

CBE 310

Molecular Concepts and Applications

Complete Molecular Partition Function

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- 0) Partition Functions and Statistical Thermodynamics
  - 1) Electronic Partition Function
  - 2) Rotational Motion and the Rotational partition function
  - 3) Complete Partition Function
  - 4) Some worked Problems

## What is the of partition function?:

The partition function is the connection between the microscopic details of the behavior of a system and the macroscopic thermodynamic properties of the system.

**\*\*The partition function tells you how the particles are *partitioned* among the possible states of the system. \*\* EVERY ENERGY MANIFOLD WILL HAVE ITS OWN FORM OF THE PARTION FUNCTION**

**\*\*The partition function counts the number of states that are *effectively accessible* at a given temperature\*\***

Translational Motion: Governed by “particle in a box” energies

Vibrational Motion: Governed by “Harmonic Oscillator” energies

Rotational Motion: Governed by “Rigid Rotor” energies

Electronic Transitions: Governed by “Electron Configuration” energies

## What is the of partition function?:



In a way, (this is an analogy), the partition function is like a thermal wavefunction, of a thermodynamics wave function.

It contains essentially all of the information about how the system responds to changes in temperature and work

We can use it to calculate any thermodynamic function of any system given that we know the quantum mechanical behavior of the molecules involved

EVERY ENERGY MANIFOLD or SET OF STATES WILL HAVE ITS OWN FORM OF THE PARTION FUNCTION