Microwave Spectroscopy of Isothiazole

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Five-membered ring structure are found in some amino acids. In addition, five-membered ring cyanocyclopentadiene has been identified toward TMC-1 [1]. Therefore isothiazole (C_3H_3NS) is a potential interstellar molecule of five-membered ring with two adjacent hetero atoms, nitrogen and sulfur. Previous studies of microwave spectroscopy have been conducted below 35 GHz including information on the dipole moment, isotopologues, and the Zeemann effect [2-4]. The *a*-axis and *b*-axis components of the dipole moment are doubled by 1.1 D and 2.2 D, respectively. Information on higher frequency range is essential for future detection.

In this study, microwave spectroscopy of isothiazole was performed in the 40-360 GHz region at room temperature at the University of Toyama and University of Wisconsin–Madison. The assignment was based on the frequency prediction using molecular constants from previous high-resolution infrared studies [5,6]. The spectra were analyzed by using AABS package.[7] Figure 1 shows an example. Over 2000 lines were assigned and analyzed using Watson's *A*-reduced Hamiltonian.

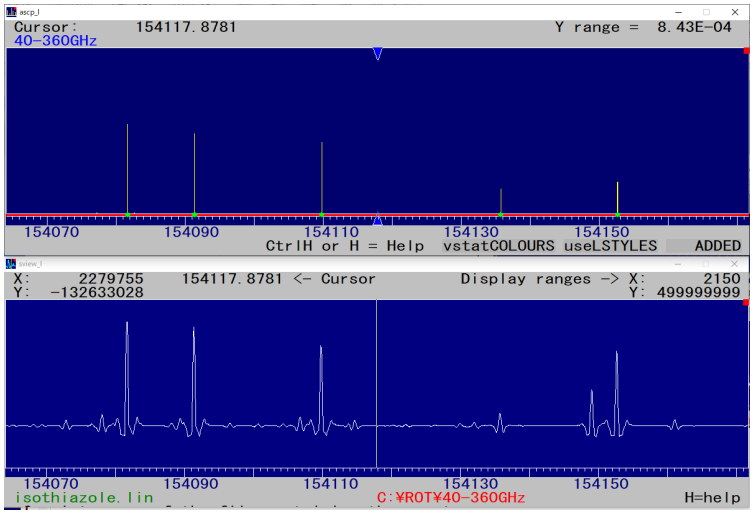

Figure 1: The spectrum and the frequency prediction of isothiazole.

References

[1] M.C. McCarthy, K.L.K. Lee, R.A. Loomis, A.M. Burkhardt, C.N. Shingledecker, S.B. Charnley, M.A. Cordiner, E. Herbst, S. Kalenskii, E.R. Willis, C. Xue, A.J. Remijan, B.A. McGuire, Nat. Astron. 5 (2021) 176–180.
[2] J.H. GRIFFITHS, A. WARDLEY, V.E. WILLIAMS, N.L. OWEN, J. SHERIDAN, Nature. 216 (1967) 1301–1301.
[3] J. Wiese, D.H. Sutter, Zeitschrift Für Naturforsch. A. 35 (1980) 712–722.
[4] J. Gripp, U. Kretschmer, H. Dreizler, The 33S Nuclear Hyperfine Structure in the Rotational Spectrum of Isothiazole, Zeitschrift Für Naturforsch. A. 49 (1994) 1059–1062.
[5] F. Hegelund, R. Wugt Larsen, R.A. Aitken, H. Kraus, F.M. Nicolaisen, M.H. Palmer, Mol. Phys. 102 (2004) 1583–1595.
[6] F. Hegelund, R.W. Larsen, R.A. Aitken, M.H. Palmer, J. Mol. Struct. 780–781 (2006) 45–56.
[7] Z.Kisiel, L.Pszczolkowski, I.R.Medvedev, M.Winnewisser, F.C.De Lucia, E.Herbst, J.Mol.Spectrosc. 233, (2005) 231-243.