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THE DATABASES IN THERMODYNAMICS OF THE COMPLEXATION.

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The original factual database on IBM PC in thermodynamics of complexation of macrocyclic polyethers with salts of alkali and alkaline-earth metals is created. The database contains more than 4,000 records. These records include the critically reviewed and evaluated thermodynamic data derived from over 60 journals covered by Chemical Abstracts (CA) from 1968 to the present. The reaction record contains the structure diagram for ligand (macrocyclic polyether, crown-ether), formula of salt of alkali or alkaline - earth metal, the solvent, concentrations of ligand and salt in solution, ionic strength, temperature, equilibrium constant $\log K$, the enthalpy ΔH , the entropy ΔS , where available, experimental methods for evaluation of thermodynamic data, references, all of which are searchable and displayable. The database is in English, except for some text fields. At present we prepare the factual database in thermodynamics of the complexation of all organic ligands with metal cations. This database will contain more than 50,000 reactions.