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Millimeter-wave observations of the NH_3–D_2 and ND_3–H_2 van der Waals complexes

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Abstract. The rotational spectra of the ND_3−H_2 and NH_3−D_2 van der Waals complexes have been observed in a supersonic molecular jet for the first time. The OROTRON intracavity spectrometer was used to detect pure rotational transitions in the frequency range from 75 to 120 GHz. The search of the spectral lines was based on the initial observation of the main isotopic species of the NH_3−H_2. The measured transition frequencies including hyperfine splitting were analyzed in order to determine the energy levels, molecular parameters and structure of the *ortho*ND_3−*ortho*H_2 and *ortho*NH_3−*para*D_2 complexes.

Since its discovery in the interstellar medium in 1969, ammonia has been widely used as a probe of the physical conditions in a variety of interstellar environments, ranging from pre-stellar cores, molecular clouds, to external galaxies. The peculiar structure of the molecule makes ammonia lines excellent tracers of the density and temperature in these environments. Thus the excitation temperature between the first two *para*-metastable (rotational) levels is an excellent probe of the gas kinetic temperature. However, the calibration of this ammonia thermometer depends on the accuracy of the collisional rates with H_2. Although a number of collisional studies have been made on the NH_3-H_2 system, laboratory data generally do not directly provide state-to-state rate coefficients. As a result, radiative transfer models can exclusively rely on theoretical estimates. On the other hand, laboratory measurements are crucial to establish the predictive abilities of theory and, in particular, of the potential energy surfaces (PES). The NH_3-H_2 system is a van der Waals complex, and the bound states of such complexes are sensitive to the interaction potential [1]. As a result, high-resolution spectroscopy on the NH_3-H_2 complex is an important tool for increasing our understanding of intermolecular forces between NH_3 and H_2.

The study of the deuterated isotopologues provides an effective new probe of the intermolecular interaction between ammonia and dihydrogen and can help to test the existing *ab initio* potential energy surface calculations. In this work, the rotational spectra of the ND_3−H_2 and NH_3−D_2 van der Waals complexes have been observed in a supersonic jet for the first time. The millimeter-wave OROTRON intracavity jet spectrometer [1] along with double resonance technique was used to detect two nuclear spin species, *ortho*ND_3−*ortho*H_2 and *ortho*NH_3−*para*D_2, in the frequency range from 75 to 120 GHz. The spectra were predicted from the initial observation of the main isotopic species of the *ortho*NH_3−*ortho*H_2 [2]. The measured line positions including hyperfine splitting due to the ^{14}N nuclear spin of

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ammonia were analyzed in order to determine the molecular parameters and structure of the *ortho*ND_3−*ortho*H_2 and *ortho*NH_3−*para*D_2 complexes.

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