Transition from Regular to Stochastic Vibrational Motion in H$_3^+$ Molecule: An ab initio Classical Trajectory Study

P. Babinec$^{a,b}$, E. Jakubíková$^a$, and J. Leszczynski$^b$

$^a$ Department of Biophysics and Chemical Physics, Comenius University, MFF UK, Mlynská dolina F1, 842 15 Bratislava, Slovakia
$^b$ Department of Chemistry, The Computational Center for Molecular Structures and Interactions, Jackson State University, Jackson, MS 39217, USA

Reprint requests to Dr. P. B.; Fax: +(421)-7-654-25-882. E-mail:babinec@fmph.uniba.sk

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An ab initio classical trajectory study of intramolecular vibrational dynamics in H$_3^+$ molecule revealed a transition from regular quasiperiodic to stochastic motion at an energy slightly higher than the zero point vibrational energy.

Key words: H$_3^+$ Molecule; Vibrational Dynamics; ab initio Stochastic Motion.