November, 1985] *© 1985 The Chemical Society of Japan* NOTES *Bull. Chem. Soc. Jpn., 58, 3401—3402 (1985)*

The 1-Octanol/Water Partition Coefficient of Mercury

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(Received February 8, 1985)

Synopsis. The 1-octanol/water partition coefficient of metallic mercury was measured as a useful parameter for predicting the environmental behavior or fate of mercury. The partition coefficient obtained was 4.15±0.20 at 298 K; it slightly decreased from 4.80 to 3.80 as the temperature rose from 278 to 308 K. The partition coefficient of metallic mercury is very low in comparison with those of such nonpolar organic compounds as benzene and tetrachloromethane. Therefore, it was found that metallic mercury has a tendency to be further concentrated in the atmosphere.

It is well known that mercury has been released to the environment1) by the combustion of fossil fuels. It has been increasingly important to predict how contaminants will behave upon their release to the environment in order to assess the potential hazards of contaminants. Several models2,3) have been developed which predict environmental behavior or fate from accessible physico-chemical properties, such as vapor pressure, aqueous solubilities, Henry's constant, the soil-sorption constant, and the bioconcentration factor. The soil-sorption constant based on the organic carbon content4,5) and, in particular, the bioconcentration factor6,7) are complicated to measure experimentally, therefore, they have been correlated to the 1-octanol/water partition coefficient,16) which is relatively measurable. The partition coefficient is, then, very useful parameter in predicting the environmental behavior of a contaminant.

In this work, the partition coefficient of metallic mercury is experimentally determined; no information on this has previously been reported.

Experimental

All the chemicals used were of an analytical-reagent grade. The metallic mercury was further purified in the usual manner.8) The 1-octanol/water was distilled twice to remove trace amounts of impurities, which tended to produce emulsions.9) Doubly distilled water was used throughout this work.

By shaking an octanol solution containing a few drops of the purified metallic mercury and 0.001 mol dm^{-3} of hydrazine used as a reducing agent to prevent the mercury oxidation,8) the mercury was dissolved into the 1-octanol (approximately 0.8 mg-mercury/cm^3). A 2-cm^3 aliquot of the 1-octanol solution and 20 cm^3 of the distilled water were then shaken for 24 h at a constant temperature in a closed 25-cm^3 centrifuge tube. After equilibrium and then centrifugation, the two phases were separated and analyzed by means of the cold-vapor atomic-absorption method.10) The mercury concentrations in the two phases were constant after 24 h of shaking and thereafter remained constant over a period of several days. The 1-octanol/water partition coefficient was determined in the temperature range from 278 to 308 K.

Results and Discussion

Figure 1 shows the effect of the temperature on the 1-octanol/water partition coefficient, K_{OW}. The partition coefficient was 4.15±0.20 at 298 K, but it slightly decreased from 4.80 to 3.80 as the temperature rose from 278 to 308 K. The K_{OW} value of metallic mercury thus obtained is very low in comparison with those of nonpolar organic compounds, for example, 1.34×10^2 11) for benzene and 4.37×10^2 11) for tetrachloromethane, and with that of 1.66×10^6 16)for PCB (aroclor 1242).

Table 1 shows the soil-sorption constant, based on the organic carbon content, K_{OC}, and the bioconcentration factor, K_B, of metallic mercury and organic compounds calculated using the correlation equations of Karickhoff *et al.*6) and Veith *et al.*5) from the partition coefficient. The sorption by a soild phase, such as soil, a suspended solid, and sediment, and the

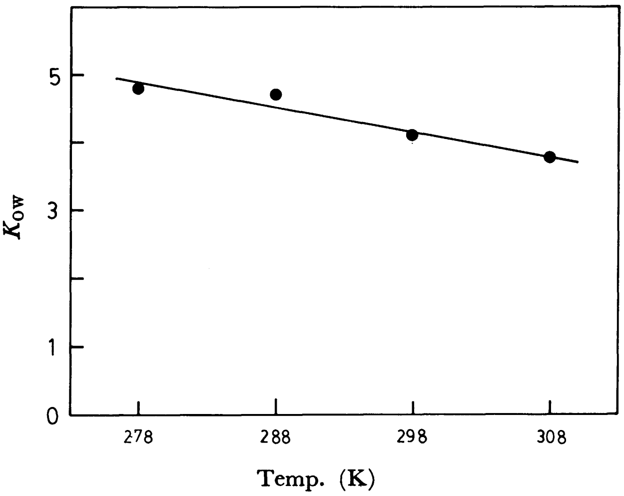

Fig. 1. Effect of temperature on the 1-octanol/water partition coefficient of metallic mercury, K_{OW}.

Table 1. The values of K_{OW}, K_{OC}, K_B, and $K_v^{(i)}/K_v^{(O_2)}$.

Contaminant	K_{ow}	K_{OC}6)	K_B5)	$K_v^{(i)}/K_v^{(O_2)}$
Mercury	4.15	2.6	6.7×10^{-1}	0.94 12)
Benzene	1.34×10^2 11)	8.3×10^1	1.3×10^1	0.56 13)
Tetrachloromethane	4.37×10^2 11)	3.0×10^2	$3.5\times10_1$	0.62 14)
PCB (aroclor 1242)	1.66×10^6 16)	1.0×10^6	3.9×10^4	0.22 15)

uptake by the aquatic-biota phase for mercury are much less than those for nonpolar organic compounds such as benzene and tetrachloromethane, and for PCB (aroclor 1242). In addition, Okouchi *et al.*[12] has reported that the volatilization rate of metallic mercury from water to the atmosphere is more rapid than those of benzene,[13] tetrachloromethane,[14] and PCB (aroclor 1242)[15] by factors of about 1.7, 1.5, and 4.3 respectively, judging from the volatility coefficient ($K_v^{(i)}/K_v^{(O_2)}$) as is shown in Table 1. The volatility coefficient represents the comparative volatilization rate of a volatile contaminant $K_v^{(i)}$ with oxygen $K_v^{(O_2)}$.

Therefore, from the 1-octanol/water partition coefficient of mercury measured in this work, it was found that metallic mercury has a tendency to be further concentrated in the atmosphere because of very low sorption by the particulate soild phase and uptake by the aquatic-biota phase.

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