Oxygen	E in Hartree			
Name	E NIST	E pred	ΔΕ	ΔE /E NIST
Ecoul	36.331102	36.333347	0.002245	0.000062
Etot	-74.473077	-74.473077	0.000000	-0.000000
2s	-0.871362	-0.873616	0.002254	-0.002587
Exc	-7.768482	-7.768832	0.000350	-0.000045
Ekin	74.116881	74.117972	0.001091	0.000015
2p	-0.338381	-0.340597	0.002216	-0.006550
1s	-18.758245	-18.760452	0.002207	-0.000118





