Title:	Structural organization and molecular self-assembly of a new class of polar and non-polar four-ring based bent-core molecules
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Abstract:	We have studied two new series of polar and non-polar four-ring based achiral bent-core molecules containing single bondCN and single bondOCH3 moiety respectively at the tip of the molecular short arm and their molecular self-assembly in crystal and liquid crystal state. Crystal structure analysis revealed the bent molecular geometry of the compounds with bent angle 151° along with fundamental intermolecular interactions such as antiparallel arrangement of the polar molecules, intermolecular hydrogen bonding, different types of π–π interactions and entangled/helical molecular arrangement in 3D space. Due to the dimeric antiparallel molecular arrangement, lower homologues of the polar compounds of series 1-n (1-8, 1-10) exhibited long range nematic phase with cybotactic clustering (Ncyb). However, the lower homologues of non-polar compounds of series 2-n (2-6, 2-8) did not form any type of clustering exhibiting normal nematic phase. Dielectric spectroscopic investigations and X-ray diffraction measurements of compound 1-8 confirmed the presence of nematic cybotacticity. Thus, the formation of clusters in nematic phase of bent-core molecules was not only due to an underlying smectic phase but also due to the combined effect of the molecular structural parameters including bent angle, molecular dipole moment and its spatial arrangement. Negative bend-splay (K33-K11) elastic constant behavior was observed in the entire nematic range.
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