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Topological Analysis of Hydrogen Bonds in Pyruvic Acid-Water Mixtures

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Abstract : The molecular geometries of the possible conformations of pyruvic acid-water complexes (PA-$(H_2O)_n$ = 1- 4) have been fully optimized at DFT/B3LYP/6-311G ++ (d, p) levels of calculation. Among several optimized molecular clusters, the most stable molecular arrangements obtained when one, two, three, and four water molecules are hydrogen-bonded to a central pyruvic acid molecule are presented in this paper. Apposite topological and geometrical parameters are considered as primary indicators of H-bond strength. Atoms in molecules (AIM) analysis shows that pyruvic acid can form a ring structure with water, and the molecular structures are stabilized by both strong O-H…O and C-H…O hydrogen bonds. In large clusters, classical O-H…O hydrogen bonds still exist between water molecules, and a cage-like structure is built around some parts of the central molecule of pyruvic acid. The electrostatic potential energy map (MEP) and the HOMO-LUMO molecular orbital (highest occupied molecular orbital-lowest unoccupied molecular orbital) analysis has been performed for all considered complexes.

Keywords : pyruvic acid, PA-water complex, hydrogen bonding, DFT, AIM, MEP, HOMO-LUMO
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