ReO2Me3

Atom	X	Y	Z (Angstrom)
1.Re	-0.003668	0.003125	0.000000
2.O	1.715683	0.016613	0.000000
3.O	-0.924449	1.456894	0.000000
4.C	-1.088121	-1.914204	0.000000
5.H	-0.912027	-2.520467	-0.894438
6.H	-0.912027	-2.520467	0.894438
7.H	-2.148093	-1.612990	0.000000
8.C	-0.300111	-0.502970	2.057761
9.H	0.076777	0.400440	2.565216
10.H	-1.350764	-0.670513	2.313662
11.H	0.302159	-1.371667	2.341618
12.C	-0.300111	-0.502970	-2.057761
13.H	-1.350764	-0.670513	-2.313662
14.H	0.076777	0.400440	-2.565216
15.H	0.302159	-1.371667	-2.341618

Bond Energy LDA -3.24806798 a.u.
Bond Energy LDA -88.38446275 eV
+ GGA-X -2.87436628 a.u.
+ GGA-X -78.21551806 eV
+ GGA-XC -3.03890841 a.u.
+ GGA-XC -82.69293890 eV

H2CReMeO2

Atom	X	Y	Z (Angstrom)
1.Re	0.000781	0.000463	0.000000
2.O	0.396083	0.726373	1.511610
3.O	0.396083	0.726373	-1.511610
4.C	0.479431	-1.830030	0.000000
5.H	0.700048	-2.369359	0.926886
6.H	0.700048	-2.369359	-0.926886
7.C	-2.104258	-0.147715	0.000000
8.H	-2.505888	0.876491	0.000000
9.H	-2.449356	-0.681354	-0.893507
10.H	-2.449356	-0.681354	0.893507

Bond Energy LDA -2.32736588 a.u.
Bond Energy LDA -63.33087362 eV
+ GGA-X -2.05661605 a.u.
+ GGA-X -55.96339288 eV
+ GGA-XC -2.17559356 a.u.
+ GGA-XC -59.20093717 eV

(H2C)2Re(O)OH

Atom	X	Y	Z (Angstrom)
1.Re	0.000363	0.002149	0.001054
2.O	1.942378	-0.009185	-0.003684
3.H	2.298068	0.899398	-0.026444
4.O	-0.686216	0.060304	-1.564433
5.C	-0.413883	-1.593917	0.926732
6.H	-0.192565	-1.716608	1.994422
7.H	-0.916519	-2.441525	0.449039
8.C	-0.516433	1.483841	1.061687
9.H	-1.014691	2.353250	0.617588
10.H	-0.391529	1.526737	2.150544

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Bond Energy LDA      -2.28430173 a.u.
Bond Energy LDA     -62.15903823 eV
         + GGA-X      -2.00918673 a.u.
         + GGA-X     -54.67277495 eV
        + GGA-XC      -2.12964468 a.u.
        + GGA-XC     -57.95060405 eV
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