MILLIMETER WAVE SPECTRUM OF ACETAMIDE

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We are reporting recent progress in measuring, assigning and fitting the millimeter wave rotational transitions of the ground torsional state (and a few lines of the first excited torsional state) of the acetamide molecule CH_3CONH_2. The new measurements of the acetamide spectrum have been carried out using the microwave spectrometer in Kharkov between 50-150 GHz. We have assigned 331 and 199 new rotational transitions belonging to the A and E species respectively and involving J up to 20 and K_a up to 10. The observed spectrum was analyzed using the so-called rho axis method (RAM) which was applied in the past to several internal rotors with success. After having removed the observed hyperfine splittings due to the quadrupole coupling, this new data along with 115 previously published measurements are fitted using 32 parameters of the RAM Hamiltonian with root-mean-square deviations of 37 kHz and 49 kHz for the 630 v_t=0 lines belonging to the ground torsional state and for the 15 v_t=1 lines belonging to the excited torsional state respectively. Separate rms deviations for the A (32 kHz) and for the E (44 kHz) species indicate similar quality of the fit for the two symmetry species. The main difficulty which is encountered now in the assignment process of the higher J and K values of the A species in the first excited torsional state and in even the ground torsional state of the E species is caused by the problem of finding a correct K label for the eigenvectors corresponding to energy levels involved in the fit (so-called labeling problem). We will discuss this problem and other aspects which make the acetamide molecule a rather typical model molecule for future studies on polypeptide mimetics.
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