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Title:	Tuning the self-assembly and photophysical properties of bi-1,3,4-thiadiazole derivatives through electron donor–acceptor interactions and their application in OLEDs†
Authors:	De, J. (/jspui/browse?type=author&value=De%2C+J.) Pal, S.K. (/jspui/browse?type=author&value=Pal%2C+S.K.)
Keywords:	Centrally Termini Anisotropic Molecules
Issue Date:	2017
Publisher:	Royal Society of Chemistry
Citation:	Journal of Materials Chemistry C, 5(36), pp.9345-9358.
Abstract:	We report several shape anisotropic molecules that contain two centrally placed 1,3,4-thiadiazole units, which vary from each other with respect to the number and length of the flexible chains at the termini. The number, position and length of the peripheral chains connected to the termini showed an impact on the thermal behavior of these compounds. The compounds with two terminal tails exhibited an enantiotropic smectic C phase, whereas the compounds with four terminal tails turned out to be crystalline. Surprisingly, among the compounds with six terminal tails, only the compound with a longer terminal chain exhibited a columnar phase with oblique symmetry. It is also to be noted that only compounds with six terminal chains exhibited gelation in long chain hydrocarbons. The xerogel of the hexacatenar with six n-decyloxy chains showed an entangled network of nanofibers of several micrometers in length. The aggregation behavior of the hexacatenar in the hydrocarbon solvent is mainly supported by the attractive π - π interactions of the aromatic cores and the van der Waals interactions offered by the peripheral flexible tails. The emission behavior is dependent on the number of peripheral tails and not on the length. Furthermore, one of the hexacatenars exhibited solvatochromic emissive behavior. This molecular design helps in the development of long molecular nanowires with a central conducting core and insulating peripheral sheath, which will be helpful for the application in organic electronic devices. The application potential of the columnar liquid crystal material was tested by the fabrication of organic light emitting diodes (OLEDs) either as a single emissive material or as a guest material in a host polymer. Higher efficiency and brightness were noticed in the host guest OLED, which exhibited a technologically important bright blue emission.
Description:	Only IISERM authors are available in the record.
URI:	https://pubs.rsc.org/en/content/articlelanding/2017/tc/c7tc01420a#!divAbstract (https://pubs.rsc.org/en/content/articlelanding/2017/tc/c7tc01420a#!divAbstract) http://hdl.handle.net/123456789/2673 (http://hdl.handle.net/123456789/2673)
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