THE ROTATIONAL SPECTRUM OF SULFANILAMIDE AND ITS HYDRATED CLUSTER [a]

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Sulfanilamide (SA, 4-aminobenzenesulfonamide) is an antibacterial drug that interferes with the conversion of para-aminobenzoic acid (PABA) to folate, preventing the synthesis of folic acid (vitamin B9), essential in multiple carbon transfer reactions. Due to its importance, in this work, we characterize sulfanilamide in the isolation conditions of a supersonic expansion using Fourier transform microwave techniques assisted by laser ablation. A single conformer of the bare molecule, stabilized by an N-H•••O=S intramolecular interaction of the sulfonyl group, has been detected. Because the docking process is controlled by the difference in Gibbs free energy between the ligands solvated by the extracellular medium and the ligand interacting with the receptor's active site, we have also studied the sulfanilamide's microsolvation process. Interestingly, a single water molecule is enough to trigger a conformational switch.

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