VIBRATIONAL QUANTUM GRAPHS AND THEIR APPLICATION TO THE QUANTUM DYNAMICS OF CH_5^+

CSABA FÁBRI, *Laboratory of Molecular Structure and Dynamics, Eötvös University, Budapest, Hungary*;
ATTILA CSÁSZÁR, *Research Group on Complex Chemical Systems, MTA-ELTE, Budapest, Hungary*.

The first application of the quantum graph model to vibrational quantum dynamics of molecules is reported. The usefulness of the approach is demonstrated for the astructural molecular ion CH_5^+, an enigmatic system of high-resolution molecular spectroscopy and molecular physics, challenging our traditional understanding of chemical structure and rovibrational quantum dynamics. The vertices of the quantum graph correspond to different versions of the molecule (120 in total for CH_5^+), while the differently colored edges represent different collective nuclear motions transforming the distinct versions into one or another. These definitions allow the mapping of the complex low-energy vibrational quantum dynamics of CH_5^+ onto the motion of a one-dimensional particle confined in a quantum graph. The quantum graph model provides a simple and intuitive qualitative understanding of the intriguing low-energy vibrational dynamics of CH_5^+ and is able to reproduce, with just two adjustable parameters related to the two different motions (indicated by the red and blue lines in the figure), the lowest vibrational energy levels of CH_5^+ (and CD_5^+) with remarkable accuracy.