

Geometry, Vibration Frequencies, Normal Coordinates and IR Absorption Intensities of [6]-Radialene

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SCF-MO calculations, using the MINDO/3-FORCES method, are reported for the equilibrium geometry, vibration frequencies and IR absorption intensities of 6-radialene, considering the planar and chair form. The chair conformation is found to be more stable. The C=C stretching frequencies of the chair form are found to be higher than those of the planar ones. The =CH₂ bending frequencies of the planar form are higher than those of the chair form. Also the PM3 method was used for the calculation of the vibration frequencies. Its results are compared with those of the MINDO/3-FORCES method.

Key words: [6]-Radialene; Vibration Frequencies; MINDO/3-FORCES.