Transition from Regular to Stochastic Vibrational Motion in H_3^+ Molecule: An ab initio Classical Trajectory Study

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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.