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Pentacene Derivatives: Electronic Structure and Spectra ROSS NETUSIL, Chemistry Department, State University of New York at Oswego, CAROLINA ILIE, THORIN KANE, Physics Department, State University of New York at Oswego, FEHMI DAMKACI, Chemistry Department, State University of New York at Oswego — The variation in composition and structure of the substituent groups of pentacene compounds promises a broad range of electronic structures and behaviors and provides a vast and alluring field of inquiry with avenues of exploration. These include the development of synthetic schema, the process of design for novel derivatives and, in order to identify those hypothesized compounds which demonstrate the desired behavior, the identification and refinement of computational tools that make accurate predictions about the electronic behavior of theoretical compounds. Two computational techniques and six pentacene derivatives are here examined. One technique was used to predict the vibrational spectra of the compounds, in order to both acquire data about the optical conductivity of the compounds and to establish a pool of theoretical data against which experimental data will be compared. The molecular orbital energy level diagram of the same six compounds was derived using a second approach, with the same goals of discerning between valid and invalid predictive schema by comparison with pending experimental data and between hypothesized compounds which show promise and those which present little potential for use in organic semiconductor technology.

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