UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
Fall 2014

COURSE: – Chemistry 701.07, Research in Applied Chemical Thermodynamics

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	PHONE	EMAIL	OFFICE HOURS
L01	TBA	TBA	SB 221	Dr. Robert Marriott	SB 221	220-2417/3144	rob.marriott@ucalgary.ca	TBA

COURSE DESCRIPTION:

The purpose of this is course is to introduce several concepts of interest to students who is studying modern experimental chemical thermodynamics. The class will be divided into three parts: (1) general concepts for the thermodynamics of chemicals in ideal gas and real fluid phases, (2) experimental techniques and (3) computational chemical thermodynamics. The course topic will emphasise the connections between theoretical chemistry (e.g., statistical mechanics), experimental techniques and applied thermodynamic modelling. Two seminar topics will be assigned taking research interests into consideration.

MATERIAL TO BE COVERED:

(1) General concepts for the thermodynamic properties of chemicals in ideal gas and real fluid phases,
- Ideal gas properties, estimation versus predictive techniques
- *Ab initio* techniques versus empirical models for intra-molecular contributions
- Inter-molecular contributions, long-range interaction potentials, the many-body problem, cubic equations-of-state and reduced Helmholtz energy equations-of-state

(2) Experimental techniques
- Partial, excess and apparent molar properties
- Advanced *p*-*V*-*T* and caloric measurement techniques

(3) Computational chemical thermodynamics
- Gibb's energy minimization for multi-component systems
- Basics of object oriented programming
- Computer programming for the application of advanced equations-of-state, literature reading and reproduction of complex models

TEXTBOOKS:
'Molecular Thermodynamics of Fluid Phase Equilibria', J. M. Prausntiz, R. N. Lichtenthaler, E. G. De Azevedo
'The Properties of Gases and Liquids', B. E. Poling, J. M. Prausnitz, J. P. O'Connell
'Physical Chemistry', Atkins
'Thermodynamics in Geochemistry, the Equilibrium Model', G. M. Anderson and D. A. Crerar

Department Approval: Approved by Department Head Date: September 5 2014