Dynamics of Conformational Transitions in Biological Molecules

J. Šebek[1], R. B. Gerber[1,2]

[1]*Institute of Chemistry and The Fritz Haber Research Center*
The Hebrew University, Jerusalem 91904, Israel
[2]*Department of Chemistry, University of California*

Many biological processes are based on conformational changes of biomolecules. Therefore detailed studies of conformational equilibria and dynamics of conformational changes in relevant systems can contribute to understanding the principles of many processes in nature. For our study we chose some simple molecules for which experimental spectra are available.

The first system of interest is 3-aminophenol. There are at least two conformers of this molecule (*cis* and *trans*) which can be separated with using an ac quadrupole m/μ selector because they significantly differ in the dipole moment.[1] This enables measurement of both rotational and vibrational spectra for each conformer in gas phase. The energies, geometries and harmonic IR spectra of both conformers were calculated at MP2/6-311++G** level and compared to the data found in literature.[2, 3] The spectroscopic data were used as a tool of identification of the conformers. The transition state geometry and the barrier were calculated to receive information about the *cis-trans* isomerization and the reaction pathway was investigated. It was found that the isomerization occurs by torsion. In future, the reaction dynamics will be investigated. On this project we cooperate with Prof. J. Manz, Dr. J. Küpper, Prof. G. Meijer and Dr. G. von Helden.

Another system convenient for the studies of simple conformation changes is the protonated dimer of glycine which is an example of a proton pump. There are several conformers of such systems which were described in the literature.[4, 5] We investigated the equilibrium geometries and energies of these conformers at both DFT and MP2 level, while each of these method identified a different structure to be energetically favored. In future we will investigate which of these structures corresponds to real systems by the means of vibrational spectroscopy and describe the dynamics of the proton exchange.

The results obtained for the two mentioned systems will be used in future studies of conformational changes in more complicated systems, such as saccharides.

[1] Filsinger, F.; Erlekam, U.; Helden, G. von; Küpper, J.; Meijer, G., *Phys. Rev. Lett.* **2008,** 100 (13), 133003.

[2] Buyukmurat, Y.; Akyuz, S., *Journal of Molecular Structure* **2005**, 744, 921–928.

[3] Unterberg, C.; Gerlach, A.; Jansen, A.; Gerhards, M.: *Chemical Physics* **2004**, 304, 237–244

[4] Raspopov, S. A.; McMahon, T. B., *J. Mass Spectrom.* **2005**; 40, 1536–1545.

[5] Atkins, C. G.; Rajabi, K.; Gillis, E. A. L.; Fridgen, T. D., *J. Phys. Chem. A* **2008**, 112 (41), 10220–10225.