HYPERFINE STRUCTURE AND TUNNELING MOTION IN ETHYLENEDIAMINE

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The first investigation[a] of the microwave spectrum of ethylenediamine (NH_2CH_2–CH_2NH_2) showed that in the gas phase this molecule occurs in two conformers which both exhibit a large amplitude tunneling motion corresponding to an interchange of the roles of the amino groups. In conformer I, the tunneling splitting is about 172 MHz while it is only 2.7 MHz in conformer II.

In the paper an analysis of the hyperfine structure of several transitions of conformer I, recorded using a pulsed molecular beam Fourier transform microwave spectrometer, will be presented. The hyperfine patterns are dominated by quadrupole hyperfine coupling at the nitrogen atoms and, unexpectedly, the molecule behaves as if this hyperfine coupling was the same for both nitrogen atoms. Such a result can be understood making use of symmetry considerations and taking into account the fact that the tunneling splitting is much larger than the hyperfine coupling. This also implies that only certain components of the effective quadrupole coupling tensors can be retrieved from the analysis of the microwave data. These theoretical results will be discussed in the paper and values for the determinable components of the effective quadrupole coupling tensors will be reported.

Microwave data, recorded with the same apparatus, are also available for the hyperfine structure of transitions belonging to conformer II. At the present time, for this second conformer, it has not yet been possible to assign the hyperfine transitions, as they do not seem to follow a usual quadrupole coupling hyperfine pattern. Work is in progress and we will try to see if, including in the hyperfine Hamiltonian matrix elements between different tunneling state, allows us to reproduce the observed hyperfine patterns.

[a] K.-M. Marstokk and H. Møllendal, *J. Molec. Struc.* **49,** 221 (1978).