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Title:	Highly Resolved Morphology of Room-Temperature Columnar Liquid Crystals Derived from Triphenylene and Multialkynylbenzene Using Reconstructed Electron Density Maps
Authors:	Gupta, Santosh Prasad (/jspui/browse?type=author&value=Gupta%2C+Santosh+Prasad) Gupta, Monika (/jspui/browse?type=author&value=Gupta%2C+Monika) Pal, S.K. (/jspui/browse?type=author&value=Pal%2C+S.K.)
Keywords:	Columnar Correlation Electron density maps
Issue Date:	2017
Publisher:	Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim
Citation:	ChemistrySelect, 2(21), pp. 6070-6077.
Abstract:	This paper demonstrates highly resolved structure of the self-assembly of dyad and triads constituted from triphenylene (T) and multialkynylbenzene (M) units linked via flexible alkyl spacers (n). Resolved structures of these systems are based on reconstructed electron density maps derived from X-ray diffraction patterns. T-M compound (dyad) exhibits columnar hexagonal (Colh) phase which is explained by its columnar layered structure. In contrast, T-M-T compounds (triads) with spacer lengths of n = 8 and 10 exhibited columnar oblique (Colob) mesophase whereas, the one with shortest spacer length, i. e., n = 6, showed a columnar oblique plastic (Colobp) phase. We also found that molecules are interdigitated within themselves for compounds having longer spacer lengths (n = 8 and 10). However, a side by side packing is observed for the compound with shortest alkyl spacer (n = 6).
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