MICROWAVE SPECTRA OF THE HCS AND THE HSC RADICALS

H. HABARA, S. YAMAMOTO, *Department of Physics, The University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan*.

The 1_{01}–0_{00} rotational transition of the HCS radical in the $\tilde{X}^2A'$ electronic ground state was observed in our laboratory using the Fourier transform millimeter-wave (FTMW) spectrometer [a]. The HCS radical was generated in a free expansion molecular gas which was prepared by discharging a hydrogen sulfide and methane mixture diluted in argon. On the basis of the measurements of the 1_{01}–0_{00} transition, we also observed higher-N rotational transitions of HCS using a conventional millimeter- and submillimeter-wave spectrometer combined with a glow discharge cell. In this case, the HCS radical was produced by discharging a gaseous mixture of hydrogen sulfide and carbon monoxide. A series of the a-type R-branch pure rotational transitions with K_a = 0 was observed up to 362 GHz. Molecular constants including hyperfine interaction terms were determined accurately from the observed frequencies. The Fermi contact term of the hydrogen nucleus of HCS is found to be 127 MHz, which is much smaller than that of HCO (389 MHz). This implies the quasi-linear nature of HCS.

During a search for the $K_a \geq 1$ lines of HCS, other strong paramagnetic lines that showed the K-structure pattern of an asymmetric free radical were observed. This strong spectrum was observed in the same experimental condition as the HCS radical. Judging from the rotational constants (A= 295 GHz, B= 21.0 GHz, and C= 19.6 GHz), we concluded that these lines are due to the HSC radical in its $\tilde{X}^2A'$ electronic ground state, which is the structural isomer of the HCS radical. There is no experimental study of the HSC radical so far. More than one hundred transitions lines including a-type R-branch and b-type Q-branch rotational transitions were measured for HSC, and nineteen molecular constants were determined accurately.

[a] H. Habara, S. Yamamoto, C. Ochsenfeld, M. Head-Gordon, R.I. Kaiser, and Y.T. Lee, J. Chem. Phys. 108, 8859 (1998).