Bonding, Electron Densities and Vibration Frequencies of [3]-, [4]-, [5]- and [6]-Radialenes; a B3LYP Density Functional Study

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B3LYP density functional treatment is reported for the [3]- to [6]-radialene. For the first two molecules the corresponding D_{nh} symmetry resulted from the treatment. For the [5]-radialene, the completely planar D_{5h} structure was found energetically a non-minimal configuration showing two imaginary vibrations. An almost planar C_1 structure of [5]-radialene emerged as the stable species. As for [6]-radialene, the planar D_{6h} structure proved to be a non-minimal structure too, showing three imaginary vibrations. The D_{3d} chair form was most stable, followed by a twisted boat form of the molecule. The chair form of [6]-radialene was more stable than the twist boat form by 0.9 kcal/mol. Variation of the bond lengths, of A_{1g} (ν_{CC} and ν_{CH}) vibration frequencies as well as of the total (ρ^{tot}) and σ (ρ^{σ}) electron densities for the four molecules, compared with those of ethylene, is discussed. To explain the results, a bonding model for the radialene rings is suggested, which assumes an sp hybridization of the ring atoms in [3]- and [4]-radialenes going over to sp^2 hybridization in [5]- and [6]-radialenes.

Key words: Radialene; Frequency; Geometry; Density.