

Experimental, Ab Initio and Density Functional Theory Studies on Sulfadiazine

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Sulfadiazine is a member of the sulfonamides or sulfa drugs and widely used as antibacterial agents. It is used for the treatment of a variety of infections, including toxoplasmosis, an infection of the brain. It can also be used to prevent certain types of meningococcal disease.

In this study combined experimental and computational study on molecular vibrations of free sulfadiazine has been reported. Harmonic and anharmonic wavenumbers of the molecule have been calculated by the aid of Gaussian03 program package and by ab initio HF and DFT methods at B3LYP/6-31++G(d,p) levels of theory. The theoretically possible stable conformers of free sulfadiazine molecule in electronically ground state were searched by means of torsion potential energy surfaces scan studies at both semi-empirical PM3 and B3LYP/3-21G levels of theory. The possible conformers of the molecule were determined by varying the dihedral angles C1-C7-S8-N9, C7-S9-N9-C10 and S8-N9-C10-N11. The geometry optimizations of the stable conformers were performed. The vibrational normal modes of each conformer and associated wavenumbers, IR intensities and Raman activities were calculated and the results were compared with those of experimental findings. The fundamental vibrational modes were assigned depending on their total energy distribution. The theoretically constructed spectra coincide satisfactorily with those of experimental spectra.

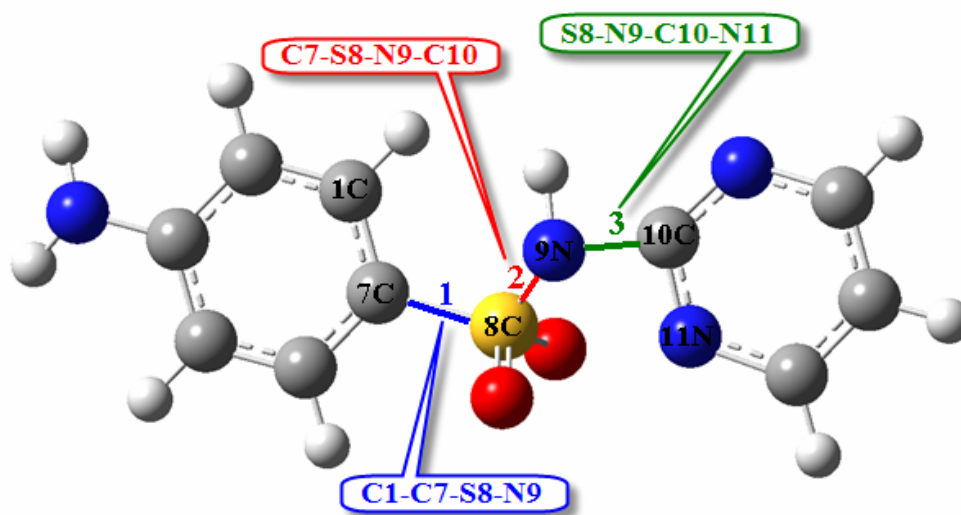


Fig. 1: The model of sulfadiazine molecule