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Determination of the Octanol−Air Partition Coefficients (K_{OA}) of Fluorotelomer Alcohols

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Octanol−air partition coefficients (K_{OA}) for five fluorotelomer alcohols (4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH, and for the first time 12:2 FTOH) were determined over a temperature range from (5 to 40) °C using a modified generator column method. Octanol-saturated air at a fixed temperature was blown over a column filled with glass spheres which were coated with an FTOH solution. FTOHs partitioning to the gas phase were collected on a trap filled with XAD-2 and eluted with acetone afterward. The concentrations of FTOH were measured by GC-MS using positive chemical ionization. The K_{OA} values were calculated as the ratio of the FTOH concentrations in the octanol to the FTOH concentrations in the air. Values of log K_{OA} at 25 °C ranged from 4.5 (4:2 FTOH) to 6.2 (12:2 FTOH). The calculated internal energies of phase change (ΔU_{OA}) ranged from 42.8 $kJ \cdot mol^{-1}$ (12:2 FTOH) to 61.1 $kJ \cdot mol^{-1}$ (4:2 FTOH). The combined uncertainty of the method applied ranged from 8.3 % (4:2 FTOH) to 10.5 % (10:2 FTOH). The expanded uncertainty ($P = 95$ %) ranged from 18.7 % (4:2 FTOH) to 38.7 % (10:2 FTOH), respectively.

Introduction

The recent determination of nonvolatile, highly persistent perfluoroalkyl carboxylic acids (PFCAs) in the fauna of pristine regions,[1–5] in Arctic snow,[6] and the observation of fluorotelomer alcohols (FTOHs) in air[7–12] strengthened the hypothesis that FTOHs are volatile precursors of PFCAs which degrade during or after transport to the persistent perfluorinated acids.[13]

Fluorotelomer alcohols are a class of linear, long-chain, polyfluorinated alcohols. FTOHs determined in this study have the generic structure $CF_3(CF_2)_nCH_2CH_2OH$, where n is 3, 5, 7, 9, or 11. Designating the number of perfluorinated carbon atoms (X) and nonsubstituted methylene groups (Y), the FTOHs are often referred to as X:Y FTOHs. Exact data describing the physical-chemical properties of FTOHs are needed to model their atmospheric distribution and transport behavior because these are governed by the compounds' properties.[14] The octanol−air partition coefficient (K_{OA}) is recognized as a key descriptor of a chemical's partitioning between the atmosphere and organic phases such as organic films on aerosols, organic carbon in soil, the waxy cuticle, or lipid portions of vegetation.[15–25]

The K_{OA} is the ratio of the solute concentration in octanol (c_O) to its concentration in air (c_A) when the octanol−air system is at equilibrium. There are different ways to determine the K_{OA}: First, by computer models using quantitative structure–property relationships (QSPRs). However, these models are often not able to take into account the unique FTOH behavior caused by the strong C−F bond and intramolecular bonds to the molecule's OH group.[26,27] Second, by gas chromatographic methods, which compare retention times of the compounds of interest to that of a standard reference compound. Gas chromatographic methods often underestimate K_{OA} values because the nonpolar stationary phase of the column used cannot form hydrogen bonds with the compounds as the octanol does.[28] Third, by the dynamic generator column method as developed by Harner and Mackay.[29] This method determines the K_{OA} directly by using octanol-saturated air at a fixed temperature which is blown over a glass wool packed column. The wool is coated with a solution of compounds in octanol. The flow and volume of the air are optimized to ensure equilibrium-like conditions. Chemicals that partitioned to the gas phase are collected on an adsorbent trap and eluted afterward. The octanol mixing is considered to be partial, and the mass transfer coefficient (MTC) is considered to be finite. The measurement of a chemical's concentration in air over experimental time results in a curve that reaches a plateau after a certain time. At this plateau, the concentration in the air and in the octanol are supposed to be at equilibrium, and the K_{OA} can be calculated as a ratio of c[FTOH (liq. soln, cO)]/c[FTOH (g soln, cA)] or short c_O/c_A.[29]

In this study, we modified and improved the generator column method. Octanol−air partition coefficients and the internal energies of phase change (ΔU_{OA}) of five FTOHs (4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH, and for the first time 12:2 FTOH) were determined.

Experimental

Instrumental Setup. The setup used in this study was similar to the generator column method developed by Harner and Mackay.[29] Instead of glass wool, glass spheres were used, and the experiments were done without an octanol trap.

The apparatus for the K_{OA} determination consisted of two 12 cm × 1 cm water-jacketed glass columns and a third glass column of 12 cm × 1 cm (Figure 1). The first column contained 2 g of Amberlite XAD-2 resin (Supleco, Munich, Germany, cleaned with acetone/dichloromethane 2:1 v/v using Soxhlet extraction) and glass spheres coated with 100 μL of octanol (99.5 %, Sigma Aldrich, Steinheim, Germany). The XAD-2 trapped potential contaminants within the compressed synthetic air (20.5 % O_2 in N_2, Messer GmbH, Krefeld, Germany) flowing

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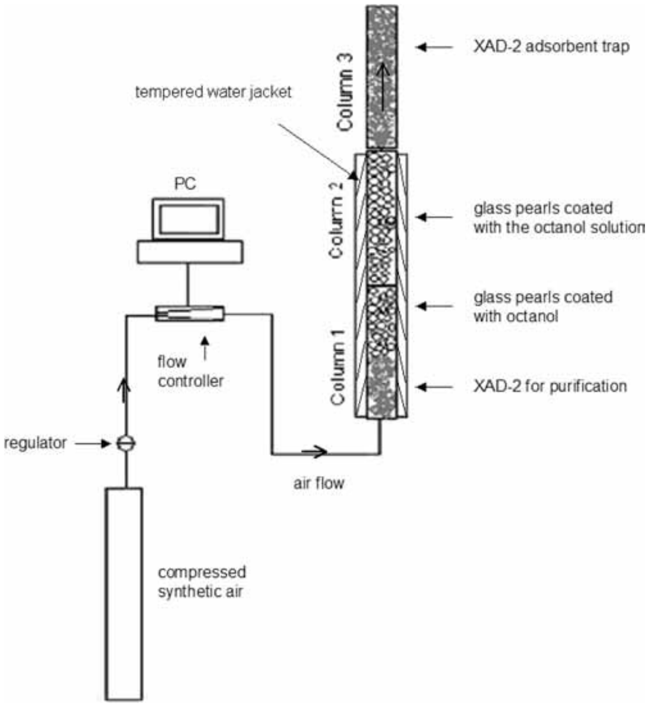

Figure 1. Instrumental setup for the determination of octanol−air partition coefficients used in this study. Explanations are within the text.

Table 1. Volumes of Synthetic Air Used for the Determination of the FTOH K_{OA} Values at Different Temperatures

air temperature °C	air volume L
5	5
10	4
15	3
20	2
25	1
30	0.75
35	0.5
40	0.2

through the system, and the octanol saturated the synthetic air. The second column contained glass spheres which were coated with a solution of five FTOHs in octanol (see below). The first and second columns were inside a circulated water bath (RTE 111, Thermo NESLAB, Karlsruhe, Germany) to ensure constant temperatures in the range of [(5 to 40) ± 0.1] °C. The third column filled with 4 g of XAD-2 was fixed on top of the second column to trap the FTOHs partitioned to the gas phase. The columns were connected by their ground spherical ball joints and fixed tightly by joint clips. The gas pipes were of copper and fixed by Swagelok connections.

The synthetic air passed through a regulator and a computer-controlled flow controller (EL-FLOW digital, Bronkhorst Mättig, Unna, Germany). Air flow and volume had been optimized by previous equilibrium tests. To ensure that the FTOH residence time was sufficiently high to establish equilibrium conditions, a flow of 0.05 $L\cdot min^{-1}$ was chosen. The volumes used for determination of the K_{OA} of 4:2 FTOH to 12:2 FTOH over a temperature range from (5 to 40) °C are shown in Table 1.

Analytical Procedure. An amount of 300 μL of a standard solution (200 $ng\cdot\mu L^{-1}$) containing 1*H*,1*H*,2*H*,2*H*-perfluorohexan-1-ol (4:2 FTOH, 97 %, Sigma Aldrich, Steinheim, Germany), 1*H*,1*H*,2*H*,2*H*-perfluorooctan-1-ol (6:2 FTOH), 1*H*,1*H*,2*H*,2*H*-perfluorodecan-1-ol (8:2 FTOH), 1*H*,1*H*,2*H*,2*H*-perfluorododecan-1-ol (10:2 FTOH), and 1*H*,1*H*,2*H*,2*H*-perfluorobutadecan-1-ol (12:2 FTOH) (all 97 %, Lancaster Synthesis, Frankfurt a.M., Germany) in octanol was added to the second column. The column was shaken for 1 min to ensure good dispersion. An amount of 200 μL of a solution ($c = 5$ $ng\cdot\mu L^{-1}$) containing 1*H*,1*H*,2*H* -perfluorooctan-1-ol (7:1 FA, 97 %), 1*H*,1*H*,2*H*-perfluorodecan-1-ol (9:1 FA, 98 %), 1*H*,1*H*,2*H*-perfluorododecan-1-ol (11:1 FA, > 90 %), and 1*H*,1*H*,2*H*-perfluorobutadecan-1-ol (13:1 FA, 96 %) (Lancaster Synthesis, Frankfurt a.M., Germany) in acetone was added as the internal standard (IS) to the top of the third column. The column was eluted with 50 mL of acetone (picograde, 99.0 %, Promochem,Wesel, Germany) in the direction opposite to the gas flow. The solvent volume was reduced to 4 mL using a rotary evaporator (Büchi, Flawil, Switzerland) and further concentrated to 200 μL with a gentle stream of nitrogen (Barkey, Leopoldshöhe, Germany). An amount of 50 μL of hexachlorobenzene (HCB, 99.5 %, Dr. Ehrenstorfer GmbH, Augsburg, Germany) in acetone ($c = 5$ $ng\cdot\mu L^{-1}$) was added as an injection standard prior to the measurement.

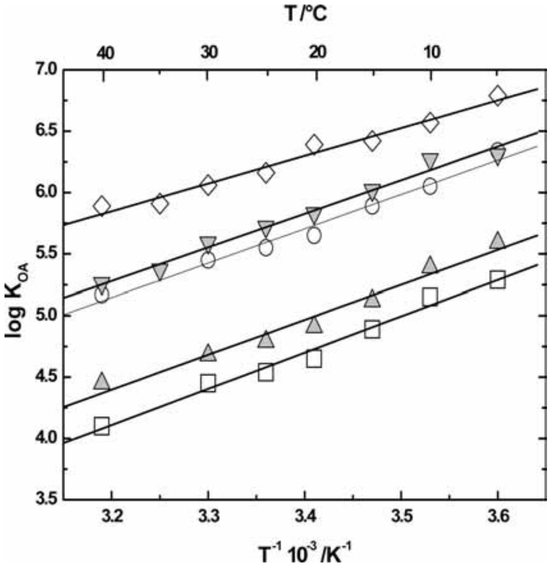

Figure 2. Log K_{OA} values of 4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH, and 12:2 FTOH at temperatures from (40 to 5) °C expressed as T^{-1}/K. □, 4:2 FTOH; ▲, 6:2 FTOH; ○, 8:2 FTOH; ▼, 10:2 FTOH; ◇, 12:2 FTOH.

FTOHs were measured using a GC-MS (6890 GC, 5973 MSD, Agilent Technologies, Waldbronn, Germany) in positive chemical ionization mode (PCI) with methane as the reactant gas. Gas chromatographic separation was performed using the parameters of Jahnke et al.[30]

Recoveries. Average recoveries of FTOHs after the elution of XAD-2 were determined at different concentration levels from (0.5 to 5) $ng\cdot\mu l^{-1}$ ($n = 6$). 7:1 FA was used to correct 4:2 FTOH, 6:2 FTOH, and 8:2 FTOH; 9:1 FA was used for the correction of 10:2 FTOH; and 13:1 FA was used for the correction of 12:2 FTOH. Because the recovery behavior of the internal standards differed slightly but constantly from that of the FTOH, a deviation factor was introduced as a correction factor accounting for these differences (see Supporting Information). Average recoveries after the XAD-2 extraction ranged from 67 % (4:2 FTOH) to 125.3 % (8:2 FTOH), and average corrected recoveries ranged from 97.2 % (12:2 FTOH) to 99.9 % (4:2 FTOH). Signal enhancement at low concentration levels was observed for FTOH of C10 and larger.

Combined Uncertainty of the Method. The combined uncertainty of the entire method for the determination of K_{OA} values at 25 °C of FTOH was calculated according to guidelines in

Table 2. Calculated log K_{OA} (log K_{OA} cal.) at 25 °C, Regression Constants (*a*, *b*), Regression Coefficients (*r*), and the Internal Energy of Phase Transfer (ΔU_{OA}) of 4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH, and 12:2 FTOH

compound	log K_{OA} cal. at 25 °C	*a*	*b*	*r*	ΔU_{OA} kJ·mol^{-1}
4:2 FTOH	4.57 ± 0.55	−5.33 ± 0.55	2949 ± 0.16	0.980	54.0 ± 0.55
6:2 FTOH	4.84 ± 0.71	−4.70 ± 0.71	2842 ± 0.21	0.976	52.0 ± 0.71
8:2 FTOH	5.58 ± 0.60	−3.79 ± 0.60	2792 ± 0.18	0.985	51.1 ± 0.60
10:2 FTOH	5.71 ± 0.47	−3.48 ± 0.47	2736 ± 0.14	0.993	50.1 ± 0.47
12:2 FTOH	6.20 ± 0.49	−1.38 ± 0.49	2259 ± 0.14	0.989	41.4 ± 0.49

GUM and EURACEM/SITAC.[31,32] It ranged from 8.3 % (4:2 FTOH) to 10.5 % (10:2 FTOH). 21.1 % of the uncertainty resulted from the impurities of the compounds used, 54.7 % from the GC-MS measurement, and 21.8 % from the uncertainty of the internal quantification. A t-distribution with a 95 % confidence interval was anticipated. Hence, the extended uncertainty (P = 95 %) ranged from 18.7 % (4:2 FTOH) to 38.7 % (10:2 FTOH), respectively.

Calculation of K_{OA} Values and ΔU_{OA}. The experimental K_{OA} at a fixed temperature was calculated as $K_{OA} = c_O/c_A = (c_OT_1)/(m_AVT_2)$, where c_O is the FTOH concentration in octanol; m_A is the calculated and recovery corrected FTOH mass in air; V is the volume of synthetic air before it enters the heated columns; T_1 is the temperature of synthetic air before it enters the heated column; and T_2 is the temperature of synthetic air in the column. The FTOH concentration in octanol is assumed to remain constant because partitioning into the air phase occurs very slowly.[28] However, it was ensured that less than 10 % of the compounds' mass was lost due to partitioning to the gas phase. Two K_{OA} values of FTOH were determined for each temperature. Each sample was measured twice and averaged afterward. The experimental data were regressed using the equation: log $K_{OA} = a + b/T = a + \Delta U_{OA}/2.303RT$, where a and b are the regression constants and T is the temperature. Regression parameters and errors were calculated using OriginPro 7.5. The temperature coefficient was expressed as an internal energy of phase change ΔU_{OA} (J·mol^{-1}), where R is the ideal gas constant.[29]

Quality Assurance. All experiments were performed in a clean laboratory (class 10.000). Perfluorinated materials or fluorinated polymers were avoided in the apparatus used and during chemical analysis. The glassware was machine-washed, heated at 250 °C for 12 h, and washed twice with acetone prior to use. Standard solutions were used at room temperature. Prior to use they were held in the ultrasonic bath for a short time. Glass adsorption of analytes was excluded by comparing K_{OA} values determined with the setup described above to those using silanized glass spheres in the setup.

The possibility of a significant breakthrough of FTOH in the trap containing 4 g of XAD-2 was excluded by the failure to determine FTOH in an additional column placed in sequence behind column three.

Internal and injection standards were used to correct for losses and irregularities during analysis and measurement. For each compound, one target ion and two qualifier ions were measured for the correct GC-MS identification of the compounds. An eight-point calibration [(0.5 to 7) ng·μL^{-1}] was used for the quantification of the FTOH. Linearity of the GC-MS measurements was determined as described in DIN 32645[33] with a regression coefficient (r) ranging from 0.9998 (4:2 FTOH) to 0.9990 (12:2 FTOH). Calibrations were checked for linearity before each batch of measurements.

Blank samples were measured to determine possible cross contamination of the entire method. Only once, signals were found, probably due to an insufficient cleaning process of XAD-2.

Results

K_{OA} values at different temperatures for five FTOHs are shown in Figure 2. Values of log K_{OA} for FTOH decreased with increasing temperature and decreasing chain length. The slope of the regression of log K_{OA} to $1/T$ slightly decreased with increasing chain length, as did the ΔU_{OA} (Table 2).

Discussion

The octanol−air partition coefficient increased linearly with reciprocal absolute temperature because FTOHs preferentially partition to organic phases at colder temperatures. This is consistent with other compounds of environmental concern, such as polychlorinated biphenyls (PCB), perfluoroalkyl sulfonamides, and polybrominated diphenyl ethers.[11,18,22,34–36] With continuous addition of $-CF_2-$ groups, FTOHs tend to partition more preferentially to the organic phase. The log K_{OA} values determined in this study demonstrate that the FTOHs are found in the gaseous phase and thus may act as volatile precursors of the persistent perfluorinated sulfonic and carboxylic acids. These results confirm studies analyzing environmental gas and the particle phase concentrations of FTOH.[8,17] In these studies, FTOHs in the particle phase were rarely detected or quantified.

The internal energy of phase transfer decreased with decreasing compound vapor pressure (increasing K_{OA}) and decreased with increasing FTOH chain length. This is unusual and in contrast to other studies in which enthalpies of phase transfer were determined for FTOH.[37,38] Treves et al.[39] observed decreasing enthalpies of phase transfer with increasing carbon chain length for two δ-hydroxy alkyl nitrates and explained this fact with different solubilities of the compounds in octanol. Maybe the influence of the FTOH's OH group is reduced by the addition of $-CF_2-$ groups similarly, leading to a smaller degree of free contact of $-OH$ to octanol and thus to a decreased compound solubility in octanol. This would also explain the difference between data of Lei et al.[37] and Krusic et al.,[38] who used the GC retention time method instead of the generator column method with octanol to calculate the octanol−air partition coefficient and the internal energy of phase transfer. Effects of interactions of FTOH with octanol were thus not accounted for. Further research is needed with respect to the FTOH's internal energies of phase transfer. Solubility of FTOH in octanol should be determined to clarify this point.

Plots of log K_{OA} values to the number of carbon atoms should result in parallel curves for homologous compound classes, because homologues grow by the same molecular fragment (in this case $-CF_2-$). The identical increment added to the overall interaction energy has thus the same influence on the slope of this plot and often serves as a quality indicator for the observed data.[28] In the case of FTOH, the unavailability of homologous

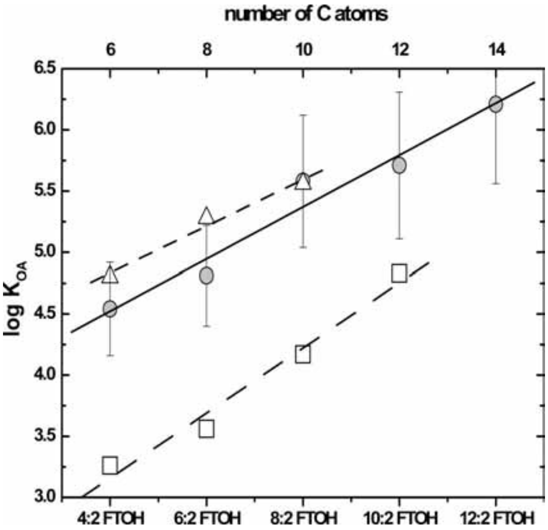

Figure 3. Calculated log K_{OA} values for FTOHs of different chain lengths at 25 °C in comparison to those of ref 28 and ref 37. Error bars show the combined uncertainty of this study's measured K_{OA} values. ■, ref 37; ●, this study; △, ref 28.

compound classes hinders this comparison and quality check of log K_{OA} values. Further research is urgently needed in this field.

Calculated K_{OA} values for FTOH at 25 °C were compared to K_{OA} values determined by Lei et al.[37] and Goss et al.[28] as shown in Figure 3.

The slope of the regression curve resulting from the plot of log K_{OA} values to the number of C-atoms in this study differed from that of Lei et al.[37] and, less pronounced, from that of Goss et al.[28] Lei et al.[37] determined lower K_{OA} values compared to this study and thus observed a lower intercept. The log K_{OA} values published by Lei et al.[37] were calculated by the comparison of GC retention times of HCB to FTOH using a nonpolar DB-1 capillary column. Because the octanol used in our study acts as an H-donor and H-acceptor, FTOH molecules are able to form H-bonds. However, FTOH cannot form H-bonds with the nonpolar stationary phase of the DB-1 column leading to an underestimation of the K_{OA}.[28] Of these three studies, Goss et al.[28] published the highest log K_{OA} values which leads to the highest intercept of the three curves shown. However, K_{OA} values were only determined for 4:2 FTOH, 6:2 FTOH, and 8:2 FTOH at three temperatures. Because Goss et al.[28] used the generator column method described by Harner and Mackay[29] and thus a method very similar to that of our study, other methodological differences might explain the observed discrepancy. The presence or absence of internal and injection standards, the number of repetitions, and/or the temperature intervals at which K_{OA} values were determined might be responsible for the observed differences. Taking the uncertainty of the methods for the determination of octanol−air partition coefficients into account, K_{OA} values published by Goss et al.[28] are still in the range of the uncertainty of our K_{OA} values, whereas those of Lei etal.[37] are out of this range. Overall, the octanol−air partition coefficients and internal energies of phase change determined in this study are reliable and present a good base for models describing the distribution of FTOH in the environment.

Supporting Information Available:

Information on the determination of instrumental settings and calculation of log K_{OA}. This material is available free of charge via the Internet at http://pubs.acs.org.

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