LABORATORY AND ASTRONOMICAL SPECTROSCOPY OF REACTIVE HYDROCARBONS

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ABSTRACT. The rotational spectra of C_3H_2, C_3H, and C_2D, molecules not previously studied, were investigated in a continuing program of mm-wave spectroscopy in space and in the laboratory of hydrocarbons of astrophysical interest. Laboratory measurements producing reactive species in a DC glow discharge through organic gases have been essential to the identification of these species.

1. INTRODUCTION

A combination of astronomical and laboratory spectroscopy of reactive molecules has been very useful in identification of "nonterrestrial" species. Here we summarize our recent work on three such molecules. Laboratory production has permitted rapid, flexible frequency measurements over most of the mm-wave band and the application of tests to assist in identification of carriers of the lines observed. We found that a DC glow discharge through gas mixtures containing acetylene produces a rich variety of reactive hydrocarbons.

2. C_3H_2: THE FIRST HYDROCARBON RING IN SPACE

The cyclopropenylidene radical, C_3H_2, a planar, oblate, asymmetric top, is the first organic ring detected in space. Its identification from a total of 27 lines (22 laboratory, 11 astronomical, 6 overlapping) is now secure. The molecular constants have been determined to high accuracy, and the frequencies of the astronomically most interesting lines can be predicted to better than one part per million (Thaddeus, Vrtilek, and Gottlieb 1985). Identification of C_3H_2 was initiated by laboratory detection of the carrier of the strong astronomical line at 85338 MHz first observed in 1976 but not assigned until now. Measurement of additional laboratory lines and assignment of further astronomical lines, including the strong, ubiquitous one at 18343 MHz (Matthews and Irvine 1985), confirmed the tentative identification as C_3H_2. There is good agreement of the molecular constants with those predicted

M. S. Vardya and S. P. Tarafdar (eds.), Astrochemistry, 87–88.

ab initio. Highly polar (3.3 D), with strong lines observed along many lines of sight in the Galaxy, C_3H_2 may be a generally useful molecular probe.

3. C_3H

The propynylidyne radical is a linear chain molecule with $^2\Pi$ electronic ground state. C_3H was identified in the mm-wave spectra of IRC+10216 and TMC-1 (Thaddeus et al. 1985), filling the gap in the sequence of linear carbon-chain molecules. Its column density in IRC+10216 is $3x10^{13}$ cm^{-2}, about an order of magnitude less than that of either C_2H or C_4H. The identification of C_3H rests on 13 frequencies measured in space and 34 in the laboratory, with 6 detected in both. An accurate set of spectroscopic constants (Gottlieb et al. 1985) allows the spectrum to be calculated into the submillimeter range to an accuracy equivalent to 0.1 km s^{-1} in radial velocity (Gottlieb et al. 1986).

4. C_2D: A NEW DEUTERATED SPECIES

We detected C_2D first in a laboratory discharge in a search based on ab initio calculation and then using the Bell Labs 7m antenna at and near the KL position in Orion (Vrtilek et al. 1985). Two rotational transitions were measured in the laboratory, N=1-2 and 2-3. The derived molecular constants are in excellent agreement with those obtained independently by Bogey, Demuynck, and Destombes (1985). In Orion, measurement of the N=2-1 transition NE of the KL position gave a C_2D column density of $1.8x10^{13}$ cm^{-2} and an isotopic ratio $N(C_2D)/N(C_2H)=0.05$, in agreement with the ratio obtained by Combes et al. (1985). Since CCD lines can be readily detected, this deuterated species should be a useful probe of deuterium fractionation and molecular cloud evolution.

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