Supplemental Material

Prediction of clearing temperatures of bent-core liquid crystals using decision trees and multivariate adaptive regression splines

Jelena Antanasijević^{1,*}, Viktor Pocajt¹, Davor Antanasijević², Nemanja Trišović¹, Katalin Fodor-Csorba³

¹ *University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia*

² *Innovation Center of the Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia*

³ *Wigner Research Centre for Physics, Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary*

* Corresponding author e-mail: jantanasijevic@tmf.bg.ac.rs

Table S1. Molecular structure of bent-core liquid crystals and their clearing temperatures

Comp.	Molecular structure	Obs. temp. (K)	Ref.

1	R = C ₆ H ₁₃	453.35	[1]
2	R = C ₈ H ₁₇	449.05	[1]
3*	R = C ₁₀ H ₂₁	444.45	[1]
4	R = C ₁₂ H ₂₅	440.85	[1]

5	R = C ₄ H ₉	409.25	[2]
6*	R = C ₅ H ₁₁	408.05	[2]
7	R = C ₆ H ₁₃	409.95	[2]
8	R = C ₇ H ₁₅	407.85	[2]
9	R = C ₈ H ₁₇	407.55	[2]
10	R = C ₉ H ₁₉	408.75	[2]
11	R = C ₁₀ H ₂₁	410.55	[2]
12	R = C ₁₁ H ₂₃	410.75	[2]
13	R = C ₁₂ H ₂₅	412.05	[2]
14	R = C ₁₄ H ₂₉	411.45	[2]
15	R = C ₁₆ H ₃₃	410.95	[2]

16	R = C ₄ H ₉	445.35	[2]
17	R = C ₅ H ₁₁	425.15	[2]
18	R = C ₆ H ₁₃	428.15	[2]
19	R = C ₇ H ₁₅	429.95	[2]
20	R = C ₈ H ₁₇	435.05	[2]
21	R = C ₉ H ₁₉	436.15	[2]
22	R = C ₁₀ H ₂₁	439.55	[2]
23	R = C ₁₁ H ₂₃	441.35	[2]
24	R = C ₁₂ H ₂₅	444.75	[2]

25	R = C ₉ H ₁₉	415.35	[2]
26	R = C ₁₀ H ₂₁	415.25	[2]
27	R = C ₁₁ H ₂₃	413.15	[2]
28	R = C ₁₂ H ₂₅	412.85	[2]

29	R = C ₆ H ₁₃	436.05	[2]
30	R = C ₇ H ₁₅	434.85	[2]
31*	R = C ₈ H ₁₇	438.55	[2]
32	R = C ₉ H ₁₉	436.25	[2]
33	R = C ₁₀ H ₂₁	435.75	[2]
34	R = C ₁₁ H ₂₃	433.55	[2]
35	R = C ₁₂ H ₂₅	433.35	[2]
36	R = C ₁₄ H ₂₉	432.15	[2]
37	R = C ₁₆ H ₃₃	428.35	[2]

38	R = C ₄ H ₉	414.95	[2]
39*	R = C ₆ H ₁₃	415.85	[2]
40*	R = C ₈ H ₁₇	408.25	[2]
41	R = C ₁₀ H ₂₁	410.55	[2]
42*	R = C ₁₂ H ₂₅	410.75	[2]

43	R = C ₁₄ H ₂₉	406.55	[2]
44	R = C ₁₆ H ₃₃	405.45	[2]
45	R = C ₁₈ H ₃₇	398.55	[2]

46	$R = C_6H_{13}$	432.75	[3]
47	$R = C_8H_{17}$	428.65	[3]
48	$R = C_{10}H_{21}$	422.65	[3]
49	$R = C_{12}H_{25}$	417.95	[3]
50*	$R = C_6H_{13}$	404.15	[4]
51*	$R = C_8H_{17}$	384.15	[4]
52	$R = C_9H_{19}$	383.15	[4]
53	$R = C_{10}H_{21}$	380.15	[4]
54	$R = C_{12}H_{25}$	382.15	[4]
55	$R = C_{14}H_{29}$	374.15	[4]
56	$R = C_{16}H_{33}$	375.15	[4]
57*	$R = C_{18}H_{37}$	376.15	[4]
58	$R = C_{20}H_{41}$	377.15	[4]
59	$R = C_6H_{13}$	385.15	[4]
60	$R = C_{14}H_{29}$	368.15	[4]
61	$R = C_{20}H_{41}$	368.15	[4]
62		352.15	[4]
63	$X = H, Y = H$	448.35	[5]
64	$X = H, Y = Cl$	417.45	[5]
65	$X = F, Y = H$	423.65	[5]
66	$X = F, Y = Cl$	416.05	[5]

67	$R = C_8H_{17}$	388.15	[6]
68*	$R = C_{10}H_{21}$	378.15	[6]
69	$R = C_{12}H_{25}$	375.15	[6]
70	$R = C_{14}H_{29}$	374.15	[6]
71	$R = C_{16}H_{33}$	378.15	[6]

72	$R = C_8H_{17}$	386.15	[6]
73	$R = C_{10}H_{21}$	368.15	[6]
74	$R = C_{12}H_{25}$	366.15	[6]
75	$R = C_{14}H_{29}$	368.15	[6]
76*	$R = C_{16}H_{33}$	371.15	[6]

77	$R = C_{16}H_{33}$	395.15	[6]

78	$R = C_6H_{13}$	399.15	[7]
79	$R = C_8H_{17}$	392.15	[7]
80	$R = C_{10}H_{21}$	379.15	[7]
81*	$R = C_{12}H_{25}$	379.15	[7]
82*	$R = C_{14}H_{29}$	381.15	[7]
83	$R = C_{16}H_{33}$	373.15	[7]
84		384.15	[7]

85		393.15	[7]
86		387.15	[7]
87*		363.15	[7]

88	R = C ₈ H ₁₇	416.15	[8]
89	R = C ₁₀ H ₂₁	409.15	[8]
90	R = C ₁₂ H ₂₅	410.15	[8]
91	R = C ₁₄ H ₂₉	412.15	[8]
92	R = C ₁₆ H ₃₃	413.15	[8]
93	R = C ₁₈ H ₃₇	415.15	[8]

94	R = C ₈ H ₁₇	389.15	[9]
95	R = C ₁₀ H ₂₁	389.15	[9]
96	R = C ₁₂ H ₂₅	387.15	[9]
97*	R = C ₁₄ H ₂₉	389.15	[9]

98	R = C ₁₂ H ₂₅ ; R ₁ = C ₁₆ H ₃₃	393.45	[10]
99	R = C ₁₆ H ₃₃ ; R ₁ = C ₁₂ H ₂₅	393.25	[10]
100	R = C ₁₆ H ₃₃ ; R ₁ = C ₁₆ H ₃₃	391.75	[10]

101	R = C ₅ H ₁₁	401.15	[10]
102	R = C ₆ H ₁₃	420.35	[10]
103	R = C ₇ H ₁₅	397.85	[10]
104	R = C ₈ H ₁₇	388.05	[10]
105	R = C ₉ H ₁₉	389.55	[10]
106	R = C ₁₁ H ₂₃	393.25	[10]
107	R = C ₁₂ H ₂₅	389.75	[10]
108	R = C ₁₄ H ₂₉	388.75	[10]
109	R = C ₁₆ H ₃₃	388.55	[10]
110	R = C ₄ H ₉	437.75	[11]
111	R = C ₅ H ₁₁	436.75	[11]
112	R = C ₆ H ₁₃	437.25	[11]
113	R = C ₇ H ₁₅	436.25	[11]
114	R = C ₈ H ₁₇	437.15	[11]
115	R = C ₉ H ₁₉	437.45	[11]
116	R = C ₁₀ H ₂₁	436.85	[11]
117*	R = C ₁₁ H ₂₃	436.25	[11]
118	R = C ₁₂ H ₂₅	436.35	[11]
119	R = C ₁₄ H ₂₉	435.25	[11]
120	R = C ₁₆ H ₃₃	433.95	[11]
121	R = C ₄ H ₉	420.45	[11]
122	R = C ₅ H ₁₁	420.45	[11]
123	R = C ₆ H ₁₃	422.45	[11]
124*	R = C ₇ H ₁₅	421.05	[11]
125*	R = C ₈ H ₁₇	419.85	[11]
126	R = C ₉ H ₁₉	421.65	[11]
127	R = C ₁₀ H ₂₁	422.65	[11]
128	R = C ₁₁ H ₂₃	423.15	[11]
129	R = C ₁₂ H ₂₅	423.65	[11]
130	R = C ₁₄ H ₂₉	424.85	[11]
131	R = C ₁₆ H ₃₃	422.15	[11]

132	R = OC ₄ H ₉	394.65	[12]
133	R = OC ₆ H ₁₃	395.15	[12]
134	R = OC ₈ H ₁₇	393.55	[12]
135	R = OC ₁₀ H ₂₁	393.95	[12]
136*	R = OC ₁₂ H ₂₅	396.05	[12]
137*	R = C ₄ H ₉	399.55	[12]
138	R = C ₆ H ₁₃	394.65	[12]
139	R = C ₈ H ₁₇	390.45	[12]
140*	R = C ₁₀ H ₂₁	388.95	[12]
141*	R = C ₁₂ H ₂₅	388.65	[12]

142	R = C ₄ H ₉	418.95	[13]
143	R = C ₆ H ₁₃	415.25	[13]
144	R = C ₈ H ₁₇	413.65	[13]
145	R = C ₁₀ H ₂₁	409.55	[13]
146	R = C ₁₂ H ₂₅	409.05	[13]
147	R = OC ₄ H ₉	431.55	[13]
148	R = OC ₆ H ₁₃	430.35	[13]
149	R = OC ₈ H ₁₇	426.55	[13]
150	R = OC ₁₀ H ₂₁	420.15	[13]
151	R = OC ₁₂ H ₂₅	415.95	[13]

152	R = C ₈ H ₁₇	407.75	[14]
153	R = C ₁₀ H ₂₁	405.45	[14]
154	R = C ₁₂ H ₂₅	404.25	[14]

155	R = C ₈ H ₁₇	414.15	[15]
156	R = C ₁₀ H ₂₁	401.15	[15]

157	$R = C_{12}H_{25}$	398.15	[15]
158	$R = C_{14}H_{29}$	397.15	[15]
159	$R = C_{16}H_{33}$	394.15	[15]

160	$R = OC_5H_{11}$	454.15	[16]
161	$R = OC_6H_{13}$	446.55	[16]
162	$R = OC_7H_{15}$	444.85	[16]
163	$R = OC_8H_{17}$	447.05	[16]
164*	$R = OC_{10}H_{21}$	446.05	[16]
165	$R = OC_{12}H_{25}$	443.05	[16]
166	$R = OC_{16}H_{33}$	436.85	[16]
167	$R = C_5H_{11}$	423.05	[16]
168	$R = C_6H_{13}$	428.75	[16]
169*	$R = C_8H_{17}$	431.25	[16]
170	$R = C_{10}H_{21}$	431.65	[16]
171	$R = C_{12}H_{25}$	429.15	[16]
172	$R = C_{14}H_{29}$	424.45	[16]

173	$R = OC_7H_{15}$	403.15	[16]
174	$R = OC_8H_{17}$	406.15	[16]
175	$R = OC_9H_{19}$	409.15	[16]
176	$R = OC_{10}H_{21}$	413.15	[16]
177	$R = OC_{12}H_{25}$	415.15	[16]
178	$R = C_8H_{17}$	392.15	[16]
179	$R = C_{10}H_{21}$	398.15	[16]
180	$R = C_{12}H_{25}$	400.15	[16]
181	$R = C_{14}H_{29}$	400.15	[16]

182	$R = OC_6H_{13}$	438.15	[16]
183	$R = OC_7H_{15}$	426.15	[16]
184	$R = OC_8H_{17}$	421.15	[16]
185*	$R = OC_9H_{19}$	416.15	[16]

186	$R = OC_{10}H_{21}$	413.15	[16]
187	$R = OC_{12}H_{25}$	410.15	[16]
188	$R = C_{14}H_{29}$	390.15	[16]

189	$R = OC_7H_{15}$	446.15	[16]
190	$R = OC_8H_{17}$	445.15	[16]
191*	$R = OC_9H_{19}$	441.15	[16]
192*	$R = OC_{10}H_{21}$	440.15	[16]
193	$R = OC_{12}H_{25}$	437.15	[16]

194	$R = OC_6H_{13}$	450.15	[16]
195*	$R = OC_7H_{15}$	449.15	[16]
196	$R = OC_8H_{17}$	450.15	[16]
197	$R = OC_9H_{19}$	447.15	[16]
198	$R = OC_{12}H_{25}$	446.15	[16]

199	$R = OC_6H_{13}$	421.15	[16]
200	$R = OC_7H_{15}$	409.15	[16]
201	$R = OC_8H_{17}$	405.15	[16]
202	$R = OC_9H_{19}$	395.15	[16]
203	$R = OC_{10}H_{21}$	390.15	[16]

204	$R = OC_6H_{13}$	403.15	[16]
205*	$R = OC_7H_{15}$	399.15	[16]
206*	$R = OC_8H_{17}$	397.15	[16]
207	$R = OC_9H_{19}$	390.15	[16]

208		394.15	[16]
209		420.15	[16]
210		424.15	[16]
211		458.15	[16]
212	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₈ H ₁₇	401.55	[16]
213	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₉ H ₁₉	406.15	[16]
214	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₁₀ H ₂₁	411.65	[16]
215	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₁₁ H ₂₃	412.15	[16]
216	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₁₂ H ₂₅	414.15	[16]
217	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₁₃ H ₂₇	414.65	[16]
218	R = OC ₁₂ H ₂₅ ; R ₁ = OC ₁₄ H ₂₉	415.15	[16]
219	R = OC ₁₀ H ₂₁ ; R ₁ = OC ₈ H ₁₇	407.15	[16]
220	R = OC ₁₀ H ₂₁ ; R ₁ = OC ₉ H ₁₉	407.15	[16]
221	R = OC ₁₀ H ₂₁ ; R ₁ = OC ₁₀ H ₂₁	405.15	[16]
222	R = C ₁₂ H ₂₅	387.55	[17]
223*	R = C ₁₃ H ₂₇	379.95	[17]

224*	$R = OC_8H_{17}$	426.05	[17]
225	$R = C_{10}H_{21}$	412.75	[17]
226	$R = C_{11}H_{23}$	409.55	[17]
227	$R = C_{12}H_{25}$	410.45	[17]
228	$R = C_{13}H_{27}$	421.95	[17]
229	$R = OC_8H_{17}$	432.85	[17]
230	$R = C_{10}H_{21}$	425.65	[17]
231	$R = C_{11}H_{23}$	427.15	[17]
232	$R = C_{12}H_{25}$	424.85	[17]
233*	$R = C_{13}H_{27}$	424.15	[17]
234	$R = C_7H_{15}$	414.65	[18]
235	$R = C_8H_{17}$	415.65	[18]
236	$R = C_9H_{19}$	416.15	[18]
237*	$R = C_{10}H_{21}$	415.65	[18]
238*	$R = C_{11}H_{23}$	415.65	[18]
239	$R = C_{12}H_{25}$	413.65	[18]
240	$R = C_{13}H_{27}$	413.65	[18]
241	$R = C_{14}H_{29}$	412.15	[18]
242	$R = C_{16}H_{33}$	411.65	[18]
243*	$R = C_{18}H_{37}$	409.15	[18]

* Compounds used in test set

References

1. Srinivasan MV, Kannan P, Roy A. Photo and electrically switchable B7 mesophase exhibiting asymmetric bent-core liquid crystals. *New J Chem*. 2013;37:1584–1590.
2. Nagaveni NG, Roy A, Prasad V. Achiral bent-core azo compounds: effect of different types of linkage groups and their direction of linking on liquid crystalline properties. *J Mater Chem*. 2012;22:8948–8959.
3. Vijay Srinivasan M, Kannan P, Roy A. Investigations on photo and electrically switchable asymmetric bent-core liquid crystals. *J Mater Sci*. 2013;48:2433–2446.
4. Alaasar M, Prehm M, Brautzsch M, Tschierske C. 4-Methylresorcinol based bent-core liquid crystals with azobenzene wings – a new class of compounds with dark conglomerate phases. *J Mater Chem C*. 2014;2:5487–5501.
5. Lutfur MR, Hegde G, Kumar S, Tschierske C, Chigrinov VG. Synthesis and characterization of bent-shaped azobenzene monomers: Guest-host effects in liquid crystals with azo dyes for optical image storage devices. *Opt Mater*. 2009;32:176–183.
6. Alaasar M, Prehm M, Tschierske C. Influence of halogen substituent on the mesomorphic properties of five-ring banana-shaped molecules with azobenzene wings. *Liq Cryst*. 2013;40:656–668.
7. Alaasar M, Prehm M, Brautzsch M, Tschierske C. Dark conglomerate phases of azobenzene derived bent-core mesogens – relationships between the molecular structure and mirror symmetry breaking in soft matter. *Soft Matter*. 2014;10:7285–7296.
8. Alaasar M, Prehm M, May K, Eremin A, Tschierske C. 4-Cyanoresorcinol-based bent-core mesogens with azobenzene wings: Emergence of sterically stabilized polar order in liquid crystalline phases. *Adv Funct Mater*. 2014;24:1703–1717.
9. Alaasar M, Prehm M, Tschierske C. A new room temperature dark conglomerate mesophase formed by bent-core molecules combining 4-iodoresorcinol with azobenzene units. *Chem Commun*. 2013;49:11062–11064.
10. Nagaveni NG, Raghuvanshi P, Roy A, Prasad V. Azo-functionalised achiral bent-core liquid crystalline materials: effect of presence of –N=N– linkage at different locations in the molecular architecture. *Liq Cryst*. 2013;40:1238–1254.
11. Nagaveni NG, Prasad V, Roy A. Azo functionalised achiral bent-core liquid crystals: observation of photo-induced effects in B7 and B2 mesophases. *Liq Cryst*. 2013;40:1405–1416.
12. Prasad V, Kang S-W, Qi X, Kumar S. Photo-responsive and electrically switchable mesophases in a novel class of achiral bent-core azo compounds. *J Mater Chem*. 2004;14:1495–1502.
13. Prasad V, Kang S-W, Kumar S. Novel examples of achiral bent-core azo compounds exhibiting B1 and anticlinic-antiferroelectric B2 mesophases. *J Mater Chem*.

2003;13:1259–1264.

14. Prasad V, Jákli A. Achiral bent-core azo compounds: observation of photoinduced effects in an antiferroelectric tilted smectic mesophase. *Liq Cryst.* 2004;31:473–479.
15. Alaasar M, Prehm M, Tschierske C. New azobenzene containing bent-core liquid crystals based on disubstituted resorcinol. *Liq Cryst.* 2014;41:126–136.
16. Pelzl G, Diele S, Weissflog W. Banana-shaped compounds - a new field of liquid crystals. *Adv Mater.* 1999;11:707–724.
17. Pyc P, Mieczkowski J, Pocięcha D, Gorecka E, Donnio B, Guillon D. Bent-core molecules with lateral halogen atoms forming tilted, synclinic and anticlinic, lamellar phases. *J Mater Chem.* 2004;14:2374–2379.
18. Umadevi S, Jákli A, Sadashiva BK. Odd-even effects in bent-core compounds containing terminal n-alkyl carboxylate groups. *Soft Matter.* 2006;2:875–885.