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ADDITIONS AND CORRECTIONS

Steps To Demarcate the Effects of Chromophore Aggregation and Planarization in Poly(phenyleneethynylene)s. 1. Rotationally Interrupted Conjugation in the Excited States of 1,4-Bis(phenylethynyl)benzene [*J. Am. Chem. Soc.* **2001**, *123*, 4259−4265]. Marcia Levitus, Kelli Schmieder, Holly Ricks, Ken D. Shimizu, Uwe H. F. Bunz,* and Miguel A. Garcia-Garibay*

Page 4259. Changes in the excitation and emission spectra of 1,4-bis(phenylethynyl)benzene (compound **3**) in dilute methylcyclohexane solutions at 298 K, in glassy matrixes at 77 K, and in polyethylene films at 298 and 77 K were interpreted in terms of structural changes associated with rotation about the phenyl−alkyne single bonds. We deduced the coexistence of two distinguishable conformer populations that we referred to as coplanar and twisted. After publication of this work, Prof. Andrew Beeby from the University of Durham in the United Kingdom brought to our attention the possible presence of an emissive impurity in the samples used in our study. Analyis of the original samples confirmed his suggestions and showed a small amount of a similar chromophore with a red shift of ca. 20 nm. Prompted by this, we repeated our measurements with freshly purified samples. We would like to report the following corrections: (1) A shoulder between 350 and 370 nm reported in the absorption spectrum of **3** published in Figure 1 (page 4261) is an impurity. The correct absorption spectrum of the pure sample has a sharp cutoff at 350 nm (Supporting Information, Figure Cl). (2) The dotted spectra shown in Figure 2 (page 4261) correspond to compound **3**, and the spectra reported in solid lines correspond to the impurity. Excitation spectra measured in dilute solution at ambient temperatures are independent of emission wavelengths and emission spectra of the excitation wavelength used (Figure C2). (3) The excitation spectrum shown with a dotted line in Figure 4 (page 4262) corresponds to the impurity. However, large changes reported in the excitation spectrum in going from solution at 298 K to glassy matrixes at 77 K are correct (Figure Cl, bottom). Changes in the absorption spectrum observed in going from solution at 298 K to polyethylene films at 298 K are correct. The dichroism of **3** in stretched polyethylene films is also correct. Additional excitation and emission measurements carried out with **3** in solvents of different viscosities and at different temperatures reveal large changes in excitation and small changes in emission spectra (Figure C3, Supporting Information). The results with compound **3** are analogous to those recently reported with 1,4-bis(9-ethynylanthryl)benzene (Schmieder et al., *J. Phys. Chem.* **2002**, *106*, 1551−1556).

In conclusion, a fluorescent impurity accounts for the spectral heterogeneity observed at ambient temperature. Although relaxation of **3** occurs within the lifetime of the excited state and fluorescence is observed from a single species, variables expected to affect the population of ground state conformers (planarization and twisting) give rise to significant changes in photophysical properties. Our general hypothesis regarding changes in photophysical properties as a function of planarization and twisting does not change.

Supporting Information Available: Supporting Information Available: Revized absorption, fluorescence excitation, and fluorescence emission spectra of 1,4-bis(phenylethynyl)benzene (PDF). This material is available free of charge via the Internet at http://www. pubs.acs.org.

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