

Supplementary Information

Theoretical and experimental studies on isotachopheresis in multi-moving chelation boundary system formed with metal ions and EDTA

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pH Change in the system

Under the electric field, the hydrogen and hydroxyl ions migrate towards the cathode and anode, respectively. And the migration of hydrogen and hydroxyl ions would induce the pH change in the system. The solubility products $K_{sp,Cu(OH)_2}$ and $K_{sp,Co(OH)_2}$ are 1.0×10^{-14} and 1.6×10^{-15} , respectively⁵³. Due to the flux of proton is almost equal to that of hydroxyl ion, the pH values under the steady state would be calculated and when the ratios of [Cu(II)] to [EDTA] were 30:10, 30:15, 30:20, 30:25, 30:30, 25:30, 20:30, 15:30 and 10:30, the pH values were 4.911, 4.919, 4.924, 4.928, 4.930, 4.927, 4.924, 4.920 and 4.911. The result manifested that the pH values were close to 5.0, and the pH change was very little and could be ignored when the system reached the steady state. So the velocities shown in Fig. 3 and Table 1 were calculated with the mobilities under pH 5.0.

Calculation of the velocity

The calculation of the theory velocity was line with Eqn. (16), namely,

$$v = i \left(\frac{\mu_{M_n}^{-\beta_n} C_{M_n}^{-\beta_n}}{\kappa^{\beta_n}} - \frac{\mu_C^{-\gamma} C_C^{-\gamma}}{\kappa^{\gamma}} \right) / \left(C_{M_n}^{-\beta_n} - C_C^{-\gamma} \right)$$

For the 2-metal mMCB system mentioned in the text, the specific conductivity was constant in the whole system (the reason had been explained at P11, Line 22-23, in the text), the specific Eqn. (6) would be:

$$v = \frac{i}{\kappa} \left(\mu_{Cu}^{-} C_{Cu}^{-} - \mu_{EDTA}^{-} C_{EDTA}^{-} \right) / \left(C_{Cu}^{-} - C_{EDTA}^{-} \right) \quad (S-1)$$

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Here, the constituent mobility $\bar{\mu}$ was calculated in line with Eqn. (5), the effective mobility of the copper ion involved in Eqn. (5) was obtained in accordance with Eqn. (18) and (19), the molar conductivity can be gained from Ref. [53]. The effective mobilities of complex and EDTA were obtained through the mobility determination by CE (Please see P12, Line 18~25). The total metal ion concentrations were obtained through multiplying the diluted folds of sample by the direct results of ICP-AES. The metal complex concentrations were achieved with multiwavelength mapping analysis method by UV-vis spectrometry and the details were given as below.

The 0.5 ml sample was detected by UV-vis spectroscopy at 208 nm, 212 nm, 226 nm, 236 nm and 261 nm wavelength. Noticeably, at 212 nm $[\text{Cu-EDTA}]^{2-}$ and $[\text{Co-EDTA}]^{2-}$ have the same molar absorption coefficient. The spectra were corrected background absorbance by subtracting the absorbance of a cell filled with the blank contrast. The molar absorptivities (ε) of $[\text{Cu-EDTA}]^{2-}$ and $[\text{Co-EDTA}]^{2-}$ at 208 nm, 212 nm, 226 nm, 236 nm and 261 nm and the ratio (f) of $\varepsilon_{[\text{Co-EDTA}]^{2-}}/\varepsilon_{[\text{Cu-EDTA}]^{2-}}$ were shown in Table S-1.

Table S-1. The molar absorptivities of $[\text{Cu-EDTA}]^{2-}$ and $[\text{Co-EDTA}]^{2-}$ and the ratio of $\varepsilon_{[\text{Co-EDTA}]^{2-}}/\varepsilon_{[\text{Cu-EDTA}]^{2-}}$ at five different wavelengths.

	208 nm	212 nm	226 nm	236 nm	261 nm
$\varepsilon_{[\text{Co-EDTA}]^{2-}}$	2.8687 $\text{mM}^{-1}\text{cm}^{-1}$	2.33 $\text{mM}^{-1}\text{cm}^{-1}$	1.174 $\text{mM}^{-1}\text{cm}^{-1}$	0.738 $\text{mM}^{-1}\text{cm}^{-1}$	0.067 $\text{mM}^{-1}\text{cm}^{-1}$
$\varepsilon_{[\text{Cu-EDTA}]^{2-}}$	2.268 $\text{mM}^{-1}\text{cm}^{-1}$	2.331 $\text{mM}^{-1}\text{cm}^{-1}$	2.954 $\text{mM}^{-1}\text{cm}^{-1}$	3.261 $\text{mM}^{-1}\text{cm}^{-1}$	2.745 $\text{mM}^{-1}\text{cm}^{-1}$
Ratio (f)	1.264	1.000	0.397	0.226	0.024

The linear relation between absorption and concentration of a single determination is given by Lambert-Beer's law.

$$A(\lambda)l^{-1} = \sum_{i=1}^n \varepsilon_i(\lambda) \cdot c_i \quad (\text{S-2})$$

Where, A_λ is the absorption of the sample at wavelength λ , l is the optical path length of the matched silica cell, i is the component i , c_i is the concentration of component i , λ is the corresponding wavelength. For a mixture in solution containing two components at concentrations c_1 and c_2 , the absorbance at any wavelength λ is, for unit path length, given by

$$A(\lambda) = c_1 \cdot \varepsilon_1(\lambda) + c_2 \cdot \varepsilon_2(\lambda) \quad (\text{S-3})$$

Both side of Equation (II) divide $\varepsilon_1(\lambda)$, the Lambert-Beer's law can be written as

$$\frac{A(\lambda)}{\varepsilon_1(\lambda)} = c_1 + c_2 \cdot \frac{\varepsilon_2(\lambda)}{\varepsilon_1(\lambda)} \quad (\text{S-4})$$

For our experiment, ε_1 is $\varepsilon_{[\text{Cu-EDTA}]^{2-}}$, ε_2 is $\varepsilon_{[\text{Co-EDTA}]^{2-}}$, c_1 is the concentration of $[\text{Cu-EDTA}]^{2-}$, c_2 is the concentration of $[\text{Co-EDTA}]^{2-}$, and $\varepsilon_2/\varepsilon_1$ is the ratio f . According to the absorptions $A(\lambda)$ of the samples at the five different wavelengths and the diluted folds, we use the ratio f as an independent variable, $A(\lambda)/\varepsilon_1(\lambda)$ as the dependent variable, and a straight line could be obtained. The slope of the straight line is c_2 , and the intercept at x axis is c_1 . After a run, one straight line would be gained for phase β' (or α').

And according to the definition of the current intensity i and the specific conductivity κ , as well as the experimental conditions, the value of i/κ was 1.208 V/m.