COMBINED MICROWAVE AND MILLIMETER WAVE STUDIES OF THE MOLECULES HYDROXYACETONE AND LACTONITRILE

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The molecules hydroxyacetone and lactonitrile are attractive candidates for astrophysical studies because they exhibit the next level of chemical complexity, yet still remain similar in size to other already identified species. Previous spectroscopic work[ab] in the early 1980s on these two species proved insufficient for interstellar searches. In each of these early studies, course measurements over a very small frequency range (10 to 40 GHz) made it impossible to accurately predict frequencies useful for astronomical observations. Last year at this conference, Braakman et al.[c] reported the rotational spectrum of hydroxyacetone at 3 mm and 1 mm wavelengths, but reported that they were having difficulties with the E-state assignment presumably owing to its low-barrier internal rotor. In March 2005, we independently measured the spectrum of hydroxyacetone at 3mm, 2mm and also in the microwave region using our newly constructed Fourier transform microwave spectrometer. The E-state microwave lines led us to several misassignments in the original spectroscopy paper. We now have a global fit of the A- and E-states of hydroxyacetone for J<31 and K<8 using a code provided by Isabella Kleiner for internal rotors. The rho-axis code included the eigenfunction decomposition method outlined in Mekhtiev and Hougen[d] and was subsequently modified with the second diagonalization routine outlined by Ilyushin[e]. We are currently working on assigning the first torsional state. Work has just started on Lactonitrile and at present we cannot located the ground state conformer. The two series reported by Corbelli and Lister did not produce lines in our cold molecular beam source; hence it is likely that those lines are from some excited vibrational states or other high energy conformers.

[a] Kattija-Ari and Harmony, (1980), Int. J. of Quant. Chem.: Quant. Chem. Symp., 14, 443
[b] Corbelli and Lister, (1981), J. Mol. Struct., 74, 39
[c] Braakman et al., (2005), The 60th International Symposium on Molecular Spectroscopy, RA07
[d] Mekhtiev and Hougen, (1998), J. Mol. Spectr., 187, 49
[e] Ilyushin, (2004), J. Mol. Spect., 227, 140