Bound states and scattering of NH_3 – noble gas complexes

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Ammonia-noble gas complexes (NH_3-NG) have been the subject of a large number of studies, both theoretical and experimental, focusing either on rotationally inelastic scattering or on the measurement and interpretation of the microwave and infrared spectra. Recent experimental advances have renewed interest in these systems by allowing the measurement of quantum-state resolved integral and differential cross sections using crossed beam scattering [1, 2], which can be directly compared to theoretical predictions based on accurate potential energy surfaces and quantum-mechanical scattering calculations. The same techniques, combined with a Stark-decelerated beam of NH_3, would allow the measurement of integral and differential cross sections at very low collision energies [3], where the cross section is dominated by resonances that are very sensitive to the details of the PES. Finally, inelastic collisions of NH_3 with He and Ne are also of interest in the simulation of the rotational cooling of ammonia in a buffer gas cell.

To study these processes, we have computed new potential energy surfaces (PESs) for the complexes formed of ammonia and all noble gases except He, for which a recent PES is available [3]. The PESs, which include the umbrella inversion motion of NH_3, were computed using the coupled cluster method with single, double and perturbative triple excitations (CCSD(T)). The PESs are used to compute the spectra of NH_3-NG complexes, which we illustrate for NH_3-Ar [4]. We then discuss the scattering of NH_3 with noble gases, focusing on the initial state $j_k^{\pm} = 1_1^-$ of ammonia, which is the most relevant in the context of the experiments described above.

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