High Resolution Study of $^{13}CH_3D$ in the region of 2000-2700 cm^{-1}

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We have previously presented extensive analyses of spectra of $^{12}CH_3D$ [1]. We have newly measured the spectra of $^{13}CH_3D$ at essentially Doppler limited resolution at low temperature in collisional cooling cell (80K) with the Zürich FTIR prototype spectrometer Bruker IFS125 (ZP2001) in the range 900 to 9000 cm^{-1} and at room temperature in the range 2000-2700 cm^{-1} with the Bruker IFS120 at the University of Oulu (Finland). We report here results of the first high resolution analysis for $^{13}CH_3D$ in the region between 2000 cm^{-1} and 2700 cm^{-1} on the basis of these spectra.

The spectra look very complicated because the eight ro-vibrational bands, v_2 (A_1), $2v_3(A_1)$, $2v_6(A_1)$, $2v_6(E)$, $v_3+v_6(A_1)$, $v_5+v_6(A_1)$, $v_5+v_6(A_2)$, and $v_5+v_6(E)$, which are located in the region studied, strongly interact with each other. Therefore, an assignment of transitions was made simultaneously with a fit of parameters of the Hamiltonian used in analysis. To simplify the analysis, we, first of all, estimated the values of the main spectroscopic parameters of the Hamiltonian on the basis of (a) isotopic relations, on the one hand, and (b) relations between some spectroscopic parameters of axially symmetric molecules from [2].

As a result of the analysis, transitions with $J^{max.}=20$ *and* $K^{max.}=14$ were assigned in the spectra, and rotational energy values of the vibrational states $(v_2=1,\ A_1)$, $(v_3=2,\ A_1)$, $(v_6=2,\ A_1)$, $(v_6=2,\ E)$, $(v_3=v_6=1,\ A_1)$, $(v_5=v_6=1,\ A_1)$, $(v_5=v_6=1,\ A_2)$, and $(v_5=v_6=1,\ E)$ were obtained. The latter were used then in a fit procedure, and a set of parameters was determined which reproduce the initial experimental data with accuracies close to experimental uncertainties.

[1]. O. N. Ulenikov, E. S. Bekhtereva, S. Albert, S. Bauerecker, H. Hollenstein, and M. Quack, *Mol. Phys.*, **2010**, 108, 1209-1240.

[2]. O. N. Ulenikov, E. S. Bekhtereva, A.L. Fomchenko, A.G. Litvinovskaya, C. Leroy, and M. Quack, „On the „Expanded Local Mode" Approach Applied to the Methane Molecule: Isotopic Substitution CH_3D – CH_4 and CHD_3 – CH_4", *paper at this meeting (Budapest, 2013)*.