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Liquid–Liquid Extraction Systems of Benzoic Acid in Water and Heptane, Methylbenzene, or Trichloroethylene as Cosolvent

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S Supporting Information

ABSTRACT: Equilibrium data at (293 ± 2) K are presented for benzoic acid in water and three different organic phases (heptane, methylbenzene, and trichloroethylene). The monomeric partition constant, K_P^{MON}, and the dimerization constant, K_D, for the organic phase were determined at 293 K. For the heptane/water benzoic acid system, K_P^{MON} equals $(0.209 \pm 0.049)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(1.33 \pm 0.68)\ m^3 \cdot mol^{-1}$. For the methylbenzene/water benzoic acid system, K_P^{MON} equals $(1.17 \pm 0.92)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(0.39 \pm 0.64)\ m^3 \cdot mol^{-1}$. For the trichloroethylene/water benzoic acid system, K_P^{MON} equals $(0.808 \pm 0.295)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(1.18 \pm 0.89)\ m^3 \cdot mol^{-1}$. Equilibrium constants were obtained from UV–vis spectroscopy and conductivity experiments. The equilibrium data of these extraction systems can be used to quantify liquid–liquid mass transfer rates with extraction systems that require low flammability risk (trichloroethylene), low costs (methylbenzene), or setups constructed from polymethyl methacrylate (heptane).

1. INTRODUCTION

The European Federation of Chemical Engineering (EFCE) Working Party on Distillation, Absorption and Extraction recommends three standard extraction systems that can be used to measure liquid–liquid mass transfer rates: (1) water/methylbenzene and propanone, (2) water/butan-1-ol and butanedioic acid, and (3) water/4-methylpentan-2-one and acetic acid.[1] The preference of these systems was based on their high flashpoint, low toxicity, availability of the components, moderate costs of the materials, and the possibility to analyze the product compositions. In this paper we present three novel extraction systems, in which benzoic acid is applied as a solute: water/heptane with benzoic acid, water/methylbenzene with benzoic acid, and water/trichloroethylene with benzoic acid. Benzoic acid is chosen as a solute because it can be measured in-line in both phases by UV–vis spectroscopy. Additionally, it has low toxicity, and it is inexpensive. Until now benzoic acid was a noncommon solute, because of its tendency to dimerize in the organic phase. This paper presents the monomeric partition constant and the dimerization constant for these three systems.

Heptane was chosen as organic solvent because it can be used in equipment that is constructed out of poly(methyl 2-methylpropenoate) (PMMA). PMMA is often used as a construction material for lab scale reactors in which visual observation of the liquid flow is desired. PMMA cannot be used with the recommended systems of the EFCE. Trichloroethylene was chosen as a solvent because of its low flammability. This allows for applications of this system in experimental setups which are not Atmosphere Explosive (ATEX) certified.

In extraction systems where benzoic acid is partitioning over water and an organic phase, three equilibria are present which are shown in Figure 1. The equilibria from Figure 1 can be described by equilibrium reactions 1, 2, and 3.

$$(\text{PhCOOH})_{\text{ORG}} \overset{K_P^{\text{MON}}}{\rightleftarrows} (\text{PhCOOH})_{\text{AQ}} \quad (1)$$

$$\text{H}_2\text{O} + (\text{PhCOOH})_{\text{AQ}} \overset{K_A}{\rightleftarrows} \text{H}_3\text{O}^+ + (\text{PhCOO}^-)_{\text{AQ}} \quad (2)$$

$$2(\text{PhCOOH})_{\text{ORG}} \overset{K_D}{\rightleftarrows} (\text{PhCOOH})_{2,\text{ORG}} \quad (3)$$

Reaction 1 represents the partitioning of the benzoic acid over the two phases, reaction 2 the acid dissociation equilibrium in the aqueous phase, and reaction 3 the dimerization equilibrium of the benzoic acid in the organic phase. When calculating the liquid–liquid mass transfer rates from extraction experiments, one needs to know the concentration difference between the two phases. When benzoic acid is used as a solute, this concentration difference is given by the difference between the monomeric species in the organic phase and the nondissociated species in the aqueous phase, as is shown in Figure 1. Therefore, the monomeric partition constant and the dimerization constant are needed for accurate mass transfer rate calculations.

The dimerization of benzoic acid in heptane was studied by various authors. The pressure dependence on dimerization was reported by Sawamura et al.[2] A spectroscopic method to determine the dimerization constant was investigated by Kubista et al.[3] A quantitative analysis of the UV spectra of benzoic acid and its derivatives was studied by Ito.[4] However, the influence of the distribution over two immiscible liquids was not described before. Hanrahan and Bruce concluded that only monomers and dimers are present in the organic phase.[5] Therefore, the formation of trimers and other oligomers is further neglected for all three systems that were discussed.

Equation 4 shows the total benzoic acid concentration in the aqueous phase, C_{AQ}^{TOT}, which is defined as the sum of the

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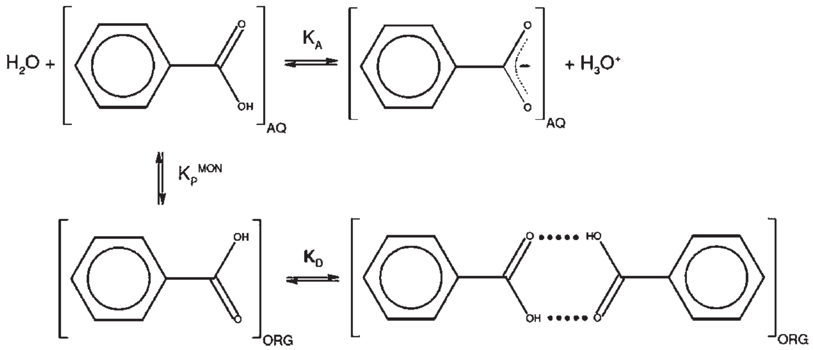

Figure 1. Equilibria present when benzoic acid is partitioning between the aqueous phase and an organic phase.

nondissociated benzoic acid, C_{AQ}^{HA}, and the dissociated benzoic acid, $C_{AQ}^{A^-}$, concentrations. Equation 5 shows the total benzoic acid concentration in the organic phase, C_{ORG}^{TOT}, which is equal to the sum of the monomer concentration, C_{ORG}^{MON}, and twice the dimer concentration, C_{ORG}^{DIM}, in the organic phase.

$$C_{AQ}^{TOT} = C_{AQ}^{HA} + C_{AQ}^{A^-} \tag{4}$$

$$C_{ORG}^{TOT} = C_{ORG}^{MON} + 2C_{ORG}^{DIM} \tag{5}$$

The observed partition constant, K_P^{OBS}, is defined as the ratio of the total benzoic acid concentration in the organic phase, over the total benzoic acid concentration in the aqueous phase. Combining the eqs 4 and 5 with the equilibrium constants of reactions 1, 2, and 3, gives an observed partition constant that is a nonlinear function of the total concentration of benzoic acid in the aqueous phase.

$$K_P^{OBS} = \frac{C_{ORG}^{TOT}}{C_{AQ}^{TOT}} = \frac{C_{ORG}^{MON} + 2C_{ORG}^{DIM}}{C_{AQ}^{HA} + C_{AQ}^{A^-}} = \frac{K_P^{MON} + 2K_D(K_P^{MON})^2 C_{AQ}^{TOT}}{1 + \sqrt{\dfrac{K_A}{C_{AQ}^{TOT}}}} \tag{6}$$

Equation 6 is rewritten into eq 7 to determine $K_P{}^{MON}$ and K_D from a linear fit of the experimental data. In eq 7, the adjusted partition constant, $K_P{}^{ADJ}$, is given by the total concentration of benzoic acid in the organic phase divided by the nondissociated benzoic acid concentration in the aqueous phase, C_{AQ}^{HA}. The difference between the adjusted partition constant and the observed partition constant is that instead of the total concentration of benzoic acid, only the nondissociated benzoic acid concentration in the water phase is used.

$$K_P^{ADJ} = \frac{C_{ORG}^{TOT}}{C_{AQ}^{HA}} = \frac{C_{ORG}^{MON} + 2C_{ORG}^{DIM}}{C_{AQ}^{HA}} = K_P^{MON} + 2K_D(K_P^{MON})^2 C_{AQ}^{HA} \tag{7}$$

The adjusted partition constant is a function of the dimerization constant, the monomeric partition constant, and the acid dissociation constant and is a linear function of the nondissociated benzoic acid concentration in the water phase.

The acid dissociation constant of benzoic acid in pure water, pK_A, is known as a function of temperature and equals 4.205 [−] at 293 K.[6] When the concentration of nondissociated benzoic acid is plotted versus the adjusted partition constant, this will result in a straight line with an intercept that equals $K_P{}^{MON}$ and a slope that is equal to 2 K_D $(K_P{}^{MON})^2$. This method is commonly applied to obtain the equilibrium constants $K_P{}^{MON}$ and K_D.[7] This graphical representation allows for easy identification of errors in the partitioning behavior and reduces the error that is introduced by the low concentration measurements. The accuracy of $K_P{}^{MON}$ and K_D increases with the concentration range. Long et al. used this method to determine $K_P{}^{MON}$ and K_D for the water/dodecane benzoic acid system and the water/hexane benzoic acid system, which are systems with comparable physical properties when compared to water/heptane benzoic acid.[8]

2. EXPERIMENTAL SECTION

2.1. Materials. Demineralized water was obtained by purification with a Millipore Elix UV-10 machine. Heptane (mass fraction, w = 0.99, Sigma-Aldrich), trichloroethylene (IUPAC systematic name 1,1,2-trichloroethylene) (w = 0.98, VWR International ProLabo), and methylbenzene (w = 0.98, VWR International ProLabo) were used in combination with benzoic acid (w = 0.995, Merck). The water content in the benzoic acid was measured by weighing a specific amount of benzoic acid before and after a 24 h period of drying at 373 K and was determined to be less than w = 0.01. Heptane, methylbenzene, and trichloroethylene were not further purified. All experiments were performed at (293 ± 2) K. The physical properties of the used chemical systems at 293 K are given in Table 1.

2.2. Analysis Procedure. The benzoic acid concentrations were determined from UV−vis absorption spectra. The absorption spectra were measured on a Shimadzu UV-1650PC UV−vis spectrophotometer. The samples were measured in quartz cuvettes, type 100-QS with an optical path length of 10 mm. Typical absorption spectra for benzoic acid in different solvents are shown in Figure 2. For heptane the peak at 275 nm, for trichloroethylene the peak at 274 nm, and for methylbenzene the peak at 283 nm were used for the determination of the benzoic acid concentration. For all three systems the linearity of the Lambert−Beer law was confirmed by calibrating over the whole range of concentration.

2.3. Determination of the Equilibrium Constants. A series of equilibrium compositions was obtained by dissolving weighed amounts of benzoic acid in a mechanically stirred $10 \cdot 10^{-5}$ m^3 volumetric flask that contained weighed amounts of $50 \cdot 10^{-6}$ m^3 water and $50 \cdot 10^{-6}$ m^3 organic phase (i.e., heptane, trichloroethylene, or methylbenzene). The flask was sealed to prevent evaporation. The mixtures were simultaneously mixed overnight

Table 1. Density, ρ/kg·m^{-3}, Viscosity, η/kg·m^{-1}·s, Benzoic Acid Solubility, S/mol %, and Interfacial Tension with Water, σ/kg·s^{-2}, at 293 K for Water, Heptane, Methylbenzene, and Trichloroethylene

	ρ		η		S		σ	
property	kg·m^{-3}	ref	kg·m^{-1}·s	ref	mol %	ref	kg·s^{-2}	ref
water	998.15		$1.02\cdot10^{-3}$		$4.95\cdot10^{-4}$	16		
heptane	683.7	17	$0.39\cdot10^{-3}$	18	1.17	19	$51.24\cdot10^{-3}$	20
methylbenzene	866.9	21	$0.55\cdot10^{-3}$	22	7.34	19	$36.1\cdot10^{-3}$	23
trichloroethylene	1451.4	24	$0.530\cdot10^{-3}$	24			$34.5\cdot10^{-3}$	25

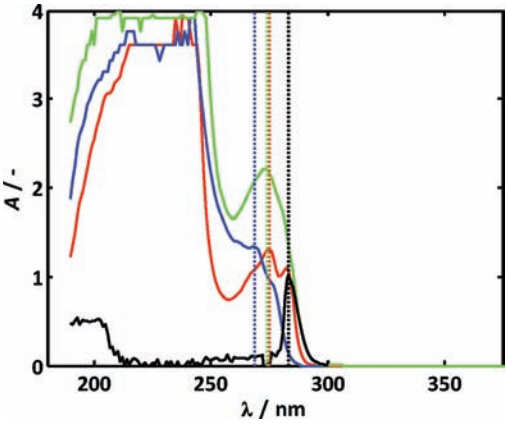

Figure 2. Typical UV–vis spectra in which the wavelength (in nm) is plotted versus the absorbance of benzoic acid in water (blue), heptane (red), trichloroethylene (green), and methylbenzene (black). The dotted lines represent the wavelengths that are selected for further measurements.

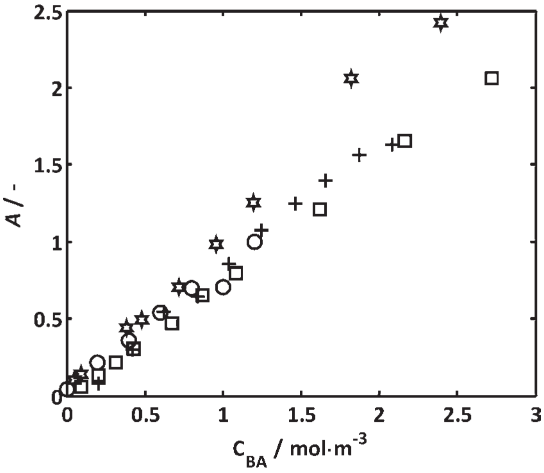

Figure 3. UV–vis calibration curves for relating the concentration of benzoic acid (C_{BA}) in □, water; ☆, heptane; ○, methylbenzene, and +, trichloroethylene to the measured absorbance, A, at 293 K (see Table 1).

at 293 K by placing them on an orbital shaker. After this mixing operation, complete phase separation was obtained by settling through gravitational force for at least 3 h. Samples were withdrawn from the settled mixtures using a $1.0\cdot10^{-6}$ m^3 Finn pipet. To achieve samples with an extinction below 2.5, all samples were diluted with a maximum factor of 20, using a $0.5\cdot10^{-6}$ m^3 Finn pipet. The benzoic acid concentration in the diluted samples was determined from the UV–vis absorption spectra. A mass balance was made for each combination of measured benzoic acid concentrations in the organic phase and the water phase. The data were omitted from the data set if the mass balance deviated more than 5 %. This way 9.1 % of the measurements was excluded from the measurements of the heptane system and 11.1 % from the methylbenzene system. For the trichloroethylene system the mass balance was constructed from the water phase concentrations only.

For the methylbenzene/water mixtures, the benzoic acid concentration was, additionally to the UV–vis measurements, determined in the aqueous phase by measuring the conductivity with a Consort K611 conductivity meter. From this aqueous phase and the initial weight amount of benzoic acid, the concentration in methylbenzene could be deduced, resulting in a set of equilibrium compositions.

3. RESULTS AND DISCUSSION

3.1. Calibration of UV–vis Equipment. UV–vis calibration results are shown for water, heptane, methylbenzene, and trichloroethylene in Figure 3. These curves were used to measure the concentrations in the diluted samples. Calibration curves for UV–vis spectroscopy had a squared correlation coefficient of 0.99 as a minimum.

3.2. Equilibrium Constants for the Heptane/Water Benzoic Acid System. The monomeric partition constant and the dimerization constant were determined for the heptane/water benzoic acid system from a set of equilibrium compositions. The prepared solutions resulted in aqueous concentrations of benzoic acid ranging from 4.0 mol·m^{-3} to 19.0 mol·m^{-3} and benzoic acid concentrations in heptane ranging from 2.0 mol·m^{-3} to 42.0 mol·m^{-3}. These values were compared with the equilibrium data from physically similar systems, hexane and dodecane,[8,9] and are plotted as a function of the total concentration in the water phase in Figure 4.

Benzoic acid distribution between water and heptane was studied by Berthod et al.,[10] for buffered acidity ranging from pH = 1 to pH = 7 at 303 K. They do not report the monomeric partition constant for nonbuffered equilibrium mixtures and do not report the accuracy of the measured concentrations. For their calculations they use the dimerization constant of benzoic acid in heptane at 303 K reported by Kubista et al.,[3] K_D = 15.9 mol·m^3. The measured equilibrium curve of the water/heptane system is located in between the equilibrium curves of the water/hexane system and the water/dodecane system, both reported by Long.[8,9] The measured concentrations in the water and organic phase are used to calculate the adjusted partition constant, K_P^{ADJ}, as defined by eq 7. In Figure 5, K_P^{ADJ} is shown as a function of the concentration of nondissociated benzoic acid. A linear curve is found with a positive intercept on the y-axis, as predicted by eq 7. A least-squares fit of eq 7 to the data in Figure 5 gives the K_D and K_P^{MON} values given in Table 2, including the 95 % confidence intervals.

Comparing the equilibrium constants of the various *n*-alkane systems in Table 2 shows that the uncertainty[11,12] ($k = 2$) in both K_P^{MON} and K_D for the heptane/water benzoic acid system are at least twice as narrow and thus that the accuracy of K_P^{MON} and K_D is higher. Also it can be seen that the monomeric partition constant seems to be in the same order of magnitude, which was also expected, since the physical properties of all three systems are rather similar.

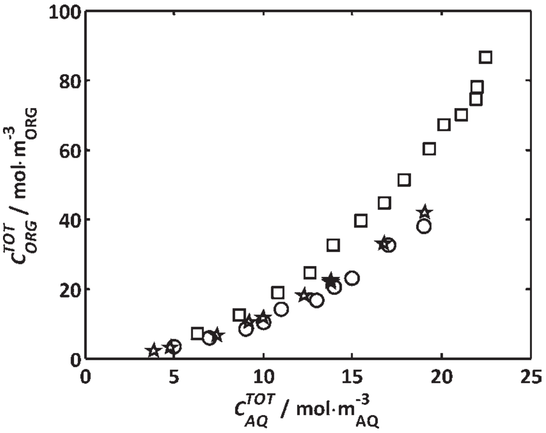

Figure 4. Total concentration of benzoic acid in the aqueous phase versus the total concentration in ☆, heptane; ○, hexane; and □, dodecane at 293 K (see Table 1). The measured concentrations for the heptane and the hexane system[9] are almost similar; dodecane[8] has somewhat higher concentrations in the organic phase.

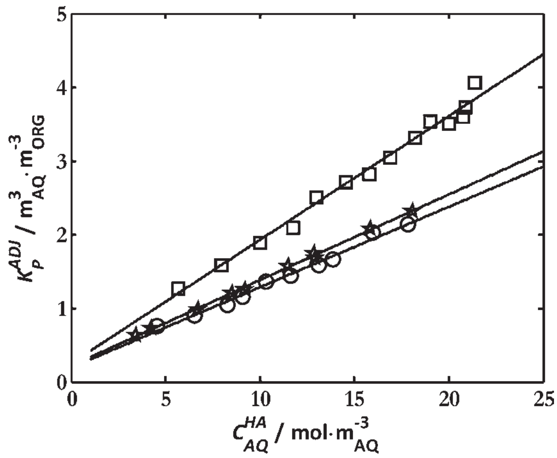

Figure 5. Adjusted partition constant as a function of the nondissociated benzoic acid concentration in the aqueous phase at 293 K (see Table 1). A linear trend is observed for □, dodecane; ○, hexane; and ☆, heptane. The fitted linear correlations of eq 7 are indicated by the lines. The fitted parameters are given in Table 2.

3.3. Equilibrium Constants for the Methylbenzene/Water Benzoic Acid System.

The prepared solutions of the methylbenzene/water benzoic acid system resulted in aqueous concentrations of benzoic acid ranging from 4.0 mol·m^{-3} to 21.0 mol·m^{-3} and benzoic acid concentrations in methylbenzene ranging from 20 mol·m^{-3} to 450 mol·m^{-3}. The measured concentrations for methylbenzene and the concentrations from literature are plotted as a function of the total concentration in the water phase in Figure 6.

The first to publish the equilibrium concentrations were Schilow and Lepin.[13] By titration they determined the equilibrium for five different samples over most of the solubility range for the aqueous phase. Fujii et al. studied the solvent effect on dimerization of benzoic acid.[14] They acidified the aqueous solution with perchloric acid to prevent acid dissociation and determined the concentration in both phases by potentiometric titration with sodium hydroxide. The counter-current extraction of benzoic acid from water, as the continuous phase, to methylbenzene, as the discontinuous phase, and vice versa was reported

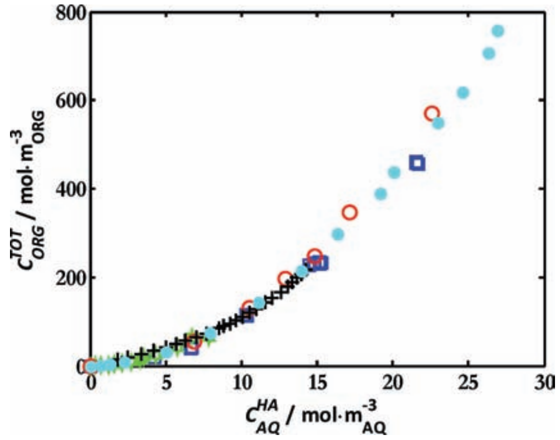

Figure 6. Total concentration of benzoic acid in the aqueous phase versus the total concentration in methylbenzene at 293 K (see Table 1). Both UV–vis based (□) and conductivity based (☆) experiments are shown. Experimental data from ○, Schilow and Lepin;[13] ●, Fujii et al.;[14] and +, Appel and Elgin[15] are also given.

Table 2. Least-Squares Fitted Monomeric Partition Constant, K_P^{MON}/m$^3_{AQ}$·m$^{-3}_{ORG}$, and Dimerization Constant, K_D/m^3·mol^{-1}, in eq 7 for Systems with Dodecane, Hexane, Heptane, Methylbenzene, and Trichloroethylene as the Organic Phase and Their Uncertainties for k = 1.984[11,12]

		T	K_P^{MON}	K_D
solvent	ref	K	m$^3_{AQ}$·m$^{-3}_{ORG}$	m^3·mol^{-1}
dodecane	Long et al.[8]	293	(0.243 ± 0.199)	(1.42 ± 2.54)
hexane	Long[9]	293	(0.185 ± 0.119)	(1.60 ± 2.21)
heptane	this work, UV–vis	293	(0.209 ± 0.049)	(1.33 ± 0.67)
methylbenzene	Schilow and Lepin[13]	293	(1.47 ± 1.72)	(0.28 ± 0.67)
methylbenzene	Fujii et al.[14]	298	(1.15 ± 1.07)	(0.30 ± 0.04)
methylbenzene	this work, UV–vis	293	(1.17 ± 0.92)	(0.39 ± 0.64)
methylbenzene	this work, conductivity	293	(1.33 ± 0.85)	(0.33 ± 0.47)
trichloroethylene	this work, UV–vis	293	(0.808 ± 0.295)	(1.18 ± 0.89)

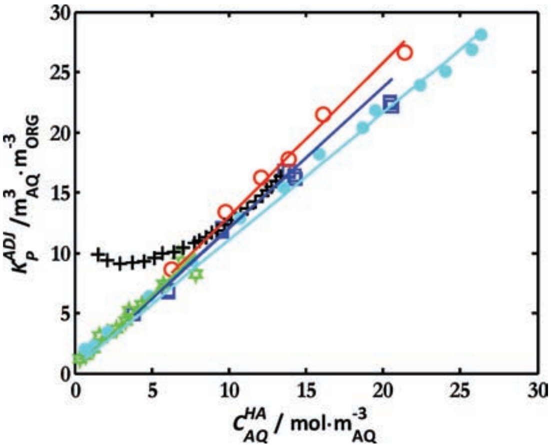

Figure 7. Adjusted partition constant as a function of the nondissociated benzoic acid concentration in the aqueous phase at 293 K (see Table 1). Both UV−vis based (☐) and conductivity based (☆) experiments are shown. Experimental data from ○, Schilow and Lepin;[13] ●, Fujii et al.;[14] and +, Appel and Elgin[15] are also given. The fitted parameters are given in Table 2.

by Appel et al.[21] For these experiments they determined the equilibrium composition for 287.5 K, 292 K, and 297 K. Their experimentally determined partition constant was reported as a "closely linear function of the water phase", which is noticeable since the data in Figure 6 (with the results at 292 K) show a clear nonlinear behavior. In their publication a trend of the compositions is shown, instead of single point measurements, which makes interpretation ambiguous. Figure 7 shows the nonlinear correlation between the nondissociated benzoic acid concentration in the water phase and the adjusted partition constant. Table 2 shows the least-squares fitted equilibrium constants in eq 7 that give the lines in Figure 7 for the methylbenzene/water benzoic acid system, with their 95 % confidence intervals.

Comparing the equilibrium constants for the methylbenzene/water benzoic acid system, from the previous studies with the current study (Table 2), shows that the UV−vis spectroscopy-based method gives a monomeric partition constant which is comparable to the values that were determined before: the 95 % confidence interval for the UV−vis based monomeric partition constant is 14 % smaller when compared to that of Fujii et al.[14] and 50 % smaller when compared to Schilow and Lepin.[13] The constant that was measured using conductivity is somewhat higher as found by UV−vis and has an even smaller confidence interval.

The dimerization constant found from the UV−vis measurements is 16 % higher when compared to the conductivity-based result, 29 % higher to the values reported by Schilow and Lepin,[13] and 22 % with the dimerization constant identified by Fujii et al.[14] Measurements at low concentrations of Appel and Elgin,[15] show different behavior when compared to the other measurements as is shown in Figure 7 and are therefore not fitted with eq 7. Therefore, the parameters that fit the measurements from Appel and Elgin were omitted from Table 2.

3.4. Equilibrium Constants for Trichloroethylene/Water Benzoic Acid System.

The prepared solutions for the trichloroethylene/water system resulted in aqueous concentrations of benzoic acid ranging from 4.0 mol·m^{-3} to 15.0 mol·m^{-3} and benzoic acid concentrations in trichloroethylene ranging from 0.02 mol·m^{-3} to 32 mol·m^{-3}. The measured benzoic acid concentrations in trichloroethylene are plotted as a function of the total concentration in the water phase in Figure 8. The linear correlation yielding the equilibrium constants is plotted in Figure 9. The monomeric partition constant and the dimerization constant of benzoic acid in the water/trichloroethylene have not been published before.

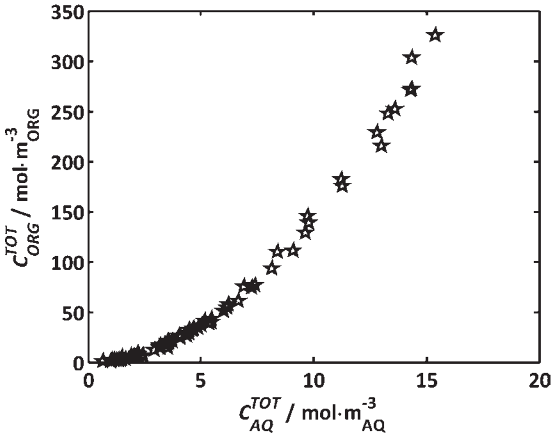

Figure 8. Total concentration of benzoic acid in the water phase versus the total concentration in the trichloroethylene phase at 293 K (see Table 1).

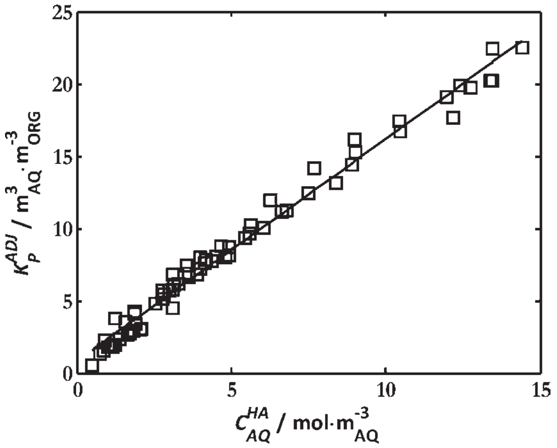

Figure 9. Adjusted partition constant, K_P^{ADJ}/m$^3_{AQ}$·m$^{-3}_{ORG}$, as a function of the nondissociated benzoic acid concentration in the aqueous phase at 293 K (see Table 1). The fitted parameters are given in Table 2.

3.5. Reproducibility and Usage.

For the methylbenzene/water system and the heptane/water system the UV−vis measurement was omitted from the data set if the mass balance deviated more than 5 %. Less than 12 % of the measurements was omitted. The narrow 95 % confidence interval shows that measurements are well-reproducible. The measured concentrations for the UV−vis calibration curves ranged from 0.1 mol·m^3 to the maximum solubility of benzoic acid for the given mixture. The reproducibility at the lowest measured concentrations was within 3 % for a three-fold measurement for all three extraction systems. This accuracy at low concentrations illustrates that, for UV-active solutes, UV−vis is a suitable analysis method which allows for in situ monitoring liquid−liquid extraction processes.

With the monomeric partition constant and the dimerization constant known, these novel extraction systems now are applicable to study liquid−liquid mass transfer rates. For this purpose two liquids are intensely contacted in a multiphase reactor, like a packed column, microreactor, or rotor-stator spinning disk reactor. In such reactors the benzoic acid will partition between the two phases. Only the nondissociated monomeric species are able to partition between water and the organic phase. The concentrations involved in the liquid−liquid mass transfer process can be calculated from the total concentrations at the reactor outlet using K_D and K_A. With K_P^{MON} known, the overall mass transfer rate can then be calculated. These mass transfer rates allow for a comparison of reactor performance, together with equipment volume, processing time, and energy input. In this way the most appropriate multiphase reactor can be selected for a given process.

4. CONCLUSIONS

The monomeric partition constant, K_P^{MON}, and the dimerization constant, K_D, for the organic phase are presented for benzoic acid in water and three different organic phases: heptane, methylbenzene, and trichloroethylene at 293 K. For the heptane/water benzoic acid system, K_P^{MON} equals $(0.209 \pm 0.049)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(1.33 \pm 0.68)\ m^3 \cdot mol^{-1}$. For the methylbenzene/water benzoic acid system, K_P^{MON} equals $(1.17 \pm 0.92)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(0.39 \pm 0.64)\ m^3 \cdot mol^{-1}$. For the trichloroethylene/water benzoic acid system, K_P^{MON} equals $(0.808 \pm 0.295)\ m^3_{AQ} \cdot m^{-3}_{ORG}$, and K_D equals $(1.18 \pm 0.89)\ m^3 \cdot mol^{-1}$. Equilibrium constants were obtained from UV−vis and conductivity experiments. The results of the heptane system were validated by comparing with physically similar systems. The results for the methylbenzene system were validated by comparison with existing literature. With the monomeric partition constant and the dimerization constant known, these novel extraction systems now are applicable to study mass transfer rates, by means of UV−vis spectroscopy. This allows for easy and fast measurements, with the option of in situ measurements for counter current equipment. The equilibrium data of these extraction systems can be used to quantify liquid−liquid mass transfer rates by using extraction systems that require low flammability risk (trichloroethylene) and low costs (methylbenzene) or setups constructed from polymethyl methacrylate (heptane).

■ ASSOCIATED CONTENT

Ⓢ Supporting Information. Data of the heptane/water benzoic acid (Table 3), methylbenzene/water benzoic acid (Table 4), and trichloroethylene/water benzoic acid (Table 5) systems. This material is available free of charge via the Internet at http://pubs.acs.org.

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