Determination of Octanol−Air Partition Coefficients (K_{OA}) of Fluorotelomer Acrylates, Perfluoroalkyl Sulfonamids, and Perfluoroalkylsulfonamido Ethanols

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Octanol−air partition coefficients (K_{OA}) for three fluorotelomer acrylates (6:2 FTA, 8:2 FTA, 10:2 FTA), two perfluoroalkyl sulfonamides (*n*-methyl perfluorooctane sulfonamide (MeFOSA), *n*-ethyl perfluorooctane sulfonamide (EtFOSA)), and two perfluoroalkyl sulfonamido ethanols (*n*-methyl perfluorooctane sulfonamido ethanol (MeFOSE), *n*-ethyl perfluorooctane sulfonamido ethanol (EtFOSE)) were determined over a temperature range from (278 to 313) K using a modified generator column method. The K_{OA} values were calculated as the ratio of the target analyte concentrations in octanol to the target analyte concentrations in octanol saturated air. Calibrated log K_{OA} values at 298 K ranged from 4.5 (6:2 FTA) to 6.7 (EtFOSE). Log K_{OA} values decreased with increasing temperature and increased in the order of 6:2 FTA, 8:2 FTA, 10:2 FTA, MeFOSA, MeFOSE, EtFOSA, EtFOSE. The combined uncertainty of the method applied ranged from 5.1 % (6:2 FTA) to 17.6 % (MeFOSA). The relative extended uncertainty ($P = 95$ %) ranged from 11.6 % (6:2 FTA) to 39.8 % (MeFOSA), respectively.

Introduction

Nonvolatile, bioaccumulative, and highly persistent perfluoroalkyl carboxylates (PFCA) and sulfonates (PFSA) have been determined in the fauna of pristine regions.[1−4] Their occurrence in Arctic snow[5] as well as observations of volatile fluorotelomer alcohols (FTOH), fluorotelomer acrylates (FTA), perfluorinated alkyl sulfonamides (FOSA), and sulfonamido ethanols (FOSE) in air[6−9] strengthen the hypothesis that atmospheric transport of volatile polyfluorinated compounds (PFC) and breakdown to the persistent acids is an important pathway of global PFCA and PFSA distribution.[10−14]

The worldwide occurrence of PFC recently increased the interest to predict the environmental fate and transport of these compounds. One key descriptor to model atmospheric distribution and transport behavior is the octanol−air partition coefficient (K_{OA}) assessing the 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.[15−20] Octanol−air partition coefficients have been determined by different methods for FTOH in several studies.[21−25] However, there is only little information on K_{OA} values for FOSA and FOSE[24,26] and none for fluorotelomer acrylates.

The aim of this study was to determine K_{OA} values and the internal enthalpies of phase change (ΔH_{OA}) of seven volatile polyfluorinated compounds (6:2 FTA, 8:2 FTA, 10:2 FTA, MeFOSA, EtFOSA, MeFOSE, EtFOSE) over a temperature range from (278 to 313) K using a modified generator column method.

Experimental Section

Instrumental Setup. The setup used in this study was the same as described by Thuens et al.[25] Briefly, the apparatus for the K_{OA} determination consisted of two water-jacketed glass columns and a third glass column. The first column contained 2 g of cleaned Amberlite XAD-2 resin (Supelco, Munich, Germany) to trap potential contaminants and glass spheres coated with 100 μL octanol (99.5 %, Sigma Aldrich, Steinheim, Germany) to saturate the air with octanol. The second column contained glass spheres which were coated with a solution of three FTA or four FOSA/FOSE in octanol (Table 1). The first and the second column were attached to the circulated water bath (RTE 111, Thermo NESLAB, Karlsruhe, Germany) to ensure constant temperatures in the range from (278 to 313) K ± 0.1 K. Compounds partitioned to the gas phase were trapped onto the third column which was filled with 4 g of XAD-2 and fixed on top of the second column. The synthetic air (20.5 % O_2 in N_2, Messer GmbH, Krefeld, Germany) flowing through the system was regulated by a computer-controlled flow controller (EL-FLOW digital, Bronkhorst Mättig, Unna, Germany). Prior to the determination of K_{OA} values, air volumes were optimized by previous equilibrium tests. To ensure that the target compounds' residence times were sufficiently high to establish equilibrium conditions, a flow of 0.05 $L\cdot min^{-1}$ was chosen. The volumes in dependence of temperature used for determination of the K_{OA} of FTA, FOSA, and FOSE are presented in Table SI6 (Supporting Information).

Analytical Procedure. Octanol−air partition coefficients of FTA and FOSA/FOSE were determined separately. An amount of 300 μL of standard solution I (6:2 FTA, 8:2 FTA, and 10:2 FTA) or II (MeFOSA, EtFOSA, MeFOSE, EtFOSE) in octanol, 200 $ng\cdot\mu L^{-1}$ each, was added to the second column. The column was shaken for 1 min to ensure good dispersion. After the partitioning of the compounds to the gas phase at a fixed temperature and their subsequent trapping by the third column, the column was eluted with 50 mL of acetone (picograde,

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Table 1. Information on the Target Compounds[a]

acronym	full compound name	formula	CAS	*m*/*z* TI
6:2 FTA	perfluorohexyl ethylacrylate	$C_8F_{13}H_4SO_3H$	17527-29-6	419
8:2 FTA	perfluorooctyl ethylacrylate	$C_{10}F_{17}H_4SO_3H$	27905-45-9	519
10:2 FTA	perfluorodecyl ethylacrylate	$C_{12}F_{21}H_4SO_3H$	17741-60-5	619
MeFOSA	*n*-methyl perfluorooctane sulfonamide	$C_8F_{17}SO_2NH(CH_3)$	31506-32-9	514
EtFOSA	*n*-ethyl perfluorooctane sulfonamide	$C_8F_{17}SO_2NH(CH_2CH_3)$	4151-50-2	528
MeFOSE	*n*-methyl perfluorooctane sulfonamidoethanol	$C_8F_{17}SO_2NH(CH_3)CH_2CH_2OH$	24448-09-7	540
EtFOSE	*n*-ethyl perfluorooctane sulfonamido ethanol	$C_8F_{17}SO_2N(CH_2CH_3)CH_2CH_2OH$	1691-99-2	554

[a] m/z TI: mass to charge ratio of the target ion determined by mass spectrometry. Details on supplier and purity can be found in the Supporting Information.

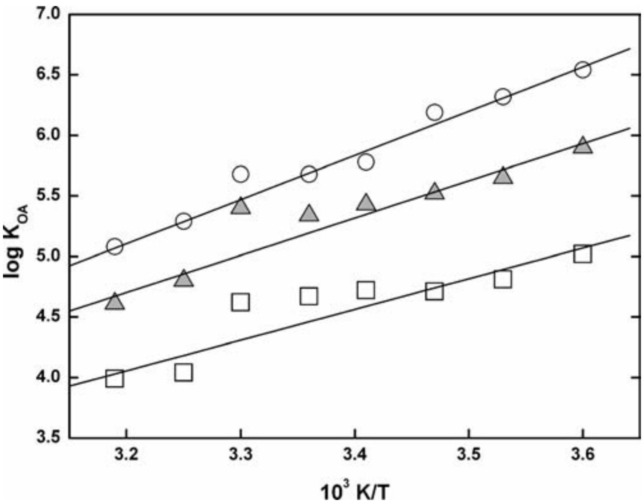

Figure 1. Mean experimental log K_{OA} values ($n = 3$) of 6:2 FTA, 8:2 FTA, and 10:2 FTA at temperatures from (278 to 313) K expressed as 10^3 K/*T*. □, 6:2 FTA; ▲, 8:2 FTA; ○, 10:2 FTA.

99.0 %, Promochem, Wesel, Germany) in the direction opposite to the gas flow. Prior to the elution, 200 μL of a solution ($c = 5$ ng$\cdot\mu$L^{-1}) containing 4:2 FTOH, 6:2 FTOH, 8:2 FTOH, MeFBSA, and MeFBSE as internal standards was added to account for losses during sample preparation. The solvent volume was reduced using a rotary evaporator (Büchi, Flawil, Switzerland) and further concentrated to 150 μL with a gentle stream of nitrogen (Barkey, Leopoldshöhe, Germany). An amount of 50 μL of trichlorobenzene in acetone ($c = 5$ ng$\cdot\mu$L^{-1}) was added as an injection standard prior to the measurement. PFC were determined by gas chromatography−mass spectrometry 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 Dreyer et al.[6]

Analyte recovery rates of the target compounds were calculated applying fluorochemicals as internal standards (see above). 4:2 FTOH was used to correct 6:2 FTA, 6:2 FTOH to correct 8:2 FTA, 8:2 FTOH to correct 10:2 FTA, MeFBSA to correct MeFOSA and EtFOSA, and MeFBSE to correct MeFOSE and EtFOSE. Average recovery rates varied between 18 % (4:2 FTOH) and 115 % (MeFBSE). To account for differences in the recovery behavior of the internal standards and the target compounds, a deviation factor was introduced as a correction factor (see Supporting Information).

Combined Uncertainty of the Method. The relative combined uncertainty of the entire method for the determination of K_{OA} values at 298 K of the target compounds was calculated according to guidelines in GUM and EURACEM/SITAC.[27,28] It ranged from 5.1 % (6:2 FTA) to 17.6 % (MeFOSA). Much of the combined uncertainty resulted from the GC−MS measurement. Anticipating a t-distribution with a 95 % confidence interval, the relative extended uncertainty ($P = 95$ %) ranged from 11.6 % (6:2 FTA) to 39.8 % (MeFOSA). The rather low uncertainties are supported by standard deviations calculated for triplicate K_{OA} determinations (Table SI4, SI5, Supporting Information). Further details on the method uncertainty are given in the Supporting Information.

Calculation of K_{OA} Values and ΔH_{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 concentration of the target compound in octanol; m_A is the calculated and recovery corrected mass of the target compound 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 concentrations of the target compounds in octanol are assumed to remain constant since partitioning into the air phase occurs very slowly.[23] K_{OA} values were determined in triplicate for each temperature. Since air concentrations were used in the calculation of the log K_{OA} values, the experimental data were regressed using the equation: $\log K_{OA} = a + b/\mathrm{T} = a + \Delta U_{OA}/2.303RT$, where a and b are the regression constants; T is the temperature; and R is the ideal gas constant.[29,30] Regression parameters and errors were calculated using OriginPro 7.5. ΔH_{OA} values were derived by $\Delta H_{OA} = \Delta U_{OA} - RT$.

Quality Assurance. All experiments were performed in a clean lab (class 10.000). Perfluorinated materials or fluorinated polymers were avoided in all laboratory utensils used for the experiments and for GC analysis. The glassware was machine-washed, heated at 250 °C for 12 h, and washed with acetone prior to use. Internal and injection standards were used to correct for losses and irregularities during extraction, volume reduction, analysis, and measurement. An eight-point calibration (0.5 ng$\cdot\mu$L^{-1} to 7 ng$\cdot\mu$L^{-1}) was used for quantification. Linearity of the calibrations was checked before each set of measurements as described by Thuens et al.[25] Breakthrough of the compounds of interest was tested by fixing a second trap on top of the actual trap. Both traps were treated equally during the experimental process. Results for breakthrough were found to be insignificant. The volumes of air used for the determination of K_{OA} values at different temperatures were thoroughly evaluated (also see Supporting Information).

Results

Log K_{OA} values at different temperatures for 3 FTA, 2 FOSA, and 2 FOSE are shown in Figures 1 and 2. Log K_{OA} values for FTA decreased with increasing temperature and decreasing chain length. The slope of the regression of log K_{OA} to $1/T$ increased with increasing chain length, as did the ΔH_{OA} (Table 3). Log K_{OA} values for FOSA and FOSE increased in the order MeFOSA, MeFOSE, EtFOSA, EtFOSE and decreased with increasing temperature. The slopes of the regressions of log K_{OA} to $1/T$ varied between the substances as did the ΔH_{OA}

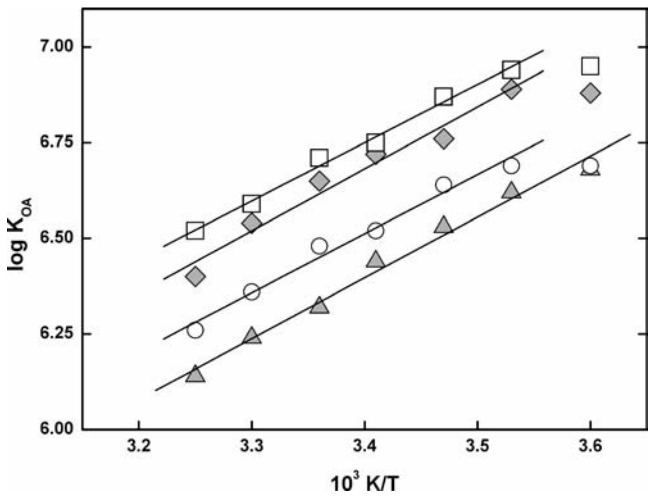

Figure 2. Mean experimental log K_{OA} values ($n = 3$) of MeFOSA, EtFOSA, MeFOSE, and EtFOSE at temperatures from (278 to 313) K expressed as 10^3 K/*T*. ▲, MeFOSA; ○, MeFOSE; ◆, EtFOSA; ●, EtFOSE. Note: the log KOA values at 313 K were not determined for this group of compounds. 278 K log K_{OA} values of MeFOSE, EtFOSA, and EtFOSE were not included in the regression analysis.

Table 2. Calculated log K_{OA} (log K_{OA} cal) at 298 K, Regression Constants (*a*, *b*), Regression Coefficients (*r*), and the Internal Enthalpy of Phase Transfer (ΔH_{OA} in kJ mol^{-1}) of 6:2 FTA, 8:2 FTA, 10:2 FTA, MeFOSA, MeFOSE, EtFOSA, and EtFOSE[a]

compound	log K_{OA} cal. T/K = 298	*a*	*b*	*r*	ΔH_{oa}
6:2 FTA	4.4 ± 1.3	−4.1 ± 1.3	2536 ± 0.4	0.903	46.1 ± 0.007
8:2 FTA	5.2 ± 0.9	−5.1 ± 0.9	3077 ± 0.2	0.933	56.4 ± 0.005
10:2 FTA	5.7 ± 0.6	−6.6 ± 0.6	3650 ± 0.2	0.984	67.4 ± 0.003
MeFOSA	6.3 ± 0.3	1.0 ± 0.3	1590 ± 0.1	0.993	28.5 ± 0.002
MeFOSE	6.4 ± 0.3	1.3 ± 0.3	1544 ± 0.1	0.991	28.0 ± 0.002
EtFOSA	6.6 ± 0.5	1.2 ± 0.5	1618 ± 0.1	0.984	27.1 ± 0.003
EtFOSE	6.7 ± 0.2	1.6 ± 0.2	1522 ± 0.1	0.996	26.7 ± 0.001

[a] Note: Errors of *a* and *b* are standard errors derived from the regression. Log K_{OA} cal and ΔH_{OA} errors are min./max. estimated values using *a* and *b* errors and the regression equation.

Table 3. Calculated log Octanol−Air Partition Coefficients at 298 K of FTA Determined in This Study and Those of FTOH Determined in Several Studies[a]

	log K_{OA} FTA (this study)	log K_{OA} FTOH (Thuens et al.[25])	log K_{OA} FTOH (Goss et al.[23])	log K_{OA} FTOH (Lei et al.[24])	log K_{OA} FTOH (Eger et al.[22])
4:2	n.a.	4.6 ± 0.5	4.8	3.3 ± 0.3	n.a.
6:2	4.4 ± 1.3	4.8 ± 0.7	5.3	3.6 ± 0.3	4.8 ± 0.2 4.8 ± 0.5
8:2	5.2 ± 0.9	5.6 ± 0.6	5.6	4.2 ± 0.3	n.a.
10:2	5.7 ± 0.6	5.7 ± 0.5	n.a.	4.8 ± 0.3	n.a.
12:2	n.a.	6.2 ± 0.5	n.a.	n.a.	n.a.

[a] n.a.: not analyzed. Note: Lei et al. used the GC retention time method to determine log K_{OA} values of FTOH which lead to lower log K_{OA} values compared to studies of Thuens et al.,[25] Goss et al.,[23] and Eger et al.[22] where an octanol phase was involved in the sampling setup.

(Table 2). Slopes and ΔH_{OA} of FOSA and FOSE were lower than those of FTA.

Discussion

As expected, the log octanol−air partition coefficients of all target compounds increased linearly with reciprocal absolute temperature showing the preferential partitioning of these PFC to organic phases at colder temperatures. This is consistent with findings for FTOH,[21,23−25] perfluoroalkyl sulfonamides,[24,26] and other compounds of environmental concern, such as polychlorinated biphenyls (PCB) and polybrominated diphenyl ethers.[17,31]

Table 4. Calculated log Octanol−Air Partition Coefficients of MeFOSA, EtFOSA, MeFOSE, and EtFOSE Determined in This and Other Studies[a]

	log K_{OA}		
compound	this study[b]	Lei et al.[24][b]	Shoeib et al.[26][b]
MeFOSA	6.3 ± 0.3	n.a.	n.a.
MeFOSE	6.4 ± 0.3	6.8 ± 0.3	7.7
EtFOSA	6.6 ± 0.5	5.9 ± 0.3	n.a.
EtFOSE	6.7 ± 0.2	7.1 ± 0.3	7.8

[a] n.a.: not analyzed. [b] At 298 K. [c] At 293 K.

Calculated log octanol−air partition coefficients of the three FTAs determined in this study were in a close range from 4.4 ± 1.3 to 5.7 ± 0.6. Taking the related errors into account, calculated log K_{OA} values for a temperature of 298 K were in the same order of magnitude as those of corresponding X:2 FTOH[22−25] (Table 3). As for the FTOH, FTA tend to partition more preferentially to the organic phase with continuous addition of $-CF_2$ groups. The log K_{OA} values determined here demonstrate that the FTA are found predominantly in the gaseous phase and thus may act as atmosphere-transported volatile precursors of the persistent perfluorinated carboxylates found in remote regions.[32] These results corroborate a study analyzing environmental gas and the particle phase concentrations of FTA.[6] In this study, FTAs were only quantifiable in the gas phase.

Calculated log K_{OA} values at 298 K of perfluorinated sulfonamides and sulfonamido ethanols ranged from 6.3 (MeFOSA) to 6.7 (EtFOSE) and hence were quite similar. Methylated substances were more volatile than their ethylated counterparts. Perfluorinated sulfonamides were more volatile than the according perfluorosulfonamido ethanols. Taking the method uncertainties into account, this studies' log K_{OA} values calculated for a temperature of 298 K were similar to those calculated by Lei et al.[24] for the same temperature but lower than those determined by Shoeib et al.[26] for a temperature of 293 K (Table 4). Octanol−air partition coefficients of perfluorinated sulfonamides and sulfonamido ethanols were up to two log units higher than those of FTA and FTOH revealing a different partitioning behavior. These findings support environmental studies in which FOSA and FOSE were quantified in the gas and particle phase of air samples.[6,7,9,33]

The internal enthalpy of phase transfer of FTA increased with decreasing compound vapor pressure (increasing K_{OA}) and increased with increasing FTA chain length. This confirms findings of tendencies of FTOH ΔH_{OA} values determined by Lei et al.[24] and is in contrast to FTOH ΔH_{OA} values determined by Thuens et al.[25] The internal enthalpies of phase transfer of FTA were significantly larger than those of FOSA and FOSE. In comparison to this study and with regard to absolute values and their corresponding errors, Lei et al.[24] and Shoeib et al.[26] determined higher ΔH_{OA} values for FOSA and FOSE. This is due to the steeper slopes of their regressions in the K_{OA}/T^{-1} plot. Maybe 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. However, since standard deviations of triplicate K_{OA} determinations and errors of ΔH_{OA} are small, this study's values appear to be reliable and will present a good base for models describing the distribution of these volatile PFC in the environment.

Supporting Information Available:

Compound information, the setup 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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