Code: **QI146**

Name: **Interações Químicas**

Name in English: **Chemical Interactions**

Name in Spanish: **Interacciones Químicas**

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 |
|---|---|---|---|---|---|---|---|---|
| **2** | **-** | **-** | **-** | **-** | **-** | **2** | **15** | **2** |

Occurrence on curriculum: **05, 50**

Pre requirement: **QG108**

**Summary:** Molecular orbital theory for polyatomic molecules. Introduction to group theory. Acids and bases.

**Program**:

**Molecular Orbitals**

Introduction to group theory: symmetry, point groups and the use of the character tables in the classification of molecules and orbitals. Symmetry adapted molecular orbitals. Molecular orbital theory for polyatomic molecules (single species: $H_3$ and $H_3^+$, $H_2O$, $NH_3$ and Walsh diagrams for molecules $EH_2$); Molecular orbitals for chains of atoms, hypervalent molecules, molecules with $\pi$ bond and electron deficient molecules (examples: $SF_6$, fragment B-H-B of boranes, $NO_2^-$)

**Acids and Bases**

Bronsted acidity: $H^+$ in $H_2O$; conjugate acids and bases; acidity and basicity of solvents. Periodic trends in Bronsted acidity: aqua-acids; oxo-acids (Pauling Rule); anhydrous oxides; amphoterism. Lewis's acids and bases: periodic trends; examples of reactions: adduct formation (correlating with the molecular orbital); displacement reactions; metathesis. Structural and steric considerations on the strength of acids and bases in several theories. Hard and soft acids and bases including f elements. The interpretation of hardness/softness and usefulness of this concept. Surface acidity, for example, silica, alumina, aluminosilicates. Generalized concept of acids and bases. Hydrides - periodic trends.

**Basic Bibliography**

1) HOUSECROFT, C.E.; SHARPE, A.G. **INORGANIC chemistry**. 4. Ed. Upper Saddle River. NJ: Prentice-Hall, 2012. 754p.

2) MIESSLER, G.L.;TFISCHER, P.J.;TARR, D.A. **Química Inorgânica**. 4.Ed.,São Paulo: Pearson,2014.649 p.

3) HUHEEY, J.E.; KEITER, E.A.; KEITER, R.L. **Inorganic chemistry: principles of structure and reactivity**. 4. Ed. New York : Harper Collins, 1993. 964p.

**Supplementary Bibliography**

1) SHRIVER, D.F.; ATKINS, P.W.; LANGFORD, C.H. **Inorganic chemistry**. 2. Ed. Oxford, UK: Oxford University Press, 1994. 819 p.

2) KETTLE, S.F.A. **Symmetry and structure**: **readable group theory for chemists**. 2. Ed. Chichester : John Wiley, 1995. 416p.

3) Cotton, F.A. **Chemical applications of group theory**. 3 Ed. New York: John Wiley, 1990. 461p.

4) OLIVEIRA, G.M. **Simetria de moléculas e cristais: fundamentos da espectroscopia vibracional**. Porto

5) OGDEN, J.S. **Introduction to molecular symmetry**. United State: Oxford University Press,2006. 90 p.