Journal Basrah Researches ((Sciences)) Vol. 34 , No. 6. 15 December 2008

Theoretical Study for the Antibacterial Activity of Sulfonamides

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ISSN -1817 -2695
((Received 5/3/2008 , Accepted 19/11/2008))

Abstract

The NH_2 stretching vibrations of a series of anilines that were used for the synthesis of sulphonamides were calculated using HF/6-31G+ level of theory. From these frequencies the N-H stretching vibration force constants were calculated. From the geometry optimized structures of the anilines the H-N-H bond angles were calculated which were then used to calculate the double-bond character of the C-N bond. The C-N bond lengths as well as the atomic charges of the atoms N and C were also calculated and correlated with biological activity of the sulphonamides synthesized from the studied anilines.

Keywords: sulfonamides, antibacterial activity, NH_2 stretching frequencies.

Introduction

Sulfonamides, also known as sulfa drugs, were the first synthetic compounds to be effective against grave bacterial infections such as meningitis, pneumonia and blood poisoning [1]. Though new antibacterial and antimicrobial drugs have been supplanted many sulfonamides, they still in widespread use because of their low cost and relatively efficient action against common bacterial diseases [2-7]. Sulfonamides are synthesized mainly from anilines [8, 9]. It has been shown that there is an approximate linear relationship between the stretching frequencies, the force constant (**k**) and the bond intensities of the N-H bonds of the amino group of the parent anilines, and the MIC of sulfa drug to show inhibition of bacterial growth [10]. The band intensity or the "s" character of the nitrogen hybrid orbital of the N-H bond was expressed as the coefficient **b** of the amine used to synthesize the sulfonamide. The constant **k** was calculated By Eq. (1) [10, 11]:

$$k = \frac{\pi^2 c^2 m'}{\frac{1}{M'} + \frac{1}{M''}} (\nu_s + \nu_a)^2 \text{ dyne cm}^{-1} \quad (1)$$

where **c** is the velocity of the light; m' is the mass of a particle with molecular weight of 1; M' and M" are the atomic weights of atom participating (for NH_2, M'= 14; M"=1); ν_s and ν_a are the symmetrical and the asymmetrical stretching vibrations of NH_2. The constant **b** was calculated by Eq. (2) [10, 12]:

$$b^2 = -\cos\theta / (1-\cos\theta) \quad (2)$$

where θ is the H-N-H angel.

In the presence of many excellent theoretical computation programs the structural properties and the vibrational frequencies of molecules can be calculated to acceptable degrees of accuracy. In this work we try to find a correlation between MIC of sulfonamides and some of theoretically estimated constants of the anilines used to synthesize the drugs.