A common spectral characteristic of several benzoyl compounds at about 0.8 THz

Zhao Hongwei, Ge Min, Han Jiaguang, Li Qingnuan, Wang Wenfeng
Shanghai Institute of Applied Physics, Chinese Academy of Sciences, 2019 Jialuo Road, Jiading, Shanghai, China
201800,zhaohongwei@sinap.ac.cn

***Abstract*-We have found that several different chemical compounds with benzoyl group have a similar absorption peak around 0.8 THz. Quantum chemical calculation results suggest the motion at about 0.8 THz is assigned as butterfly mode between the two phenyl rings.**

I. INTRODUCTION

Terahertz time-domain spectroscopy (THz-TDS) can provide useful THz fingerprint information of materials [1]. Compounds with benzoyl group are a kind of popular chemical materials which are always used in organic synthesis and pharmaceutical intermediates. Investigating the low-frequency characteristic of these compounds will help understanding their structures and dynamic behaviors.

II. EXPERIMENT AND DISCUSSION

Benzophenone (1), Benzamide (2), 2-Hydrobenzophenone (3), 4,4'-Dihydroxybenzophenone (4), 4,4'-Dimethoxybenzophenone (5), 2,2'-Dihydroxy-4,4'-dimethoxybenzophenone (6) were purchased from Acros and used without further purification. The samples were prepared by milling with spectral purity polyethylene powder and made into pellets with thickness about 1.5 mm. THz-TDS apparatus used in our experiments and corresponding experimental data analysis method have been discussed in previous reports [2]. All experiments were carried out at room temperature.

THz absorption spectra of the compounds mentioned above are shown in Fig. 1. Different absorption spectra have been measured in those compounds. It indicates THz-TDS is sensitive to ingredient and structure of chemical compounds. An interesting phenomenon is all of these compounds have a common absorption peak at about 0.8 THz.

Quantum chemical calculations and simulations have been used to study those molecular geometric structures and low-frequency vibrations to insight into their vibrational modes and THz spectra. The calculation results suggest that the common motion at about 0.8 THz is assigned as butterfly mode between the two phenyl rings. Whether the common absorption is a universal and particular characteristic of this kind of structural compounds is undergoing study.

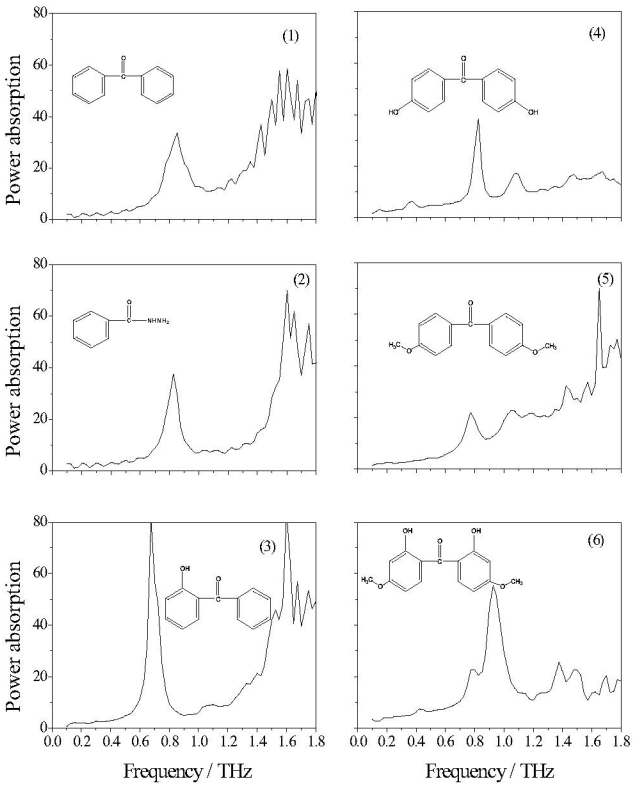

Figure 1. THz absorption spectra and structures of the title compounds.

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