COMPLEX-FORMATION SOLUTION-EQUILIBRIA BETWEEN METALS AND LIGANDS OF BIOLOGICAL AND/OR PHARMACOLOGICAL SIGNIFICANCE

Many metals are involved in the biological processes that support plant and animal life. Some of them are called "minor" metals, since they are present only in trace amounts although they are part of fundamental molecules of life, such as metal-proteins and metal-enzymes. The formation of these complexes is regulated by a large number of environmental factors including the competition of other ligands and metal ions. Therefore, it is important to understand the behavior of these systems under dynamic conditions, such as those occurring in solution, in biological fluids.

GOALS

The main goals of this research are as follows: a) measurement of acid/base properties of the considered ligands; b) definition of the speciation model relative to complex species formed between the ligands and metals investigated; c) calculation of distribution and competition diagrams; d) study of the structure in solution of the main complexes. This scheme of investigation has recently been applied in different fields: metal-peptide equilibria (used as models for metal-protein complexes, e.g. SPARC or Prion proteins); potential drugs for chelation therapy (used in the treatment of heavy-metal poisoning); macro-chelate complexes (e.g. metallacrowns), possible candidates as contrast agents in diagnostic imaging.

INSTRUMENTS AND METHODS

The most widely used method for studying solution equilibria involving molecules with acid-base properties is potentiometry with the glass electrode. In special cases other electrodes can be used, e.g. electrodes sensitive to the metal ion. The laboratory has two automatic titrators, each consisting of a motor-driven microburette and a precision pH-meter, both operated by a computer. In order to complete the thermodynamic characterization of solution equilibria, the laboratory has an isoperibol titration microcalorimeter (Tronac, mod. 450). To obtain information about the structure of the species formed in solution several spectroscopic techniques are used, including UV-Vis spectrophotometry (available in the lab), circular dichroism spectroscopy, EPR and NMR spectroscopies. In addition, among the techniques available in our Department, the following are also widely employed: ESI-MS spectrometry, useful to confirm the stoichiometry of the species in solution, and the X-rays diffraction, giving the solid state structure of complex species. In collaboration with the Department of Life Sciences and Biotechnology tests of biological activity in vitro of both the ligands and complexes are performed.

MAIN SUBJECTS

Analytical Chemistry, Physical Chemistry, Bioinorganic Chemistry, Organic Chemistry, Biochemistry.

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