THE OBSERVATION AND PROPERTIES OF $(H_2O\cdots HCl)\cdots Ar$

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The trimer $(H_2O\cdots HCl)\cdots Ar$ was observed in this laboratory by supersonic expansion cavity-FTMW spectroscopy, during the work carried out on H_2O...HCl[a] and $(H_2O)_2$HCl.[b] The title trimer appears to be useful test-bed for detailed assessment of the effect of complexing a Rare-gas atom to the more strongly bound $H_2O\cdots HCl$ subunit. $(H_2O\cdots HCl)\cdots Ar$ is near-planar and since the $H_2O\cdots HCl$ unit is oriented at $\approx 27^\circ$ to the b-inertial axis both the μ_b and the μ_a dipole moment components are appreciable, giving rise to a rich rotational spectrum. Presently we present a summary of the information obtained for this trimer.

Five different isotopomers of the trimer, resulting from ^{37}Cl, D, and ^{18}O substitution, have been observed. In addition to the usual spectroscopic constants it was possible to determine accurate values of the χ_{ab} nuclear quadrupolar splitting constant for the chlorine nucleus, and thus the principal nuclear quadrupole tensor and the associated rotation angle. Electric dipole moment of the trimer was measured and supporting $ab\ initio$ calculations at the MP2/aug-cc-pVTZ level were carried out. Following a recent test of the applicability of the r_m method to weakly bound complexes[c] we derived such a geometry for $(H_2O\cdots HCl)\cdots Ar$ and find it to be in satisfactory agreement with the $ab\ initio$ calculations. Comparison of results obtained for the trimer with the accurate data available for $H_2O\cdots HCl$ allow the effects of this first step in inert-gas matrix isolation of $H_2O\cdots HCl$ to be identified.

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