HALOGEN BOND AND INTERNAL DYNAMICS IN $CClF_3$-H2O

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The pure rotational spectra of $CF_3{}^{35}Cl$-H_2O, $CF_3{}^{37}Cl$-H_2O, $CF_3{}^{35}Cl$-$H_2{}^{18}O$, $CF_3{}^{35}Cl$-OHD, $CF_3{}^{35}Cl$-D_2O isotopologues have been investigated by pulsed supersonic-jet FT-microwave spectroscopy. We assigned the m = 0 and m = 1 (for the first 2 isotopologues) states and the spectra, for all, are characteristic of a symmetric top of evenly spaced band. A substitution analysis was made for the m = 0 state of the dimers with $H_2{}^{18}O$ and D_2O. Ab initio calculation (MP2 level of electron correlation and 6-311++G** basis set) have been carried out in order to obtain information about the structure and relative stability. The interaction between the subunits occurs via C-Cl$\cdots$O(H_2O) halogen bond.