SRM UNIVERSITY

DEPARTMENT OF CHEMISTRY
FACULTYOF SCIENCE & HUMANITIES
SRM UNIVERSITY
KATTANKULATHUR

LESSON PLAN
Academic year 2017 – 18

Program : M.Sc. Chemistry
Subject Title : Classical and Statistical Thermodynamics
Subject Code : 17PCY102
Total No. of Hours: 60
Semester : I

UNIT No.& Title	TOPICS	LECTURE NO.	REFERENCE BOOKS
I. Classical Thermodynamics – I	First law of thermodynamics, concept of work and heat	1	1. P. W. Atkins, J. De Paula, *Physical Chemistry*, 9th Ed., Oxford University Press, Oxford, 2010. 2. J. Rajaram and J.C.Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Ed., S.L.N. Chand and Co, Jalandhar, 1993.
	Concept of enthalpy and heat capacities – solving numerical	2	
	Second law of thermodynamics, physical significance of entropy	3	
	Direction of spontaneous change and dispersal of energy	4	
	Carnot cycle – Deriving the expression of work done by the heat engine	5	
	Efficiency of heat engine and numerical related to that	6	
	Coefficient of performance of heat engine	7	
	Gibbs and Helmholtz functions	8	
	Gibbs–Helmholtz equation and solving numerical	9	
	Maxwell relations	10	
	Maxwell relations – continuation and solving problems	11	
	Discussing the questions about first and second laws of thermodynamics	12	
II. Classical Thermodynamics – II	Thermodynamic equation of state	13	1. P. W. Atkins, J. De Paula, *Physical Chemistry*, 9th Ed., Oxford University Press, Oxford, 2010. 2. J. Rajaram and J.C.Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Ed., S.L.N. Chand and Co, Jalandhar, 1993.
	Thermodynamics of systems of variable composition	14	
	Partial molar quantities, partial molar volume, Partial molar free energy etc.	15	
	Chemical potential, Gibbs-Duhem equation	16	
	Correlation of chemical potential with temperature and pressure	17	
	Experimental determination of fugacity of real gases	18	
	Solving problems related to chemical potential	19	
	Third law of thermodynamics, Nernst Heat theorem	20	

	Absolute entropies & determination	21	3. S. Glasstone *Thermodynamics for Chemists*, Litton Educational Publishing Inc., New York, 2012.
	Exceptions to third law, unattainability of absolute zero	22	
	Solving numerical related to third law of thermodynamics	23	
	Evaluating the student's knowledge by conducting a descriptive test	24	
III. Statistical Thermodynamics – I	Introduction: Macro and micro states	25	1. J. Rajaram and J.C.Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Ed., S.L.N. Chand and Co, Jalandhar, 1993. 2.M.C. Gupta, *Statistical Thermodynamics*, New Age International, Pvt. Ltd, New Delhi, 1995. 3. P. W. Atkins, J. De Paula, *Physical Chemistry*, 9th Ed., Oxford University Press, Oxford, 2010.
	Ensembles (microcanonical and canonical)	26	
	Maxwell-Boltzmann statistics	27	
	Boltzmann- Planck equation	28	
	Fermi-Dirac Statistics	29	
	Bose-Einstein statistics	30	
	Solving problems	31	
	Negative absolute temperatures	32	
	Partition function and evaluation of the partition function translational partition function	33	
	Evaluation of rotational partition function	34	
	Evaluation of vibrational partition function and electronic partition function	35	
	Nuclear partition function and problems related to partition function	36	
IV. Statistical Thermodynamics – II	Thermodynamic functions in terms of the partition function- internal energy, entropy, Helmholtz function	37	1. P. W. Atkins, J. De Paula, *Physical Chemistry*, 9th Ed., Oxford University Press, Oxford, 2010. 2. M.C. Gupta, *Statistical Thermodynamics*, New Age International, Pvt. Ltd, New Delhi, 1995. 3. D.A. McQuarrie and J.D. Simon, *Physical Chemistry, A Molecular Approach*, Viva Books Pvt. Ltd., New Delhi, 1999
	Continuation of partition funcions-Pressure, Gibbs function, residual entropy, equilibrium constant, isotope effects	38	
	Molecular interpretation of the basic laws of thermodynamics	39	
	Solving problems	40	
	Average energies and equipartition principle	41	
	Heat capacity of monoatomic gases, population inversion, negative Kelvin temperature	42	
	Einstein's and Debye's theories of heat capacities of solids	43	
	Nuclear spin statistics and solving problems	44	
	Statistical basis of entropy of H_2 gas, ortho and para nuclear states	45	
	Calculation of entropy in terms of ortho- para ratio	46	
	Residual entropy of H_2 at 0 K	47	

	Evaluating the student's knowledge on Statistical thermodynamics by interaction and discussion	48	
V. Non-equilibrium Thermodynamics	Introduction, near equilibrium process	49	1. C. Kalidas and M.V.Sangaranarayanan, Non equilibrium thermodynamics- principles and applications, Macmillan, India, 2004. 2. J. Rajaram and J.C.Kuriacose, *Thermodynamics For Students of Chemistry*, 2nd Ed., S.L.N. Chand and Co, Jalandhar, 1993. 3. P. W. Atkins, J. De Paula, *Physical Chemistry*, 9th Ed., Oxford University Press, Oxford, 2010.
	General theory, conservation of mass and energy	50	
	Entropy production in chemical reactions	51	
	Entropy production and entropy flow in open systems	52	
	Transformation properties of rates and affinities	53	
	Onsager's theory	54	
	Solving problems	55	
	Introduction to irreversible thermodynamics	56	
	Irreversible thermodynamics and biological systems	57	
	Oscillatory reactions	58	
	Solving numerical	59	
	Discussing and solving the previous year question papers	60	

STAFF DETAILS

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HOD/Chemistry 26/7/17