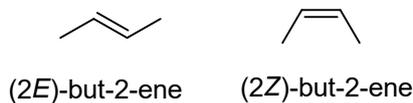


TD3 – Density Functional Theory

The goal of this tutorial is to use DFT to determine which isomer of butene should be the most abundant at room temperature.



1. Login with your amU account into ChemCompute (chemcompute.org).
2. Execute a geometry optimization of the *E* isomer with the B3LYP functional and the 3-21G basis set.
3. Collect the final total energy in the Table below.
4. Repeat the steps above for the *Z* isomer.
5. Evaluate the quantities required in the Table.
6. Compute the Boltzmann relative population of the two isomers at $T = 300$ K. This quantity is given by

$$\frac{P_E}{P_Z} = \exp\left(-\frac{|E_E - E_Z|}{k_B T}\right)$$

where k_B is the Boltzmann constant.

E_Z (au)	E_E (au)	$E_Z - E_E$ (au)	$E_Z - E_E$ (kcal/mol)