INFRARED SPECTRUM OF THE ν_1 FUNDAMENTAL BAND OF H_3O^+

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Infrared spectrum of H_3O^+ has been observed by a difference frequency laser spectrometer with positive column discharges of H_2/O_2 gas mixtures, which gave a spectrum remarkably simpler than the previous one with H_2/O_2/He discharges.[a] After extending the previous assignment of the ν_3 fundamental bands to higher J, K transitions, vibration-rotation structures due to the $\nu_1^+ \leftarrow 0^-$ and $\nu_1^- \leftarrow 0^+$ bands of H_3O^+ were identified with the band origins of 3389.66 cm^{-1} and 3491.17 cm^{-1}, respectively, in the region of the strong $\nu_3^\pm \leftarrow 0^\pm$ bands. Molecular constants for the $\nu_1^\pm \leftarrow 0^\mp$ bands were obtained by the least-squares fittings for the observed frequencies. Coriolis interactions between the ν_1 and ν_3 vibrations have been considered to explain some large deviations of the observed transitions from the calculated frequencies in the ν_1 and ν_3 bands.

[a] W. C. Ho, C. J. Pursell, and T. Oka, J. Mol. Spectrosc. 149, 530 (1991).