

Rotational spectrum of the NH₃–He van der Waals complex

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Abstract. The interaction between ammonia and helium has attracted considerable interest over many years, partly because of the observation of interstellar ammonia. The rate coefficients of NH₃–He scattering are an important ingredient for numerical modeling of astrochemical environments. Another, though quite different application in which the NH₃–He interaction can play an important role is the doping of helium clusters with NH₃ molecules to perform high-resolution spectroscopy. Such experiments are directed on the detection of non-classical response of molecular rotation in helium clusters addressing fundamental questions related to the microscopic nature of superfluidity. High-resolution spectroscopy on the NH₃–He complex is an important tool for increasing our understanding of intermolecular forces between NH₃ and He.

The experimental spectra of NH₃–He would be of great importance to test the accuracy of available potential energy surfaces used in the analysis of the role of resonances in low energy collisions [1, 2]. The rate coefficients of NH₃–He scattering are an important ingredient for numerical modeling of astrochemical environments. This is one of the reasons why NH₃–He interactions have been studied experimentally and theoretically by several groups (see [1, 2] and Refs. therein). Recently, a new four-dimensional potential energy surface (PES), based on a high-quality fit of 4180 *ab initio* points, was calculated [1]. The potential has a well depth of $D_e = 35.08 \text{ cm}^{-1}$, which is to be compared with the well depth of 33.46 cm^{-1} for the earlier potential of Hodges and Wheatley [3]. Although this difference is not very large, it was found that small differences in the potential can have profound consequences for the observed resonance structures at low scattering energies. High-resolution spectra of the NH₃–He complex could be an additional test of the PES's quality, but these spectra have not been observed yet. High-resolution infrared and/or microwave spectra of the related NH₃–Ar (see [4] and Refs. there) and NH₃–Ne [5] in the gas phase have been reported, but no comparable data exist for helium.

A very different experiment in which the NH₃–He interaction plays an important role, is the trapping of NH₃ molecules inside He nanodroplets to perform high resolution spectroscopy. Such experiments are directed on the detection of a superfluid response of molecular rotation in helium clusters [6, 7]. It was shown that the lighter probe molecules allow one to measure the effective inertia of He clusters while maintaining a maximum

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superfluid response with respect to dopant rotation [8]. Ammonia opens an additional possibility in such experiments to study the inversion motion in dependence of the helium cluster size. Infrared [9] and microwave [10] spectra of NH₃ in large (> 1000 He atoms) superfluid helium droplets were already observed.

Recently all bound rovibrational levels of the weakly bound NH₃-He complex have been calculated by A. van der Avoird [11] for total angular momentum $J = 0 \dots 6$ on the new intermolecular potential surface [1]. The energy levels were obtained for two different nuclear spin states of NH₃-He arising from combinations of He with (*ortho*)-NH₃ and (*para*)-NH₃. The (*o*)-NH₃ and (*p*)-NH₃ complexes behave as different molecules, because they do not interconvert at the time scale of the experiment, due to the different nuclear spin statistics.

The rotation-inversion spectra of (*o*)-NH₃-He and (*p*)-NH₃-He in the frequency range of 5-25 GHz are under study guided by the bound state calculations. The experimental data on the rotational levels will be compared with the theoretical results.

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