THE UNIVERSITY of ADELAIDE

Infrared Spectroscopy of Astrophysically Relevant Molecules

Masters of Philosophy Thesis

School of Physical Sciences (Chemistry)

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Abstract

This thesis involves use of the Terahertz & Far-Infrared Beamline facility at the Australian Synchrotron to record spectra and try to resolve the rotational fine structure of species having astrophysical relevance. The primordial nature of hydrogen makes understanding its interaction with other species interesting in terms of the origin and evolution of interstellar media and planetary systems. The interaction of molecular hydrogen with rare gas atoms constituted some of the first spectroscopic experiments on van der Waals complexes, and part of this thesis involves extending this body of work to the far-infrared spectra of H_2/D_2–Xe. The high polarisability of Xe makes the complex an "easy" spectroscopic target, and attempts at collecting high resolution spectra of the H_2/D_2–Xe complexes were successful. From rare gas species the field evolved into the interaction of H_2 with other homonuclear diatomics such as N_2 and O_2, and this thesis expands on a previous far-infrared study on H_2–O_2 by providing and analysing the mid-infrared spectra of H_2–O_2 and the far-infrared spectra of D_2–O_2. Spectroscopic signatures of interstellar molecules provide the foundation for experimental studies into astronomically relevant systems such as vinyl alcohol, which was observed towards Sagittarius B2(N) in 2001. The second and major component of this thesis involves the analysis of the torsional bands of vinyl alcohol. The fundamental and first two hot bands of *syn*-vinyl alcohol are observed, along with the first infrared observation of the *anti* rotamer, including the fundamental and first hot band. High resolution far-infrared spectroscopy is used, with the assistance of computational calculations and a spectral analysis program, to refine the ground state, and provide accurate excited state, rotational and centrifugal distortion constants as well as the determination of relative rotamer abundance. Far-infrared spectra of monodeuterated vinyl alcohol, CH_2CHOD, is also presented, similarly showing the OD torsional fundamental and first two hot bands of *syn* rotamer, and the fundamental and first hot band of the *anti* rotamer.

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