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Theoretical studies of the vibrational properties of the 3,4,9,10,-perylene tetracarboxylic dianhydride (PTCDA) molecule

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Abstract

The vibrational properties of the 3,4,9,10,-perylene tetracarboxylic dianhydride (PTCDA) molecule have been computed using different DFT methods, and the resulting vibrational frequencies are assigned to experimental Raman and IR modes of bulk crystals and thin films. For some Raman active B_{3g} modes, this assignment is performed for the first time. A comparison based on the scalar product of eigenvectors is presented for the different methods of calculation. The best agreement between unscaled calculated frequencies and experimental mode positions in terms of root mean square deviations is obtained for the Becke three parameter Lee–Yang–Parr functional (B3LYP) and the 3-21G basis set.

Author Keywords: PTCDA; B3LYP; Density functional theory; Vibrational modes

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