Energy as a function of nuclei configuration for H₂O with 6-311G basis 125 -75.5 120 -75.6 115 -75.7110 -75.8 θ [$^{\circ}$] 105 -75.9100 -7695 -76.190 - 1.5 -76.2 1.6 1.7 1.8 1.9 2 2.1 r [a.u.]