Internal rotation and ^{14}N quadrupole coupling in N,N-diethylacetamide

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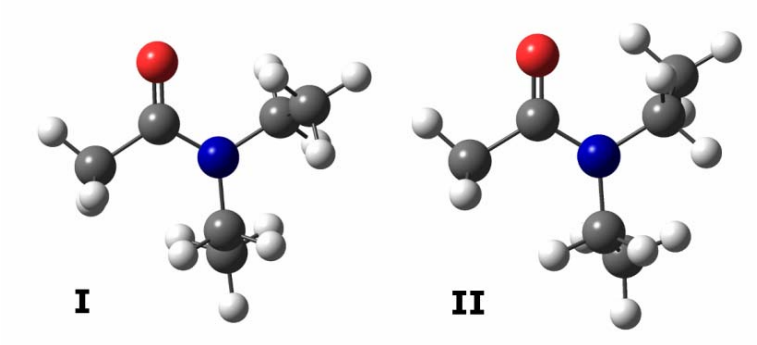
The conformational analysis of *N,N-diethylacetamide* which has been carried out at the MP2/6-311++G(d,p) level of theory using the program *Gaussian09* yielded five stable conformers. The two most energetically favorable conformers (conformer **I** and **II**) were found in the microwave spectrum within a frequency range from 9 to 15 GHz.

The spectrum of this molecule is extremely complicated due to a combination of two effects, the internal rotation of the acetyl methyl group and the quadrupole coupling of the nitrogen atom. These two effects cause splittings on the same order of magnitude, which made the assignment difficult. Due to internal rotation, all rotational transitions split into A-E doublets. Each of these symmetry species splits into triplets, quintets or septets, depending on the respective transitions, due to ^{14}N quadrupole coupling. Using the program XIAM, totally 450 transitions of conformer I and 262 transitions of conformer II were fitted to standard deviations of 14.5 kHz and 1.9 kHz, respectively. The rotational constants, centrifugal distorstion constants, quadrupole coupling constants, and internal rotation parameters could be determined. The barrier to internal rotation of *N,N-diethyl-acetamide* was compared to the one found in *N-methylacetamide* [1] and *N,N-dimethylacetamide* [2]. Quantum chemical calculations using different methods and basis sets were carried out and some molecular parameters were compared to the experimental ones in order to find out the best method and basis set.



[1] N. Ohashi, J. T. Hougen, R. D. Suenram, F. J. Lovas, Y. Kawashima, M. Fujitake, J. Pyka, *J. Mol. Spectrosc.* **2004**, *227*, 28.
[2] M. Fujitake, Y. Kubota, N. Ohashi, *J. Mol. Spectrosc.* **2006**, *236*, 97.