ReO3Et

Atom	X	Y	Z (Angstrom)
1.Re	0.003607	0.000689	-0.000052
2.O	1.728069	-0.003641	-0.035517
3.O	-0.665475	1.590324	0.009013
4.O	-0.697716	-1.019075	-1.201140
5.C	-0.530055	-0.851136	1.840883
6.C	-0.000100	-0.091981	3.062488
7.H	-0.381443	0.936800	3.095743
8.H	1.096784	-0.051479	3.068698
9.H	-0.323673	-0.600987	3.982838
10.H	-0.153951	-1.886512	1.801869
11.H	-1.631188	-0.899565	1.829459

Bond Energy LDA -2.65092600 a.u.
Bond Energy LDA -72.13539624 eV
+ GGA-X -2.33493969 a.u.
+ GGA-X -63.53696760 eV
+ GGA-XC -2.47270385 a.u.
+ GGA-XC -67.28572284 eV