

# Microwave spectrum and nuclear quadrupole structure analysis of the $\text{NH}_3\text{-N}_2$ van der Waals complex

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The pure rotational transitions of the  $\text{NH}_3\text{-N}_2$  van der Waals complex and its deuterated isotopologues ( $\text{ND}_3\text{-N}_2$ ,  $\text{NHD}_2\text{-N}_2$ ,  $\text{NH}_2\text{D-N}_2$ ) have been observed in the frequency range of 6–26 GHz using chirped-pulse Fourier-transform microwave (CP-FTMW) technique. Complicated hyperfine structure due to three quadrupole  $^{14}\text{N}$  nuclei was resolved and examined for the first time, thus supplementing the previous pure rotational analysis of the only main isotopic species of  $\text{NH}_3\text{-N}_2$  [1, 2, 3]. In the earlier papers [2, 3] six series of the millimeter-wave transitions have been assigned to the  $K = 0$  or  $K = 1$  states of the complex involving all combinations of the nuclear spin isomers of the parent molecules, *ortho/para*-ammonia and *ortho/para*-nitrogen. In our study one of the two detected  $K = 0$  series belongs to already known ground state of the *ortho*- $\text{NH}_3$ -*ortho*- $\text{N}_2$  spin isomer [1–3], while another  $K = 0$  series assigned to the *para*- $\text{NH}_3$ -*para*- $\text{N}_2$  spin isomer was not reported before. Two other  $K = 0$  series were expected for *para*- $\text{NH}_3$ -*para*- $\text{N}_2$  and *para*- $\text{NH}_3$ -*ortho*- $\text{N}_2$  from earlier analysis [2], but current experiment calls their assignment into question. The hyperfine splitting patterns for all observed isotopic and nuclear spin species were examined in order to obtain the dynamical information about the orientation of the ammonia and nitrogen units within the van der Waals complex.

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[2] K.A. Walker, A.R.W. Mckellar, *Mol. Phys.*, 2001, **99**, 1391.

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# New millimeter-wave study of the CO–N<sub>2</sub> van der Waals complex

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Recently, new CO–N<sub>2</sub> intermolecular potential energy surface has been carried out at the explicitly correlated coupled cluster level of theory with single, double, and perturbative triple excitations [1]. The accompanying bound state computations resulted in further progress in assignments of the measured rotational spectra of the CO–N<sub>2</sub> complex. Guided by these *ab initio* calculations a new millimeter-wave survey in the frequency range of 100–145 GHz was performed using the intracavity OROTRON jet spectrometer described elsewhere [2]. Newly observed lines were assigned to the *P*- and *R*-branches of the  $K = 0 - 0$  subband correlating with the  $j_{\text{CO}} = 2 - 1, j_{\text{N}_2} = 0$  internal rotor states of the CO–*ortho*N<sub>2</sub> nuclear spin modification. Experimental transitions with partly resolved hyperfine splitting due to nuclear spins of two <sup>14</sup>N atoms were analyzed in order to determine the molecular parameters and structure of the complex in the  $K = 0, (j_{\text{CO}}, j_{\text{N}_2}) = (2, 0)$  state detected for the first time.

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# Microsolvation of ethyl carbamate conformers: a rotational spectroscopy study

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The microwave spectra of complexes between ethyl carbamate and up to three molecules of water generated in a supersonic expansion have been studied using both a chirped-pulse and a molecular beam spectrometers covering the 2–13 GHz frequency range. The monomer of ethyl carbamate shows an equilibrium in the gas phase between two close in energy conformations connected by a low interconversion barrier.[1, 2] The observation of these forms and their correspondent complexes depends on the carrier gas used due to collisional relaxation in the supersonic jet. While using argon only the most stable form and its complexes are observed, using neon both forms and their corresponding complexes can be observed. The structures of six new complexes have been characterized and in all cases water closes sequential cycles with the H–N–C=O amide group. They show a remarkable similarity in both structure and dynamics to those observed in related systems, as for example in formamide–(H<sub>2</sub>O)<sub>n</sub> clusters.

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# Study of the molecular structure and microsolvation ( $\text{H}_2\text{O}$ N=1–3) of 2-Phenylpyridine by rotational spectroscopy

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Conjugated organic ligands are usually used in devices as light emitting diodes or semiconductors due to their electronic and optical properties associated to its structure. One of the most employed conjugated organic ligand is 2-phenylpyridine (2ppy). We present the study of this molecule and its complexes with  $n$  water molecules ( $n=1-3$ ) by rotational spectroscopy using a molecular beam Fourier transform microwave spectrometer (MB-FTMW) and a chirp pulse Fourier transform microwave spectrometer (CP-FTMW). For the monomer and the one water complex we have also assigned all their  $^{13}\text{C}$  and  $^{15}\text{N}$  single isotopologues in their natural abundance. These measures have enabled a direct structural comparison between the bare molecule and its water complex, determining not only the structure of 2ppy but also how the water affects to it.

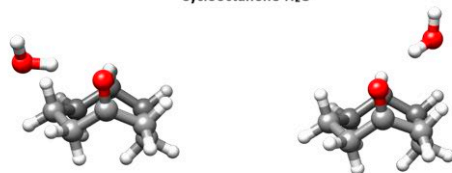
# Structures of the complexes of Cyclooctanone with water

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Water is present in the air with a concentration of up to 4 %, and also in the olfactory mucosa, where it has the role of protecting the olfactory epithelium. Odorants are thus very likely to interact with water before reaching the receptor, which may affect their conformational properties or even produce a reaction. The study of complexes of cyclooctanone with water constitutes a first step towards understanding how larger macrocyclic compounds interact with water before they reach the olfactory receptors. Two complexes of the most abundant conformer of cyclooctanone with one water molecule, and two complexes with two water molecules have been characterised using chirped-pulse Fourier Transform Microwave (CP-FTMW) spectroscopy. The observation of all <sup>13</sup>C and some <sup>18</sup>O isotopic species of the cyclooctanone ring in the complexes in their natural abundances, and of the <sup>18</sup>O species of the water molecules using isotopically enriched water allowed us to calculate the substitution structures of the complexes. These have been compared with the effective structures of the complexes and with that of cyclooctanone to determine any changes undergone by cyclooctanone upon complexation. In the cyclooctanone-H<sub>2</sub>O complexes, water forms a O-H...O hydrogen bond with the carbonyl oxygen of cyclooctanone and two O...H-C hydrogen bonds with the -CH<sub>2</sub> groups in the cyclooctanone ring. In the cyclooctanone-(H<sub>2</sub>O)<sub>2</sub> complexes, the second molecule of water binds primarily to the first molecule of water through hydrogen bonding, whilst also forming secondary interactions with the -CH<sub>2</sub> groups in the ring.

Cyclooctanone-H<sub>2</sub>O



Cyclooctanone-(H<sub>2</sub>O)<sub>2</sub>

