Molecular spectroscopy using ion traps

1. Introduction

For the spectroscopy of charged molecules, ion trap setups can be used. They offer the advantages of cooling to cryogenic temperatures and mass selection. In this experiment, the linear molecular cation $HCCCO^+$ is investigated by its C-C stretching in the 5µm region. For this, a novel technique, called leak-out-spectroscopy (LOS), is applied.

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2. Experimental Setup

The typical setup for spectroscopic experiments in ion traps is shown above. Ions are generated in an ion source by electron bombardment of a suitable precursor (gas or vapour), and pulses of these ion bunches are extracted, mass selected in a first quadrupole mass selector (QMS I), and steered via a quadrupole bender (QB) into the ion trap. There, they are cooled via He buffer gas to low temperatures, and stored for several 100 ms. During this storage time, the massselected ions are exposed to a high-resolution laser beam crossing the ion trap. In case the laser frequency is resonant with a rovibrational transition of the stored ion, a part of the initial photon energy may be transferred to kinetic energy of the ion (see details below). This accelerated ion may then escape the trap in the direction of the second quadrupole mass selector (QMS II) and be counted in the high-efficiency ion detector. By repeating these storage cycles (at typically 1 Hz), and counting the escaping ions as a function of the excitation frequency, an action spectrum can be recorded.

3. The method: leak-out-spectroscopy



The spectroscopic method used here is called leak-out-spectroscopy (LOS). It is based on the collision-induced transfer of vibrational energy into kinetic energy which is illustrated in the Figure above. Imagine a molecular ion stored in a cryogenic ion trap. Upon resonant absorption of a laser photon, the molecular ion can be lifted into a vibrationally excited state. If this excited ion collides with a neutral non-reactive particle (e.g. N₂ or Ne), a part of this energy may be released into kinetic energy of the two collision partners. The accelerated ion can then escape, or leak out of the trap (hence the name of the method) along the direction of QMS II (see the Setup) to the ion detector, where it is counted. This produces spectra with very low background counts and thus high signal-to-noise ratio.

4. Typical results



Rovibrational Leak–Out Spectrum of the v₃ C–C Streching Mode of HC₃O⁺

The aim of the experiment is to measure (a part of) the ro-vibrational C-C-stretching vibration of the linear ion HCCCO⁺ (see Figure above). As light source, a quantum cascade laser operating in the 5 μ m region (about 2000 cm⁻¹) is applied.