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Complexation of [*S*,*S*] and mixed stereoisomers of *N*,*N*′-ethylenediaminedisuccinic acid (EDDS) with Fe(III), Cu(II), Zn(II) and Mn(II) ions in aqueous solution

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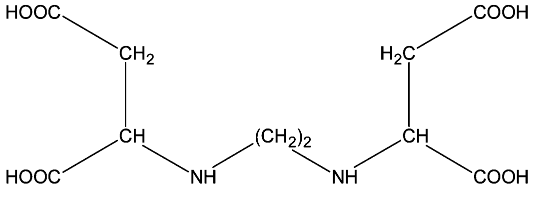
The protonation and complex formation equilibria of *N*,*N*′-ethylenediaminedisuccinic acid (EDDS) in the isomeric form [*S*,*S*] and a mixture of EDDS isomers (25% [*S*,*S*], 50% [*R*,*S*], 25% [*R*,*R*]) with Fe(III), Cu(II), Zn(II) and Mn(II) have been studied in aqueous 0.1 M NaCl solution at 25 °C by potentiometric titrations. The calculations were carried out with the computer program SUPERQUAD.

Introduction

The ability of aminopolycarboxylates and aminopolyphosphonates to form stable metal complexes has been widely utilized in analytical chemistry and industrial applications. The best known example is ethylenediaminetetraacetic acid (EDTA) which has for more than 60 years been extensively used as a chelating agent for a variety of large volume applications from detergents to agrochemicals. The persistence of EDTA and its metal complexes in the nature may, however, cause environmental harm.[1] Thus replacement of EDTA for a ligand showing comparable or even more effective complex-forming properties but being substantially more biodegradable would be of great value.

One plausible example of a such compound is *N*,*N*′-ethylenediaminedisuccinic acid (EDDS), a potentially hexadentate ligand which, due to its two chiral carbon atoms, can exist in the three stereoisomeric forms [*S*,*S*], [*S*,*R*/*R*,*S*] and [*R*,*R*] depending on the absolute configuration of its aspartate units.



EDDS

The biodegradation and mineralization stereospecific tests executed on the different isomers of EDDS have revealed that the [*S*,*S*] form is rapidly and completely mineralized in different environmental compartments whereas the others are degraded to only a limited extent.[2]

The different EDDS stereoisomers may have an effect not only on the biodegradation process but also on the set of metal complexes formed in the solution as well as on the values of their equilibrium constants. In the present paper the protonation of EDDS and its complexation with Fe(III),Cu(II), Zn(II) and Mn(II) ions has been studied systematically by a potentiometric titration method in aqueous solution over a wide pH range.

Although there are some previous equilibrium studies on complex formation between EDDS and these metals, the results obtainable from the literature[3] are contradictory, and no attention has been paid to the possible stereospecificity in these systems. The aim of this investigation was to obtain a reliable picture on the complexing models of EDDS with the metals involved, to obtain accurate values of the stability constants of the complexes formed, and to find out whether any stereoselective effects result. For this purpose one of the optically active forms (*S*,*S*) and a mixture of EDDS isomers (25% [*S*,*S*], 50% [*R*,*S*], 25% [*R*,*R*]), which can be easily prepared, have been used in the measurements.

Experimental

Reagents

EDDS was synthesized from ethylenediamine and maleic anhydride. This route yields a mixture of the isomers consisting of 25% [*S*,*S*], 50% [*R*,*S*], and 25% [*R*,*R*] form.[4]

The single [*S*,*S*]-stereoisomer of EDDS was prepared using 1,2-dibromoethane and L-aspartic acid as described Neal and Rose.[5]

The purity of the preparations was checked by NMR methods and potentiometric titration.

The metal concentrations in the metal chloride stock solutions were standardized against EDTA and by ion exchange using a cation-exchange resin followed by neutralization titration of the free acid liberated with known NaOH. The copper(II) content was also determined electrogravimetrically.

Potentiometric measurements

The protonation and complex formation equilibria were studied in aqueous 0.1 M NaCl at 25.0 °C through a series of potentiometric EMF titrations by use of a Schott-Geräte GmbH Titrator TPC2000, titration software TR600, version 5.00.

The cell arrangement for the measurement of the hydrogen ion concentration, $[H^+]$, was as follows

$$-\mathrm{RE} \mid \text{equilibrium solution} \mid \mathrm{GE}+ \quad (1)$$

where GE denotes a glass electrode, Schott N2680, and RE = $Hg,Hg_2Cl_2 \,||\, 0.1$ M NaCl. Assuming the activity coefficients to be constant, the expression (2) is valid:

$$E = E_o + 59.157 \log[H^+] + j_H[H^+] + j_{OH}[OH^-] \quad (2)$$

Table 1 Protonation constants of EDTA and [*S*,*S*] and mixed stereoisomers of EDDS and their stability constants of Fe(III), Cu(II), Zn(II) and Mn(II) complexes in aqueous 0.1 M NaCl at 25 °C. The stereoisomers are not defined in the literature values

Reaction	log *K* EDTA[3]	log (*K* + 3σ) [*S*,*S*]-EDDS	log (*K* + 3σ) EDDS mix	log *K* EDDS[3]
H^+				
$L^{4-} + H^+ \longrightarrow HL^{3-}$	9.5–10.4	10.1 ± 0.1	10.1 ± 0.1	10.0
$HL^{3-} + H^+ \longrightarrow H_2L^{2-}$	6.13	6.91 ± 0.02	6.94 ± 0.01	6.84
$H_2L^{2-} + H^+ \longrightarrow H_3L^-$	2.69	3.84 ± 0.02	3.85 ± 0.01	3.86
$H_3L^- + H^+ \longrightarrow H_4L$	2.00	3.05 ± 0.02	3.08 ± 0.01	2.95
$H_4L + H^+ \longrightarrow H_5L^+$	1.5	1.4 ± 0.2	1.6 ± 0.1	
$H_5L^+ + H^+ \longrightarrow H_6L^{2+}$	0.0	2.1 ± 0.2	1.6 ± 0.2	
No. of points/titrations		287/4	321/4	
Fe(III)				
$Fe^{3+} + L^{4-} \longrightarrow FeL^-$	25.1	20.6 ± 0.2	20.1 ± 0.2	22.0[a]
$Fe(OH)L^{2-} + H^+ \longrightarrow FeL^-$	7.37	7.9 ± 0.1	7.3 ± 0.1	
$Fe(OH)_2L^{3-} + H^+ \longrightarrow Fe(OH)L^{2-}$		9.9 ± 0.2	9.7 ± 0.2	
No. of points/titrations		283/9	325/8	
Cu(II)				
$Cu^{2+} + L^{4-} \longrightarrow CuL^{2-}$	18.8	18.7 ± 0.1	18.3 ± 0.1	18.4
$CuL^{2-} + H^+ \longrightarrow CuHL^-$	3.1	3.6 ± 0.1	3.8 ± 0.1	3.6
$CuHL^- + H^+ \longrightarrow CuH_2L$	2.0	2.3 ± 0.1	2.5 ± 0.1	
$Cu(OH)L^{3-} + H^+ \longrightarrow CuL^{2-}$	11.4	11.1 ± 0.2	11.0 ± 0.2	10.4
$CuL^{2-} + Cu^{2+} \longrightarrow Cu_2L$		2.4 ± 0.2	2.2 ± 0.3	
$CuL^{2-} + HL^{3-} \longrightarrow CuL(HL)^{5-}$		2.5 ± 0.2	2.4 ± 0.3	
$CuL(HL)^{5-} + H^+ \longrightarrow Cu(HL)_2{}^{4-}$		7.1 ± 0.2	7.4 ± 0.2	
$Cu(HL)_2{}^{4-} + H^+ \longrightarrow Cu(HL)(H_2L)^{3-}$		3.7 ± 0.2	4.0 ± 0.2	
$Cu(HL)(H_2L)^{3-} + H^+ \longrightarrow Cu(H_2L)_2{}^{3-}$		3.5 ± 0.2	3.3 ± 0.2	
No. of points/titrations		303/5	345/5	
Zn(II)				
$Zn^{2+} + L^{4-} \longrightarrow ZnL^{2-}$	16.5	13.58 ± 0.03	13.15 ± 0.03	13.4[a]
$ZnL^{2-} + H^+ \longrightarrow ZnHL^-$	3.0	3.67 ± 0.03	4.18 ± 0.03	
$ZnHL^- + 2H^+ \longrightarrow ZnH_3L^+$		5.9 ± 0.1	6.0 ± 0.1	
$Zn(OH)L^{3-} + H^+ \longrightarrow ZnL^{2-}$	11.6	11.3 ± 0.2	11.1 ± 0.2	
$ZnHL^- + HL^{3-} \longrightarrow Zn(HL)_2{}^{4-}$		5.5 ± 0.1	5.4 ± 0.1	
No. of points/titrations		276/5	378/5	
Mn(II)				
$Mn^{2+} + L^{4-} \longrightarrow MnL^{2-}$	13.89	8.97 ± 0.03	8.69 ± 0.03	8.57
$MnL^{2-} + H^+ \longrightarrow MnHL^{2-}$	3.1	4.7 ± 0.1	5.0 ± 0.1	
$MnHL^- + HL^{3-} \longrightarrow Mn(HL)_2{}^{4-}$		4.0 ± 0.2	4.0 ± 0.2	
No. of points/titrations		180/5	173/5	

[a] At 20 °C.

The cell parameter E_o and the liquid junction coefficient j_H valid in acidic solutions were determined for each titration by addition of a known amount of HCl to the background electrolyte. The value of the coefficient j_{OH} was assumed to be constant (230 mV M^{-1}).

During the measurements of the metal complex equilibria aqueous NaOH or HCl were added to the solution. The ratio between the total concentrations of metal, C_M, and ligand C_L, was usually held constant. The initial concentrations were varied within the limits $0.0007 \le C_M \le 0.0032$ M and $0.0015 \le C_L \le 0.0063$ M, covering the metal-to-ligand ratios 1:1, 1:2 and 1:4. In some runs aqueous metal chloride was also used as the titrant. For each system 5–9 independent titrations were carried out. The number of data points used in the calculation of the stability constants varied between 173 and 378 from the pH (= $-\log[H^+]$) ranges 2.7–10.4 (Fe), 1.9–10.5 (Cu), 2.0–10.5 (Zn) and 4.8–9.2 (Mn). The concentration ranges were restricted by the relatively low solubility of EDDS in acidic solutions; in some titrations the upper pH values were limited by the appearance of a precipitate or very slow attainment of equilibria. The reproducibility and reversibility of the equilibria were tested by performing forward (increasing pH) and backward (decreasing pH) titrations.

Data treatment

To visualize the experimental data sets, Z_H *versus* pH was drawn. Z_H is defined as the average number of OH^- ions reacted per ligand and is given by the relation $Z_H = ([H^+] - C_H - k_w[H^+]^{-1})/C_L$, where C_H denotes the total concentration of protons calculated over the zero level H_4L, H_2O and M^{n+}.

In evaluating the equilibrium constants the following two-component equilibria were considered:

$$H_4L \rightleftharpoons H_{4-p}L^{p-} + pH^+, \quad p = 1\text{–}4; \quad \beta_{-p01} \qquad (3)$$

$$pH^+ + H_4L \rightleftharpoons H_{4+p}L^{p+}, \quad p = 1,2; \quad \beta_{p01} \qquad (4)$$

$$pH^+ + qM^{n+} \rightleftharpoons (H^+)p(M^{n+})q; \quad \beta_{pq0} \qquad (5)$$

During the calculations the values for the metal ion hydrolysis constants [reaction (5)] were considered as known.[6]

The metal complex formation can be characterized by the general three-component equilibrium:

$$pH^+ + qM^{n+} + r(H_4L) \rightleftharpoons (H^+)_p(M^{n+})_q(H_4L)_r; \quad \beta_{pqr} \qquad (6)$$

The mathematical analysis of the systems involves the search for the complex models (*pqr*-triplets) and the equilibrium constants of the complexes that best describe the experimental data. The calculations were carried out using the computer program SUPERQUAD.[7] The sample standard deviation, *s*, and the χ^2-statistics used as criteria in selection of the complex models were those given by the program.[7] To facilitate comparison between the results obtained for EDTA from the literature[3] the final results given in Table 1 are presented in the form of the stepwise stability constants.

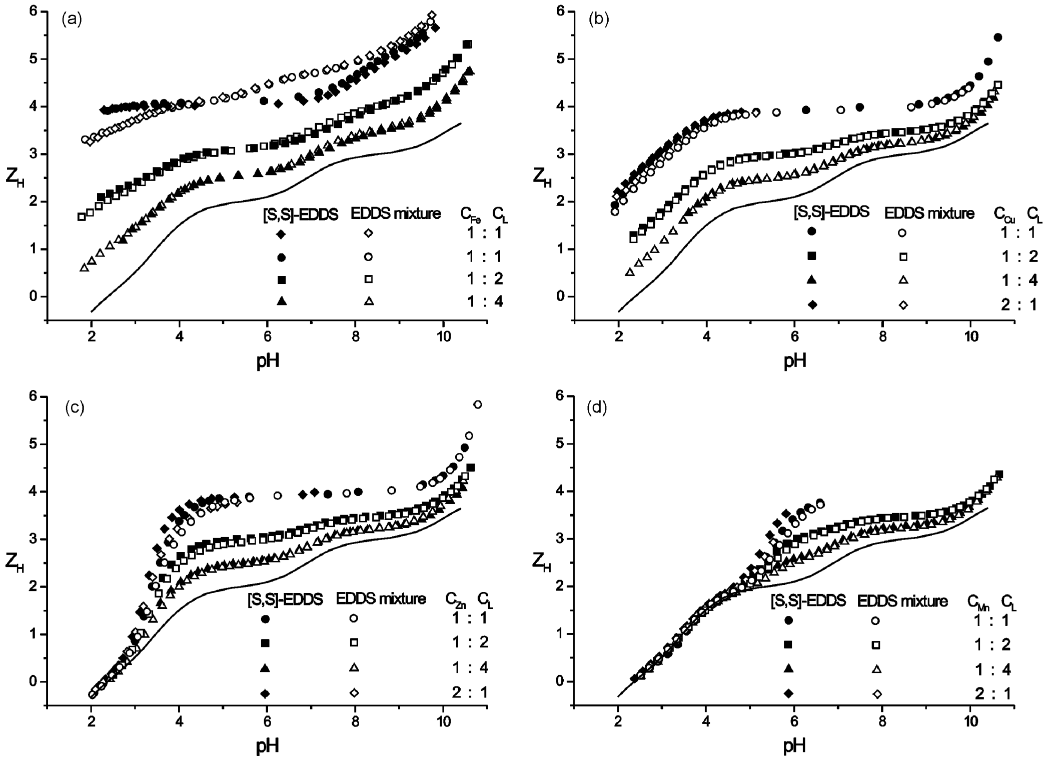


Fig. 1 Z_H *versus* pH for complexation with [*S*,*S*]-EDDS and the EDDS mixture for (a) Fe(III), (b) Cu(II), (c) Zn(II), and (d) Mn(II) complexes. (For all plots, Z_H *versus* pH for EDDS = full line.)

Results

Acidity of EDDS

The neutralization titrations show the stepwise deprotonation of H_4L to L^{4-} occurs in the pH range 2.5–10.5. The negative Z_H values reached only in solutions of very high acidity show that the basicity of H_4L is very weak. The equilibrium constants for reactions (3) and (4) obtained in the final refinements are listed in Table 1 (s = 0.82, χ^2 = 59.8 for [*S*,*S*]-EDDS and s = 0.76, χ^2 = 78.0 for the isomeric mixture).

Complexation with Fe(III)

Addition of iron(III) ions to the EDDS solution leads to a nearly quantitative dissociation of protons from the ligand. Consequently the complex formation has already started in very acidic solutions [Fig. 1(a)]. The coincidence of all curves with [*S*,*S*]-EDDS and the mixture of EDDS stereoisomers indicates the same complexing model in both systems. The displacement of the four ligand protons per metal ion, almost complete already at pH = 2, gives evidence for the formation of a very stable species with $p,q,r = -4,1,1$. With a 1:1 ligand-to-metal ratio, precipitation of $Fe(OH)_3$ occurs in slightly acidic solution whereas with greater C_L:C_M ratios the Z_H values readily exceed 4 and 5 in alkaline conditions. This suggests the presence of the hydrolyzed complex species −5,1,1 and −6,1,1 in the solutions. The refinement of the complex model consisting of these three species gave very low values for the sample standard deviation (s = 0.94 and 1.02, for [*S*,*S*]-EDDS and the isomeric mixture, respectively). Although the χ^2 statistics were somewhat high (χ^2 = 80.5 and 86.5) explanation of the experimental data can be regarded as quite satisfactory. Several additional complexes (bis or binuclear) were also tested but no significant improvement to the fit was obtained. We therefore suggest the set of mononuclear complexes FeL^-, $Fe(OH)L^{2-}$ and $Fe(OH)_2L^{3-}$ as a final complexing model for both EDDS compositions. The stability constants of the complexes are given in Table 1.

Complexation with Cu(II)

The plots Z_H *versus* pH in Fig. 1(b) show that with Cu(II) the dissociation of ligand protons does not occur as easily as with Fe(III). At pH = 2 the Z_H values give evidence of the major species with p,q,r notation −2,1,1 in the solution. At pH 5–6 the number of the dissociated protons increases from two to four. For pH > 9 the deprotonation is continued, obviously due to the formation of some hydroxo complex. In this respect, too, the behavior of both EDDS systems is identical. In the computational analysis the mononuclear complexes −2,1,1, −3,1,1, −4,1,1 and −5,1,1 gave a quite satisfactory fit to the experimental data (s = 1.63, χ^2 = 47.6 for [*S*,*S*]-EDDS, and s = 1.97, χ^2 = 61.6 for the isomeric mixture).

A better explanation was, however, obtained when a series of the bis complexes −4,1,2, −5,1,2, −6,1,2 and −7,1,2 was included in the model (s = 1.20, χ^2 = 30.4, and s = 1.13, χ^2 = 15.1). Addition of the binuclear species −4,2,1 further resulted in a slight but significant improvement of the fit (s = 1.09, χ^2 = 22.2, and s = 1.08, χ^2 = 16.0). In all, the best model for both of the isomeric systems was that assuming the complexes $Cu(H_2L)$, $Cu(HL)^-$, CuL^{2-}, $Cu(OH)L^{3-}$, $Cu(H_2L)_2{}^{2-}$, $Cu(H_2L)(HL)^{3-}$, $Cu(HL)_2{}^{4-}$, $Cu(HL)L^{5-}$ and Cu_2L with the stability constants given in Table 1.

Complexation with Zn(II)

Fig. 1(c) shows the complex formation to begin at *ca.* pH = 3 when the Z_H values for the metal–ligand titrations start to differ from the respective values of the mere ligand. The steepness of Z_H between pH 3 and 4 together with the following long plateau that can be found in the C_M: C_L = 1:1 conditions is also noteworthy. The curve corresponds to the removal of a total of four protons from EDDS per Zn(II) and implies the formation of a deprotonated complex −4,1,1 as a predominating species. As with the previous metals, Z_H values greater than four can be reached in alkaline solutions. In the calculations at least the following four mononuclear species had to be included in the model: $Zn(H_3L)^+$, $Zn(HL)^-$, ZnL^{2-} and $Zn(OH)L^{3-}$ (s = 1.50, χ^2 = 51.3, and s = 2.27, χ^2 = 58.1). When a number of other

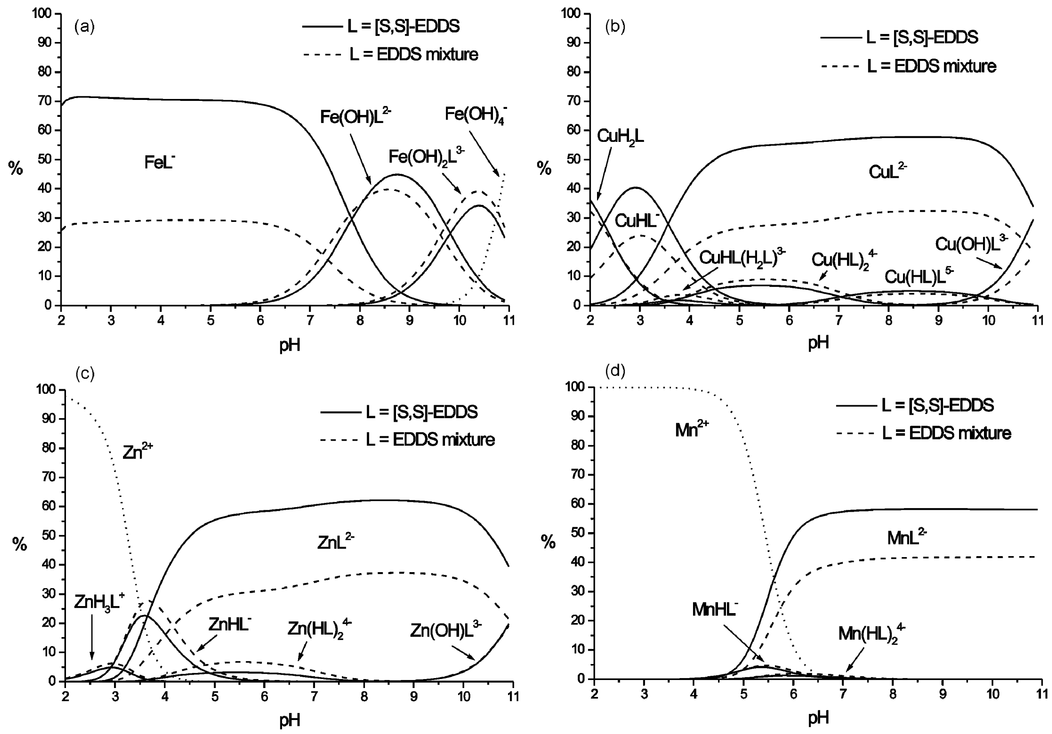


Fig. 2 Percentage distribution of different complexes *versus* pH for (a) Fe(III), (b) Cu(II), (c) Zn(II), and (d) Mn(II).

complexes were tested, significant improvement to the fit was obtained only when a bis complex $-6,1,2$ [= $Zn(HL)_2^{4-}$] was accepted. All other mononuclear and polynuclear complexes were rejected. The final refinements assuming the above-mentioned five complex species were ceased at s = 1.13, χ^2 = 42.4, and s = 1.67, χ^2 = 18.4 for [*S*,*S*]-EDDS and the isomer mixture, respectively, indicating a good explanation of the experimental data. The stability constants of the complexes are shown in Table 1.

Complexation with Mn(II)

With manganese(II) ions the complex formation begins when the pH of the solution is increased to *ca.* 5, as can be found from Fig. 1(d). The Z_H values greater than four cannot be reached until precipitation occurs. The analysis showed that the mononuclear complexes $-3,1,1$ and $-4,1,1$ alone could explain the experimental data fairly well (s = 1.72, χ^2 = 10.6, and s = 1.56, χ^2 = 46.5 for [*S*,*S*]-EDDS and the isomeric mixture, respectively) but a slightly better fit was obtained when a bis complex $-6,1,2$ was also added (s = 1.63, χ^2 = 11.6, and s = 1.35, χ^2 = 20.5) in the calculations. As the best explanation of the data in the studied pH range we suggest the model comprising the three complexes $Mn(HL)^-$, MnL^{2-} and $Mn(HL)_2^{4-}$ with the stability constants given in Table 1.

Discussion

The values of the protonation constants of the [*S*,*S*]-EDDS and the isomeric mixture of EDDS (25% [*S*,*S*], 50% [*R*,*S*], 25% [*R*,*R*]) are given in Table 1. The values that refer to the deprotonation of the first two carboxylic acid groups are only approximate while the rest of the four acidity constants can be obtained with great accuracy. In both systems studied, the corresponding values are equal within experimental error, and the acid properties of the diastereoisomers are thus similar. The values of the acidity constants found here are in very good agreement with those given earlier in the literature.[3] It may be noted that the acidities of the carboxylic acid groups in EDTA are somewhat stronger than for the aspartic acid groups in EDDS.[3]

The complexes formed with the enantiomers [*S*,*S*] and [*R*,*R*] are likely to be identical by symmetry whereas the [*R*,*S*] form may differ from [*S*,*S*] and [*R*,*R*]. The results obtained here (Table 1) show that the different chiralities of the EDDS molecules have no distinct effect on the complexation models; with all metal ions the same complex species were found in the isomeric systems studied.

As can be well expected, very stable mono complexes FeL^- and ML^{2-} (M = Cu, Zn, Mn) dominate the complex formation with this potentially hexadentate ligand. The coordination geometries of the [*S*,*S*] or [*R*,*S*] forms of EDDS with Fe(III), Co(III), Cu(II) and Ni(II) are known in the solid state from X-ray diffraction studies.[8–11] Although there are some structural variations, in all these complexes the central metal atom is coordinated by two imine nitrogen atoms and by one oxygen atom from each of the four carboxylate groups of the ligand. There is hardly any doubt that the basic structure of the solid complexes and the above-mentioned aqueous species are similar.

In the case of Cu(II), Zn(II) and Mn(II) a variety of acidic mono complexes $M(H_pL)^{p-2}$ was also found. It is evident that in these structures some of the carboxylic acid groups are still protonated and do not bind the partly hydrated metal ions. With Fe(III) the formation of the major species FeL^- is already formed in solutions of very low pH so that detection of any acidic iron complexes was not possible.

It was of interest to find that the mono complexes FeL^-, CuL^{2-} and ZnL^{2-} are still able to deprotonate after all four carboxylic acid groups have lost their protons. The same phenomenon has also been observed for the corresponding EDTA complexes. With [*S*,*S*]-EDDS the conventional pK_a values of the complexes are 7.9, 11.1 and 11.3 for Fe, Cu and Zn, respectively. With the isomeric mixture the same values are 7.3, 11.0 and 11.1. It is likely that these species can be classified as hydroxo complexes, *i.e.* dissociation occurs at the coordinated water molecules rather than at the coordinated imino NH groups. The appearance of precipitation already at relatively low pH presumably prevented the verification of such species with manganese.

In addition to the mono complexes, bis complexes of the type $M(HL)_2^{4-}$ are formed with Cu, Zn and Mn in solution with high C_L:C_M ratios. With copper a whole series of acidic bis complexes is formed. The only polynuclear species found in this study is Cu_2L. The structure of this binuclear complex is uncertain but it may be noted that a chelate of similar composition has been verified in the solid state with nickel(II). The crystal structure of Ni_2L consists of the complex anions $[Ni(S,S)\text{-EDDS}]^{2-}$ and pentahydrated cations $[Ni(H_2O)_5]^{2+}$ mutually connected by the acetate group of the six-membered chelate ring to form a discrete binuclear complex unit.[11]

By comparing the values of the stability constants of the corresponding complexes given in Table 1 it can be found that there are only minor differences between the two isomeric systems. It is, however, noteworthy that with all these metal ions the stability of the major species $ML^{(4-n)-}$ formed with the [*S*,*S*] form of EDDS is 0.3–0.5 log units higher than the corresponding complex formed with the isomer mixture. This indicates the existence of a small stereospecificity due to the differences in the coordination geometry between the [*S*,*S*] and [*R*,*S*] forms of the ligand.

In the mono complexes $ML^{(4-n)-}$ the ligand is hexadentate, all carboxylic groups of the ligand being deprotonated and bound to the central metal ion. With the acidic mono complexes $M(H_pL)^{(n+p-4)}$ where all carboxylic donor groups of EDDS are evidently not in use, stabilities of the complexes are nearly equal and no clear stereoselective effects can be found. The predominating role of the $ML^{(4-n)-}$ complexes over a wide pH range in solutions with a metal-to-ligand ratio of 1:1 as well as the effect of stereoselectivity is illustrated in Fig. 2 which shows the distribution of the different complexes *versus* pH ($C_M = C_{[S,S]\text{-EDDS}} = C_{\text{EDDS mixture}} = 1$ mM). With Fe(III), where the binary hydrolysis of the metal ion is very strong, the complex distribution is greatly dependent on the concentration of the metal, and the presence of the various $Fe(OH)_s^{(3-s)+}$ species in the solution is markedly increased by dilution.

In industrial applications it is usually more practical to consider conditional stability constants instead of the conventional stability constants. The conditional stability constant K'_{ML} for the major complex species $ML^{(4-n)-}$ is given by the relation

$$K'_{ML} = \frac{\alpha_{ML}}{\alpha_M \cdot \alpha_L} \cdot K_{ML} \tag{7}$$

where the side reaction coefficients α_M, α_L and α_{ML} are defined as follows:

$$\alpha_M = \frac{\Sigma(H^+)_p(M^{n+})_q}{\left[M^{n+}\right]} \tag{8}$$

$$\alpha_L = \frac{\Sigma(H^+)(L^{4-})}{\left[L^{4-}\right]} \tag{9}$$

$$\alpha_{ML} = \frac{\Sigma(H^+)_p(M^{n+})_q(L^{4-})_r}{\left[ML^{n-4}\right]} \tag{10}$$

$$K_{ML} = K(M^{n+} + L^{4-} \rightleftharpoons ML^{n-4}) \tag{11}$$

The values of the conditional stability constants of the [*S*,*S*]-EDDS complexes, as calculated with the aid of the equilibrium constants determined in this study and with the aid of the binary hydrolysis of the metal ions given in the literature,[6] vary as a function of pH as shown in Fig. 3(a). For comparison, the same plot for the respective EDTA complexes is also included in Fig. 3(b).

The values of $\log K'_{ML} \geq 6$ are often considered as a criterion for an efficient complexation. With this assumption the approximate pH ranges suitable for the use of EDDS and EDTA as a chelating agent in the metal transition are given in Table 2.

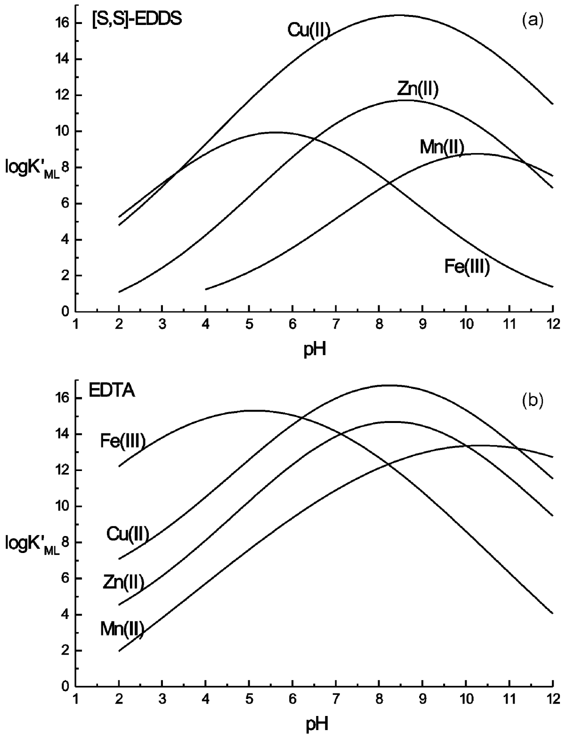


Fig. 3 Conditional stability constants for ML complexes of (a) [*S*,*S*]-EDDS *vs.* pH, and (b) EDTA *vs.* pH.

Table 2 Approximate pH ranges suitable for chelation

	EDDS	EDTA
Fe(III)	3–9	2–11
Cu(II)	3–12	2–12
Zn(II)	5–12	3–12
Mn(II)	8–12	5–12

The present metal complexes are somewhat lower in stability than the corresponding EDTA complexes. This results in some narrowing of the useful chelating range so that somewhat higher pH values are needed for EDDS. In the case of iron(III) the upper pH limit for useful complexation is also somewhat higher for EDTA that for EDDS.

It is, however, clear that the stabilities of the EDDS chelates are great enough for most practical applications. In forming the $ML^{(4-n)-}$ complexes there is a slight extra stabilization of the [*S*,*S*] form of the ligand relative to the [*R*,*S*] isomer. From the environmental perspective the readily biodegradable [*S*,*S*] stereoisomer is also recommended.

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