Global Dynamics of nonrigid triatomic molecular systems of three degrees of freedom

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Abstract

In this contribution we present the global dynamical structure of the vibrational motions of triatomic molecular systems such as HO2 and HCP, described by realistic models with three degrees of freedom. Molecules can be considered as hamiltonian systems formed by a collection of nonlinear anharmonic coupled oscillators. For this purpose we construct the frequency map of these systems at different values of the excitation energy. At low energies the frequency maps look like very regular and the frequency lines are very easily identified, while at higher energies, invariant tori are destroyed and spread points due to the presence of chaotic motions appears in certain regions of the frequency map. The subyacent structure of the chaotic region is evident and many resonance lines have been detected to govern the dynamical behavior of the system. The temporal evolution of several trajectories starting at different regions of the phase space have been followed. For Chaotic trajectories the Arnold diffussion has been observed. Finally, we would like to stress that the global picture provided by the frequency analysis makes research in intramolecular dynamics much more efficient, by allowing researchers to target dynamically interesting regions using the map shown in this contribution.