

Diss. Nr. 4916

**Beitrag zur theoretischen Erfassung
der Alkali- und Erdalkalitionen
von Trägerantibiotika und Modellverbindungen**

ABHANDLUNG

zur Erlangung
der Würde eines Doktors der technischen Wissenschaften
der
EIDGENÖSSISCHEN TECHNISCHEN HOCHSCHULE
ZÜRICH

vorgelegt von

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Angenommen auf Antrag von
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Juris Druck + Verlag Zürich
1972

7. SUMMARY

- 7.1. A model for the computation of free energies of hydration and coordination numbers of cations using easily available parameters is described. For 27 mono-, di- and trivalent cations the mean deviation of the calculated from the experimental ΔG_H^0 -values is 3,9%. All of the computed coordination numbers agree with experimental ones.
- 7.2. Using model calculations, the influence of the coordination number, the properties of ligand groups, the dimension of the ligand, steric interactions and the solvent on the complexation of alkali- and alkaline earth metal cations by electrically neutral ligands (carrier antibiotics, model compounds) is discussed. Information is given on the molecular parameters needed to achieve a given ion selectivity in view of the use of such ligands as carriers in ion selective membranes.
- 7.3. In order to explain the cation selectivity of ion exchangers, a modified theory of interionic interactions in solution (ion association) is applied. Several analytically useful cation exchangers are briefly discussed.
- 7.4. The alkali cation selectivity of negatively charged multidentate ligands is studied by means of model calculations. The influence of the coordination number (coordination geometry) and the distance between cation and anionic ligand group on the relative complex stability is discussed. It was established that the inverse selectivity sequence in regard to Na^+ and K^+ exhibited by the carrier antibiotics nigericin and monensin is caused by differing steric interactions in the framework of the ligand.