COURSE: – Chemistry 701.xx, Research in Applied Chemical Thermodynamics

COURSE DESCRIPTION:

The purpose of this course is to introduce several concepts of interest to a student 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 emphasize 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. Prausnitz, R. N. Lichtenthaler, E. G. De Azevedo
‘Physical Chemistry’, Atkins
‘Thermodynamics in Geochemistry, the Equilibrium Model’, G. M. Anderson and D. A. Crerar

Department Approval: _______Approved by Department Head______ Date: __ January 7, 2019______