Vibration Frequencies and Normal Coordinates of 3Radialene

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SCF-MO calculations of the vibration frequencies and IR absorption intensities of 3radialene are reported. Complete normal coordinate analysis for the molecule was done. The C=C str. frequencies of 3radialene are found to be intermediate between the values for ethylene and acetylene. The results are explained in terms of a modified Förster-Walsh model for the 3ring in which the central carbon atoms show sp hybridization.

Key words: 3Radialene; Vibration Frequencies; MINDO/3-FORCES.