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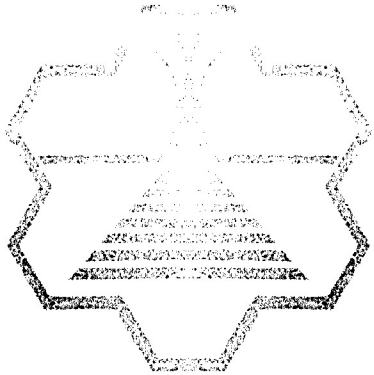

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Abstracts

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THERMODYNAMICS OF COMPLEXATION OF SALTS OF ALKALI AND ALKALINE-EARTH CATIONS WITH MACROCYCLIC LIGANDS.

V.P.Solov'ev, N.N.Strakhova, L.V.Govorkova, O.A.Raevsky

Institute of Physiologically Active Compounds,
USSR Academy of Sciences, 142432 Chernogolovka

Thermodynamic parameters such as free energy and enthalpy and entropy of complexation between macrocyclic ligands and alkali and alkali-earth cations in different media were evaluated. It was studied for the purpose of understanding the interactions governing complexation, search for ligands with optimum complex stability and the selectivity of interaction, for designing quantitative models between the structure of the ligands and thermodynamic values.

A computer programs was written in FORTRAN for the IBM family of personal computer. A program involve of solution of a problem of designing the best equilibrium model of the system, i.e. of determining the number of complexes in solution, their stoichiometry, stability constant and enthalpies.These values were determined in H_2O, C_2H_5OH and CH_3CN at 298 K for the complexation of macrocyclic ligands and podands containing ether, carbonyl and phosphoryl oxygen as donor atoms. Methods of calorimetric titration, IR and NMR spectroscopy were used for the calculation of the thermodynamic values.

The complexes of ligands containing phosphoryl group in the polyether ring are less stable when compared with the unsubstituted benzo-crown ethers. Phosphoryl containing podands are to form more stable complexes with lithium and magnesium cations in comparison with macrocyclic polyethers. The thermodynamic values of complexation were found to be dependent on the anion present. This effect counteranion on complex formation is not explained only by presence of associated cation with anion .

A factual database on IBM PC in thermodynamics of complexation of macrocyclic polyethers with salts of alkali and alkaline-earth metals was created.