UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QG108	Theoretical General Chemistry

Vector
OF:S-5 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement	None

Summary

Atomic structure; periodicity of atomic properties; models of chemical bond (ionic and covalent); molecular geometry; intermolecular interactions, general properties of solids, liquids and gases. Notions of thermodynamics.

Program

1. Atomic structure
Atomic models. Wave functions and energy levels. Quantum numbers and atomic orbitals. Electron spin. Orbital energy. Magnetism and Paramagnetism. Hund's rule and Pauli's exclusion principle. Filling orbitals and electron configuration of atoms.
2. Periodicity of the atomic properties
Electronic configuration and the periodic table. Effective nuclear charge. Periodicity of atomic properties: atomic radius, ionic radius, ionization energy, electron affinity and its anomalies. Main groups of elements.
3. Chemical bond models (ionic and covalent) and molecular geometry
General introduction to the concepts of chemical bond: Ionic and covalent bonds. Ionic connection. Electronic configuration of ions, ionization energy and electronic affinity. Born-Haber Cycle. Structure and energy of crystalline lattice. Covalent character in predominantly ionic bonds (bond distance, solubility, thermal stability, melting point and sublimation) Covalent Bond. Lewis structures. Molecular geometry: VSEPR model. Valence bond theory and orbital hybridization model. Hybrid orbitals involving d-orbitals. Multiple connections. Limitations of the valence bond theory. Chemical bonding properties: enthalpy and bond length. Order of the link. Resonance structures. Polarity of chemical bonds. Electronegativity. Molecular orbitals for homonuclear and heteronuclear diatomic molecules.
4. Intermolecular interactions
Ion-ion interactions; ion-dipole; dipole-dipole and induced dipoles. Hydrogen bond. Effects of these interactions on melting, boiling and solubility. General structure of liquids. Ideal gas and real gases.
5. Notions of thermodynamics and chemical equilibrium
The laws of thermodynamics; spontaneity criteria; Gibbs energy. Equilibrium constants; equilibrium response to changes in conditions.
6. Chemical kinetics
Order of reaction. First and second order reactions. Half-life time. Influence of temperature on reaction rate; activation energy

Bibliography

-ATKINS, P., JONES, L. Princípios de química: questionando a vida moderna e o meio ambiente. Porto Alegre: Bookman, 2001.

-BROWN, T.L., LeMAY Jr., H.E., BURSTEN, B.E., BURDGE, J.R. Química - a ciência central. 9ª. edição. São Paulo : Pearson Prentice Hall, 2005
-KOTZ, J. C.; TREICHEL, P. Química e reações químicas. 3ª edição, Volumes 1 e 2. Rio de Janeiro: Livros Técnicos e Científicos, 1998.
-RUSSEL, J. B. Química geral. 2ª edição, Volumes 1 e 2. São Paulo: Makron Books, 1994
SANTOS FILHO, P.F. Estrutura atômica e ligação química. Campinas: Unicamp, 2000.
-LEE, J. D. Química Inorgânica não tão concisa. 5ª ed., São Paulo: Edgard Blücher, 1999.
-CHANG, R, CRUICKSHANK, R. Chemistry. 8th edition. Boston: McGraw-Hill. 2005.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.