

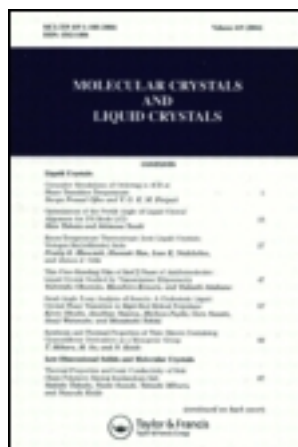
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Molecular Crystals and Liquid Crystals

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Heterocycles derivatives

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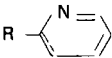
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HETEROCYCLES DERIVATIVES

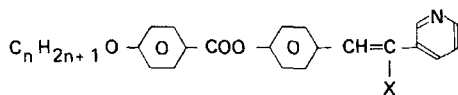
- 2-substituted pyridins



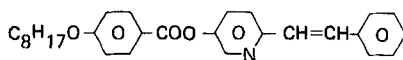
R	K ₂	K ₁	S ₃	S _B (1)	S _A (1)	N (1)	i	Ref.
CH ₃ O-  -COO-  -CH=CH-	-	• 151 6.11	-	-	-	• 179 0.07	•	5
C ₈ H ₁₇ O-  -COO-  -CH=CH-	• 92 4.40	• 112 2.34	-	-	-	• 153 0.14	•	5
CH ₃ O-  -  -N=CH-	-	• 116.8 4.89	-	-	-	• 118.8 0.47	•	36, 1, 83
C ₈ H ₁₇ O-  -  -N=CH-	-	• 82 3.10	• 112.5 0.33	• 116 1.34	• 119.5 0.16	• 123.5	•	5

(1) S_B, S_A, N : from textures.

• 3-substituted pyridins

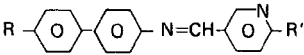


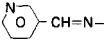
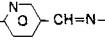
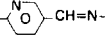
n	X	K ₂		K ₁		N		I	Ref.
1	-CN	•	154 4.59	•	162 3.03	•	194 0.07	•	5
8	-H	—		•	54 7.61	•	65 0.06	•	5
8	-CN	—		•	112 11.66	•	159 0.09	•	5



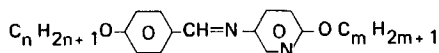
K₂ 49 3.06 K₁ 62 9.96 S_A (1) 64 2.18 I Ref. 5

(1) From texture.



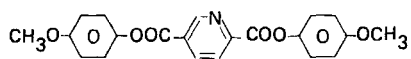
R	R'	K ₂	K ₁	S ₃	S _B (1)	S _A (1)	N	I	Ref.
CH ₃ O	H	—	• 175.7 3.70	—	—	—	• 195.2 0.095	•	36, 1, 83
C ₈ H ₁₇ O	H	—	• 107 6.21	• 164 0.66	• 175 0.39	• 194 2.48	—	•	5
	H	• 144 1.31	• 244 3.86	—	—	—	• 324 0.09	•	5
CH ₃ - 	-CH ₃	• 179	• 215 4.90	—	—	—	• 258 0.14	•	5
CH ₃ O - 	-OCH ₃	• 166 1.11	• 190 8.14	—	—	—	• 267 0.18	•	5

(1) From texture.



n	m	K	S _B	S _A	N	I	Ref.
1	1	• 94 7.73	—	—	—	•	86
4		• 70.6 6.97	—	• 75.0 2.23	—	•	86
6		• 65.0 5.76	• 68.0 0.68	• 78.0 1.64	—	•	86
7		• 62.8 6.98	• 69.0 0.59	• 81 1.85	—	•	86
2	2	• 84.0 7.75	—	—	• 87.0	•	86
3		• 89.5 9.37	—	—	—	•	86
4		• 81.7 5.94	• 86 1.08	• 91.5 1.91	—	•	86
5		• 62.8 7.27	• 84.0 1.28	• 91.0 2.0	—	•	86
6		• 83.0 7.13	• 85 1.35	• 97.0 2.11	—	•	86
7		• 70.8 8.56	•	• 97.0 1.94	—	•	86
1	3	• 55.6 7.44	—	—	• [18.0]	•	86
2		• 67.0 5.93	—	• [61]	• 71	•	86
3		• 80.0 6.85	—	—	• [75.0]	•	86
4		• 75.2 3.18	• 90.5 0.99	• 93.0 1.65	—	•	86
5		• 52.5 3.06	• 84.5 1.18	• 93.0 1.88	—	•	86
6		• 51.3 4.32	• 86.0 1.35	• 96.0 2.00	—	•	86
7		• 78.2 8.71	• 83.0 1.68	• 94.0 2.08	—	•	86

n	m	K	S_B	S_A	N	I	Ref.
1	4	• 60.0 8.63	—	—	• [43.0]	•	86
2		• 76.0 3.85	—	• [69]	• 84.0 0.09	•	86
3		• 69 5.85	• [65]	• 77	— 1.92	•	86
4		• 62.0 6.37	• 82.0 0.99	• 96.0 1.76	—	•	86
5		• 55.8 5.61	• 79.0 1.11	• 93.0 1.65	—	•	86
6		• 66.7 6.20	• 84.0 1.24	• 99.0 1.96	—	•	86
7		• 72.5 6.54	• 83.0 1.35	• 98.0 1.76	—	•	86
1	5	• 51.0 7.09	—	—	• [35.5]	•	86
2		• 60.0 6.33	—	• 67.0 0.23	• 78.5 0.16	•	86
4		• 60.5 7.35	• 81.0 0.84	• 94.0 1.96	—	•	86
5		• 65.0 6.32	• 76.0 1.19	• 91.0 1.69	—	•	86
6		• 52.4 4.59	• 78.0 1.53	• 96.0 2.40	—	•	86
7		• 62.5 6.69	• 79.0 1.51	• 95.0 2.11	—	•	86
1	6	• 53.0 9.83	—	• [28.0]	• [42]	•	86
2		• 56.0 7.43	• [48]	• 69.0 0.09	• 82.0 0.23	•	86
3		• 58.2 5.56	• 64.0 1.02	• 78.0 1.31	—	•	86
4		• 47.7 5.89	• 77.0 0.92	• 95.0 1.87	—	•	86
5		• 57.2 5.60	• 72.5 0.93	• 91.0 1.90	—	•	86
6		• 57.0 5.34	• 77.0 0.99	• 97.0 1.99	—	•	86
7		• 69.2 5.22	• 75.0 0.94	• 96.0 1.78	—	•	86



K	173.2	N	255.3 0.311	I	Ref. 21
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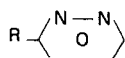
● Pyridines substituées en 4



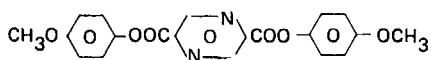
R	K ₂	K ₁	S ₃	S _B (1)	S _A (1)	N (1)	I	Ref.
<chem>CH3O-c1ccc(cc1)-c2ccc(cc2)-N=CH-</chem>	—	● 193.8 8.65	—	—	—	● [181.3] 0.084	●	83, 1
<chem>C8H17O-c1ccc(cc1)-c2ccc(cc2)-N=CH-</chem>	—	● 108 6.67	● 173 0.48	● 182 0.56	● 187.5 2.28	—	●	
<chem>CH3O-c1ccc(cc1)-COO-c2ccc(cc2)-CH=CH-</chem>	● 65 4.31	● 140 5.63	—	—	—	● 230 0.28	●	5
<chem>C8H17O-c1ccc(cc1)-COO-c2ccc(cc2)-CH=CH-</chem>	● 95 4.58	● 117 0.32	—	—	—	● 214 0.25	●	5

(1) From texture.

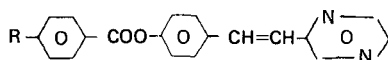
• Pyrimidine



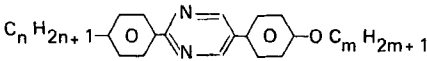
R	K	N	I	Ref.
$\text{CH}_3\text{O}-\text{C}_6\text{H}_4-\text{COO}-\text{C}_6\text{H}_4-\text{CH}=\text{CH}-$	• 189 8.80	• 238 0.02	•	5
$\text{C}_8\text{H}_{17}\text{O}-\text{C}_6\text{H}_4-\text{COO}-\text{C}_6\text{H}_4-\text{CH}=\text{CH}-$	• 139 8.41	• 210 0.21	•	5



K	202.6	N	249.5 0.316	I	Ref. 21
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R	K	N	I	Ref.
CH ₃	• 192 8.39	• 213 0.09	•	5
C ₈ H ₁₇ O	• 132 9.05	• 172 0.16	•	5

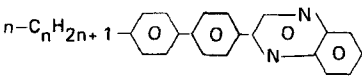


n	m	K	s_G	s_F	s_C	s_A	N	I	Ref. (1)
1	1	• 179 183–184 5.3	—	—	—	—	• 214–219 210–211 0.22	•	169
2	2	• 146 4.8	—	—	—	—	• 226.5 0.24	•	169
3	3	• 132.2 4.5	• [124.2] 0.05	—	—	• 205 0.53	• 216.5 0.24	•	169
3	5	• 104.5 104.4 4.1	• 130.3 130.4 0.79	—	• 145.3 145.1 (a)	• 216 215.5 1.7	—	•	169
4	4	(b) • 90.3 4.1	• 113.7 0.60	•	• 120.7 120.6 0.16	• 215 1.7	—	•	169
4	5	• 81 81.9 4.5	• 123.8 124 0.31	—	• 153 153.5 0.10	• 212 211 1.2	—	•	169
5	5 (2)	(b) • 79.5 79.4 5.7	• 102.4 102.4 0.06	• 113.2 113 0.17	• 144.8 144.5 0.04	• 210.2 211 1.7	—	•	169
5	6	• 65 65.1 5.7	• 98.8 99.1 0.06	• 116.5 117 0.17	• 153.5 153.8 0.03	• 211 210.6 2.0	—	•	169
6	5	• 79.2 80.5 7.4	• 80.3 80 0.014	• 107.9 109 0.14	• 136.8 136 0.03	• 207 207.7 1.9	—	•	169
6	6	• 76.5 77 6.7	• 80.0 80 0.012	• 116.5 116 0.18	• 153.2 152 0.04	• 206 206 2.0	—	•	169
7	5	• 79.5 80.1 7.2	• [62] [62.5] 0.005	• 102.9 104.2 0.11	• 125.8 125.7 (a)	• 205 206.4 2.0	—	•	169
7	7	• 80.5 81 7.9	• 84.5 84 0.004	• 124.7 124 0.22	• 171.8 171 0.07	• 200 200 2.1	—	•	169
8	5	• 73 73.6 8.6	—	• 101.7 102 0.22	• 114.2 112.8 (a)	• 203 203.8 2.2	—	•	169

n	m	K	S _G	S _F	S _C	S _A	N	I	Ref. (1)
8	6	• 77 78.4 9.1	—	• 114.8 114.9 0.23	• 135 134.2 (a)	• 202 203.4 2.2	—	•	169
8	8	• 76.5 76–77 9.1	• 88–89 88.3–89.3 0.001	• 129 130.2 0.55	• 177 176.7 0.13	• 195.2 194.9 2.4	—	•	169
9	5	• 74.3 74.7 8.4	—	• 98 97.5 0.22	• 107.7 107.5 (a)	• 200.5 200.5 2.2	—	•	169
9	9	• 88.5 88.9 12	• 92–93 (c) (c)	• 130.6 131 0.62	• 180.2 180.1 0.17	• 189 189.2 2.4	—	•	169
10	5	• 75.2 75.6 9.6	—	• 96 96.1 (d)	• 98 97.4 (d)	• 197.9 198.6 2.3	—	•	169
10	10	• 86 87.3 12.4	• 117.7 117.7 < 0.001	• 132.8 132.6 0.84	• 179.4 179.6 0.19	• 183.5 183.8 2.6	—	•	169

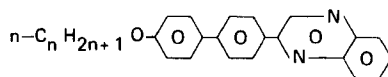
- (1) For each compound :
 First line : transition temperatures according to the microscopic observation.
 Second line : transition temperatures from the DSC investigations.
- (a) : S_C/S_A transition without latent heat only a jump in the C_p curve.
- (b) $\leftrightarrow$ k : With decreasing temperature transition in n, m = 4.4 at 73°C and n, m = 5.5 at 61.5°C to an additional smectic phase, classified as smectic H by L. Richter, H. Sackmann et al (to be published).
- (c) $\leftrightarrow$ e : S_G-S_F transition : only observed by microscopy.
- (d) $\leftrightarrow$ f : The transitions S_F-S_C , and S_C-S_A showed a double peak which could not be split into two parts.
- (2) See ref. 87.

• Quinoxalins



n	K		S _E (1)		S _A (1)		I	Ref.
1	•	122 8.03	—		•	152 0.074	•	88
2	•	122 3.22	—		•	165 1.32	•	88
3	•	121 2.73	—		•	175 1.32	•	88
4	•	120 5.90	—		•	167 1.02	•	88
5	•	112 2.37	—		•	171 1.22	•	88
6	•	99 2.02	—		•	173 1.14	•	88
7	•	86 2.43	•	88 0.87	•	170 0.98	•	88
8	•	60 5.48	•	82 0.76	•	176 0.33	•	88
10	•	53 5.26	•	83 0.88	•	171 1.79	•	88

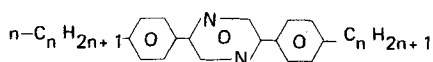
(1) Identified by isomorphy Ref. 88.



n	K	S_E (1)	S_A (1)	N	I	Ref.
1	• 169 6.8	—	• [163] 0.75	• 203 0.09	•	88
2	• 175 1.69	—	• 202 1.39	• 216 0.13	•	88
3	• 157 3.02	—	• 204 1.83	—	•	88
5	• 145 4.89	• [130] 1.09	• 206 1.79	—	•	88
8	• 96 2.10	• 115 1.07	• 195 1.64	—	•	88
10	• 98 2.44	• 119 1.34	• 191 2.18	—	•	88

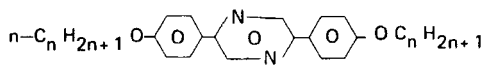
(1) Identified by isomorphy.

• Pyrazines



n	K	S_C (1)	S_A (1)	N	I	Ref.
2	• 163.8 6.22	—	—	• 176.2 0.08	•	76
3	• 157.3 4.88	—	—	• 200.7 0.26	•	76
4	• 161.3 5.35	• 166.4 0.85	—	• 181.9 0.23	•	76
5	• 134.3 4.29	• 173.6 0.08	• 182.2 0.29	• 191.3 0.36	•	76
6	• 116.1 3.97	• 172.3 0.09	• 179.2 1.17	—	•	76
7	• 109.6 4.34	• 175.0 0.08	• 187.0 1.76	—	•	76
8	• 104.6 3.46	• 178.0 2.38	• 187.0 1.79	—	•	76
9	• 108.8 4.85	• 177.0 2.38	—	—	•	76
10	• 111.2 6.88	• 171.5 2.14	—	—	•	76

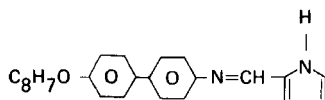
(1) Identified by isomorphy Ref. 76 ter.



n	K ₂	K ₁	S _B (1)	S _C (1)	N	I	Ref.
1	—	• 228 9.40	—	—	• 274 0.32	•	76
2	—	• 221 8.65	—	—	• 280 0.42	•	76
3	• 155	• 202 8.49	—	—	• 242 0.45	•	76
4	• 155 1.41	• 170.3 2.69	—	• 218 0.96	• 246 0.38	•	76
5	• 56	• 153.4 4.66	—	• 211 1.18	• 224 0.39	•	76
6	• 130 0.75	• 135.7 1.83	• 139.6 2.38	• 212 1.21	• 220 0.58	•	76
7	—	• 126 3.62	• 128.5 1.41	• 211 1.57	• 212 0.59	•	76
8	—	• 118.8 3.17	• 121.1 1.37	• 209 2.93	—	•	76
9	—	• 118.7 12.26	—	• 204 2.78	—	•	76
10	• 75	• 113.0 11.81	—	• 201 3.47	—	•	76

(1) Identified by isomorphy Ref. 76 quater.

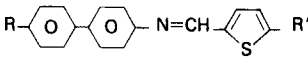
• Pyrrole



K ₂	94 1.92	K ₁	119 3.65	S _A (2)	189 3.69	I	Ref. 5
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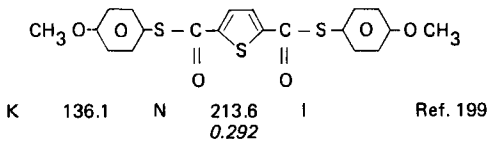
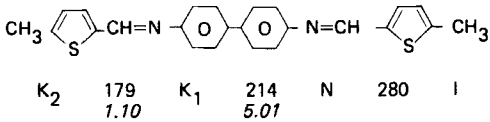
(1) From texture Ref. 5.

• Thiophenes



R	R'	K	S ₃	S _B (1)	S _A (1)	N	I	Ref.
CH ₃ O-	CH ₃ -	• 160.1 7.51	-	-	-	• 211.0 0.153	•	1, 83, 5
C ₈ H ₁₇ O-	H	• 132 2.68	• 152 0.09	• 157	- 157 3.95	-	•	5
C ₈ H ₁₇ O-	CH ₃ -	• 150 2.96	-	-	-	• 181 0.13	•	5

(1) Identified from textures.



• Furane

