SUPPORTING INFORMATION

Towards a global Greener process: From Solvent-Less Synthesis of Molybdenum(VI) ONO Schiff Base Complexes to catalyzed olefins epoxidation under organic-solvent-free conditions .

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Figure S17. Mercury rendered crystal packing patterns in complexes **2a, 3, 6, 7, 9**. Hydrogen bonds are denoted as orange dashed lines (for detailed metrical parameteres of hydrogen bonds see **Table S7**).

a) Formation of centrosymmetric puckered 15-membered ring *via* C13-H13···O2 intermolecular hydrogen bond in **3**. Assembling with supramolecular 8-membered hydrogen bonded ring into infinite puckered ribbons of rings in the alternating AB manner.

b) The chains in **2a** are cross over interlinked *via* C-H···O type of intermolecular hydrogen bonds between methanol solvent molecule and C4A-H4A phenyl group. The C7A-H7A···O2A intermolecular hydrogen bond additionally supported infinite 1D chain formation along *a* axis.

c) Assembling of mutually condensed infinite ribbon of alternating AB rings and the ribbon of alternating CD rings in **7**.

acceptor) and O6-H6···O2 (proton donor) intermolecular hydrogen bonds.

d) Bridging of chains in **9** *via* C16-H16···O2 hydrogen bond which form 22-membered hydrogen bonded ring.

Table S4. General and crystallographic data for compounds **2a, 3, 6, 7** and **9** and preliminary data for compound **4**.

Table S5. Selected bond distances (Å) and angles (°) within molybdenum atoms primary coordination sphere (complexes **2a, 3, 6, 7, 9**).

Table S6. Dihderal angles (°) between planes defined by the atoms of equatorial octahedral plane and peripheral rings [I: O1, O3, O4, N1; II: C1 – C6; III: C8 – C13 (or C8 - C17 in **7** and **9**)]

Table S7. Hydrogen bond and interaction geometry (Å,°) for complexes **2a, 3, 6, 7, 9**.

Synthesis of ligands

All ligands were prepared by a) solution method and by b) grinding experiments.

a) Equimolar quantities of aldehyde (1 mmol) and ammine (1 mmol) were refluxed in ethanol for one hour.

b) The manual, neat grinding experiments were performed in an agate mortar. Equimolar quantities of aldehyde (1 mmol) and ammine (1 mmol) were ground for 30 minutes at 20 °C.

The obtained products were characterized by means of chemical analysis, IR spectroscopy and PXRD data.

Table S1 Analytical and spectral data for ligands prepared by a) solution method and b) by grinding

Analysis found (calcd.)						Selected IR data (cm^{-1})		
	Ligands		%C	%H	%N	N − H···O (w, b)	C − N (s)	C = C (s, m)
H_2L^1	$C_{13}H_{11}O_2N$	a	72.99 (73.23)	5.12 (5.20)	6.50 (6.57)	3452, 3440	1633	1596−1504
		b	73.12 (73.23)	5.09 (5.20)	6.47 (6.57)	3451,3439	1628	1592−1501
H_2L^2	$C_{14}H_{13}O_2N$	a	73.92 (73.99)	5.72 (5.76)	6.11 (6.16)	3449,3413	1631	1600−1508
		b	73.98 (73.99)	5.80 (5.76)	6.23 (6.16)	3440,3429	1626	1596−1500
H_2L^3	$C_{14}H_{13}O_2N$	a	73.80 (73.99)	5.78 (5.76)	6.16 (6.16)	3447,3429	1639	1598−1523
		b	73.95 (73.99)	5.72 (5.76)	6.21 (6.16)	3446,3429	1638	1598−1521
H_2L^4	$C_{14}H_{15}O_2N$	a	73.20 (73.23)	6.61 (6.59)	6.10 (6.11)	3442,3437	1634	1593−1521
		b	73.09 (73.23)	6.52 (6.59)	6.02 (6.11)	3442,3430	1632	1594−1520
H_2L^5	$C_{15}H_{15}O_2N$	a	74.59 (74.67)	6.20 (6.27)	5.82 (5.80)	3448,3418	1627	1598−1516
		b	74.48 (74.67)	6.18 (6.27)	5.65 (5.80)	3440,3421	1631	1601−1523
H_2L^6	$C_{15}H_{15}O_2N$	a	74.51 (74.67)	6.09 (6.27)	5.80 (5.80)	3454,3426	1636	1578−1522
		b	74.41 (74.67)	6.25 (6.27)	5.70 (5.80)	3455,3425	1636	1577−1530
H_2L^7	$C_{17}H_{13}O_2N$	a	76.99 (77.56)	5.00 (4.98)	5.13 (5.32)	3443,3427	1634	1567−1529
		b	77.45 (77.56)	4.78 (4.98)	5.35 (5.32)	3432,3411	1637	1562−1518
H_2L^8	$C_{18}H_{15}O_2N$	a	77.82 (77.96)	5.44 (5.45)	4.98 (5.05)	3441,3422	1635	1560−1520
		b	77.90 (77.96)	5.36 (5.45)	5.00 (5.05)	3442,3430	1632	1557−1524
H_2L^9	$C_{18}H_{15}O_2N$	a	77.88 (77.96)	5.38 (5.45)	5.12 (5.05)	3439,3421	1628	1549−1515
		b	77.91 (77.96)	5.40 (5.45)	4.92 (5.05)	3437,3421	1624	1559−1509

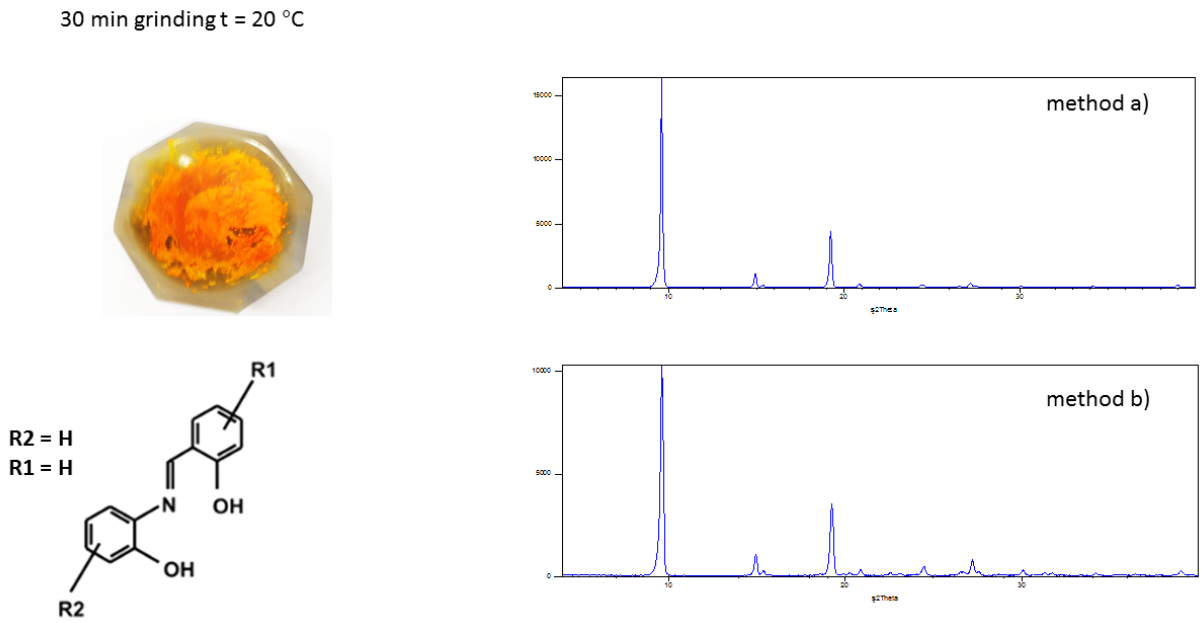


Figure S1: Ligand H_2L^1 prepared by a) solution method b) grinding

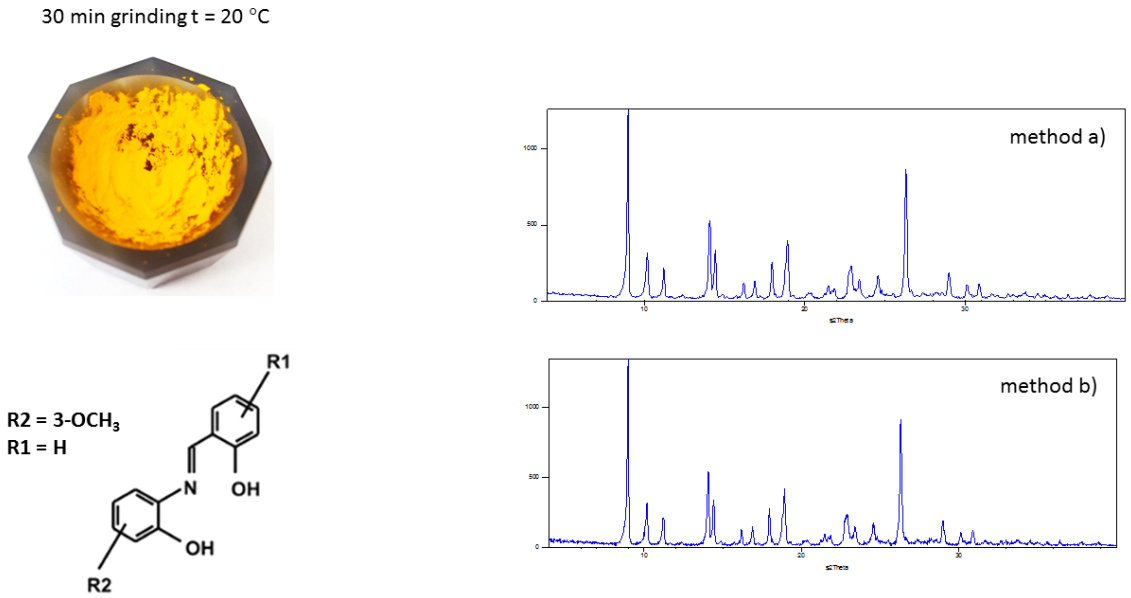


Figure S2: Ligand H_2L^4 prepared by a) solution method b) grinding

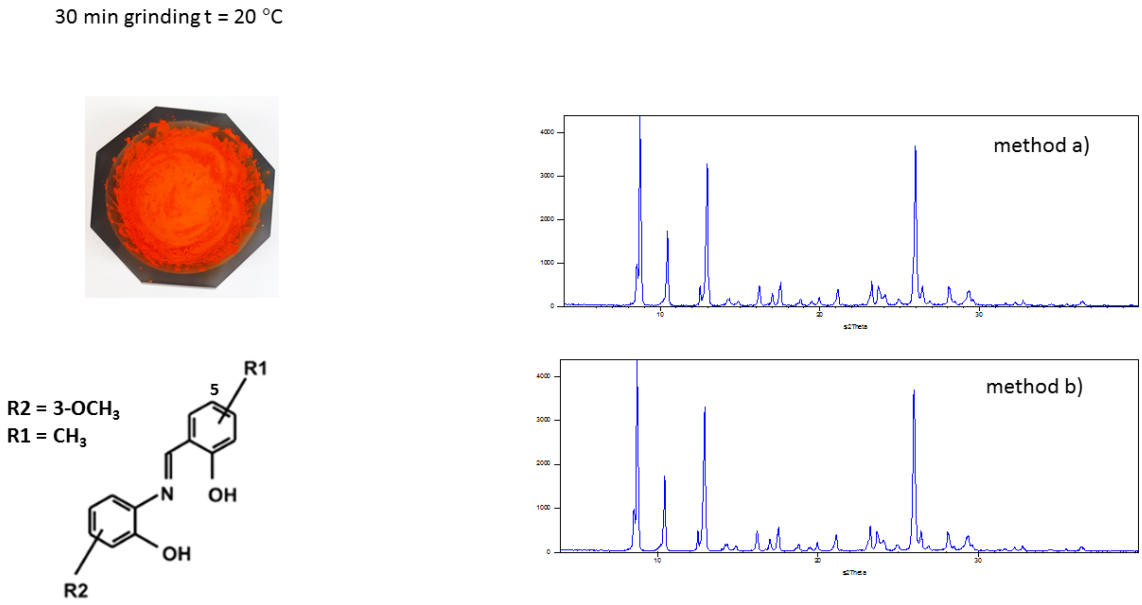


Figure S3: Ligand H_2L^5 prepared by a) solution method b) grinding

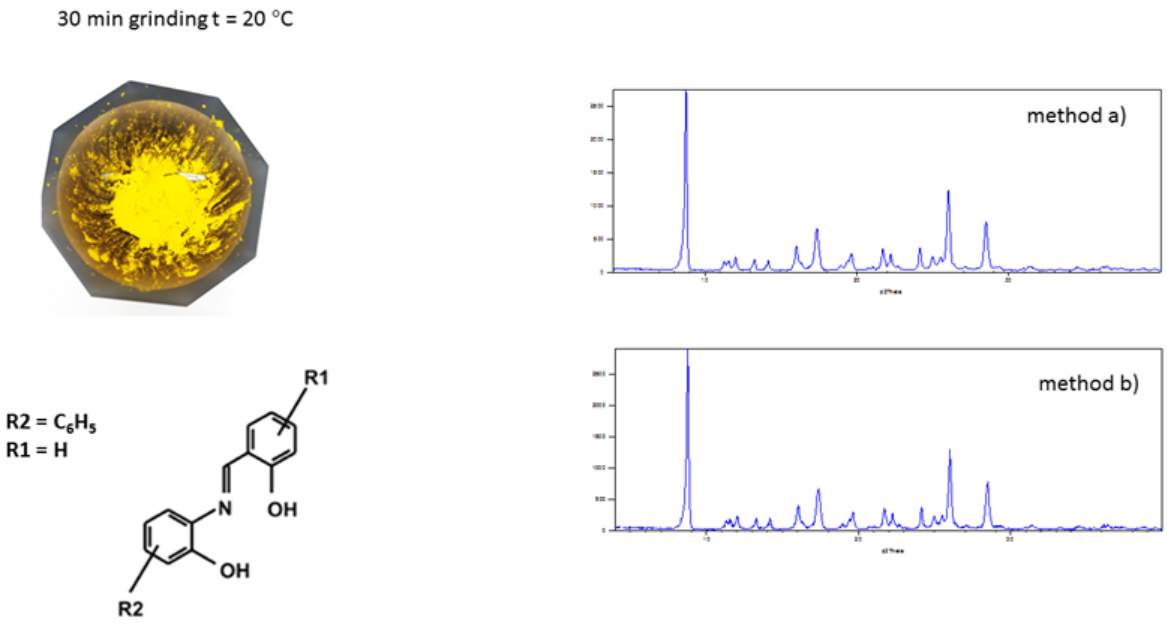
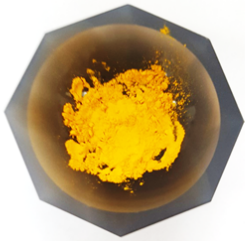
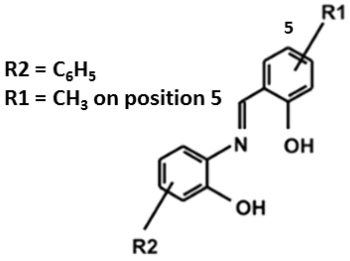
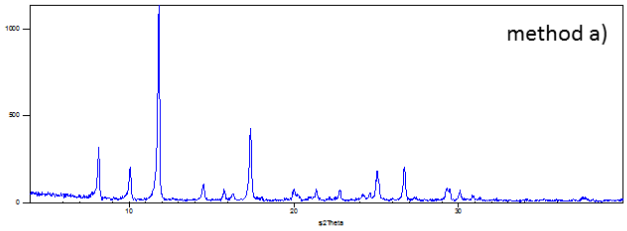


Figure S4: Ligand H_2L^7 prepared by a) solution method b) grinding

30 min grinding t = 20 °C







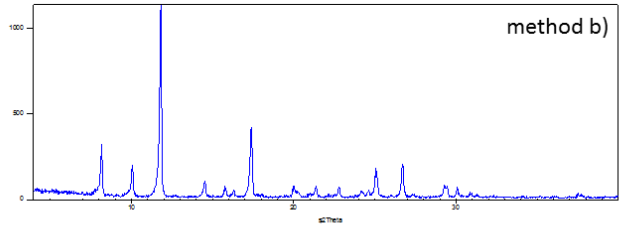
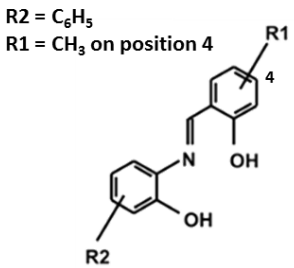
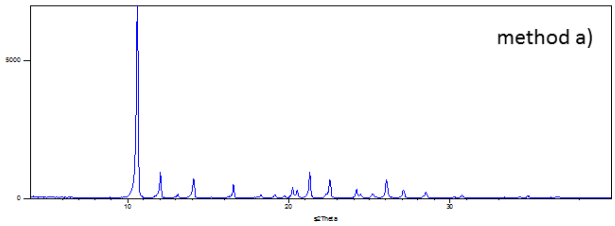


Figure S5: Ligand H_2L^8 prepared by a) solution method b) grinding

30 min grinding t = 20 °C





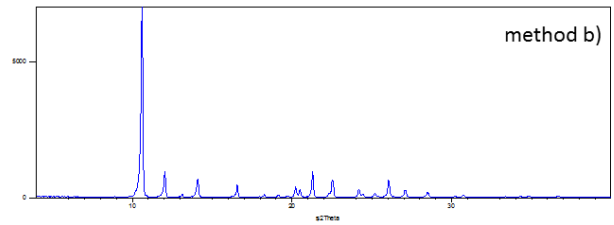


Figure S6: Ligand H_2L^9 prepared by a) solution method b) grinding

Thermal analysis

Table S2 Results of thermal analysis of Mo(VI) complexes prepared by two synthetic methods

		First step		Second step	
Method	Complexes	ω(CH_3OH) % exp./calcd.	$t_{init.}$-$t_{fin.}$ °C	ω(Mo) % exp./(calcd)	$t_{init.}$-$t_{fin.}$ °C
a)	$[MoO_2L^1(CH_3OH)]$	8.50/8.59	64 – 158	25.58/25.71	271 – 586
b)	$[MoO_2L^1(CH_3OH)]$	8.56/8.59	69 – 142	25.58/24.71	222 – 600
a)	$[MoO_2L^2(CH_3OH)]$	9.12/8.32	42 – 110	24.74/24.91	287 – 561
b)	$[MoO_2L^2(CH_3OH)]$	8.05/8.32	53 – 180	23.88/24.91	228 – 546
a)	$[MoO_2L^{2a}(CH_3OH)]\cdot CH_3OH$	15.15/15.35	53 – 117	22.74/22.99	300 – 538
a)	$[MoO_2L^3(CH_3OH)]\cdot CH_3OH$	14.15/15.35	38 – 169	21.81/22.99	245 – 545
b)	$[MoO_2L^3(CH_3OH)$	8.13/8.32	43 – 193	22.96/24.91	191 – 551
a)	$[MoO_2L^4(CH_3OH)]$	7.79/7.93	60 – 123	23.48/23.73	218 – 123
b)	$[MoO_2L^4]_2$		65 – 580*	22.98/25.98	
a)	$[MoO_2L^5(CH_3OH)]$	7.56/7.31	43 – 154	21.88/23.10	159 – 551
b)	$[MoO_2L^5(CH_3OH)]$	7.39/7.71	40 – 143	21.44/23.10	143 – 553
a)	$[MoO_2L^6(CH_3OH)]\cdot CH_3OH$	13.03/14.33	52 – 143	21.71/21.45	223 – 531
b)	$[MoO_2L^6(CH_3OH)]$	7.84/7.71	46 – 155	23.60/23.10	234 – 556
a)	$[MoO_2L^7(CH_3OH)]$	7.99/8.35	48 – 125	21.94/22.77	283 – 514
b)	$[MoO_2L^7]_2$		53 – 538*	22.64/23.79	
a)	$[MoO_2L^8]_2$		266 – 514*	23.39/23.79	
b)	$[MoO_2L^8]_2$		246 – 525*	22.95/23.79	
a)	$[MoO_2L^9(CH_3OH)]\cdot CH_3OH$	13.13/13.69	50 – 232	19.86/20.53	230 – 552
b)	$[MoO_2L^9(CH_3OH)]$	7.61/7.36	48 – 150	24.15/22.05	149 – 528

IR Spectroscopy

All complexes were characterized by IR spectroscopyand results are compared to the literature data.[i,ii]

Table S3 Selected bands from the IR spectra of prepared complexes (**1-9**) by solution method a) and by grinding b)

Selected IR data (cm^{-1})					
	complexes	method	C = N	Mo − O	Mo − O ⋯ Mo
1	$[MoO_2L^1(CH_3OH)]$	a	1616	935, 934	
	$[MoO_2L^1(CH_3OH)]$	b	1611	935, 907	
2	$[MoO_2L^2(CH_3OH)]\cdot CH_3OH$	a	1599	940, 917	
	$[MoO_2L^2(CH_3OH)]$	b	1604	935, 907	
3	$[MoO_2L^2(CH_3OH)]\cdot CH_3OH$	a	1613	946, 911	
	$[MoO_2L^2(CH_3OH)]$	b	1614	934, 896	
4	$[MoO_2L^4(CH_3OH)]$	a	1609	949, 926	
	$[MoO_2L^4]_2$	b	1625		816, 750
5	$[MoO_2L^5(CH_3OH)]$	a	1614	949, 926	
	$[MoO_2L^5(CH_3OH)]$	b	1617	931,899	
6	$[MoO_2L^6(CH_3OH)]\cdot CH_3OH$	a	1615	965, 899	
	$[MoO_2L^6(CH_3OH)]$	b	1624	935, 902	
7	$[MoO_2L^7(CH_3OH)]$	a	1609	980, 934	
	$[MoO_2L^7]_2$	b	1590		812, 742
8	$[MoO_2L^8]_2$	a	1619		863, 774
	$[MoO_2L^8]_2$	b	1619		824, 767
9	$[MoO_2L^9(CH_3OH)]\cdot CH_3OH$	a	1631	900, 885	
	$[MoO_2L^9(CH_3OH)]$	b	1619	942, 900	

[1] K. Yamanuchi, S. Yamada, *Inorg. Chim. Acta,* 1974, **9**, 161; W. E. Hill, N. Atabay, C. A. McAuliffe, F. P. McCoullough, S. M. Rozohi, *Inorg. Chim Acta,* 1979, **35**, 35.

[1] J. R. Dilworth, C. A. McAuliffe, B. J. Sayle, *J. Chem. Soc., Dalton Trans.,* 1977, 849.

PXRD for Mo(VI) complexes prepared by two methods a) solution-based synthesis and b) liquid-assisted mechanosynthesis

In order to monitor the efficacy of mechanochemical synthesis (LAG) in preparation of (method b) and to qualitatively identify the products powder X-ray diffraction (PXRD) experiments were performed on a PHILIPS PW 1840 X-ray diffractometer with $CuK_{\alpha 1}$(1.54056 Å) radiation at 40 mA and 40 kV. The scattered intensities were measured with a scintillation counter. The angular range (2θ) was from 5 to 45 ° with steps of 0.02 ° and the measuring time was 0.5 s per step.
The obtained PXRD patterns were compared with those generated from SCXRD data.

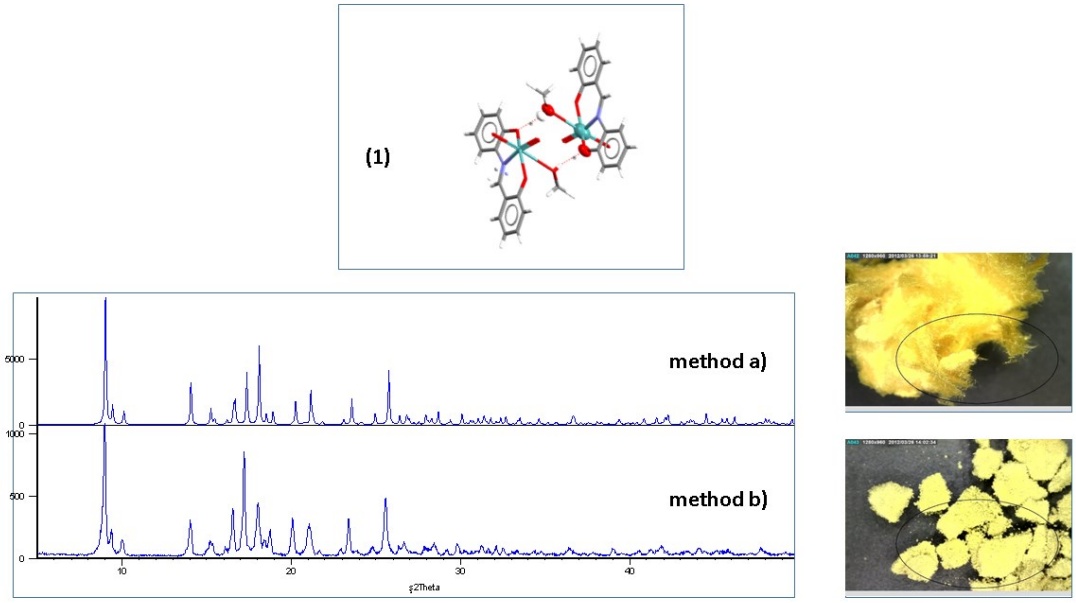


Figure S7: a) $[MoO_2L^1(CH_3OH)]$ (generated from SCXRD) and b) $[MoO_2L^1(CH_3OH)]$

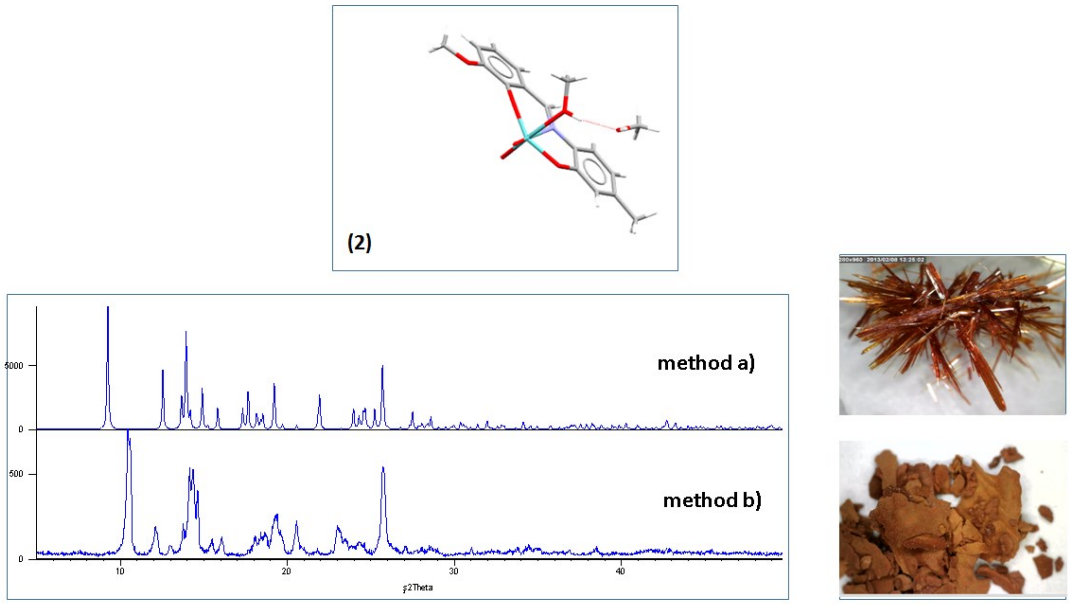


Figure S8: a) $[MoO_2L^2(CH_3OH)]$ (generated from SCXRD) and b) $[MoO_2L^2(CH_3OH)]$

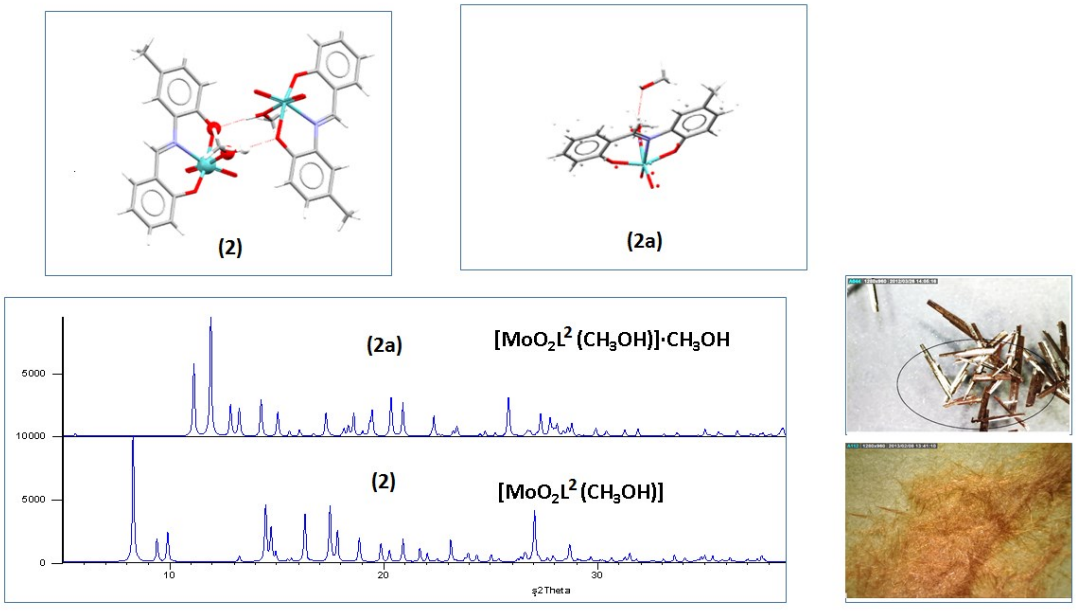


Figure 8a: a) $[MoO_2L^2(CH_3OH)] \cdot CH_3OH$ (generated from SCXRD) (2a) and b) $[MoO_2L^2(CH_3OH)]$

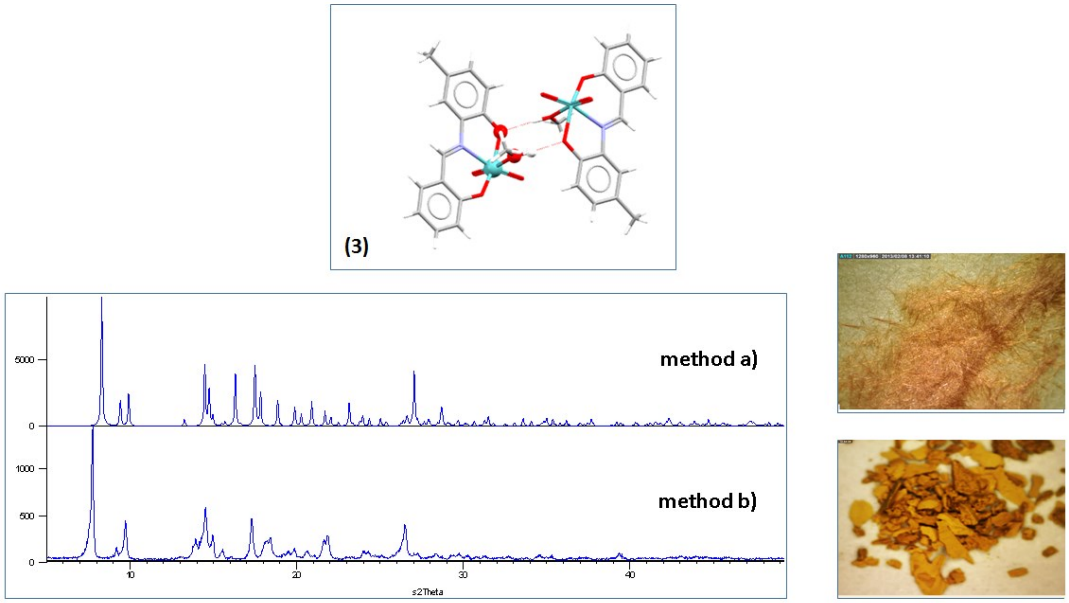


Figure S9: a) $[MoO_2L^3(CH_3OH)] \cdot CH_3OH$ (generated from SCXRD) and b) $[MoO_2L^3(CH_3OH)]$

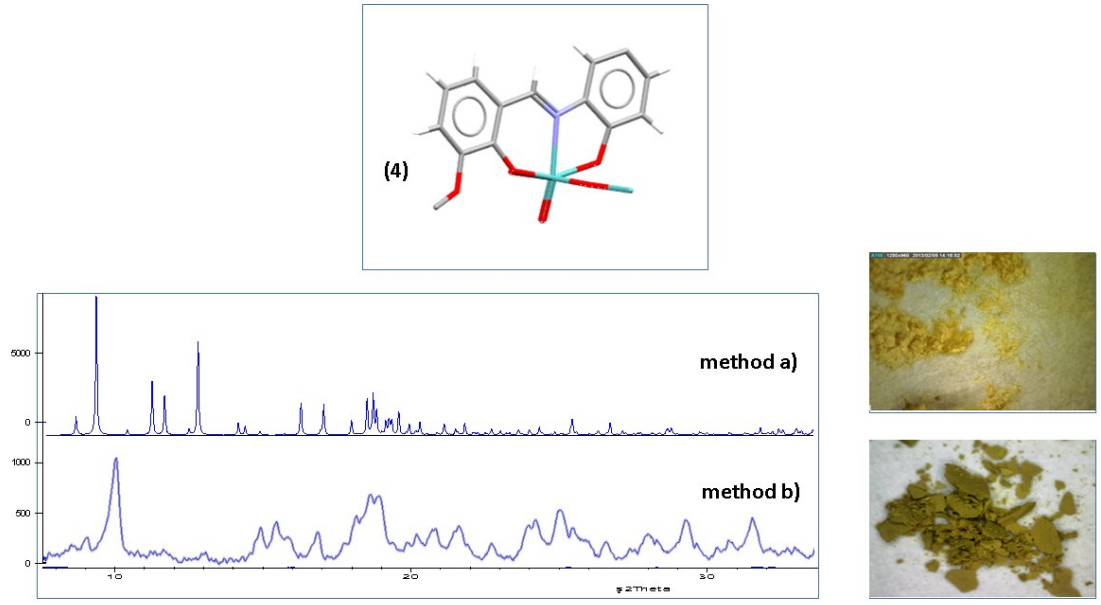


Figure S10: $[MoO_2L^4(CH_3OH)]$ (generated from SCXRD) and $[MoO_2L^4]_2$

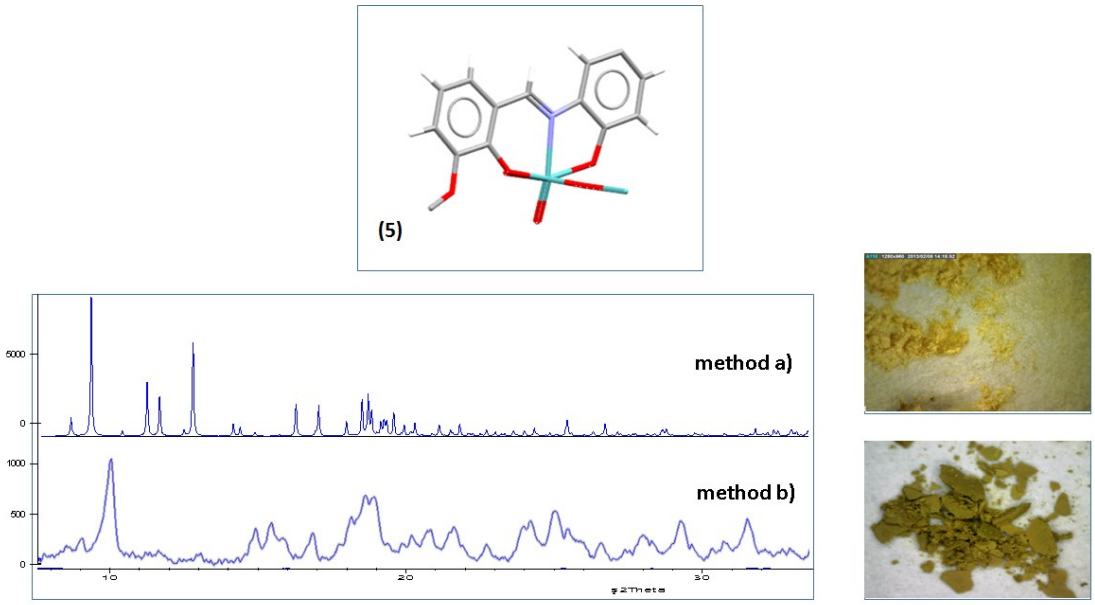


Figure S11: a) $[MoO_2L^5(CH_3OH)]$ (generated from SCXRD) and b) $[MoO_2L^5(CH_3OH)]$

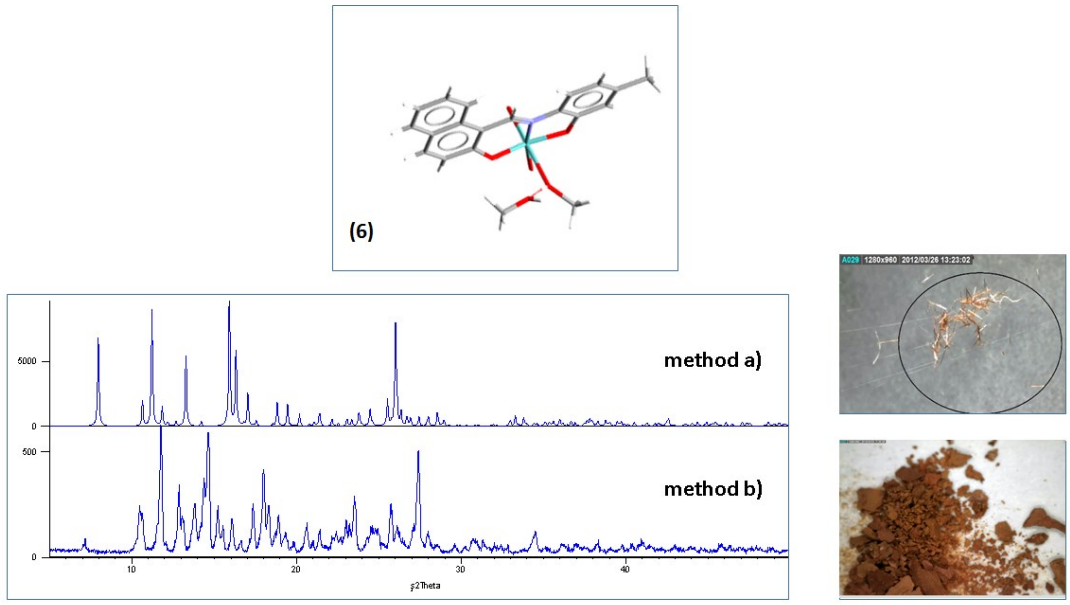


Figure S12: a) $[MoO_2L^6(CH_3OH)] \cdot CH_3OH$ (generated from SCXRD) and b) $[MoO_2L^6(CH_3OH)]$

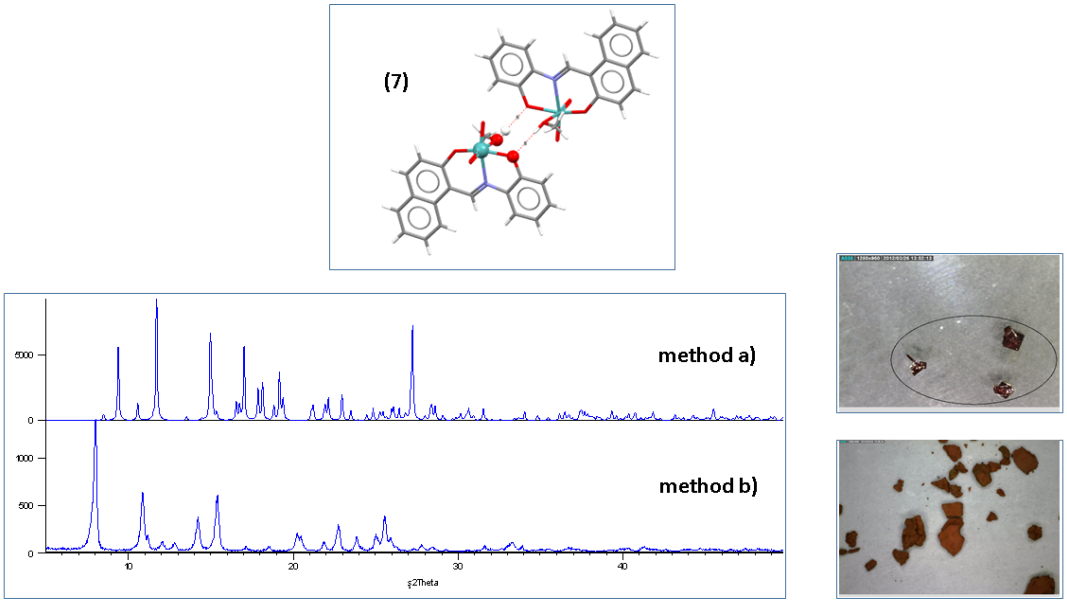


Figure S13: $[MoO_2L^7(CH_3OH)]$ (generated from SCXRD) and $[MoO_2L^7]_2$

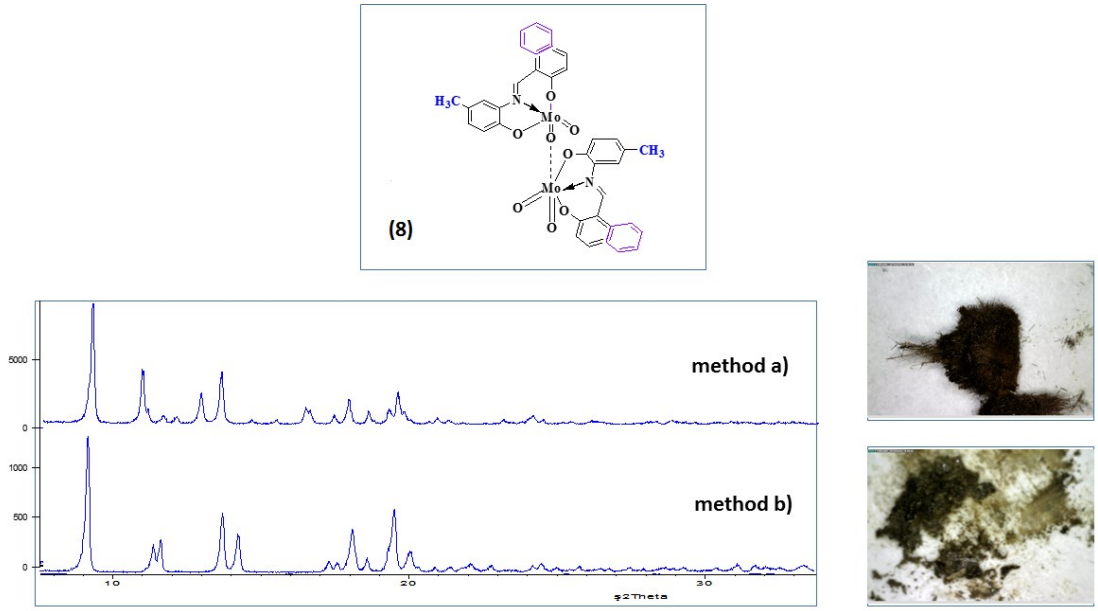


Figure S14: a) and b) $[MoO_2L^8]_2$

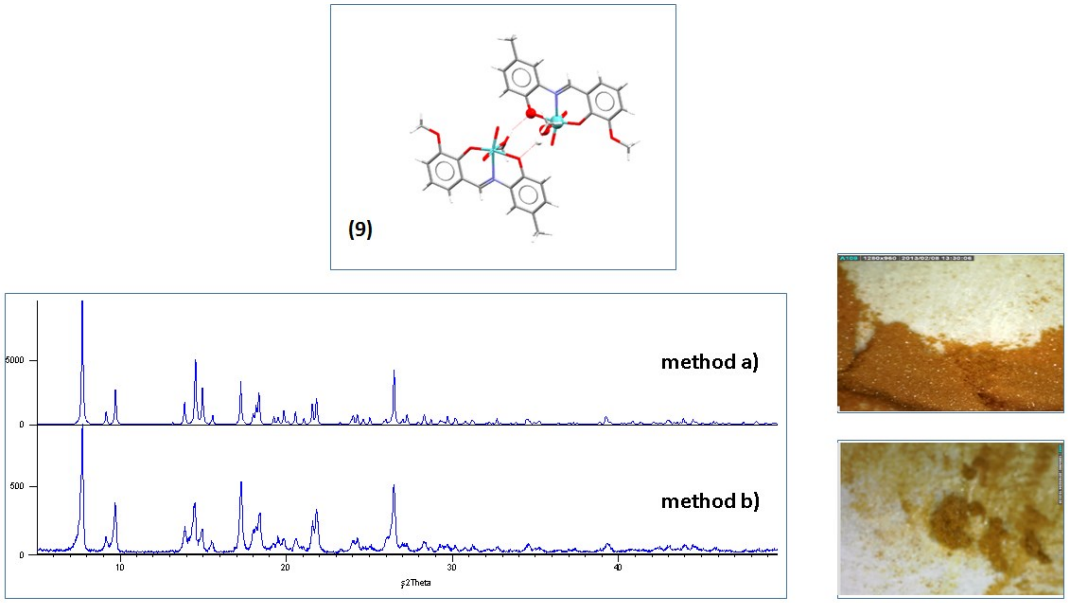
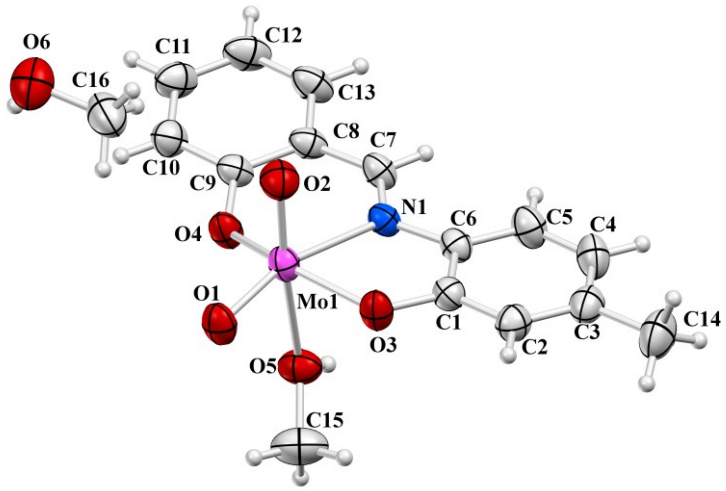


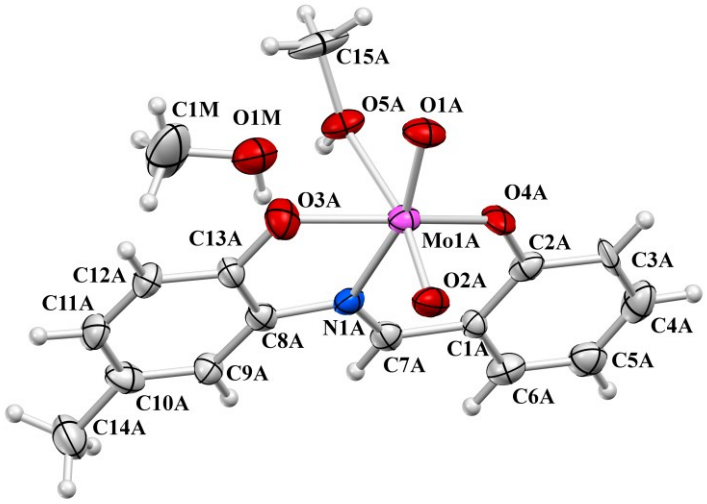
Figure S15: a) $[MoO_2L^9(CH_3OH)] \cdot CH_3OH$ (generated from SCXRD) and b) $[MoO_2L^9(CH_3OH)]$

Exp_2552_3



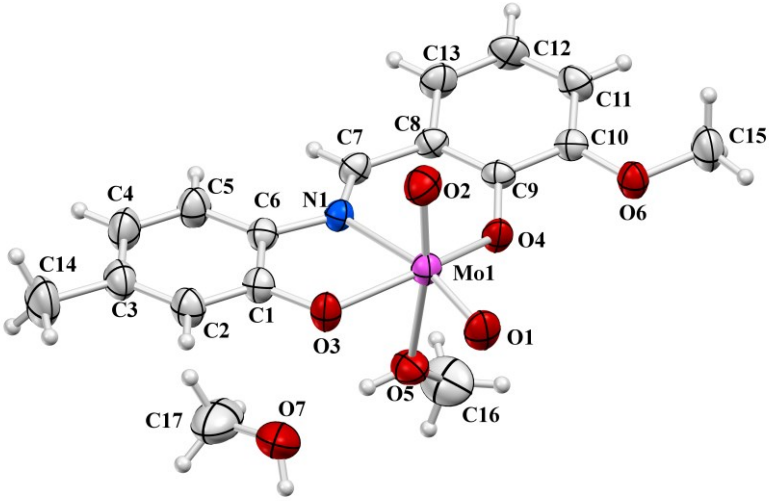
a)

Exp_2879_2a



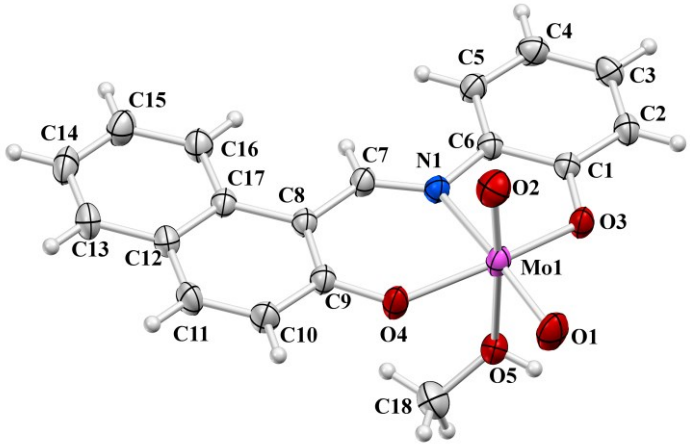
b)

Exp_2550_6



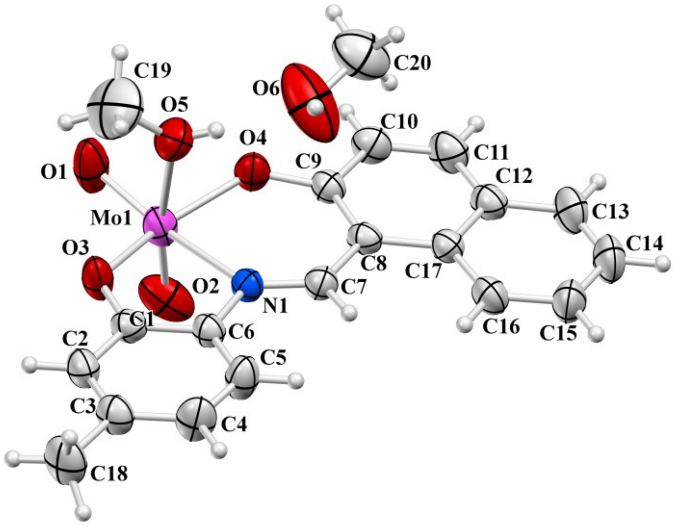
c)

Exp_2545_7



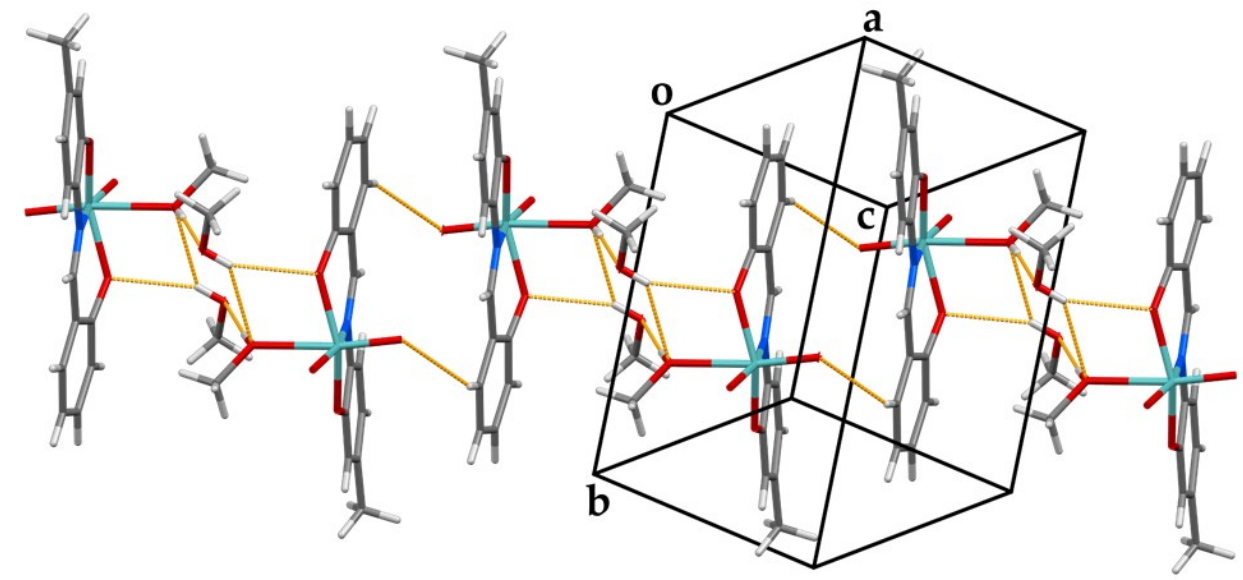
d)

Exp_2608_9

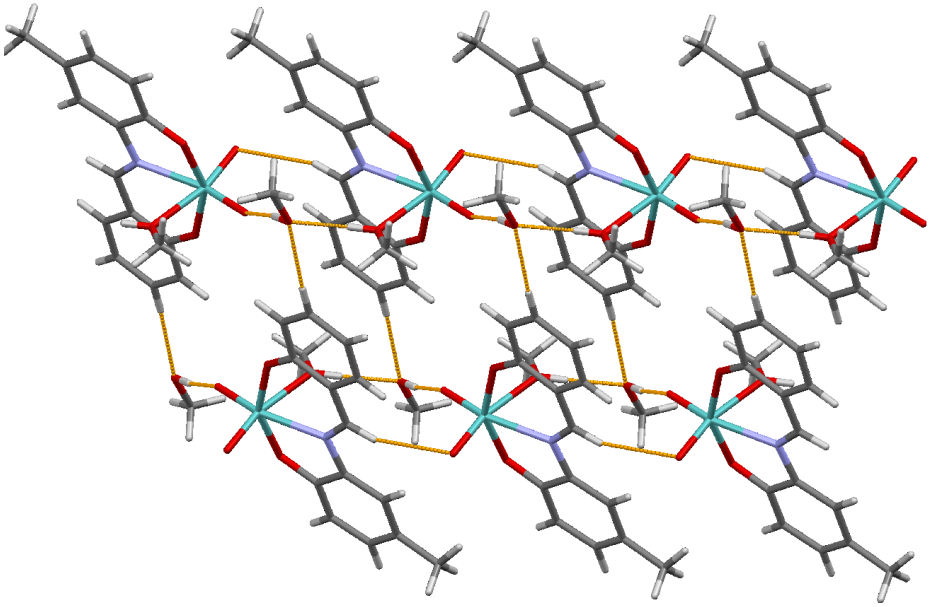


e)

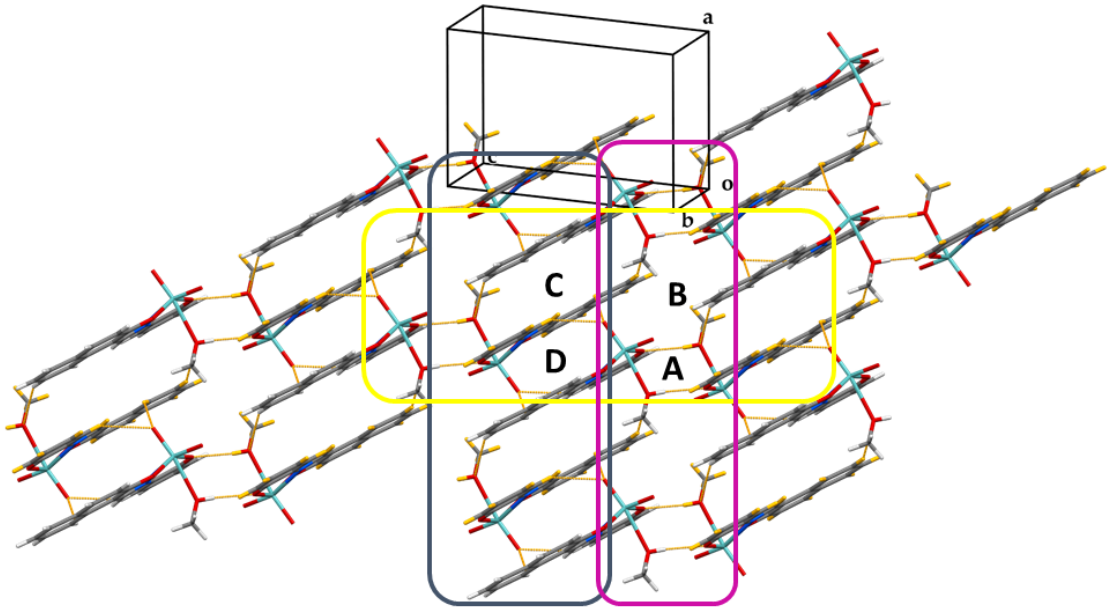
Figure S16. a) – e) Mercury rendered ORTEP view of the asymmetric unit of the complexes **2a, 3, 6, 7, 9** with the analogous atom-numbering scheme for all complexes. For complex **2a** (b) only major component A is shown. Displacement ellipsoids are drawn at the 50% probability level (296(2) K). Hydrogen atoms are presented as spheres of arbitrary small radii.



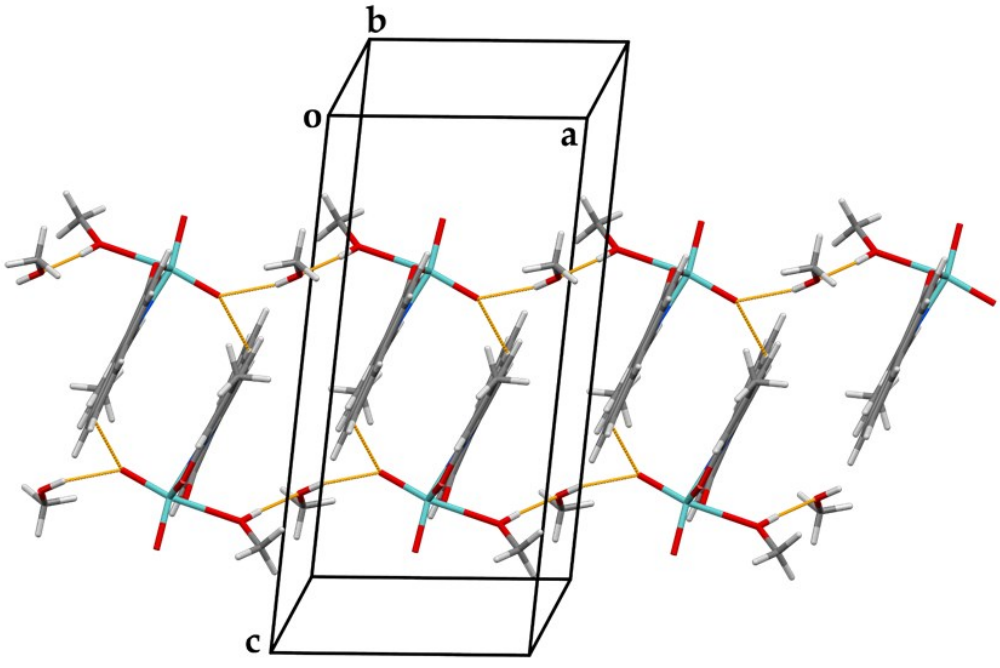
a)



b)



c)



d)

Figure S17. Mercury rendered crystal packing patterns in complexes **2a, 3, 6, 7, 9**. Hydrogen bonds are denoted as orange dashed lines (for detailed metrical parameteres of hydrogen bonds see **Table S7** in ESI).

a) Formation of centrosymmetric puckered 15-membered ring *via* C13-H13···O2 intermolecular hydrogen bond in **3**. Assembling with supramolecular 8-membered hydrogen bonded ring into infinite puckered ribbons of rings in the alternating AB manner.

b) The chains in **2a** are cross over interlinked *via* C-H···O type of intermolecular hydrogen bonds between methanol solvent molecule and C4A-H4A phenyl group. The C7A-H7A···O2A intermolecular hydrogen bond additionally supported infinite 1D chain formation along *a* axis.

c) Assembling of mutually condensed infinite ribbon of alternating AB rings and the ribbon of alternating CD rings in **7**.

acceptor) and O6-H6···O2 (proton donor) intermolecular hydrogen bonds.

d) Bridging of chains in **9** *via* C16-H16···O2 hydrogen bond which form 22-membered hydrogen bonded ring.

Table S4. General and crystallographic data for compounds **2a, 3, 6, 7, 9**.

[a] $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; [b] $w = 1/[\sigma^2(F_o^2) + (g_1P)^2 + g_2P]$ where $P = (F_o^2 + 2F_c^2)/3$
[c] $wR = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ [d] $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(N_r - N_p)\}^{1/2}$ where N_r = number of independent reflections, N_p = number of refined parameter.

	2a_2879	**3_2552**	**6_2550**	**7_2545**	**9_2608**
Brutto chemical formula	$C_{16}H_{19}MoNO_6$	$C_{16}H_{19}MoNO_6$	$C_{17}H_{21}MoNO_7$	$C_{18}H_{15}MoNO_5$	$C_{20}H_{21}MoNO_6$
Moiety formula	$C_{15}H_{15}MoNO_5\times CH_3OH$	$C_{15}H_{15}MoNO_5\times CH_3OH$	$C_{16}H_{17}MoNO_6\times CH_3OH$	$C_{16}H_{17}MoNO_6$	$C_{19}H_{17}MoNO_5\times CH_3OH$
M_r	417.27	417.26	447.29	421.25	467.32
Crystal system, color and habit	Monoclinic, dark red needle	Triclinic, orange prismatic block	Monoclinic, dark red-brown hexagonal prism	Triclinic, dark red tetragonal prism	Monoclinic, dark red plate
Crystal dimensions (mm^3)	0.48 × 0.18 × 0.15	0.44 × 0.32 × 0.15	0.57 × 0.41 × 0.26	0.32 × 0.28 × 0.25	0.27 × 0.21 × 0.19
Space group	$P\,2_1/n$	$P\,\bar{1}$	$P\,2_1/c$	$P\,\bar{1}$	$P\,2_1/c$
Z	4	2	4	2	4
a /Å	6.9126(14)	8.7538(5)	19.6100(7)	7.6444(5)	7.9476(13)
b /Å	7.6578(15)	10.0269(5)	7.5974(4)	9.9107(5)	14.9809(14)
c /Å	31.895(6)	10.7193(6)	12.7835(5)	11.0535(6)	16.765(3)
α /°	90	97.063(4)	90	82.196(5)	90
β /°	92.22(3)	111.466(5)	102.178(4)	82.196(5)	96.268(19)
γ /°	90	95.831(4)	90	88.111(5)	90
V /Å^3	1687.1(6)	857.95(8)	1861.70(15)	789.61(8)	1984.1(5)
ρ(calculated) / g cm^{-3}	1.643	1.615	1.596	1.772	1.564
T /K	296(2)	296(2)	296(2)	296(2)	296(2)
Reflections collected, unique, R_{int}, observed [$I \geq 2\sigma(I)$]	11403 3635(0.031), 2890	8408 4985(0.0190), 3858	10356 5409(0.023), 3797	7922 4590(0.0142), 4029	7285 4084(0.0366), 2347
R_1[a] [$I \geq 2\sigma(I)$]	0.0321	0.0281	0.0303	0.0229	0.0393
wR_2[b] (all data)	0.0699	0.0593	0.0744	0.0654	0.0811
Goodness of fit on F^2, S[c]	1.045	0.924	0.894	1.053	0.85
Max., and min. electron density (e Å^{-3})	0.264, −0.337	0.345, −0.367	0.587, −0.422	0.384, −0.509	0.417, −0.485

Preliminary crystallographic data data for compound **4**: Space group P $2_1/n$; a /Å = 15.564; b /Å = 21.594; c /Å = 3.768 β /° = 95.56

Table S5. Selected bond distances (Å) and angles (°) within molybdenum atoms primary coordination sphere (complexes **2a, 3, 6, 7, 9**).

	2a	**3**	**6**	**7**	**9**
			Bond distances		
Mo1=O_t[2]	1.722(6)	1.6944(12)	1.6924(14)	1.6973(13)	1.686(2)
	1.698(10)	1.6920(14)	1.7035(17)	1.7023(15)	1.701(3)
Mo1-N1	2.245(7)	2.2830(14)	2.3046(16)	2.2697(13)	2.274(3)
Mo1-O3[3]	1.952(4)	1.9550(12)	1.9591(14)	1.9802(12)	1.943(2)
Mo1-O4[4]	1.932(6)	1.9553(13)	1.9358(14)	1.9317(12)	1.926(2)
Mo1-D[5]	2.281(12)	2.3548(15)	2.3091(17)	2.4087(14)	2.314(3)
			Bond angles		
O1=Mo1=O2	104.6(5)	106.00(7)	105.79(8)	105.69(7)	106.36(14)
O_t =Mo1-O3	95.7(2)	96.64(6)	97.62(7)	95.55(6)	96.74(11)
	98.5(3)	100.92(7)	99.00(8)	100.70(6)	99.47(12)
O_t =Mo1-O4	101.6(2)	100.65(6)	101.30(7)	101.75(6)	101.26(11)
	96.8(3)	97.80(6)	98.76(8)	99.84(6)	97.22(12)
O_t =Mo1-N1	161.0(3)	161.10(6)	164.37(8)	161.43(7)	161.14(13)
	93.4(5)	92.29(6)	89.00(7)	91.98(6)	92.01(11)
O_t =Mo1-D	86.2(4)	83.27(6)	87.11(8)	84.28(6)	84.80(13)
	167.7(5)	170.08(6)	166.98(7)	169.96(5)	168.67(11)

[1] The values for compound **2a** is given for major component A. The corresponding distance values in component B are: 1.691(13) and 1.708(8) Å; 2.286(9) Å; 1.945(7) Å; 1.939(8) Å; 2.418(16) Å. The corresponding angle values are: 105.2(6)°; 96.3(3)°; 99.2(4)°; 102.0(3)°; 96.6(4)°; 159.8(4)°; 94.3(6)°; 82.3(5)°; 169.5(6)°; [2] O_t - terminal oxido oxygen atoms O1 and O2; [3] O3 – the hydroxy oxygen atom from imino *N*-substituent part of the ligand; [4] O4 – the phenolate oxygen atom from aldiminato part of the ligand; [5] D - monodentate neutral Lewis base *i.e.* its donor atom (O from CH_3OH in all complexes).

Table S6. Dihderal angles (°) between planes defined by the atoms of equatorial octahedral plane and peripheral rings [I: O1, O3, O4, N1; II: C1 – C6; III: C8 – C13 (or C8 - C17 in **7** and **8**)]

Compound	∠I,II	∠II, III
2a*	0.5(2)	4.5(2)
3	7.07(11)	10.23(14)
5	1.36(8)	11.67(11)
7	2.43(8)	2.27(7)
8	6.11(15)	6.06(14)

*Calculated for the major component A of disordered complex molecule.

Table S7. Hydrogen bond and interaction geometry (Å,°) for complexes **2a**, **3**, **6, 7, 9**.

D–H···A	D–H	H···A	D···A	∠D–H···A	Symmetry code
			3		
O5- H1O5···O6	0.77(2)	1.88(2)	2.645(2)	173(3)	−1+x,y,z
O6- H1O6···O4	0.79(2)	2.37(2)	3.113(2)	157(3)	1−x,1−y,−z
O6- H1O6···O5	0.79(2)	2.43(3)	3.004(2)	131(3)	1−x,1−y,−z
C12-H12···O3	0.93	2.570	3.442(2)	157	x,−1+y,z
C10 -H10···O4	0.93	2.957	3.877(3)	170	−x+1,−y+1,−z
C11-H11···O1	0.93	2.810	3.392(3)	122	−x+1,−y+1,−z
C10-H10···O1	0.93	2.650	3.309(3)	128	−x+1,−y+1,−z
C14 -H14···O1	0.96	2.828	3.523(3)	130	−x+1,−y+2,−z+1
C2-H2···O2	0.93	2.805	3.667(2)	155	−x+1,−y+2,−z+1
C7-H7···O2	0.93	2.724	3.418(3)	132	−x+1,−y+1,−z+1
C13-H13···O2	0.93	2.654	3.391(3)	137	−x+1,−y+1,−z+1
C12-H12···O1	0.93	2.685	3.446(3)	137	x,+y−1,+z
			2a*		
O1M-H1M···O1A	0.66(4)	2.14(4)	2.795(6)	167(5)	−1+x,y,z
O5A-H5AA···O1M	0.82(1)	1.74(1)	2.544(13)	166(1)	-
C3A-H3A···O4A	0.93	2.919	3.816(10)	163(1)	−x+1,−y+1,−z
C4A-H4A···O1M	0.93	2.724	3.651(9)	174(1)	−x,-y+1, −z
C6A-H6A···O2A	0.93	2.752	3.583(12)	149(1)	x−1,+y,+z
C7A-H7A···O2A	0.93	2.590	3.469(13)	158	−1+x,y,z
C9A-H9A···O2A	0.93	2.918	3.830(12)	167(1)	x−1,+y,+z

			6		
O5- H1O5···O7	0.82(2)	1.82(2)	2.624(3)	169	–
O7- H1O7···O2	0.83(3)	1.94(3)	2.747(3)	165	x,–1+y,z
C12- H12···O6	0.93	2.540	3.456(3)	167	x,3/2–y,–1/2+z
C16 -H16A ···O1	0.96	2.873	3.708(4)	146	x,–y+1/2+1,+z+1/2
C5-H5···O3	0.93	2.677	3.367(3)	132	x,–y+1/2+1,+z+1/2
C11-H11···O6	0.93	2.967	3.564(3)	123	–x,+y+1/2,–z+1/2
C15-H15B···O4	0.96	2.642	3.539(3)	156	–x,–y+2,–z
C15-H15B···O6	0.96	2.787	3.438(3)	126	–x,–y+2,–z
			7		
O5-H1O5···O3	0.77(2)	1.99(2)	2.761(2)	175(2)	–x,2–y,–z
C5-H5··· O2	0.93	2.60	3.436(2)	150	–x,2–y,1–z
C3-H3···O1	0.93	2.845	3.636(2)	144	x,+y+1,+z
C4-H4···O4	0.93	2.769	3.668(2)	163	x,+y+1,+z
C16-H16···O2	0.93	2.605	3.394(2)	143	–x,–y+2,–z+1
C5-H5···O2	0.93	2.600	3.435(2)	150	–x,–y+2,–z+1
C7-H7···O2	0.93	2.923	3.717(3)	144	–x,–y+2,–z+1
C11-H11···O2	0.93	2.816	3.474(2)	129	–x,–y+1,–z+1
C10-H10···O2	0.93	2.958	3.540(2)	122	–x,–y+1,–z+1
C14-H14···O1	0.93	2.729	3.513(3)	143	x–1,+y,+z+1
C15-H15···O5	0.93	2.630	3.478(3)	152	–x–1,–y+2,–z+1
C18-H18C···O2	0.96	2.844	3.524(3)	129	x–1,+y,+z
			9		
O5-H1O5···O6	0.80(3)	1.81(3)	2.609(5)	176(3)	–
O6-H1O6···O2	0.81(5)	1.88(4)	2.665(4)	163(6)	–1+x,y,z
C10-H10···O3	0.93	2.550	3.440(4)	160	1–x,1/2+y,1/2–z
C11- H11···O1	0.93	2.570	3.350(4)	142	1–x,1/2+y,1/2–z
C16-H16··· O2	0.93	2.520	3.278(4)	139	1–x,–y,1–z
C5-H5···O2	0.93	2.895	3.643(5)	138	–x+1,–y,–z+1
C7-H7···O2	0.93	2.880	3.652(5)	141	–x+1,–y,–z+1
C14-H14 ···O5	0.93	2.784	3.689(5)	165	x,–y+1/2,+z+1/2
C18-H18C···O1	0.96	2.617	3.576(5)	177	–x+1,+y–1/2,–z+1/2

*Calculated for the major component A of disordered complex molecule.