High Resolution Infrared Spectroscopy in Molecular Astrophysics: Observation of H_3^+ in Various Astronomical Objects

Takeshi Oka

Department of Astronomy and Astrophysics and Department of Chemistry, The Enrico Fermi Institute, The University of Chicago, Chicago, IL, USA

Because of the efficient ion-neutral reaction $H_2^+ + H_2 \rightarrow H_3^+ + H$, the H3+molecular ion is the most abundantly produced ion in H2 dominated plasmas. The intense and pure H_3^+ emission from Jupiter has now been well established as a useful probe to study Jovian plasma activity.

Recently H_3^+ with column density of $(1.7\text{-}5.5) \times 10^{14}$ cm^{-2} has been detected in absorption towards the direction of young stellar objects that are deeply embedded in molecular clouds (1,2). Quite unexpectedly, H_3^+ with similar column density has also been detected in diffuse clouds towards the visible star Cygnus OB2 No.12 (3) and with one order of magnitude higher column density towards the galactic center(4).

The H_3^+ chemistry in those clouds together with its astrophysical implication will be discussed.

(1) T.R.Geballe and T.Oka, Nature 384,334 (1996)
(2) B.J.McCall, T.R.Geballe, and T.Oka manuscript in preparation.
(3) B.J.McCall, T.R.Geballe, K.H.Hinkle, and T.Oka, Science 279,1910(1998)
(4) T.R.Geballe, B.J.McCall, K.H.Hinkle, and T.Oka, Ap.J. submitted

QUANTUM MECHANICAL AND SEMICLASSICAL DESCRIPTION OF ROVIBRATIONAL DYNAMICS OF FLOPPY MOLECULES

JAN MAKAREWICZ

Faculty of Chemistry, A. Mickiewicz University, PL-60780 Poland

e-mail: jasiu@rovib.amu.edu.pl

Large amplitude motions, tunnelling splitting and strong centrifugal deformation in floppy molecules are discussed using theoretical tools based on the adiabatic separation of various mode motions and on the self-consistent field treatment of the inter-mode interactions. The quantum molecular states are calculated from the potential energy surfaces (PES) of molecules by employing approximate as well as highly accurate procedures. An analysis of the PES for some triatomic and four-atomic molecules reveals bifurcations which determine a change in the character of the large amplitude motions in excited molecular states.

Qualitative features of the ro-vibrational spectra are discussed in terms of a semiclassical ro-vibrational energy surface (RVES) calculated directly from the PES of a molecule. The bifurcations found in the RVES describe a change in the topology of the surface .As a consequence, a change in the structure of the ro-vibrational energy spectrum is predicted from the RVES. A deep insight into the energy level clusterization effect is gained for symmetric water-like triatomic molecules. The critical values of the angular momentum quantum number and values of the energy barrier responsible for the cluster formation are determined for the ground and excited bending states.

An interesting reorganization of the vibrational polyads in rotationally excited triatomic molecules is revealed and explained on the grounds of the quantum and semiclassical theory.