

Course: Organic Chemistry and Soil Coordination Compounds

Identification Code: SOL 859

Credits: 4 (3 hours theory -1 hour practice)

Level: Master and Doctorate

Professor: Leandro Souza da Silva **System:** Annual (II semester)

Discipline objectives

To provide students with knowledge of the basic concepts of organic chemistry to relate them to the nature of organic matter and its biological, physical, and chemical properties. To provide students with knowledge of coordination compounds in soil chemistry to identify, characterize, and relate the factors that act on the formation, structuring, and stability of organic and inorganic complexes in the soil solution and at the solid-solution interface. To provide a theoretical foundation to understand soil and water quality, agricultural production, and agroecosystem sustainability.

Syllabus

Fundamentals of coordination compounds and organic chemistry; coordination compounds in soil solution; coordination compounds at the solid-solution interface; chemistry of soil organic matter; evaluation and characterization of organic substances; interactions of organic matter in the soil.

Methodology and/or teaching instruments

Lectures, individual seminars, discussion of scientific articles (overhead projector and blackboard).

Forms of evaluation

Written exams, seminars, activity reports, and class participation.

Program - Title and Breakdown of Units

Unit 1

Fundamentals of organic chemistry

- 1.1 Introduction to organic chemistry
 - 1.1.1 Hybridization of carbon orbitals
 - 1.1.2 Structural and geometric representations
- 1.2 Nomenclature and characterization
 - 1.2.1 Alkanes
 - 1.2.2 Alkenes
 - 1.2.3 Alkynes
 - 1.2.4 Aromatic compounds
- 1.3 Main groups of organic compounds
 - 1.3.1 Halides
 - 1.3.2 Alcohols
 - 1.3.3 Phenols
 - 1.3.4 Ethers
 - 1.3.5 Amines
 - 1.3.6 Aldehydes and ketones
 - 1.3.7 Carboxylic acids

Unit 2

Chemistry of soil organic matter

- 2.1 Importance and functions of organic matter
- 2.2 Formation and decomposition of organic matter



- 2.2.1 Organic matter compartments and their characterization
- 2.2.2 Physical and chemical fractionation of organic matter and its relationship with soil dynamics
- 2.3 Structure and reactions of organic matter and its relationship with soil properties

Unit 3

Evaluation and characterization of organic substances

- 3.1 Quantitative analysis of carbon in soil and solution
- 3.2 Using spectroscopic techniques to characterize organic matter
 - 3.2.1 UV-Visible
 - 3.2.2 Infrared
 - 3.2.3 NMR and EPR

Unit 4

Fundamentals of coordination compounds

- 4.1 Introduction to coordination compounds
 - 4.1.1 Importance of coordination compounds and their relationship with the environment
 - 4.1.2 Historical aspects of coordination compounds
- 4.2 Basic concepts
 - 4.2.1 Complex, central atom, and ligands
 - 4.2.2 Types of ligands and coordination numbers
- 4.3 Models in the study of coordination compounds
 - 4.3.1 Valence bond theory
 - 4.3.2 Crystal field theory
 - 4.3.3 Molecular orbital theory

Unit 5

Coordination compounds in soil solution

- 5.1 Cations in aqueous media and their dynamics in the soil solution
 - 5.1.1 Coordinated cations with water
 - 5.1.2 Oxo-hydroxo and aquo-ion forms
- 5.2 Types of complexes in the soil solution and interactions
 - 5.2.1 "Free" ions
 - 5.2.2 Outer-sphere complexes (ionic pairs)
 - 5.2.3 Inner-sphere complexes
- 5.3 Main inorganic complexes in solution
- 5.4 Main organic complexes in solution
- 5.5 Speciation in the soil solution
 - 5.5.1 Importance of speciation in the activity of nutrients and toxic elements
 - 5.5.2 Soil solution extraction and characterization
 - 5.5.3 Use of computer programs for soil solution speciation

Unit 6

Coordination compounds at the solid-solution interface

- 6.1 Characteristics of the surface of soil particles
 - 6.1.1 Charges and functional groups
 - 6.1.2 Protonation
- 6.2 Surface complexes and the availability of nutrients and toxic elements
 - 6.2.1 Outer-sphere complexes (exchange reactions)
 - 6.2.2 Inner-sphere complexes (specific adsorption)
- 6.3 Coordination compounds and the solubility of minerals in the soil
 - 6.3.1 Dissolution by protonation



6.3.2 - Dissolution by binders

Unit 7

Organic matter interactions in soil

- 7.1 Interactions of organic matter with inorganic colloids and their relation with soil dynamics
- 7.2 Interactions of organic matter with anthropogenic compounds and their relationship with the environment

Recommended literature

ALLINGER, N.L.; CAVA, M.P.; DE JONGH, D.; JOHNSON, C.R.; LEBEL, N.A.; STEVENS, C.A. **Química Orgânica.** Rio de Janeiro: Editora Guanabara Koogan S.A. 1978. 322p.

BARROS, H.L.C. Química inorgânica: uma introdução. Belo Horizonte: Editora UFMG, 1992. 509p.

CADISCH, G., GILLER, K.E. **Driven by nature: plant litter quality and decomposition**. Cambridge: CAB Intl. 1997. 120p.

SANTOS, G.A.; SILVA, L.S.; CANELLAS, L.P.; CAMARGO, F.A.O, (Eds.) **Fundamentos da matéria orgânica do solo**: ecossistemas tropicais e subtropicais, 2 ed. Porto Alegre: Metrópole, 2008. 636p.

COLEMAN, D.C., OADES, J.M., UEHARA, G. **Dynamics of soil organic matter in tropical ecosystems**. Honolulu: University of Hawaii, 1989. 524 p.

CORNELL, R.M.; SHWERTMANN, U. The iron oxides: structure, properties, reactions, occurrence and uses. Weinheim: VCH Verlagsgesellschaft Gmbh. 1996.

HUANG, P.M.; SCHNITZER, M. (Eds). Interactions of soil minerals with natural organics and microbes. Madison: Soil Science Society of America, 1986. 606p.

McBRIDE, M.B. Environmental chemistry of soil. New York: Oxford University Press. 1994. 406p.

MacCARTHY, P., CLAPP, C.E., MALCOLM R.L., et al. **Humic substances in soil and crop sciences**. Madison: American Society of Agronomy, 1990. 281p.

MAGDOFF, F.R.; TABATABAI, M.A.; HANLON Jr, E.A. (Eds.) **Soil organic matter: analysis and interpretation**. Madison: Soil Science Society of America, 1996. 67p.

PAUL, E.A., CLARK, F.E. **Soil microbiology and biochemistry**. San Diego: Academic Press, Inc., 1996. 276 p.

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SILVERSTEIN, R.M., BASSLER, G.C., MORRILL, T.C. Identificação espectrométrica de compostos orgânicos. Rio de Janeiro: Editora Guanabara, 1979. 299 p.

SPARKS, D.L. Environmental Soil Chemistry. California: Academic Press. 1995. 267p.



SPOSITO, G. The chemistry of soil. New York: Oxford University Press. 1989. 277p.

SPOSITO, G. Environmental chemistry of aluminium. (2nd ed.) Boca Raton: CRC Press. 1996. 464p.

STEVENSON, F.J. **Humus chemistry: genesis, composition, reaction**. (2nd ed.) New York: J. Wiley, 1994. 496p.

STUMM, W; MORGAN, J.J. Aquatic chemistry. (3th ed.) New York: John Wiley & Sons. 1996. 1022p.

STUMM, W. Chemistry of the soil-water interface. New York: John Wiley & Sons. 1992. 428p.

TABATABAI, M.A.; SPARKS, D.L. (Eds.) **Chemical processes in soils**. Madison: Soil Science Society of America, 2005. 723p.

URE, A.M.; DAVIDSON, C.M. **Chemical speciation in the environmental**. (5th ed.) Glasgow: Blackie Academic & Professional. 1995. 408p.

WOLT, J. Soil solution chemistry. New York: John Wiley & Sons. 1994. 345p.