Theoretical study on the interaction potential and bound states of the Ne-BeH complex

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Abstract. The first two-dimensional potential energy surface for the Ne-BeH van der Waals interaction is calculated by the single and double excitation coupled-cluster theory with noniterative treatment of triple excitations [CCSD(T)]. Mixed basis sets, aug-cc-pVQZ for the Be , H and Ne atom, with an additional $(3s3p2d1f1g)$ set of midbond functions are used. There is a single global minimum at $R_e = 6.95a_0$ and $\theta_e = 72.5°$ with well depth -34.43607 cm^{-1}. Based on the potential, the rovibrational energy level structure of the Ne-BeH complex is also investigated.

1 Introduction

The nonbonding interaction potential, mainly resulted from van der Waals (vdW) interaction, plays a crucial role to understand the structures and properties of gases, liquids, solids, as well as any other in condensed phase. In the past several decades, there were a lot of experimental and theoretical studies for the closed-shell and open-shell vdW systems [1–6].

Recent progress in the development of experimental methods for the cooling and trapping of atoms and molecules may provide an opportunity for high resolution spectroscopy, accurate determination of intermolecular potential, and the study of reactive and inelastic collision at ultralow temperature [7,8]. Several methods have been proposed for creating translationally cold molecules. A successful demonstration of trapping CaH in a magnetic trap was carried out by Doyle and co-workers [9]. A cold buffer gas of ^{3}He was used to cool molecules to a temperature of about 240 mK. Molecules, slowed down by elastic collisions with the buffer gas, were further trapped in an inhomogeneous magnetic field. The open-shell molecule is paramagnetic molecules and hence suitable for the magnetic trapping from viewpoint of experiment.

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In 2003, Groenenboom and Balakrishnan [2] reported the interaction potential of the He-CaH vdW complex for the first time. The calculation was performed by RCCSD(T) and supermolecule approach. The interaction energy for 3732 geometries was analytically fitted to a three-dimensional potential model. In the accompanying paper [10], they reported quantum scattering calculations of rovibrational transitions in CaH induced by collisions with 3He atom over a wide range of temperatures and compared the data with the experimental results of Doyle and co-workers.

To our knowledge, there is no theoretical and experimental study on the structures and dynamics of the Ne-BeH complex. In this paper, we report the two-dimensional interaction potential of the Ne-BeH vdW complex using CCSD(T) method and big basis set extended with an additional $(3s3p2d1f1g)$ set of midbond functions. The rovibrational energy level structure of the Ne-BeH complex is also investigated based on the potential.

2 Computational details

Jacobi coordinates are used throughout the present work. In these coordinates, r_{BeH} is the BeH bond length, R refers to the distance between the Ne atom and the center of mass of BeH molecule, and θ is the angle between R and r_{BeH} with $\theta = 0°$ referring to the Ne-H-Be linear configuration.

2.1 Ab initio calculation

The interaction potential energy surface of the Ne-BeH complex is calculated by the single and double excitation coupled-cluster theory with noniterative perturbational treatment of triple excitations [CCSD(T)] [11–13]. We employ the augmented correlation-consistent polarized valence quadruple zeta (aug-cc-pVQZ) basis set for the H ,Be and Ne atom with the additional set of $(3s3p2d1f1g)$ midbond functions (denoted by BF) centered in the middle of the van der Waals bond. The midbond functions are well known to improve the basis set convergence very efficiently. The exponents of these midbond functions are 0.90, 0.30, 0.10 for the $3s$ and $3p$ functions, 0.60, 0.20 for the $2d$ functions, and 0.30 for the $1f$ and $1g$ functions [14]. We denote this basis set as avqz +33211. It is found if the avqz +33211 basis set is used directly the calculation will encounter the convergence problem in the step of CCSD(T) computation of complex. In order to overcome this difficulty, we firstly perform Hartree-Fock calculation using a small basis set, the cc-pVDZ for the H and Be atom and the cc-pVTZ for the Ne atom, and save the orbit. In the second step we then use the saved orbit as the initial guess orbit in the following calculation with avqz +33211 basis set.

The supermolecule approach is adopted to get the intermolecular potential energy for each configuration. The full function counterpoise method of Boys-Bernardi [15] is invoked to correct for the basis set superposition error (BSSE). Calculations are performed over 19 values of the intermolecular separation R: {5.0,5.5,6.0,6.5,7.0,7.5,8.0, 8.5,9.0,10.0,11.0,12.0,13.0,15.0,17.0,19.0,22.0,25.0,30.0} a_0, and over 12 angles θ