of the crystal structures of a) methanol complexes and b) imidazole complexes. Carbon atoms are represented by black, molybdenum by cyan, oxygen by red and nitrogen by blue numbers. Hydrogen atoms have the same number as its parent atom.

Table S4. Selected bond lengths (in Å) in reported crystal structures. Atoms are numbered according to Figure S3.

Bond	**1a**	**1b·CH_3CN**	**5a·CH_3OH**	**5a'·0.64CH_3OH**	**5b·CH_3CN**	**6a**	**6b·2CH_3CN**
Mo1–O1	1.907(5), 1.903(5)	1.916(2)	1.911(2)	1.916(4)	1.9057(16)	1.908(2)	1.917(2)
Mo1–N1	2.276(5), 2.271(5)	2.277(3)	2.275(2)	2.279(5)	2.2913(17)	2.287(3)	2.280(3)
Mo1–O2	1.999(4), 1.999(4)	1.996(2)	2.014(2)	2.015(4)	2.0173(16)	2.000(2)	2.007(2)
Mo1–O4	1.689(6), 1.698(5)	1.710(3)	1.699(2)	1.702(5)	1.7118(17)	1.694(3)	1.706(3)
Mo1–O5	1.701(5), 1.709(5)	1.702(2)	1.7121(18)	1.712(4)	1.7022(16)	1.705(3)	1.704(2)
Mo1–O10	2.358(5), 2.302(5)	N/A	2.251(2)	2.268(5)	N/A	2.316(3)	N/A
Mo1–N5	N/A	2.295(4)	N/A	N/A	2.306(2)	N/A	2.353(3)
Mo2–N2	2.103(5), 2.121(5)	2.142(3)	2.109(2)	2.123(6)	2.1556(17)	2.106(3)	2.114(3)
Mo2–N4	2.251(6), 2.249(5)	2.244(3)	2.228(2)	2.242(5)	2.2561(17)	2.231(3)	2.243(3)
Mo2–O3	1.926(5), 1.926(5)	1.942(2)	1.916(2)	1.914(5)	1.9339(15)	1.923(2)	1.951(2)
Mo2–O6	1.691(5), 1.688(5)	1.696(3)	1.692(2)	1.688(6), 1.703(9)	1.6954(17)	1.691(3)	1.720(3)
Mo2–O7	1.702(5), 1.698(5)	1.707(3)	1.701(2)	1.693(5), 1.718(7)	1.7098(16)	1.703(3)	1.707(2)
Mo2–O11	2.342(5), 2.344(4)	N/A	2.388(2)	2.416(7), 2.255(10)	N/A	2.364(3)	N/A
Mo2–N7	N/A	2.372(4)	N/A	N/A	2.3577(17)	N/A	2.325(3)
O1–C2	1.361(8), 1.357(8)	1.358(4)	1.353(3)	1.364(6)	1.352(3)	1.341(5)	1.352(4)

O2–C8	1.301(7), 1.306(7)	1.315(4)	1.301(3)	1.317(9)	1.308(3)	1.305(5)	1.314(5)
O3–C11	1.344(9), 1.347(8)	1.344(5)	1.340(3)	1.354(8)	1.347(3)	1.349(5)	1.344(4)
N1–C7	1.281(9), 1.270(8)	1.283(5)	1.291(3)	1.275(8)	1.284(3)	1.289(5)	1.287(4)
N1–N2	1.392(7), 1.396(7)	1.397(4)	1.385(3)	1.378(7)	1.395(2)	1.396(4)	1.396(4)
N2–C8	1.384(7), 1.358(7)	1.370(5)	1.369(3)	1.374(8)	1.359(3)	1.367(5)	1.384(4)
N3–C8	1.312(7), 1.317(7)	1.315(5)	1.314(4)	1.320(9)	1.323(3)	1.302(5)	1.304(4)
N3–N4	1.398(8), 1.397(7)	1.400(4)	1.393(3)	1.401(8)	1.399(2)	1.401(4)	1.395(4)
N4–C9	1.286(9), 1.295(8)	1.292(5)	1.294(4)	1.307(9)	1.291(3)	1.290(5)	1.287(4)
C1–C7	1.446(11), 1.466(8)	1.448(5)	1.453(4)	1.458(9)	1.453(3)	1.440(5)	1.446(5)
C9–C10	1.429(10), 1.445(8)	1.445(5)	1.437(4)	1.441(10)	1.446(3)	1.436(6)	1.442(6)

Table S5. Selected angles (in °) in reported crystal structures. Atoms are numbered according to Figure S3.

Angle	**1a**	**1b·CH$_3$CN**	**5a·CH$_3$OH**	**5a'·0.64CH$_3$OH**	**5b·CH$_3$CN**	**6a**	**6b·2CH$_3$CN**
O1–Mo1–O2	148.16(19), 150.46(19)	150.66(10)	151.28(8)	150.59(18)	151.56(7)	150.49(10)	151.29(10)
O1–Mo1–N1	80.75(19), 82.46(18)	82.55(11)	81.56(8)	82.11(18)	82.86(6)	82.27(10)	82.54(10)
O2–Mo1–O5	99.4(2), 94.4(2)	95.85(11)	95.05(9)	94.77(18)	95.11(7)	95.00(11)	95.81(10)
O4–Mo1–O5	105.8(3), 105.3(2)	105.53(12)	105.79(11)	106.1(2)	105.90(8)	105.85(14)	105.26(12)
O5–Mo1–N1	160.6(2), 160.1(2)	162.97(12)	159.35(10)	160.71(19)	161.43(7)	159.09(12)	161.24(11)
O1–Mo1–O4	99.1(2), 97.2(2)	96.10(11)	99.08(10)	97.73(18)	99.14(8)	99.22(12)	98.23(12)
O2–Mo1–N1	71.37(18), 71.82(18)	72.01(11)	72.49(7)	72.42(17)	72.02(6)	72.16(9)	72.47(9)
O4–Mo1–N1	92.5(2), 91.1(2)	88.23(12)	91.72(9)	90.07(19)	88.58(7)	92.20(12)	90.80(11)
O1–Mo1–O5	102.2(2), 106.1(2)	105.40(11)	105.78(9)	105.54(19)	105.65(7)	104.62(12)	104.19(11)
O2–Mo1–O4	97.2(2), 97.6(2)	97.44(11)	93.89(9)	96.78(19)	93.47(8)	96.28(11)	96.07(12)
O3–Mo2–O6	99.7(2), 100.4(2)	97.34(12)	100.55(10)	93.4(5), 103.2(3)	99.82(8)	100.54(12)	96.18(12)
O3–Mo2–N4	81.36(19), 81.84(19)	80.77(10)	82.42(8)	82.0(2)	81.35(6)	81.95(10)	82.50(10)
O6–Mo2–N2	98.5(2), 96.1(2)	97.06(13)	93.57(10)	91.7(3)	94.28(7)	93.91(12)	97.92(11)
O7–Mo2–N2	96.8(2), 94.8(2)	97.57(12)	93.69(9)	93.7(2), 99.9(4)	98.09(7)	96.56(12)	94.25(11)
N2–Mo2–N4	70.18(18), 70.66(18)	70.49(12)	70.97(8)	71.3(2)	70.66(6)	71.43(10)	71.18(10)
O3–Mo2–O7	105.1(2), 104.7(2)	105.44(11)	105.69(10)	105.6(4), 103.8(2)	104.45(7)	103.03(11)	106.66(11)

O6–Mo2–N4	93.8(2), 98.3(2)	91.62(12)	101.35(9)	89.5(5), 101.2(3)	90.65(7)	102.15(12)	92.81(10)
O7–Mo2–N4	159.5(2), 153.1(2)	159.80(13)	150.10(9)	169.7(4), 146.6(2)	160.65(7)	74.86(10)	158.30(11)
O3–Mo2–N2	147.1(2), 149.65(19)	148.08(12)	151.89(8)	151.6(2)	148.73(7)	151.87(10)	150.61(10)
O6–Mo2–O7	104.0(2), 105.9(2)	106.32(13)	105.19(10)	96.9(6), 109.2(3)	106.20(8)	104.15(13)	105.38(11)
Mo1–N1–C7	125.0(5), 124.9(4)	125.5(3)	126.82(18)	125.8(4)	126.37(14)	126.3(2)	124.8(2)
N2–N1–C7	119.5(6), 120.7(5)	120.1(3)	119.2(2)	120.0(5)	119.94(17)	120.3(3)	121.0(3)
Mo1–N1–N2	115.0(4), 114.1(3)	114.3(2)	113.61(15)	114.1(4)	113.67(12)	113.35(19)	113.83(17)
Mo2–N2–C8	119.2(4), 117.8(4)	117.0(2)	118.38(17)	117.3(4)	117.43(13)	118.1(2)	117.1(2)
N1–N2–C8	109.7(4), 110.4(4)	110.8(3)	111.4(2)	111.5(5)	111.25(16)	111.3(3)	111.5(3)
Mo2–N2–N1	130.9(4), 131.8(3)	131.6(3)	130.15(16)	130.2(4)	131.20(13)	130.5(2)	131.19(19)
N4–N3–C8	109.5(5), 109.9(4)	109.4(3)	110.99(19)	109.8(5)	110.34(16)	111.3(3)	110.4(3)
Mo2–N4–N3	119.5(4), 118.1(4)	119.0(2)	118.20(14)	118.5(4)	118.61(12)	117.5(2)	118.17(18)
Mo2–N4–C9	125.0(5), 126.4(4)	124.8(3)	126.31(17)	127.1(5)	125.69(14)	127.7(3)	125.6(2)
N3–N4–C9	115.3(6), 115.3(5)	115.9(3)	115.5(2)	114.3(5)	115.32(17)	114.6(3)	116.3(3)
Mo1–O1–C2	129.3(5), 130.3(4)	129.7(2)	135.45(18)	130.0(4)	135.81(14)	137.2(2)	132.2(2)
Mo1–O2–C8	123.4(4), 122.8(4)	123.2(2)	121.49(17)	121.5(4)	122.02(14)	122.5(2)	122.81(18)
Mo2–O3–C11	134.8(4), 136.8(4)	128.4(2)	136.38(19)	134.7(4)	131.63(14)	139.0(2)	129.8(2)
O1–C2–C1	120.8(7), 121.1(6)	121.1(3)	122.9(3)	122.4(5)	123.12(19)	122.2(3)	122.3(3)
N1–C7–C1	122.6(6), 122.8(6)	123.2(3)	123.8(2)	123.9(6)	124.05(18)	124.7(3)	124.2(3)

O2–C8–N2	119.7(5), 120.1(5)	119.7(3)	120.4(2)	119.9(6)	71.58(10)	71.58(10)	119.4(3)
O2–C8–N3	118.7(5), 117.3(5)	117.3(3)	118.7(2)	117.2(6)	116.21(18)	118.3(3)	118.1(3)
N2–C8–N3	121.6(5), 122.6(5)	123.0(3)	120.9(2)	122.9(6)	122.89(19)	121.7(3)	122.5(3)
N4–C9–C10	125.3(6), 125.3(6)	123.4(3)	125.8(2)	124.4(6)	124.9(2)	125.7(4)	124.7(3)
O3–C11–C10	122.4(7), 122.6(5)	121.6(3)	122.2(2)	122.4(6)	122.83(19)	121.1(3)	122.0(3)

Table S6. Selected geometric parameters of planes generated in reported crystal structures. Atoms are numbered according to Figure S3. Planes are defined in following manner:

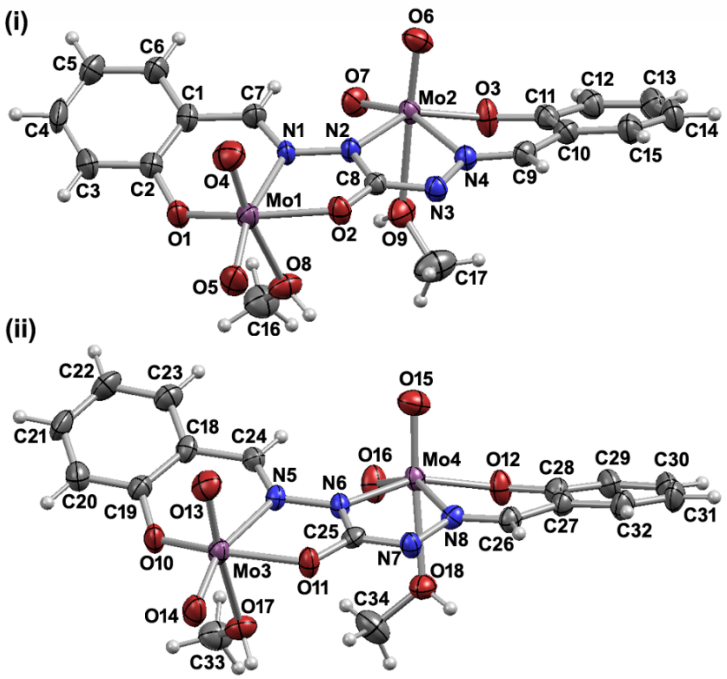
R1 – L.S. plane defined by the atoms C1 C2 C3 C4 C5 C6

R2 – L.S. plane defined by the atoms C10 C11 C12 C13 C14 C15

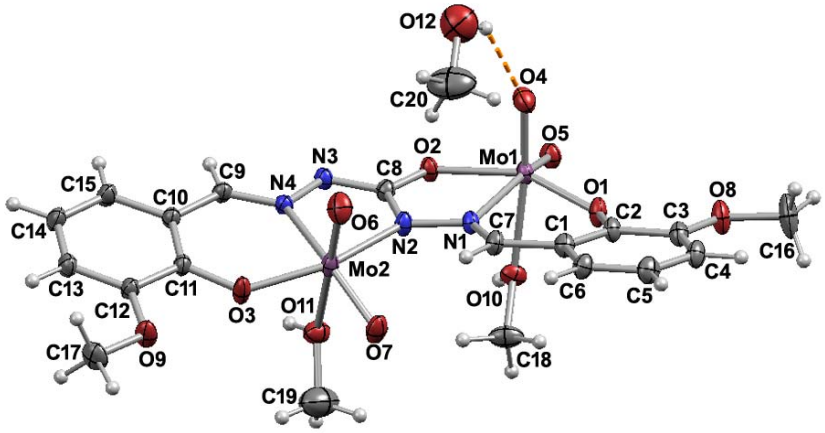
L1 – exact plane defined by the atoms O1 N1 O2

L2 – exact plane defined by the atoms N2 N4 O3

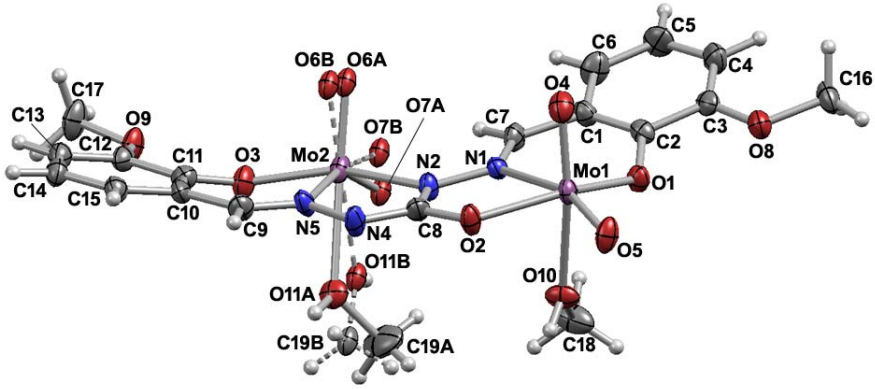
Geometric parameter	**1a**	**1b·CH$_3$CN**	**5a·CH$_3$OH**	**5a'·0.64CH$_3$OH**	**5b·CH$_3$CN**	**6a**	**6b·2CH$_3$CN**
d(Mo1–L1) / Å	0.320(4) 0.297(4)	0.299(3)	0.2551(18)	0.303(4)	0.2735(16)	0.301(2)	0.290(2)
d(Mo2–L2) / Å	0.361(5) 0.280(5)	0.309(3)	0.196(2)	0.212(4)	0.3082(16)	0.196(3)	0.285(2)
∡(R1–L1) / °	20.6(3) 19.1(3)	19.87(14)	8.54(9)	18.2(2)	4.04(10)	2.93(14)	13.36(15)
∡(R2–L2) / °	8.6(2) 6.1(3)	21.8(2)	7.90(12)	12.7(3)	14.35(14)	3.03(16)	17.30(15)
∡(L1–L2) / °	29.77(18) 26.7(2)	15.4(2)	17.41(10)	13.2(2)	9.40(11)	11.18(14)	23.64(10)


(i)
O6
C6
C5
O7
Mo2
O3
C12
C13
C1
C7
C11
C14
C4
N1
N2
C10
C15
O4
C8
N4
C9
C3
C2
Mo1
N3
O1
O2
O9
O8
C17
O5
C16
(ii)
C22
C23
O15
C21
C18
C24
O16
Mo4
O12
C28
C29
C30
N5
N6
C20
C19
O13
C25
N8
C26
C27
C32
C31
O10
N7
Mo3
O11
O18
O14
O17
C34
C33

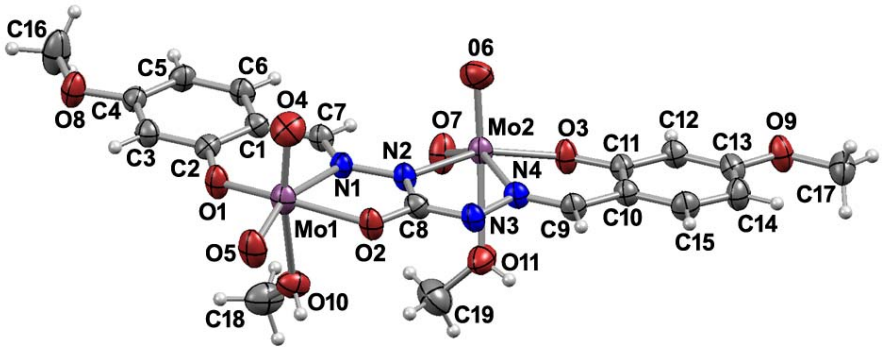
(a)


O12
O4
C20
O2
Mo1
O5
N3
C8
C9
N4
C15
C10
O1
C2
C3
O8
C14
O6
C7
C1
N2
N1
C16
Mo2
C4
C13
C11
C6
C5
O3
O11
O10
C12
O7
C17
O9
C18
C19

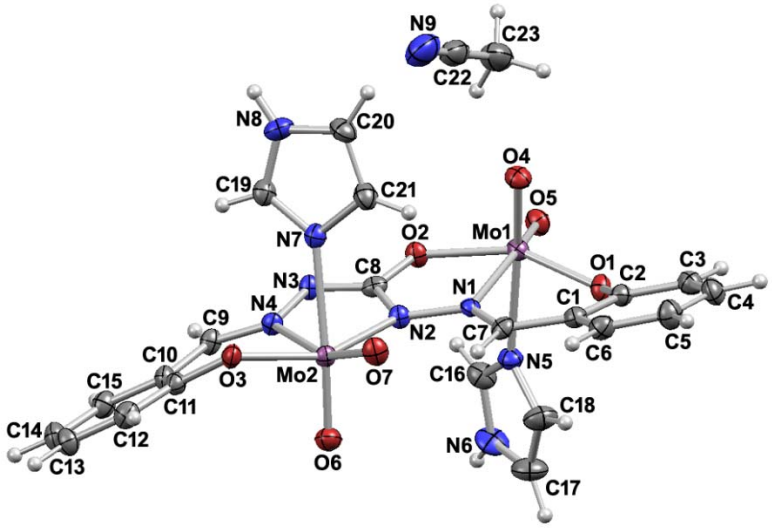
(b)


O6B
O6A
C5
C6
C17
O4
C4
C16
C13
O9
O7A
C7
O7B
C1
C2
C3
C12
C11
O3
Mo2
N2
N1
O8
C14
C15
Mo1
O1
C10
C9
N5
N4
C8
O2
O5
O11B
O10
O11A
C19B
C19A
C18

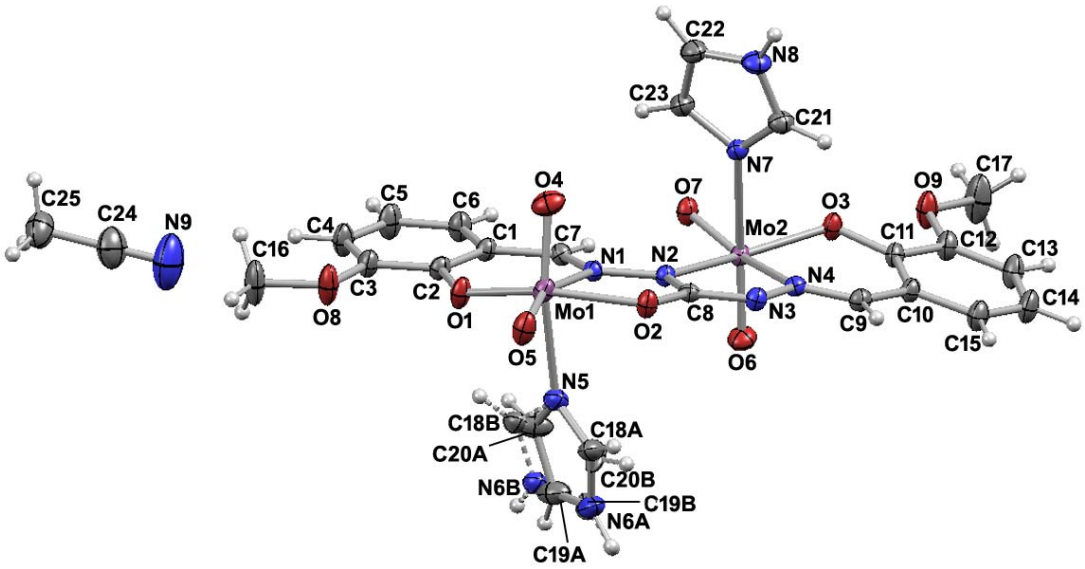
(c)


C16
C5
C6
O6
O8
C4
O4
C7
O7
Mo2
O3
C11
C12
C13
O9
C3
C2
C1
N2
N4
C17
O1
N1
C10
Mo1
C8
N3
C9
C15
C14
O5
O2
O11
O10
C18
C19

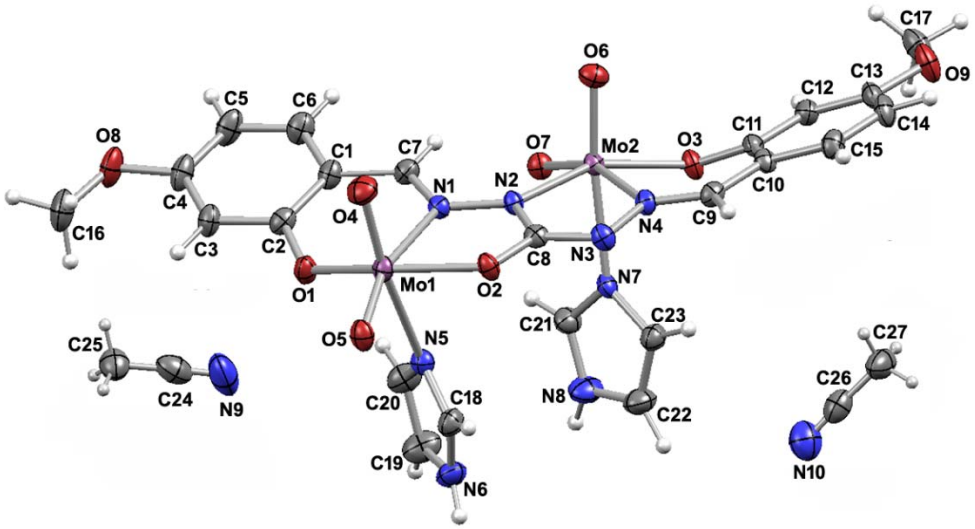
(d)


N9
C23
C22
N8
C20
O4
C19
C21
O5
N7
O2
Mo1
C8
O1
C2
C3
N3
N1
C4
N4
C1
C9
N2
C7
C5
C10
O3
Mo2
O7
N5
C6
C16
C15
C11
C18
C14
C12
N6
C13
O6
C17

(e)


C22
N8
C23
C21
N7
C25
C24
N9
O4
O7
O9
C17
C5
C6
O3
C4
C1
C7
Mo2
C11
C12
C13
C16
N1
N2
N4
C3
C2
O8
O1
Mo1
O2
C8
N3
C9
C10
C14
C15
O5
O6
N5
C18B
C18A
C20A
C20B
N6B
C19B
N6A
C19A

(f)



(g)

Figure S4. Mercury-ORTEP view of molecular structures of: (**a**) **1a**, showing both molecules ((i) and (ii)) of the asymmetric unit (for clarity, molecules are not shown in their true position within the asymmetric unit); (**b**) **5a·CH$_3$OH**; **(c) 5a'·0.64CH$_3$OH**; **(d) 6a; (e) 1b·CH$_3$CN**; **(f) 5b·CH$_3$CN, and (g) 6b·2CH$_3$CN.** For clarity, in (a) and (g) molecules constituting the asymmetric unit are not shown in their true position. The displacement ellipsoids are drawn at 50% probability level. Hydrogen atoms are presented as spheres of arbitrary small radii.

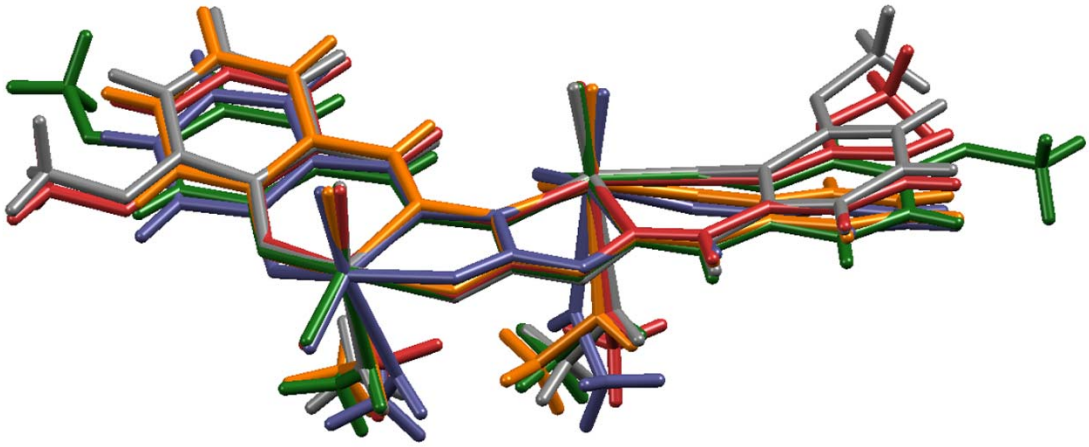


Figure S5. Overlapping diagram for methanol-based complexes described in this work, **1a** (molecule (i**)** - blue, molecule **(**ii)-orange**), 5a·CH$_3$OH** (red), **5a'·0.64CH$_3$OH** (gray) and **6a** (green).

Table S7. Geometry of hydrogen bonds and C–H···O interactions (Å, º) for **1a**, **5a·CH₃OH, 5a'·0.64CH₃OH, 6a, 1b·CH₃CN, 5b·CH₃CN** and **6b·2CH₃CN**

D–H···A	D–H	H···A	D···A	∠D–H···A	Symmetry code
1a					
O8–H8O···N3	0.84(4)	2.00(4)	2.801(7)	160(5)	2−*x*, −*y*, −*z*
O9–H9O···O7	0.83(3)	2.18(6)	2.929(7)	149(5)	2−*x*, 1−*y*, −*z*
O17–H17O···N7	0.84(3)	1.84(2)	2.665(7)	166(4)	−*x*, 1−*y*, 1−*z*
O18–H18O···O14	0.84(5)	2.01(5)	2.795(6)	155(4)	−*x*, 1−*y*, 1−*z*
C4–H4···O14	0.9300	2.5500	3.360(9)	146.00	1−*x*, 1−*y*, −*z*
C21–H2···O5(*parst*)	0.9300	2.690	3.5608(1)	156.30(1)	−*x*+1, −*y*, −*z*
C17–H17A···O2	0.9600	2.5100	3.284(9)	138.00	2−*x*, −*y*, −*z*
C17–H17C···O6	0.9600	2.3200	3.144(10)	144.00	1+*x*, *y*, *z*
C26–H26···O13	0.9300	2.4500	3.305(8)	152.00	1−*x*, 1−*y*, 1−*z*
C34–H34A···O11	0.9600	2.5900	3.340(9)	135.00	−*x*, 1−*y*, 1−*z*
5a·CH₃OH					
O10–H10O···N3	0.81(3)	1.82(3)	2.611(3)	166(3)	1−*x*, −*y*, −*z*
O11–H11O···O5	0.81(3)	2.09(3)	2.876(3)	163(3)	1−*x*, −*y*, −*z*
O12–H12O···O4	0.88(3)	2.25(5)	3.004(4)	144(5)	
C6–H6···O6	0.9500	2.4200	3.195(3)	138.00	1−*x*, 1−*y*, 1−*z*
C14–H14···O7	0.9500	2.4400	3.128(4)	129.00	1+*x*, *y*, *z*
C16–H16C···O4	0.9800	2.5600	3.028(5)	109.00	−*x*, 1−*y*, −*z*
C17–H17B···O8	0.9800	2.4000	3.147(3)	132.00	1+*x*, *y*, 1+*z*
5a'·0.64CH₃OH					
O10–H10 ···N3	0.84(3)	1.80(4)	2.627(7)	167(7)	1−*x*, 1−*y*, 2−*z*
O11A–H11A···O5	0.84(2)	2.12(3)	2.940(8)	164(12)	1−*x*, 1−*y*, 2−*z*
C9–H9···O4	0.9500	2.5800	3.343(8)	138.00	2−*x*, 1−*y*, 2−*z*

C15−H15···O4	0.9500	2.4900	3.310(9)	145.00	2−*x*, 1−*y*, 2−*z*
C17−H17B···O8	0.9800	2.5200	3.245(9)	130.00	1+*x*, 1+*y*, *z*
C18−H18B···O6A	0.9800	2.5700	3.315(11)	132.00	−1+*x*, *y*, *z*
C18−H18B···O6B	0.9800	2.4800	3.301(18)	142.00	−1+*x*, *y*, *z*
6a					
O10−H10O···N3	0.79(3)	1.87(3)	2.653(4)	172(3)	2−*x*, 1−*y*, 1−*z*
O11−H11O···O5	0.79(3)	2.36(4)	3.060(4)	148(3)	2−*x*, 1−*y*, 1−*z*
C3−H3···O5	0.9300	2.5400	3.444(5)	166.00	2−*x*, −*y*, 1−*z*
C12−H12···O7	0.9300	2.5800	3.487(5)	165.00	1−*x*, 1−*y*, −*z*
C15−H15···O4	0.930	3.4027(1)	2.6005(1)	144.75	−*x*+1, −*y*+1, −*z*+1
1b·CH$_3$CN					
N6−H6N···O4	0.87(3)	1.95(3)	2.782(4)	159(4)	−1+*x*, *y*, *z*
N8−H8N···N3	0.87(4)	2.09(4)	2.945(5)	168(4)	2−*x*, 1−*y*, 2−*z*
C13−H13···O4	0.9500	2.5700	3.507(5)	168.00	3/2−*x*, −1/2+*y*, 3/2−*z*
C15−H15···O2	0.9500	2.5000	3.434(5)	167.00	1−*x*, 1−*y*, 2−*z*
C23−H23B···O1	0.9800	2.5400	3.267(6)	131.00	1/2+*x*, 3/2−*y*, 1/2+*z*
5b·CH$_3$CN					
N8−H8N···N3	0.89(3)	1.97(3)	2.841(3)	169(3)	−*x*, 2−*y*, 1−*z*
N6A−H6NA···O4	0.88(8)	2.002(2)	2.807(10)	151.45(50)	1+*x*, *y*, *z*
N6B−H6NB···O3	0.88(2)	2.685(2)	3.287(20)	127(1)	−*x*+1, −*y*+1, −*z*+1
C15−H15···O2	0.9500	2.5200	3.471(3)	174.00	1−*x*, 2−*y*, 1−*z*
C17−H17A···O5	0.9800	2.5800	3.358(4)	137.00	*x*, *y*, −1+*z*
C17−H17B···O8	0.9800	2.4100	3.315(4)	153.00	*x*, *y*, −1+*z*
6b·2CH$_3$CN					
N6−H6N···N3	0.84(4)	2.09(4)	2.867(5)	154(4)	2−*x*, 1−*y*, −*z*

N8−H8N···O6	0.91(4)	2.00(4)	2.824(5)	149(5)	1+*x, y, z*
C6−H6···O7	0.9500	2.5300	3.122(6)	121.00	1−*x,* 1−*y,* 1−*z*
C17−H17C···O4	0.9800	2.4100	3.344(6)	159.00	*x,* 1+*y, z*
C19−H19···O6	0.9500	2.6000	3.276(6)	129.00	1+*x, y, z*
C22−H22···O5	0.9500	2.4500	3.193(5)	135.00	2−*x,* 1−*y,* −*z*
C25−H25A···O6	0.9800	2.5400	3.351(7)	140.00	–
C27−H27B···O5	0.9800	2.5900	3.446(7)	147.00	1−*x,* −*y,* 1−*z*

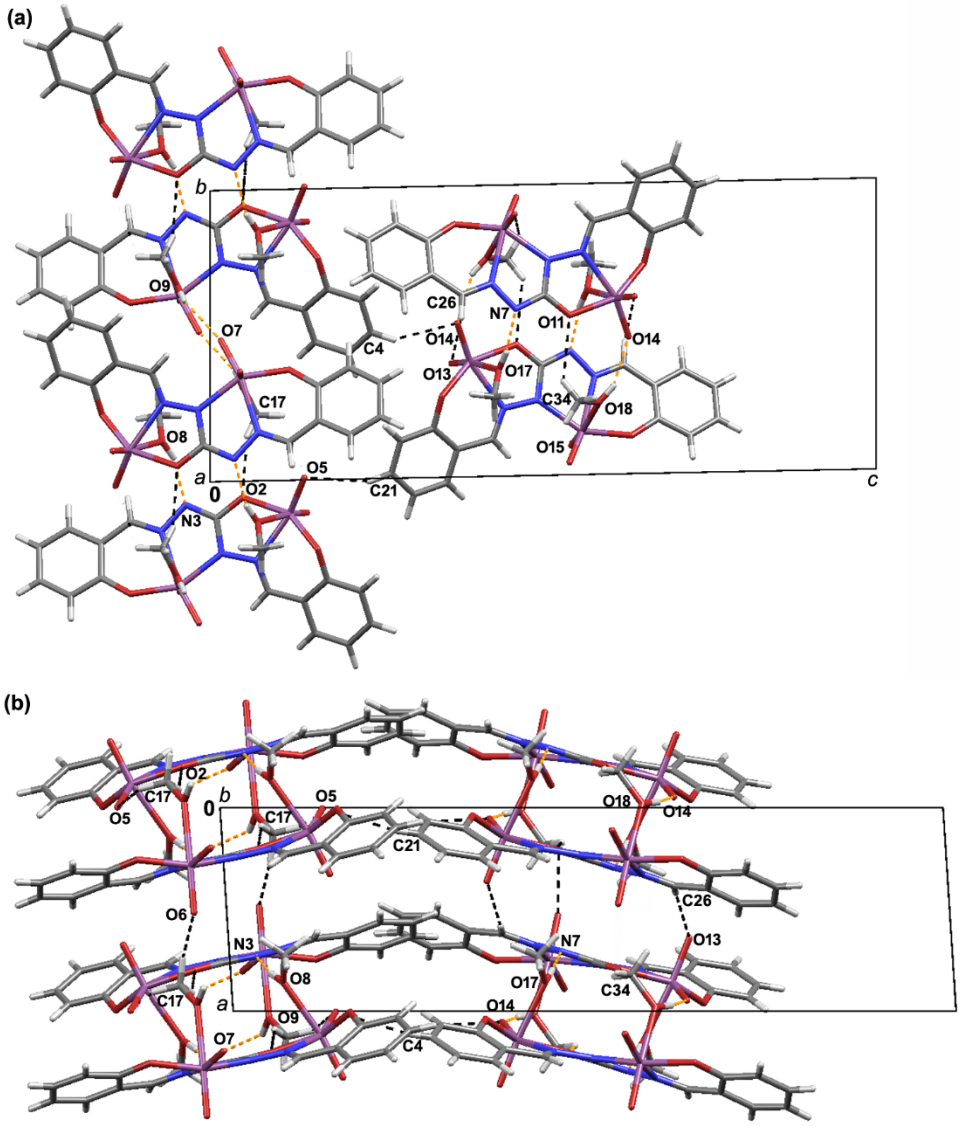


Figure S6. Crystal packing in **1a** shown down the: (a) *a*-axis; and (b) *b*-axis. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, while C–H···O interactions are highlighted as black dashed lines. Supramolecular chains form through O8–H8···N3 ($R_2^2(12)$ motif) and O9–H9···O7 ($R_2^2(8)$ motif) hydrogen bonds, whereas the dimers rely on O17–H17O···N7 ($R_2^2(12)$ motif) and O18–H18O···O14 ($R_2^2(14)$ motif) hydrogen bonds.[1]

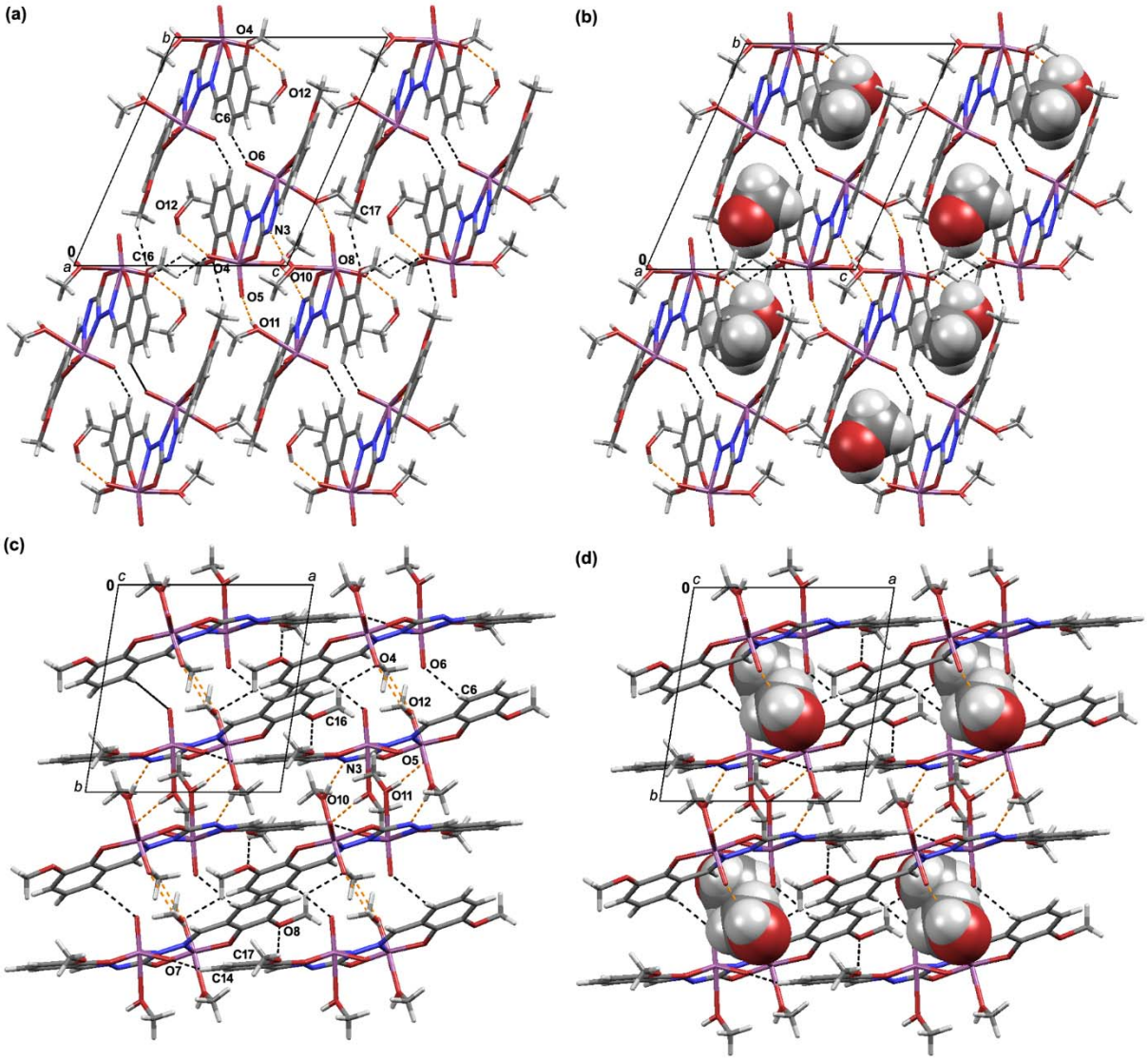


Figure S7. Crystal packing in **5a·CH₃OH** shown down the: (a) and (b) *b*-axis; and (c) and (d) *c*-axis. Crystal solvent (methanol) molecules are depicted in a spacefill style. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, whereas C–H···O interactions are highlighted as black dashed lines. Supramolecular dimers form through O10–H10O···N3 ($R_2^2(12)$ motif) and O11–H11O···O5 ($R_2^2(14)$ motif) hydrogen bonds.[1]

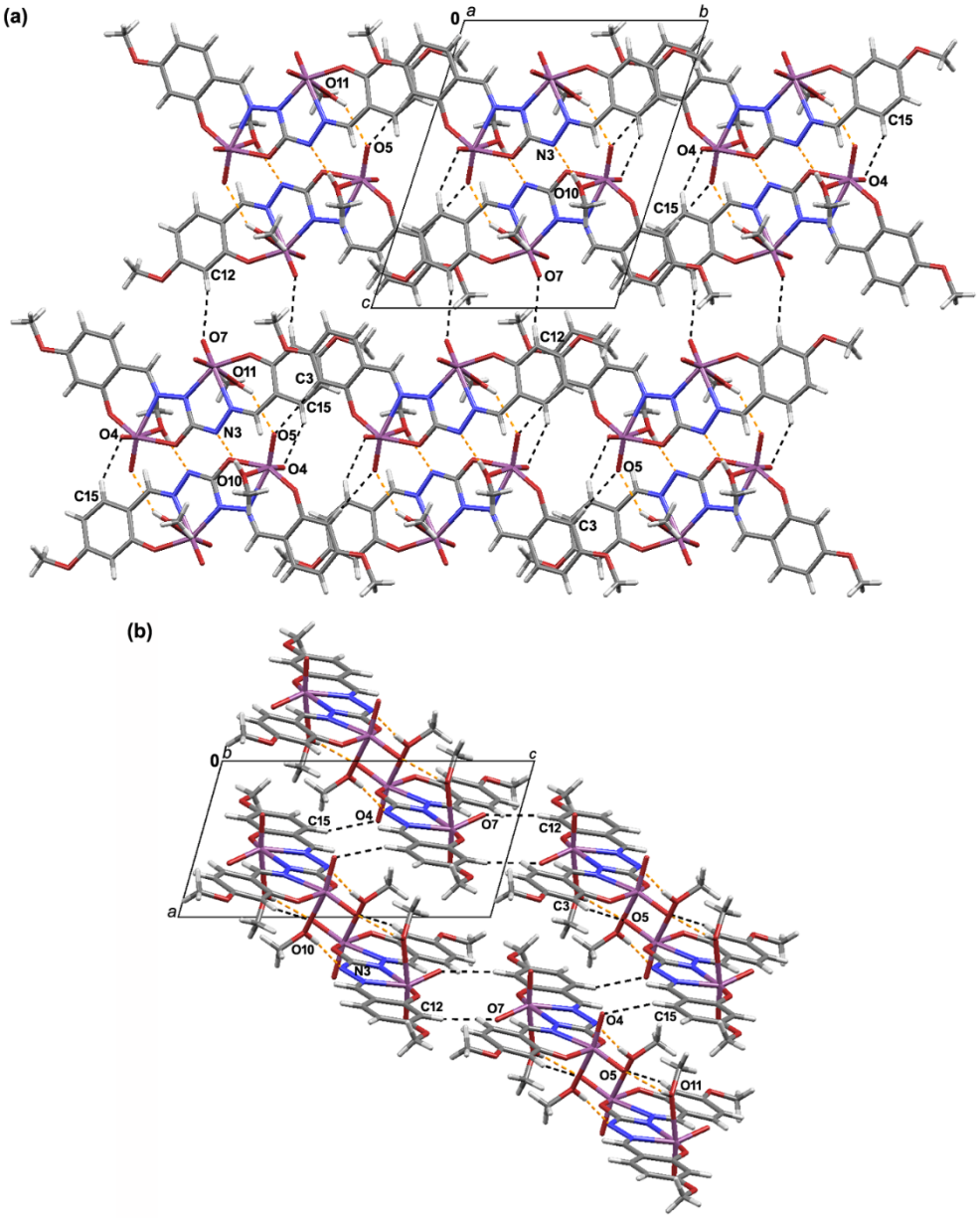


Figure S8. Crystal packing in **6a** shown down the: (a) *a*-axis; and (b) *b*-axis. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, while C–H···O interactions are highlighted as black dashed lines. Supramolecular dimers form through O10–H10O···N3 ($R_2^2(12)$ motif) and O11–H11O···O5 ($R_2^2(14)$ motif) hydrogen bonds.[1]

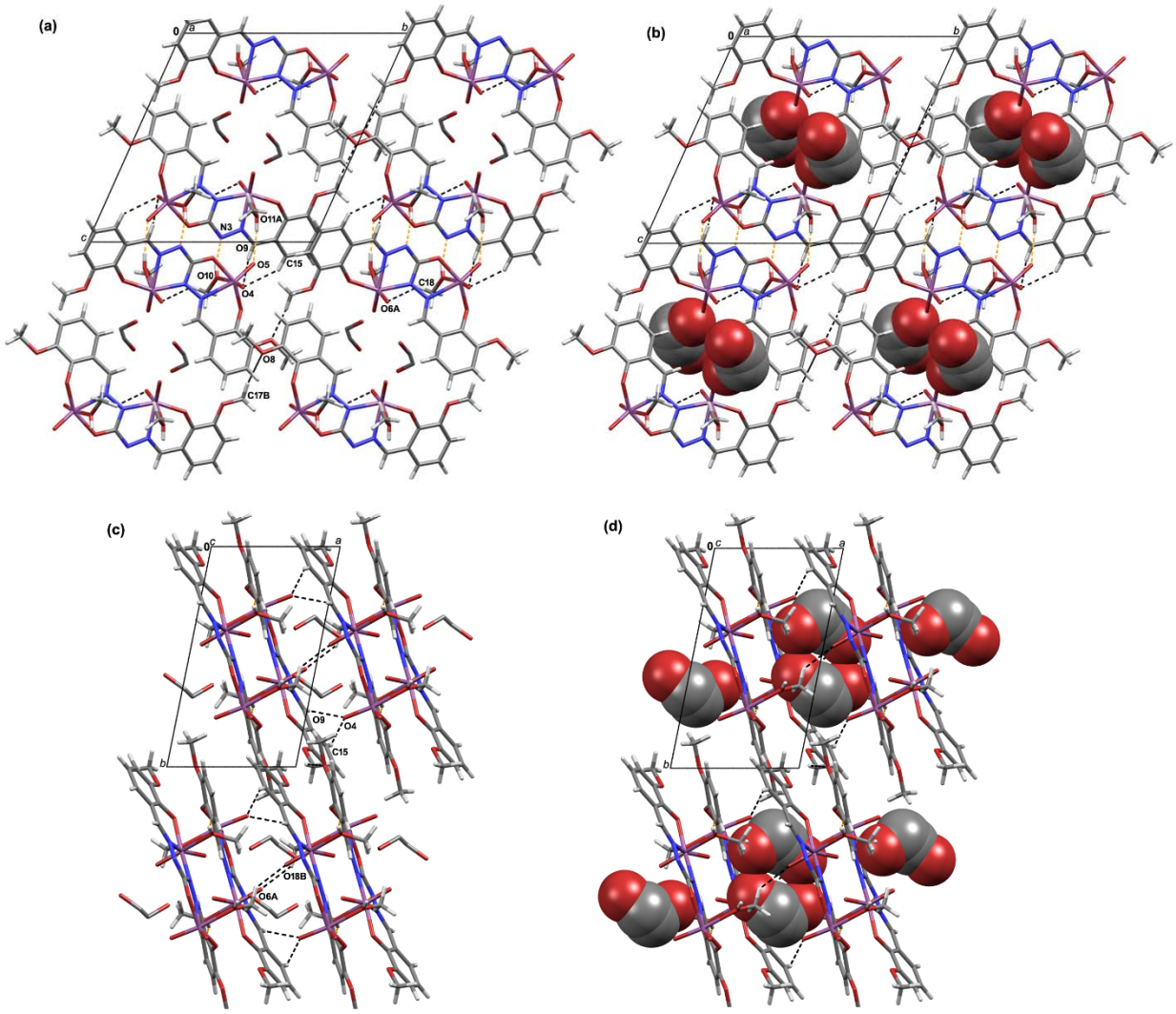


Figure S9. Crystal packing in **5a'·0.64CH$_3$OH** shown down the: (a) and (b) *b*-axis; and (c) and (d) *c*-axis. Disordered solvent (methanol) molecules (in both positions A and B) are depicted in a spacefill style. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, whereas C–H···O interactions are highlighted as black dashed lines. Supramolecular dimers form *via* O10–H10O···N3 ($R_2^2(12)$ motif) and O11A–H11A···O5 ($R_2^2(14)$ motif) hydrogen bonds.[1]

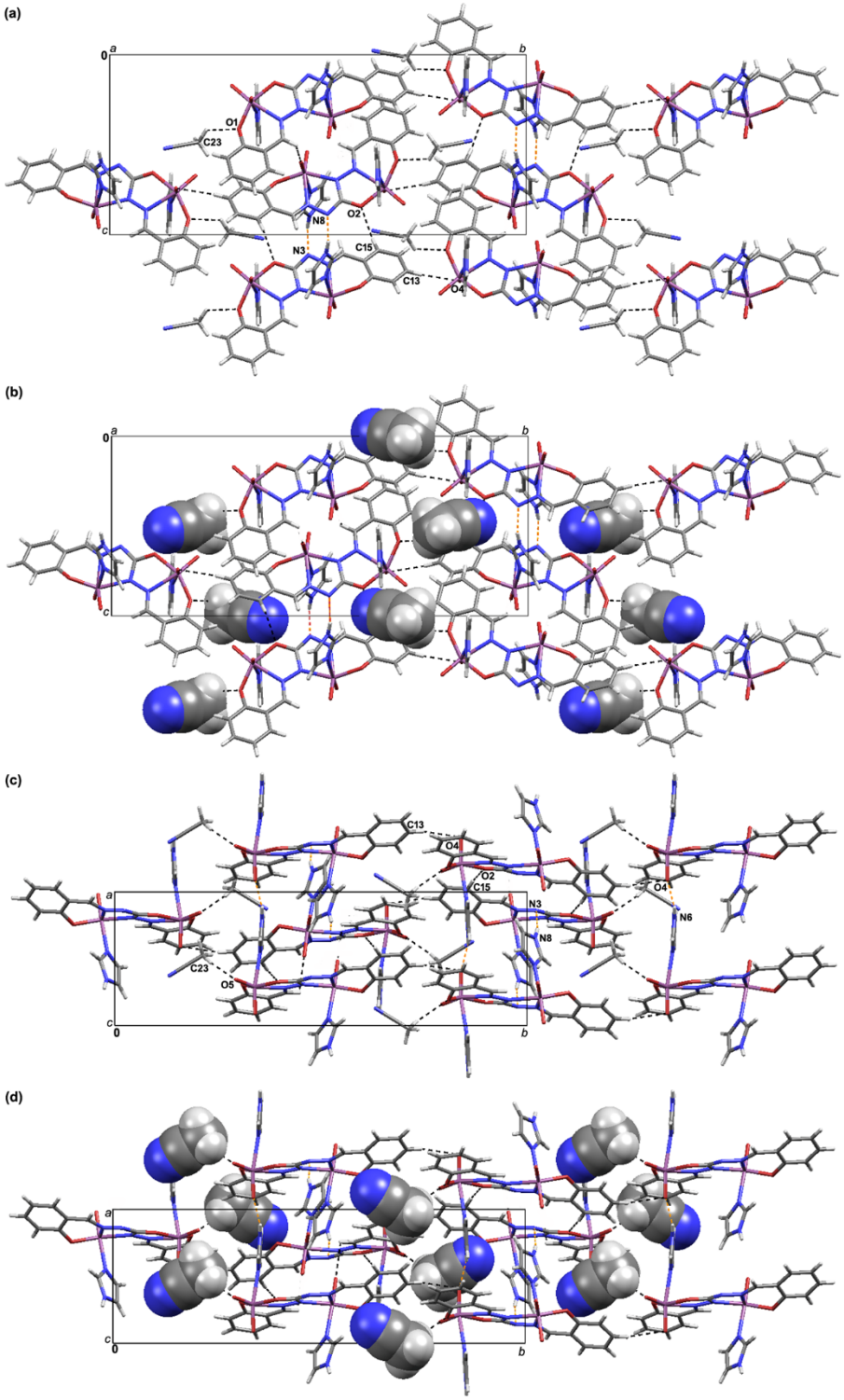


Figure S10. Crystal packing in **1b·CH₃CN** shown down the: (a) and (b) *a*-axis; and (c) and (d) *c*-axis. Crystal solvent (acetonitrile) molecules are depicted in a spacefill style. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, whereas C–H···O interactions are highlighted as black dashed lines. Supramolecular chains form through N8–H8N···N3 ($R_2^2(14)$ motif) and N6–H6N···O4 ($C_1^1(6)$ motif) hydrogen bonds.[1]

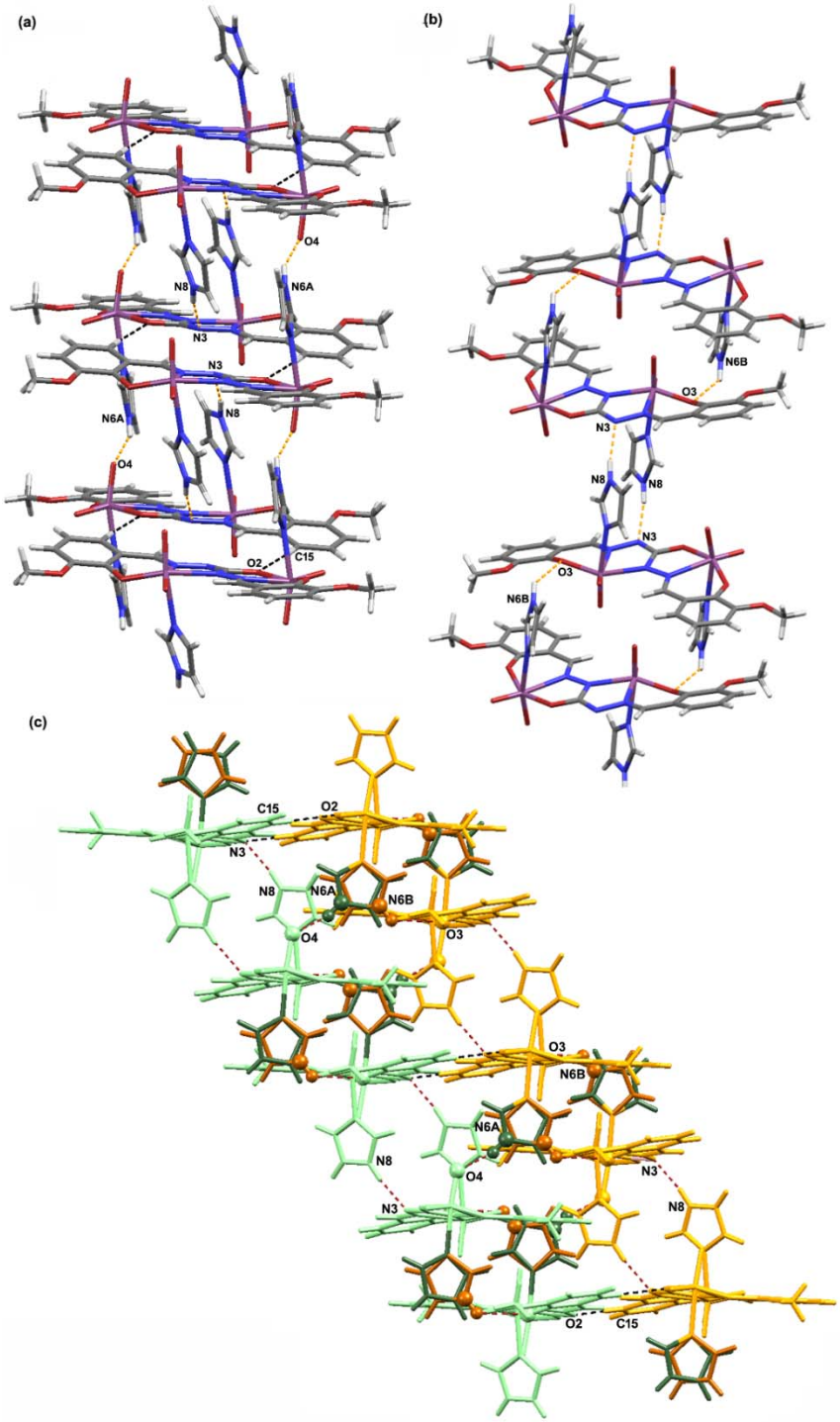


Figure S11. Chains found in **5b·CH$_3$CN** when considering: (a) only major component A; (b) only minor component B; (c) both components, with chains in (a) depicted in green, and chains in (b) in orange color. In (a) and (b) hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, while C–H···O interactions are highlighted as black dashed lines. In (c) hydrogen bonds of the N–H···N and O–H···N type are presented as red dashed lines C–H···O interactions as black dashed lines. Supramolecular chains form through N8–H8N···N3 ($R_2^2(14)$ motif) and N6–H6N···O4 ($C_1^1(6)$ motif) hydrogen bonds.[1]

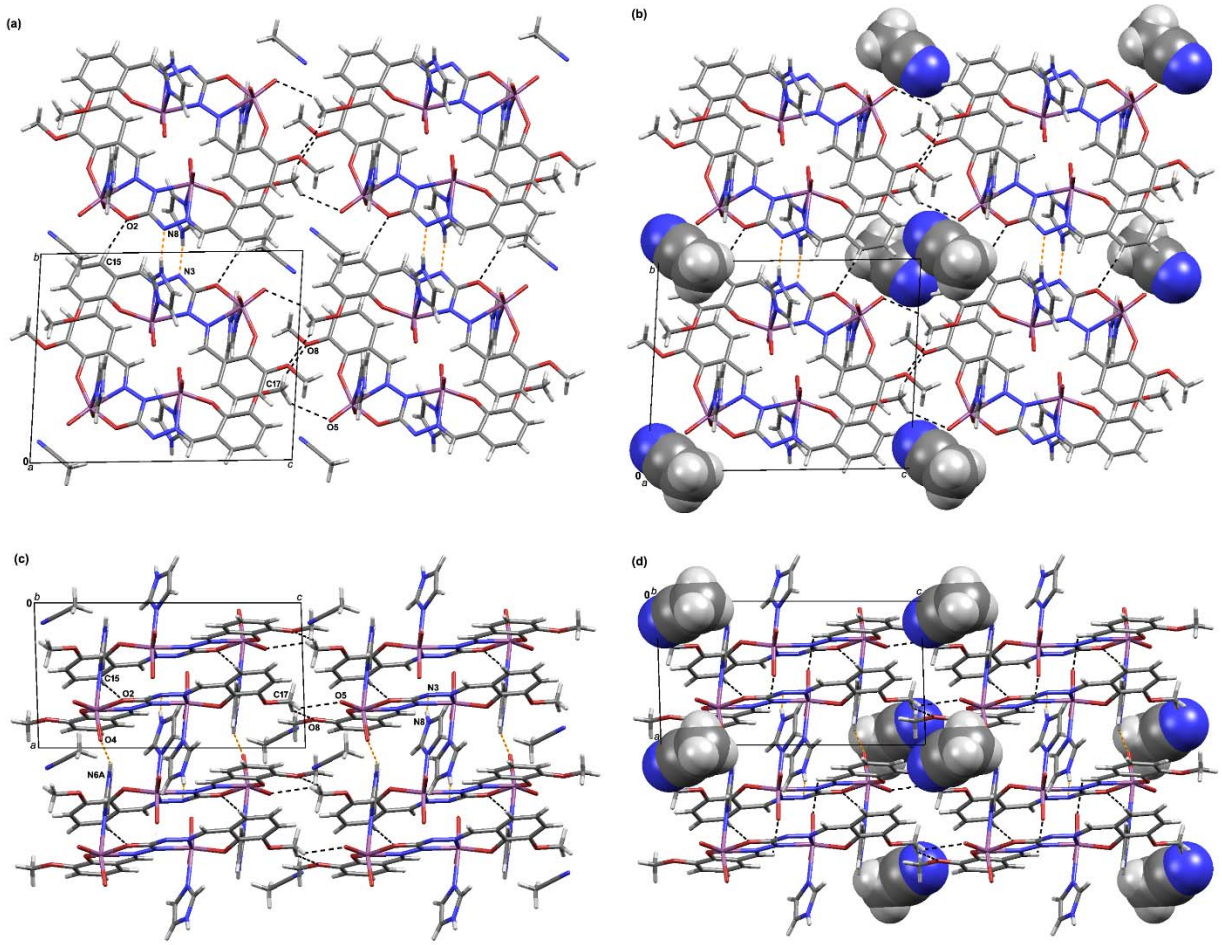


Figure S12. Crystal packing in **5b·CH$_3$CN** shown down the: (a) and (b) *a*-axis; and (c) and (d) *b*-axis. Crystal solvent (acetonitrile) molecules are depicted in a spacefill style. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, whereas C–H···O interactions are highlighted as black dashed lines.

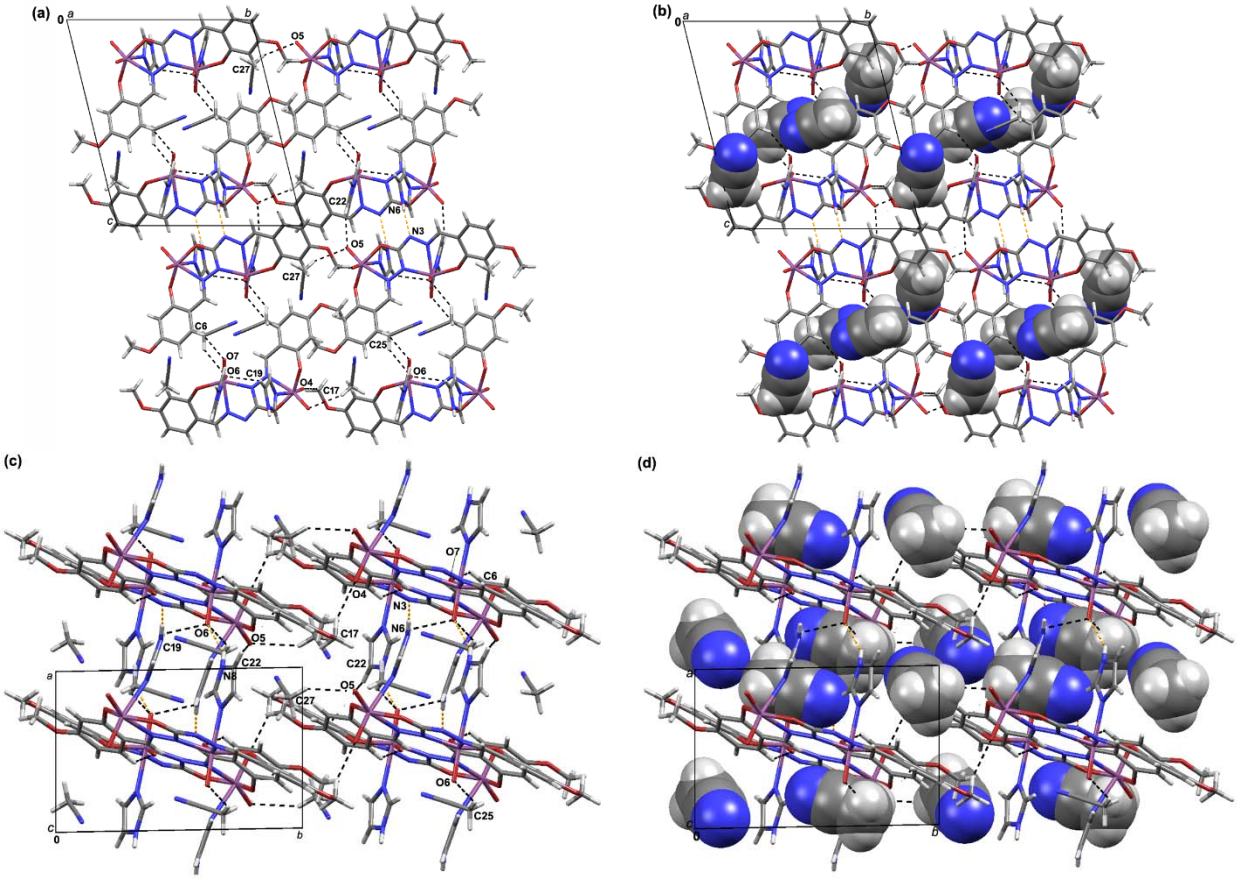


Figure S13. Crystal packing in **6b·2CH$_3$CN** shown down the: (a) and (b) *a*-axis; and (c) and (d) *c*-axis. Crystal solvent (acetonitrile) molecules are depicted in a spacefill style. Hydrogen bonds of the N–H···N and O–H···N type are presented by orange dashed lines, whereas C–H···O interactions are highlighted as black dashed lines.

Spectroscopic characterization

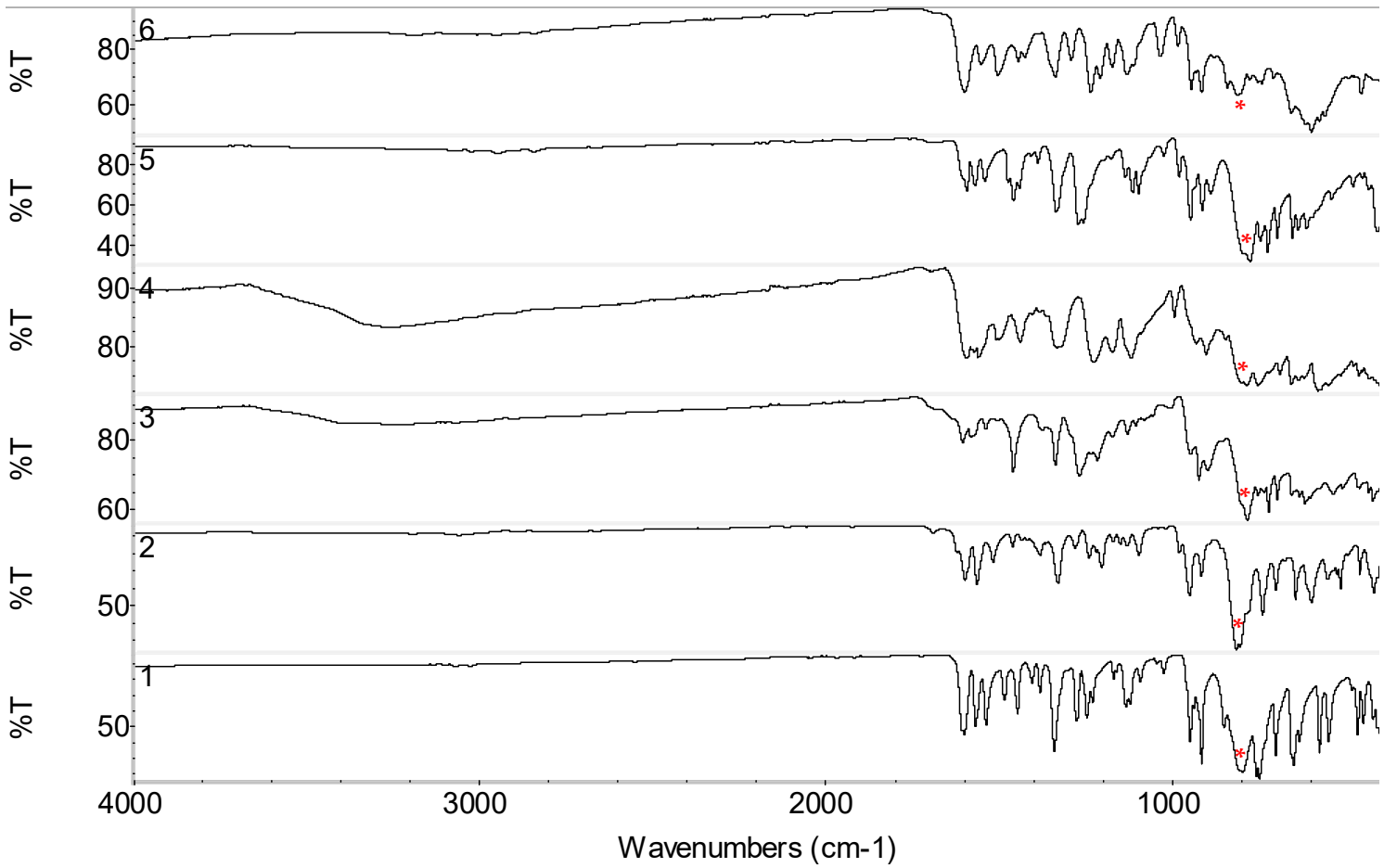


Figure S14. ATR-FTIR spectra of **1**, **2**, **3**, **4**, **5** and **6.** All polynuclear complexes show characteristic Mo=O···Mo bands at ~800 cm^{-1}, marked by asterisk (*).

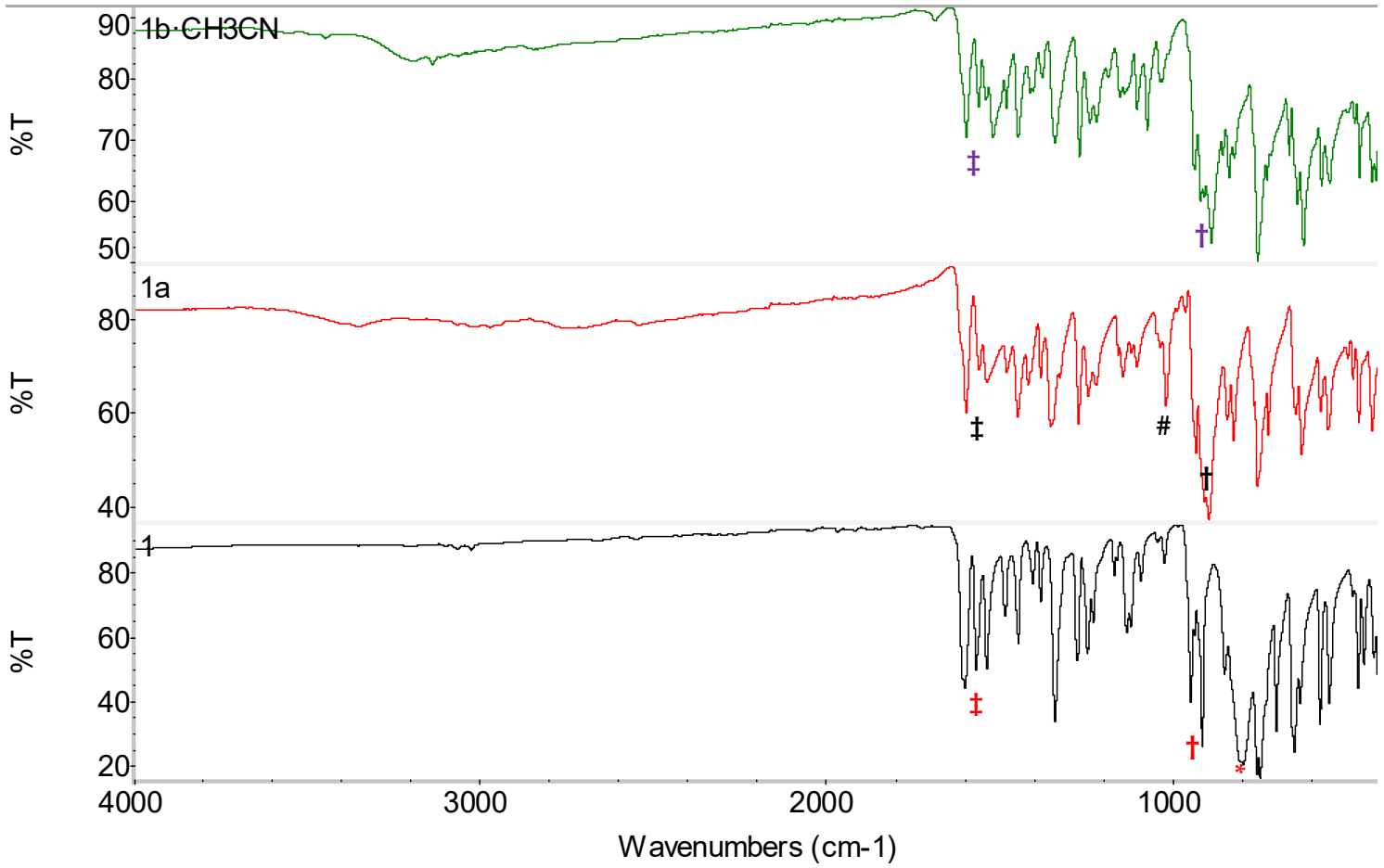


Figure S15. ATR-FTIR spectra of **1**, **1a** and **1b·CH$_3$CN**. Mo=O···Mo bands are represented by asterisk (*), $\{MoO_2\}^{2+}$ asymmetric stretching band by dagger (†), methanolic C–O stretching band by hash (#) and C=C, C=N stretching bands by double dagger (‡). Spectra of **1a** and **1b·CH$_3$CN** show no characteristic Mo=O···Mo bands.

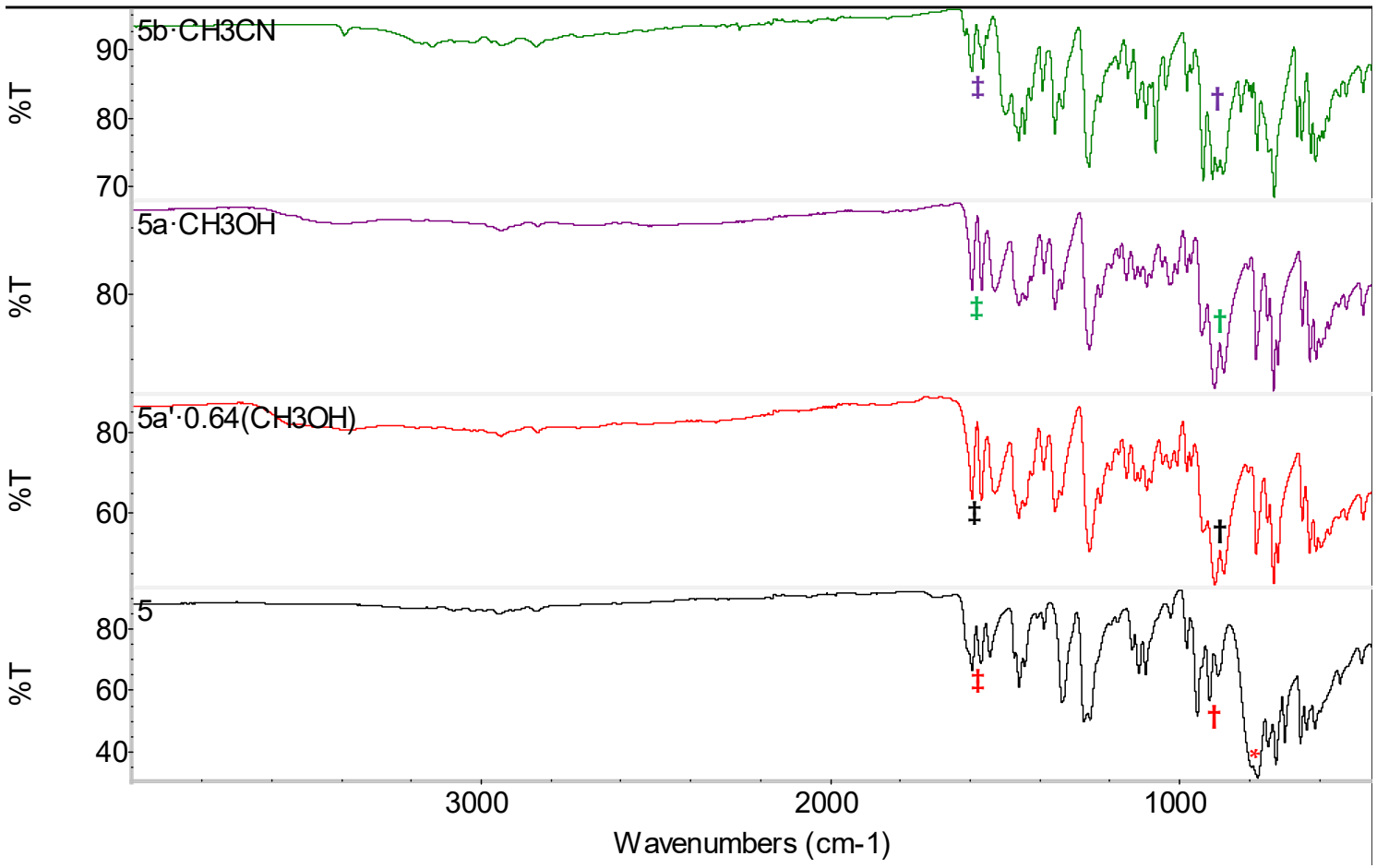


Figure S16. ATR-FTIR spectra of **5**, **5a·CH_3OH, 5a'·0.64CH_3OH** and **5b·CH_3CN**. Mo=O···Mo bands are represented by asterisk (*), $\{MoO_2\}^{2+}$ asymmetric stretching band by dagger (†) and C=C, C=N stretching bands by double dagger (‡). Spectra of **5a·CH_3OH, 5a'·0.64CH_3OH** and **5b·CH_3CN** show no characteristic Mo=O···Mo bands.

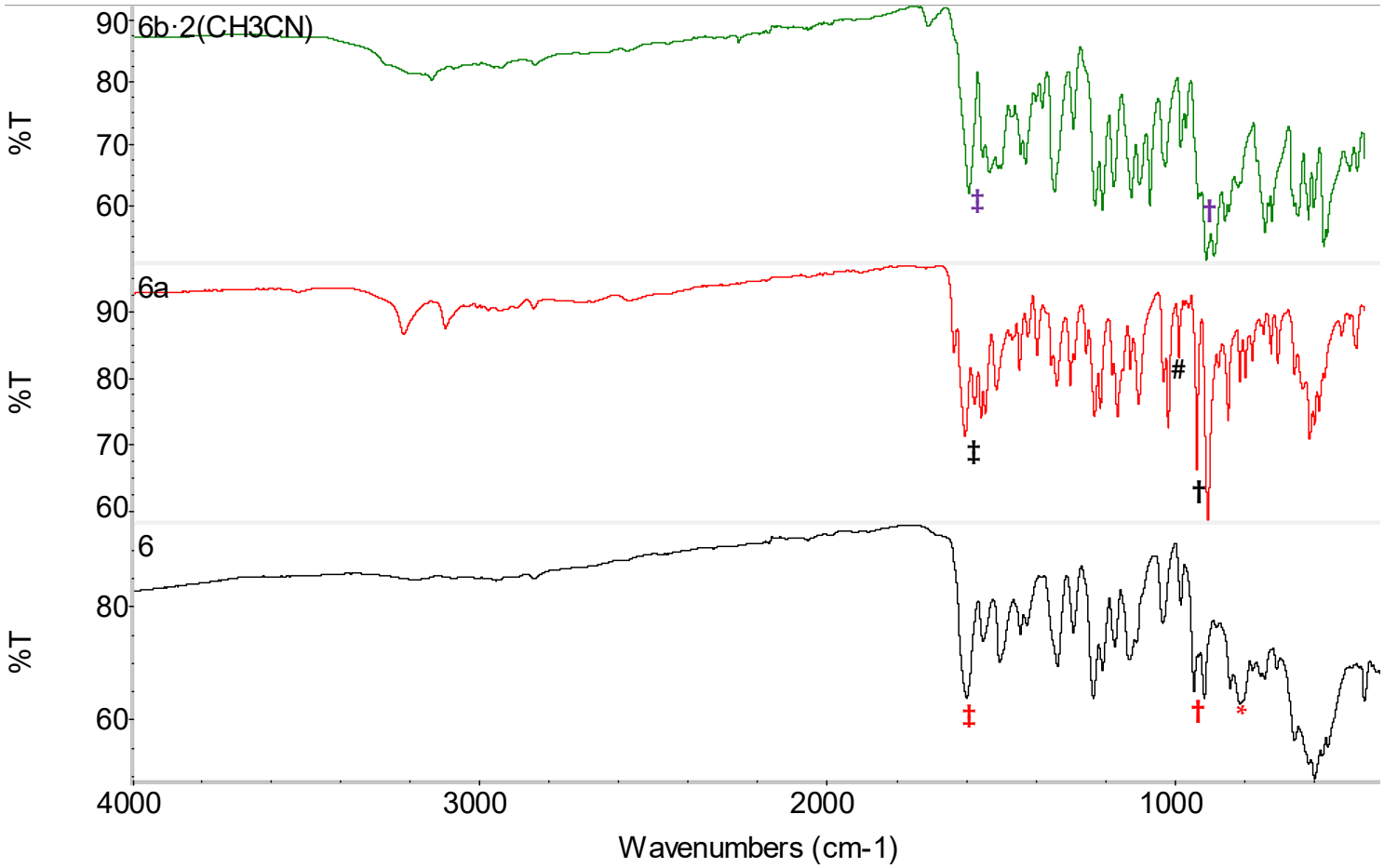


Figure S17. ATR-FTIR spectra of **6**, **6a** and **6b·2CH$_3$CN**. Mo=O···Mo bands are represented by asterisk (*), $\{MoO_2\}^{2+}$ asymmetric stretching band by dagger (†), methanolic C–O stretching band by hash (#) and C=C, C=N stretching bands by double dagger (‡). Spectra of **6a** and **6b·2CH$_3$CN** show no characteristic Mo=O···Mo bands, but significant differences arise in their spectra, which is an indication that two do have different structures.

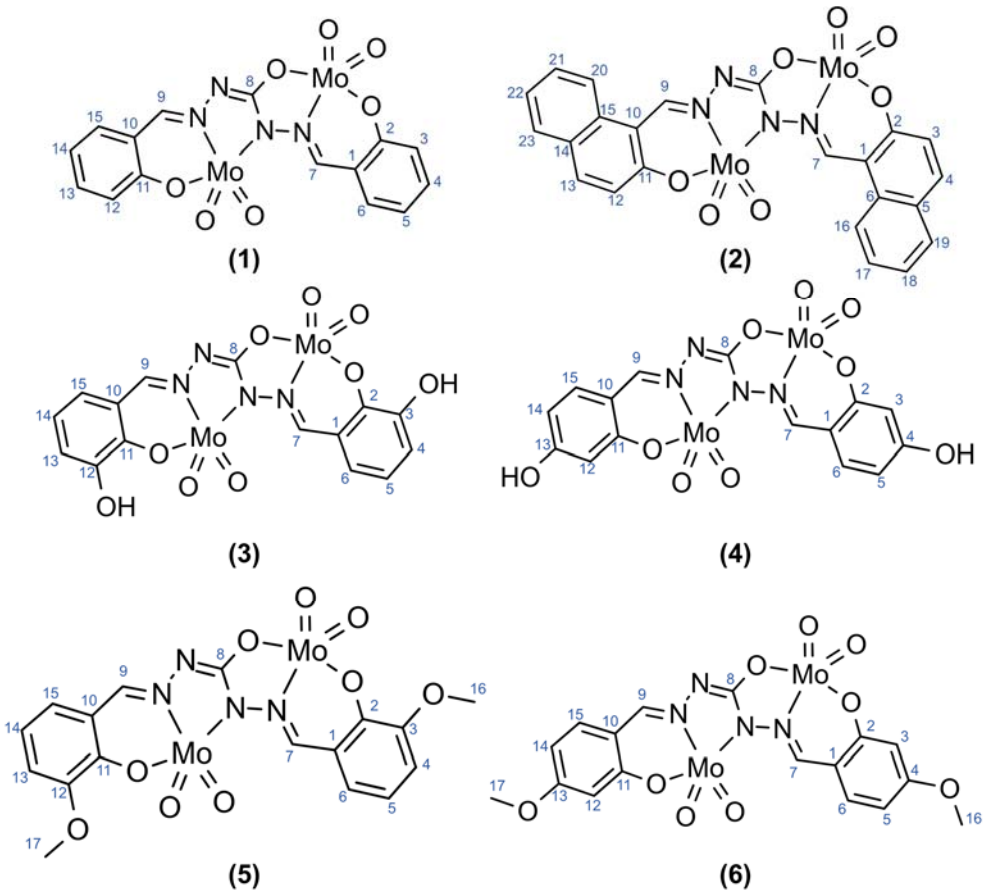


Figure S18. The NMR numbering scheme.

Table S8. ^{1}H and ^{13}C chemical shifts for $H_4L^{1–6}$ and **1**–**6** in DMSO–d_6 at 298 K.

Atoms	H_4L^1		**1**		H_4L^2		**2**	
	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm
1, 10	–	120.1	– –	121.0 121.6	–	109.4	– –	112.3 112.9
2, 11	–	152.4	– –	158.9 159.3	–	156.7	– –	159.3 160.0
3, 12	6.92	116.7	6.99 6.95	118.7 118.1	7.24	118.6	7.27 7.22	119.8 120.4
4, 13	7.26	128.6	7.49 7.49	133.9 133.9	7.90	131.9	8.10 8.11	134.6 135.3
5, 14	6.90	119.6	7.12 7.07	122.5 122.3	–	127.9	– –	129.6 129.5
6, 15	7.71	128.4	7.68 7.66	133.9 134.4	–	131.5	– –	132.6 132.5
16, 20					8.35	121.7	8.24 8.45	121.0 122.3
17, 21					7.60	127.6	7.78 7.65	129.2 128.9
18, 22					7.40	123.4	7.55 7.50	125.3 125.2
19, 23					7.88	128.7	8.02 7.96	129.8 129.4
7, 9	8.48	144.3	8.63 8.60	150.8 144.3	9.20	143.2	9.63 9.43	140.3 147.3
8	–	157.1	–	171.2	–	151.6	–	171.0
OH(2)	10.86	–	–	–	11.88	–	–	–

Atoms	H_4L^3		**3**		H_4L^4		**4**	
	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm
1, 10	–	120.0	– –	121.6 122.1	–	111.5	– –	113.2 113.7
2, 11	–	145.3	– –	147.7 148.0	–	158.4	– –	160.5 161.2
3, 12	–	145.6	– –	146.4 146.1	6.30	102.5	6.33 6.28	104.9 104.3
4, 13	6.82	116.5	7.07 7.09	120.5 120.0	–	160.0	– –	163.1 163.8
5, 14	6.72	119.0	6.93 6.87	122.3 122.5	6.34	107.5	6.48 6.54	110.8 110.5
6, 15	7.13	118.6	7.03 7.01	123.8 123.9	7.44	129.7	7.44 7.45	135.2 135.3
7, 9	8.42	144.1	8.60 8.51	144.4 150.8	8.28	144.3	8.47 8.40	144.5 150.9
8	–	152.0	–	171.2	–	152.1	–	170.4
OH(2)	10.25	–	–	–	10.73	–	–	–
OH(3)	9.28	–	9.44	–	9.76	–	10.40 10.42	–

Atoms	H_4L^5		**5**		H_4L^6		**6**	
	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm	δ_H, ppm	δ_C, ppm
1, 10	–	120.4	–	121.3	–	113.2	–	114.3

			–	121.9			–	114.8
2, 11	–	146.7	– –	148.4 148.7	–	158.7	– –	160.5 161.1
3, 12	–	148.4	– –	148.7 149.0	6.46	101.4	6.55 6.59	102.8 103.4
4, 13	6.83	113.4	7.19 7.22	116.1 126.7	–	161.9	– –	164.2 164.8
5, 14	6.98	119.3	7.00 7.06	122.2 122.2	6.49	106.6	6.71, 6.69 6.67, 6.65	109.7 109.8
6, 15	7.33	120.1	7.20 7.24	124.9 125.0	7.57	129.9	7.56 7.58	134.8 134.9
7, 9	8.47	140.6	8.56 8.61	144.2 150.8	8.33	141.8	8.48 8.53	144.2 150.7
8	–	152.4	–	171.2	–	152.4	–	170.5
OH(2)	10.87	–	–	–	10.67	–	–	–
16, 17	3.82	56.3	3.82 3.83	56.4	3.76	55.6	3.82 3.83	56.2

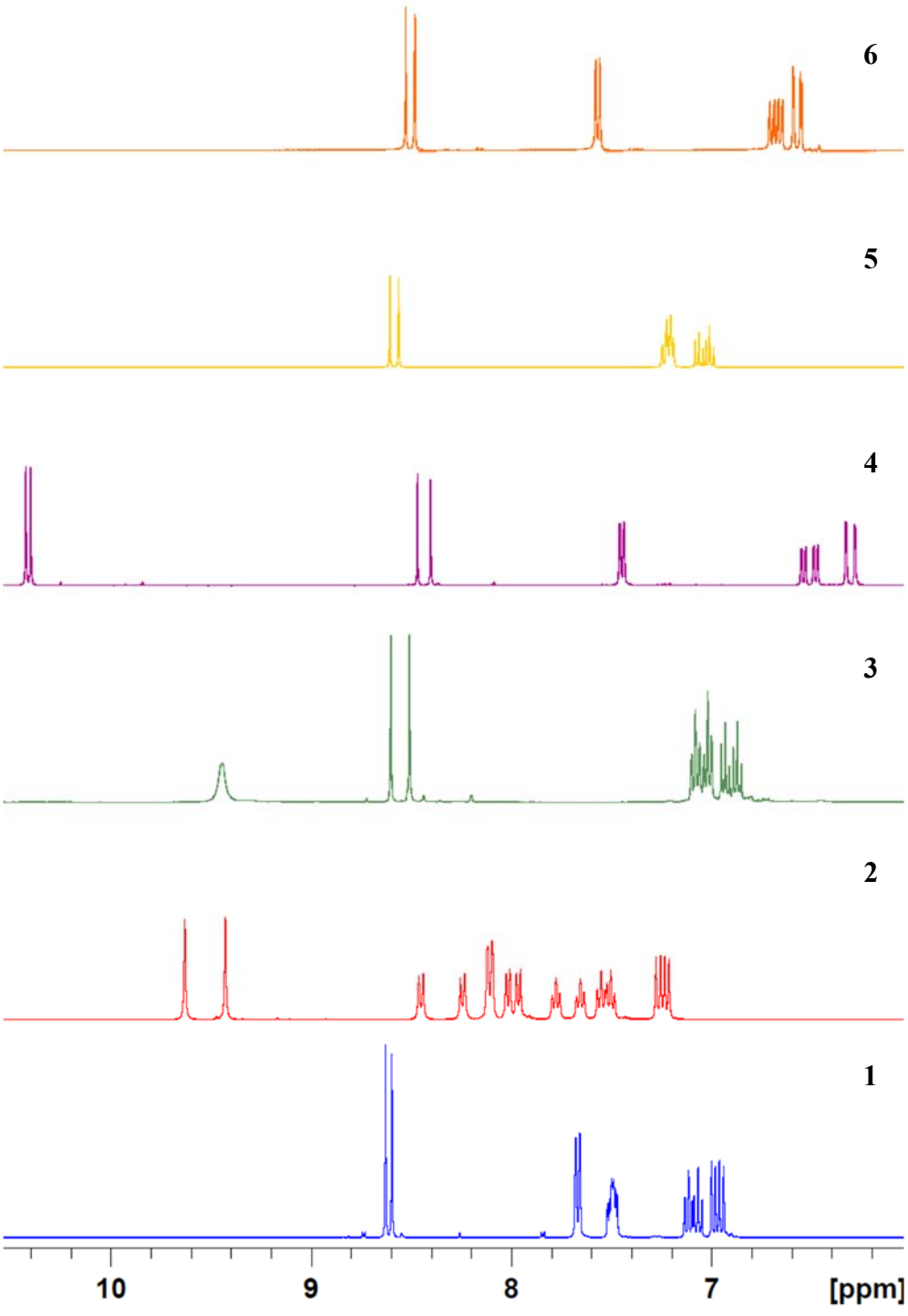


Figure S19. ^{1}H NMR spectra of (from bottom to top): **1**, **2** ,**3, 4**, **5** and **6** in DMSO–d_6 at room temperature.

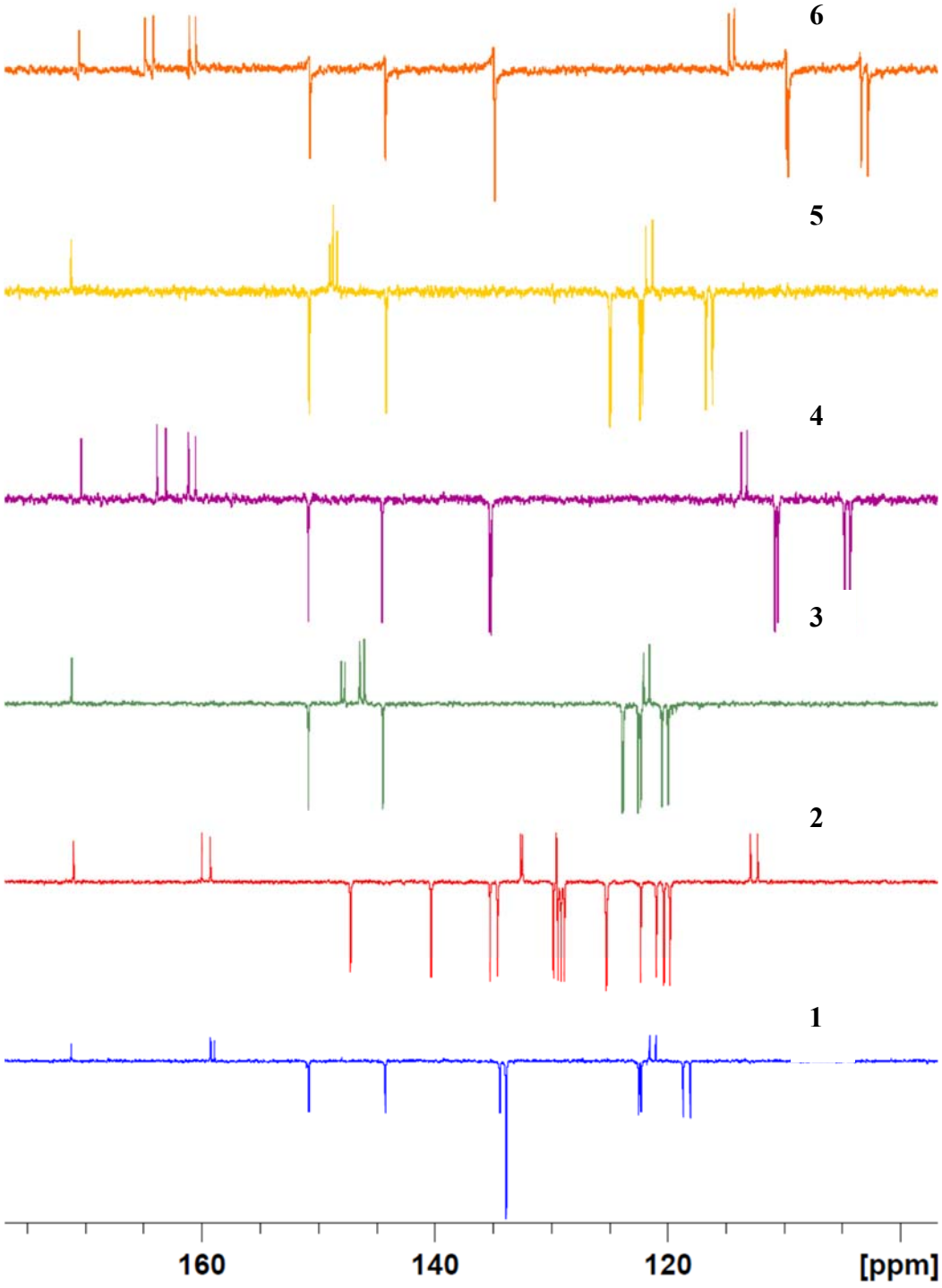


Figure S20. DEPTQ ^{13}C NMR spectra of (from bottom to top): **1**, **2** ,**3, 4**, **5** and **6** in DMSO–d_6 at room temperature.

Stability study of complexes

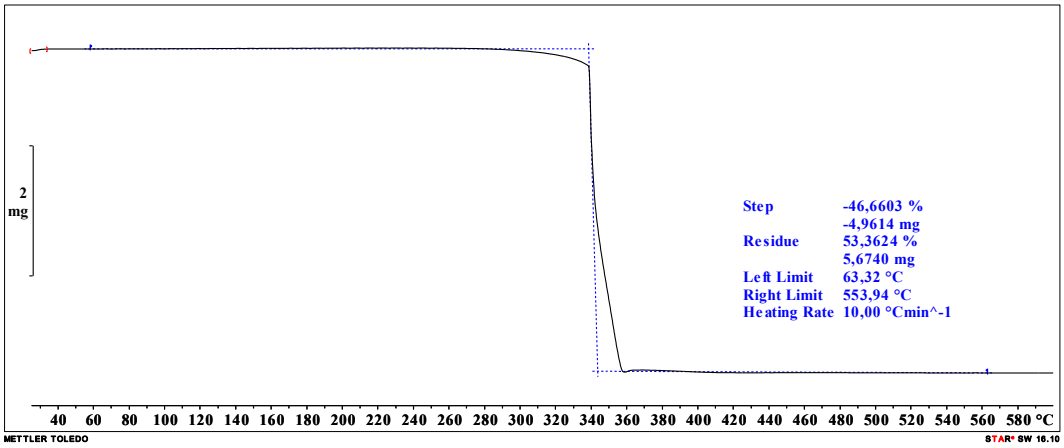


Figure S21. TG curve of **1**.

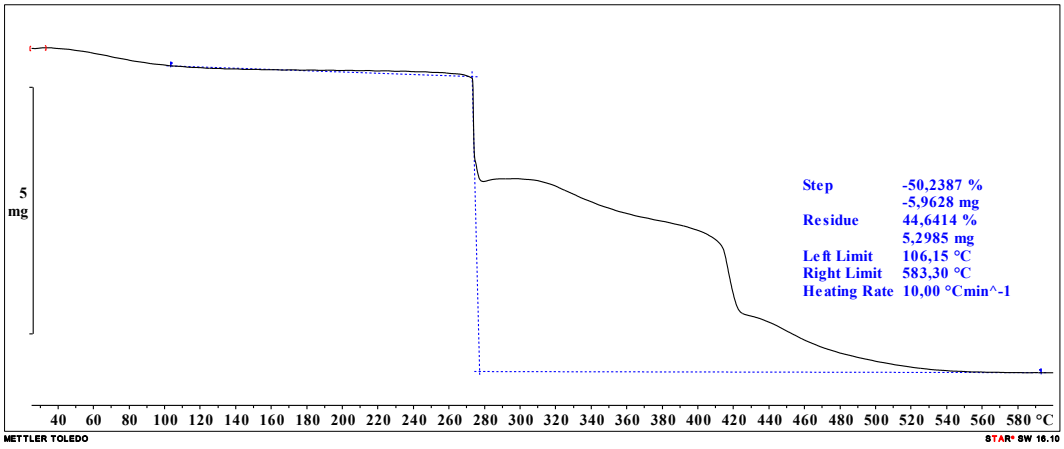


Figure S22. TG curve of **2**.

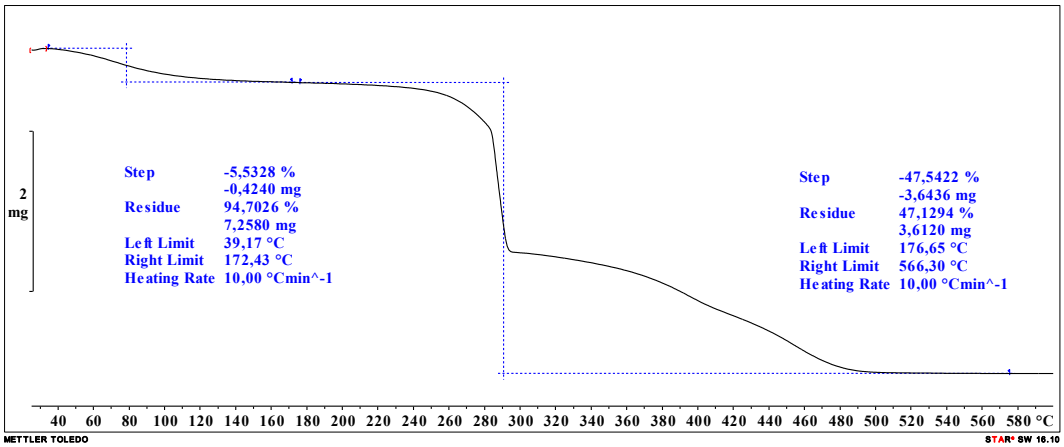


Figure S23. TG curve of **3**. (MoO_3 content is calculated by dividing step 2 residue with step 1 residue.)

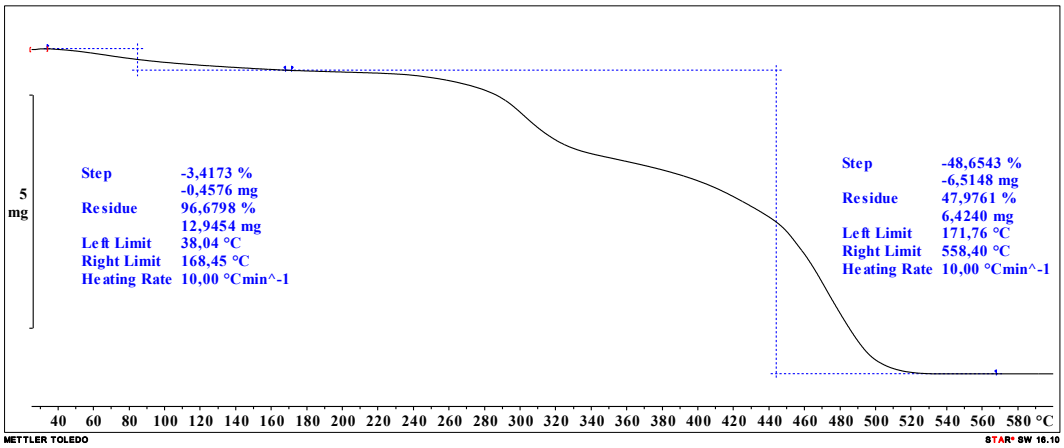


Figure S24. TG curve of **4**. (MoO_3 content is calculated by dividing Step 2 residue by Step 1 residue.)

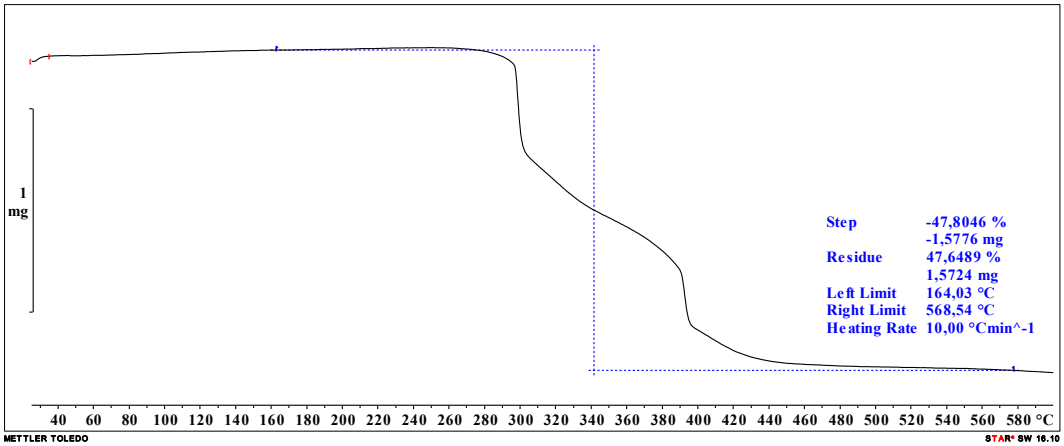


Figure S25. TG curve of **5**.

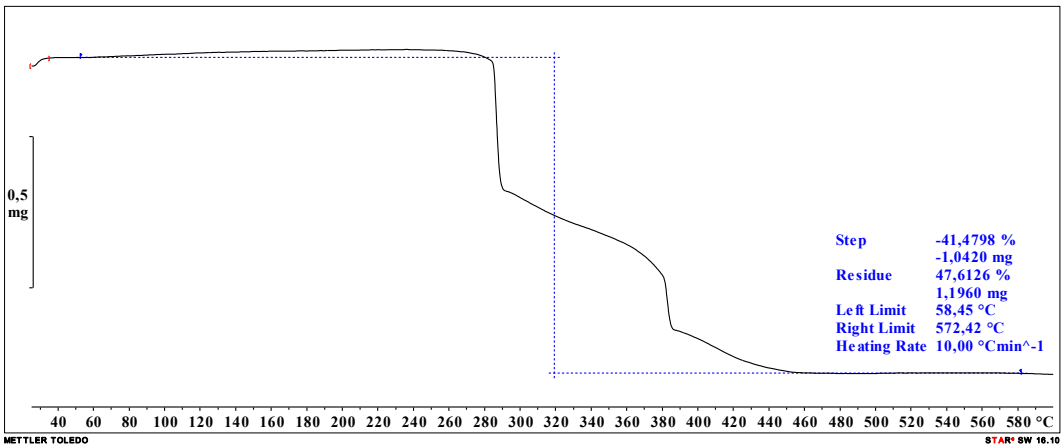


Figure S26. TG curve of **6**.

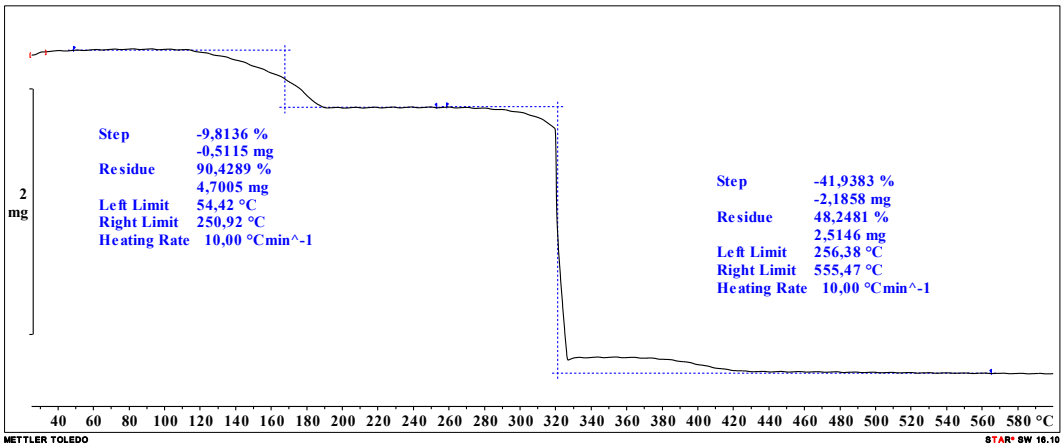


Figure S27. TG curve of **1a**.

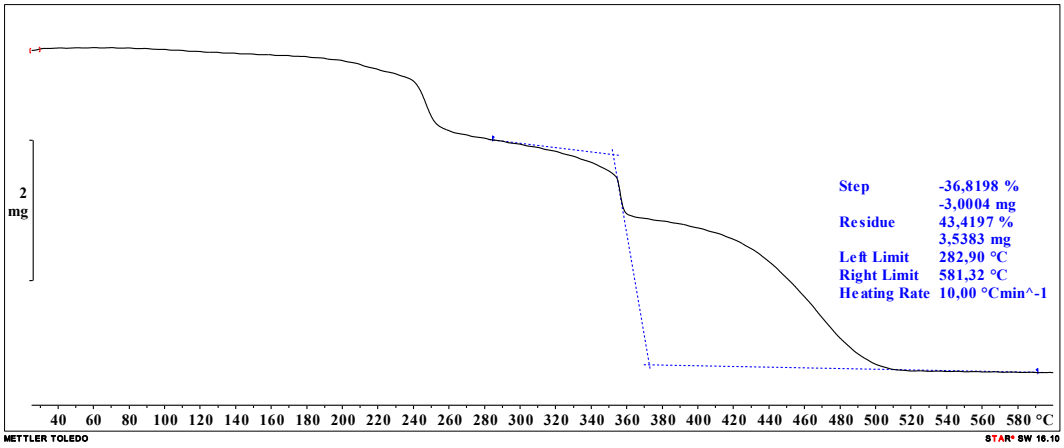


Figure S28. TG curve of **1b·CH_3CN**.

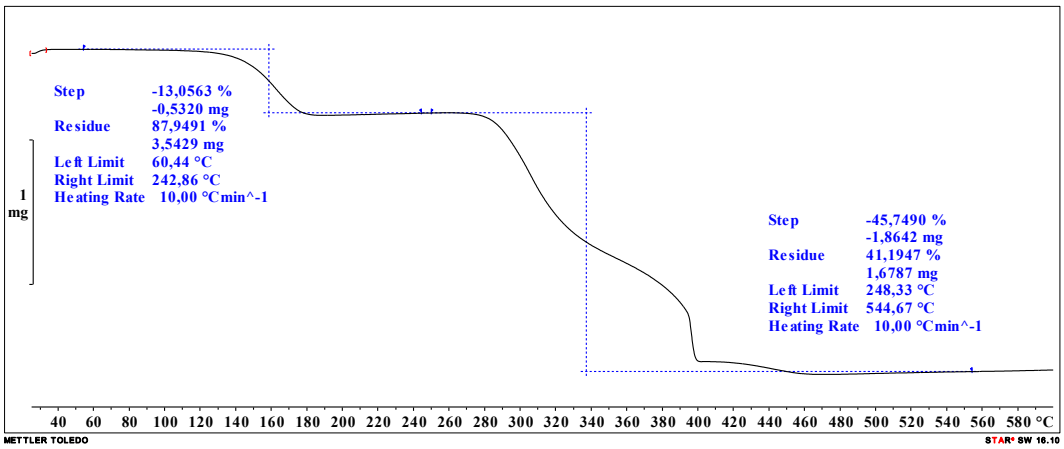


Figure S29. TG curve of **5a·CH_3OH**.

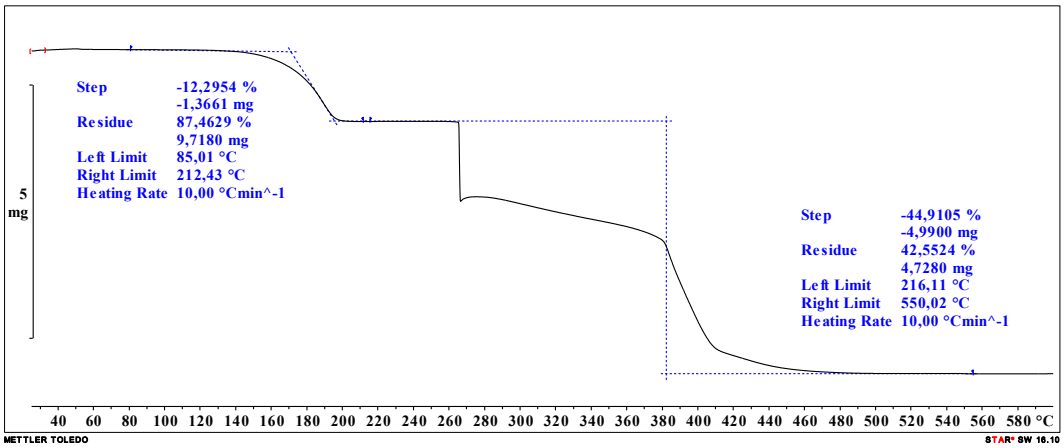


Figure S30. TG curve of **5a'·0.64CH_3OH**.

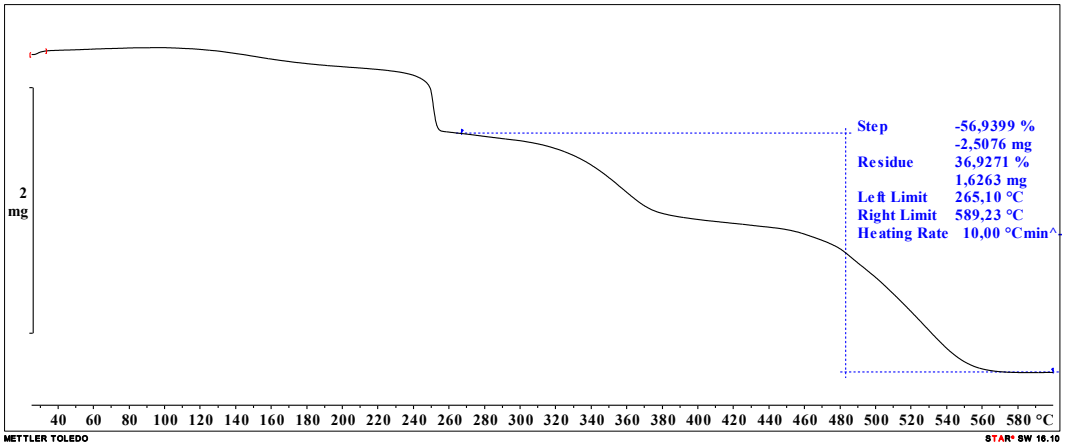


Figure S31. TG curve of **5b·CH_3CN**.

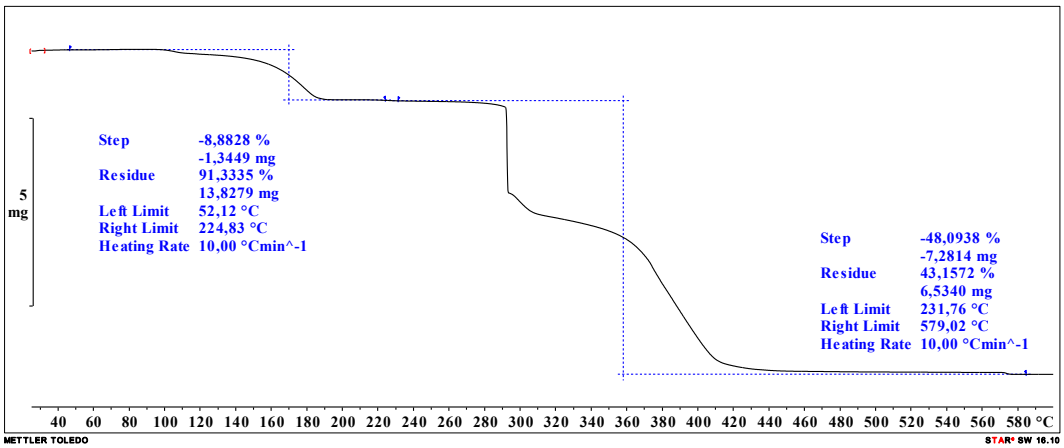


Figure S32. TG curve of **6a.**

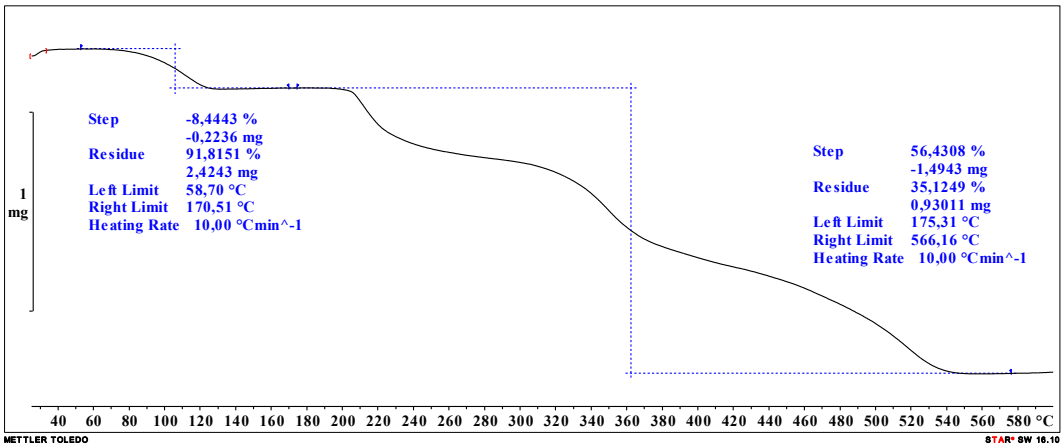


Figure S33. TG curve of **6b·2CH$_3$CN**

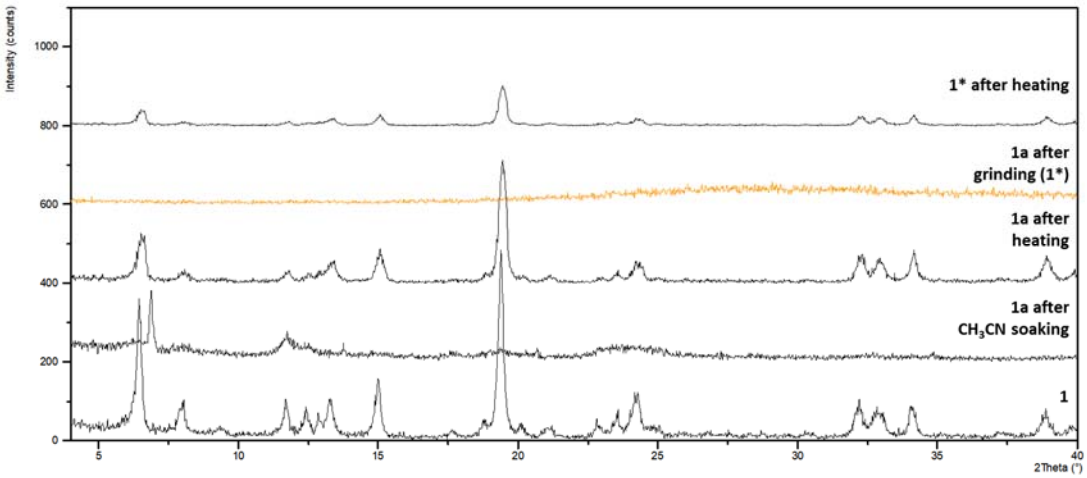


Figure S34. PXRD patterns of (from bottom to top) **1**, **1a** after soaking in acetonitrile, **1a** after heating to 180 °C, **1a** after grinding (**1***) and **1*** after heating.

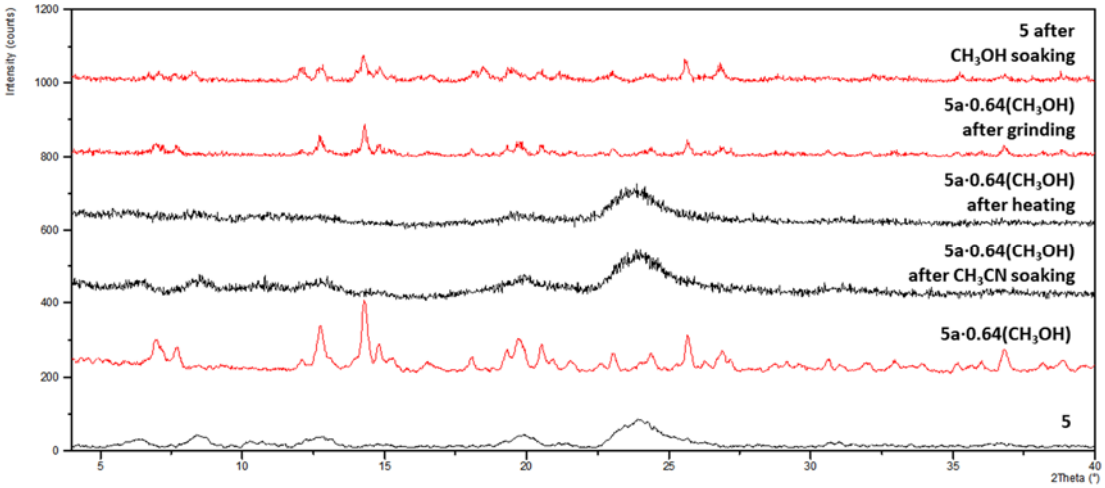


Figure S35. PXRD patterns of (from bottom to top) **5**, **5a'·0.64CH$_3$OH, 5a'·0.64CH$_3$OH** after soaking in acetonitrile, **5a'·0.64CH$_3$OH** after heating to 180 °C, **5a'·0.64CH$_3$OH** after grinding and **5** after soaking in methanol.

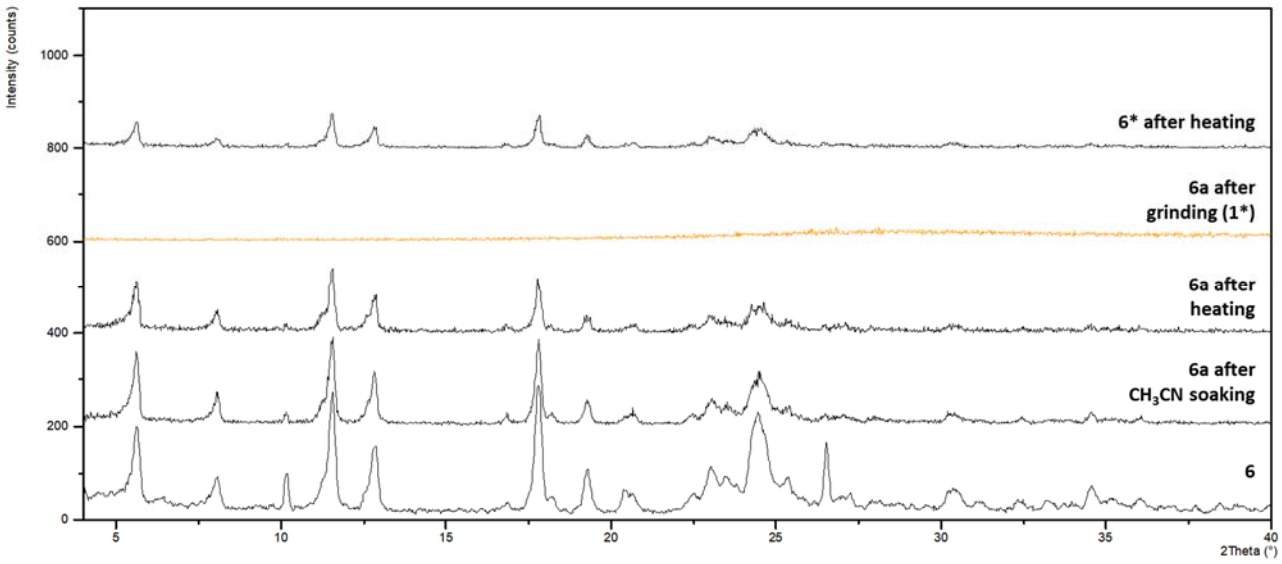


Figure S36. PXRD patterns of (from bottom to top) **6**, **6a** after soaking in acetonitrile, **6a** after heating to 180 °C, **6a** after grinding (**6***) and **6*** after heating.

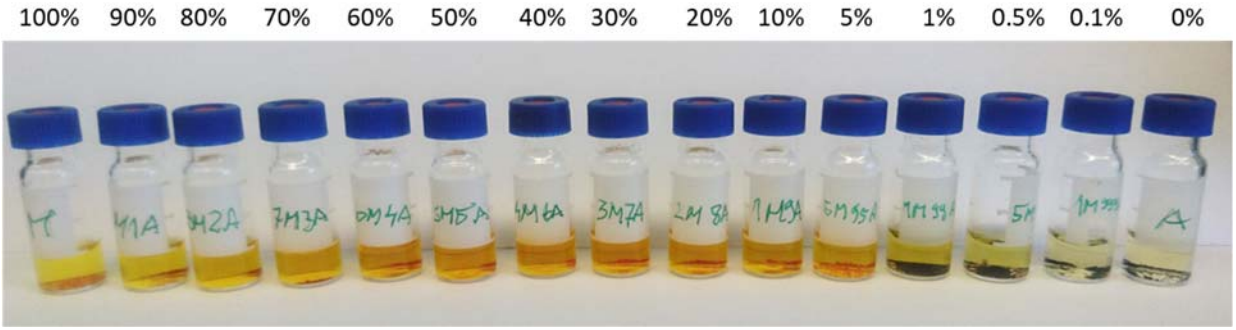


Figure S37. Soaking experiments with **5a'·0.64CH$_3$OH**, with percent value above each flask representing the volume ratio of methanol in mixture with acetonitrile. Experiments with **1a** and **6a** yielded similar results.

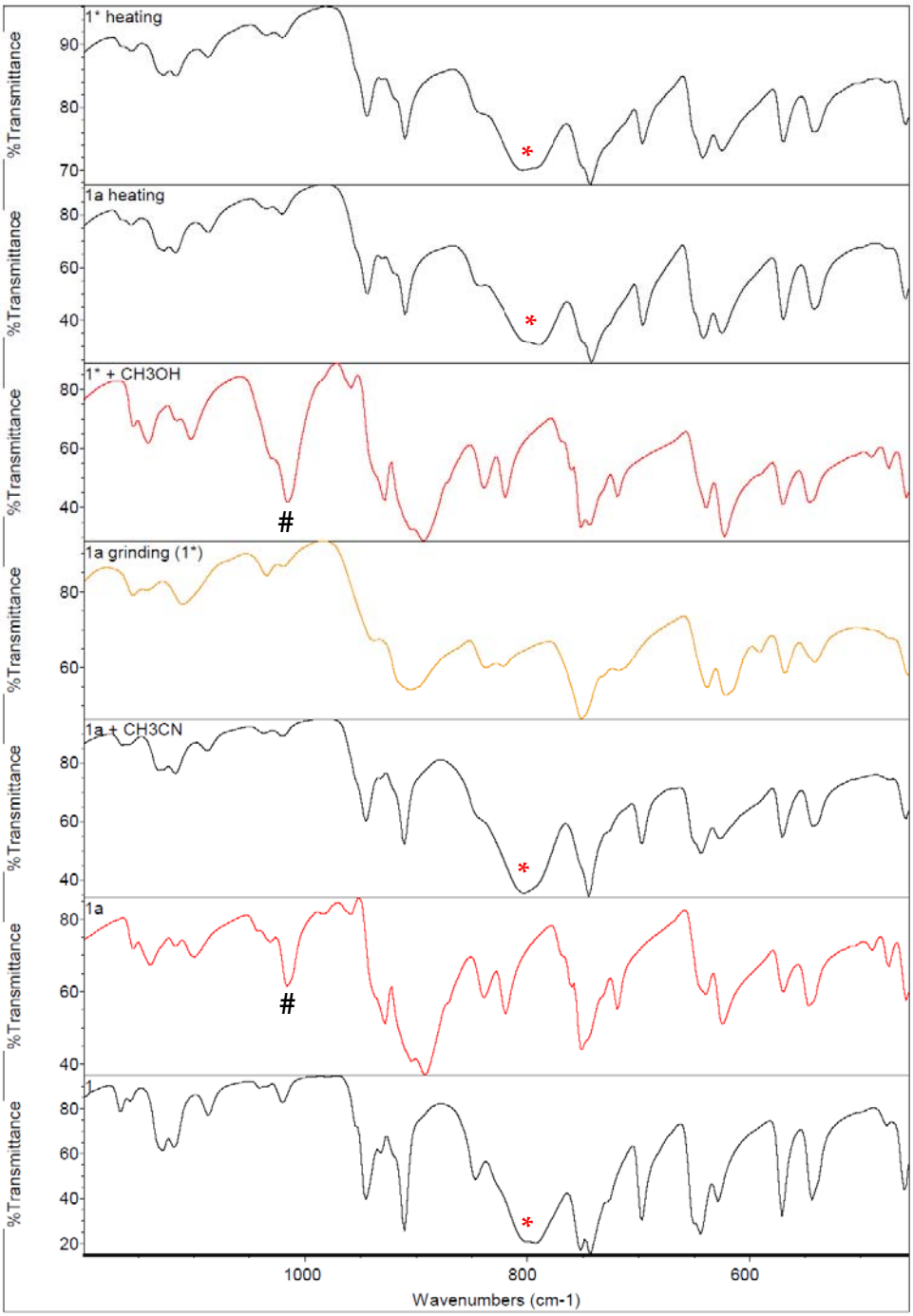


Figure S38. ATR-FTIR spectra of compounds (from bottom to top): **1**, **1a**, **1a** after soaking in acetonitrile, **1a** after grinding (**1***), **1*** after soaking in methanol, **1a** after desolvation by heating to 180 °C and **1*** after heating at 180 °C**.** Strong broad peak at ~800 cm^{-1} marked with asterisk (*) corresponds to Mo=O···Mo interactions present in polymeric **1**. Peak marked with hash (#) corresponds to coordinated methanol C–O stretch present in **1a.** Both peaks are absent in **1***, which corroborates that **1*** is coordinatively unsaturated dinuclear complex.

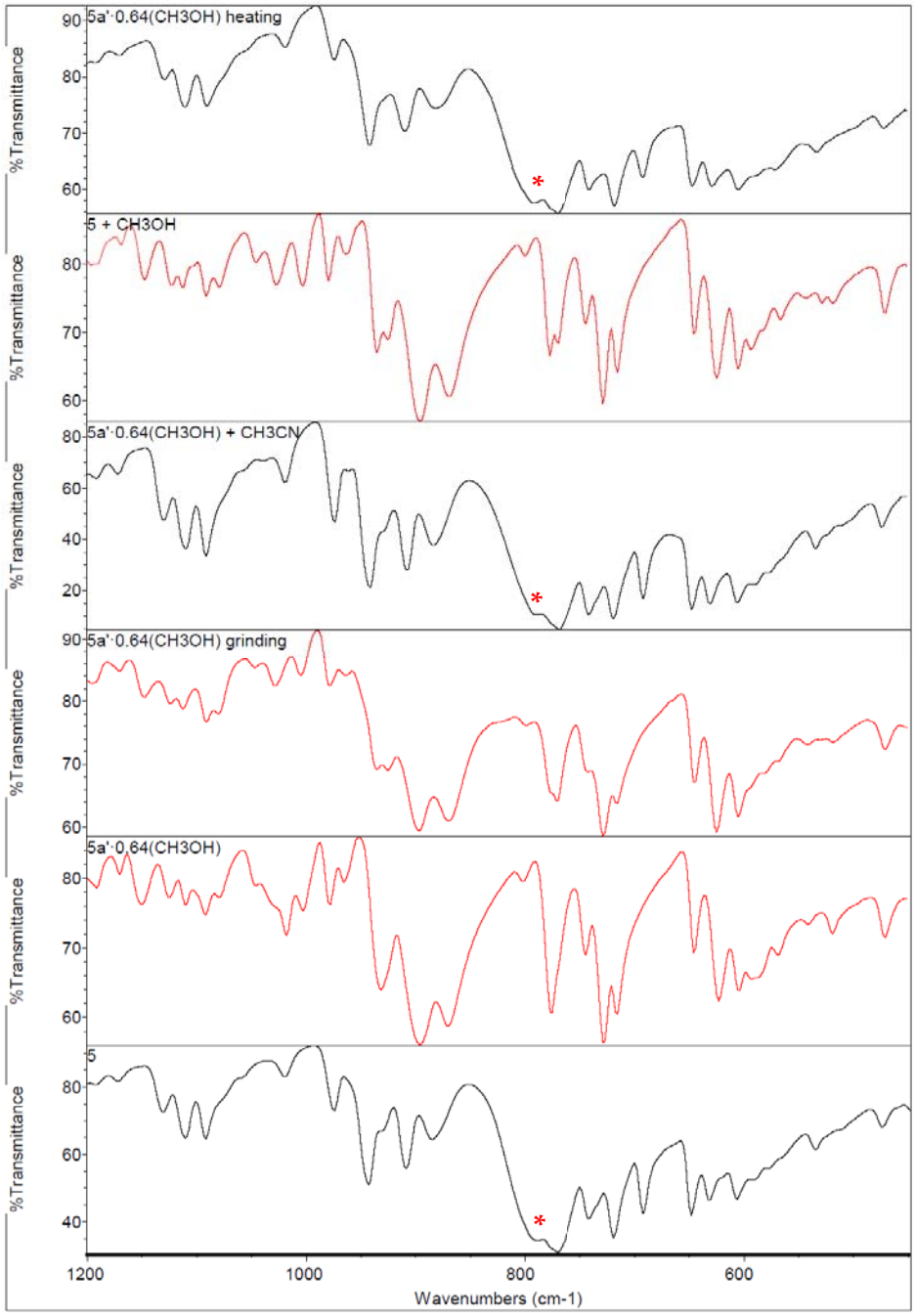


Figure S39. ATR-FTIR spectra of (from bottom to top) **5**, **5a'·0.64CH$_3$OH**, **5a'·0.64CH$_3$OH** after grinding, **5a'·0.64CH$_3$OH** after soaking in acetonitrile, **5** after soaking in methanol and **5a'·0.64CH$_3$OH** after desolvation by heating to 180 °C. Strong broad peak at ~780 cm^{-1} marked with asterisk (*) corresponds to Mo=O···Mo interactions present in polymeric **5**.

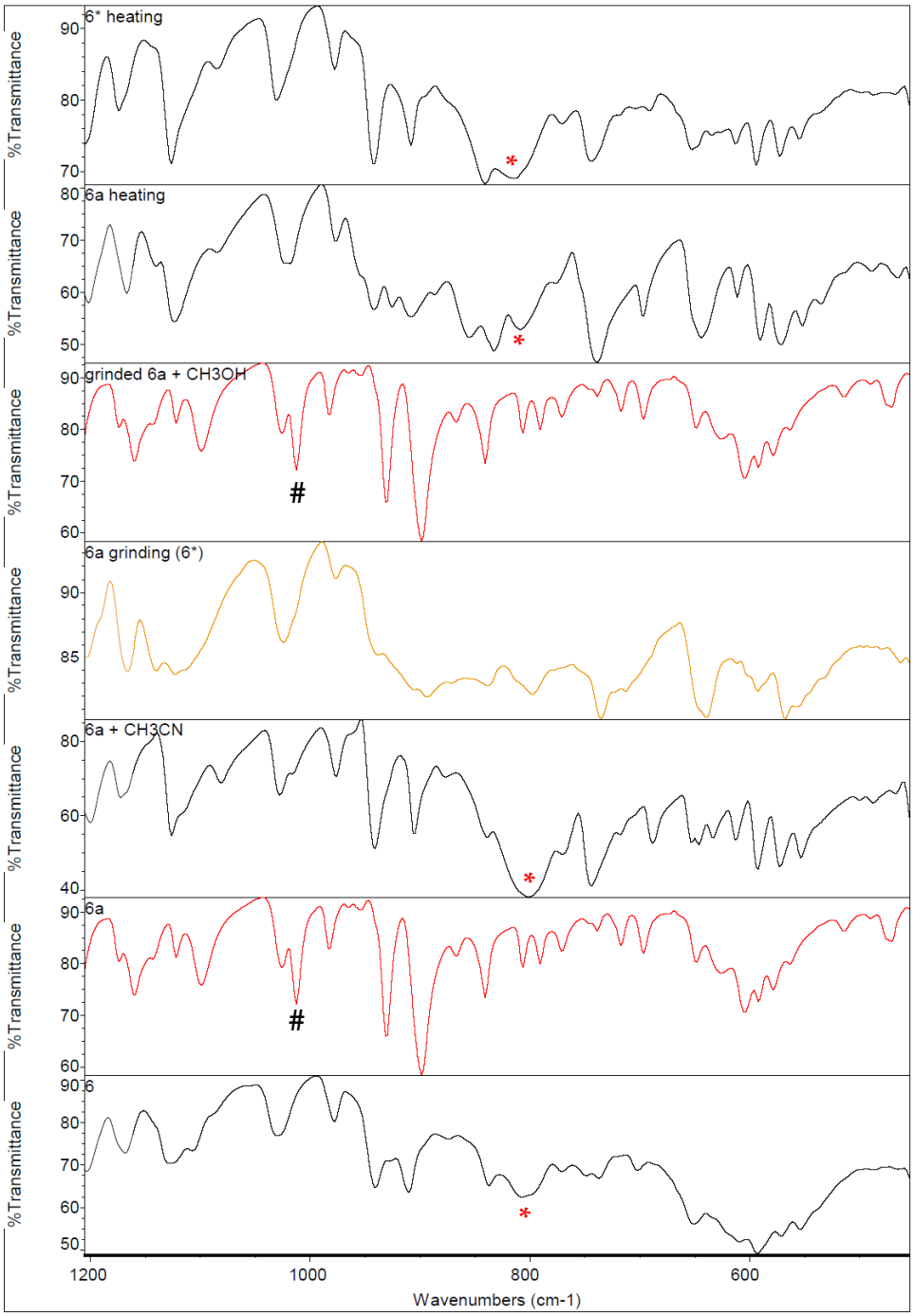


Figure S40. ATR-FTIR spectra of (from bottom to top) **6**, **6a**, **6a** after soaking in acetonitrile, **6a** after grinding (**6***), **6*** after soaking in methanol, **6a** after desolvation by heating to 180 °C and **6*** after heating at 180 °C**.** Strong broad peak at ~800 cm^{-1} marked with asterisk (*) corresponds to Mo=O···Mo interactions present in polymeric **6**. Peak marked with hash (#) corresponds to coordinated methanol C–O stretch present in **6a.** Both peaks are very weakly expressed, if not absent in **6***, which corroborates that **6*** is coordinatively unsaturated dinuclear complex.

Theoretical calculations

Table S9. Relative enthalpies and enthalpy differences $\Delta H_{cis\text{-trans}}$ of the different species (in kcal mol^{-1}).

H(kcal mol^{-1})	L^1		L^5		L^6	
	Gas	PCM	Gas	PCM	Gas	PCM
cis-[$(MoO_2)_2(L^i)$]	0	0	0	0	0	0
trans-[$(MoO_2)_2(L^i)$]	–0.1	+0.7	–0.1	+0.2	+1.5	+1.4
$\Delta H_{cis–trans}$	+0.1	–0.7	+0.1	–0.2	–1.5	–1.4
cis-[$(MoO_2)_2(L^i)(Im^{ONO})$]	–16.2	–13.3	–15.6	–12.8	–15.3	–12.7
trans-[$(MoO_2)_2(L^i)(Im^{ONO})$]	–15.5	–12.3	–15.1	–12.3	–13.2	–10.8
$\Delta H_{cis–trans}$	–0.7	–1.0	–0.5	–0.5	–2.1	–1.9
cis-[$(MoO_2)_2(L^i)(Im)_2$]	–26.0	–21.2	–25.2	–21.1	–24.5	–20.0
trans-[$(MoO_2)_2(L^i)(Im)_2$]	–28.8	–21.1	–28.1	–20.5	–25.7	–18.6
$\Delta H_{cis–trans}$	+2.8	–0.1	+2.9	–0.6	+1.3	–1.4

Experimental data

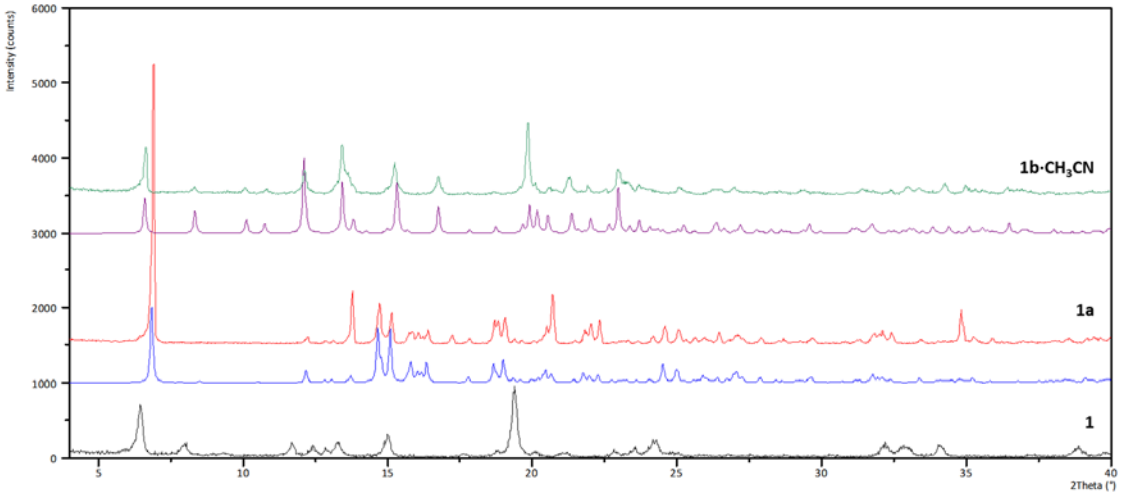


Figure S41. PXRD patterns of (from bottom to top): **1**, **1a** (calculated from crystal structure), **1a**, **1b·CH$_3$CN** (calculated from crystal structure) and **1b·CH$_3$CN.**

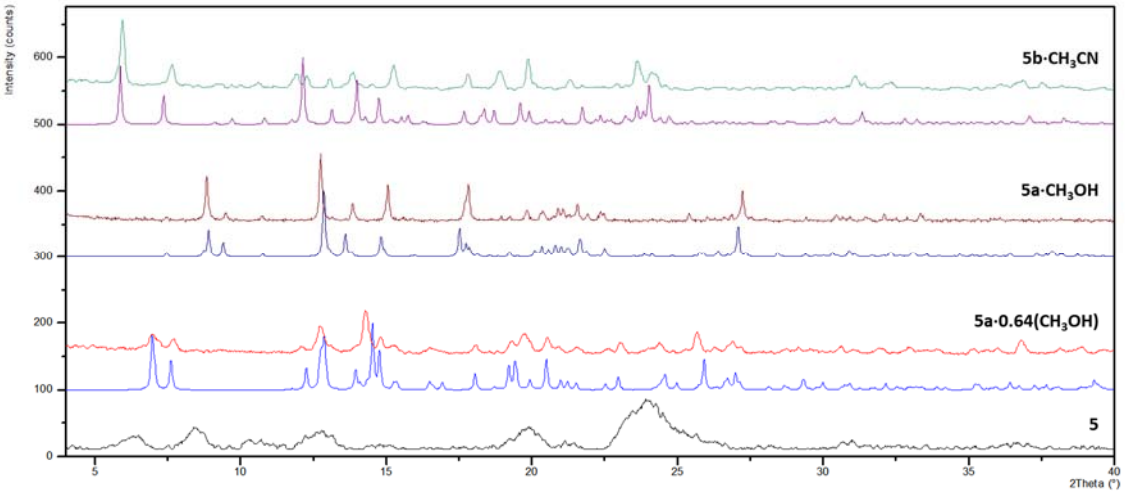


Figure S42. PXRD patterns of (from bottom to top) **5**, **5a'·0.64CH$_3$OH** (calculated from crystal structure), **5a'·0.64CH$_3$OH**, **5a·CH$_3$OH** (calculated from crystal structure), **5a·CH$_3$OH**, **5b·CH$_3$CN** (calculated from crystal structure) and **5b·CH$_3$CN**. Slight differences between calculated and experimental patterns for **5a'·0.64CH$_3$OH**, **5a·CH$_3$OH** and **5b·CH$_3$CN** can be ascribed to differences in diffraction experiment temperatures.

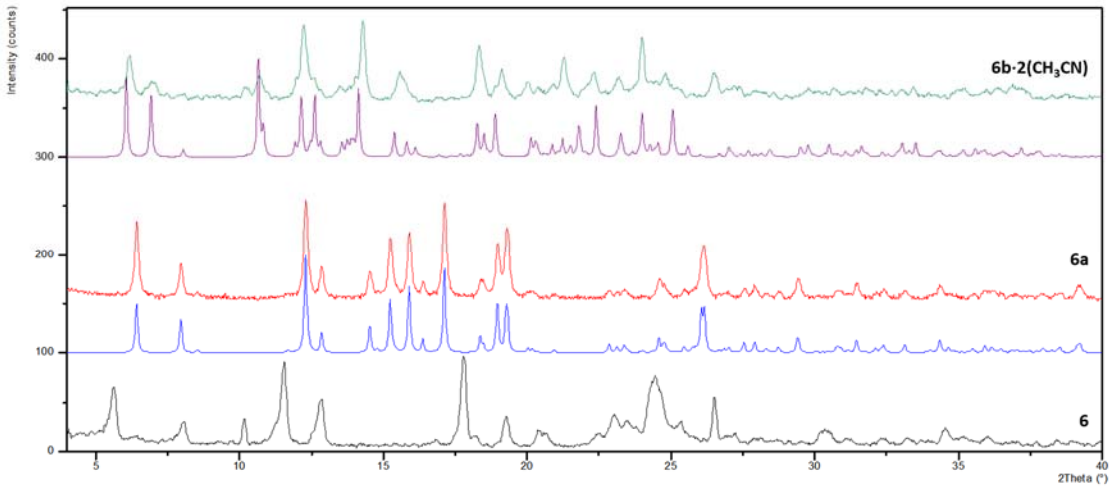


Figure S43. PXRD patterns of (from bottom to top) **6**, **6a** (calculated from crystal structure), **6a**, **6b·2CH$_3$CN** (calculated from crystal structure) and **6b·2CH$_3$CN**. Slight differences between calculated and experimental patterns for **6b·2CH$_3$CN** can be ascribed to differences in diffraction experiment temperatures as well as possible sample desolvation

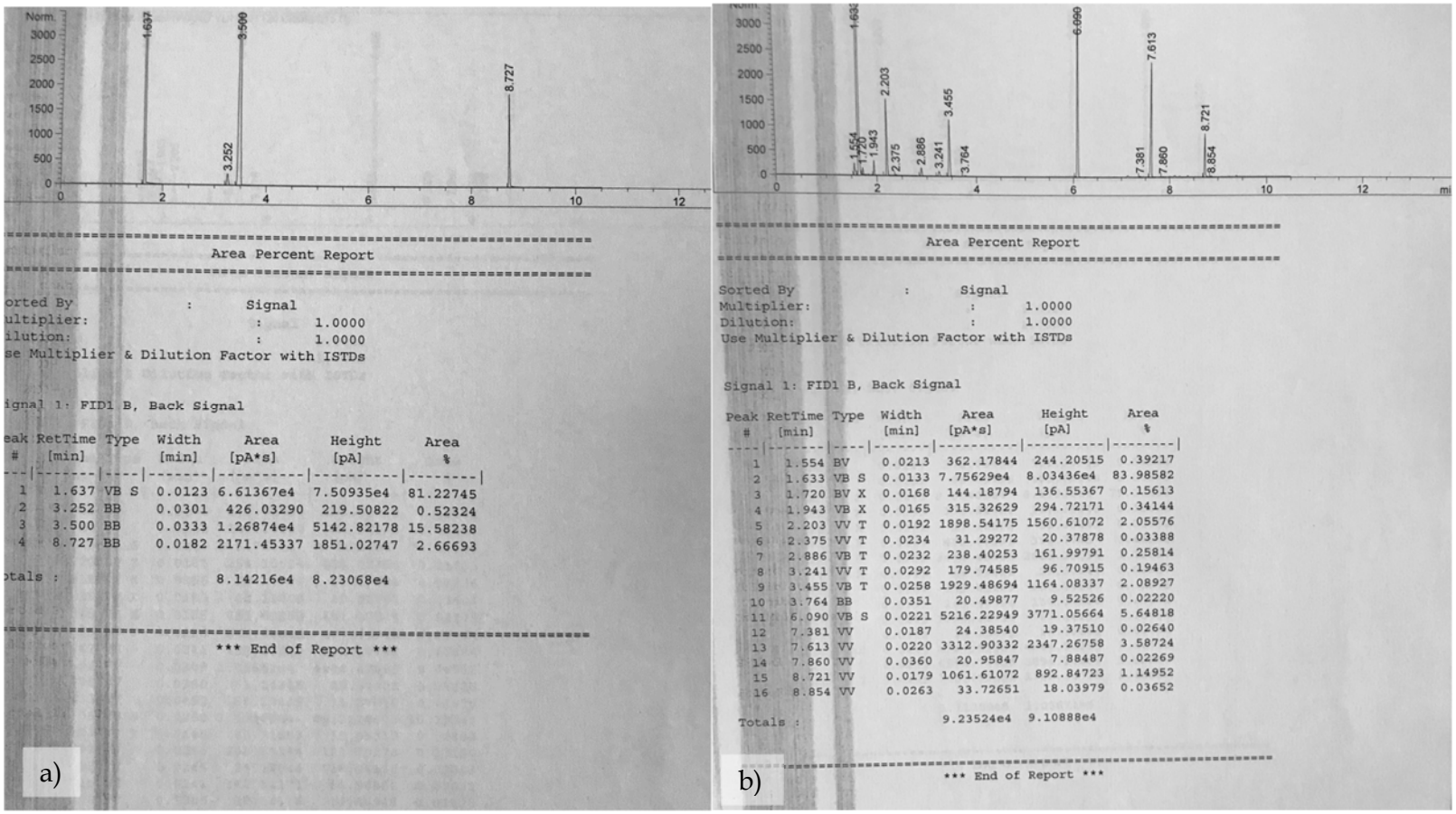
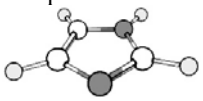
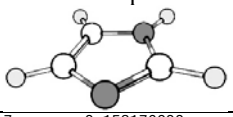


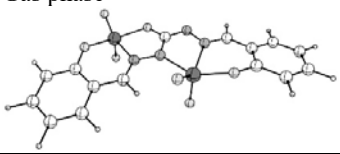
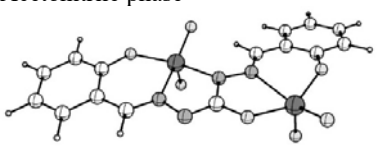
Figure S44. GC spectra for general cyclooctene epoxidation reaction: a) start of the investigated reaction, and b) the end of the investigated reaction. Retention time 1.633 min corresponds to diethyl ether, 3.500 min to cyclooctene, 6.090 min to cyclooctene oxide, and 8.727 min to acetophenone (the internal reference).

Table S10. Structures optimized by DFT calculation in gaseous phase and acetonitrile solution. Numerical data represent atomic number followed by Cartesian coordinates (in Å) of atoms in the structure.

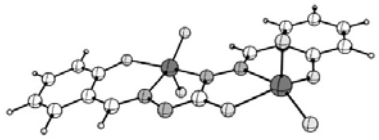
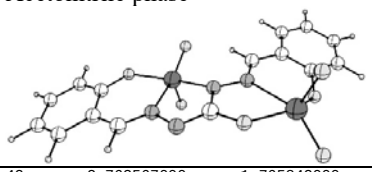
Imidazole

Gas phase				Acetonitrile phase			
							
7	0.146041000	-1.226478000	0.000034000	7	0.158176000	-1.225544000	-0.000236000
7	-0.765321000	0.799051000	-0.000005000	7	-0.770397000	0.787479000	-0.000376000
1	-1.470107000	1.521821000	0.000063000	1	-1.483968000	1.507156000	0.002448000
6	-0.982277000	-0.551200000	-0.000022000	6	-0.981898000	-0.556344000	0.000109000
1	-1.977006000	-0.976883000	-0.000049000	1	-1.974068000	-0.986033000	-0.000035000
6	1.139427000	-0.271043000	-0.000016000	6	1.146180000	-0.260053000	0.000413000
1	2.184705000	-0.549327000	-0.000056000	1	2.195687000	-0.524609000	0.000422000
6	0.601970000	0.992051000	0.000014000	6	0.590712000	0.996689000	-0.000151000
1	1.042655000	1.977532000	-0.000018000	1	1.017933000	1.988186000	-0.000776000

cis-[$(MoO_2)_2(L^1)$]

Gas phase				Acetonitrile phase			
							
42	-2.767242000	-1.793974000	0.049513000	42	-2.764257000	-1.784708000	0.006163000
42	1.653721000	1.010846000	0.024152000	42	1.654262000	0.997822000	-0.005058000
8	-0.887223000	-2.392216000	-0.234544000	8	-0.880959000	-2.420472000	-0.196173000
8	3.524050000	1.273135000	-0.400889000	8	3.525088000	1.292314000	-0.382239000
8	-4.000586000	-0.439992000	-0.565967000	8	-4.044607000	-0.445834000	-0.514094000
8	-3.456987000	-3.136097000	-0.719461000	8	-3.485979000	-3.176461000	-0.668327000
8	0.936442000	2.160413000	-1.010571000	8	0.937437000	2.267066000	-0.907239000
8	1.478800000	1.528735000	1.630935000	8	1.519644000	1.396042000	1.642548000
7	-0.034004000	-0.249206000	-0.110945000	7	-0.041003000	-0.258713000	-0.172727000
8	-3.024230000	-1.912582000	1.718593000	8	-2.974558000	-1.859199000	1.688908000
7	2.313711000	-1.130827000	-0.100322000	7	2.323678000	-1.137805000	-0.064900000
7	1.363861000	-2.130653000	-0.169331000	7	1.364874000	-2.137698000	-0.117275000
7	-1.375428000	0.066689000	-0.071817000	7	-1.387471000	0.056469000	-0.121078000
6	0.165193000	-1.614490000	-0.157889000	6	0.168466000	-1.621101000	-0.151987000
6	3.547093000	-1.562344000	-0.050877000	6	3.557539000	-1.563003000	-0.006988000
1	3.659353000	-2.646097000	-0.030563000	1	3.693408000	-2.642913000	0.037540000
6	5.874977000	1.391720000	-0.204996000	6	5.875694000	1.404733000	-0.215029000
1	5.812373000	2.465078000	-0.349508000	1	5.816960000	2.477084000	-0.372563000
6	-1.760193000	1.306340000	0.022143000	6	-1.774776000	1.296107000	-0.030018000
1	-1.008646000	2.087162000	0.100043000	1	-1.027390000	2.081858000	0.034171000
6	4.735206000	-0.758751000	-0.024226000	6	4.737914000	-0.746104000	0.000753000
6	4.691122000	0.645119000	-0.199210000	6	4.694341000	0.656525000	-0.188397000
6	-3.136600000	1.734372000	0.006760000	6	-3.149174000	1.730552000	-0.014332000
6	-4.209507000	0.858344000	-0.284918000	6	-4.239589000	0.861493000	-0.249293000
6	5.990189000	-1.385023000	0.140464000	6	5.995646000	-1.370082000	0.159869000
1	6.022745000	-2.463804000	0.269330000	1	6.027751000	-2.446980000	0.299622000
6	7.096619000	0.748488000	-0.029360000	6	7.100603000	0.763204000	-0.045819000
6	-5.520923000	1.347027000	-0.336078000	6	-5.549981000	1.350485000	-0.252847000
1	-6.320989000	0.653342000	-0.572107000	1	-6.366811000	0.661813000	-0.444160000
6	-3.419243000	3.097309000	0.243030000	6	-3.414168000	3.099110000	0.213314000
1	-2.593824000	3.770703000	0.459469000	1	-2.575963000	3.768419000	0.386776000
6	7.160554000	-0.642466000	0.144379000	6	7.165894000	-0.625682000	0.142725000
1	8.118850000	-1.133837000	0.278158000	1	8.126017000	-1.115404000	0.270348000
6	-5.770676000	2.692439000	-0.086309000	6	-5.782050000	2.702243000	-0.011251000
6	-4.720027000	3.574751000	0.205258000	6	-4.714756000	3.581999000	0.221797000
1	-4.922133000	4.623669000	0.396974000	1	-4.904062000	4.634661000	0.406080000
1	8.010815000	1.335313000	-0.031015000	1	8.013981000	1.350924000	-0.066399000
1	-6.792474000	3.059636000	-0.121622000	1	-6.802829000	3.073470000	-0.008016000

trans-[$(MoO_2)_2(L^1)$]

Gas phase				Acetonitrile phase			
							
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8	2.928545000	-1.902428000	1.797048000	8	3.370871000	-1.912258000	1.590853000
7	-2.312147000	-1.122481000	-0.095220000	7	-2.329508000	-1.134984000	0.133405000
7	0.038294000	-0.232502000	-0.064588000	7	0.036949000	-0.233366000	0.202930000
7	1.383970000	0.078458000	-0.041852000	7	1.391060000	0.063219000	0.119980000
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6	-0.161574000	-1.595426000	-0.169507000	6	-0.171542000	-1.595269000	0.236747000
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6	3.157428000	1.734459000	-0.016717000	6	3.176479000	1.710227000	0.080638000
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6	5.548366000	1.314688000	-0.262315000	6	5.505122000	1.324725000	-0.541393000
1	6.349251000	0.605298000	-0.442236000	1	6.268687000	0.649874000	-0.914965000
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1	6.827783000	3.025099000	-0.079330000	1	6.823883000	3.001378000	-0.319207000
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1	-8.129044000	-1.133134000	-0.133890000	1	-8.115540000	-1.140102000	-0.370778000
6	4.750088000	3.569918000	0.152766000	6	4.805133000	3.511091000	0.258453000
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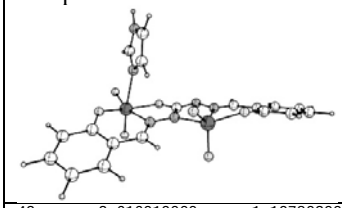
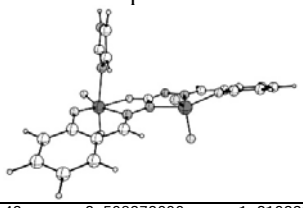
1	-6.034549000	-2.450427000	-0.335294000	1	-6.013980000	-2.464414000	-0.293103000

cis-[$(MoO_2)_2(L^1)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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8	0.727788000	-1.886064000	-1.297213000	8	0.712466000	-1.916698000	-1.242264000
8	-3.734932000	0.965609000	0.852692000	8	-3.759564000	0.992618000	0.861965000
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8	3.428424000	-2.695625000	-1.011562000	8	3.416589000	-2.716787000	-1.080227000
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8	-1.931198000	2.352416000	-0.941151000	8	-2.027869000	2.205672000	-1.061870000
7	-0.211589000	0.052305000	-0.439925000	7	-0.216994000	0.027707000	-0.378860000
8	2.833228000	-0.507672000	-2.541278000	8	2.735342000	-0.499724000	-2.535430000
7	2.008152000	-1.891319000	1.280324000	7	2.102227000	-1.872380000	1.271203000
7	-2.503312000	-0.888077000	-0.692719000	7	-2.529542000	-0.919003000	-0.640439000
7	-1.528137000	-1.759972000	-1.121847000	7	-1.538090000	-1.791707000	-1.049651000
7	1.100379000	0.456221000	-0.376019000	7	1.098963000	0.432437000	-0.348571000
7	1.873989000	-3.290204000	2.973011000	7	1.845190000	-3.197241000	3.006112000
1	1.967881000	-4.139251000	3.511293000	1	1.798700000	-4.046874000	3.557607000
6	-0.340093000	-1.223205000	-0.972843000	6	-0.357161000	-1.246338000	-0.903246000
6	-3.729152000	-1.292138000	-0.899033000	6	-3.751534000	-1.331195000	-0.838566000
1	-3.824535000	-2.235147000	-1.436849000	1	-3.864143000	-2.284748000	-1.353756000
6	2.274739000	-3.120346000	1.689597000	6	2.118399000	-3.134814000	1.687817000
1	2.751495000	-3.881810000	1.091100000	1	2.330037000	-3.997843000	1.075664000
6	-6.095531000	1.075518000	0.825305000	6	-6.119757000	1.097373000	0.807538000
1	-6.042112000	1.921826000	1.502115000	1	-6.078009000	1.961744000	1.462753000
6	1.411957000	-1.244338000	2.346019000	6	1.807329000	-1.100735000	2.382598000
1	1.090110000	-0.216082000	2.279246000	1	1.740856000	-0.024874000	2.327932000
6	1.410458000	1.691381000	-0.128235000	6	1.417122000	1.670888000	-0.132352000
1	0.621311000	2.431926000	-0.019068000	1	0.638297000	2.419892000	-0.014532000
6	-4.931396000	-0.626642000	-0.479571000	6	-4.948446000	-0.644103000	-0.438797000
6	1.319619000	-2.101470000	3.408936000	6	1.643615000	-1.915601000	3.470617000
1	0.923932000	-1.978821000	4.404960000	1	1.412126000	-1.708090000	4.504049000
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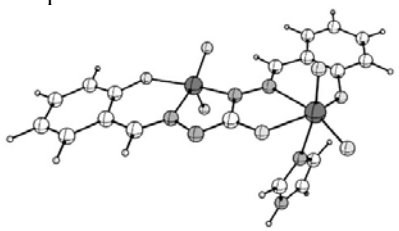
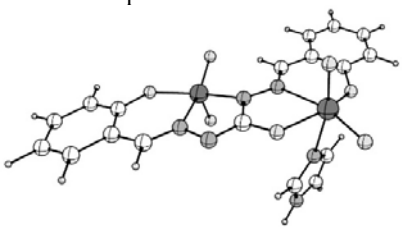
trans-[$(MoO_2)_2(L^1)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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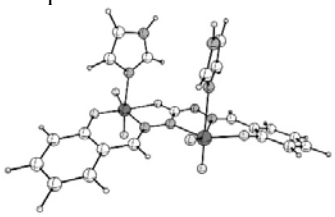
cis-[$(MoO_2)_2(L^1)(Im)_2$]

Gas phase



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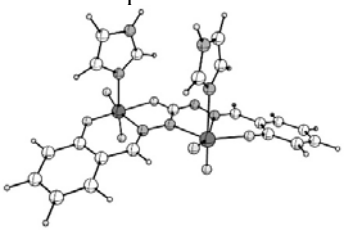
Acetonitrile phase



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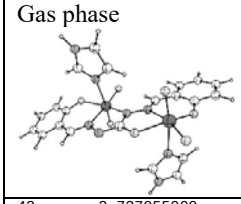
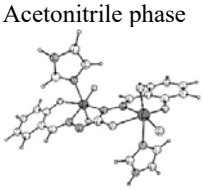
trans-[$(MoO_2)_2(L^1)(Im)_2$]

Gas phase				Acetonitrile phase			
							
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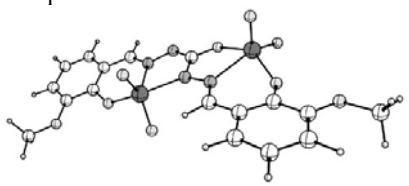
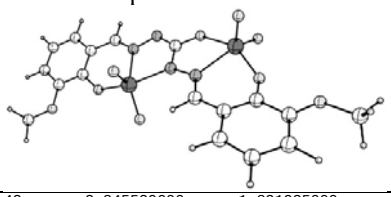
cis-[$(MoO_2)_2(L^5)$]

Gas phase				Acetonitrile phase			
							
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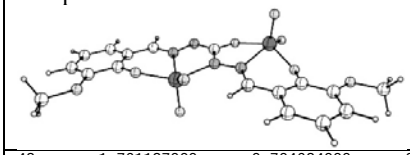
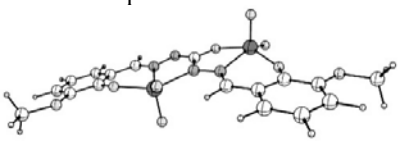
trans-[$(MoO_2)_2(L^5)$]

Gas phase				Acetonitrile phase			
							
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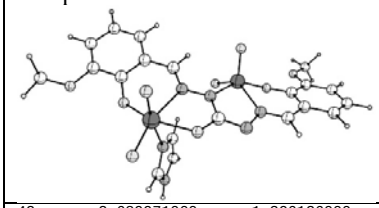
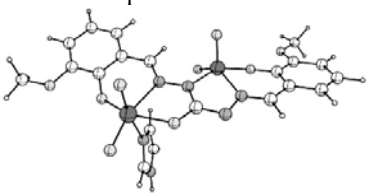
cis-[$(MoO_2)_2(L^5)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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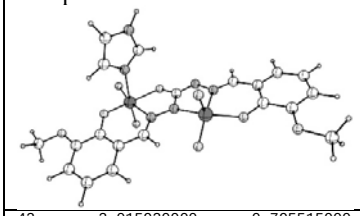
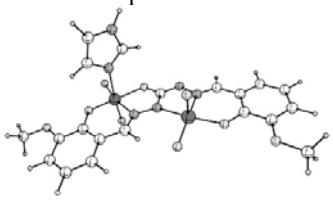
trans-[$(MoO_2)_2(L^5)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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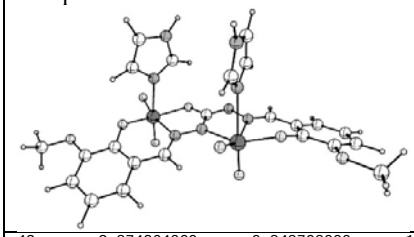
cis-[$(MoO_2)_2(L^5)(Im)_2$]

Gas phase



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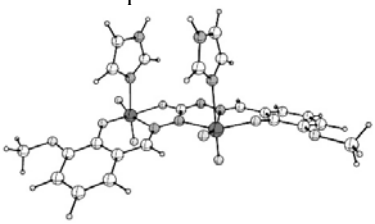
Acetonitrile phase



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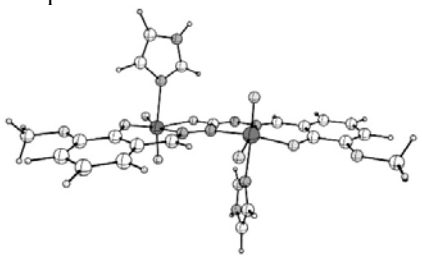
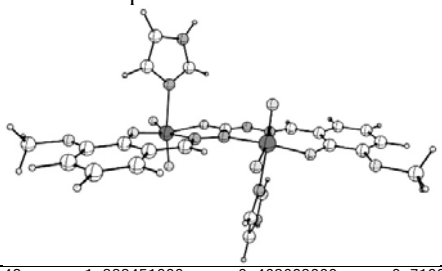
trans-[$(MoO_2)_2(L^5)(Im)_2$]

Gas phase				Acetonitrile phase			
							
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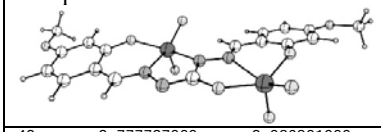
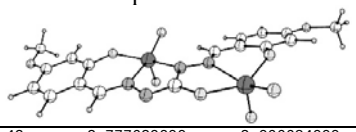
cis-[$(MoO_2)_2(L^6)$]

Gas phase				Acetonitrile phase			
							
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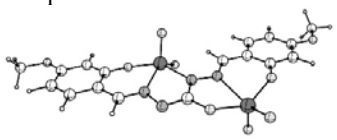
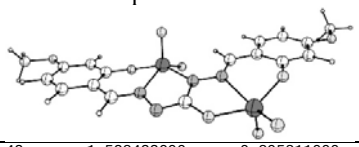
trans-[$(MoO_2)_2(L^6)$]

Gas phase				Acetonitrile phase			
							
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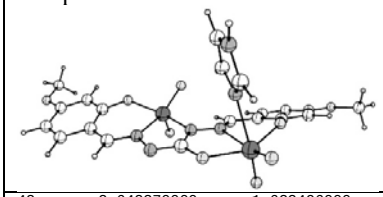
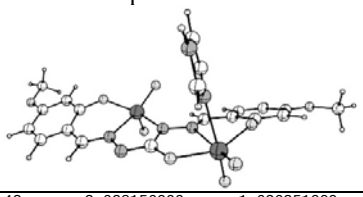
cis-[$(MoO_2)_2(L^6)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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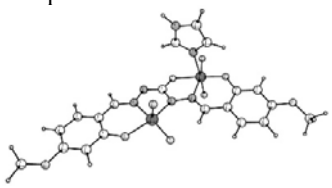
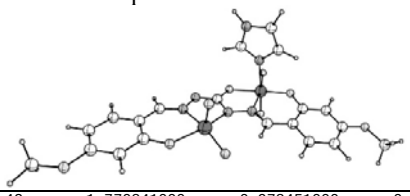
trans-[$(MoO_2)_2(L^6)(Im^{ONO})$]

Gas phase				Acetonitrile phase			
							
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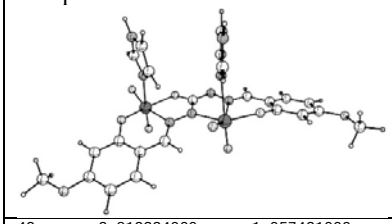
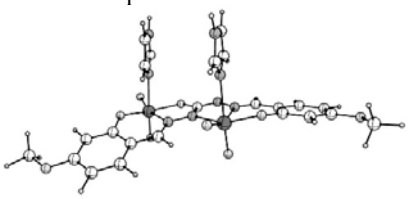
cis-[$(MoO_2)_2(L^6)(Im)_2$]

Gas phase				Acetonitrile phase			
							
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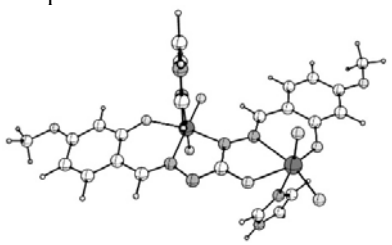
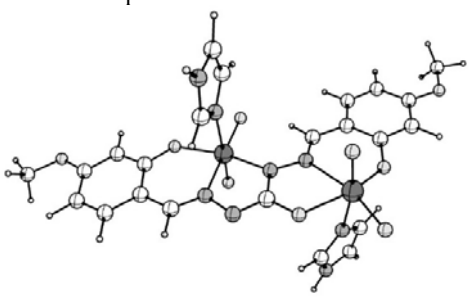
1	2.425803000	3.872313000	0.974095000	1	-2.540200000	-3.893224000	0.599580000
6	-7.094063000	0.214929000	-1.528684000	6	7.153200000	0.208093000	-1.323056000
1	-8.028994000	0.056988000	-2.054831000	1	8.101413000	0.524498000	-1.744706000
6	5.666607000	2.883357000	0.779108000	6	-5.755877000	-2.795345000	0.585111000
6	8.045253000	2.659933000	0.795000000	6	-8.124770000	-2.481091000	0.755638000
1	8.119560000	2.375486000	-0.262053000	1	-8.251718000	-2.074315000	-0.254142000
1	8.889026000	3.299420000	1.059748000	1	-8.975805000	-3.119114000	0.999851000
1	8.064899000	1.754864000	1.415552000	1	-8.062611000	-1.660714000	1.479812000
6	4.555347000	3.714701000	1.027638000	6	-4.663099000	-3.679129000	0.718738000
1	4.725149000	4.717633000	1.403443000	1	-4.849442000	-4.708603000	1.006426000

trans-[$(MoO_2)_2(L^6)(Im)_2$]

Gas phase	Acetonitrile phase
	

42	1.638666000	-0.683628000	-0.737031000	42	1.642818000	-0.654960000	-0.753273000
42	-2.716666000	1.499334000	1.334292000	42	-2.693289000	1.500680000	1.356308000
8	3.533278000	-1.139066000	-0.660285000	8	3.538390000	-1.089479000	-0.738038000
8	-0.801520000	2.111750000	1.389082000	8	-0.804713000	2.159044000	1.337111000
8	0.884984000	-2.197127000	-1.026649000	8	0.884813000	-2.163380000	-1.073311000
8	-4.127290000	0.655459000	0.287136000	8	-4.136403000	0.584719000	0.448602000
8	1.590690000	0.167361000	-2.210079000	8	1.581172000	0.216645000	-2.225075000
7	-0.045301000	0.298981000	0.144898000	7	-0.045695000	0.320836000	0.129723000
7	2.360159000	1.093602000	0.481795000	7	2.364767000	1.125534000	0.442787000
8	-2.665299000	0.422452000	2.652768000	8	-2.533531000	0.448056000	2.697903000
7	1.712222000	-1.602566000	1.585311000	7	1.778632000	-1.607580000	1.509465000
7	1.419349000	1.894483000	1.094573000	7	1.416159000	1.938943000	1.037738000
7	-1.395581000	0.014535000	0.083538000	7	-1.398465000	0.028391000	0.090912000
8	-3.449983000	2.926348000	1.897957000	8	-3.441351000	2.917819000	1.954885000
7	1.628236000	-1.907361000	3.763372000	7	2.140474000	-2.019126000	3.640648000
1	1.552731000	-1.693474000	4.747306000	1	2.399822000	-1.870899000	4.609371000
7	-2.466351000	2.674240000	-0.811526000	7	-2.619383000	2.624978000	-0.794186000
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6	-3.231613000	-1.397632000	-0.637325000	6	-3.234436000	-1.399859000	-0.610040000
6	-1.835453000	-1.031753000	-0.538792000	6	-1.844240000	-1.012365000	-0.539814000
1	-1.121093000	-1.707387000	-1.006211000	1	-1.137492000	-1.670340000	-1.041230000
6	1.664890000	-0.996550000	2.759880000	6	2.195827000	-1.091963000	2.661222000
1	1.639719000	0.071710000	2.918942000	1	2.528762000	-0.078345000	2.820024000
6	5.850803000	-1.080523000	-1.006978000	6	5.862305000	-1.037731000	-1.047592000
6	4.686621000	-0.472756000	-0.539710000	6	4.697125000	-0.428781000	-0.589346000
6	1.702533000	-2.958612000	1.846166000	6	1.442332000	-2.924538000	1.777847000
1	1.721737000	-3.676866000	1.041125000	1	1.068637000	-3.575070000	1.002156000
6	3.593914000	1.488182000	0.598888000	6	3.598803000	1.526398000	0.557870000
1	3.751749000	2.423460000	1.138884000	1	3.764116000	2.464990000	1.088110000
6	4.750367000	0.808775000	0.077964000	6	4.754700000	0.844442000	0.044812000
6	-3.542946000	-2.642243000	-1.215170000	6	-3.542459000	-2.626161000	-1.233091000
1	-2.724137000	-3.273972000	-1.550487000	1	-2.725017000	-3.223011000	-1.629297000
6	1.650148000	-3.167723000	3.197411000	6	1.663754000	-3.193427000	3.101646000
1	1.623178000	-4.067198000	3.792268000	1	1.529791000	-4.085313000	3.694404000
6	-4.313689000	-0.576168000	-0.212457000	6	-4.318335000	-0.626633000	-0.109771000
6	7.089788000	-0.441352000	-0.877150000	6	7.105591000	-0.405115000	-0.889277000
6	-5.901069000	-2.269420000	-0.929810000	6	-5.897148000	-2.323464000	-0.837669000
6	-5.627670000	-1.018869000	-0.364311000	6	-5.627231000	-1.089573000	-0.226906000
6	-4.847861000	-3.092689000	-1.363880000	6	-4.841530000	-3.099357000	-1.351621000
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6	6.012046000	1.419070000	0.200598000	6	6.019398000	1.449002000	0.195071000
1	6.070987000	2.395953000	0.674575000	1	6.073381000	2.418649000	0.682951000
7	-1.705005000	4.035407000	-2.361669000	7	-2.091059000	4.042903000	-2.389425000
1	-1.094813000	4.684922000	-2.836097000	1	-1.591921000	4.766523000	-2.894511000
6	7.175440000	0.822739000	-0.266166000	6	7.185794000	0.852782000	-0.260692000
1	8.124349000	1.332555000	-0.155186000	1	8.136343000	1.354288000	-0.127909000
6	-3.334494000	2.655268000	-1.884094000	6	-3.535471000	2.501252000	-1.824668000
1	-4.222785000	2.043622000	-1.867639000	1	-4.353670000	1.799953000	-1.772572000
6	-2.875054000	3.495975000	-2.861096000	6	-3.216416000	3.379277000	-2.825548000
1	-3.258112000	3.752662000	-3.836298000	1	-3.672362000	3.587378000	-3.781383000
6	-1.496462000	3.515273000	-1.127310000	6	-1.762317000	3.568412000	-1.169816000
1	-0.653473000	3.764066000	-0.500695000	1	-0.918251000	3.919881000	-0.597354000
1	-6.445235000	-0.384909000	-0.040071000	1	-6.445927000	-0.487294000	0.152952000
1	5.796540000	-2.058011000	-1.472472000	1	5.812123000	-2.011580000	-1.523212000
8	-7.218277000	-2.593749000	-1.022257000	8	-7.202142000	-2.674715000	-0.889010000
6	-7.570063000	-3.851614000	-1.579261000	6	-7.555247000	-3.921366000	-1.497069000
1	-7.231591000	-3.940557000	-2.619683000	1	-7.261360000	-3.945193000	-2.552540000
1	-7.156800000	-4.681603000	-0.991876000	1	-7.100377000	-4.765483000	-0.966330000
1	-8.660131000	-3.895680000	-1.549330000	1	-8.641992000	-3.987309000	-1.421562000
8	8.153644000	-1.128158000	-1.369373000	8	8.168574000	-1.087959000	-1.368376000
6	9.444050000	-0.541330000	-1.279544000	6	9.473167000	-0.513576000	-1.235954000
1	9.494263000	0.406099000	-1.831242000	1	9.546982000	0.434003000	-1.781473000
1	9.736129000	-0.369339000	-0.235601000	1	9.732713000	-0.356475000	-0.183045000
1	10.129192000	-1.259795000	-1.732564000	1	10.159516000	-1.239823000	-1.674754000

References

[1] For the graph-set analysis of hydrogen-bonding patterns see for example: a) M. C. Etter, J. MacDonald and J. Bernstein, *Acta Cryst.,* 1990, **B46**, 256; b) J. Bernstein, R. E. Davis, L. Shimoni and N.L. Chang *Angew. Chem. Int. Ed Eng.* 1995, **34**, 1555.