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Abstract

Quinoline-3-carbonitrile is an important constituent in a variety of pharmaceutical compounds. DFT/CAM-B3LYP with 6-311++G(d,p) basis set calculations in gas phase and in solvents using the PCM for newly synthesized 4-[4-(dimethylamino) phenyl]-2-oxo-1,2,5,6 tetrahydrobenzo[*h*]quinoline-3-carbonitrile (MAPC) have been performed. Efforts to simulate the complex formation of MAPC with water have also been performed. The electron density and its Laplacian have been computed at H-bonds BCP of water-MAPC complexes. The protonation and deprotonation of MAPC as important chemical and biochemical processes are examined. Their forms and energies are computed, analyzed and discussed. The NBO analysis and the stabilization energy of the MAPC in their neutral, cation and anion forms due to their internal donor–acceptor orbital interactions were analyzed. The 1,3-intramolecular proton transfer between the keto-enol interconversion has been investigated and the thermodynamic parameters of the process have been analysed.

Keywords: Quinoline-3-carbonitrile; water complexes; protonation and deprotonation; proton transfer; DFT/PCM calculations.