Oxygen	E in Hartree			
Name	E NIST	E pred	ΔΕ	ΔE /E NIST
Ecoul	36.331102	36.385742	0.054640	0.001504
Etot	-74.473077	-74.470546	0.002531	-0.000034
2s	-0.871362	-0.867825	0.003537	-0.004059
Exc	-7.768482	-7.775777	0.007295	-0.000939
Ekin	74.116881	74.138542	0.021661	0.000292
2р	-0.338381	-0.334438	0.003943	-0.011653
1s	-18.758245	-18.752198	0.006047	-0.000322





