Code: **QG108**

Name: **Química Geral Teórica**

Name in English: **General Theoretical Chemistry**

Name in Spanish: **Química General Teórica**

Subject type: **Weekly**

Approval Type: **Grade and Frequency**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semestral / All periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
4	**-**	**-**	**-**	**-**	**-**	**4**	**15**	**4**

Occurrence on curriculum: **05, 50, 56, 63**

Pre requirement:

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. Basics of thermodynamics.

Program:

1. Atomic structure:

Atomic models. Wavefunctions and energy levels. Quantum numbers and atomic orbitals. Electron spin; Orbital energy. Magnetism and Paramagnetism. Hund's rule and Pauli exclusion principle. Filling of atomic orbitals and electronic configuration of atoms.

2. Periodicity of 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 the elements.

3. Models of chemical bond (ionic and covalent) and molecular geometry:

General introduction to the concepts of chemical bond: ionic and covalent.

Ionic bond. Electron configurations of ions, ionization energy and electron affinity. Born-Haber cycle. Structure and energies of crystalline lattices. Covalent character in predominantly ionic bonds (bond length, solubility, thermal stability, melting point and sublimation).

Covalenet bond. Lewis structures. Molecular geometry: VSEPR model. Valence bond theory and the hybridization model of orbitals. Hybrid orbitals involving d-orbitals. Multiple bonds. Limitations of valence bond theory.

Chemical bond properties: enthalpy and bond length. Bond order. Resonance structures. Chemical bond polarity. Electronegativity.

Molecular orbitals for homonuclear and heteronuclear diatomic molecules.

4. Intermolecular interactions

Ion-ion, ion-dipole, dipole-dipole and induced dipole interactions. Hydrogen bond. Intermolecular interaction effects on melting and boiling points and on solubilities. General structure of liquids. Ideal and real gases.

5. Basics of thermodynamics and chemical equilibrium
The laws of thermodynamics; criteria for spontaneity; Gibbs energy. Equilibrium constants; Equilibrium response to changes.
6. Chemical kinetics
Reaction order. First and second-order reactions. Half-life time. Temperature effects on reaction rate; activation energy.

Basic Bibliography

1) ATKINS, P.W.; JONES, L. **Princípios de química: questionando a vida moderna e o meio ambiente**, Obs: O Sistema de Bibliotecas da Unicamp dispõe de e-books e diversos exemplares das edições de 2001; 2006 (3. Ed), 2012 (5. Ed), 2018 (7.ed.).
2) KOTZ, J. C. TREICHEL JR, P. **Química e reações químicas**, 3ª edição, Volumes 1 e 2. RJ: Livros Técnicos e Científicos, 1998. (e 4ª edição, Volumes 1 e 2. RJ: Livros Técnicos e Científicos, 2002).
3) BROWN, T.L.; LEMAY JR., H.E.; BURSTEN, B.E.; BURGE, J.R. **Química - a ciência central**. 9ª. edição. São Paulo: Pearson Prentice Hall, 2005

Supplementary Bibliography

1) CHANG, R. **Química geral: conceitos essenciais**, 4a edição, Porto Alegre, RS AMGH, 2010 (livro impresso e e-book)
2) RUSSEL, J. B. **Química geral**, 2ª edição, Volumes 1 e 2. São Paulo: Makron Books, 1994
3) FILHO, P.F.S. **Estrutura atômica e ligação química** Campinas: Unicamp, 2000.
4) LEE, J. D. **Química Inorgânica não tão concisa**. 5ª ed., São Paulo: Edgard Blücher, 1999.
5) BRADY, J.E. **Química Geral.** 2ª ed., Volumes 1 e 2. Rio de Janeiro: LTC, 1986.