

Vibration Frequencies and Normal Coordinates of Benzo(c)phenanthrene

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MINDO/3-FORCES quantum mechanical calculations yielded non-planar (C_2) geometry of Benzo(c)phenanthrene. The result agrees with the majority of published results but disagrees with others in which a planar (C_{2v}) structure was accepted in order to simplify the analysis of certain spectroscopic data. Vibration frequencies and IR absorption intensities were calculated then, applying the non-planar (C_2) structure. A complete normal coordinate analysis for the molecule is reported. Inspection of these coordinates allowed the discovery of some useful comparative relations between them, which are reported in the paper.

Key words: Benzo(c)phenanthrene, Vibration Frequencies, MINDO/3-FORCES.