Molecular Dynamics Involving Ammonia and Noble-Gases

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INTRODUCTION

Ammonia was the first polyatomic molecule detected in interstellar medium space, and has proved to be an invaluable spectroscopic tool in the study of interstellar medium [1]. And besides, the detailed characterization of intermolecular potentials and the development of suitable analytical functions for their formulation provide the foundation on which microscopic and macroscopic properties of matter can be described and extensive molecular dynamics simulations can be built. Specifically, the study of the intermolecular interaction between hydrogenated molecules and neutral species is of great interest for understanding presence and role of hydrogen bonding in various environments [2]. In this work, we present a study about the dynamics of the systems that involve ammonia (NH_3) and noble-gases (Ar, He, Kr, Ne, and Xe). More precisely, we determined the ro-vibrational energies and spectroscopic constants of these systems. All this study was based on the potential energy curves (PEC) of the kind Improved Lennard-Jones (IJL) with experimentally adjusted parameters.

METHODS

Ro-vibrational spectroscopic constants involving ammonia and noble-gases were determined by using two different approaches: discrete variable representation (DVR) and Dunham methods. In both cases, it was used the ILJ PEC given by the following expression:

$$V(r) = \varepsilon\left[\frac{6}{n(r)-6}\left(\frac{r_m}{r}\right)^{n(r)} - \frac{n(r)}{n(r)-6}\left(\frac{r_m}{r}\right)^{6}\right] \quad (1)$$

where $n(r) = \beta + 4\left(\frac{r}{r_m}\right)^2$. In the equation (1), the first and second terms represent the repulsion and the attraction, respectively. The parameter ε is the depth of the potential well, r_m the equilibrium distance and β is associated with the resistance of the chemical species involved.

RESULTS AND DISCUSSIONS

The ro-vibrational constants (ω_e, $\omega_e x_e$, $\omega_e y_e$, α_e, and γ_e) obtained using Dunham and DVR methodologies are in an excellent agreement. This

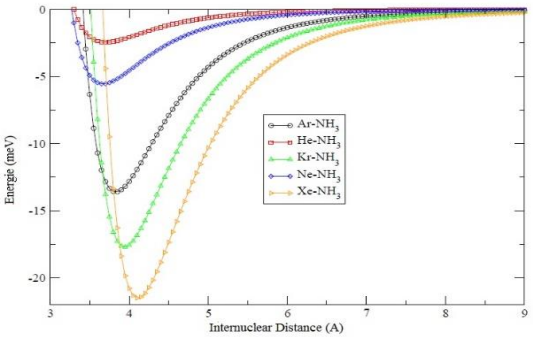

Figure 1: Potential energy curves for the interaction of ammonia with noble-gases.

fact indicates a good quality of our results and the suitable of both methods to treat the NH_3-Ng systems. Furthermore, we determined the first fifteen vibrational states for these systems using the DVR approach. From these calculations, it was observed that the NH_3-He system can remain bonded even with a small dissociation energy.

CONCLUSIONS

It was the first time that the NH_3-Ng ro-vibrational energies and spectroscopic constants calculations are presented in the literature. The current predictions are expected to be useful in the future experimental investigations.

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