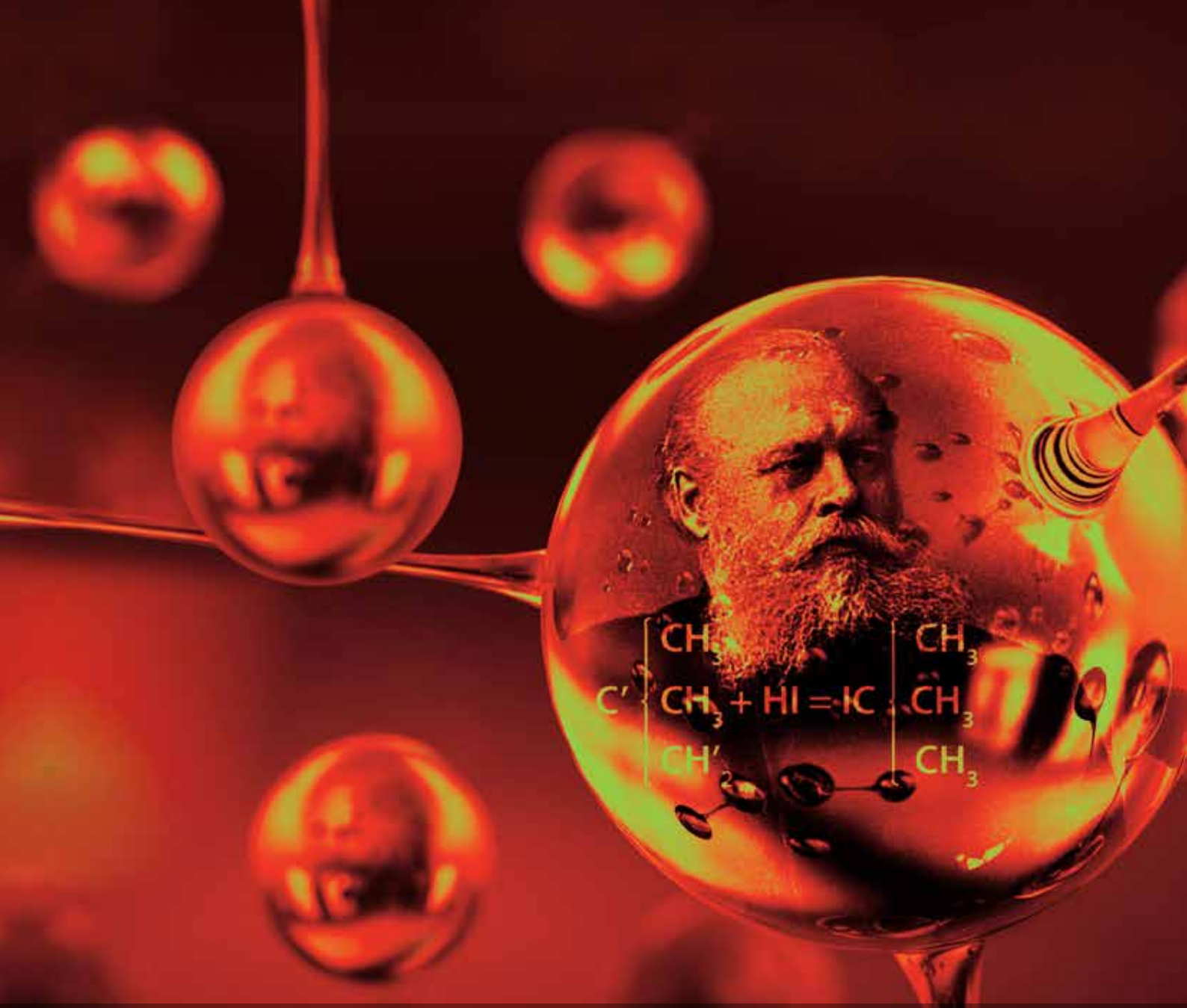

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BOOK OF ABSTRACTS

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PREDICTING THE STABILITY CONSTANTS OF LANTHANIDE COMPLEXES BY CHARACTERISTICS OF COMPLEXATION SIMILARITY

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We present a simple method of predicting the stability constants $\log\beta_1$ and $\log\beta_2$ of the ML and ML_2 complexes of lanthanide ions M (from Ce^{3+} to Lu^{3+}) with diverse organic ligands (L) in water derived from linear free energy relationships. This method assesses the stability constants within predictable uncertainties compatible with those in known experimental values for most ligands. Two complexation characteristics e_1 and e_2 for every lanthanide ions were derived for an accurate prediction of stability constant for jth lanthanide ion using stability constant for ith lanthanide ion by the relationships $\log\beta_1^j = e_1^j/e_1^i.\log\beta_1^i$ and $\log\beta_2^j = e_2^j/e_2^i.\log\beta_2^i$ for given ligand.

Three thousands of new $\log\beta_1$ values and one thousand of new $\log\beta_2$ values of potential complexes were predicted for the numerous metal/ligand combinations. The standard deviation of the predictions varies from 0,3 to 1,0 for $\log\beta_1$ and from 0,4 to 1,2 for $\log\beta_2$ as a linear function of the difference of ionic radii (Δr_M) of two metal ions involved in the calculations: $s_1 = 0{,}27 + 4{,}25\Delta r_M$ for $\log\beta_1$ and $s_2 = 0{,}39 + 5{,}16\Delta r_M$ for $\log\beta_2$. The characteristics e_1 and e_2 correlate with ionic radii for lanthanide ions. Studied experimental data included 2854 $\log\beta_1$ values for 445 organic ligands and 947 $\log\beta_2$ values for 156 organic ligands and 13 metal datasets.

A predictor of the stability constants $\log\beta_1$ ($\log\beta_2$) of the ML (ML_2) complexes of lanthanide ions M^{3+} with diverse organic ligands (L) in water was created on the base of the complexation characteristics e_1 and e_2. The predictor is freely available as the program LanComSim (Lanthanide Complexation Similarity) under Windows operating systems.