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Ab initio potential energy curves and transition dipole moments for the low-lying electronic states of GeH⁺

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Introduction

The germanium hydrides containing GeH_n and GeH_n⁺ are important source materials for the growth of semiconductor films using chemical vapor deposition method. The GeH⁺ cation have been the topic of many theoretical and experimental investigations that focused on its spectroscopic properties. The a³Π-X¹Σ⁺ and A¹Π-X¹Σ⁺ band systems of GeH⁺ have been recorded in emission [1-3]. Since GeH⁺ contains the heavy atom Ge, the effect of spin-orbit coupling (SOC), which may play a significant role in the spectroscopic and dynamic characterizes of electronic states, should be considered. In a very recent theoretical study [4], multi-reference configuration interaction was used for 8 Λ-S states and 23 Ω states of GeH⁺: Ge⁺(²P^o) + H(²S) → ^{1,3}Σ⁺, ^{1,3}Π that made the ground state asymptote and Ge⁺(⁴P) + H(²S) → ^{3,5}Σ⁻, ^{3,5}Π, which lies at 51600 cm⁻¹ above the ground state asymptote. However, the two asymptote Ge(³P)+H⁺(¹S) → ³Σ⁻, ³Π and Ge(¹D) + H⁺(¹S) → ¹Σ⁺, ¹Π, ¹Δ lie at about 46000 and 53090 cm⁻¹ above the ground state asymptote, respectively; the electronic states of the second asymptote were ignored in Ref. [4].

In this work we considered 13 Λ-S states and 50 Ω states of GeH⁺ and plotted potential energy curves, dipole moments and transition dipole moments between different electronic states with spin-orbit coupling.

Computational methods

All calculations were carried out using the ORCA 2.9.0 quantum chemistry program. The augmented correlation-consistent polarized valence quadruple zeta (aug-cc-pVQZ) basis sets of Woon and Dunning were used for both Ge (22s17p13d3f2g) and H (7s4p3d2f) atoms. Scalar relativistic effects were included through the second-order Douglas-Kroll-Hess (DKH) Hamiltonian. These calculations were performed for different Ge-H distances. Ab initio points of the potential curves were imported in program LEVEL in order to compute

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Einstein A coefficients, vibrational energy levels of all the electronic states, equilibrium internuclear distances (r_e), vibrational constants ω_e , $\omega_e x_e$ and other spectroscopic constants.

Results and discussion

The $a^3\Pi$ excited state of GeH^+ is split into $a0^+$, $a0^-$, $a1$ and $a2$ states by spin-orbit interaction. The ab initio potential energy curves (PECs) at the MRCISD level for these split excited states are plotted in Fig.1. Matrix elements of the dipole moment operator between the $X0^+$ ground state and the $a0^+$ and $a1$ excited state wavefunctions, i.e., transition dipole moments, were computed. The results are displayed in Fig. 2.

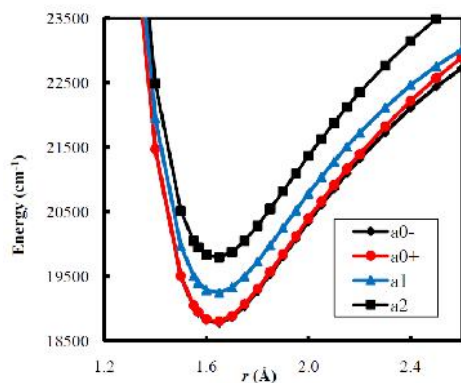


Fig. 1. Potential energy curves for the $a^3\Pi$ ($a0^-$, $a0^+$, $a1$ and $a2$) excited state of GeH^+ with the spin-orbit correction included.

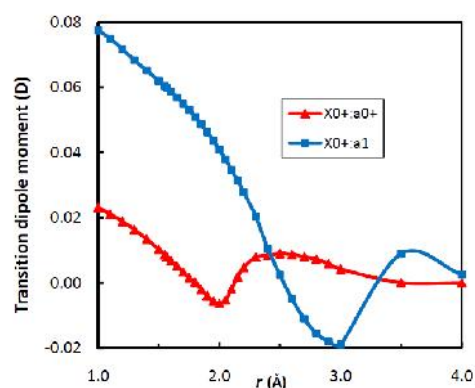


Fig. 2. Ab initio transition dipole moments for transitions from the $X^1\Sigma^+$ ($X0^+$) ground state to the $a^3\Pi$ ($a0^+$ and $a1$) states of GeH^+ .

Conclusions

Ab initio potential energy curves and transition dipole moments for the low-lying states of GeH^+ were calculated at the MRCI level of theory with large active space and basis sets, including the scalar-relativistic and spin-orbit corrections.

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