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Title:	Influence of terminal halogen moieties on the phase structure of short-core achiral hockey-stick-shaped mesogens: design, synthesis and structure–property relationship
Authors:	Kaur, Supreet (/jspui/browse?type=author&value=Kaur%2C+Supreet) Mohiuddin, G. (/jspui/browse?type=author&value=Mohiuddin%2C+G.) Punjani, V. (/jspui/browse?type=author&value=Punjani%2C+V.) Pal, S.K. (/jspui/browse?type=author&value=Pal%2C+S.K.)
Keywords:	Density functional theory Nematic liquid crystals Chemical bonds Intermolecular H-bonding
Issue Date:	2018
Publisher:	Royal Society of Chemistry
Citation:	Molecular Systems Design and Engineering, 3(5), pp. 839-852
Abstract:	An extensive study of the effect of terminal halogens on the structure–property relationship in three series of polar short-core hockey-stick-shaped or L-shaped mesogens has been elucidated. The behaviour of the halogens at the tip of the short arm and the role of the end alkyl chain at the long arm in the phase structure of the mesogens have been characterised explicitly. The compounds are shown to exhibit a long-range nematic phase composed of cybotactic clusters (Ncyb) along with an underlying orthogonal smectic phase that has a tendency to align in defect-free fashion in the planar cell. Investigations of X-ray diffraction and dielectric spectroscopy confirm the presence of cybotacticity. The measured elastic constants (K11 and K33) exhibited the usual behaviour (like bent-core mesogens) in the Iso–N phase; however, a trend reversal was observed towards smectic transition. Temperature-dependent Raman study confirms the formation of intermolecular H-bonding (via –C[double bond, length as m-dash]O) in the crystalline phase that systematically weakens and is finally disrupted as the system transforms through the smectic to nematic and isotropic phases. Density functional theory (DFT) study reveals the important molecular parameters that correlate with the experimental findings of the self-assembled structures.
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