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Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
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COURSE SYLLABUS

1. Identification

Code and title: QUP 336 - Advanced Analytical Chemistry
Professor: João Henrique Zimnoch dos Santos
Level: Master and Doctorate
Credit hours: 3
Revised: August_2021

2. Summary

Statistical methods applied to Analytical Chemistry. Errors and data treatment. Validation of analytical methodology. Calibration. Activity coefficient and Debye-Hückel theory. Advanced studies of chemical equilibrium involving acid-base, solubility, complexation and oxy-reduction. Analytical chemistry in non-aqueous solvents.

3. Objective

To deepen the knowledge of the postgraduate student in Quantitative Analytical Chemistry, through the broad approach of theoretical foundations already established in the area and theories under construction.

4. Contents

- Statistics for Analytical Chemistry: Analytical Problems, Statistics of repeated measurements and Analytical figures of merit, Significance tests, Validation of Analytical Methods, Errors in quantitative analysis, Calibration methods: regression and correlation, Introduction to Multivariate analysis, The quality of analytical measurements
- Effect of electrolytes on chemical balances: Ionic force, Activity and activity coefficient, Debye Hückel's Theory (Extended Equation and Limit Law), Davies Equation, Balance calculations using activity coefficients
- Non-aqueous solvents: Physical properties of solvents (cohesive forces, solubility parameters, dielectric constant, refractive index), Chemical properties (donor number, acceptor number, solvatochromism) , Classification of solvents, Leveling and differentiating effect of solvents on acid and base strength, Determination of organic and inorganic species in non-aqueous media by different analytical techniques.
- Acid-base equilibrium: Monoprotic acids and bases, Polyfunctional acids and bases. Species distribution. Composition of polyprotic acid solutions as a function of pH (α - values). Logarithmic concentration diagrams, Graphical representation of acid-base equilibrium.
- Solubility equilibrium: Influence of various factors on equilibrium (pH, common ion, other ions, hydrolysis)
- Complexation equilibrium: Distribution of species in equilibrium. Formation constants, Influence of pH on complexation equilibrium, Equilibrium of complexation and solubility.
- Equilibrium in oxy-reduction reactions: Mechanisms of oxy-reduction reactions, Spontaneity of oxy-reduction reactions, Simultaneous equilibrium involving oxy-reduction, acid-base, complexation and solubility.

5. Assessment

Exercise lists, Presentation and discussion of scientific articles and Theoretical tests. The student who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:
A: grade equal to or above 9.0
B: grade equal to or above 7.5 and below 9.0
C: grade equal to or above 5.0 and below 7.5
D: grade below 5
FF: lack of frequency

6. Methodology

Theoretical lectures. Use of statistical treatment softwares.

7. Bibliography

- Compton, R. G., Sanders, G. H. W., Electrode Potentials, Oxford University Press, 1996 (Reprinted 2009)
- Ellison, S. L. R., Barwick, V. J., Farrant, T. J. D, Practical statistics for the Analytical Scientist. A bench guide, 2 ed. RCS, 2009.
- Hair, Black, Babin, Anderson, Tathan, Análise Multivariada de Dados, Bookman, 6ª Ed., 2009.
- Meites, L., An Introduction to Chemical Equilibrium and Kinetics, Pergamon Press, 1981.
- Miller, J. N., Miller, J. C. Statistics and chemometrics for Analytical Chemistry, Prentice Hall, 7ª ed., 2018.
- Petrozzi, S., Practical Instrumental Analysis. Methods, Quality Assurance and Laboratoy Manegement, Wiley, 2013.
- Skoog, F., West, Holler, Crouch, Fundamentos de Química Analítica, Thomson Learning, 8ª ed., 2011.