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Thermodynamic Analysis and Prediction of Chemical Synergy in Complex Aqueous Chemical Processes

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INTRODUCTION & AIM

The authors have proved, for all chemical processes used in different physico-chemical methods of analysis and research and in various fields of applications, that the common feature of the synergism phenomenon is the formation of a mixed compound. A prior knowledge of this common feature offers the possibility of a deeper understanding of this phenomenon and of the directed search or prediction of the necessary or pre-planned synergistic effects. For a better understanding of the synergism phenomenon, examples of synergistic processes in other disciplines have been given. The authors have formulated the following rule: the formation of mixed complexes is a necessary, but not sufficient condition to explain the occurrence of the chemical synergism. To prove the synergistic effect, it is necessary to measure a certain physicochemical or physical quantity, which proves the superiority of the non-additivity phenomenon over a simple summation of the properties of individual components. In other words, the theory of chemical equilibrium cannot serve as a basis for predicting synergy, but it can be post-proof of this phenomenon.

RESULTS & DISCUSSION

It has been proven that some chemical processes exhibit a common characteristic: the formation of a mixed compound [1]. In reference [1], the nature of the synergistic effect of total buffering action in heterogeneous mixtures was explained. For instance, the authors have found that when hexanoic acid (HA) and decanoic acid (HB) combine in benzene (the organic phase) to create the mixed complex HAHB, this compound enhances the overall buffering effect. This notion is supported by other researchers who propose that in solvent extraction processes, the synergistic effect primarily arises from the formation of mixed metal complex compounds involving all extracting molecules.

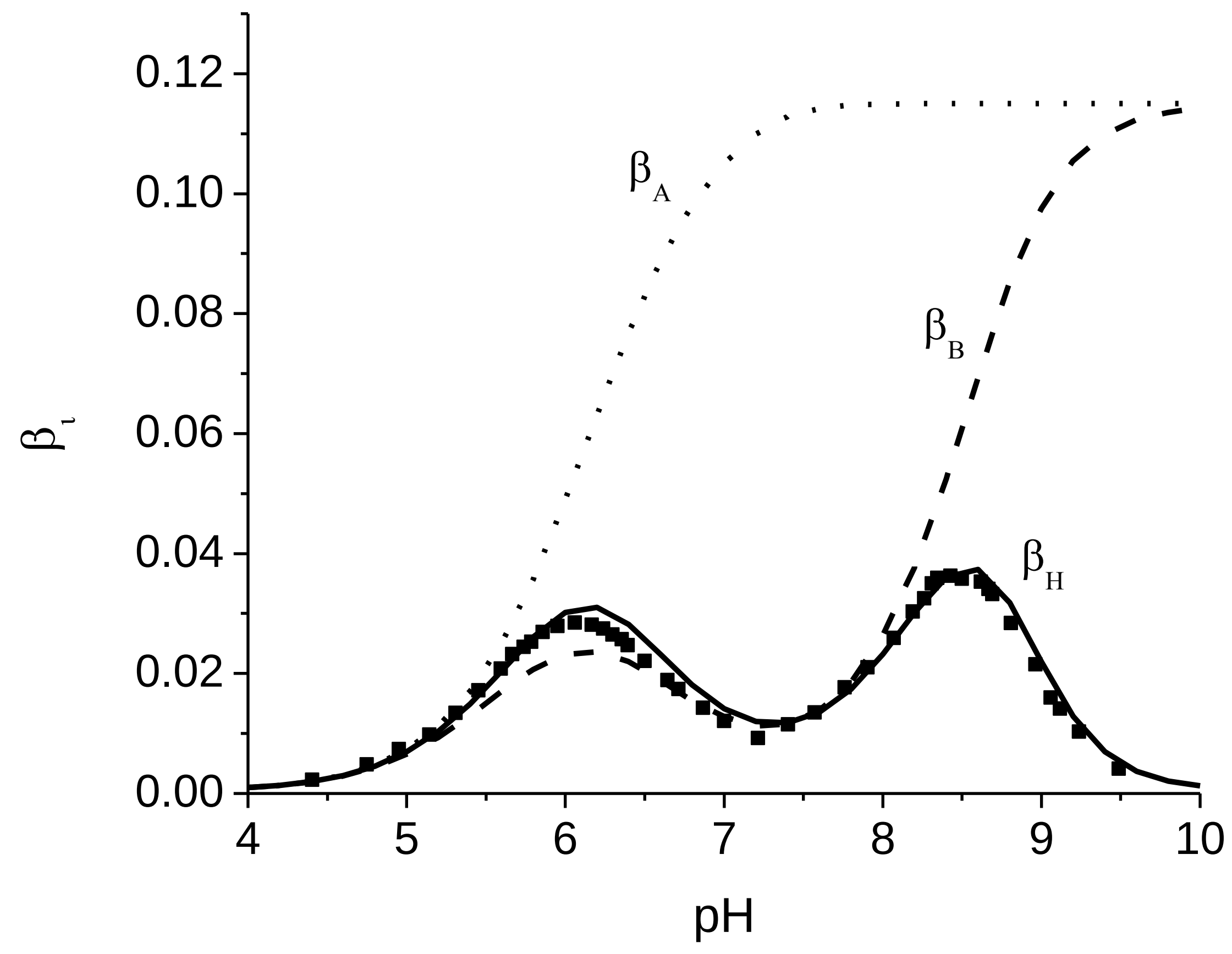

Fig. 1. Curves β_H = f(pH), β_A = f(pH) and β_B = f(pH) for the two-component two-phase buffer system, containing hexanoic and decanoic acids. $C_A^0 = C_B^0 =$ 0.05 mol L^{-1}, I = 0.1, t = 25°C. $V(C_6H_6) \div V(H_2O) = 1 \div 1$

In reference [2], the formation of mixed complex compounds with precious metals was found to significantly accelerate their dissolution rates (see Fig. 2). Consequently, the process of forming mixed complex compounds could be applied for the oxidative dissolution of gold. For example, the addition of small amounts of ammonium thiosulfate to ammonium solutions has a synergistic effect on the dissolution of gold. This results in a higher dissolution rate compared to using thiosulfate or ammonium solutions separately at the same concentrations as those in the mixture.

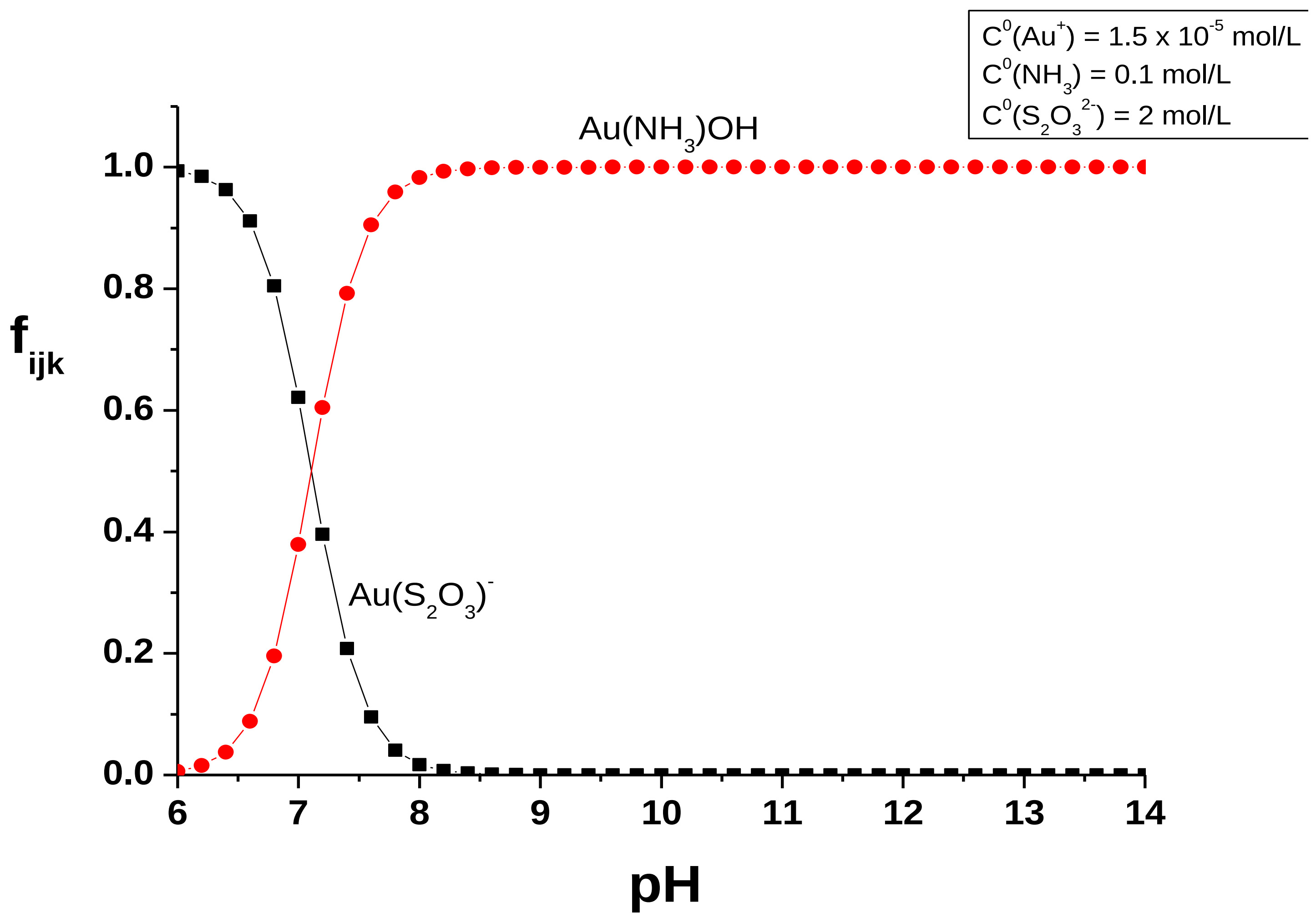

Fig. 2. Curves of distribution of the *Au(I)* species versus pH in homogeneous system $Au(I) - NH_3 – S_2O_3^{2-} - H_2O$. Concentrations, mol L^{-1}: $C^0_{Au^+} = 1.5 \cdot 10^{-5}; C^0_{NH_3} = 0.1; C^0_{S_2O_3^{2-}} = 2$

CONCLUSION

Through rigorous thermodynamic analysis, the phenomenon of chemical synergy in complex chemical processes has been elucidated. Chemical synergy informs and enhances numerical and experimental methods, as well as data analyses, in water sciences by providing a more comprehensive understanding of the complex interactions between chemical components in water systems. Chemical synergy manifests in various ways, depending on factors such as reactant structures and process energies. Essentially, any chemical interaction depends on the chemical composition of the reaction mixture, temperature, and pressure.

REFERENCES/ ACKNOWLEDGMENTS

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1. Povar, I., & Spinu, O. (2015). Acid-Base Buffer Properties of Heterogeneous Multicomponent Extraction Systems. Solvent Extraction and Ion Exchange, 33(2), 196-209.
2. Povar, I., Ubaldini, S., Spinu, O., & Lupascu, T. (2019). Thermodynamic analysis of the copper (I) homogeneous and heterogeneous speciation in ammonium thiosulfate leaching systems. Canadian Journal of Chemistry, 97(9), 651-658.