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Iron Aspartate Complexes and Model Processes of Their Formation

M. M. Rakhimova*, T. M. Nurmatov, N. Z. Yusupov, Dzh. A. Davlatshoeva,
M. A. Ismailova, and A. Ismatov

Research Institute, Tajik National University, Dushanbe, Tajikistan

**e-mail: muboshira09@mail.ru*

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Abstract—Complexation of iron(II) and iron(III) ions with aspartate anions was studied by measuring oxidative potentials. The empirical formulas, stability constants, pH ranges, and mole fractions of the resulting iron aspartate complexes were determined using an oxidative function and a new concept of modeling complexation equilibria.

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INTRODUCTION

In the presence of polybasic acids or polyfunctional ligands, when the formation of heterovalent complexes and composite heteroleptic complexes with protonated ligands becomes more probable, novel approaches and procedures for thermodynamic calculations are required to obtain, in a short period of time, reproducible and accurate data. The goal of this study was to determine the empirical formulas, stability constants, pH ranges, and mole fractions of iron aspartate complexes that are of practical interest from experimental redox data, using an oxidative function described below and a new concept of modeling complexation equilibria [1, 2].

EXPERIMENTAL

The oxidative potential of the system iron(II)–iron(III)–aspartic acid–water was measured on a setup [2] with three galvanic cells consisting of: (1) a redox electrode and SCE for measuring the emf of the circuit, (2) SCE and a glass electrode for determining the pH of solutions, and (3) platinum and glass electrodes for checking the readings of the first and second circuits. The emf produced in the galvanic cells was measured with an EV-74 ionomer. Standard electrode potentials and the quantity $\upsilon = 2.303RT/F$ at necessary temperatures were taken from [3]. The electrodes were prepared properly as described in [2]. The pH values of the solutions under study were checked using a glass electrode and a calibration curve obtained from the pH values of standard buffer solutions.

Iron(II) and iron(III) perchlorates with the poorest complexing ability [2] were prepared as described in [4] and used as the starting salts. The concentrations of the components of the system were determined according to appropriate procedures [5, 6]. An equimolar mixture of solutions of iron(II) and iron(III) perchlorates was prepared in 1 M $HClO_4$; their total concentration was determined by reduction of Fe(III) to Fe(II) with a reducing agent containing amalgamated zinc [7].

The empirical formulas of the resulting iron complexes were determined by analyzing the experimental plots of the oxidative potential of the system versus one of the following parameters: pH, pc_o, pc_r, pc_{HL}, and $p(c_o = c_r)$, the others being kept constant. The slopes of the curves correspond to the numbers of atoms of the oxidized and reduced species and the total number of ligands and coordinated hydroxyl groups in tentative formulas of the complexes. The overall equation of the oxidative potential was derived with consideration for the formulas and constants of formation of the complexes, which then were calculated using an iterative procedure.

The accumulated experimental and theoretical data on complexation in redox systems showed that the redox method works well only with the simplest systems containing variable valence metals and monobasic ligands in an acidic pH range, where no heterovalent complexes are formed. With an increase in pH, which favors the formation of heteroleptic, polynuclear, and heterovalent complexes, this method should be supplemented with new, improved approaches to thermodynamic calculations that would make allowance for the formation of all possible complexes. The method developed in [8] is used to accomplish rapid and exact calculations with modern computer software and a proposed new oxidative function f.

According to [8], the general equation of oxidative potential φ for the formation of heterovalent heteroleptic complexes has the form:

$$\begin{gathered}\varphi = \varphi^0 + \upsilon/e \log c_\mathrm{o}/c_r + \upsilon/e \\ \times \log \sum_1^q \sum_0^p \sum_0^s \sum_0^l \sum_0^k pq\beta_{qpslk}^{1/p} G_{qpslk}^{(g-1)/g} [\mathrm{H}_{b-n}\mathrm{L}^{n-}]^{1/p} h^{-k/} \\ \times [\mathrm{M}^{z+}]^{p/q} - \upsilon/e \log \sum_0^q \sum_1^p \sum_0^s \sum_0^l \sum_0^k qp\beta_{qpslk}^{1/q} P_{qpslk}^{(p-1)/} \\ \times [\mathrm{H}_{b-n}\mathrm{L}^{n-}]^{1/q} h^{-k/q} [\mathrm{M}^{(z-e)+}]^{q/p},\end{gathered} \tag{1}$$

where φ^0 is the standard oxidative potential; c_o is the total concentration of the oxidized metal species; c_r is the total concentration of the reduced metal species; G_{qpslk} and P_{qpslk} are the concentrations of the complexes of the oxidized and reduced metal species, respectively; $\upsilon = 2.303RT/F$; q is the number of metal atoms in the oxidized species (nuclear number of the complex); k is the number of protonated groups in the complex; p is the number of metal atoms in the reduced species (nuclear number of the complex); l is the number of protonated groups in the complex.

The activity of water for the dilute solutions studied is constant and taken to be unity. The quantities r, m, u, and n are related to others by the following expressions:

$$\begin{gathered} r = 6q - 2x - y; \quad m = (n+)q - x - y; \\ w = 6p - u - v; \quad n = 2p - u - v, \end{gathered} \tag{2}$$

where x is the number of groups A^{b-}, y is the number of coordinated hydroxyl groups, r is the number of coordinated water molecules, m is the charge of the complex of the oxidized metal species, u is the number of coordinated ligands A, v is the number of coordinated hydroxyl groups, w is the number of coordinated water molecules, and n is the charge of the complex of the reduced metal species.

Equilibrium between metal ions in aqueous solutions can be represented as follows:

$$\mathrm{M(H_2O)}_6^{z+} + \mathrm{e}^- = \mathrm{M(H_2O)}_6^{(z-e)+}. \tag{3}$$

An experimental oxidative function is calculated from experimental plots of oxidative potential versus pH according to Eq. (4):

$$f_\mathrm{exp}^0 = (c_r/c_\mathrm{o})\exp[(\varphi - \varphi^0)n/\theta]. \tag{4}$$

This is followed by plotting f_exp^0 versus pH. The number of linear segments on this curve corresponds to the number of the complexes formed and the lengths of the segments correspond to their pH ranges.

The theoretical oxidative function [8] has the form:

$$\begin{gathered} f_T^0 = (c_r/c_\mathrm{o}) \left\{ \left(\sum_0^q \sum_1^p \sum_0^s \sum_0^l \sum_0^k pq\beta_{qpslk}^{1/p} P_{qpslk}^{(p-1)/p} \right.\right. \\ \left. \times \left[\mathrm{H}_s\mathrm{L}^{n-}\right]^{1/p} h^{-k/p} \left[\mathrm{M}^{Z+}\right]^{q/p} \right) \Bigg/ \left(\sum_1^q \sum_0^p \sum_0^s \sum_0^l \sum_0^k qp \right. \\ \left.\left. \times \beta_{qpslk}^{1/q} G_{qpslk}^{(q-1)/q} [\mathrm{H}_s\mathrm{L}^{n-}]^{l/q} h^{-k/q} [\mathrm{M}^{(z-e)+}]^{p/q} \right) \right\}, \end{gathered} \tag{5}$$

where all the quantities correspond to the designations cited in Eqs. (1) and (2). Each sum deals with the fragments of the equation for an individual complex in agreement with the slopes (coefficients) of the experimental plots, which are determined by comparing their values with the derivatives of the oxidative potential with respect to one of the aforementioned parameters. The true constants of formation of the complexes are determined by iteration of the theoretical oxidative function with the experimental one using the Excel program. The calculations do not stop until the theoretical and experimental pH-dependences of the oxidative function come as close together as possible (usually, eight to ten iterations are required). Thus, the oxidative function allows one to determine the empirical formulas of the complexes, perform calculations of their constants of formation within a shorter period of time, and obtain more reliable data.

It is easier to calculate the constants of formation of complexes using a model of chemical equilibria. This is a matrix consisting of the number of basic species, the tentative formulas of the complexes, and the equations of the complexation reactions. This must be preceded by compiling a general table (stoichiometric matrix) of all equilibria present in the system, with numerical values of the slopes of the experimental oxidative potential plots φ–pH, φ–pc_o, φ–pc_r, and φ–pc_L. To reduce the number of similar linear plots with different slopes, one should construct a stoichiometric matrix for the whole pH range of complexation (Table 1). The tabulated data are used to construct a chemical model with a columnar representation of the basic species: the nuclear numbers of the complexes for oxidized and reduced metal species, the number of coordinated ligands, and the numbers of protons and hydroxyl groups in them (q, p, s, l, and k, respectively), which are determined by comparing the experimental slopes of the curves and the partial derivatives of the general oxidative potential equation (1) with respect to the concentration variables. For instance, for the plot φ–pH, we obtain

$$(\partial\varphi/\partial\mathrm{pH})_{\mathrm{p}c_\mathrm{o},\mathrm{p}c_r,\mathrm{p}c_\mathrm{L}} = (\upsilon/e)[(k+nl)/p - (k+nl)/q]. \tag{6}$$

If the basicity of an acid is b, then we obtain $(n+1)$ partial derivatives ($n = 0, 1, 2, \ldots$) from Eq. (6), which allows quantifying the total number of protons of the proton-donating ligand $\mathrm{H}_{b-n}\mathrm{L}^{n-1}$ in a complex. How-

Table 1. Experimental slopes of the plot of the oxidative potential on the concentration variables (stoichiometric matrix) for the system Fe(II)–Fe(III)–DL-aspartic acid–water at 298.16 K ($I = 0.5$, $c_{Fe(III)} = c_{Fe(II)} = 1 \times 10^{-3}$ mol/L, $c_L = 1 \times 10^{-2}$ mol/L)

pH range of the slope	Stoichiometric matrix				Tentative empirical formulas of the complexes	β_{qpslk}
	pH	pc_o	pc_r	pc_L		
0.2–3.8	$-\upsilon$	$-\upsilon$	0	$+\upsilon$	$[FeHL]^{2+}$	β_{10110}
1.6–4.0	-2υ	$-\upsilon$	0	$+\upsilon$	$[FeL]^{+}$	β_{10010}
1.2–4.2	-2υ	$-\upsilon, -\upsilon/2$	0	$+\upsilon$	$[Fe_2L_2]^{2+}$	β_{20020}
2.8–6.2	-2υ	$-\upsilon/2$	0	$+\upsilon$	$[Fe_2L_2(OH)_2]^0$	β_{20022}
5.0–7.0	$-\upsilon$	$-\upsilon/3$	0	$-\upsilon$	$[Fe_3L_3(OH)_3]^0$	β_{30033}
4.6–8.8	υ	$-\upsilon/2$	$+\upsilon$	$-\upsilon$	$[Fe^{III}Fe^{II}L_2OH]^0$	β_{11021}
5.8–10.5	$-\upsilon$	$-\upsilon/2$	$+\upsilon$	$-\upsilon$	$[Fe_2^{III}Fe^{II}L_3(OH)_2]^0$	β_{21032}
2.2–5.0	υ	0	$+\upsilon$	$-\upsilon$	$[FeHL]^{+}$	β_{01110}
3.2–8.0	$-\upsilon$	0	$-\upsilon/2$	$-\upsilon$	$[FeL]^0$	β_{01010}
8.5–10.5	$-\upsilon$	0	$-\upsilon/2$	$-\upsilon$	$[Fe_2L(OH)_2]^0$	β_{02012}

Table 2. Chemical model of formation of the Fe(III) DL-aspartate complexes at 298.16 K ($I = 0.5$, $c_{Fe(III)} = c_{Fe(II)} = 1 \times 10^{-3}$ mol/L, $c_L = 1 \times 10^{-2}$ mol/L)

Fe(III)	Fe(II)	H	L	OH	Empirical formula of the complex	Complexation reactions
q	p	s	l	k		
1	0	1	1	0	$[FeHL]^{2+}$	$[Fe(H_2O)_6]^{3+} + HL^- \rightleftharpoons [FeHL(H_2O)_5]^{2+} + H_2O$
1	0	0	1	0	$[FeL]^+$	$[Fe(H_2O)_6]^{3+} + L^{2-} \rightleftharpoons [FeL(H_2O)_4]^+ + 2H_2O$
2	0	0	2	0	$[Fe_2L_2]^{2+}$	$2[FeL(H_2O)_4]^+ \rightleftharpoons [Fe_2L_2(H_2O)_8]^{2+}$
2	0	0	2	2	$[Fe_2L_2(OH)_2]^0$	$[Fe_2L_2(H_2O)_8]^{2+} + 2H_2O \rightleftharpoons [Fe_2L_2(OH)_2(H_2O)_6]^0 + 2H_3O^+$
3	0	0	3	3	$[Fe_3L_3(OH)_3]^0$	$[Fe_2L_2(H_2O)_8]^{2+} + [FeL(H_2O)_4]^+ \rightleftharpoons [Fe_3L_3(OH)_3(H_2O)_9]^0 + 3H_2O$
1	1	0	2	1	$[Fe^{III}Fe^{II}L_2OH]^0$	$[FeL(H_2O)_4]^+ + [FeL(H_2O)_4]^0 + H_2O \rightleftharpoons [Fe^{III}Fe^{II}L_2(OH)(H_2O)_7]^0 + H_3O^+$
2	1	0	3	2	$[Fe_2^{III}Fe^{II}L_3(OH)_2]^0$	$[Fe_2L_2(OH)_2(H_2O)_6]^0 + [FeL(H_2O)_4]^+ \rightleftharpoons [Fe_2^{III}Fe^{II}L_3(OH)_2(H_2O)_{10}]^0$

ever, for more accurate determination of the equilibrium species generated by ionization of the acid, we should consider a partial derivative of the oxidative potential with respect to pc_L:

$$(\partial\varphi/\partial pc_L)_{pH,pc_o,pc_r} = (\upsilon/e)[1/q - 1/p]. \tag{7}$$

The partial derivatives with respect to the logarithmic concentration indices of the oxidized and reduced metal species take the following form:

$$(\partial\varphi/\partial pc_o)_{pH,pc_L,pc_r} = -\upsilon/eq, \tag{8}$$

$$(\partial\varphi/\partial pc_r)_{pH,pc_L,pc_o} = \upsilon/ep. \tag{9}$$

The numerical values of the basic species q, p, s, l, and k, from Table 2 (chemical model) are used as subscripts to the constants of formation of the complexes, which simplifies the notation of their composition. According to the set of numbers q, p, s, l, and k of each row, we obtain equations for a separate linear segment the summation of which provides a general expression for the theoretical oxidative function of the system studied.

All subsequent calculations of the constants of formation of the complexes were performed using the oxidative function described above and the Excel program. Then we calculated the mole fractions of the resulting complexes by the following equations:

$$\alpha_{compl} = c_{compl}/c_o \quad \text{and} \quad \alpha_{i\ Fe(III)} = c_{Fe(III)}/c_o, \tag{10}$$

$$\alpha_{compl} = c_{compl}/c_r \quad \text{and} \quad \alpha_{i\ Fe(II)} = c_{Fe(II)}/c_r, \tag{11}$$

where α_i are the mole fractions of the equilibrium species of the components of the complexation, $c_{Fe(III)}$ and $c_{Fe(II)}$ are the equilibrium concentrations of free iron ions, and c_o and c_r are the total concentrations of the oxidized and reduced iron species. The calculated stability constant, the maximum mole fraction, the pH range, and the fragments of the oxidative potential equation are unique to each complex and written as a separate table of model parameters.

RESULTS AND DISCUSSION

For the system Fe(II)–Fe(III)–DL-aspartic acid–water, we plotted the measured oxidative potential φ versus one of the following parameters: pH, pc_o, pc_r, pc_{HL}, and $p(c_o = c_r)$, the others being kept constant (the concentration conditions are specified in Tables 1–3). The data obtained were analyzed with consideration that DL-aspartic (DL-aminosuccinic, $HOOCCH_2CH(NH_2)COOH$) acid is a potential tribasic acid. The numerical values required for calcu-

Table 3. Chemical model of formation of the Fe(II) DL-aspartate complexes at 298.16 K ($I = 0.5$, $c_{\mathrm{Fe(III)}} = c_{\mathrm{Fe(II)}} = 1 \times 10^{-3}$ mol/L, $c_{\mathrm{L}} = 1 \times 10^{-2}$ mol/L)

Fe(III)	Fe(II)	H	L	OH	Empirical formula of the complex	Complexation reactions
q	p	s	l	k		
0	1	1	1	0	$[FeHL]^+$	$[Fe(H_2O)_6]^{2+} + HL^- \rightleftharpoons [FeHL(H_2O)_5]^+ + H_2O$
0	1	0	1	0	$[FeL]^0$	$[Fe(H_2O)_6]^{2+} + L^{2-} \rightleftharpoons [FeL(H_2O)_4]^0 + 2H_2O$
0	2	0	1	2	$[Fe_2L(OH)_2]^0$	$2[Fe(H_2O)_6]^{2+} + L^{2-} \rightleftharpoons [Fe_2L(OH)_2(H_2O)_8]^0 + 2H_3O^+$
1	1	0	2	1	$[Fe^{III}Fe^{II}L_2OH]^0$	$[FeL(H_2O)_4]^+ + [FeL(H_2O)_4]^0 + H_2O \rightleftharpoons [Fe^{III}Fe^{II}L_2(OH)(H_2O)_7]^0 + H_3O^+$
2	1	0	3	2	$[Fe_2^{III}Fe^{II}L_3(OH)_2]^0$	$[Fe_2L_2(OH)_2(H_2O)_6]^0 + [FeL(H_2O)_4]^+ \rightleftharpoons [Fe_2^{III}Fe^{II}L_3(OH)_2(H_2O)_4]^0 + 6H_2O$

Table 4. Model parameters of the Fe(III) aspartate complexes at 298.16 K ($I = 0.5$, $c_{\mathrm{Fe(III)}} = c_{\mathrm{Fe(II)}} = 1 \times 10^{-4}$ mol/L, $c_{\mathrm{L}} = 1 \times 10^{-2}$ mol/L)

Empirical formula of the complex	pH range of the complex	$\log\beta_{qpslk} \pm 0.02$	$\alpha_{\max}$, %	pH	Fragments of the equations of the oxidative potential of the system
$[FeHL]^{2+}$	0.2–3.8	2.55	18.0	2.0	$\upsilon lq(h^5 + \beta_{10110}K_2c_{2a}h^4)$
$[FeL]^+$	1.6–4.0	4.46	15.0	2.8	$\upsilon lq(h^5 + \beta_{10010}K_2K_3c_{2a}h^3)$
$[Fe_2L_2]^{2+}$	1.2–4.2	15.18	84.0	2.8	$\upsilon lq(h^5 + 2\beta_{20020}^{1/2}\,Q_{20020}^{1/2}\,K_2K_3c_{2a}h^3)$
$[Fe_2L_2(OH)_2]^0$	2.8–6.2	11.74	98.0	4.4	$\upsilon lq(h^5 + 2\beta_{20022}^{1/2}\,Q_{20022}^{1/2}\,K_2K_3c_{2a})$
$[Fe_3L_3(OH)_3]^0$	5.0–7.0	27.55	99.0	6.0	$\upsilon lq(h^5 + 3\beta_{30033}^{1/3}\,Q_{30033}^{1/3}\,K_2K_3c_{2a})$
$[Fe^{III}Fe^{II}L_2OH]^0$	6.6–8.8	12.67	38.0	7.4	$\upsilon lq\{h^5 + 2\beta_{11021}^{1/2}\,Q_{11021}^{1/2}\,(K_2K_3c_{2a})^2[Fe^{2+}]\}$
$[Fe_2^{III}Fe^{II}L_3(OH)_2]^0$	5.8–10.5	22.54	98.0	8.0	$\upsilon lq\{h^5 + 3\beta_{21032}^{1/3}\,G_{21032}^{1/3}\,(K_2K_3c_{2a})^2[Fe^{2+}]^{1/2}\}$

lations ($pK_1 = 1.88$ (α-COOH), $pK_2 = 3.64$ (β-COOH), and $pK_3 = 13.32$ (NH_2)) were determined under the experimental conditions by pH-metric titration.

In accordance with the redox method, we analyzed the slopes of all the above plots to construct a stoichiometric matrix (Table 1). By comparing the experimental slopes of the curves (see Table 1, columns 3–6) with the partial derivatives of the oxidative potential equation (Eqs. (6)–(9)), we calculated numerical values of the basic species, compiled a table for a complexation model (Table 2), and formulated the resulting complexes as $[FeHL]^{2+}$, $[FeL]^+$, $[Fe_2L_2]^{2+}$, $[Fe_2L_2(OH)_2]^0$, $[Fe_3L_3(OH)_3]^0$, $[Fe^{III}Fe^{II}L_2OH]^0$, $[Fe_2^{III}Fe^{II}L_3(OH)_2]^0$, $[FeHL]^+$, $[FeL]^0$, and $[Fe_2L(OH)_2]^0$.

In an acid pH range, the predominant ligand HL^- (first-step dissociation product of aspartic acid) forms a complex with trivalent iron, $[FeHL]^{2+}$. With an increase in pH, aspartic acid undergoes second-step dissociation, thus producing the mononuclear complex $[FeL]^+$ and then a binuclear one. As pH increases, the latter adds two OH groups and the trinuclear complex $[Fe_3L_3(OH)_3]^0$ is formed. The formation of heterovalent complexes with Fe(III) : Fe(II) ratios of 1 : 1 and 2 : 1 occurs at pH 4.5–11.0. Divalent iron yields the complexes $[FeHL]^+$, $[FeL]^0$, and $[Fe_2L(OH)_2]^0$, the mononuclear one being dominant at pH 3.2–8.0.

The constructed model of the formation of iron(III) and iron(II) aspartate complexes (Tables 2, 3) comprises the number of basic species of the system, the empirical formulas of the resulting complexes, and the equilibrium equations with stoichiometric coefficients. This model allows calculations of the stability constants of complexes from the oxidative function [8] using the aforementioned iterative procedure. The mole fractions determined from Eqs. (11) and (12) are used to find the maximum mole fraction of the complex. This is followed by filling the table of the model parameters of the complexes with the fragments of the oxidative potential equations employed in their calculations (Tables 4, 5).

According to the calculated model parameters (Table 4), the first two complexes are less stable than the others and exist in a narrow pH range, and their mole fractions are low (15.0–18.0%). The Fe(III) bi- and trinuclear complexes $[Fe_2L_2]^{2+}$, $[Fe_2L_2(OH)_2]^0$, and $[Fe_3L_3(OH)_3]^0$ are most stable (logβ = 15.18, 11.74, and 27.55, respectively) and dominate over a wide pH range, their mole fractions varying from 84.0

Table 5. Model parameters of the Fe(II) aspartate complexes at 298.16 K ($I = 0.5$, $c_{\mathrm{Fe(III)}} = c_{\mathrm{Fe(II)}} = 1 \times 10^{-4}$ mol/L, $c_{\mathrm{L}} = 1 \times 10^{-2}$ mol/L)

Empirical formula of the complex	pH range of the complex	$\log\beta_{qpslk} \pm 0.02$	$\alpha_{\max}$, %	pH	Fragments of the equations of the oxidative potential of the system
$[\mathrm{FeHL}]^+$	2.2–5.0	2.26	78.0	3.4	$\upsilon lq(h^5 + \beta_{01110}K_2c_{2a}h^4)$
$[\mathrm{FeL}]^0$	3.2–8.0	3.08	99.0	5.4	$\upsilon lq(h^5 + \beta_{01010}K_2K_3c_{2a}h^3)$
$[\mathrm{Fe_2L(OH)_2}]^0$	8.5–10.5	11.74	98.0	10.5	$\upsilon lq(h^5 + 2\beta_{02012}^{1/2}P_{02012}^{1/2}K_2K_3c_{2a}h^2)$
$[\mathrm{Fe^{III}Fe^{II}L_2OH}]^0$	6.6–8.8	12.67	38.0	7.4	$\upsilon lq\{h^5 + 2\beta_{11021}^{1/2}G_{11021}^{1/2}(K_2K_3c_{2a})^2[\mathrm{Fe}^{3+}]\}$
$[\mathrm{Fe_2^{III}Fe^{II}L_3(OH)_2}]^0$	5.8–10.5	22.54	98.0	8.0	$\upsilon lq\{h^5 + 3\beta_{21032}^{1/3}G_{21032}^{1/3}(K_2K_3c_{2a})^{2/3}[\mathrm{Fe}^{3+}]\}$

to 99.0%. Because of such parameters, the synthesis of these complexes is very feasible.

The heterovalent complex $[\mathrm{Fe_2^{III}Fe^{II}L_3(OH)_2}]^0$ with a maximum mole fraction of 98% is one of the most stable complexes ($\log\beta = 22.54$) and exists over a wide pH range from 5.8 to 10.5. Iron aspartate complexes are known to exhibit biological activity; for this reason, the calculated model parameters of the most stable complexes $[\mathrm{Fe_3L_3(OH)_3}]^0$ and $[\mathrm{Fe_2^{III}Fe^{II}L_3(OH)_2}]^0$ were used to optimize the conditions for their isolation from solutions. The complexes were produced in larger amounts and employed in wetting and pelleting of medium-staple and fine-staple cotton seeds prior to sowing. It turned out that these iron aspartate complexes promote plant growth. The field germinating power of cotton seeds increases by 7% compared to the plants in a control group. The other benefits include more fruiting structures, an increased weight of raw cotton, and more cotton bolls, which affords an additional crop of, on average, 350 kg per hectare [9, 10].

The iron(II) aspartate complexes $[\mathrm{FeHL}]^+$ and $[\mathrm{FeL}]^0$ are less stable ($\log\beta = 2.26$ and 3.08) than the binuclear complex $[\mathrm{Fe_2L(OH)_2}]^0$ ($\log\beta = 11.74$), which agrees with the literature data. The degrees of their accumulation are high (78.0–99.0%).

To sum up, by measuring the oxidative potential and using the proposed oxidative function and concept of modeling complexation equilibria in systems, we determined the empirical formulas, stability constants, pH ranges, and mole fractions of ten iron aspartate complexes: $[\mathrm{FeHL}]^{2+}$, $[\mathrm{FeL}]^+$, $[\mathrm{Fe_2L_2}]^{2+}$, $[\mathrm{Fe_2L_2(OH)_2}]^0$, $[\mathrm{Fe_3L_3(OH)_3}]^0$, $[\mathrm{Fe^{III}Fe^{II}L_2OH}]^0$, $[\mathrm{Fe_2^{III}Fe^{II}L_3(OH)_2}]^0$, $[\mathrm{FeHL}]^+$, $[\mathrm{FeL}]^0$, and $[\mathrm{Fe_2L(OH)_2}]^0$. We successfully applied the oxidative function and the system-modeling concept to polyfunctional aminosuccinic acid, with a substantial gain in both the time and accuracy of the calculations. The calculated model parameters of the complexes allowed distinct demarcation of the pH ranges of existence and isolation of stable complexes with high mole fractions from solutions for subsequent use of the results obtained as reference data for targeted syntheses.

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