Syllabus CHEM531

No	List of Topics	Contact Hours
	CHEM 531: ADVANCED THERMODYNAMIC	
1	**I. The distribution of molecular states** ***I.1 Configurations and weights*** I.1.1 Instantaneous configurations I.1.2 The Boltzmann distribution ***I.2 The molecular partition function*** I.2.1 An interpretation of the partition function I.2.2 Approximations and factorizations	5
2	**II. The internal energy and the entropy** ***II.1 The internal energy*** II.1.1 The relation between U and q II.1.2 The value of b ***II.2 The statistical entropy*** II.2.1 Impact on technology	5
3	**III. The canonical partition function** **III.1 The canonical ensemble** III.1.1 The concept of ensemble III.1.2 Dominating configurations III.1.3 Fluctuations from the most probable distribution **III.2 The thermodynamic information in the partition function** III.2.1 The internal energy III.2.2 The entropy **III.3 Independent molecules** III.2.3 Distinguishable and indistinguishable molecules III.2.4 The entropy of a monatomic gas **Exercises**	6
	MED term 1	2
4	**IV Fundamental relations** **IV.1 The thermodynamic functions** IV.1.1 Helmholtz energy IV.1.2 The pressure IV.1.3 The enthalpy IV.1.3 The Gibbs energy **IV.2 The molecular partition function** IV.2.1 The translational contribution IV.2.2 The rotational contribution IV.2.3 The vibrational contribution IV.2.3 The electronic contribution IV.2.4 The overall partition function	6

	MED Term 2	2
5	**V Using statistical thermodynamics** **V.1 Mean energies** V.1.1 The mean translational energy V.1.2 The mean rotational energy V.1.3 The mean vibrational energy **V.2 Heat capacities** V.2.1 The individual contributions V.2.2 The overall heat capacity **V.3 Equations of state** **V.4 Molecular interactions in liquids** V.4.1 The radial distribution function V.4.2 The calculation of g(r) V.4.3 The thermodynamic properties of liquids **V.5 Residual entropies** **V.6 Equilibrium constants** V.6.1 The relation between K and the partition function V. 6.2 A dissociation equilibrium V.6.3 Contributions to the equilibrium constant **Exercises**	8
	Revision	2
	Final EXAM	3
Total		37