THE H_2O-CH_3F COMPLEX: A COMBINED MICROWAVE AND INFRARED SPECTROSCOPIC STUDY SUPPORTED BY STRUCTURE CALCULATIONS

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The H_2O-CH_3F complex could have two geometries, one with a hydrogen bond and one with the newly proposed carbon bond[a]. While in general carbon bonds are weaker than hydrogen bonds, this complex appears to have comparable energies for the two structures. Infrared (IR) and microwave (MW) spectroscopic measurements using, respectively, the Jet-AILES apparatus[b] and the FTMW spectrometer at the PhLAM laboratory[c], have been carried out to determine the structure of this complex. The IR spectrum shows the formation of the CH_3F- H_2O hydrogen bonded complex and small red-shifts in OH frequency most probably due to $(CH_3F)_m$-$(H_2O)_n$ clusters. Noticeably, addition of CH_3F in the mixture promotes the formation of small water clusters. Preliminary MW spectroscopic measurements indicate the formation of the hydrogen bonded complex. So far, we have no experimental evidence for the carbon bonded structure. However, calculations of the Ar-CH_3F complex show three energetically equivalent structures: a T-shape, a "fluorine" bond and a carbon bond. The MW spectrum of the $(Ar)_n$-CH_3F complexes is currently under analysis.

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