Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supplementary Information

# -for-

# Physical model for temperature-dependent dielectric properties of anisotropic nematic liquid crystals

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**S1. Four-parameter model for $\varepsilon_e(T)$ and $\varepsilon_o(T)$**

When we follow the conventional four-parameter refractive index model in deriving a physical analytic model for the temperature-dependent dielectric parameters of nematic liquid crystals (NLCs), the temperature-dependent extraordinary and ordinary dielectric constants– $\varepsilon_e$ and $\varepsilon_o$, respectively– can be written by employing eqn (5) as follows, with similar formulas to eqn (7) and (8):

$$\varepsilon_e(T) = A + BT + \frac{2}{3}(\Delta\varepsilon)_0\left(1-\frac{T}{T_{NI}}\right)^{\lambda_\varepsilon} \tag{S1}$$

$$\varepsilon_o(T) = A + BT - \frac{1}{3}(\Delta\varepsilon)_0\left(1-\frac{T}{T_{NI}}\right)^{\lambda_\varepsilon} \tag{S2}$$

where $(\Delta\varepsilon)_0$ is defined as follows similar to eqn (6).

$$\Delta\varepsilon = (\Delta\varepsilon)_\circ\left(1-\frac{T}{T_{NI}}\right)^{\lambda_\varepsilon} \tag{S3}$$

In this case, the mean dielectric value of the temperature-dependent NLC can be expressed with eqn (S1) and (S2) as follows, which also have a similar form to eqn (5).

$$<\varepsilon(T)>= A + BT \tag{S4}$$

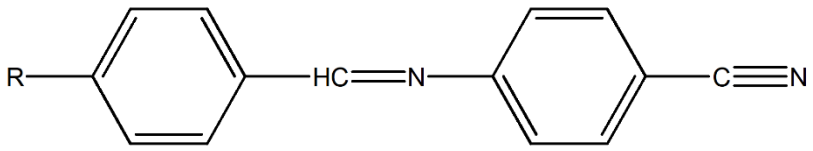
The analytic curves for the temperature-dependent mean dielectric values and dielectric constants obtained by the four-parameter dielectric models are co-plotted as the dotted lines with the fitting results obtained by the six-parameter dielectric models in Figs. 4 and 5. The physical parameters extracted from the four-parameter dielectric model of eqn (S1), (S2), and (S4) for the four fluorinated NLCs are listed in Table S1.

**Table S1**. Fitting parameters for the four fluorinated NLCs, where the parameters are obtained by using the four-parameter dielectric model.

| LC material | $A_\varepsilon$ | $B_\varepsilon$ ($\times 10^{-2}$ K$^{-1}$) | $(\Delta\varepsilon)_o$ | $\lambda_\varepsilon$ |
|---|---|---|---|---|
| 3PBC$^{3,5}$F$_2$ | 5.95±0.02 | − 0.68±0.04 | 5.25±0.03 | 0.224±0.02 |
| 5PBC$^{3,5}$F$_2$ | 5.79±0.03 | − 0.63±0.05 | 4.46±0.05 | 0.202±0.03 |
| 3PBC$^{3,4,5}$F$_3$ | 18.40±0.01 | − 3.27±0.01 | 15.45±0.09 | 0.238±0.02 |
| 5PBC$^{3,4,5}$F$_3$ | 15.62±0.02 | − 2.67±0.03 | 14.12±0.1 | 0.230±0.04 |

**S2. Fitting results of six-parameter dielectric model for aminobenzonitrile NLCs**

The fitting accuracy of the six-parameter dielectric model derived in our work was checked by applying our model to different sets of NLCs. In this evaluation, three types of aminobenzonitrile NLCs[1] were used as shown in Fig. S1. Their fitting results for the temperature-dependent dielectric constants and dielectric anisotropies are shown in Fig. S2 and S3, respectively. The fitting parameter values obtained by the six-parameter dielectric models are listed in Table S2.




**$R_1$= *n*-$C_4H_9$-O- ($T_{NI}$= 370.75 K),**

**$R_2$= *n*-$C_3H_{13}$-O- ($T_{NI}$= 374.05 K),**

**$R_3$= *n*-$C_7H_{15}$-COO ($T_{NI}$= 383.62 K).**

**Fig. S1** Chemical structures of three types of aminobenzonitrile NLCs[1] and their phase transition temperatures ($T_{NI}$).

**Table S2**. Fitting parameters of $\varepsilon^*$, $A_\varepsilon$, $B_\varepsilon$, $T^*$, $(\Delta\varepsilon)_o$ and $\lambda_\varepsilon$ for three types of aminobenzonitrile NLCs, which were extracted from the temperature-dependent average dielectric constants[1] $<\varepsilon(T)>$ and dielectric anisotropies[1] ($\Delta\varepsilon(T)$) using eqn (14) and (15), respectively, to obtain the six-parameter dielectric permittivity models of eqn (16) and (17).

| LC | $\varepsilon^*$ | $A_\varepsilon$ ($\times 10^{-3}$ K$^{-1}$) | $B_\varepsilon$ (K$^{-0.5}$) | $(\Delta\varepsilon)_o$ | $\lambda_\varepsilon$ | $T^*$ (K) |
|---|---|---|---|---|---|---|
| $R_1$ | 13.9±0.002 | − 0.4±0.2 | 0.095±0.003 | 34.27±0.07 | 0.25±0.01 | 373.6±0.02 |
| $R_2$ | 12.4±0.004 | − 0.1±0.1 | 0.090±0.001 | 24.3±0.09 | 0.18±0.02 | 374.01±0.03 |
| $R_3$ | 10.8±0.003 | − 0.5±0.3 | 0.099±0.002 | 17.8±0.10 | 0.16±0.03 | 383.6±0.04 |

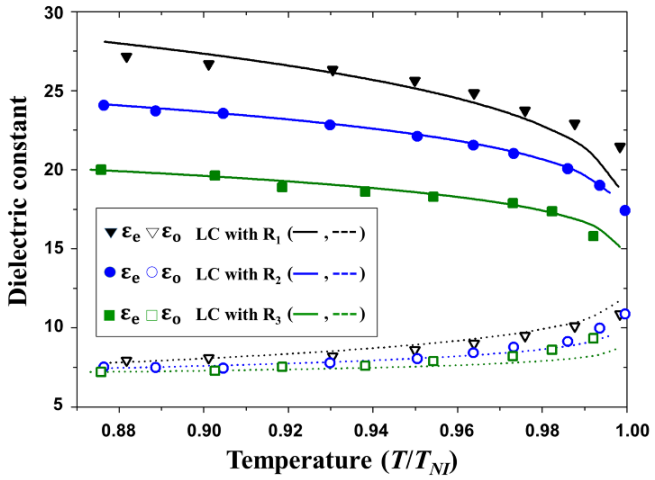



**Fig. S2** Temperature-dependent dielectric constants ($\varepsilon_e(T)$, $\varepsilon_o(T)$) of the aminobenzonitrile NLCs. The experimental data[1] and the fitted curves are presented as symbols and solid lines, respectively. The fitting curves are obtained with the six-parameter dielectric model of eqn (16) and (17) and the physical parameters listed in Table S2.

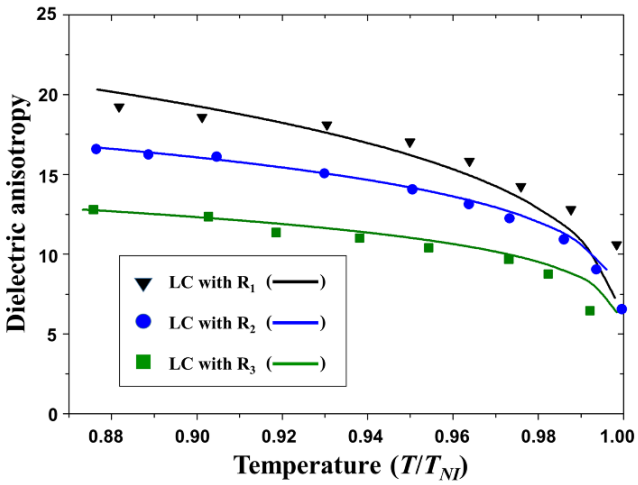



**Fig. S3** Temperature-dependent dielectric anisotropy ($\Delta\varepsilon(T)$) of the aminobenzonitrile NLCs, where the symbols and solid lines represent the experimental data[1] and the fitted curves obtained by using eqn (15), respectively.

**S3. Fitting results of threshold voltages and splay elastic constants obtained from the four-parameter dielectric model using four fluorinated NLCs**

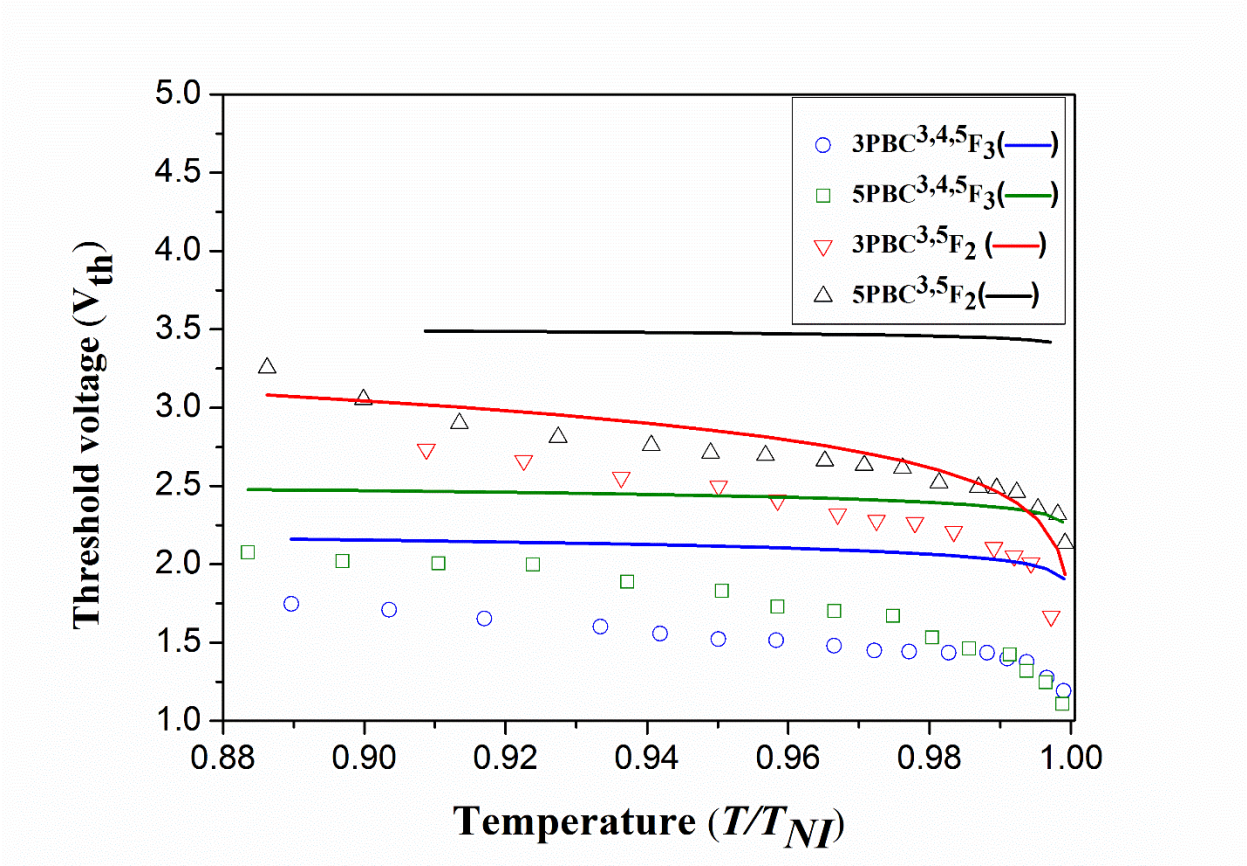



**Fig. S4** Temperature-dependent threshold voltage ($V_{th}$) properties of the four fluorinated NLCs, where the experimental data and analytic curves are presented as symbols and solid lines, respectively. The analytic curves were obtained using the equation $V_{th} = (V_{th})_o ((1-T/T_{NI})^{\beta - \lambda_\varepsilon/2}$, where the $\beta$ values were obtained from the Haller approximation method shown in eqn (6) and the $\lambda_\varepsilon$ values listed in Table S1 were used.

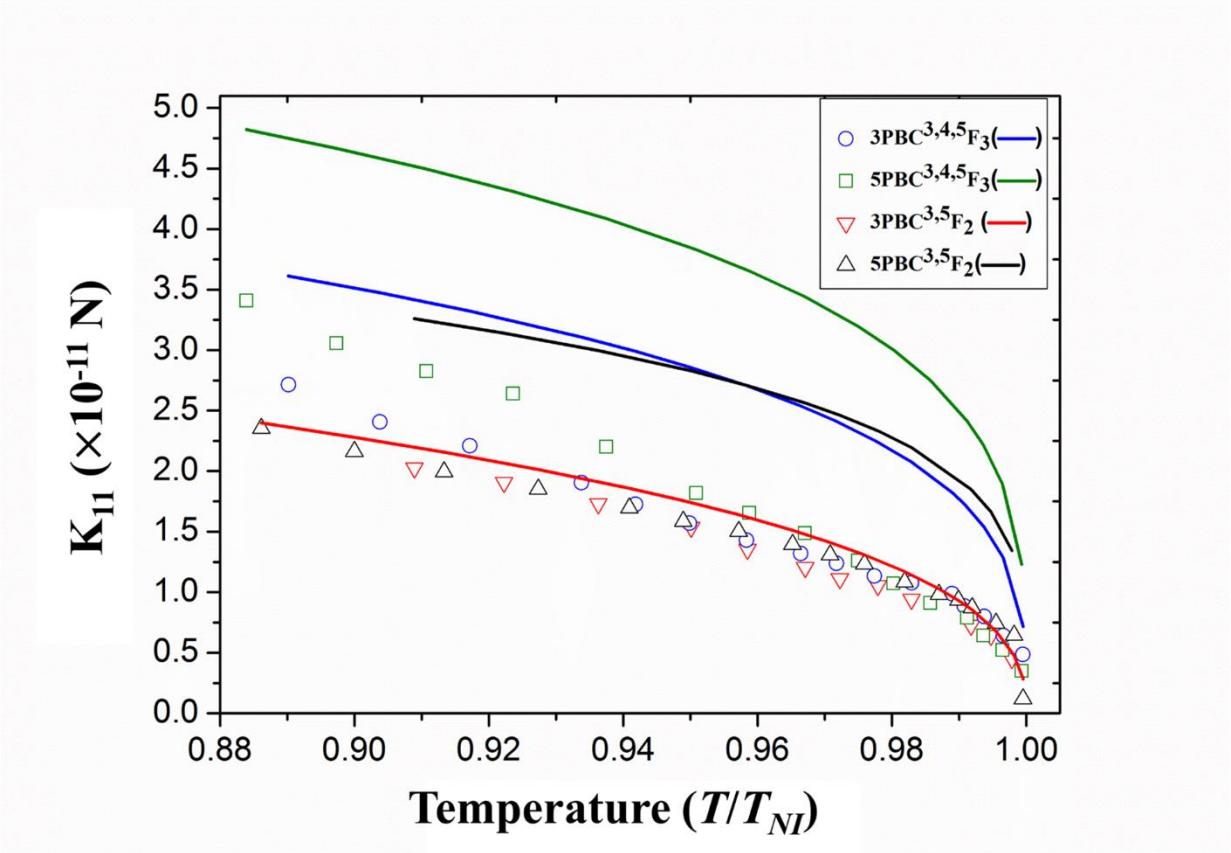



**Fig. S5** Temperature-dependent splay elastic constant ($K_{11}$) properties of the four fluorinated NLCs, where the experimental data and analytic curves are presented as the symbols and solid lines, respectively. The analytic curves were obtained using the equation $K_{11}=(K_{11})_0((1-T/T_{NI})^{2\beta}$ and the physical parameters are based on the four-parameter refractive index model.

## References

1 M. Schadt, *J. Chem. Phys.*, 1972, **56,** 1494-1497.