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Chain Conformations and Photoluminescence in Poly(di-*n*-octylfluorene)[1] MICHAEL WINOKUR, WITHOON CHUNWACHIRASIRI, BOY TANTO, DAVID HUBER, Department of Physics, University of Wisconsin — The diverse steady-state spectroscopic properties of poly(di-*n*-octylfluorene) are addressed from a molecular-level perspective. Modeling of representative oligomers support the experimental observation of at least three distinguishable classes of conformational isomers with differing chain torsion angles. One class appears to be populated by a single compact structural isomer and this appears to conform to the so called β phase. A rigorous Franck-Condon analysis of the photoluminescence in conjunction with Frenkel-type exciton band structure calculations are performed. These results accurately reproduce all major spectral features of the photoabsorption and those of singlet exciton emission.

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