

Structural and Vibrational Study of 4-(2'-Furyl)-1-Methylimidazole

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The 4-(2'-furyl)-1-methylimidazole (**1**) has been synthesized and its molecular structure is observed in the Figure. The compound was characterized by infrared, Raman, multidimensional nuclear magnetic resonance and mass spectroscopy. The infrared and Raman spectra were registered in solid state, and the RMN ¹H, ¹³C, COSY spectra were registered in a DMSO-d₆ solution. The corresponding geometry for the compound was calculated using the Gaussian 03 [1] program at theory level B3LYP. The harmonic vibrational frequencies for the optimized geometry of the compound were calculated using 6-31G* and 6-311++G** basis sets in the approximation of the isolated molecule. Then, in order to get a good assignment of the IR and Raman spectra in solid phase of (**1**) the best fit possible between the calculated and recorded frequencies was carry out and the corresponding force field was scaled using the Pulay et al. SQMFF methodology.

The force constants were calculated for the compound using the Pulay et al. [2] methodology from the Scaling Quantum Mechanic Force Field (SQM). The assignment of the observed bands in the vibrational spectra was performed. Furthermore, the analysis of the Natural Bond Orbitals (NBO) [3] was carried out to study the charge transference interactions between the furan and imidazole rings of the compound.

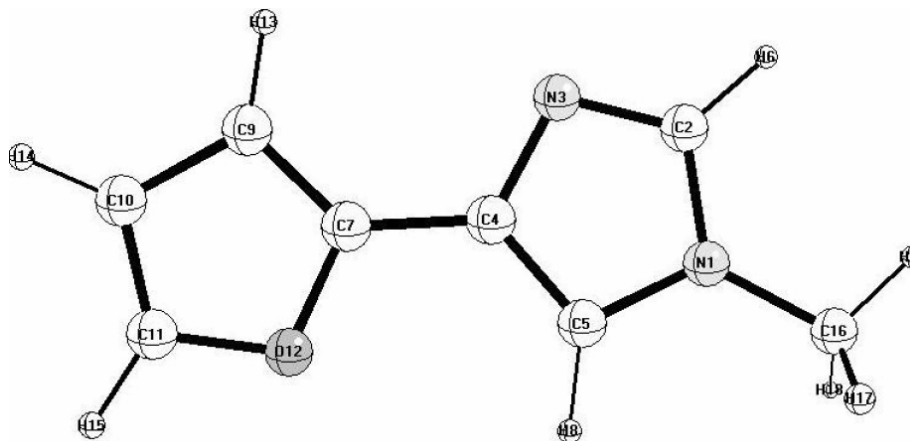


Fig. 1: Structure of 4-(2'-furyl)-1-methylimidazole.

[1] Program Gaussian 03, GAUSSIAN, Inc. Pittsburgh, PAA, USA, 2003.

[2] G. Fogarasi, X. Zhou, P.W. Taylor and P. Pulay, J. Am. Chem. Soc. 105 (1992) 7037.

[3] E.D. Gledening, J.K. Badenhoop, A.D. Reed, J.E. Carpenter, F.F. Weinhold, NBO 3.1; Theoretical Chemistry Institute, University of Wisconsin; Madison, WI, 1998.