Electronic Supplementary Information

Design, synthesis and mesomorphic behaviour of four-ring achiral bent-core liquid crystal in the nematic phase.

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Table 1: DFT calculated bend angle θ as shown in **Figure 1** , dihedral angles, dipole moment components (μ_X, μ_Y, μ_Z), and the resultant dipole moment (μ).

Compound	Dipole moment (Debye)				E (a. u.) (RB3LYP)	Dihedral angle °	Bend angle (°) θ
	μ_x	μ_y	μ_z	$\mu_{resultant} = (\mu_x^2+\mu_y^2+\mu_z^2)^{1/2}$			
GK3	-1.94	0.50	-4.37	4.80	-1936.17038134	102, 137	142
GK4	-1.94	0.56	-4.43	4.87	-1975.49460944	102, 137	142
GK3up	2.08	0.36	4.62	5.08	-1936.17041798	104, 136	142
GK4up	2.09	0.39	4.69	5.15	-1975.49464247	104, 136	142
GK5	-1.33	1.83	-4.32	4.87	-1936.16898438	135, 138	148
GK6	-1.33	1.70	-4.45	4.94	-1975.49320973	135, 137	148
GK5up	1.58	3.05	3.86	5.15	-1936.16533011	138, 138	146
GK6up	1.57	3.04	3.95	5.23	-1975.48953659	138, 138	146
GK1	-1.58	1.87	-4.69	5.29	-1896.84218270	136,137	146
GK2	-1.57	1.74	-4.81	5.36	-1936.16640494	136,137	146

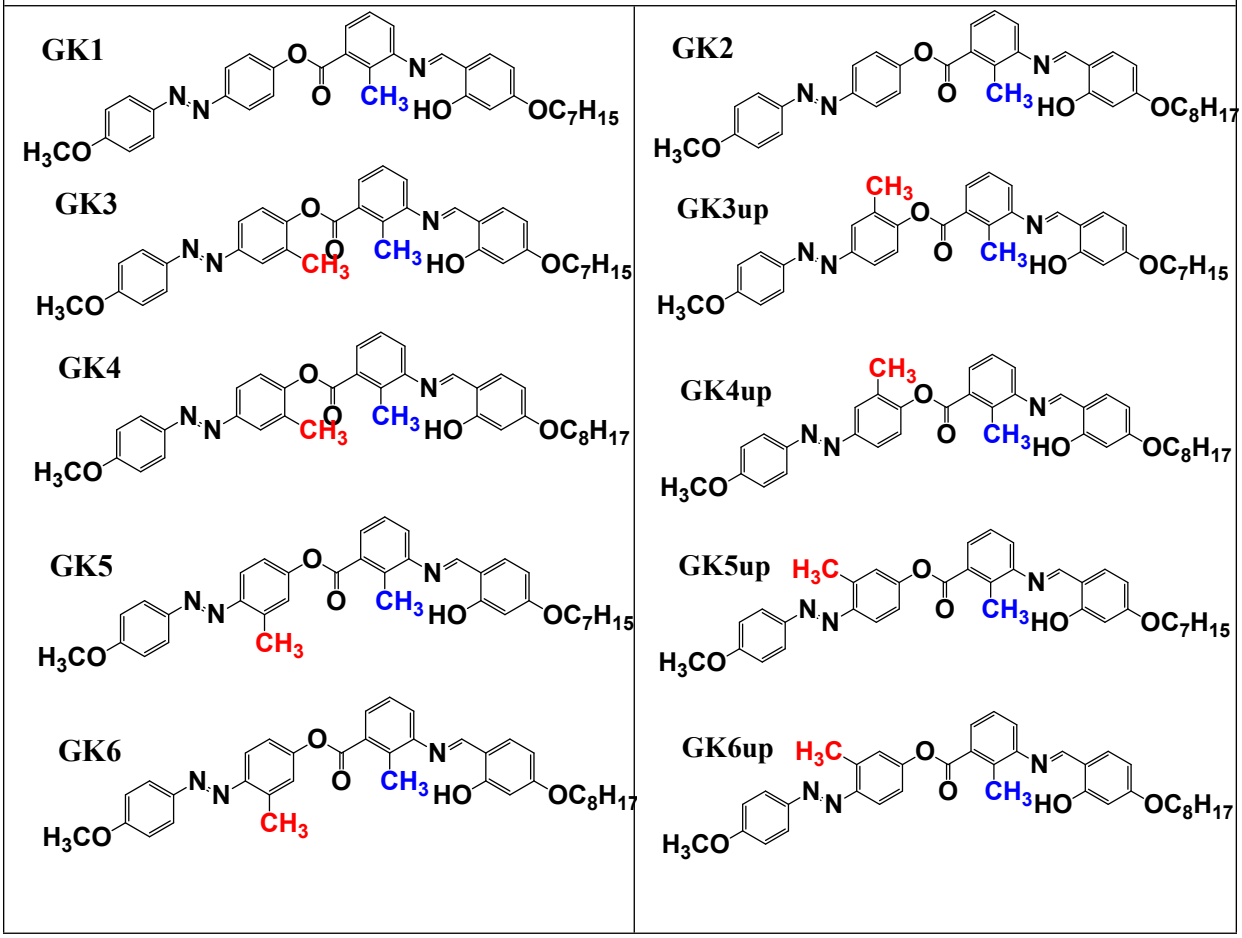
The values relative to angles and dipole moment are expressed in degree (°) and Debye (D) respectively.

Table 2: DFT calculated principal polarizability components[a] (α_{XX}, α_{YY}, α_{ZZ}), isotropic polarizability $\alpha^{iso} = (\alpha_{XX} + \alpha_{YY} + \alpha_{ZZ})/3$, Polarizability anisotropy $\Delta\alpha = [\alpha_{XX} - (\alpha_{YY} + \alpha_{ZZ})/2]$, and asymmetry parameter, $\eta = [(\alpha_{YY} - \alpha_{ZZ})/ (\alpha_{XX} - \alpha^{iso})]$. Parameters relative to the molecular polarizability tensor in the Cartesian Reference frame

Compound	α_{XX}	α_{YY}	α_{ZZ}	α_{iso}	$\Delta\alpha$	η_α
GK3up	955	360	344	553	603	0.0398
GK4up	969	373	353	566	606	0.0496
GK5	1004	326	357	563	660	0.0703
GK6	1020	335	370	575	667	0.0786
GK1	991	315	340	549	663	0.0565
GK2	1007	324	353	561	668	0.0632

[a]All polarizability components and the anisotropy parameter are calculated in Bohr^3 (with 1 Bohr = 0.52917 Å).

S1:Planar molecular structures for optimisation in DFT studies



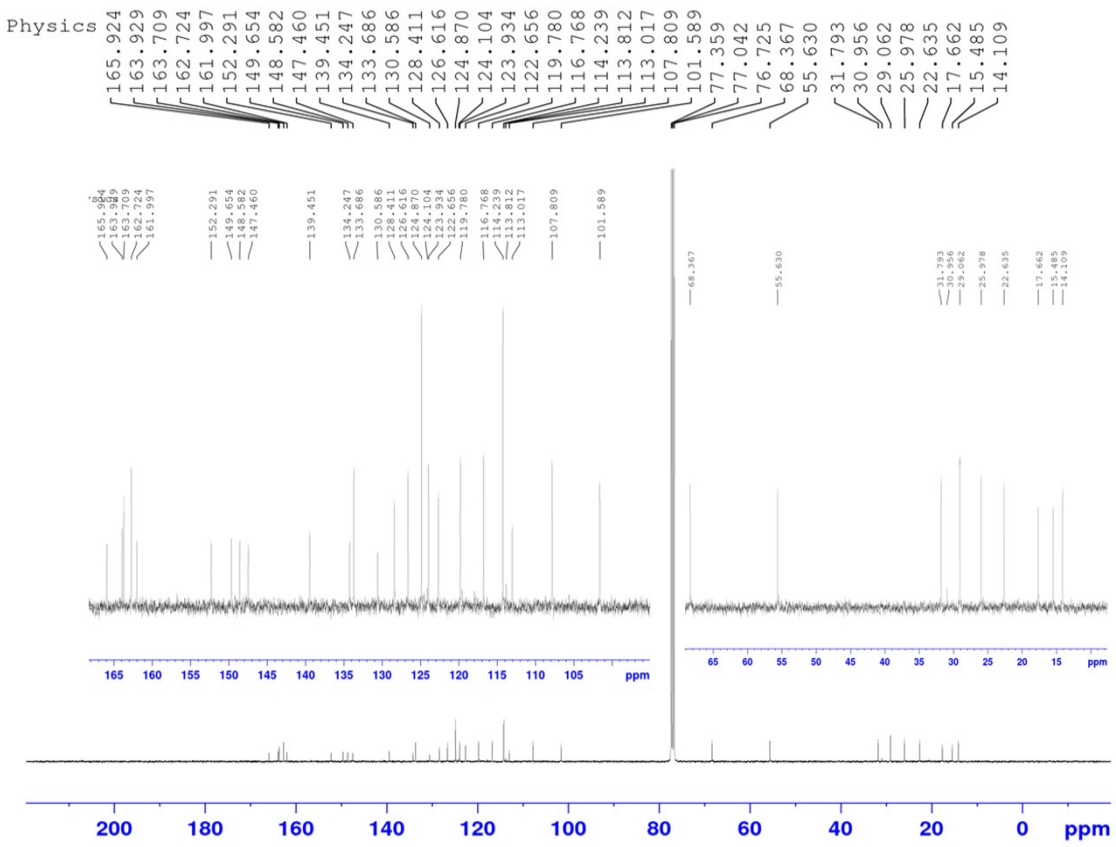


Figure S2: 13C NMR spectra of compounds GK5 recorded on Bruker Avance AV- III 400 MHz NMR spectrometer.