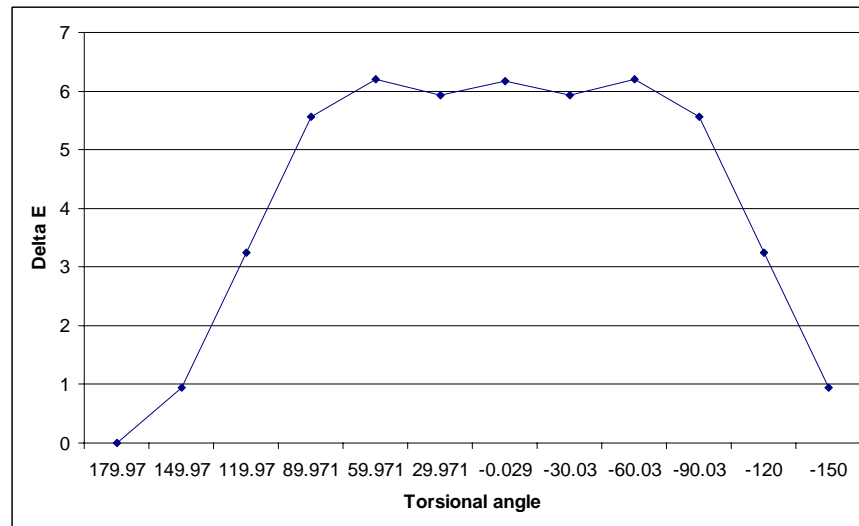
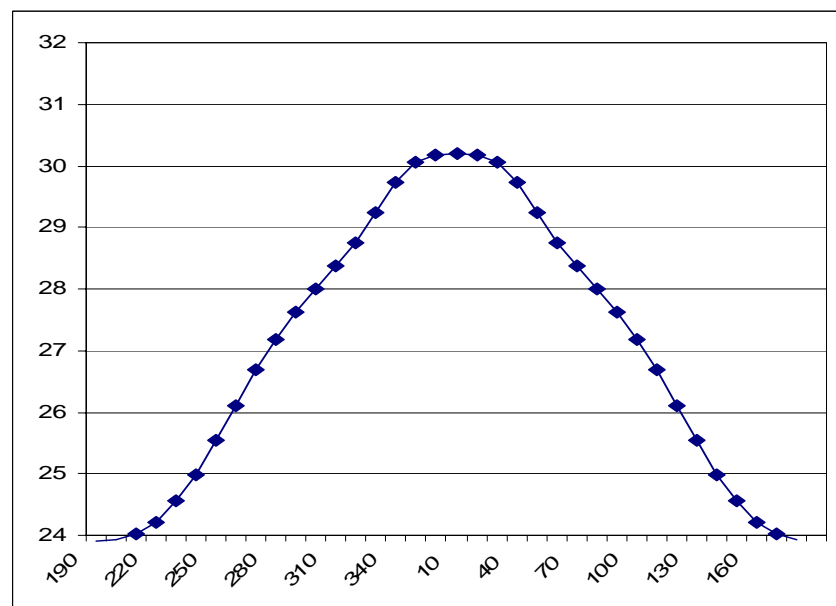


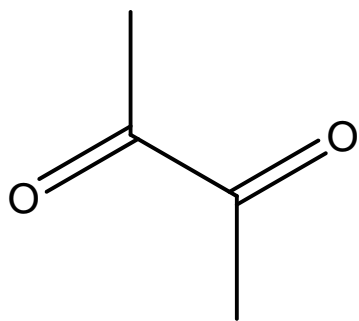
Biacetyl – model molecule



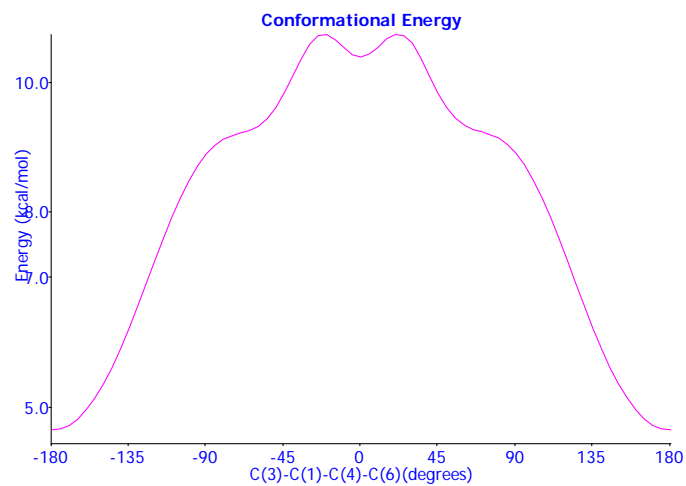
QM



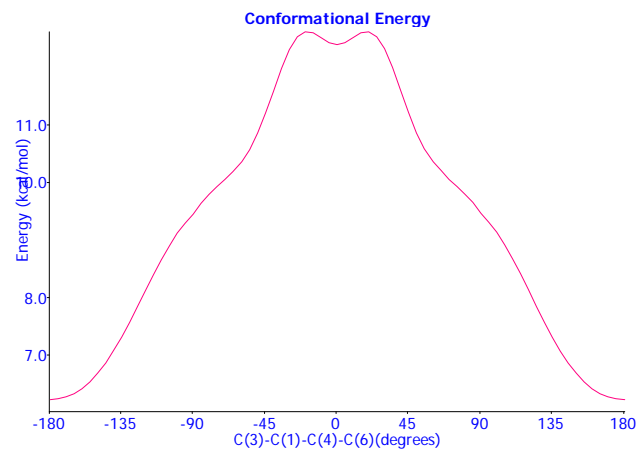
GAFF



Biacetyl – model molecule



MM2



MMFF