ANOMALOUS CENTRIFUGAL DISTORTION IN NH_2

MARIE-ALINE MARTIN-DRUMEL, OLIVIER PIRALI, L. H. COUDERT, *Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, Orsay, France*.

The NH_2 radical spectrum, first observed by Herzberg and Ramsay,[a] is dominated by a strong Renner-Teller effect[b] giving rise to two electronic states: the bent $X\,^2B_1$ ground state and the quasi-linear $A\,^2A_1$ excited state. The NH_2 radical has been the subject of numerous high-resolution investigations and its electronic and ro-vibrational transitions[c] have been measured. Using synchrotron radiation, new rotational transitions have been recently recorded and a value of the rotational quantum number N as large as 26 could be reached.[d] In the $X\,^2B_1$ ground state, the NH_2 radical behaves like a triatomic molecule displaying spin-rotation splittings. Due to the lightness of the molecule, a strong coupling between the overall rotation and the bending mode arises whose effects increase with N and lead to the anomalous centrifugal distortion evidenced in the new measurements.[d]

In this talk the Bending-Rotation approach[e] developed to account for the anomalous centrifugal distortion of the water molecule is modified to include spin-rotation coupling and applied to the fitting of high-resolution data pertaining to the ground electronic state of NH_2. A preliminary line position analysis of the available data[c,d] allowed us to account for 1681 transitions with a unitless standard deviation of 1.2. New transitions could also be assigned in the spectrum recorded by Martin-Drumel *et al.*[d] In the talk, the results obtained with the new theoretical approach will be compared to those retrieved with a Watson-type Hamiltonian and the effects of the vibronic coupling between the ground $X\,^2B_1$ and the excited $A\,^2A_1$ electronic state will be discussed.

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[a] Herzberg and Ramsay, *J. Chem. Phys.* **20** (1952) 347

[b] Dressler and Ramsay, *Phil. Trans. R. Soc. A* **25** (1959) 553

[c] Hadj Bachir, Huet, Destombes, and Vervloet, *J. Molec. Spectrosc.* **193** (1999) 326; McKellar, Vervloet, Burkholder, and Howard, *J. Molec. Spectrosc.* **142** (1990) 319; Morino and Kawaguchi, *J. Molec. Spectrosc.* **182** (1997) 428

[d] Martin-Drumel, Pirali, and Vervloet, *J. Phys. Chem. A* **118** (2014) 1331

[e] Coudert, *J. Molec. Spectrosc.* **165** (1994) 406