MOLECULAR ORBITAL STUDY OF THE HYDRATED CLUSTERS OF STRONG ACIDS WITH WATER MOLECULES

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The molecular structures and vibrational frequencies of the hydrated clusters of the strong acids, $HCl\bullet(H_2O)_n$ and $H_2SO_4\bullet(H_2O)_n$; n=1∼5, are examined by employing the density functional molecular orbital method. When the number of water molecules is small, the hydrated clusters take the hydrogen-bonded structures without proton transfer. In the cases of $n\geq4$, the proton transferred forms become dominant and there are many isomeric forms for both the direct ion-pair $X^-\bullet H_3O^+\bullet(H_2O)_{n-1}$, and indirect ion-pair $X^-\bullet(H_2O)_{n-1}\bullet H_3O^+$ structures, where X=Cl, HSO_4. The calculated IR spectra of the stable clusters clearly indicate the large red-shifts of the stretching frequencies of the H-Cl and the O-H bond of H_2SO_4. The difference of the hydrated clusters of HCl, H_2SO_4, and HF is also discussed.