Supporting information for the article

Liquid-Liquid Equilibria of 5-Methyl-2-pyrazinecarboxylic Acid for Solvents with Trioctylamine at Increased Ionic Strength

Ján Marták, Ľubica Kubišová, Štefan Schlosser

Table S1. Summary table of complexes in extraction from ternary solutions (organic acid + inorganic acid or salt + H_2O). These complexes were proposed in papers of Schunk *et al.*[1] and Schunk and Maurer.[2-4] The stoichiometry is (*p, r, q, s*) where the coefficients are *p* for organic acid, *r* for mineral acid, *q* for TOA and *s* for water. The abbreviations are MIBK for methylisobutyl ketone, H_3Cit for citric acid and HAc for acetic acid.

diluent	toluene	MIBK	MIBK
mineral acid	HCl		H_2SO_4
H_3Cit	(1, 2, 3, 3)	(2, 1, 3, 9) (1, 2, 3, 2)	
HAc	(1, 2, 3, 2) (1, 2, 2, 0) (2, 2, 2, 2)	(1, 2, 3, 2) (2, 2, 3, 6) (4, 2, 3, 8)	(2, 1, 4, 2) (4, 1, 4, 8) (10, 1, 4, 12)

Table S2. Summary table of complexes in extraction from ternary aqueous solutions containing two organic acids. These complexes were proposed in papers of Kirsch and Maurer[5-7] and Maurer.[8] The stochiometric coefficients are p_{Ac} for acetic acid, p_{Cit} for citric acid, p_{Ox} for oxalic acid, *q* for TOA and *s* for water. MIBK is methylisobutyl ketone.

diluent	toluene	MIBK	$CHCl_3$
(p_{Ac}, p_{Ox}, q, s)	(1, 1, 1, 1)		(1, 1, 1, 0)
(p_{Ox}, p_{Cit}, q, s)		(1, 1, 1, 5)	
(p_{Ac}, p_{Cit}, q, s)	(1, 2, 3, 2)		(1, 1, 2, 1)

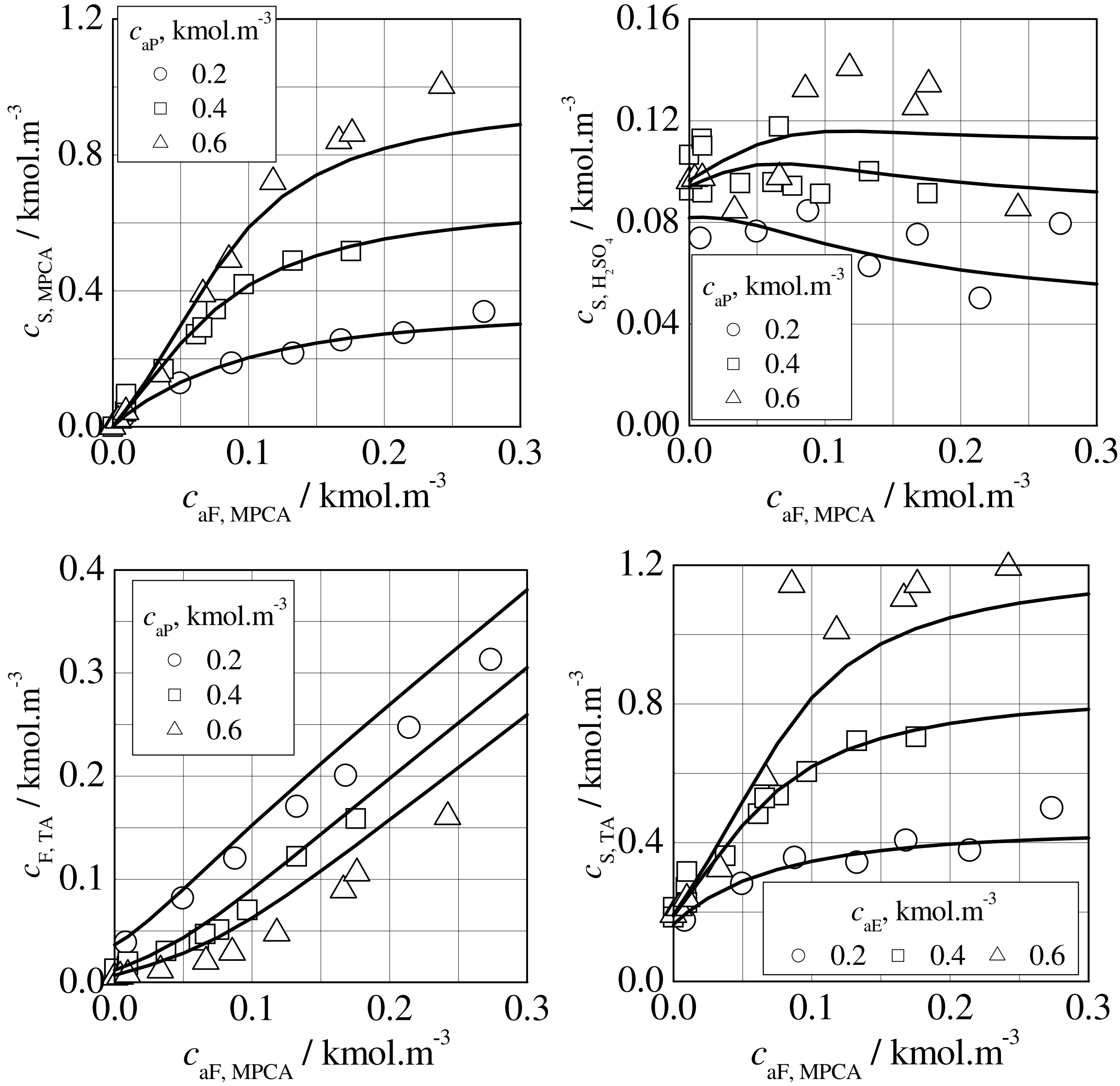

Figure S1. Results of fitting of the first set of data. Fitted dependent variables vs. equilibrium concentration of MPCA, $c_{aF, MPCA}$, for solvent (TOA + xylene) with three different concentrations of TOA, c_{Eo} = (0.2, 0.4 and 0.6) kmol.m^{-3} (Table 2). MPCA was extracted from aqueous solution (MPCA + H_2SO_4 + Na_2SO_4 + H_2O) with c_{Fo, H_2SO_4} = 0.1 kmol.m^{-3} and c_{Fo, Na_2SO_4} = 1 kmol.m^{-3}. The lines were calculated according to the model 2 in Table 5.

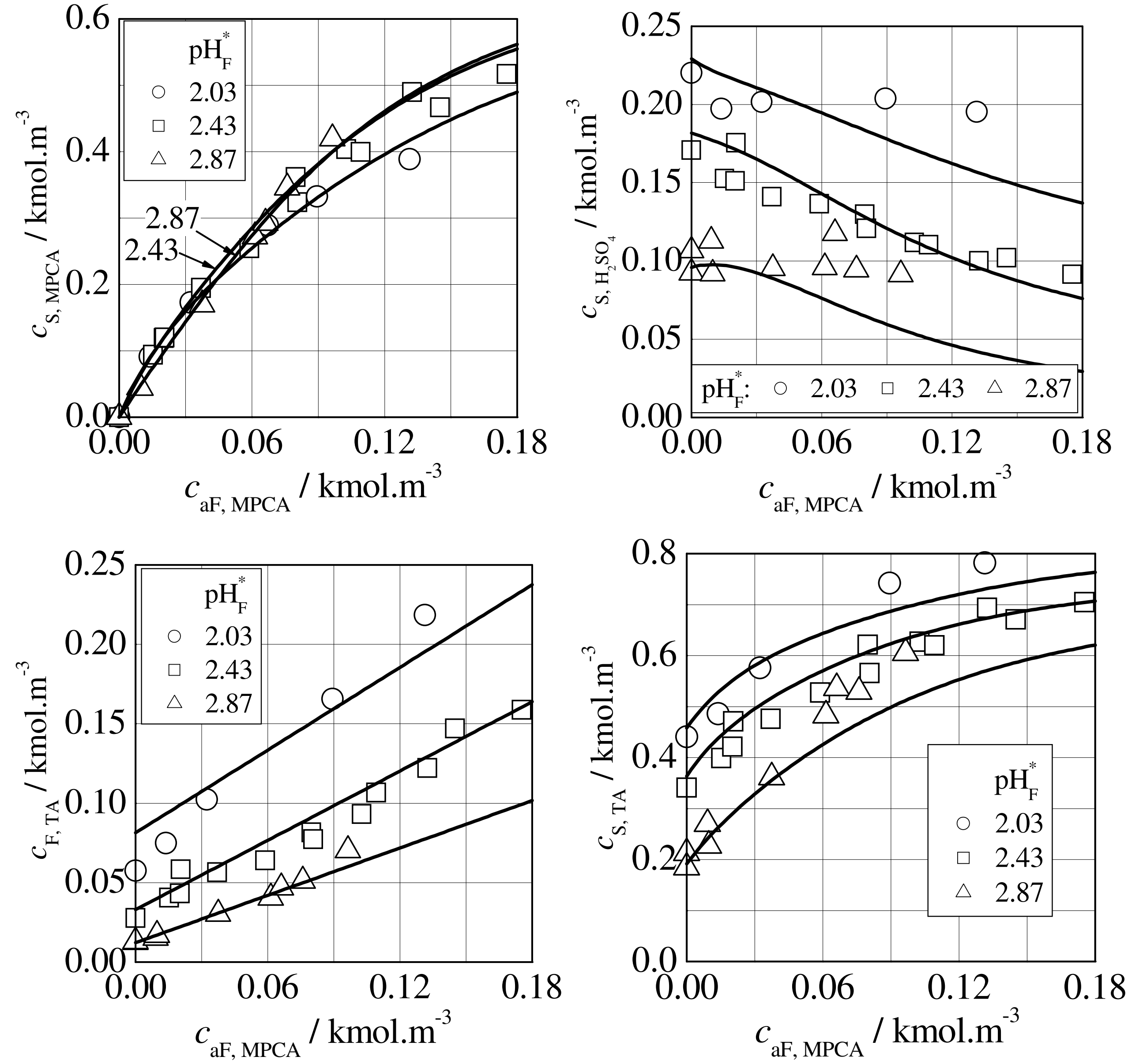

Figure S2. Results of fitting of the second set of data. Fitted dependent variables vs. equilibrium concentration of MPCA, $c_{aF,\,MPCA}$, at three different equilibrium pH. MPCA was extracted from aqueous solution (MPCA + Na_2SO_4 + H_2O) with $c_{Fo,\,Na_2SO_4}$ = 1 kmol.m^{-3} to the solvent (TOA + xylene) with c_{Eo} = 0.4 kmol.m^{-3} (Table 3). The lines were calculated according to the model 2 in Table 5.

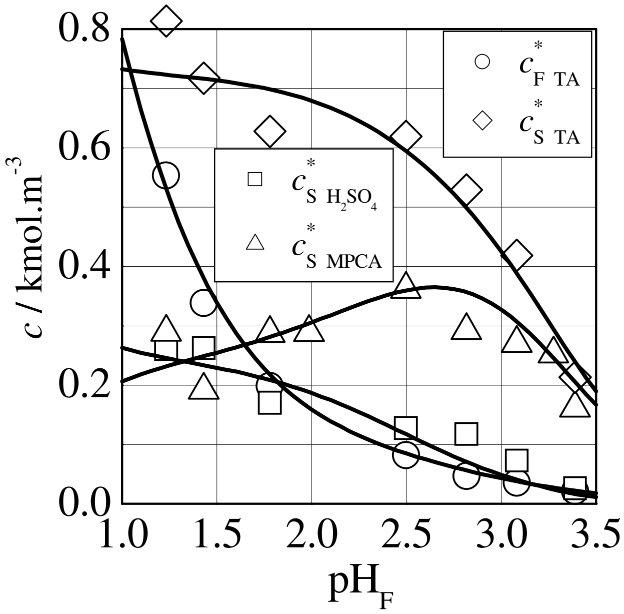

Figure S3. Results of fitting of the second set of data. Fitted dependent variables vs. equilibrium pH in the aqueous phase. The same system as in Figure S2 was used. $c_{\mathrm{aF,\,MPCA}}$ = 0.081 kmol.m^{-3}. The lines were calculated according to the model 2 in Table 5.

1. Schunk, A.; Menert, A.; Maurer, G., On the influence of some inorganic salts on the partitioning of citric acid between water and organic solutions of tri-n-octylamine Part I: Methyl isobutyl ketone as organic solvent. *Fluid Phase Equilibria* **2004,** 224, 55-72.
2. Schunk, A.; Maurer, G., On the influence of some inorganic salts on the partitioning of citric acid between water and organic solutions of tri-n-octylamine. Part II: Toluene as organic solvent. *Industrial & Engineering Chemistry Research* **2005,** 44, 8837-8851.
3. Schunk, A.; Maurer, G., On the influence of some strong electrolytes on the partitioning of acetic acid to aqueous/organic two-phase systems in the presence of tri-n-octylamine Part 1: Methyl isobutyl ketone as organic solvent. *Fluid Phase Equilibria* **2006,** 239, 223-239.
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5. Kirsch, T.; Maurer, G., Distribution of binary mixtures of citric, acetic and oxalic acid between water and organic solutions of tri-n-octylamine.1. Organic solvent toluene. *Fluid Phase Equilibria* **1997,** 131, 213-231.
6. Kirsch, T.; Maurer, G., Distribution of binary mixtures of citric, acetic and oxalic acid between water and organic solutions of tri-n-octylamine - Part II. Organic solvent methylisobutylketone. *Fluid Phase Equilibria* **1998,** 142, 215-230.
7. Kirsch, T.; Maurer, G., Distribution of binary mixtures of citric, acetic and oxalic acid between water and organic solutions of tri-n-octylamine Part III. Organic solvent chloroform. *Fluid Phase Equilibria* **1998,** 146, 297-313.
8. Maurer, G., Modeling the liquid-liquid equilibrium for the recovery of carboxylic acids from aqueous solutions. *Fluid Phase Equilibria* **2006,** 241, 86-95.