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AGE OF NETWORKING
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and Better Human Life

SCIENTIFIC PROGRAM
EXTENDED ABSTRACTS
AND PROCEEDINGS

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SOLVENT EFFECTS ON CROWN ETHER COMPLEXATIONS

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A systematic study of the complexation between potassium cation and 18-crown-6 in 14 different solvents shows that stability constant K increases by $> 10^4$ from water to pure methanol or to propylene carbonate (PC), with constants increasing in the order $H_2O < HMPT < DMSO < DMF < MeCHOHMe < MeCN < Me_2CO < MeOH < PC$. The calorimetrically determined thermodynamic values of the complexation (ΔG , ΔH , ΔS) are compared with a large range of available solvent properties. The best linear correlations ($R \approx 0.95$) are obtained for ΔG of metal cation - macro cyclic ligand systems with the standard Gibbs transfer energies ΔG° of the metal ion from water to the given solvent, to a lesser degree ($R \approx 0.9$) with values characterizing the electron donor capacity of the solvent. The reaction enthalpies ΔH for $K^+/18C6$ system vary much more than ΔG , for instance from 12 kJ mol^{-1} (in MeCN) to 68 kJ mol^{-1} (in Me_2CHOH), without meaningful correlations to known solvent properties, or between ΔG and ΔH . An exception is the correlation of ΔH with the solvent polarity index π^* with $R = 0.996$ if MeCN is excluded.