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Aggregation Properties and Liquid Crystal Phase of a Dye Based on Naphthalenetetracarboxylic Acid MICHELLE TOMASIK, PETER COLLINGS, Swarthmore College — R003 is a dye produced for thin film optical components by Optiva, Inc.[1] made from the sulfonation of the dibenzimidazole derivative of naphthalenetetracarboxylic acid. Its molecular structure is very different from the aggregating food dye previously investigated in our laboratory[2] and R003 forms a liquid crystal phase at significantly lower concentrations. We have performed polarizing microscopy, absorption spectroscopy, and x-ray diffraction experiments in order to determine the phase diagram and aggregate structure. In addition, we have included both translational and orientational entropy in the theoretical analysis of the aggregation process, and have used a more realistic lineshape in analyzing the absorption data. Our results indicate that the "bond energy" for molecules in an aggregate is even larger than for the previously studied dye and that the aggregate structure has a cross-sectional area equal to two or three molecular areas rather than one.

[1]Lazarev, P., N. Ovchinnikova, M. Paukshto, SID Int. Symp. Digest of Tech. Papers, San Jose, California, June XXXII, 571 (2001).

[2]V. R. Horowitz, L. A. Janowitz, A. L. Modic, P. A. Heiney, and P. J. Collings, Phys. Rev. E 72, 041710 (2005).

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