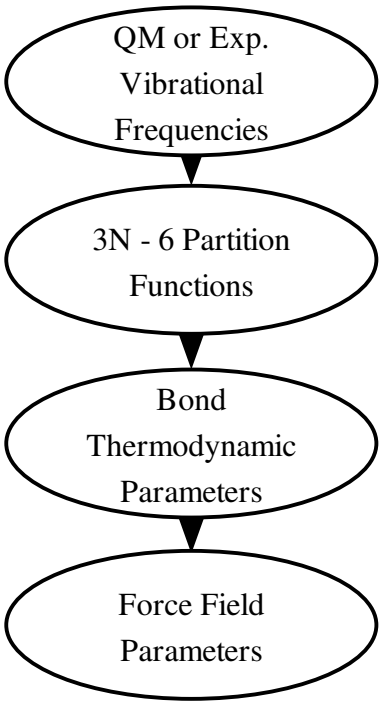
Force Field Development Via the Molecular Partition Function

James H. McConnell '07, Karl N. Kirschner, George C. Shields
Department of Chemistry, Hamilton College, Clinton, NY 13323

The molecular partition function is composed of four functions that describe the rotational, electronic, translational, and vibrational energy of a molecule. While each of the four partition functions helps characterize the thermodynamic properties of the molecule, the vibrational partition function is derived from internal vibration and thus each 3N – 6 vibration contributes to thermodynamic values. By following force field development methodology, bond types will be characterized by the vibrational partition function:



To this end, several simple hydrocarbons have been examined to characterize carbon-carbon and carbon-hydrogen stretching frequencies. Ultimately, we plan to expand the test set to include the necessary bond type parameters for a robust molecular mechanics force field.