Prediction of Adsorption Isotherms of Organic Compounds from Water on Activated Carbons. II.[1] Relative Adsorbabilities of Elements

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Synopsis. In order to predict the adsorbability of organic compounds out of water onto activated carbon, the contribution of individual atoms to the adsorbability is calculated. The contribution of the carbon atom is positive, that of nitrogen and oxygen atoms is negative, and that of the hydrogen atom is very small.

Adsorption onto activated carbon provides a technique for purification of municipal and industrial wastewaters. In the design of such water purification facilities, equilibrium adsorption information is required. To reduce experimental work, it is desirable to predict the adsorbability of organic compounds.

In a previous paper,[2] the partition coefficients (α) of 93 organic compounds between the solution and the adsorbed phases at an infinite dilution have been calculated and correlated with the molecular weight (MW). Further details of the relationship between $\log \alpha$ and MW are illustrated in Fig. 1. For 52 aliphatic monofunctional compounds, a good linear relationship has been obtained, with a high correlation coefficient (r). Furthermore, the standard deviation (s), the t-value in the Student test, and the over-all goodness of fit expressed by means of the F-value indicate that the relationship is statistically significant. The adsorbability of the multifunctional compounds is lower than that of the monofunctional compounds. This result suggests that the adsorbability of oxygen and nitrogen atoms constituting the functional group is lower than that of the carbon atom. The over-all correlation coefficient is low for this reason.

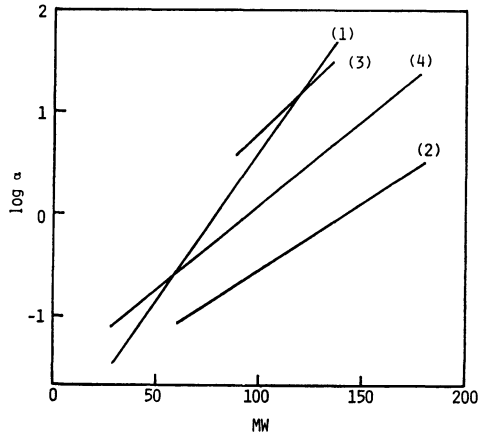

Fig. 1. Relationship between log α and molecular weight (MW).
(1): Aliphatic monofunctional compounds,
$n=52, r=0.9512, s=0.2635, F=475.0^{***}, t=21.79^{***}$.
(2): Aliphatic multifunctional compounds,
$n=27, r=0.6459, s=0.5614, F=17.89^{***}, t=4.230^{***}$.
(3): Aromatic compounds,
$n=14, r=0.6024, s=0.4263, F=6.834^{*}, t=2.614^{*}$.
(4): All compounds,
$n=93, r=0.6051, s=0.6867, F=52.58^{***}, t=7.251^{***}$.
Significance level: $^{*}<0.05$, $^{**}<0.01$, $^{***}<0.001$.

The relationship between adsorbability and molecular weight can be expressed by the following equation:

$$\log \alpha = aMW + b = a(12N_C + 1N_H + 14N_N + 16N_O + \cdots) + b, \quad (1)$$

where N_C, N_H, N_N, and N_O are the number of carbon, hydrogen, nitrogen, and oxygen atoms, respectively, in a molecule, and a and b are constants. Equation 1 assumes that the individual atoms contribute to the adsorbability of the molecule by the relative magnitude of atomic weight.

In order to estimate the exact contribution of the individual atoms to the adsorbability, the a coefficients in Eq. 2 have been calculated by multiple regression analysis. The relative magnitude of these coefficients is a measure of the contribution to the adsorbability.

$$\log \alpha = a_C N_C + a_H N_H + a_N N_N + a_O N_O + \cdots + b. \quad (2)$$

The data of 91 compounds, excluding two halogenated compounds, have been processed by a SHARP PC-7300 computer, and Eq. 3 has been derived. Table 1 shows

Table 1. Squared correlation matrix for independent variables in Eq. 3

	N_C	N_H	N_N	N_O
N_C	1.000			
N_H	0.458	1.000		
N_N	0.005	0.011	1.000	
N_O	0.013	0.084	0.122	1.000

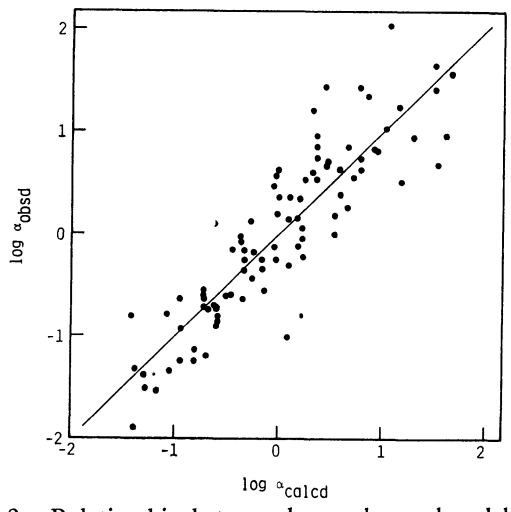

Fig. 2. Relationship between log α observed and log α calculated using Eq. 3.
$\log \alpha_{obsd} = 0.9998 \log \alpha_{calcd} - 0.0002$,
$n=91, r=0.8803, s=0.4090, F=306.3^{***}, t=17.50^{***}$.

$$\log \alpha = 0.4370N_C - 0.04465N_H - 0.2050N_N - 0.1302N_O - 1.501 \quad (3)$$

(n=91, r=0.8803, s=0.4161, F=74.01***, $t(N_C)$=13.60***, $t(N_H)$=−2.659**, $t(N_N)$=−2.104*, $t(N_O)$=−2.490*)

the squared correlation matrix for degree of collinearity between the variables used in Eq. 3.

A comparison of the coefficients in Eq. 3 yields the following conclusions. The presence of carbon atom in a molecule increases the adsorbability of the molecule. Nitrogen and oxygen atoms decrease the adsorbability. The contribution of hydrogen atom is much smaller than those of the other atoms.

Figure 2 shows the relationship between log α observed and log α calculated using Eq. 3. For the same 91 compounds, the relation between log α and the molecular weight is expressed by Eq. 4:

$$\log \alpha = 0.01639MW - 1.558. \quad (4)$$

(n=91, r=0.6050, s=0.6864, F=51.39***, t=7.169***)

These results indicate that Eq. 3 provide a better approximation than Eq. 4. The adsorbability of many compounds can be predicted from the molecular formula alone.

References

1) Part I: I. Abe, K. Hayashi, and M. Kitagawa, *Bull. Chem. Soc. Jpn.*, **54**, 2819 (1981).

2) I. Abe, K. Hayashi, M. Kitagawa, and T. Urahata, *Bull. Chem. Soc. Jpn.*, **53**, 1199 (1980).