UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2017

1. Course: Chemistry 689, Molecular Driving Forces

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01	T / Th	12:30–1:45	ST027A	Justin MacCallum Peter Kusalik	BI 557 SB323	justin.maccallum@ pkusalik@	By appointment

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2. Course Description: In this introduction to statistical mechanics we will explore the basis from which to understand molecular driving forces. We will also examine how this formalism is applied within computer simulations of liquids, solids and solutions. The emphasis will be on physical models and interpretations, with applications to systems of chemical and biochemical interest. Selected topics from the recent literature will also be included. We will closely follow the required text, *Molecular Driving Forces* by Dill and Bromberg.

3. Required Textbook(s): *Molecular Driving Forces*, Ken A. Dill and Sarina Bromberg, Garland Science. Second Edition is preferable, but the First is also acceptable..

4. Topics Covered and Suggested Readings:

Course Content	**Chapter in Textbook**
MATHEMATICAL TOOLS Probability Extremum principles Multivariate calculus	Chapters 1, 2, and 4
FUNDAMENTALS OF STATISTICAL THERMODYNAMICS Heat, work, and energy Entropy and the Boltzmann law Thermodynamic driving forces The logic of thermodynamics Laboratory conditions and free energy Maxwell's relations and mixtures The Boltzmann distribution law Temperature and heat capacity	Chapters 3, 5–10, 12
SIMPLE APPLICATIONS OF STATISTICAL THERMODYNAMCS The statistical mechanics of simple solids, liquids, and gases Chemical equilibria Equilibria between solids, liquids, and gases Solutions and mixtures	11, 13–15
ADVANCED APPLICATIONS Selected advanced topics depending on class background and interests, examples: • Physical kinetics and diffusion • Microscopic dynamics • Electrostatic forces • Intermolecular interactions • Cooperativity and phase transitions	Selected from Chapters 16–30

Department Approval: Approved by Department Head Date: January 6, 2017