IR ROTATIONAL SPECTRUM OF METHYLAMINE

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In the current work a recent progress is reported on assignment and fitting the rotational spectrum of the ground vibrational state, the first and the second torsional states. It was possible to assign in the IR spectrum the complete 'R and 'Q series for higher values of K and J, and all symmetry species. The IR spectra were recorded with a resolution of 0.00125 cm⁻¹ using Bruker IFS-120HR spectrometer at the University of Oulu. New series of pure rotational lines in the ground state of the IR spectrum were identified and fitted. In comparison to previous pure rotational spectrum ¹, it was possible to assign and fit about 5000 new rotational transitions up to K=20 and J=50. All available data in the ground state were taken into account in the global fit (microwave, rotational and combination differences from the torsional band). The experimental data were fitted using the group-theoretical formalism ². The standard deviation for microwave and infrared transitions was 0.86 MHz and 0.0004 cm⁻¹, respectively. In the first excited torsional state of methylamine, a number of pure rotational transitions was also assigned. Previously, there were 86 pure rotational reported in the first excited torsional state ³ (of B and E₁ symmetry only) whereas in our study about 2350 new rotational lines for all symmetry species were identified and fitted together with microwave and rovibrational transitions. The standard deviation for pure rotational transitions was 0.0008 cm⁻¹. About 1300 new pure rotational transitions were then assigned in the second torsional state and their assignments were confirmed with the Lower States Combination Differences. The transitions were assigned to all symmetry species for different values of K and J. Previously, 35 pure rotational lines were assigned in this state ⁴, and all of them were of B symmetry species only. The pure rotational lines ν₁₅=2→2 were fitted together with transitions of a hot band ν₁₅=2→1, and with an overtone band ν₁₅=2→0. The standard deviation of the fit was 0.006 cm⁻¹. The simulated spectra were generated in the LWW.