THE ROTATIONAL, RO-VIBRATIONAL EXPERIMENTAL AND COMPUTATIONAL INVESTIGATION OF MONODEUTERATED CHLOROMETHANE

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The comprehensive description of our spectroscopic analyses and ab initio calculations for the mono-deuterated chloromethane, $CH_2D^{37}Cl$, is presented. It includes the detection of ν_4 and ν_8 ro-vibrational fundamental bands between 1170 and 1370 cm^{-1} in the recently recorded high-resolution FTIR spectra (P. Stoppa et al., High resolution FTIR spectrum of $CH_2D^{37}Cl$: ν_4 and ν_8 fundamental bands, accepted in JQSRT) and our detailed previous analysis of ν_5, ν_6 and ν_9 fundamentals between 650 and 1100 cm^{-1} (doi:10.1016/j.jqsrt.2021.107719, P. Stoppa et al., High resolution FTIR study of the ν_5, ν_6 and ν_9 fundamental bands of $CH_2D^{37}Cl$, JQSRT 270, 107719, 2021). The vibration analyses from the medium resolution (up to 0.1 cm^{-1}) gas-phase infrared spectra of CH_2DCl, investigated in the region 600-9000 cm^{-1}, are also reported (doi:10.1364/AO.39.003984, A. Pietropolli Charmet, Computational, rotational and ro-vibrational experimental investigation of monodeuterated chloromethane, JQSRT 305, 108624, 2023). All most important spectral features have been assigned in terms of fundamental, overtone and combination bands, achieving an accurate description of the vibrational structure.

The rotational spectra of the ^{13}C species have been recorded for the first time in the 250-300 GHz frequency range and, for the two isotopologues $^{12}CH_2D^{35}Cl$ and $^{12}CH_2D^{37}Cl$, the knowledge has been extended up to 520 GHz. In addition, very accurate ab initio calculations have been performed in order to derive reliable predictions of the equilibrium structure, rotational constants, and centrifugal distortion terms for the $^{12/13}C$ and $^{35/37}Cl$ isotopologues. The accurate semi-experimental equilibrium structure of chloromethane has been derived. This extended experimental and computational spectroscopic work will be useful to assist the detection of CH_2DCl in remote environments.