School of Chemistry

Module Aims: Session 2023-2024, Semester 1

Module CH3717: Statistical Mechanics and Computational Chemistry

Course Title: Introduction to Statistical Mechanics

Duration: 10 hours

Lecturer: Dr J. B. O. Mitchell

Aims: The aim of this course is to provide an introduction to the basic ideas of statistical mechanics, the essence of which is the description and interpretation of macroscopic thermodynamic quantities in microscopic / atomistic terms.

Objectives:

1. To understand the concepts of microstates and configurations and the idea of the predominant configuration.
2. To understand the Boltzmann Distribution Law and its significance in chemistry.
3. To know the form of and understand the meaning of partition functions, and to become familiar with molecular translational, rotational, vibrational and electronic partition functions.
4. To understand the pivotal relationship between partition functions and thermodynamic quantities and the notion of thermal averages. To understand how macroscopic thermodynamic quantities such as internal energy and entropy can be computed from partition functions.
5. To know how partition functions are defined and computed for molecules having multiple degrees of freedom.
6. To understand how partition functions are calculated for systems comprising many molecules. To consider the effect of distinguishability and indistinguishability on partition functions.
7. To know how and when thermodynamic quantities can be calculated easily from equipartition. To understand heat capacities.
8. To be able to calculate equilibrium constants from partition functions.
9. To have an overview of transition state theory.
10. To be aware of applications of statistical mechanics and statistical thermodynamics in the sciences.

Recommended reading:

1. ***Physical Chemistry***, P.W. Atkins, 5th Edition, Oxford
2. ***Statistical Thermodynamics***, A. Maczek, Oxford Chemistry Primers, Oxford
3. ***An Introduction to Statistical Thermodynamics***, R.P.H. Gasser and W.G. Richards, World Scientific
4. ***Statistical Mechanics***, G.S. Rushbrooke, Oxford