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Comparison of Experimental and Theoretical Vibrational Spectra for Pentacene Derivatives GREGORY MASLAK, MARK STEWART, LILLIE GHOBRIAL, WES LAURION, Dept. of Physics, SUNY Oswego, JINYUE JIANG, LI TAN, Dept. of Engineering Mechanics, UNL, CAROLINA C. ILIE, Dept. of Physics, SUNY Oswego — The practical use of pentacene in the area of organic field-effect transistors is limited by its sensitivity to oxygen and poor solubility in organic solvents. To overcome these disadvantages, new organic semiconductors as 2,3,9,10-tetrakis(3,5-di-t-butylphenylethynyl)-6,13- bis (trimethylsilylethynyl) pentacene are synthesized. The new pentacene derivatives may be useful for electronic devices such as organic field-effect transistors or organic light-emitting diodes. Here we compare the calculated vibrational spectra to the experimental data in order to characterize the new derivative. The methods and similarities between the theoretical calculations and the experimental data are discussed.

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