

TOWARD POLAR 1,4-DIPHENYLBUTADIENE MATERIALS

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ABSTRACT

The fast response time of π -electrons makes organic materials increasingly interesting as highly anisotropic materials. We are especially interested in dipole parallel-aligned crystals because of the much higher chromophore density as compared to polymers. Our group achieved several near-perfectly and perfectly dipole parallel-aligned crystals of acetophenone azines, and two assumptions to guide the design. One is that arene-arene T-contacts work as lateral synthons and help to align polar molecules, and, secondly, the azine spacer functions as a conjugation stopper and provides quadrupolarity. To deeply analyze and support these suppositions, the intramolecular features and intermolecular bonding of 1,4-diphenylbutadiene and its derivatives have now been studied.

In Chapter 1, we illustrate the difficulty of achieving dipole parallel-aligned crystals, the solution to the problem, and the research in our group. In Chapter 2, (E,E)-1,4-diphenyl-1,3-butadiene is analyzed by computations in gas phase, dissections in its two polymorphs, and comparisons of the crystal structure of benzene, in Chapter 3, Unsymmetrical syntheses of (E,E)-2,5-diphenyl-2,4-hexadienes are discussed.

The last chapter of the thesis is concerned with an entirely different topic, namely the challenges of preparing college students for science communication. In Chapter 4, the design and development of a webtool is described to support the *Chemistry Is in the News* project.