THE INFRARED SPECTRUM OF CH_5^+

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Protonated methane, CH_5^+, has unusual C-H bondings and is a new prototype of spectroscopic specimen. While all of the five protons are strongly bound to the central carbon atom with well defined C-H stretch potentials, angles between C-H bonds are highly fluxional. Ab initio theory predicts lowest energy for an "equilibrium structure" with C_s symmetry but the barriers separating the 24 equivalent structures are extremely low and almost non-existent when zero point vibrations are taken into account.[a,b]

We have identified nearly 1000 spectral lines of CH_5^+ in a liquid N_2-cooled hydrogen dominated plasma using a gas mixture of H_2:CH_4 $\sim$ 100:1.[c] The spectral lines are weak and do not show obvious symmetry or regular pattern. The identification required extensive studies of the spectra of other carbocations CH_3^+ (and CH_2^+) and $C_2H_3^+$ (and $C_2H_2^+$) whose spectra appear in the same wavelength region with much higher intensities. Spectroscopy and plasma chemistry of those carbocations will be discussed and the raw observed spectrum of CH_5^+ will be presented without assignment nor even qualitative understanding.

[a] P. R. Schreiner et al., J.Chem.Phys. 99, 3716 (1993)
[b] H. Mueller et al., J.Chem.Phys. 106, 1863 (1997)
[c] E. T. White, J. Tang and T. Oka, Science 284, 135 (1999)