INFRARED SPECTROSCOPY OF CH_5^+

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Ab initio calculations predict that protonated methane, CH_5^+, has three low energy structures that are practically equal in energy and that barriers separating their 120 equivalent minima are low[a]. Thus CH_5^+ provides a new prototype of spectroscopic specimen in which the five equivalent protons are attached to the central carbon atom[b]. We reported preliminary observations of a CH stretch vibration-rotation spectrum of CH_5^+ in the 1997 International Symposium on Molecular Spectroscopy at the Ohio State University. We have now completed the observation and have identified transitions of CH_5^+ based upon plasma chemical behavior and line widths. Contamination by transitions of other single carbon cations has been ruled out by plasma chemical behavior, comparison with known spectra, by quantitative modeling of the plasma, and by previous mass spectrometric studies of similar plasmas[c] Contamination by transitions of 2 carbon cations has been ruled out by line width and also by unsuccessful attempts at observing such spectra using plasma chemistry strongly favoring the production of cations containing 2 carbons. Contamination by heavier cations can be ruled out definitively by line width. Altogether, **700** spectral lines have been measured between 3130 cm^{-1} and 2770 cm^{-1}. The overall spectral pattern agrees approximately with the low resolution spectrum of the CH_5^+ substructure in CH_7^+[d]. Detailed analysis of the CH_5^+ spectrum appears hopeless at this stage due to large tunneling splitting. An attempt is being made to observe the spectrum of CD_4H^+ with the hope that it may be simpler. Our current progress will be reported.

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[c] J. C. Owrutsky, Ph.D. Thesis, University of California, Berkeley, 1989.
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