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.

(2*E*)-but-2-ene (2*Z*)-but-2-ene

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)