

Sheet1

HF 6-31+GxxC

	C3H8	O2	CO2	H2O	Before	After	Diff
Ene	-118.27692666	-149.62206638	-187.63878676	-76.03123056	-866.38725856	-867.04128252	-0.65402396
Ene+ZPE	-118.17789866	-149.61799572	-187.62730856	-76.01032322	-866.26787726	-866.92321856	-0.65534130
Ene(298K)	-118.17327779	-149.61563379	-187.62469530	-76.00748690	-866.25144674	-866.90403350	-0.65258676
Entalpy(298K)	-118.17233360	-149.61468960	-187.62375111	-76.00654272	-866.24578160	-866.89742421	-0.65164261
							-1710.88743877

B3LYP3 6-31+GxxC

Ene	-119.15912695	-150.32757684	-188.59040402	-76.43404501	-870.79701115	-871.50739210	-0.71038095
Ene+ZPE	-119.05952607	-150.32397799	-188.57924466	-76.41351533	-870.67941602	-871.39179530	-0.71237928
Ene(298K)	-119.05493997	-150.32161401	-188.57658417	-76.41067867	-870.66301002	-871.37246719	-0.70945717
Entalpy(298K)	-119.05399578	-150.32066983	-188.57563998	-76.40973449	-870.65734493	-871.36585790	-0.70851297
							-1860.20054855