DOES WATER PREFER TO DONATE A PROTON TO AN F OR TO a Cl ATOM? - A ROTATIONAL STUDY OF $CH_3CHClF...H_2O$

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We measured the molecular beam Fourier transform microwave spectra of six isotopologues of the 1:1 adduct of CH_3CHClF with water. The water prefers to form an O-H...F rather than an O-H...Cl hydrogen bond. This is exactly the contrary of what observed in the chlorofluoromethane-water adduct, where a O-H...Cl link was formed [a]. Besides the rotational constants, the quadrupole coupling constants of the chlorine atom have been determined. In addition, information on the internal dynamics has been obtained.

[a] W.Caminati, S.Melandri, A.Maris and P.Ottaviani, Angew. Chem. Int. Ed. 45, 2438-2442 (2006)