

論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Theoretical and Experimental Study of the Radiative Ortho-Para Transition in Disulfur Dichloride
著者(和文)	デ`ガ`ニクワテイセ`イナブ`
Author(English)	Zeinab Dehghanitafti
出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第10928号, 授与年月日:2018年7月31日, 学位の種別:課程博士, 審査員:金森 英人,上妻 幹旺,松下 道雄,西田 祐介,相川 清隆,旭 耕一郎, 遠藤 泰樹
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第10928号, Conferred date:2018/7/31, Degree Type:Course doctor, Examiner:,,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

(論文博士)
(Dissertation Doctorate)

論 文 要 旨 (英 文) (800語程度)

Dissertation Summary (approx. 800 words in English)

報告番号 For administrative use only	乙 第 号	氏 名 Name	Zeinab DEGHANI TAFTI
---	-------	-------------	----------------------

(要 旨)

(Summary)

Transition between the pure *ortho* and *para* states is theoretically impossible. Nevertheless, some inner perturbation effects, as collision and hyperfine interactions, can change the pure symmetrical character of molecular wave function to an impure character. In such cases, the electric dipole transition between two molecular states with opposite symmetries is theoretically possible, by intensity borrowing.

The present dissertation mainly aimed to respond theoretically and experimentally to this question that “which physical and spectroscopic parameters could determine possibility of the radiative *ortho-para* transition in an asymmetric top molecule via study of S_2Cl_2 .”

Chapter 1 proposes a review concerning the previous studies conducted on the *ortho-para* interaction in order to provide a background for the study. Moreover, a review on microwave spectroscopy of disulfur dichloride is discussed. Chapter 2 explains the general theories applied in this study, involving the proposed rotational and nuclear quadrupole Hamiltonian for symmetric rotors. In fact, they demonstrate a common way to find the asymmetric top Hamiltonian in the symmetric rotor basis set. In addition, this chapter demonstrates the method to find the transition moment in symmetric and asymmetric top molecules as well as the selection rules.

The millimeter wave spectroscopy is done for determination of the spectroscopic parameters of S_2Cl_2 . Gas cell and supersonic jet spectroscopies involve the two different experimental setups being applied in the present study. As a result of microwave spectroscopy, all rotational molecular constants including fourth and sixth order centrifugal distortion constants of disulfur dichloride were determined for the first time. The measured frequency region was from 75GHz to 100GHz and the highest determined quantum numbers were $J = 55$ and $K_a = 12$. Chapter 3 describes the experimental techniques used in this study, consisting of supersonic jet and gas cell experiments. The techniques applied in these setups are also explained in this chapter, involving supersonic jet expansion, lock-in amplifier, and frequency modulation. Chapter 4 discusses details of millimeter wave spectroscopy of disulfur dichloride. By analyzing the data obtained in this step, the rotational and hyperfine constants of S_2Cl_2 in the millimeter wave region can be obtained. In fact, these spectroscopic constants are utilized in the following chapters to investigate the *ortho-para* interaction. Identifying the rotational spectroscopic constants in the millimeter wave region caused the matrix elements of disulfur dichloride molecular Hamiltonian to be calculated. By knowing the Hamiltonian matrix

elements of this molecule, the term energies and molecular wave functions were determined. These molecular wave functions were used in regard with finding the *ortho-para* mixed states. The molecular wave functions were directly used in order to find the *ortho-para* mixing coefficients for the first time. Chapter 5 proposes the *ortho-para* interaction theoretically. The theory of finding the *ortho-para* mixed states is improved, by which a list of *ortho-para* mixed states is calculated. The study results concerning the *ortho-para* mixed states search reveal the *ortho-para* mixing coefficients for some K_a -doubling states of disulfur dichloride in the millimeter wave region are so high that direct observation of the radiative *ortho-para* transition could be regarded possible. Lists of the *ortho-para* mixed states were given as candidates with respect to direct observation of the *ortho-para* transition. It is worth mentioning that for the first time, a molecule is introduced as a candidate regarding direct observation of the radiative *ortho-para* transition. As a matter of fact, a criterion is suggested for the *ortho-para* mixing coefficients for the first time. Using this criterion, by knowing the molecular spectroscopic parameters of a molecule, it seems to be possible to predict that whether this molecule serves as a good candidate regarding direct observation of *ortho-para* transitions. Regarding, a simple model for the Hamiltonian matrix, several criteria were derived to have the prediction about the magnitude of the *ortho-para* mixing coefficients. Three parameters were prominently taken into account according to this criterion including: splitting of the *ortho-para* K -doubling states, (ΔE_1), existence of at least the third state in the *ortho-para* mixing process, and the magnitudes of interaction of the third, fourth,... interacting states with the *ortho-para* K -doubling states (h_{op}). For a certain case, the energy difference of the third, fourth,... interacting state with the *ortho-para* K -doubling states, (ΔE_2), determines the magnitude of the *ortho-para* mixing coefficient. Dependency of the *ortho-para* mixing coefficient to F , J and K_a quantum numbers is demonstrated to be the same as that of ΔE_1 , ΔE_2 and h_{op} to these quantum numbers. Finally, Chapter 6 presents a conclusion for the presently reported work and offers some suggestions for future extensions.

備考：論文要旨は、和文2000字と英文300語を1部ずつ提出するか、もしくは英文800語を1部提出してください。

Note: Dissertation summaries must be written in either of the following formats: (A) both in Japanese (approx. 2000 characters) and in English (approx. 300 words), or (B) in English (approx. 800 words). Submit one copy of each.

注意：論文要旨は、東工大リサーチリポジトリ (T2R2) にてインターネット公表されますので、公表可能な範囲の内容で作成してください。

Important: Dissertation summaries will be published online in the Tokyo Tech Research Repository (T2R2). Do not include information treated as confidential under certain circumstances.