Oxygen	E in Hartree			
Name	E NIST	E pred	ΔΕ	ΔE /E NIST
Ecoul	36.331102	36.327422	0.003680	0.000101
Etot	-74.473077	-74.473077	0.000000	-0.000000
2s	-0.871362	-0.871820	0.000458	-0.000526
Exc	-7.768482	-7.768109	0.000373	-0.000048
Ekin	74.116881	74.112326	0.004555	0.000061
2p	-0.338381	-0.338826	0.000445	-0.001315
1s	-18.758245	-18.758906	0.000661	-0.000035





