HOW MUCH DO WE KNOW (AND STILL NEED TO LEARN) ABOUT THE METHANOL MOLECULE?

LI-HONG XU, *Department of Physical Sciences, University of New Brunswick, Saint John, N.B., Canada E2L 4L5.*

The spectroscopy of methanol has acquired great importance in a wide number of areas and applications in recent years. This talk will give an overview of our current knowledge from a fundamental high-resolution spectroscopic point of view. Details of the topics covered are outlined below: 1. Methanol and most of its isotopomers have been systematically studied in the MW and FIR regions for the ground state. Recently, efforts have been directed successfully towards global modeling of the first two torsional levels using a one-dimensional large-amplitude Hamiltonian in order to obtain reliable molecular parameters, ground-state energies and transition strengths, and to consolidate our extensive ground-state information to be most useful to the astronomical community. 2. The CO-stretch fundamental overlaps well with the CO_2 laser bands so has important application for IR pumping of FIR lasers. To extend the range of IR tuning coincidences, almost every existing methanol isotopomer has been examined exhaustively for CO_2-pumped FIR laser emission. So far, the CO-stretch spectra also have been studied for the majority of the isotopomers, allowing us to contribute extensively to identification of the laser transitions. 3. Above the strong CO-stretch fundamental in methanol lies a broad and ambiguous region of weak bands including the methyl rock and deformation and the OH bend. We are now making steady progress in this rich but messy region of long-standing mystery in terns of subband analysis. However, the question of the detailed vibrational and even torsional assignment of the upper-state levels sometimes remains undetermined. 4. Most recently, the 3 μm methanol spectral bands have been revisited with both molecular beam and FT techniques, and a more complete energy picture with substantial K coverage is now emerging. A driving force behind this is the dramatic observations of these bands in recent comets and the increased needs from the cometary community. It is fair to say that the ground state of methanol is largely under control, providing firm ground for IR band analysis. In contrast, none of the assigned IR bands, even the lowest-lying CO-stretch, has been interpreted successfully with a global approach. We are not satisfied with this situation! Thus, $abinitio$ tools are being adapted to explore the torsional dependence of atomic displacements and vibrational force constants. This should give the information needed to model the methanol fundamentals with a newly designed formalism.