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Title: Aromatic  $\pi$ – $\pi$  driven supergelation, aggregation induced emission and columnar self-assembly of

star-shaped 1,2,4-oxadiazole derivatives

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Abstract:

A new family of star shaped 1,2,4-oxadiazole derivatives with the variation in the number of flexible peripheral tails have been synthesized and characterized. It is interesting to note that the number of flexible tails at the periphery dictated the self-assembly and the photophysical behavior. The compound with three flexible tails stabilized the crystalline state with lamellar packing, and did not show organogelation, but showed blue emission in crystalline and thin film states. The compound with six flexible tails stabilized the hexagonal columnar liquid crystalline state and it showed the ability to gelate in nonpolar solvents at a concentration less than 1 weight percent. qualifying it as a supergelator, where  $\pi - \pi$  interactions play a major role. This phenomenon is very rare, in comparison to earlier reports where supergelation is supported by H-bonding interactions. Besides its capability to form a self-standing, moldable gel, this compound also exhibited aggregation-induced emission (AIE), which persisted even in the xerogel state. X-ray diffraction studies unraveled the rectangular columnar self-assembly in the gel state. The columnar order and emissive nature in the liquid crystal and xerogel states makes this molecule promising for application in emissive displays. Compounds with nine alkyl tails stabilized a long range columnar hexagonal phase. This report emphasizes the importance of various non-covalent interactions in deciding the nature of self-assembly.

Description: Only IISERM authors are available in the record.

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