

Frequencies and Normal Modes of Benz(a)anthracene. A MINDO/3-FORCES Treatment

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Quantum mechanical calculations, based on the MINDO/3-FORCES method, of the vibration frequencies and IR absorption intensities of benz(a)anthracene are reported and compared with calculated vibration frequencies of that molecule. For the first time a complete normal coordinate analysis for the molecule is reported. Interesting correlations between vibration motions of the same type but different symmetries are reported.

Key words: Benz(a)anthracene, Vibration Frequencies, MINDO/3-FORCES.