The Microwave Spectroscopy of Ground State CD_3SH

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Methyl mercaptan (methanethiol, CH_3SH) is an interstellar organic molecule containing sulfur. We have studied an isotopologue, CD_3SH by using microwave spectroscopy. In this study, 484 A-species transitions up to $J = 46$ and $K_a = 10$ and 581 E-species transitions up to $J = 46$ and $K_a = 10$ in the ground state were least-squares-analyzed by using the pseudo-principal axis method (PAM) Hamiltonian with 22 parameters consisting of rotational, centrifugal distortion, and internal-rotational constants.

The methyl mercaptan molecule has similar molecular structure to methanol and its rotational spectra has also similar characteristics including torsional-rotational interaction. This molecule was also identified in interstellar Sgr B2 in 1979 [1]. The triply-deuterated methanol, CD_3OH was found in IRAS 16293-2422 [2] encouraged us to study this CD_3SH molecule. Previous microwave studies on this molecule are limited [3-5].

We also introduced pseudo-principal axis method (pseudo-PAM) [6], which was successfully applied to the analysis of the $HCOOCH_3$ in the second torsional excited state. The internal-rotation parameter ρ of methyl formate is about 0.08, which is fairly small, while CD_3SH has much larger ρ of about 0.8.

The spectra was taken by the conventional Stark/source-modulation microwave spectrometer. The enriched sample was purchased from the manufacturer (MSD isotopes) and used without further purification. The 12-240 GHz frequency region was observed at room temperature without gap. Fig. 1 shows an example spectrum.

Based on the preceding studies, we were able to make predictions and to extend the assignments. In total, we analyzed 1065 transitions by using the pseudo-PAM method. The comparison with the rho-axis method (RAM) will be shown.

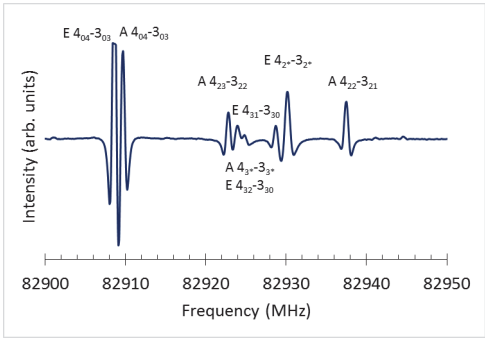

Fig. 1 Spectrum of CD3SH in the ground state. The asterisk denotes the unresolved K doublets.

References

[1] R. A. Linke, M. A. Frerking, and P. Thaddeus, 234 (1979) Astrophys. J., L139-L142.
[2] B. Parise, A. Castets, E.Herbst, E.Caux, C. Ceccarelli, I. Mukhopadhyay, and A. G. G. M. Tielens, 416 (2004) Astron. Astrophys., 159.
[3] T. Kojima, J. Phys. Soc. Jpn., 15 (1960) 1284-1291.
[4] Akihiro Kimura, University of Toyama, Master's Thesis (1983).
[5] Tomoaki Hayashi, University of Toyama, Master's Thesis (1990).
[6] K. Kobayashi, K. Takamura, Y. Sakai, S. Tsunekawa, H. Odashima, N. Ohashi, Astrophys. J. Suppl. Ser. 205 (2013) 9-15.