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**DETERMINATION OF n-OCTANOL/WATER PARTITION COEFFICIENTS
OF TETRACHLOROBENZYL TOLUENES INDIVIDUALLY AND IN A MIXTURE BY
THE SLOW STIRRING METHOD.**

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ABSTRACT

Experimentally obtained n-octanol/water partition coefficients (K_{ow}) are presented for nine TCBT isomers individually and in an eight isomers mixture. The K_{ow} values were determined with the slow stirring method, which can provide K_{ow} values for very hydrophobic compounds. The log K_{ow} values of isomers determined individually ranged from 6.725 to 7.538 with standard deviations between 0.089 and 0.356. The log K_{ow} values of TCBTs determined in the mixture ranged from 6.030 to 6.435 with standard deviations between 0.083 and 0.334. Reproducibility, isomer resolution and differences between mixture and individual measurements are discussed.

INTRODUCTION

Distribution of hydrophobic chemicals in the natural environment can often be described with physicochemical properties which are determined in the laboratory. The n-octanol/water partition coefficient has become a key parameter in the assessment and management of environmental effects of organic chemicals. n-Octanol is considered a surrogate for biotic lipid since these substances have rather similar polarities. K_{ow} represents an abiotic approximation to a biotic lipid/water partition coefficient (Chiou et al., 1977), which, however, is bearing a nonlinear character in the case of very hydrophobic compounds (Connell and Hawker, 1988; Hawker, 1990). Relationships are described between partition coefficients and other structural and physicochemical properties, such as water solubility (Miller et al., 1985) and organic carbon-water partition coefficients (Karickhoff, 1981). Values of K_{ow} are also required in mathematical simulation models that are used to predict

the environmental fate of organic chemicals (Mackay, 1984).

Many papers evaluate the different methods to determine the n-octanol/water partition coefficient for hydrophobic compounds (Eadsforth and Moser, 1983; Brooke et al., 1986; Doucette and Andren, 1988; De Bruijn et al., 1989; Chessells et al., 1991; Noble, 1993). In the log K_{ow} range from 2.0 to 5.5 there is little difference between the mean values of log K_{ow} determined by the different methods but major differences occur for compounds having log $K_{ow} > 5.5$.

The classical measurement for log K_{ow} is the shake flask method (OECD, 1981) where a compound is shaken in n-octanol/water. After establishment of the equilibrium the concentration is measured in one or both phases. This method can determine a range of log K_{ow} from -2.5 to 4.5 and is applicable to most classes of compounds. However, it is not suitable for compounds with high partition coefficients (log $K_{ow} > 5$) (Chessells et al., 1991). The water concentration may be inaccurate due to formation of micelles and the analytical difficulties inherent to the determination of the extremely low aqueous concentrations. Modifications of the shake flask method have been shown to overcome some of these problems for compounds having log K_{ow} values in the range in between 4.0 and 5.0 (De Voogt et al., 1988).

An easy and extensively used method of measuring the K_{ow} values is based upon reversed-phase high-performance liquid chromatography (RP-HPLC) (Opperhuizen et al., 1987; Weber et al., 1986; Rapaport and Eisenreich, 1984). To find an unknown log K_{ow} , a set of reference compounds of known log K_{ow} needs to be run under the same circumstances to find a calibrated relationship between a compound's log K_{ow} value and its RP-HPLC retention parameter. The disadvantages of this method are that it requires calibration, it is an indirect method and that it can only be used for a range of log K_{ow} from 0 to 6 (Noble, 1993). Reversed-phase thin-layer chromatography (RP-TLC) is also an indirect method needing reference compounds of known log K_{ow} . It has a range of 0 to 12 and is fast, but less reproducible than HPLC and is less accurate than the shake flask method (Eadsforth and Moser, 1983).

A direct method to measure K_{ow} values of very hydrophobic compounds has been developed by using the generator column technique, which avoids problems such as colloidal suspension, absorption, and volatilization of the solute (Hawker and Connell, 1988; Miller et al., 1984; De Voe et al., 1981). With this technique an n-octanol solution of the compound is sorbed to a solid support in a column. The quantity of the compound in the mobile phase of water or n-octanol/saturated water, which is passed through, is determined. Although the generator column method is suitable for log K_{ow} determinations ranging up to 8.5, an important disadvantage is its laboriousness.

Some years ago a slow stirring method has been successfully introduced to determine experimental K_{ow} values as high as 10^8 (Brooke et al., 1986; De Bruijn et al., 1989). In this method, the water and n-octanol phases are equilibrated by stirring them slowly. By careful stirring and close temperature control, the formation of micelles can be prevented and very high partition coefficients can be determined. The method is slow, 2-8 days are required for equilibrium to be achieved, but it is a direct method with high accuracy and good reproducibility.

lity (De Bruijn et al., 1989).

In the present study the slow stirring method is used to determine K_{ow} values of tetrachlorobenzyltoluenes (TCBTs), for which no experimental data are available.

Fig.1. Molecular structure of TCBTs.

TCBTs, known under the trade name Ugilec 141, are used as a replacement of PCBs as a hydraulic fluid in the mining industry. Theoretically 96 TCBT isomers are possible. Log K_{ow} values of nine commercially available individual TCBT isomers are determined by the slow stirring method. In order to save time, to get more reproducible results and to allow isomer resolution *n*-octanol-water partition coefficients are also measured of TCBTs added to the *n*-octanol as a mixture. Determined, calculated and literature data are compared. Reproducibility of the data and isomer resolution are evaluated. The possible utility of determining the TCBT-isomers as a mixture will be discussed.

MATERIALS AND METHODS

Chemicals

Nine TCBTs were purchased from Promochem; no 28, 2,2',4,6'-5; no 25, 2,2',4,5'-5 ; no 36, 2,2',5,5'-4 ; no 22, 2,2',4,4'-5; no 27, 2,2',4,6'-3; no 80, 2',3,4,6'-6; no 21, 2,2',4,4'-3; no 52, 2,3',4,4'-5; no 74, 2',3,4,4-6 (numbering according to Ehmann and Ballschmitter, 1989; numbers before and after the hyphen refer to positions of the chlorine- and methyl groups). Hexachlorobenzene and 1,2,3,4-tetrachlorobenzene were obtained from Aldrich. Silica (60, 70-230 mesh) was purchased from Merck. *n*-Hexane was obtained from Janssen Chimica and 2,2,4-trimethylpentane was purchased from Rathburn. Both solvents were redistilled before use. *n*-Octanol was obtained from Merck with a stated purity of > 99%. The water throughout the experiments was distilled in an all-glass apparatus.

Experimental set up

The log K_{ow} of 1,2,3,4-chlorobenzene was determined to validate the method by comparing this value with literature data (De Bruijn et al., 1989). The experimental determination of log K_{ow} of 1,2,3,4 tetrachlorobenzene was done in triplicate during a time course of three days. To examine the time needed to reach equilibrium for TCBTs an experiment was performed with TCBT 80 during a time course of 7 days, starting the measurements on day 4. The *n*-octanol/water partition coefficients of nine individual TCBT isomers were determined, at least in duplicate, after 7 days of slow stirring in separate experiments. In the same way a duplicate experiment with

a mixture of 8 TCBTs was carried out, using 1 of the 9 TCBT isomers as a recovery standard.

In the slow stirring method the water and n-octanol phases are equilibrated under conditions of slow stirring and close temperature control. The experiments took place in reaction vessels of about 900 ml. The reaction vessel consisted of a double walled flask through which water of constant temperature was pumped. The temperature of the circulating water was controlled carefully (25 ± 0.1 °C). Simultaneous experiments were done by connecting the outside ring of the double walled flask to another flask by plastic tubes. One pump circulated the 25°C water through the double walls of the flasks. Approximately 700 ml water was brought into the inner chamber of the reaction vessel together with a magnetic bar. The experiment was started when the water in the flask reached the temperature of 25 °C. Under slow stirring a solution of the test chemical in n-octanol was added very carefully to the water with a fixed pasteur pipette filled with some glass wool to prevent the formation of micelles of n-octanol in the water. As test chemicals 50 mg 1,2,3,4-tetrachlorobenzene, 0.5 mg TCBT isomers individually and 0.5 mg of each TCBT isomer added together as a mixture were dissolved in 50, 4 and 10.2 ml of n-octanol, respectively. The flasks were covered by a glass stopper and wrapped in aluminium foil to avoid influence of daylight. To establish equilibrium between the two phases the stirring continued 4 and 7 days for 1,2,3,4-tetrachlorobenzene and TCBTs respectively.

Sampling, extraction and clean-up

Duplicate samples of n-octanol and water were taken from each flask during time course or when equilibrium was reached. Aliquots of n-octanol were taken with a pasteur pipette and transferred to a vial. Around 0.01 g n-octanol was taken from this vial and diluted with 50 ml 2,2',4-trimethylpentane. Pentachlorobenzene or a TCBT isomer was used as a recovery standard. 250 ml water samples were taken at the same time from a glass tap at the bottom of the flask was connected with the inner chamber of the flask. The sampling of both water and n-octanol was done very carefully to prevent formation of micelles of n-octanol in the water. After adding the recovery standard, the water samples were extracted with 15 ml of n-hexane. The organic fraction was eluted through a column of silica-sulphuric acid (22% and 44% by weight) and silica sodium hydroxide (1N, 33% by weight) using 35 ml n-hexane. The eluate was concentrated by evaporation until 1 ml. Before analysis an internal standard, hexachlorobenzene or a TCBT isomer, was added.

The efficiencies of the dilution step of n-octanol samples were always between 80 and 100 %. Analysis of samples spiked with standard solutions of TCBTs in hexane demonstrated a recovery for the extraction of 71.4% and for the acid-base column 83%.

Gas Chromatographic Analysis

For analysis, 1 µl of the extract of the n-octanol or water sample was injected automatically three times into a Hewlett-Packard 5890A gas chromatograph, equipped with a ^{63}Ni electron capture detector and an on-column injector with autosampler A200S (Carlo Erba). The GC was connected to a HP 3396A integrator. A 30-m J&W DB-5 0.32 mm i.d. fused silica capillary column (film thickness: 0.25 µm) was used with a 2 m 0.53 mm

retention gap. The carrier gas was helium and the make-up gas was Ar/CH₄ 0.5-5%. The temperature program was: 120°C - 0.4 min - 70°C/min - 200°C - 1 min - 1°C/min - 211°C - 0 min - 40°C/min- 320°C - 6 min.

RESULTS AND DISCUSSION

Establishment of equilibrium, deviation from literature data and reproducibility

The results in Table I show the log K_{ow} of 1,2,3,4-tetrachlorobenzene and TCBT 80 during time course. The values of 1,2,3,4 tetrachlorobenzene are based on three separate experiments, from which three samples are taken for both phases. Due to a small temperature control deviation the temperature during the experiment with 1,2,3,4-chlorobenzene appeared to be 29 °C ($\pm 0.1^\circ\text{C}$) instead of 25°C. After two days the chlorobenzene turns out to have reached equilibrium. This is in good agreement with results from the literature. Brooke et al. (1986) reported achievement of equilibrium generally after 2 to 3 days, De Bruijn et al. (1989) stated that for compounds with log K_{ow} less than 4 to 5, equilibrium occurs within 1 to 2 days, and for compounds with higher log K_{ow} (> 5) within 3 to 4 days. The log K_{ow} values for TCBT 80 during time course, as is shown in Table I, confirm these results. The time to reach equilibrium is measured for TCBT 80 in one flask during a time course of four days, starting at day 4. An equilibrium is reached after day 4, as log K_{ow} values measured at subsequent days are not significantly different.

Table I. Determination of log K_{ow} of 1,2,3,4-tetrachlorobenzene after 2,3 and 4 days at 29 °C and determination of log K_{ow} of TCBT 80 after 4,5,6,7 days at 25 °C.

time	logKow of 1,2,3,4-tetrachlorobenzene				logKow of TCBT 80
	flask			mean	
	1	2	3		
day 1					
day 2	4.518	4.550	4.551	4.526 ± 0.021	
day 3	4.735	4.601	4.475	4.604 ± 0.130	
day 4	4.561	4.563	4.565	4.563 ± 0.002	7.15
day 5					7.07
day 6					7.10
day 7					7.06
overall mean	4.564 ± 0.074				7.10 ± 0.040

The log K_{ow} value of 1,2,3,4-tetrachlorobenzene determined by the slow stirring method from the literature is

4.635 ± 0.004 (at 25 °C) (De Bruijn et al., 1989). The value determined here is 4.564 ± 0.074 (at 29 °C). The difference of 0.07 log unit may be largely due to the difference in temperature. Sangster (1989) has listed the temperature dependence of $\log K_{ow}$ of some compounds at room temperature. After correction for the difference in temperature our $\log K_{ow}$ value is only 0.02 higher than the value of De Bruijn et al. (1989). Moreover, De Bruijn et al. (1989) concluded that standard deviations of 0.05 to 0.1 can be expected. The difference of 0.07 log unit, therefore, is quite acceptable.

The reproducibility of the method can be inferred from the $\log K_{ow}$ values of 1,2,3,4-tetrachlorobenzene. Mean results of three separate experiments on three different days are tabulated with a standard deviation of between 0.002 and 0.130. The standard deviation of the overall mean value is 0.074, which is again between 0.05 and 0.1, in accordance with De Bruijn et al. (1989).

Log K_{ow} values of TCBTs

Table II shows the results of $\log K_{ow}$ determinations of TCBTs. The values of the individual $\log K_{ow}$ determinations are means of n replicate samples. Generally at least two flasks were used per isomer and two samples were taken from each flask. The $\log K_{ow}$ values of the mixture of 8 TCBTs are means of two flasks, taking two samples from each flask again. No outliers were found with the Dixon's outlier test for both individual and mixture measurements.

Table II. Determination of $\log K_{ow}$ of 9 TCBT added individually and as a mixture.

TCBT	$\log K_{ow}$ individual	$\log K_{ow}$ mixture (n=4)
28	6.725 ± 0.356 (n=4)	6.132 ± 0.091
25	7.538 ± 0.089 (n=6)	6.089 ± 0.277
36	7.476 ± 0.098 (n=5)	6.146 ± 0.047
22	7.426 ± 0.346 (n=6)	*
27	7.203 ± 0.212 (n=3)	6.352 ± 0.083
80	7.150 ± 0.279 (n=8)	6.030 ± 0.141
21	7.200 ± 0.334 (n=3)	6.323 ± 0.103
52	7.262 ± 0.134 (n=6)	6.435 ± 0.334
74	7.405 ± 0.155 (n=5)	6.177 ± 0.137
overall mean	7.265 ± 0.244	6.211 ± 0.142

* not in the mixture; used as an internal standard

The standard deviations of the measurements shown in Table II are higher than the deviations reported by De Bruijn et al. (1989). This might be partly due to the fact that the log K_{ow} values of this study are means of more than one independent experiment, whereas values reported in the study of De Bruijn et al. (1989) are in general the mean of samples from one experiment only. The standard deviation of log K_{ow} values of p,p'-DDT from five independent experiments (De Bruijn et al., 1989), however, is still lower than the standard deviations reported here.

According to the fragmental system of Rekker (1977), the calculation of log K_{ow} of a tetrachlorobenzyltoluene isomer is 7.71, 0.44 log units higher than the overall mean log K_{ow} value of TCBTs, determined individually (Table II). The log K_{ow} of tetra-, penta-, and hexachlorobiphenyl calculated by the fragmental system is 5.901, 7.411 and 8.15 respectively. The corresponding mean isomer values determined by the slow-stirring method are 6.302, 6.754 and 7.284 (De Bruijn et al., 1989). Hence, the difference between determined and calculated log K_{ow} values of TCBT is comparable with such differences of 0.40, 0.66 and 0.87 log units for tetra-, penta- and hexachlorobiphenyl respectively.

The log K_{ow} values derived from the experiments with the mixture of TCBTs are, as the overall mean is concerned, 1.05 log units lower than the corresponding log K_{ow} values of the individually determined TCBTs. No literature could be found on differences between partition coefficients of congeners determined individually and in a mixture. The log K_{ow} determinations by the slow stirring method reported in literature (De Bruijn et al, 1989; Brooke et al, 1986) concern individually determined congeners only. However, Sijm et al. (1989) determined the log K_{ow} values in a mixture of polychlorinated dibenzo-p-dioxins and dibenzofurans by the slow stirring method. The values from this mixture are lower than log K_{ow} values of the same compounds determined individually by other methods (Webster et al., 1985; Shiu et al., 1988; Burkhard and Kuehl, 1986). The authors explained the lower values by the formation of micelles in the water. These lower values might be a confirmation of our lower mixture values. Our results, however, are determined by the same method. Micelle formation, therefore, will occur to the same extent for individual and mixture measurements. The total amount of TCBTs added as a mixture to n-octanol is about eight times as much as the amount of one TCBT added in individual experiments. These differences in concentrations might affect the K_{ow} values, although the TCBT concentrations are not higher than the maximum solubility in n-octanol. An explanation for the discrepancy between the lower log K_{ow} values determined in a mixture of compounds could be cosolvent effects of one isomer with respect to another in the mixture of compounds, which might affect solubilities in the water phase to different extents.

Further, differences in log K_{ow} values determined by the slow stirring method are found in literature. Brooke et al. (1986) found much lower log K_{ow} values for p,p'-DDT and dieldrin than those reported in the study of De Bruijn et al. (1989).

Finally, no clear systematic isomer correlation can be found between n-octanol/water partition coefficients determined individually or in a mixture (Table II). Only two isomers (TCBT 28 and 25) have a log K_{ow} value determined individually, which is significantly different from the overall mean log K_{ow} value determined

individually. TCBT 52 is the only isomer, whose log K_{ow} value, determined in a mixture, differs significantly from the overall mean value determined in a mixture. The log K_{ow} values range in between 0.813 log units and 0.405 log units for isomers determined individually or in a mixture respectively. In future research the log K_{ow} values measured will be used in order to predict the log K_{ow} values of all TCBT isomers. To this end the SOFA model (Govers, 1993) will be applied.

CONCLUSIONS

n-Octanol water partition coefficients of individual TCBTs were determined successfully for the first time. The log K_{ow} values for TCBT isomers were between 6.725 and 7.538. The results confirm the utility of the slow stirring method for determining very hydrophobic compounds. The reproducibility of the method was good. Replacing the more laborious determination of individual compounds by using a mixture of the same compounds cannot be recommended according to the results of this study. A substantial decrease in mean K_{ow} value of more than one order of magnitude was found when TCBTs were administered as a mixture to the slow stirring system.

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