PRO-TEK™ ORGANIC VAPOR G-AA AIR MONITORING BADGE
NO. 2
TECHNICAL BULLETIN
CALCULATED DIFFUSION COEFFICIENTS

If sampling rates for your particular compound are not available in the PRO-TEK™ Calculation Guide, they can be determined by using a calculated value for the diffusion coefficient from the Gilliland equation[1][2] or other equations[3] and the $\frac{A}{L}$ value of 14.8 cm for the badge (See Page 2, PRO-TEK™ Calculation Guide). It should be recognized, however, that sampling rates determined from calculated rather than experimental diffusion coefficients can be in error by as much as ± 20% (see sample calculations). The use of calculated diffusion coefficients is recommended where no good experimental data exist, but, where possible, reliable experimental data should be determined.

The Gilliland equation is expressed as follows:

$$D, \frac{cm^2}{sec} = \frac{0.0043 \times T^{3/2} \times \left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2}}{(V_A{}^{1/3} + V_B{}^{1/3})^2 \times P}$$

where M_A and M_B are the molecular weights of the air and the contaminant gas, and V_A and V_B are the molar volumes at the boiling point. Assuming the molar volume for air is 29.9 cm^3/g-mole[2] and T = 298°K, P = 1 atmosphere and M_A = 29.0 the equation can be reduced to the following:

$$D = \frac{22.120 \times \sqrt{\frac{1}{M_B} + 0.0345}}{(3.103 + V_B{}^{1/3})^2}$$

Molar volumes can be estimated for organic compounds through the use of Kopp's law of additive columns with the rules and values for each element given by Le Bas[4][5]. These values and rules are summarized in Table 1.

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(1) Gilliland, E. R., Ind. Eng. Chem., 26, 681 (1934).

(2) Nelson, G. O., *Controlled Test Atmospheres,* Ann Arbor Science Publications, 1971, p. 133.

(3) Reid, R. C. et al., *The Properties of Gases and Liquids,* McGraw-Hill, 1977, pp. 544-601.

(4) Arnold, Ind. Eng. Chem., 22, 1091 (1930).

(5) Reid, R. C., et al., *The Properties of Gases and Liquids,* McGraw-Hill, 1977, p. 58.

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TABLE 1
LE BAS ADDITIVITY VALUES AND RULES
MOLAR VALUES = Σ ATOMIC VOLUMES

Element		Atomic Volume
Carbon		14.8
Oxygen		7.4
Chlorine		24.6
Iodine		37.0
Hydrogen		3.7
Bromine		27.0
Sulfur		25.6
Fluorine		8.7
Oxygen in		
Aldehydes and Ketones	$R-\overset{\overset{O}{\|}}{C}-H,\ C-\overset{\overset{O}{\|}}{C}-C$	7.4
Methyl esters	$CH_3-O-\overset{\overset{O}{\|}}{C}-R$	9.1
Methyl ethers	$CH_3-O-C-R$	9.9
High esters and ethers	$(C_n-H_n)-\overset{\overset{O}{\|}}{C}-O-(C_nH_n),\ (C_n-H_n)-C-O-(C_nH_n)$	11.0
Acids	$R-\overset{\overset{O}{\|}}{C}-OH$	12.0
Nitrogen in		
Double and triple bonded	$R-N=N-CR,\ C\equiv N$	15.6
In primary amines	$R-NH_2$	10.5
In secondary amines	$R-NH-R$	12.0

Special Rules: (1) Deduct 6 for three-membered ring.

(2) Deduct 8 for four-membered ring.

(3) Deduct 11.5 for five-membered ring.

(4) Deduct 15 for six-membered ring.

(5) Deduct 30 for naphthalene ring.

Definition: $R = C_nH_{n+2}$ or C_nH_n or C_nH_{n-1}

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Table 1 (CONTINUED)

Examples (Molar Volume):

Benzene, C_6H_6; MW = 78

Molar Volume = 6 x 14.8 + 6 x 3.7 − 15 = 96.0

Acrylonitrile, CH_2 CHCN; MW = 53

Molar Volume = 3 x 14.8 + 3 x 3.7 + 15.6 = 71.1

Amyl acetate, CH_3 COO $(CH_2)_4$ CH_3; MW = 130

Molar Volume = 7 x 14.8 + 14 x 3.7 + 2 x 9.1 = 173.6

Examples (Diffusion Coefficients):

Benzene

$$D = \frac{22.120 \times \sqrt{\frac{1}{78} + 0.0345}}{(3.103 + 96.0^{1/3})^2} = 0.0815 \ \frac{cm^2}{sec}$$

Acrylonitrile

$$D = \frac{22.120 \times \sqrt{\frac{1}{71.1} \times 0.0345}}{(3.103 + 71.1^{1/3})^2} = 0.0928 \ \frac{cm^2}{sec}$$

Amyl acetate

$$D = \frac{22.120 \times \sqrt{\frac{1}{130} + 0.0345}}{(3.103 + 173.6^{1/3})^2} = 0.0603 \ \frac{cm^2}{sec}$$

Comparison with experimental values [Lugg, G. A., Anal. Chem., 40, 1072 (1968)] are shown in Table II.

TABLE II
CALCULATED VS. EXPERIMENTAL
DIFFUSION COEFFICIENTS $\frac{cm^2}{sec.}$

Compound	Calc.	Exp.	% Deviation From Exp.
Benzene	0.0815	0.0932	−14
Acrylonitrile	0.0928	0.1059	−14
Amyl Acetate	0.0603	0.0610	− 1

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For more information on Du Pont's PRO-TEK™ badge system, contact:

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NOTICE

The recommended procedures and product performance described herein have been developed and are the result of primary research completed by Du Pont, as well as the current state of the art knowledge.

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