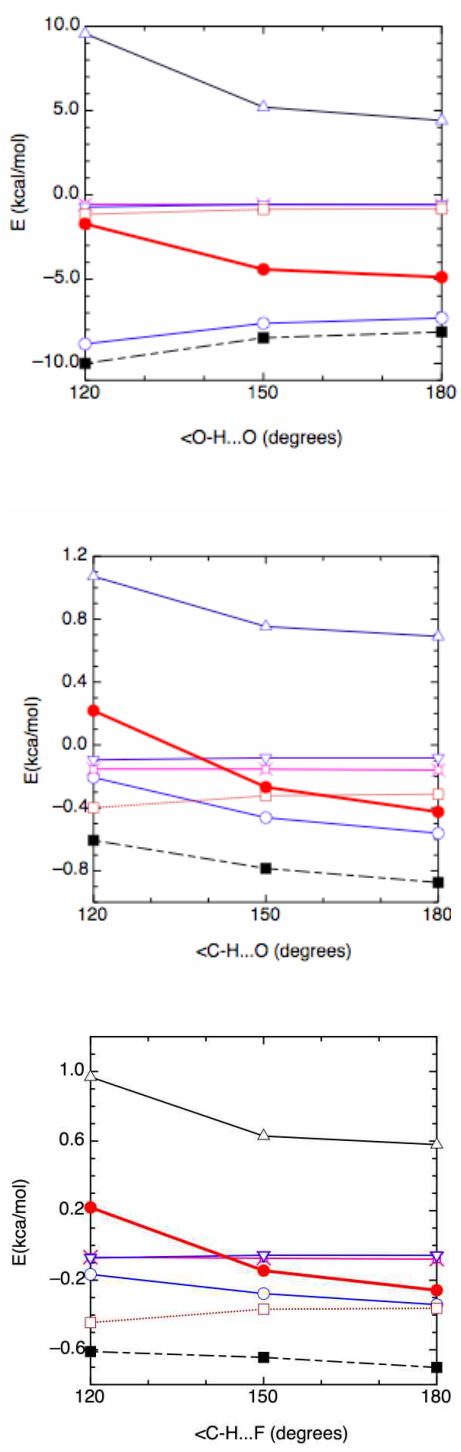

Figure S1. Variation of the interaction energy of the water dimer, methane-water and methane-fluromethane complex and its components with the <O-H···O, <C-H···O and <C-H···F angles. The following symbols are used to indicate each IMPT component: ○ for the electrostatic, △ for the exchange-repulsion, P for the polarization, ▽for the charge-transfer, and □ for the dispersion one). The total interaction energy (●, obtained by adding all components) and the sum of the electrostatic and dispersion components (■) are also given for comparison.