Ab initio study on the ground and low-lying excited states of GaH

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Abstract

A multireference configuration interaction (MRCI) study has been carried out on GaH. Potential energy curves and spectroscopic constants of the $X^1\Sigma^+$, $a^3\Pi_0^{\rho=0,1,2}$, $A^1\Pi_1$ and a Rydberg state of $^1\Sigma^+(\Pi)$ are obtained. The observed open-structure absorption bands of GaH in the region 41 650–46 300 cm$^{-1}$ can be ascribed to the transitions from this Rydberg state at about 45 000 cm$^{-1}$ to the ground state. Breit–Pauli operator is used for spin–orbit coupling effect calculations. Four $\Omega$ components of the bound $a^3\Pi_0^{\rho=0,1,2}$ state are calculated for the first time. The transition properties of the excited states, including the transition dipole moments, the radiative lifetimes and the Franck–Condon factors, are predicted.

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1. Introduction

In recent decades, gallium containing systems become more and more important in the compound semiconductor industry. As the simplest heteronuclear molecule involving the Ga atom, GaH has been extensively investigated not only by experimental methods, but also theoretically as well. The first spectrum of GaH was observed by Garton [1] in 1951. They reported the ultraviolet absorption bands which are probably due to InH and GaH molecules. In subsequent experimental work, Neuhaus [2,3] observed the band spectrum of GaH and GaD. Ginter [4,5] observed the band spectrum of the GaH molecule and calculated its potential curves by the Rydberg–Klein–Rees method. Poynor et al. [6] studied the $a^3\Pi_0^{\rho=0,1,2} \rightarrow X^1\Sigma^+$ transition of the GaH molecule. Kroughvist et al. [7] researched the $A^1\Pi \rightarrow X^1\Sigma^+$ transition in the spectra of GaH and GaD. Rajamanickam et al. [8] researched the Frank–Condon factors of the $a^3\Pi_1 \rightarrow X^1\Sigma^+$ transition of GaH molecule. Most of these works had been summarized by Herzberg [9].

In recent years, with the development of ab initio electronic-structure calculation theory and computer technology, theoretical studies on the electronic state structures of GaH have been more