Politechnika Wrocławska

DISSERTATION ABSTRACT

„Calcium complexes with carbohydrates and their derivatives - interaction analysis”

Mgr inż. Dariusz Toczek

Promoter: Prof. dr hab. inż. Roman Gancarz

This thesis contains results of interaction analysis between calcium cations and carbohydrates and their derivatives (alditols, sugar acids, sulphonate derivatives, glucosamine and phosphonate derivatives) in the molar ratio 1:1. Potential binding sites were designated for each combination ligand-Ca^{2+} and described by parameters enabling assessment of the investigated interactions due to strength, stability and equilibrium for complex formation.

A theoretical model was applied, thanks to which reliable structural mapping of potential complexes was obtained. A computational model was devised, which allowed determination of the overall and local solvent influences on the interactions investigated. Local influence can be defined by highlighting the interactions occurring at the boundary of the ligand-H_2O and cation-H_2O. Moreover, identification of relatively strong or weak individual O-Ca^{2+} interactions, was possible by completion of the first coordination sphere of the calcium cation.

Structural properties suchas ligand conformation or spatial arrangement were investigated in the context of interaction energy, stability and equilibrium constant. Furthermore, two elementary functions related to spatial arrangement of donor oxygen atoms were described. Additionally, the effect of the chemical nature (eg, hydroxyl, carboxylic, carboxylate, phosphonic, phosphonate, sulphonic) of the donor oxygen atom on the studied interactions was determined. The average energy values of individual O-Ca^{2+} interaction were estimated.

The results obtained results allow to formation of a scheme for designing new ligands with given complexing properties.