Equations for Correlating Homolog Viscosities with Chain Length

Sir:

The advantages of equations that correlate homolog properties with chain length include space economy (much information in little space), new data calculated by interpolation or prudent extrapolation, identification of grossly inaccurate (nonfitting) data, and general evaluation of data quality (accurate data give high correlation coefficients).

Simple Equation 1, which has the additional advantage of being user-friendly, was used to correlate viscosities (η, cP, or mPa·s) with total carbons, C, of 20 homologous series. Equations for hydrocarbon, nitrogen, sulfur, and halogen homologs are in Table 1; equations for oxygen homologs are in Table 2.

$$\eta^e = b + mC \quad [1]$$

where exponent *e* is frequently about 0.20, *b* is the intercept, and *m* is the slope.

The exponent 0.20 is adequate for many, but not all, homologous series (Tables 1 and 2). Because of alternation, both odd- and even-carbon-number equations are given for *n*-FA, *n*-alcohols, and *n*-alkylamines. Both polar and nonpolar compounds of low or high M.W. were used, and hence Equation 1 appears to be generally applicable and useful.

Equation 2, based on methyl *n*-alkanoate data (25°C) (1), was formed by plotting *C* against $\eta^{0.20}$ (equivalent to plotting *C* against $1/\phi^{0.2}$, where $\phi^{0.2}$ is $1/\eta^{0.2}$). Equation 3, from rearrangement of Equation 2, suggests that the limiting fluidity (fluidity of an amorphous, infinite-length homolog) is zero. Equation 4 can be used to calculate viscosities of methyl *n*-alkanoates.

$$C = -14.85 + 22.69/\phi^{0.2} \quad [2]$$

At 25°C, for C_7–C_{13}, $r = 0.999978$.

$$\phi^{0.2} = 22.69/(C + 14.85) \quad [3]$$

$$\eta = [(C + 14.85)/22.69]^5 \quad [4]$$

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TABLE 1
Equations[a] Correlating Homolog Viscosities, η, with Total Number of Carbons, C: Hydrocarbons and Nitrogen, Halogen, and Sulfur Compounds[b,c]

	Carbons (C)	Temp. (°C)	Exponent (*e*)	Intercept (*b*)	Slope (*m*)	Corr. coeff. (*r*)	Ref.
n-Alkanes	7–17	20	0.20	0.4905	0.04958	4, 79	2
″	6–20	35	0.23	0.4452	0.04918	4, 79	2
1-Alkenes	6–19	20	0.22	0.4329	0.05076	5, 83	2
R Cyclohexanes	9–14	20	0.20	0.4864	0.05713	4, 60	2
RNH_2	4–10	25	0.20	0.6689	0.04698	4, 07	3
″	5–9	25	0.20	0.6508	0.05019	3, 90	3
″	4–10	50	0.20	0.6536	0.03820	4, 82	3
″	5–9	50	0.20	0.6433	0.04018	4, 68	3
R_2NH	8–14	25	0.20	0.6335	0.04432	4, 62	4
R_3N[d]	9–24	25	0.28	0.2873	0.06582	4, 20	4
RCN[e]	3–8	30	0.20	0.6876	0.04692	5, 35	5
RCl	4–8	25	0.10	0.8233	0.02368	4, 81	6
RBr	6–10	20	0.20	0.6955	0.05099	4, 77	7
R_2S	2–8	20	0.10	0.8412	0.02043	3, 69	6

[a]$\eta^e = b + mC$, where η is the homolog viscosity, *e* is an exponent, *b* is the intercept, *m* is the slope, and C is the total number of homolog carbons.
[b]R is normal alkyl.
[c]Correlation coefficient, *r*, of 0.999979 given as 4, 79.
[d]C_{21} viscosity not used in equation formation.
[e]C_6 viscosity not used in equation formation.

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TABLE 2
Equations[a] Correlating Homolog Viscosities, η, with Total Number of Carbons, C: Oxygen Compounds[b,c]

	Carbons (C)	Temp. (°C)	Exponent (*e*)	Intercept (*b*)	Slope (*m*)	Corr. coeff. (*r*)	Ref.
ROR	4–10	15	0.20	0.5716	0.04636	4, 42	6
ROR	6–10	30	0.20	0.5801	0.04039	5, 63	5,6
RCOOMe	7–13	25	0.20	0.6542	0.04406	4, 78	1
″	7–13	75	0.20	0.6548	0.02885	5, 25	1
RCOOEt	9–14	25	0.20	0.6034	0.04630	4, 09	8
″	8–18	35	0.20	0.6514	0.03876	4, 80	9
RCOOBu	7,8,22	25	0.20	0.6822	0.03833	5, 44	6,10
MeCOOR	12–20	35	0.20	0.6936	0.03844	4, 74	9
″	12–20	50	0.20	0.7050	0.03249	3, 80	9
$RCOOC_6H_{11}$	9–18	20	0.12	0.8656	0.02493	3, 83	11
TG	39–57	75	0.20	1.045	0.01310	4, 16	8
″	27–57[d]	75	0.20	1.075	0.01254	4, 58	12
″	39–57	85	0.20	1.016	0.01204	4, 12	8
MeCOR	5–11	30	0.20	0.6384	0.04193	4, 22	6
ROH	4–10[e]	25	0.40	0.6889	0.1910	4, 84	10
″	3–9[f]	25	0.30	0.8678	0.1191	3, 81	10
RCOOH	5–9[f]	25	0.20	0.7308	0.08275	4, 86	10
″	4–8[e]	25	0.20	0.7681	0.07675	4, 13	10
″	3–9[f]	50	0.15	0.8278	0.04334	5, 19	13
″	4–10[e]	50	0.10	0.8917	0.02653	4, 06	13
″	8–14[e]	60	0.25	0.7079	0.06753	4, 75	14

[a]$\eta^e = b + mC$, where *e* is an exponent, *b* is the intercept, and *m* is the slope.
[b]R is normal alkyl.
[c]Correlation coefficient, *r*, of 0.999942 given as 4, 42.
[d]Viscosities from Reference 12 equation [η (75°C) = 0.0576 C^2 – 0.2339 C + 3.8424] were used.
[e]Even carbons.
[f]Odd carbons.

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