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论文

中药冬虫夏草二维红外光谱理论研究

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摘要:

冬虫夏草是一种名贵的中药材,有非常广泛的用途.为了探索这种中药整体的药理特征,本文将这种中药作为一个整体,将其一维线性谱的吸收峰视为简正模.在假定各模式之间的相互作用与偶极矩的大小后,建立了激光与冬虫夏草相互作用微观模型.在此基础上,理论计算了冬虫夏草的二维非线性激光谱,并将所得光谱图与实验结果比较,从而确定冬虫夏草的能级结构与各简正模式间的耦合强度以及其偶极矩的大小等,为深入研究这种名贵中药提供了一个全新的思路与方法.

关键词: 冬虫夏草 二维红外光谱 简正模式 激子模型

Theoretical Studies of Two-dimensional IR Spectroscopy for Traditional Chinese Medicine Cordyceps Sinensis

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Abstract:

Cordyceps sinensis is a kind of precious Chinese herbal medicine that is good for medical treatment and health care. The pharmacological characteristics of this kind of medicine is not based on a single or few kinds of chemical substances but on the whole constituted with all elements. In order to explore the pharmacological characteristics, this paper takes the Chinese herbal medicine, cordyceps sinensis as the whole, and the absorption peaks of the one-dimensional linear spectrum of the medicine as normal modes. The Hamiltonian of interaction between laser and cordyceps sinensis is modeled based on assuming the interaction intensity between modes and the size of the dipole moment resulting from laser irradiation. Then the two-dimensional third-order nonlinear laser spectra of the cordyceps sinensis are calculated. The theoretical spectra are adjusted with the experimental ones, thus the level structure, the coupling strength between each normal modes, and the dipole moment of each mode for the cordyceps sinensis can be obtained. This is a new method of the pharmacological researches for the valuable Chinese herbal medicine.

Keywords: Cordyceps sinensis Two-dimentional IR spectroscopy Normal modes Exciton model

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