

Discotic Liquid Crystals Do NOT Require Tails

Robert J. Twieg¹, Zhe Li¹, Kunlun Wang¹, Parikshit Guragain¹, Scott Bunge¹
Dena Agra-Koojiman², Mitchell Powers³, Lewis Sharpnack³, Brett Ellman³, Satyendra Kumar⁴

¹Kent State University, Department of Chemistry and Biochemistry, Kent, Ohio, USA

²Kent State University, Advanced Materials and Liquid Crystal Institute, Kent, Ohio, USA

³Kent State University, Department of Physics, Kent, Ohio, USA

⁴SUNY Albany, Department of Physics, Albany, New York, USA

Nearly a century ago Vorländer had the remarkable insight to anticipate mesogenic activity in simple disk-like polynuclear aromatic substances like triphenylene but he found no examples and none have been described since then.[1] Later, Chandrasekhar demonstrated that the addition of multiple flexible tails to even a simple benzene core induced discotic behavior.[2] During the intervening time many thousands of discotic substances with multiple tails have been described and lore has evolved that tails are required to deliver discotic behavior (in spite of evidence otherwise).[3] Well, after all, Vorländer was right and simple triphenylene discotics sans tails do, in fact, exist. In the course of our studies of fluorinated polynuclear aromatics as organic semiconductors synthesized via photocyclodehydrofluorination (PCDHF) we have discovered a remarkable set of triphenylenes bearing small substituents that possess discotic behavior.[4] The materials studied thus far have halogen content (usually fluorine) and sometimes one or more additional small substituents (nitrile, trifluoromethyl, etc., although such substituents are not mandatory). A challenge is to understand the origins of the mesogenic behavior of these systems. Details of the synthesis methodology critical for the preparation of these no-tail discotic materials, their mesomorphic properties and a preliminary evaluation of charge transport in these tail free systems will all be presented. As discotic liquid crystals have already played a significant role in the development and understanding of organic semiconductors, it is anticipated that these new tail free systems will play an important role. Evidence is accumulating that the design principles studied here on triphenylene will also apply to still larger discotic aromatic polynuclear systems and are also relevant to crystalline materials as well.

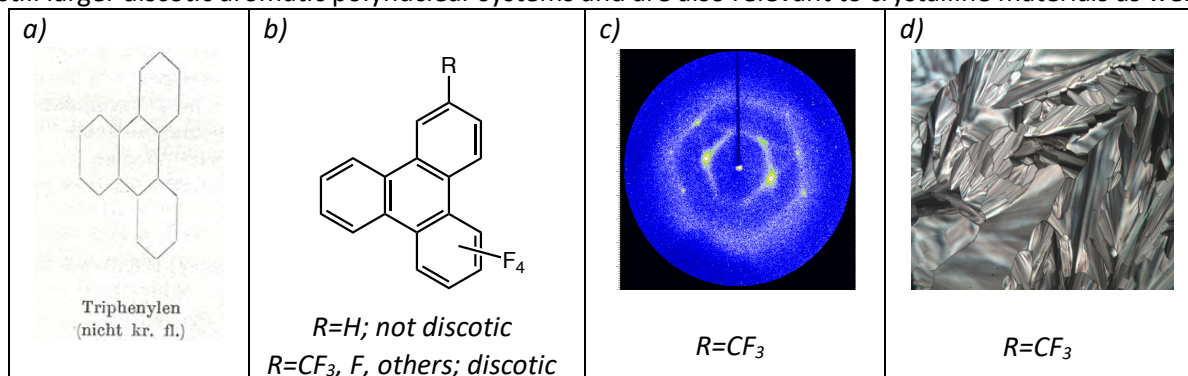


Fig. a) Vorländer's insight. [1] b) Substituent dependent phase behavior: R=H K 205 I 193 K; R=CF₃ K 167 D 176 I 174 D 115 K; R=F K 190 D 204 I 202 D 199 K' 181 K. c) XRD of R=CF₃ D phase at 176°C, d) POM texture of R=CF₃ D phase at 135°C.

[1] D. Vorländer, *Chemische Kristallographie der Flüssigkeiten*; Akademische Verlagsgesellschaft: Leipzig (1924).

[2] S. Chandrasekhar, B. K. Sadashiva, K. A. Suresh, *Pramana*, **9**, 471 (1977).

[3] S. Basurto, S. García, A. G. Neo, T. Torroba, C. F. Marcos, D. Miguel, J. Barberá, M. B. Ros, M. R. de la Fuente, *Chem. Eur. J.*, **11**, 5362 (2005).

[4] Z. Li, R. J. Twieg, *Chem. Eur. J.*, **21**, 15534 (2015).