A MOLECULAR DYNAMICS SIMULATION METHOD FOR THE REPRODUCTION OF THE MOTION OF FLEXIBLE MACROMOLECULES IN ION MOBILITY SPECTROMETRY

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In the present study, using a Nonequilibrium Molecular Dynamics Simulation method [1], we study the effect of the temperature on the structure of flexible macromolecules in inert gases under the influence of an electric field. Specifically, we examine the behavior of the vibrational motion and transport phenomena of flexible molecules at various temperatures and field strengths that apply ion mobility spectrometry. Because experimentally it appears that the flexible peptides have different structures at low and high temperatures [2], the question was raised whether a single intermolecular potential is sufficient to describe the appearance of the structures at all temperatures or the temperature is modifying permanently the structures, thus requiring the consideration of two or more potentials for the description of the motion.

We have calculated the average velocity and the cross sections of the ions in the gas, as well as other molecular properties. We observed that, although one ion-atom intramolecular potential can describe well the transport through the drift tube, the use of two different potentials for the vibration of the peptides reproduces the experimental results much better.

1. I.Litinas and A. D. Koutselos, Structure Distribution of Gaseous Ions in Strong Electrostatic Fields, *J. Phys. Chem. A* **123**, 5683-5691 (2019).

2. Lloyd W. Zilch, David T. Kaleta, Motoya Kohtani, Ranjani Krishnan, and Martin F. Jarrold. Folding and Unfolding of Helix-Turn-Helix Motifs in the Gas Phase. *J. Am. Soc. Mass Spectrom* ,18, 1239-1248 (2007).