Abstract

In the present work, we carried out a conformational analysis of cis-3-aminoindan-1-ol and evaluated the role of the intramolecular hydrogen bond in the stabilization of various conformers using quantum mechanical DFT (B3LYP) and MP2 methods. On the basis of relative energies, we have found nine conformational minima, which can interchange through the ring-puckering and the internal rotation of the OH and NH_2 groups on the five-membered ring. The intramolecular hydrogen bonds such as OH....π, NH....π, NH....OH and HN....HO are expected to be of critical importance for the conformational stabilities. The intramolecular interactions of the minima have been analyzed by calculation of electron density (ρ) and Laplacian (ρ) at the bond critical points (BCPs) using atoms-in-molecule (AIM) theory. The existence or absence of OH....π and NH....π in cis-3-aminoindan-1-ol remains unclear since the geometrical investigation has not been confirmed by topological criteria. The results of theoretical calculations demonstrate that this compound exists predominantly in one ring-puckering form stabilized by strong hydrogen bond HN....HO Interaction