

Abstract

Ab initio and density functional theory (DFT) have been applied to study the conformational species of *cis*-1,3-indanediol. We found five quasi-degenerate conformational minima, which can interchange through the ring-puckering and the internal rotation of the OH groups on the five-membered ring. The intramolecular OH $\cdots\pi$ and OH \cdots OH hydrogen bonding have been found of critical importance for the conformational stabilities. Using DFT methods, the relative stability ordering of *cis*-1,3-indanediol reveal the delicate basis set dependence. Furthermore, the order of stability of the conformers appears to be dependent of the calculation methods used (DFT and ab initio). Among five conformers of the *cis*-1,3-indanediol, there are four conformers possessing OH $\cdots\pi$ and/or OH \cdots OH H-bonds. Finally, the chemical shifts of *cis*-1,3-indanediol have been calculated using Gauge-Independent Atomic Orbital (GIAO) method and obtained results have been compared with experimental data. Experimental ^1H and ^{13}C NMR spectra of the *cis*-1,3-indanediol were measured in DMSO- d_6 solution. A complex consisting of two DMSO molecules connected with the *cis*-1,3-indanediol molecule by $\text{—O—H}\cdots\text{O}=\text{S}(\text{CH}_3)_2$ hydrogen bonds has been built and used for NMR calculations. Theoretical calculations predict a significant downfield shift for hydroxyl protons of *cis*-1,3-indanediol involved in intermolecular $\text{—O—H}\cdots\text{DMSO}$ hydrogen bonds