

Sheet1

HF 6-31+GxxC

	CH4	O2	CO2	H2O	Before	After	Diff
Ene	-40.20213114	-149.62206638	-187.63878676	-76.03123056	-339.44626390	-339.70124788	-0.25498398
Ene+ZPE	-40.15942297	-149.61799572	-187.62730856	-76.01032322	-339.39541441	-339.64795500	-0.25254059
Ene(298K)	-40.15655043	-149.61563379	-187.62469530	-76.00748690	-339.38781801	-339.63966910	-0.25185109
Entalpy(298K)	-40.15560625	-149.61468960	-187.62375111	-76.00654272	-339.38498545	-339.63683655	-0.25185110
							-661.23494644

B3LYP3 6-31+GxxC

Ene	-40.52617952	-150.32757684	-188.59040402	-76.43404501	-341.18133320	-341.45849404	-0.27716084
Ene+ZPE	-40.48294187	-150.32397799	-188.57924466	-76.41351533	-341.13089785	-341.40627532	-0.27537747
Ene(298K)	-40.48006656	-150.32161401	-188.57658417	-76.41067867	-341.12329458	-341.39794151	-0.27464693
Entalpy(298K)	-40.47912238	-150.32066983	-188.57563998	-76.40973449	-341.12046204	-341.39510896	-0.27464692
							-721.08541618