

Absorption spectroscopy of the electronic transition of thiophenoxy radical

H. Sato, M. Negishi, M. Araki, T. Oyama and K. Tsukiyama

Department of Chemistry, Tokyo University of Science, Japan

Diffuse Interstellar Bands (DIBs) are absorption bands by molecular cloud between the earth and stars. Several hundreds of bands have been detected, but no bands have been assigned except for the five ones of C_{60}^+ . Recently benzonitrile C_6H_5CN was firstly discovered in a dark cloud by radio observations. Hence, we focus on the thiophenoxy radical C_6H_5S as a candidate of DIBs. To compare DIBs with the thiophenoxy radical, the strongest peaks of this radical need to be measured in a laboratory. Shibuya *et al.* reported fluorescence excitation spectra of the ${}^2A_2-X{}^2B_1$ electronic transition of this radical [1]. From their spectra, it was mentioned that the origin band produces the strongest peak. However, Araki *et al.* observed absorption spectrum of phenoxy radical C_6H_5O and found that the vibronic bands are stronger than the origin band [2]. The fact suggests that intensities of higher vibronic bands of the thiophenoxy radical are lost by radiationless transitions in the fluorescence excitation spectra. Thus, absorption lines of vibronic bands of the thiophenoxy radical were expected to be stronger than that of the origin band. We observed the high-resolution absorption spectrum of C_6H_5S by cavity ring down spectroscopy in the resolution of 0.005 \AA in a laboratory. The radical was produced by pulsed discharge with a hollow cathode using a gas mixture of thiophenol C_6H_5SH and helium in a cell. The absorption bands were measured in the $4721\text{--}5168 \text{ \AA}$ region as shown in Figure 1. The observed strong bands were assigned to the $6a$ and $6b$ mode based on the previous works [3-5] and our quantum chemical calculation (B3LYP/6-311++G(d,p)). We found that the strongest band in the ${}^2A_2-X{}^2B_1$ electronic transition of this radical is the $6a_0^26b_0^1$ vibronic band. This band may appear as DIB if sufficient amount of this radical exists in interstellar medium.

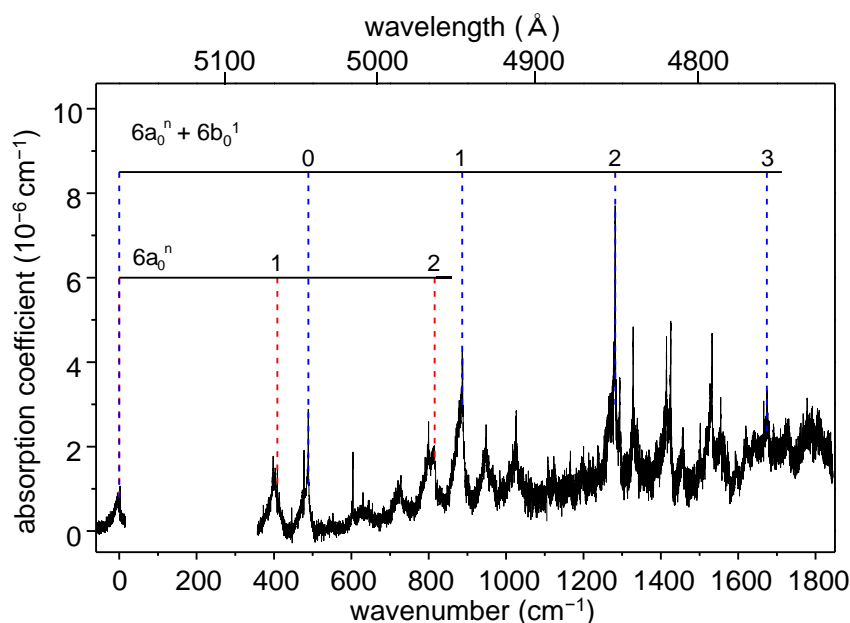


Figure 1: Absorption spectrum of the ${}^2A_2-X{}^2B_1$ electronic transition of thiophenoxy radical

References

- [1] K. Shibuya *et al.*, 1988, Chem. Phys. 121, 237. [2] M. Araki *et al.*, 2015, AJ 150, 113. [3] J. Spanget-Larsen *et al.*, 2001, J. Am. Chem. Soc. 123, 11253. [4] M. Araki *et al.*, 2014, AJ 148, 87. [5] M. Fukushima *et al.*, 2005, SPSJ, Proceedings, Spring, 125.