Energy as a function of nuclei configuration for H₂O with 3–21G basis 120 -75.54 Minimum value -75.545 115 -75.55-75.555 110 -75.56 -75.565 105 -75.57 -75.575 100 -75.5895 1.6 -75.585 1.7 1.8 1.9 2 2.1 r [a.u.]