THE HIGH RESOLUTION SPECTRUM OF JET-COOLED METHYL ACETATE IN THE C=O STRETCH REGION

FUMIE X. SUNAHORI, NICOLE BORHO, XUNCHEN LIU, AND YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2*.

Methyl acetate (MA) has two inequivalent methyl tops, i.e., the acetyl CH_3 and methoxy CH_3 groups, which have significantly different internal rotation barrier.[a] One previous study[b] has reported that coupling of the carbonyl stretching mode with the methyl rotor modes in MA plays significant roles in internal vibrational redistribution (IVR), whose effect has been observed in the FT-IR spectrum of carbonyl band of MA. Surprisingly, the jet-cooled high resolution ro-vibrational spectrum of MA in the C=O stretch region we recorded does not show strong IVR effect. The spectrum was measured by a rapid scan infared laser spectrometer equipped with an astigmatic multipass cell. Using the ground state combination differences calculated from the rotational constants of the vibrational ground state determined by a global fit of the microwave and millimeterwave lines,[c] the spectral assignment of the C=O stretching band has been made. The spectroscopic constants of the vibrationally excited state have been determined. The spectrum of deuterated MA has been also recorded in high resolution, and the difference in the degree of IVR in the isotopically substituted MA will be discussed.

[a] J. Sheldan, W. Bossert, and A. Bauder *J. Mol. Spectrosc.* **80**(1), 1980.
[b] V. A. Walters, S. D. Colson, D. L. Snavely, K. B. Wiberg, and B. M. Jamison *J. Phys. Chem.* **89**(3857), 1985.
[c] M. Tudorie and I. Kleiner, private communication.