Evaluating and Predicting n-Fatty Acid Properties

Charles H. Fisher
Chemistry Department, Roanoke College, Salem, VA 24153

Two types of equation, one correlating properties (P) with number of n-fatty acid carbons (N_c) and the other correlating properties of individual acids with temperature (t,C), were developed and used to evaluate and predict properties of the n-fatty acids. Equations correlating n-fatty acid properties with number of carbons are reported for freezing points, melting points, boiling points, densities, molar volumes, refractivities, dielectric constants, dipole moments, surface tensions and solubility parameters. Equations also are reported that correlate n-fatty acid properties with temperature.

The present paper describes a simple method, based largely upon the use of limiting properties (properties of an amorphous infinite-length n-alkane), for (a) evaluating published physical and thermodynamic properties (P) of the n-fatty acids and (b) estimating properties of new or additional acids. The method uses two types of equation: P vs molecular weight, M, or number of carbons, N_c and P vs temperature, t,C. The method assumes that n-fatty acid properties that are compatible with limiting properties (P_∞) in expressions such as Eqs. 1-3 are at least reasonably accurate. Conversely, properties that are substantially or grossly incompatible with the appropriate P_∞ may be inaccurate. The two types of equation (P vs M or N_c and P vs t) are suitable, presumably, for calculating many properties of all the n-fatty acids (exclusive of a few lower ones) over a wide temperature range.

Limiting properties. Limiting properties (1-5) (P_∞ in Tables 1 and 2) appear as parameters in Eqs. 1-3, where m is slope, L is chain length (either M or N_c), b is intercept and k and a are adjustable parameters.

$$P = P_\infty + m/(L + k) \quad [1]$$

$$P(L + k) = b + P_\infty L \quad [2]$$

$$(L + a)/P = b + L/P_\infty \quad [3]$$

Limiting properties can be calculated from the methylene increments (6-8) (slopes m and m′) in Eqs. 4 and 5, where 14.027 is the formula weight of CH_2:

$$MP = b + mN_c;\ P_\infty = m/14.027 \quad [4]$$

$$M/P = b' + m'N_c;\ P_\infty = 14.027/m' \quad [5]$$

Limiting properties calculated from recently published (6) methylene increments (for heats of formation and vaporization, entropy, heat capacity and molar volume, molar refraction and critical volume) are given in Table 2.

Some limiting properties are zero or approximately zero, e.g., dipole moments, vapor pressure, fluidity, iodine number, saponification value, acid strength, functional groups and water solubility.

The temperature dependence of the limiting densities, limiting refractivities and limiting dielectric constants are defined by Eqs. 6-8, where t is C (4):

$$d_\infty^t = 0.86544 - 0.00057636\ t \quad [6]$$

$$N_D^\infty = 0.48377 - 0.00034179\ t \quad [7]$$

$$\varepsilon_\infty^t = 2.2011 - 0.00099378\ t \quad [8]$$

Several advantages may be had from using limiting properties in developing Eqs. 1-3. It is helpful to know, in advance, one of the parameters. When P_∞ is used in constructing the equations, a suitable adjustable parameter (k or a) is provided. This avoids the need to make

TABLE 1

Limiting Properties (P_∞)

Property	P_∞	Ref
Melting point, T_m, K	414.3	1
Density, d_4^{20}, g/cm^3	0.8541	2
Density, d_4^{25}, g/cm^3	0.8509	3
Density, d_4^{40}, g/cm^3	0.8423	2
Refractivity, $N_D^{20} = n_D^{20} - 1$	0.4770	2
Refractivity, $N_D^{25} = n_D^{25} - 1$	0.4751	3
Refractivity, $N_D^{40} = n_D^{40} - 1$	0.4701	2
Dielectric constant (ε_{20})[a]	2.182[a]	4
Surface tension, γ20, dynes/cm	35.2	4
Solubility parameter (Hildebrands)[b]	8.0	4
Solubility parameter, S.I. units[c]	16.37	5

[a]Square of $n_{D\infty}^{20}$: $(1.477)^2 = 2.182$.
[b](cal/cm^3)$^{1/2}$.
[c](J/cm^3)$^{1/2}$.

TABLE 2

Methylene (CH_2) Values (m)[a] and Limiting Properties (P_∞)[b] at 25 C

	Property	State	m[a]	m[c]	P_∞[b]
1	fH°/kJmol^{-1}	g	-20.668	-20.61	-1.473
2	fH°/kJmol^{-1}	l	-25.627		-1.827
3	vH°/kJ mol^{-1}	l	4.959	4.974	0.3535
4	S°/JK^{-1} mol^{-1}	g	39.205	38.95	2.795
5	S°/JK^{-1} mol^{-1}	l	32.219		2.297
6	C_p°/JK^{-1} mol^{-1}	g	22.624		1.613
7	C_p°/JK^{-1} mol^{-1}	l	31.733	30.4	2.262
8	V/cm^3 mol^{-1} (20 C)	l	16.428		0.8539
9	V/cm^3 mol^{-1}	l	16.486	16.45	0.8508
10[d]	R/cm^3 mol^{-1} (20 C)	l	4.638		0.3307
11[d]	R/cm^3 mol^{-1}	l	4.640	4.65	0.3308
12[e]	-x/10^{-6} emu mol^{-1}	l	11.330	11.35	0.8077
13	P (parachor)	l	40.007	40.0	2.852
14	Vc/cm^3 mol^{-1}	l	59.622	57.4	0.2353

[a]From Reference 6.
[b]P_∞, m/14.027, except for V = 14.027/m.
[c]From References 7 and 8.
[d]Molar refraction, Lorentz-Lorenz.
[e]Magnetic susceptibility.

a search, frequently tedious, for suitable k or a values. A programmed calculator is adequate for developing least-squares equations based upon P_∞.

Limiting properties are applicable to all homologous series [$H(CH_2)_nG$, where G is the functional group] because all infinite-length homologs have the same composition [$(CH_2)_\infty$] and hence the same properties.

Some limiting properties are similar to those of amorphous, linear polyethylene, and hence may be useful in estimating polyethylene properties (4).

Equations correlating homolog properties (P) with chain length (L), and based upon P_∞, may be constructed as follows:

Eq. 9, based upon P_∞, may be developed by plotting L (M or N_c) against $1/(P - P_\infty$ to get $L = -k + m/(P - P_\infty)$ and rearranging it to:

$$P = P_\infty + m/(L + k) \quad [9]$$

Eq. 10, based upon P_∞, may be developed by plotting $(PL - P_\infty L)$ against P to get $PL - P_\infty L = b - kP$ and rearranging it to:

$$P(L + k) = b + P_\infty L \quad [10]$$

Eq. 11 may be developed by plotting $L/P - L/P_\infty$ vs 1/P to get $L/P - L/P_\infty = b - a/P$ and rearranging it to

$$(L + a)/P = b + L/P_\infty \quad [11]$$

RESULTS AND DISCUSSION

Freezing, melting and normal boiling points. The first four coefficients of the equation in Table 3 were developed by plotting N_c of the n-fatty acids against $1/(P - P_\infty)$ to get expressions that were rearranged to $P = P_\infty + m/(N_c + k)$. As indicated by the high correlation coefficients (r), the agreement between calculated and literature properties (10,11) is good.

The boiling point equation in Table 3 is a "best-fit" equation that correlates normal boiling points (12) of the fatty acids with carbons. The hypothetical limiting boiling point (1179 C at 760 torr) suggested by the intercept value is much higher than the limiting boiling point (805 C) proposed previously (9).

Densities and molar volumes. n-Fatty acid densities at 20 and 25 C from the literature (11-15) (Table 4) of the C_4 - C_9 fatty acids (liquids at room temperature) were used in developing d vs $1/N_c$ equations. Densities at 50, 75 and 80 C were available for the acids up to and including lauric and stearic acids (11,12,15). Densities at 100 C have been published (10) for the even-carbon C_{20}-C_{28} n-fatty acids: C_{20}, 0.8240; C_{22}, 0.8221; C_{24}, 0.8207; C_{26}, 0.8198; C_{28} 0.8191. The C_{30} density (0.8181) at 100 C was calculated from Eq. 12 correlating d^{100} with N_D. The limiting density (0.808) at 100 C was calculated from Eq. 6.

$$d^{100} = 1.1547 - 0.77863\ N_D^{100} \quad [12]$$

(C_{20}-C_{28}; r = -0.99503)

TABLE 3

n-Fatty Acids: Coefficients of the Equation[a] Correlating Freezing, Melting and Normal Boiling Points With Number of Carbons

Property	Carbon range[b]	Adj par, k	P_∞	Slope, m	Corr coeff, r	Ref[c]
t_f, °C	12-24	5.118	141	-1661.1	-0.99995	10
t_f, °C	11-25	3.808	141	-1672.5	-0.99997	10
t_m, °C	10-24	5.073	141	-1649.2	-0.99996	11
t_m, °C	11-23	3.488	141	-1635.0	-0.99981	11
t_b, °C	6-18	50.89[d]	1179.1	-55,345	-0.99997	12

[a]$P = P_\infty + m/(N_c + k)$.
[b]In addition to P_∞ at C_∞.
[c]Data source.
[d]Adjustable parameter (k) selected to give the best fit.

TABLE 4

n-Fatty Acids: Literature Densities (d)[a]

Number of carbons	Temperature (°C)					
	20[b]	25[b]	30[b,c]	50[d]	75[e]	80[f]
4	0.9582	0.9532	0.9478	0.9292	0.9043	
5	0.9390	0.9345	0.9300			
6	0.9272	0.9230	0.9183		0.8796	0.8751
7	0.9181					0.8670
8	0.9106	0.9066	0.9025	0.8864	0.8662	0.8615
9	0.9052	0.9013		0.8813		0.8570
10				0.8782	0.8583	0.8531
11				0.8741		
12				0.8706	0.8516	0.8477
14					0.8481	0.8439
16					0.8446	0.8414
18					0.8431	0.8390
∞	0.854	0.851	0.848	0.837	0.822	0.819

[a]The C_{10} and higher n-fatty acids are solids at room temperature.
[b]Ref. 13.
[c]Ref. 14.
[d]Ref. 11.
[e]Ref. 15.
[f]Ref. 12.

Coefficients of an equation correlating fatty acid densities with the number of carbons (at seven temperatures) are given in Table 5. The high correlation coefficients (r) show (a) the agreement between calculated and literature values is good, and (b) the proposed limiting densities are compatible with the literature densities.

Literature densities (11-15) were used in developing coefficients of the d vs t,C equation (Table 6) for the C_4 - C_9 fatty acids; densities calculated by the Table 5 equation were used (except for the 100 C densities) to develop the C_{10}-C_{30} coefficients.

The d vs. t equation (C_7-C_∞) converge at about 0.721 density and 250 C. This means that the density at only one temperature (e.g., 20 C) can be used with the hypothetical convergence density (0.721) to construct d vs. t,C equations similar to that in Table 6.

Coefficients of an n-fatty acid molar volume (16) equation ($V = M/d = b + mN_c$) at eight temperatures

TABLE 5

n-Fatty Acids: Coefficients of the Equation[a] Correlating Densities (d) With Number of Carbons

Temp, °C	Carbon range[b]	Adj param, k	P_∞	Slope, m	Corr coeff, r
20	5-9	1.0112	0.854	0.51169	0.99992
25	5-9	1.046	0.851	0.50438	0.99994
30	4-8	0.8490	0.848	0.48178	0.99993
50	4-12	0.7042	0.837	0.43212	0.99984
75	4-18	0.737	0.822	0.38574	0.99874
80	8-18	1.043	0.819	0.37903	0.99937
100	20-28	-1.782	0.808	0.28706	0.99519

[a] $d = d_\infty + m/(N_c + k)$.
[b] In addition to d_∞ at C_∞.

TABLE 6

n-Fatty Acids: Coefficients of the Equation[a] Correlating Densities (d) With Temperature (t,C)

Number of carbons	Temp range, °C	Intercept, b	Slope, $\times 10^{-4}$, m	Corr coeff, r
4	20-75	0.97752	-9.7439	-0.99989
5	20-30	0.95700	-9.0000	-1.0000
6	20-80	0.94464	-8.6820	-0.99999
7	20-80	0.93513	-8.5167	-1.0000
8	20-80	0.92693	-8.1410	-0.99995
9	20-80	0.92136	-8.0375	-0.99999
10	20-80	0.91611	-7.8030	-0.99989
12	20-80	0.90828	-7.4916	-0.99993
14	20-80	0.90256	-7.2704	-0.99993
16	20-80	0.89828	-7.1163	-0.99994
18	20-80	0.89481	-6.9729	-0.99995
20	20-80	0.89206	-6.8690	-0.99994
22	20-80	0.88971	-6.7729	-0.99995
24	20-80	0.88780	-6.7000	-0.99995
26	20-80	0.88609	-6.6256	-0.99994
28	20-80	0.88471	-6.5704	-0.99994
30	20-80	0.88347	-6.5266	-0.99994

[a] $d = b + m\ t,C$.

TABLE 7

n-Fatty Acids: Coefficients of the Equation[a] Correlating Molar Volumes (V) With Number of Carbons[b]

Temp, °C	Carbon range	Intercept, b	Slope, m	Corr coeff, r	Limiting density 14.027/m	Limiting density Eq. 6
20	5-9	26.177	16.519	0.99999	0.8491	0.854
25	5-9	26.399	16.578	0.99999	0.8461	0.851
50	9-18	28.731	16.772	0.99997	0.8363	0.837
60	12-17	28.648	16.948	0.99995	0.8276	0.831
70	14-18	30.714	16.962	0.99988	0.8270	0.825
75	10-18	29.978	17.091	0.99999	0.8207	0.822
80	10-18	30.514	17.135	0.99999	0.8186	0.819
100	22-28	32.125	17.375	0.99999	0.8073	0.808

[a] $V = M/d = b + mN_c$.
[b] The 50 C, 60 C and 70 C data (16).

are given in Table 7. The limiting densities suggested by these coefficients are similar to the d_∞ values calculated by Eq. 6.

Two-parameter molar volume equations can be transformed into expressions [Eq. 15] that are convenient for calculating densities; Eq. 13 is divided by Eq. 14 to get Eq. 15 (which does not require M):

$$M = b' + 14.027N_c \quad [13]$$

$$M/d = b + mN_c \quad [14]$$

$$d(N_c + b/m) = b'/m + 14.027N_c/m \quad [15]$$

n-Fatty acid refractivities. The literature refractivities ($N_D = n_D - 1$) in Table 8 were used to develop the equation in Table 9. The correlation coefficients (r) indicate the agreement between calculated and literature refractivities (11-15) is good; the literature refractivities are compatible with the limiting refractivities.

The C_6-C_9 expressions in Table 10 were developed with the literature refractivities in Table 8. The C_{10}-C_{30} expressions were developed with literature refractivities where these were available and with calculated refractivities (by Table 9 equation) where literature values were lacking.

The data pair of 0.9335 at -1297 C, compatible with the refractivity-temperature equation (Table 10), may be considered the convergence point.

n-Fatty acid dielectric constants. The usual technique (plotting N_c against $1/(P-P_\infty)$ was used to develop expressions that correlate dielectric constants (e) at 20 C (13) and 71 C (17) with number of carbons (Table 11):

$$e_{20} = 2.18 + 1.6704/(N_c - 1.740) \quad [16]$$

$$(C_4\text{-}C_8;\ r = 0.99567)$$

$$e_{71} = 2.13 + 3.5217/(N_c + 0.4737) \quad [17]$$

$$(C_6\text{-}C_{18};\ r = 0.99912)$$

n-Fatty acid dipole moments. Eq. 18 was constructed by plotting N_c against $1/\mu$ on the assumption the limiting dipole moment ($\mu\infty$) is zero; Eq. 18 was rearranged to Eq. 19. The agreement of calculated with literature values (18) is shown in Table 12.

$$N_c = -6.0332 + 16.169/\mu \quad [18]$$

$$(C_3\text{-}C_8;\ r = 0.99650)$$

$$\mu = 16.169/(N_c + 6.033) \quad [19]$$

Surface tensions and parachors. Literature surface tensions (13) (γ_{20}) and the limiting surface tension (4) at 20 C (35.2 dynes/cm) were used to construct Eqs. 20 and 21; the calculated values agree with the literature (13) surface tensions (Table 13).

The n-fatty acid parachors (Pr) calculated as $\gamma^{1/4}$ agree reasonably well (Table 13) with the parachors calculated with the Quayle (19) group values (CH_3 = 55.5; COOH = 73.8; and CH_2 = 40). Eq. 22 is based on Quayle group values.

TABLE 8

n-Fatty Acids: Literature Refractivities (N_D^t)[a]

Number of carbons	Temperature (°C)						
	20	25	30	50	70	75	80
4	0.3980	0.3958				0.3758	
5	0.4080	0.4060					
6	0.4168	0.4148	0.4132	0.4054	0.3972	0.3944	0.3931
7	0.4230	0.4209	0.4192	0.4114	0.4037		0.3993
8	0.4280	0.4261	0.4243	0.4167	0.4089	0.4069	0.4049
9	0.4322	0.4302	0.4287	0.4210	0.4132		0.4092
10				0.4248	0.4169	0.4149	0.4130
12				0.4304	0.4230	0.4208	0.4191
14					0.4273	0.4251	0.4236
16					0.4309	0.4288	0.4272
18					0.4337	0.4318	0.4299
∞	0.477	0.475	0.474	0.467	0.460	0.458	0.456

[a]Data from Refs. 11-15.

TABLE 9

n-Fatty Acids: Coefficients of the Equation[a] Correlating Refractivities (N_D^t) With Number of Carbons

Temp, °C	Carbon range[b]	Intercept, b	Slope, m	Adj param, k	Corr coeff, r	Ref[c]
20	4-9	0.477	-0.51523	2.513	-0.99987	13
25	4-9	0.475	-0.51302	2.475	-0.99987	13
50	6-13	0.467	-0.53576	2.667	-0.99994	12
70	6-18	0.460	-0.54226	2.617	-0.99997	11
75	4-18	0.458	-0.54047	2.536	-0.99992	15
80	6-18	0.456	-0.53248	2.432	-0.99997	12
100	20-30	0.450	-0.60417	4.267	-0.99966	10

[a]$N_D = b + m/(N_c + k)$, where b is N_D^∞.
[b]In addition to N_D^∞ and C_∞.
[c]Data source.

TABLE 10

n-RCOOH: Coefficients of the Equation[a] Correlating Refractivities (N_D^t) With Temperature (t,C)[b]

Number of carbons	Intercept, b	Slope $\times 10^{-4}$	Corr coeff, r
6	0.42500	-4.0026	-0.99944
7	0.43084	-3.9111	-0.99982
8	0.43578	-3.8468	-0.99995
9	0.43996	-3.8278	-0.99984
10	0.44353	-3.8052	-0.99988
12	0.44903	-3.7403	-0.99993
14	0.45331	-3.7247	-0.99986
16	0.45654	-3.6727	-0.99991
18	0.45918	-3.6481	-0.99993
20	0.46142	-3.6390	-0.99993
22	0.46325	-3.6208	-0.99990
24	0.46482	-3.6130	-0.99991
26	0.46614	-3.5935	-0.99991
28	0.46734	-3.5935	-0.99991
30	0.46835	-3.5818	-0.99989

[a]$N_D^t = b + m\ t,C$.
[b]Temperature range, 20-80 C.

TABLE 11

n-Fatty Acids: Dielectric Constants (ε)

	Number of carbons						
	2	4	5	6	8	16	18
Lit ($e_{20\ C}$)[a]	6.17	2.97	2.66		2.45		
Eq. 16		2.92	2.69	2.57	2.45	2.297	2.283
Lit ($e_{71\ C}$)[b]				2.665	2.548	2.348	2.318
Eq. 17				2.674	2.546	2.344	2.321

[a]Ref. 13.
[b]Ref. 17.

TABLE 12

n-Fatty Acid Dipole Moments (μ)[a]

	Number of carbons						
	2	3	4	5	6	7	8
μ, 20 C	1.74	1.75	1.65				1.15
Eq. 19		1.79	1.612	1.466	1.344	1.241	1.152

[a]From Ref. 18.

TABLE 13

Literature and Calculated Solpars[a]

	Number of carbons							
	3	4	5	6	7	8	9	10
Lit[b]	26.1	24.7	23.8	23.0	22.4	21.9	21.5	21.2
Eq. 24	25.93	24.73	23.80	23.05	22.45	21.94	21.51	21.14

[a]Solubility parameters.
[b]Data source, Ref. 21.

TABLE 14

n-Fatty Acids: Surface Tensions (γ) and Parachors (Pr)[a]

	γ20		V_{20}	Pr	
Number of carbons	Lit[a]	Eq. 21		γ1/4V	Eq. 22
2	27.42		57.22	130.9	129.3
3	26.70		74.57	169.5	169.3
4	26.74	26.68	91.97	209.1	209.3
5		27.47	108.8		249.3
6	28.05	28.13	125.3	288.4	289.3
7		28.69			329.3
8	29.2	29.17	158.4	368.2	369.3
9	29.57	29.58	174.8	407.6	409.3

[a]From Ref. 13.

$$N_c = -5.701 - 82.683/(\gamma - 35.2) \quad [20]$$

$$(C_4\text{-}C_9;\ r = -0.99896)$$

$$\gamma_{20} = 35.2 - 82.683/(N_c + 5.701) \quad [21]$$

$$Pr = 49.300 + 40.000N_c \quad [22]$$

Solubility parameters. The proposed (20) limiting solubility parameter of 16.37, $(J/cm^3)^{1/2}$, was used to develop Eqs. 23 and 24, which correlate, with good agreement, the literature solubility parameters (21) (Sp) with car- bons:

$$N_c = -3.974 + 66.668/(Sp - 16.37) \quad [23]$$

$$(C_3\text{-}C_{10};\ r = 0.99922)$$

$$Sp = 16.37 + 66.668/(N_c + 3.974) \quad [24]$$

ACKNOWLEDGMENT

Vernon R. and Vernon C. Miller developed the excellent computer program used in the work.

REFERENCES

1. Broadhurst, M.G., *J. Res. Nat'l Bur. Stds. 70A*:481 (1966).
2. Gouw, T.H., and J.C. Vlugter, *J. Am. Oil Chem. Soc. 41*:426 (1964).
3. Rossini, F.D., Kun Li, R.L. Arnett, M.B. Epstein, R.B. Ries, L.P. Bitler and J.M. Lynch, *J. Phys. Chem. 60*:1400 (1956).
4. Fisher, C.H., *Proceedings of the ACS Division of Polymeric Materials: Science & Engineering 53*:746 (Fall 1958).
5. Fisher, C.H., *J. Coatings Techn. 54*:67 (1982).
6. Somayajulu, G.R., *Thermodynamic Research Center (Texas) Bulletin*, Sept. 1984-Mar. 1985, pp. 478, 574.
7. Van Krevelen, D.W., with the collaboration of P.J. Hoftyzer, *Properties of Polymers*, Elsevier Scientific Publishing Co., New York, 1976.
8. Stull, D.R., E.F. Westrum Jr. and G.C. Sinke, *Chemical Thermodynamics of Organic Compounds*, John Wiley & Sons, Inc., New York, 1969, pp. 240, 242, 411.
9. Kreglewski, A., and B.J. Zwolinski, *J. Phys. Chem. 65*:1050 (1961).
10. *Fatty Acids, Part 4*, edited by K.S. Markley, John Wiley & Sons, Inc., New York, 1967, p. 2588.
11. *Bailey's Industrial Oil and Fat Products, Vol. 1*, 4th edn., edited by Daniel Swern, John Wiley & Sons, Inc., New York, 1979, p. 194.
12. *Fatty Acids, Part 1*, edited by K.S. Markley, Interscience Publishers, Inc., New York, 1960, p. 514.
13. Riddick, J.A., W.B. Bunger and T.K. Sakano, *Organic Solvents*, 4th edn., John Wiley & Sons, Inc., New York, 1986, pp. 365-375.
14. Dreisbach, R.R., *Physical Properties of Chemical Compounds*, American Chemical Society, Washington, D.C., 1961, pp. 437-441.
15. Gros, A.T., and R.O. Feuge, *J. Am. Oil Chem. Soc. 29*:313 (1952).
16. Berchiesi, G., M.A. Berchiesi and D. Leonesi, *J. Thermal Analysis 9*:455 (1976).
17. *Fatty Acids, Part 5*, edited by K.S. Markely, John Wiley & Sons, Inc., New York, 1968, p. 3441.
18. *Lange's Handbook of Chemistry*, 13th edn., edited by J.A. Dean, McGraw-Hill Book Co., New York, 1985, pp. 10-103.
19. Reid, R.C., J.M. Prausnitz and B.E. Poling, *Properties of Liquids & Gases*, 4th edn., McGraw-Hill Book Co., New York, 1987, p. 601.
20. Fisher, C.H., *Proceedings of the ACS Division PMSE 51*:588 (Aug. 1984).
21. Fujii, Y., and M. Tanaka, *Bull. Chem. Soc. Japan 54*:3696 (Dec. 1981).

[Received July 10, 1987; accepted April 17, 1988]