Isosteric substitution of B\textsuperscript{3},N\textsuperscript{+} for C,C: A unique tool for studying of polarity and coulombic effects on phase stability.

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Two series of isosteric non-polar (a) – polar (b) pairs of nematogens derived from 10-vertex (1) and 12-vertex (2) clusters were prepared and investigated. The replacement of the C–C fragment in a with the isosteric polar group \textsuperscript{N}\textsuperscript{+}–B\textsuperscript{–} in b increased the longitudinal dipole moment by 12 D and 11 D in series 1 and 2, respectively, without affecting molecular geometry. The substitution resulted in an increase of nematic phase stability in both series 1 and 2, which is attributed to the stabilizing dipole–dipole interactions. The strong dipole moment in compounds 1b and 2b gives rise to large dielectric anisotropy reaching a value of \(\Delta \varepsilon = 113\) for the cyanophenol ester [1]. Using the same concept of isosteric polar replacement, the effect of coulombic interactions on phase stability was probed in ILC, and clearing temperatures for ion pairs 3b and 4b were compared with those of the analogous non-ionic equimolar mixtures 3a and 4a. The magnitude of these dipole-dipole and coulombic interactions was assessed using DFT computational methods.

References:

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