Difficulties in Laboratory Studies and Astronomical Observations of Organic Molecules: Hydroxyacetone and Lactic Acid

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Abstract

Organic molecules in interstellar space likely play a role in prebiotic chemistry. Hence, it is very important to properly identify the organic species present and to accurately evaluate their abundance. Owing to the rich molecular spectra found in many interstellar sources, accurate laboratory rest frequency measurements are crucial to accomplish these goals.

Two key molecules are hydroxyacetone and lactic acid. A previous study on hydroxyacetone by Kattija-Ari and Harmony (1980) was not extensive enough to accurately predict even the A-state of this molecule, which has a methyl internal rotor. The E-state proved even more difficult as they found the molecule to possess a very low barrier to internal rotation. A more recent study by Braakman et al. (2005) provided rest frequencies for the A-state by measuring its spectrum at 3 mm and 1 mm, but they too reported that a definitive assignment of the E-state was proving difficult. Just prior to that time, we started measuring the microwave spectrum of hydroxyacetone, which was critical for the assignment of the E-state. We have now extended those measurements to cover the entire spectrum at 3 and 2 mm, where the strongest low-K interstellar transitions are predicted. Using the methods described for fitting low-barrier molecules by Hougan and co-workers and a modified computer code provided by Kliener et al., we now have fitted rotational constants that reproduce the data to experimental accuracy in both the A- and E-states simultaneously. The application of these methods will be described.

An extensive interstellar search has been conducted for hydroxyacetone based on these new laboratory results, as well as for lactic acid. Upper limits to the abundance of these species will be reported along with a discussion of problems in identifying these and other organic species owing to a high degree of spectral confusion.

Reference:

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Kattija-Ari and Harmony, Inter. J. Quant. Chem., 14, 443 (1980)
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