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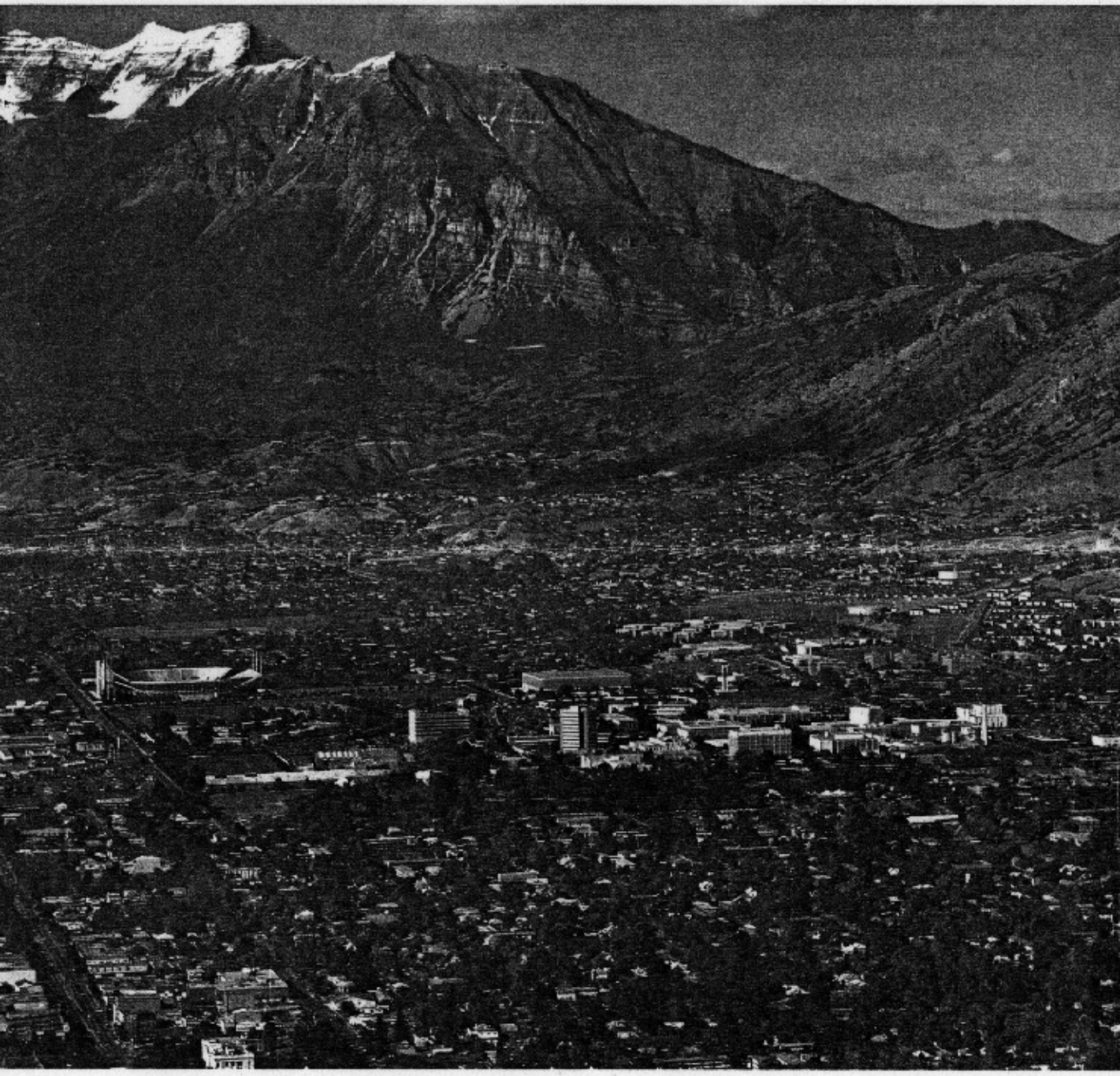
XVII INTERNATIONAL SYMPOSIUM ON MACROCYCLIC CHEMISTRY



9 - 14 August 1992
Seven Peaks Resort Excelsior Hotel
Provo, Utah U.S.A.

THE PREDICTION OF THERMODYNAMIC VALUES OF THE COMPLEXATION UPON THE MEASURE OF INTERLIGAND STRUCTURAL SIMILARITY.

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Mathematical modeling techniques is used with machine-readable files of macrocyclic and podand ligands characterized by substructural fragments. The type of substructure is defined in terms of the atomic environments and shortest path separations between all pairs of atoms in the topological representation of a chemical structure. The prediction of thermodynamic values of the complexation are based upon the program TRAIL for the calculation of a measure of interligand substructural similarity. The program correlate searched molecular substructural fragments with a corresponding contribution to a thermodynamic property (stability constant, the enthalpy ΔH, the entropy ΔS). It allow to design additive-multiplicative correlation between the thermodynamic property and substructure contributions. Such correlation was detected between stability constants of the complexation of crown-ethers with sodium chloride in methanol, and open-chain analogs of crown ethers (podands) with alkali cations in $THF + CHCl_3$ solutions.

Solov'ev V. P. The prediction of thermodynamic values of the complexation upon the measure of interligand structural similarity.// Abstr. of XVII International Symposium on Macrocyclic Chemistry. Provo (Utath, USA), August 9-14, 1992. - Provo. - 1992. - P. 99.