A new building block for electroactive organic materials? Synthesis, cyclic voltammetry, single crystal X-ray structure, and DFT treatment of a unique boron-based viologen

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SUPPORTING INFORMATION

Synthesis and characterization of 1.

In air, commercial trimethylamine-borane (Aldrich; 1.0g, 0.0137 mol) is dissolved in 50.0 mL of toluene, and to this solution solid iodine (1.7g, 0.00685 mol) is added in small portions over 30 m. Brisk H_2 evolution ensues, and the solution gradually fades from dark yellow-brown to pale amber. After stirring for 30 minutes more, 1.09g (0.00685 mol) of 4,4'-bipyridyl (Aldrich) is added in one portion. A condenser is fitted, and the mixture refluxed from 24-72 hours (Progress of the reaction is readily monitored by ^{1}H-NMR of the toluene phase using a coaxial NMR tube with a deuterated solvent, e.g., DMSO-d^6, as a lock a reference). During this time, the solution gradually darkens to deep red and considerable solid precipitates. After cooling, filtration, and washing (ether), **1** is isolated as a bright orange microcrystalline solid. Note that the crystalline product is vapochromic, and when fully dried is typically bright yellow. Exposure to various solvent vapors can lead to reversible changes in the crystal color that can range in shade from yellow to red. Yield: 3.42g (90.2%). ^{1}H-NMR (300 mHz, DMSO-d^6): d 2.68 (s, 18 H, 2 x NMe_3), 8.55 (d, 4H, pyridinium ring), 9.11 (d, 4H, pyridinium ring); BH_2 not obsvd. ^{13}C-NMR (75.56 mHz, DMSO-d^6): 50.1 (NMe_3), 126.1 (pyridinium ring), 148.9 (pyridinium ring), 150.6 (pyridinium ring).