ACCURATE TORSIONAL BARRIER HEIGHT OF TRIFLUROACETIC ACID

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Trifluoroacetic acid (TFA, $CF_3C(O)OH$) is the final degradation product of many hydrochlorofluorocarbons (HCFCs), hydrofluorocarbons (HFCs), and hydrofluoroolifines (HFOs) in the troposphere. While a recent assessment of the TFA impact on the health of humans and the environment shows that its concentration is too small to be a risk, TFA still warrants continued attention, in part because of its very long environmental lifetime.[a] The ultimate sink of TFA is in surface waters in which it forms salts that are extremely stable and are likely to have half-lives of centuries. From the spectroscopic point of view, TFA is an interesting case of the internal rotation of a heavy C_{3v} top. The presence of the CF_3 internal rotor leads to relatively strong coupling between internal and overall rotation, $\rho = 0.68$. However, owing to the high mass of the top, the tunneling probability is low; the $A-E$ splittings are hardly observable in the rotational spectrum, despite relatively low barrier of about 230 cm^{-1}. In the previous studies, the splittings were observed only in the $v_t = 4$ excited torsional state,[b] and were not observed in the ground state using molecular beam Fourier transform microwave spectroscopy which typical resolution is few kHz.[c] We present new global analysis of the rotational spectrum of TFA using the rho axis method and RAM36 code. The rotational spectrum of TFA was recorded in the range from 50 to 330 GHz. The joint analysis of the $v_t = 0$, 1, and 2 states resulted in accurate determination of the V_3 and V_6 potential energy terms, 230.36(92) cm^{-1} and -4.736(82) cm^{-1} respectively. However, the potential energy terms are strongly correlated with the intrenal rotation constant F that is kept fixed in the fit. Up to now no $A-E$ splittings were observed in the Doppler-limited resolution spectra. The analysis will be extended to $v_t = 3$ and $v_t = 4$ states in which we expect to observe the splittings that will permit to remove the correlation between V and F terms. The latest results will be presented.

The present work was funded by the French ANR Labex CaPPA through the PIA contract ANR-11-LABX-0005-01

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[b] Stolwijk, W. M. and van Eijck, B. P., 1985, *J. Mol. Spec.*, **113**, 196.

[c] Antolinez, S., *et al.*, 1999, *Z. Naturforsch. A*, **54**, 524.