Supplementary Material (ESI) for Soft Matter

Rigid Tetracatenar Liquid Crystals Derived from 1,10-Penanthroline

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Supporting Information

1. NMR and IR Data

Benzaldehyde 1a

δ_H (300 MHz, $CDCl_3$): 0.91 (t, 6H, CH_3), 1.35-1.49 (m, 12H, CH_2), 1.80-1.89 (m, 4H, C**H**$_2$-CH_2-O), 4.04-4.11 (m, 4H, CH_2-O), 6.97 (d, 1H, H-aryl, J_o = 7.9 Hz), 7.40-7.43 (m, 2H, H-aryl), 9.84 (s, 1H, CH=O).

Dibromo Vinylic Compound 2a

Yellow oil. Yield: 57%. δ_H (300 MHz, $CDCl_3$): 0.90 (t, 6H, CH_3), 1.26-1.49 (m, 12H, CH_2), 1.77-1.86 (m, 4H, C**H**$_2$-CH_2-O), 3.97-4.02 (m, 4H, CH_2-O), 6.85 (d, 1H, H-aryl, J_o = 8.3 Hz), 7.04 (dd, 1H, H-aryl, J_o = 8.3 Hz, J_m = 1.3 Hz), 7.18 (d, 1H, H-aryl, J_m = 1.3 Hz), 7.38 (s, 1H, CH=CBr_2).

Acetylene 3a

δ_H (300 MHz, $CDCl_3$): 0.90 (t, 6H, CH_3), 1.33-1.48 (m, 12H, CH_2), 1.76-1.85 (m, 4H, C**H**$_2$-CH_2-O), 2.98 (s, 1H, C=C-H), 3.95-4.01 (m, 4H, CH_2-O), 6.80 (d, 1H, H-aryl, J_o = 8.3 Hz), 6.99 (d, 1H, H-aryl, J_m = 1.3 Hz), 7.04 (dd, 1H, H-aryl, J_o = 8.3 Hz, J_m = 1.3 Hz).

Alkyne 4a

δ_H (300 MHz, $CDCl_3$): 0.27 (s, 9H, CH_3), 0.85-0.95 (m, 6H, CH_3), 1.36-1.49 (m, 12H, CH_2), 1.80-1.89 (m, 4H, C**H**$_2$-CH_2-O), 3.98-4.05 (m, 4H, CH_2-O), 6.86 (d, 1H, H-aryl, J_o = 8.3 Hz), 7.05 (d, 1H, H-aryl, J_m = 2.1 Hz), 7.09 (dd, 1H, H-aryl, J_o = 8.3 Hz, J_m = 2.1 Hz), 7.45 (s, 4H, H-aryl).

Acetylene 5a

δ_H (300 MHz, $CDCl_3$): 0.91 (t, 6H, CH_3), 1.34-1.50 (m, 12H, CH_2), 1.78-1.87 (m, 4H, C**H**$_2$-CH_2-O), 3.18 (s, 1H, C≡C-H), 4.01 (t, 4H, CH_2-O), 6.84 (d, 1H, H-aryl, J_o = 8.3 Hz), 7.03 (s, 1H, H-aryl), 7.08 (d, 1H, H-aryl, J_o = 8.3 Hz), 7.45 (s, 4H, H-aryl).

Ligand 6a

δ_H (400 MHz, $CDCl_3$): 0.91-0.93 (m, 12H, CH_3), 1.36-1.50 (m, 24H, CH_2), 1.79-1.87 (m, 8H, C**H**$_2$-CH_2-O), 4.02 (t, 8H, CH_2-O), 6.85 (d, 2H, H-aryl, J_o = 8.3 Hz), 7.05 (s, 2H, H-aryl), 7.10 (d, 2H, H-aryl, J_o = 8.3 Hz), 7.52-7.60 (m, 8H, H-aryl), 7.81 (s, 2H, H-aryl), 8.38 (d, 2H, H-aryl, J_m = 1.6 Hz), 9.29 (d, 2H, H-aryl, J_m = 1.6 Hz). δ_C (100 MHz, $CDCl_3$): 13.97, 22.58, 25.67, 29.21, 31.56, 69.21, 69.36, 87.46, 88.00, 92.28, 113.38, 114.99, 116.84, 119.74, 121.72, 124.39, 125.15, 126.90, 128.13, 131.48, 131.72, 138.01, 144.55, 148.87, 150.10, 152.43.

Rhenium(I) Complex 7a

δ_H (400 MHz, $CDCl_3$): 0.92-0.94 (m, 12H, CH_3), 1.33-1.51 (m, 24H, CH_2), 1.76-1.85 (m, 8H, C**H**$_2$-CH_2-O), 3.96-4.03 (m, 8H, CH_2-O), 6.82 (d, 2H, H-aryl, J_o = 8.3 Hz), 7.00-7.03 (m, 4H, H-aryl), 7.44-7.52 (m, 8H, H-aryl), 7.86 (s, 2H, H-aryl), 8.30 (s, 2H, H-aryl), 9.36 (s, 2H, H-aryl). δ_C (100 MHz, $CDCl_3$): 13.98, 22.58, 25.66, 25.70, 29.18, 29.25, 31.59, 69.18, 69.40, 85.50, 87.31, 93.01, 97.05, 113.28, 114.71, 116.82, 120.32, 122.61, 125.29, 127.83, 130.17, 131.54, 131.96, 138.94, 144.86, 148.86, 150.25, 154.85, 188.49, 196.23. IR (KBr-pellet, cm^{-1}): 3441 (m, ν(N–H)), 2953, 2926, 2856 (s, aliphatic C–H stretch), 2018, 1920, 1896 (s, ν(CO)).

2. Yields and CHN Analysis Results

Precursors

Compound	*n*	Yield (%)
1a	6	70
1b	8	90
1c	10	87
1d	12	82
1e	14	75
2a	6	57
2b	8	61
2c	10	62
2d	12	55
2e	14	59
3a	6	73
3b	8	76
3c	10	69
3d	12	71
3e	14	79
4a	6	55
4b	8	67
4c	10	62
4d	12	61
4e	14	69
5a	6	74
5b	8	71
5c	10	80
5d	12	69
5e	14	74

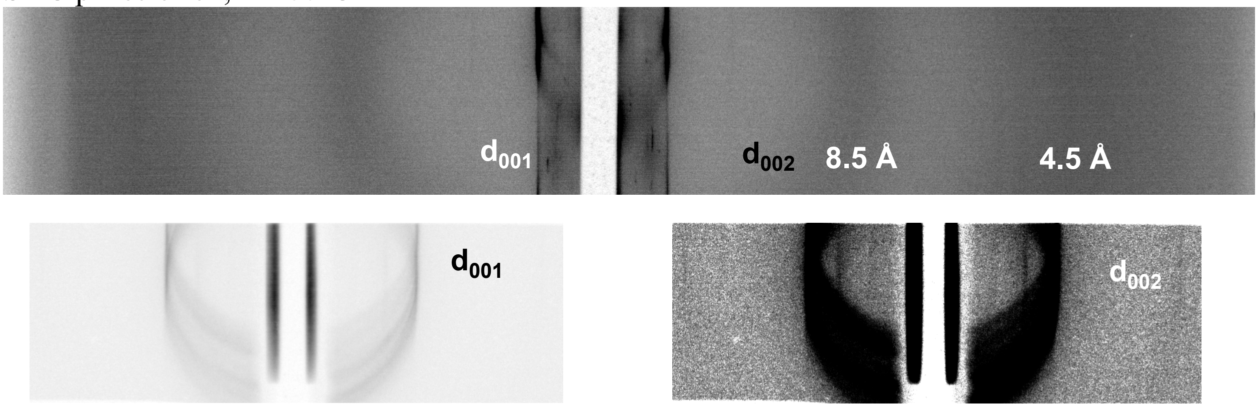
Ligands and Corresponding Metal Complexes

				Analysis (%)[a]		
Compound	*n*	Molecular Formula	Yield (%)	C	H	N
6a	6	$C_{68}H_{72}N_2O_4 \cdot H_2O$	75	82.2 (81.7)	7.8 (7.5)	2.8 (2.8)
6b	8	$C_{76}H_{88}N_2O_4 \cdot H_2O$	71	82.6 (82.1)	8.6 (8.2)	2.5 (2.5)
6c	10	$C_{84}H_{104}N_2O_4 \cdot H_2O$	76	82.6 (82.4)	8.6 (8.7)	2.3 (2.3)
6d	12	$C_{92}H_{120}N_2O_4 \cdot H_2O$	78	82.4 (82.7)	9.4 (9.2)	2.0 (2.1)
6e	14	$C_{100}H_{136}N_2O_4 \cdot H_2O$	74	82.6 (82.9)	9.9 (9.6)	1.9 (1.9)
7a	6	$C_{71}H_{72}BrN_2O_7Re \cdot H_2O$	60	62.9 (63.1)	5.6 (5.5)	2.1 (2.1)
7b	8	$C_{79}H_{88}BrN_2O_7Re \cdot H_2O$	54	64.9 (64.9)	6.4 (6.2)	1.9 (1.9)
7c	10	$C_{87}H_{104}BrN_2O_7Re$	55	67.2 (67.2)	7.2 (6.7)	1.8 (1.8)
7d	12	$C_{95}H_{120}BrN_2O_7Re \cdot H_2O$	52	67.8 (67.7)	7.4 (7.5)	1.7 (1.7)
7e	14	$C_{103}H_{136}BrN_2O_7Re \cdot H_2O$	53	68.8 (68.8)	8.1 (7.7)	1.6 (1.6)

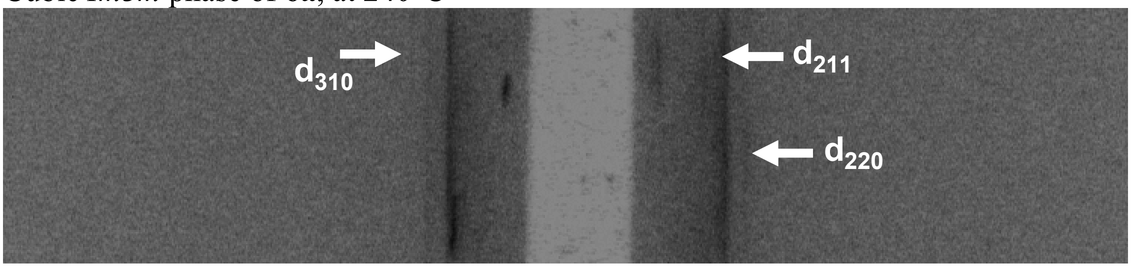
[a] Calculated values in parentheses

3. Image plates of the principal mesophases shown by the ligands 6a-6e, recorded on two different set-ups

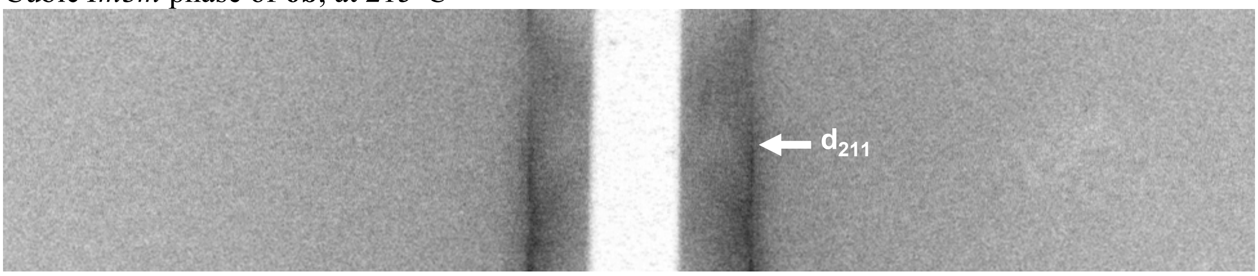
SmC phase of **6a**, at 180°C



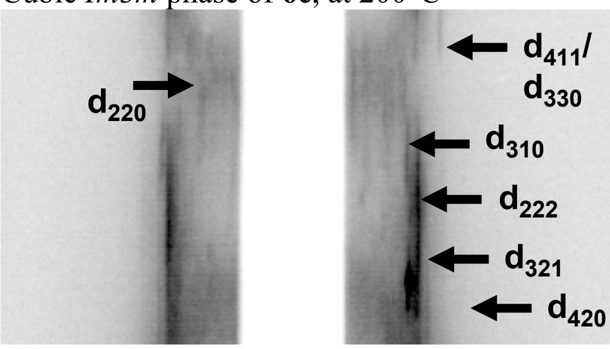
Cubic *Im*3*m* phase of **6a**, at 240°C



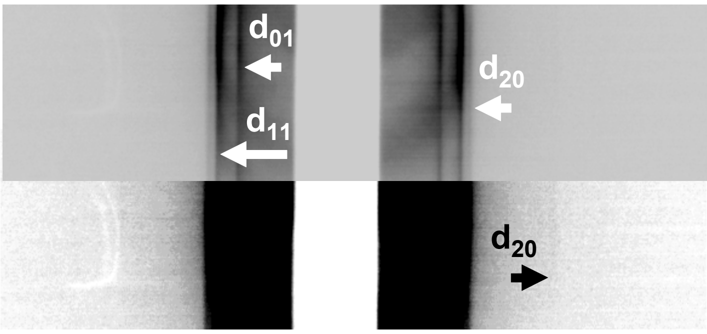
Cubic *Im*3*m* phase of **6b**, at 215°C



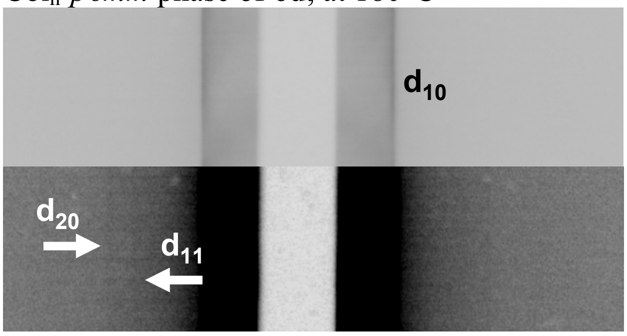
Cubic *Im*3*m* phase of **6c**, at 200°C



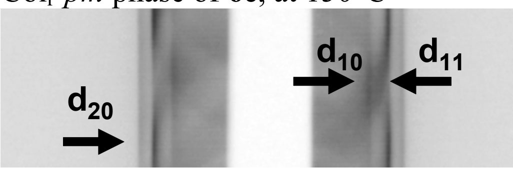
Col$_r$-*pm* phase of **6d**, at 140°C



Col$_h$-*p*6*mm* phase of **6d**, at 180°C



Col$_r$-*pm* phase of **6e**, at 150°C



Col$_h$-*p*6*mm* phase of **6e**, at 200°C