In later work it has been demonstrated that these same functionals are also universal among some nonpolar, polyatomic gases, their mixtures with each other and with the monatomic species (*1, 5, 7, 8*). In particular, the scaling parameters σ_{ij} and ϵ_{ij} for each binary interaction in the system N_2, O_2, Ar, CO_2 have been found which ensure the best representation of their functionals by eq 3. The values of these parameters are listed in Table I. Thus eq 2–4 together with the parameters of Table I immediately allow prediction of the viscosity of any mixtures of these gases over the large temperature range indicated by the limits on eq 3 and 4.

Results

The calculation scheme described in the previous section was utilized to predict the viscosity of the combustion products of carbon in dry air. The results are given in Table II for the temperature range 0–1000 °C and for air-to-fuel ratios extending from the stoichiometric value ($\alpha = 0$) to infinity (pure air). The results are also shown graphically in Figures 2 and 3. Basing our estimate of the possible uncertainty in the calculated values upon the previous success of the prediction scheme for other mixtures of complex gases (*5, 6, 8*) we estimate the accuracy of the data to be within ±0.3%. Figure 2 shows that the temperature dependence of the viscosity of the combustion products differs very little from that of air. The maximum difference between the viscosity of the combustion products and that of air does not exceed 5%.

The equations (1) to (4), given earlier, allow accurate interpolation and extrapolation in the temperature–composition space subject only to the limitations imposed by eq 3 and 4 and by the onset of molecular dissociation. However, the complexity of the equations necessitates the use of a digital computer. For the purpose of performing quick calculations of the viscosity of the combustion products as a function of temperature and excess air factors, $\mu(T, \alpha)$, we propose the much simpler formula

$$\mu(T, \alpha) = \mu(T, 0) + \alpha/[(1 + \alpha)(0.9313 - (0.3167 \times 10^{-3})T)] \quad (5)$$

where

$$\mu(T, 0) = T^{1/2}\{0.627 + 128.38(1/T) - 5818.8(1/T)^2\}^{-1} \quad (6)$$

with T in K and μ in μPa s. Equations 5 and 6 reproduce the data of Table II to within ±0.4% for $100 \leq T \leq 1000$ °C and $0 \leq \alpha \leq \infty$. The difference increases to 0.9% at $T = 0$ °C as $\alpha \rightarrow \infty$.

Literature Cited

(1) Hellemans, J., Kestin, J., Ro, S. T., *Physica* (*Utrecht*), **65**, 362 (1973).
(2) Hellemans, J., Kestin, J., Ro, S. T., *Physica* (*Utrecht*), **71**, 1 (1974).
(3) Hirschfelder, J. O., Curtiss, C. F., Bird, R. B., "The Molecular Theory of Gases and Liquids", Wiley, New York, N.Y., 1964.
(4) Kestin, J., "A Course in Thermodynamics", Vol. II, Blaisdell, Waltham, Mass., 1968.
(5) Kestin, J., Khalifa, H. E., Ro, S. T., Wakeham, W. A., *Physica* (*Utrecht*), in press.
(6) Kestin, J., Khalifa, H. E., Wakeham, W. A., *J. Chem. Phys.*, **65**, 5186 (1977).
(7) Kestin, J., Mason, E. A., *AIP Conf. Proc.*, **No. 11**, 137 (1973).
(8) Kestin, J., Ro, S. T., *Ber. Bunsenges. Phys. Chem.*, **78**, 20 (1974).
(9) Kestin, J., Ro, S. T., Wakeham, W. A., *Physica* (*Utrecht*), **58**, 165 (1972).
(10) Kestin, J., Ro, S. T., Wakeham, W. A., *J. Chem. Phys.*, **56**, 4119 (1972).
(11) Monchick, L., Yun, K. W., Mason, E. A., *J. Chem. Phys.*, **39**, 696 (1963).

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A Critical Review of Equations for Predicting Saturated Liquid Density

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An extensive evaluation of recently published generalized methods for predicting the saturated liquid density of pure compounds has been made with a large set of critically evaluated experimental density data. Results of these evaluations are given. The Spencer–Danner version of the Rackett equation with one adjustable constant, Z_{RA}, determined from the experimental data is shown to be slightly more accurate on an overall basis than the other equations. This equation also compares favorably to the other equations in terms of availability of input parameters, range of application, and ease of use. Updated values of Z_{RA} are given for 75 hydrocarbons, 71 other organic compounds, and 19 inorganics. With these values one can predict accurately the variation of the saturated liquid density over the entire temperature range from the triple point to the critical point. It is also shown that for highly associated compounds the Joffe–Zudkevitch equation is superior.

An important input parameter to most process design calculations is the liquid density and in particular the saturated liquid density of the pure component or mixture at hand. For example, accurate liquid densities are required in calculating the capacity of storage tanks, tower heights, pressure corrections to liquid fugacities, and compressor loads, for custody transfers, and in some cases, to estimate other physical properties such as surface tension (*107, 123*).

The prediction of orthobaric liquid density has been the subject of numerous studies over the last 100 years. Therefore, unlike many other physical properties where both data and correlations which do not have important limitations are relatively scarce, both correlations and data are plentiful. In 1972, Spencer and Danner (*102*) made an extensive evaluation of the available methods for predicting saturated liquid density of pure compounds as a function of temperature. They concluded that the simplest and most accurate means of prediction was a slightly modified version of the Rackett equation (*81*). In addition, they developed values of Z_{RA}, the single adjustable input parameter required for this equation, for 64 hydrocarbons, 36 organics, and 11 inorganics. The work described herein has a threefold purpose: to review and evaluate liquid density correlations that have been published since 1972, to update the recommended values of Z_{RA}, to expand compound coverage based on recently published data.

Only pure component saturated liquid density correlations are considered in this work. Extension of the final recommended equation to mixtures at both saturated and subcooled conditions is considered elsewhere (*101*).

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Table I. Summary of Correlations Evaluated

Gunn and Yamada (*41*)

$$\frac{1}{\rho_s} = V_s = V_r^{(0)}\{1 - \omega V_r^{(1)}\}\left[\frac{V_{0.6}}{(0.3862 - 0.0866\omega)}\right]$$

where $V_r^{(i)}$'s are generalized functions of T_r

Gunn and Yamada (*42*)

$$1/\rho_s = V_{scr}(0.29056 - 0.08775\omega)^{(1-T_r)^{2/7}}$$

where V_{scr}, the scaling volume, is a specified constant for each compound

Chiu et al. (*16*)

$$\frac{1}{\rho_s} = V_s = [1 + \alpha(1 - T_r) + \beta(1 - T_r)^{1/3}]\frac{V_{0.6}}{(0.3862 - 0.0866\omega)}$$

where α and β are generalized as functions of ω

Joffe and Zudkevitch (*49*)

$$\rho_s = \rho_{r,s}[\rho_{Ref}/\rho_{r,Ref}] \quad \text{(Watson relation)}$$

$$\rho_r = 1 + 0.85(1 - T_r) + (1.6916 + 0.9846\psi)(1 - T_r)^{1/3}$$

$$\psi = \psi_{Ref} + S(T_r - T_{r,}\ \text{Ref})$$

where ψ_{Ref} and S are specified constants for each compound (for nonpolar compounds $S = 0$ and ψ_{Ref} is determined from a single reliable density reference point)

Modified Rackett (*102*)

$$1/\rho_s = [RT_c/p_c]\,Z_{RA}^{[1+(1-T_r)^{2/7}]}$$

where Z_{RA} is a specified constant for each compound

Data Sources

Saturated liquid density data published prior to 1972 were obtained from the literature sources given in API Documentation Report No. 6-72, Liquid Density (*104*), prepared by the chemical engineering staff at Pennsylvania State University, who, under the auspices of the API Subcommittee on Technical Data, works on the revision of the API Technical Data Book (*4*). After an extensive literature search covering the period from 1972 to the present, this data set was supplemented with experimental data for pure hydrocarbons, as well as other organic and inorganic compounds. (The data sources are given as part of Table V).

In the compilation of the data set, only experimental values were considered to be useful. Data that were calculated or obtained by extrapolation from a nomograph were not used. For many of the compounds, especially those where multiple sources were available, the data were plotted as a function of temperature so that conflicting data sets or erroneous data points could be eliminated. The final data set included 2455 data points for 75 hydrocarbons and 1924 data points for 71 other organic and 19 inorganic liquids.

Selection and Description of Available Correlations

When selecting correlations for evaluation as well as in making the final recommendations, particular attention was given to such criteria as (1) ease of use, (2) availability of input parameters, (3) range of application, and (4) accuracy. Because current process design work is strongly computer oriented, consideration was also given to how well the designated equation could be incorporated with a computerized physical property data bank or commercial physical property prediction package, which functions as a subprogram in an overall design program. In this respect, point (2) is of utmost importance. It would obviously be advantageous to adopt an equation for liquid density which utilizes only those conventional parameters that are, in general, available in most data banks such as the pure component critical properties, normal boiling points, etc.

Most of the recently published density correlations appear to be accurate enough for design calculations. Therefore, points (1) through (3) were given the same level of importance as ac-

Table III. Comparison of Results for Selected Pure Polar Compounds

Compd	No. of data points	Average % deviation[a] Joffe and Zudkevitch	Modified Rackett (present work)
Dimethyl ether	9	2.10	0.59
Diethyl ether	21	0.22	0.25
Acetone	34	0.38	0.51
Methyl isobutyl ketone	6	0.08	0.07
Methanol	46	0.39	2.89
Ethanol	34	0.31	2.09
1-Propanol	31	0.46	1.60
2-Propanol	30	1.12	1.05
1-Butanol	58	1.96	0.63
1-Pentanol	13	0.22	1.33
Acetic acid	28	0.37	2.74
Propionic acid	7	0.21	0.25
Acetonitrile	19	0.97	1.58
Methyl chloride	71	0.71	0.33

[a] $[100/NP]\sum|(\text{calcd value} - \text{exptl value})/(\text{exptl value})|$.

Table IV. Input Parameters for the Joffe-Zudkevitch Equation [a]

Compd	T_{Ref}, K	ρ_{Ref}, g/cm^3	ψ_{Ref}	S
Dimethyl ether	293.16	0.6689	0.095	0.160
Diethyl ether	293.16	0.7133	0.229	0.034
Acetone	293.16	0.7899	0.282	−0.100
Methyl isobutyl ketone	293.16	0.8008	0.175	0.013
Methanol	293.16	0.7930	0.370	0.658
Ethanol	288.76	0.7940	0.288	0.616
1-Propanol	293.16	0.8037	0.337	0.618
2-Propanol	293.16	0.7849	0.329	0.598
1-Butanol	293.16	0.8097	0.353	0.520
1-Pentanol	293.16	0.8133	0.313	0.490
Acetic acid	293.16	1.0492	0.265	0.164
Propionic acid	293.16	0.9934	0.377	0.040
Acetonitrile	298.16	0.7770	0.776	−0.284
Methyl chloride	293.16	0.9180	0.152	0.078

[a] Reference 49.

Table II. Summary of Evaluation of the Five Selected Correlations with the Saturated Liquid Density Data Set

	No. of compd treated	No. of data points	Average % Deviation[a] Gunn and Yamada	Gunn and Yamada[c]	Chiu et al.	Joffe and Zudkevitch	Modified Rackett (present work)
Hydrocarbons	75	2455	0.58	0.59	0.62	0.74	0.42
Organics	71	1502	1.22	1.29	1.26	0.76[b]	0.63
Alcohols	8	240	2.43	3.21	2.67		1.49
Acids	5	101	1.18	1.20	1.01		1.17
Inorganics	19	422	1.26	1.20	1.23		0.73

[a] $(100/NP)\sum|(\text{calcd value} - \text{exptl value})/(\text{exptl value})|$. [b] Limited testing, results for 14 compounds encompassing 407 data points only. See text and Table III for more detailed information. [c] Reference 42.

Table V. Modified Rackett Equation Input Parameters and Description of Data Set

Compd	NP	T_r range	Av % dev	Z_{RA}	Critical temp K	Critical pressure, atm	Lit. sources
				Hydrocarbons			
Methane	38	0.466–0.997	0.18	0.28941	190.54	45.43	39, 54
Ethane	31	0.290–0.997	0.657	0.28128	305.43	48.15	33, 54
Propane	48	0.240–0.998	0.406	0.27664	369.82	41.93	6, 23, 54, 58
Butane	46	0.337–0.997	0.28	0.27331	425.15	37.46	6, 24
Isobutane	27	0.473–0.996	0.587	0.27569	408.15	35.99	6, 25
Pentane	104	0.390–0.998	0.199	0.26853	469.65	33.24	6, 14, 32, 47, 61, 87–90, 114
2-Methylbutane	61	0.326–0.989	0.389	0.27167	460.43	33.36	5, 7, 32, 47, 48
Neopentane	21	0.584–0.995	0.196	0.27570	433.76	31.56	6
Hexane	61	0.361–0.985	0.40	0.26355	507.43	29.72	6, 47, 52, 80, 106, 122
2,3-Dimethylbutane	4	0.686–0.946	0.386	0.26937	499.98	30.85	5
Heptane	58	0.339–0.996	0.366	0.26074	540.26	26.99	6, 32, 37, 47, 67, 80
2-Methylhexane	17	0.685–0.986	0.73	0.26288	530.32	26.97	67
3-Methylhexane	17	0.697–0.996	0.90	0.26103	535.26	27.76	67
3-Ethylpentane	18	0.690–0.995	0.68	0.26641	540.65	28.52	67
2,2-Dimethylpentane	33	0.390–0.986	0.892	0.26733	520.48	27.36	67
2,3-Dimethylpentane	18	0.676–0.992	0.92	0.25987	537.37	28.69	67
2,4-Dimethylpentane	37	0.579–0.987	0.83	0.26539	519.76	27.00	67, 79
3,3-Dimethylpentane	17	0.677–0.994	0.361	0.27348	536.43	29.06	67
2,2,3-Trimethylbutane	16	0.703–0.985	0.569	0.26978	531.15	29.14	67
Octane	62	0.392–0.996	0.521	0.25678	568.82	24.53	6, 13, 32, 35, 47, 80, 87
2-Methylheptane	17	0.703–0.988	0.32	0.25806	559.65	24.51	67
3-Methylheptane	18	0.698–0.990	0.92	0.25763	563.65	25.12	67
4-Methylheptane	16	0.718–0.985	0.19	0.25884	561.76	25.08	67
3-Ethylhexane	18	0.695–0.996	1.05	0.25853	565.48	25.73	67
2,2-Dimethylhexane	17	0.715–0.997	0.39	0.26393	549.87	24.95	67
2,3-Dimethylhexane	18	0.698–0.991	0.65	0.2622	563.48	25.93	67
2,4-Dimethylhexane	18	0.691–0.981	1.06	0.26579	553.54	25.22	67
2,5-Dimethylhexane	16	0.715–0.987	0.136	0.26143	550.04	24.53	67
3,3-Dimethylhexane	17	0.700–0.984	1.36	0.26007	561.98	26.18	67
3,4-Dimethylhexane	17	0.709–0.990	0.34	0.26322	568.87	26.56	67
2-Methyl-3-Ethylpentane	17	0.711–0.993	0.95	0.26122	567.09	26.64	67
3-Methyl-3-Ethylpentane	19	0.682–0.994	0.58	0.26657	576.59	27.70	67
2,2,3-Trimethylpentane	17	0.698–0.982	1.06	0.26494	563.48	26.93	67
2,2,4-Trimethylpentane	23	0.554–0.980	0.50	0.26719	543.98	25.33	67, 79
2,3,3-Trimethylpentane	19	0.685–0.991	0.59	0.26855	573.54	27.82	67
2,3,4-Trimethylpentane	18	0.694–0.994	0.34	0.26558	566.43	26.93	67
2,2,3,3-Tetramethybutane	24	0.647–0.898	0.44	0.27450	567.93	28.29	67
Nonane	69	0.369–0.897	0.32	0.25456	594.65	22.59	6, 13, 32, 80
2,2,5-Trimethylhexane	17	0.692–0.965	0.31	0.26365	568.04	22.99	5, 32, 37
Decane	68	0.394–0.997	0.23	0.25074	617.65	20.68	6, 37, 80
Undecane	34	0.396–0.897	0.127	0.24990	638.71	19.39	6
Dodecane	40	0.400–0.962	0.13	0.24692	658.26	18.00	6, 32, 37
Tridecane	34	0.404–0.878	0.64	0.24698	675.76	17.01	6
Tetradecane	29	0.409–0.800	0.82	0.24322	691.87	15.99	6
Heptadecane	34	0.400–0.836	0.18	0.23431	733.37	12.99	6
Octadecane	33	0.404–0.823	0.61	0.22917	745.04	11.97	6
Eicosane	13	0.404–0.552	0.14	0.22811	767.04	11.02	6
Ethylene	32	0.368–0.996	0.32	0.28054	282.37	49.65	3
Propylene	57	0.548–0.996	0.71	0.27821	364.76	45.51	5, 14, 32, 34, 44, 47, 61, 69, 89, 117, 129
1-Butene	73	0.465–0.991	0.50	0.27351	419.56	39.66	5, 9, 14, 17, 32, 61, 69, 73, 89, 119
cis-2-Butene	21	0.447–0.811	0.16	0.27044	435.59	41.50	5, 32, 47, 69, 119
trans-2-Butene	20	0.521–0.824	0.18	0.27212	428.65	40.48	5, 17, 32, 69, 119
2-Methylpropene	106	0.486–0.997	0.44	0.27277	417.93	39.46	5, 37, 45, 69, 119
1-Pentene	20	0.587–0.996	0.36	0.27035	465.04	35.05	125
Propadiene	15	0.494–0.771	0.098	0.27283	393.15	53.95	110
1,3-Butadiene	70	0.386–0.971	0.25	0.27130	425.37	42.72	5, 28, 32, 92
Acetylene	13	0.624–0.973	0.35	0.27063	308.32	60.57	5, 29
Propyne	27	0.541–0.915	0.292	0.27027	402.37	55.52	5, 32, 118
Cyclopropane	21	0.736–0.987	0.24	0.27429	398.25	55.01	98
Cyclobutane	21	0.506–0.724	0.05	0.27634	460.37	49.18	110
Cyclopentane	14	0.573–0.993	3.31	0.26824	511.61	44.41	53
Cyclohexane	27	0.506–0.956	0.14	0.27286	553.54	40.20	5, 32, 37, 79
Methylcyclohexane	32	0.477–0.932	0.386	0.26986	572.21	34.25	5, 32, 37
Cycloheptane	9	0.790–0.960	0.843	0.26957	604.26	37.89	127
Cyclooctane	5	0.879–0.986	1.01	0.26672	647.15	35.17	127
Benzene	137	0.486–0.993	0.26	0.26967	562.15	48.33	5, 12, 32, 37, 38, 40, 47, 74, 97, 99, 116
Methylbenzene	73	0.301–0.977	0.33	0.26455	591.82	40.54	5, 12, 32, 37, 47, 115
Ethylbenzene	23	0.289–0.633	0.25	0.26186	617.15	35.61	5, 32, 77

Table V (*continued*)

Compd	NP	T_r range	Av % dev	Z_{RA}	Critical temp K	Critical pressure, atm	Lit. sources
1,2-Dimethylbenzene	15	0.465–0.965	0.80	0.26326	630.37	36.83	5, 32, 37, 47, 97
1,3-Dimethylbenzene	55	0.397–0.977	0.47	0.25919	617.04	34.94	5, 32, 37, 47, 97, 114
1,4-Dimethylbenzene	61	0.443–0.995	0.316	0.25888	616.26	34.64	5, 32, 37, 47, 97
Propylbenzene	24	0.279–0.584	0.16	0.25990	638.37	31.57	5, 32, 114
Isopropylbenzene	19	0.433–0.674	0.061	0.26164	631.15	31.66	5, 32, 77
Biphenyl	20	0.420–0.816	0.45	0.27432	789.26	37.96	5, 32, 66
Naphthalene	31	0.445–0.632	0.10	0.26100	748.43	39.97	5, 32, 68
				Organics			
Dimethyl ether	9	0.683–0.995	0.594	0.27420	400.0	53.0	112
Methyl ethyl ether	10	0.624–0.985	0.916	0.26728	437.8	43.4	112
Diethyl ether	21	0.585–0.992	0.253	0.26444	466.71	35.9	112
Ethylamine	6	0.599–0.922	0.101	0.26419	456.15	55.5	78
Propylamine	11	0.429–0.831	0.371	0.26444	496.95	46.8	21
Isopropylamine	9	0.452–0.791	0.175	0.26849	471.85	44.8	21
Butylamine	12	0.407–0.826	0.786	0.26581	524.15	41.0	21
Isobutylamine	12	0.413–0.839	0.495	0.27347	516.0	42.0	21
Diethylamine	9	0.510–0.832	0.940	0.25677	496.65	36.6	21, 108
Dipropylamine	13	0.387–0.824	0.358	0.26909	550.15	31.0	21
Trimethylamine	4	0.630–0.711	0.067	0.27148	433.26	40.2	108
Triethylamine	12	0.398–0.809	0.319	0.26934	535.15	30.0	21
Aniline	15	0.391–0.791	0.506	0.26165	699.0	52.4	21
N-Methylaniline	16	0.361–0.789	0.207	0.28490	701.21	51.3	21
N,N-Dimethylaniline	14	0.427–0.805	0.569	0.25577	687.1	35.8	21
Methyl formate	21	0.561–0.971	0.278	0.25778	487.15	59.2	112
Ethyl formate	23	0.537–0.970	0.280	0.25863	508.43	46.8	112
n-Propyl formate	27	0.508–0.991	0.213	0.25910	538.04	40.1	112
Methyl acetate	23	0.539–0.973	0.401	0.25523	506.87	46.3	112
Ethyl acetate	30	0.522–0.962	0.371	0.25389	523.3	37.8	1, 112
n-Propyl acetate	27	0.497–0.970	0.411	0.25264	549.37	32.9	112
Methyl propionate	26	0.515–0.986	0.334	0.25656	530.54	39.5	112
Ethyl propionate	25	0.500–0.976	0.179	0.25459	546.04	33.2	112
Methyl *n*-butyrate	28	0.493–0.980	0.355	0.25627	554.43	34.3	112
Methyl isobutyrate	27	0.505–0.986	0.213	0.25848	540.76	33.9	112
Acetone	34	0.352–0.996	0.504	0.24494	508.15	46.4	112, 113, 116
Methyl isobutyl ketone	6	0.513–0.654	0.071	0.25892	571.00	32.3	113
Ethylene oxide	17	0.497–0.983	0.658	0.25762	468.98	71.0	62, 120
Propylene oxide	24	0.560–0.972	0.360	0.26221	488.15	53.7	86
Acetonitrile	19	0.542–0.990	0.575	0.19866	547.87	47.7	110, 112
Propionitrile	12	0.484–0.660	0.093	0.21690	564.37	41.3	112
Butyronitrile	10	0.469–0.633	0.086	0.22873	582.21	37.4	112
Nitromethane	13	0.506–0.810	0.350	0.23126	587.98	62.3	11
Methyl fluoride	22	0.419–0.993	0.629	0.24909	317.80	58.0	94
Difluoromethane	20	0.407–0.987	0.473	0.24651	351.60	57.5	63
Trifluoromethane	22	0.394–0.997	0.400	0.25871	299.07	47.7	94
Carbon tetrafluoride	48	0.401–0.991	0.270	0.28008	227.6	36.9	55, 94, 109
1,1-Difluoroethane	23	0.500–0.995	0.365	0.25335	386.65	44.4	94
1,1,1-Trifluoroethane	15	0.673–0.994	1.043	0.25183	346.26	37.0	94
Perfluorocyclobutane	21	0.600–0.985	0.884	0.27048	388.37	27.4	65
Perfluoro-*n*-butane	5	0.823–0.927	0.451	0.26988	386.37	22.9	36
Fluorobenzene	10	0.488–0.979	0.442	0.26616	560.09	44.9	31
Hexafluorobenzene	5	0.771–0.964	0.157	0.25667	516.73	32.6	30
Hexafluoroacetone	13	0.590–0.824	0.316	0.26641	357.14	28.0	70
Trifluoroacetonitrile	18	0.619–0.927	0.194	0.26636	311.11	35.7	70
Methyl chloride	71	0.421–0.995	0.328	0.26793	416.26	65.9	46, 95, 126
Dichloromethane	23	0.349–0.751	0.214	0.26184	510.0	60.0	95
Chloroform	30	0.391–0.640	0.270	0.27498	536.37	54.0	95, 112
Tetrachloromethane	34	0.455–0.996	0.216	0.27222	556.37	45.0	95, 112
Chloroethane	44	0.246–0.995	1.421	0.26540	460.43	52.0	76, 95
Chlorobenzene	28	0.432–0.859	0.248	0.26510	632.37	44.6	112
Chlorodifluoromethane	14	0.740–0.958	0.059	0.26800	369.2	49.11	128
Chlorotrifluoromethane	11	0.433–0.989	0.507	0.27971	302.1	38.7	2
Trichlorofluoromethane	27	0.424–0.985	0.217	0.27560	471.15	43.50	10
Dichlorotetrafluoromethane	18	0.468–0.992	0.151	0.27526	418.6	32.6	64
Ethyl bromide	7	0.321–0.602	0.613	0.28962	503.93	61.5	112
Bromobenzene	28	0.408–0.810	0.182	0.26370	670.15	44.6	112
Iodobenzene	20	0.379–0.517	0.121	0.26453	721.15	44.6	112
Methanol	46	0.509–0.997	2.885	0.23230	512.65	79.9	57, 100, 110
Ethanol	34	0.462–0.990	2.089	0.25041	516.15	62.9	82, 112, 113
1-Propanol	31	0.476–0.993	1.603	0.25272	536.78	51.0	19, 56, 112, 113
2-Propanol	30	0.524–0.994	1.052	0.24962	508.32	47.0	110

Table V (*continued*)

Compd	NP	T_r range	Av % dev	Z_{RA}	Critical temp K	Critical pressure, atm	Lit. sources
1-Butanol	58	0.450–0.991	0.627	0.25380	563.05	43.7	110, 113
1-Pentanol	13	0.362–0.770	1.327	0.25960	588.15	38.6	113
1-Hexanol	14	0.415–0.841	1.021	0.25748	610.37	34.1	113
1-Decanol	14	0.419–0.790	0.313	0.26274	700.37	25.0	113
Acetic acid	28	0.496–0.993	2.742	0.22253	592.71	57.1	20, 112
Propionic acid	7	0.446–0.512	0.248	0.24906	612.04	53.0	112
Butyric acid	24	0.433–0.840	0.197	0.27426	628.15	52.0	20, 112
Isobutyric acid	26	0.351–0.834	0.971	0.24027	609.15	40.0	20, 112
Valeric acid	16	0.358–0.819	0.589	0.24882	650.98	38.0	20
				Inorganics			
Ammonia	39	0.486–0.994	0.228	0.24658	405.54	111.3	26, 27, 43, 59
Argon	19	0.568–0.957	0.450	0.29216	150.76	48.1	29, 109
Carbon dioxide	32	0.717–0.997	0.54	0.27275	304.21	72.83	71, 76
Carbon disulfide	14	0.442–0.567	0.193	0.28492	552.15	78.0	105
Carbon monoxide	37	0.513–0.989	0.543	0.28966	132.93	34.5	60, 105, 112
Chlorine	37	0.415–0.998	0.534	0.27676	417.15	76.1	93
Fluorine	11	0.371–0.992	0.295	0.28867	144.3	51.5	93
Hydrogen	13	0.416–0.957	0.963	0.31997	33.26	12.8	90
Hydrogen chloride	33	0.503–0.996	0.506	0.26568	324.6	82.0	93, 111
Hydrogen fluoride	26	0.411–0.961	3.526	0.14514	461.0	64.0	93
Hydrogen sulfide	22	0.757–0.987	1.12	0.28476	372.54	88.88	89, 126
Krypton	12	0.562–0.775	0.049	0.29007	209.43	54.3	109
Neon	8	0.559–0.935	0.482	0.30852	44.37	27.2	8
Nitrogen	24	0.506–0.990	0.31	0.28971	126.26	33.53	85
Nitrous oxide	16	0.785–0.997	0.432	0.27592	309.59	71.50	18, 22
Oxygen	26	0.393–0.968	0.365	0.28962	154.59	49.8	76, 90, 109
Phosgene	16	0.580–0.732	0.221	0.27931	455.15	56.0	76
Sulfur dioxide	21	0.750–0.982	0.952	0.26729	430.80	77.8	50
Xenon	16	0.566–0.984	1.743	0.28288	289.71	57.6	72, 109

curacy. In other words, a specific correlation for liquid density may be very accurate (0.2–0.3 %), yet require four or five nongeneralized constants for each compound. Simply, is it practical to retain, particularly in the case of computer calculations, this number of constants for each compound of industrial importance? Perhaps for a property such as ideal gas enthalpy it is, but certainly not for saturated liquid density, unless of course, for a few compounds which happen to be one's major product.

Based on these standards an appropriate equation for liquid density is one that is simple in form, has been constructed within a corresponding states framework, and requires a minimum of arbitrary (unconventional) constants. It should be able to yield reasonable results from the triple point to the critical point for most compounds. In addition, the functional form must well describe the smooth, almost linear, behavior of density in the low reduced temperature range, and sharp decrease in density near the critical point ($0.85 \leq T_r \leq 1.00$). Also, the equation must have some application to mixtures.

The correlations scrutinized in this work are reiterated in Table I. With the exception of the modified Rackett equation, the Gunn–Yamada method is the only one of the 13 equations included in the aforementioned review by Spencer and Danner (*102*) which has been reevaluated. Their review stated that the Gunn–Yamada equation was superior to any of the other corresponding states approaches, and therefore, it has been included for additional study.

With respect to input requirements all five equations require the critical temperature, and all, except the Joffe–Zudkevitch equation (*49*), either directly or indirectly utilize the critical pressure. The acentric factor is not needed in the modified Rackett equation; however, this is not a particular advantage with respect to point (2), because acentric factors are usually available for those compounds having a known critical pressure and critical temperature. In fact, with the recent publication of numerous data compilations and computer prediction packages all three parameters, critical temperature, critical pressure, and acentric factor, are readily available for a large number of compounds.

Use of the Joffe–Zudkevitch equation, a modification of the original Riedel equation (*83, 84*), demands that the critical density of the compound be available. This requirement is a shortcoming of the aforementioned equation, because experimental critical densities are lacking or inaccurate for many compounds. However, by employing the Watson relationship (*121*), as shown in Table I, Joffe and Zudkevitch have minimized some of the effects of an erroneous critical density. This parameter is used in establishing the correlation parameter ψ from the available data but is not required in the final prediction procedure.

All the correlations except Joffe–Zudkevitch require one arbitrary constant. The liquid volume at a reduced temperature of 0.6, $V_{0.6}$, has been published for a number of the compounds included in this study. When this value was not known for a compound, it was obtained by interpolating the available experimental data. The scaling volume, V_{scr}, was established from the following equation

$$V_{scr} = V' \exp[-(1 - T_r')^{2/7} \ln (0.29056 - 0.08775\omega)] \quad (1)$$

where V' and T_r', the liquid density reference conditions, were set equal to $V_{0.6}$ and 0.6, respectively. It should be mentioned that Gunn and Yamada do not recommend these particular reference selections, stating only that T_r' should be chosen in a region in which liquid density is known with the greatest accuracy.

Chiu et al. (*16*) have published the optimum values of α and β for a number of compounds; however, this approach does compromise the very desirable property of a minimum number of arbitrary constants (three vs. one) with improved accuracy. Certainly with respect to earlier comments the generalized version is far more appealing.

Spencer and Danner determined the optimum values of Z_{RA}

from the respective experimental data by rearranging the modified Rackett equation as follows

$$\log \rho_s = \log (p_c/RT_c) - [1 + (1 - T_r)^{2/7}] \log Z_{RA} \quad (2)$$

Z_{RA} was then obtained by performing a linear regression of the following form

$$\log Z_{RA} = \frac{\Sigma X_i Y_i}{\Sigma (X_i)^2} \quad (3)$$

where

$$X_i = 1 + (1 - T_{ri})^{2/7} \quad (4)$$

$$Y_i = \log (p_c/RT_c\rho_{si}) \quad (5)$$

where ρ_{si} and T_{ri} are the respective values for each data point. Although by this linearization technique one is actually minimizing the sum of the square of the difference in the logs of the predicted and experimental densities, the density values in general vary only from 0.2 to 0.9 g/cm^3 and thus no important uneven weighing of the data is encountered. The same procedure was also used in this work to redetermine Z_{RA} for each compound in the data set. These Z_{RA}'s, the critical parameters used in obtaining them, and the resulting average deviations are listed in Table V. To maintain the stated accuracy for each compound, especially in the critical region, the respective tabulated critical values must be used. When Z_{RA} is not available for a compound, Z_c may be used. This will of course decrease the accuracy of the predicted value but will provide an estimate which in general is in error by no more than 3 or 4% (*102*).

For polar compounds two arbitrary constants, ψ_{Ref} and S, are needed via the Joffe-Zudkevitch technique. These values can be determined from two liquid density reference points. Because it was outside the scope of this work to obtain correlation parameters for more than one method, the Joffe-Zudkevitch equation was evaluated only for those polar compounds where both constants were provided. In utilizing this method for design calculations, it may be necessary only to list and, in the case of computer calculations, store the value of S for each respective polar component. In practice physical property data banks contain at least one temperature-density value, normally at 60 °F. Therefore, ψ_{Ref} can be calculated from this value and the critical density. However, if a density value is not available in the property bank, both constants must be stored for each polar component. In this situation the other four equations are more appealing, because only a single arbitrary constant is required. For nonpolar compounds $S = 0$ and ψ_{Ref} can be established from a single temperature-density value. In this study the respective liquid density at 60 °F was employed to determine ψ_{Ref}. For compounds that are not liquids at 60 °F, lower subcritical temperature-density values were selected.

A correlation recently developed by Othmer and Sze (*75*) was not considered in detail in this work. This equation has its own particular merit, and preliminary evaluations for a small set of compounds have shown that it compares favorably with the five equations that have been included in this study. However, with respect to the criteria established earlier, it is less appropriate than the other equations particularly because two arbitrary constants are required as input.

Evaluation and Comparison of Available Correlations

Each correlation was tested with the hydrocarbon portion of the data set. The overall results, which are given in Table II, clearly indicate that the modified Rackett equation is slightly more accurate than the other four equations. However, in general, all the correlations are excellent for this type (hydrocarbons) of compound. The detailed results for each respective hydrocarbon, which are available on request from the author, show that the predicted densities for most compounds are in error by less than 1% over the entire saturation range, no matter what method was applied. Errors are somewhat higher for the Joffe-Zudkevitch equation when the critical volume of the compound is questionable, such as in the case of the heavier *n*-paraffins and also for some of the branched paraffins. For these compounds the predicted densities varied from about 1.5 to 3.0%. However, in all fairness to these investigators the results for these compounds could possibly have been improved, if the reference density was selected from the respective liquid density data for each compound.

All the correlations, except Joffe-Zudkevitch, were also evaluated with the nonhydrocarbon organic and inorganic portion of the saturated liquid density data set. The overall results, which are given in Table II, show that the modified Rackett equation is superior for these types of compounds. As shown in Table V, the densities obtained from this equation vary by less than 1% from the experimental values for almost all of the nonassociated organic compounds and inorganic compounds. It should be pointed out that although utilization of the other three equations is not fully recommended by their advocates for polar compounds, reasonable predictions were obtained for many of the compounds in the organic portion of the data set. The detailed results of this portion of the work are also available from the author.

As shown in Table II all four of the equations are less accurate for associating polar organic compounds, such as alcohols and acids. This was expected for the three correlations utilizing the acentric factor, because associated compounds are not well correlated via a three-parameter approach. As pointed out by Rackett (*81*) and supported by Joffe and Zudkevitch, associated liquids do not conform to the functional form of the Rackett equation. Although this fact is not prominent in the work of Spencer and Danner, it is strongly reinforced by the results of this study. With an adjusted Z_{RA} it is possible to improve predictions for limited temperature ranges but not over the entire saturation range.

A comparison between the Joffe-Zudkevitch equation and the modified Rackett equation for a few selected associated and nonassociated organic compounds is given in Table III. Joffe-Zudkevitch correlating parameters for these compounds are given in Table IV. The Joffe-Zudkevitch equation is clearly superior for the low molecular weight associated liquids. This equation is accurate for these type of compounds, because the temperature-dependent correlation parameter, ψ, accounts for the variation of the liquid attractive forces due to hydrogen bonding with temperature. For the other organic compounds listed in Table III, the two methods are essentially equivalent.

Conclusion

On the basis of the evidence presented above, it has been concluded that the modified Rackett equation is as accurate as, or more accurate than, presently available generalized correlations for predicting the effect of temperature on saturated liquid density. It is recommended for both pure hydrocarbon and nonhydrocarbon compounds. However, in situations requiring a high level of accuracy for polar associated compounds, the Joffe-Zudkevitch equation should be used, because it is superior to the modified Rackett equation for this type of compound. In terms of the other selection criteria, all five of the equations are quite easy to use, are shown to have a wide range of application, and require only a single adjustable (unconventional) input parameter. None of the equations presents any particular problems with respect to use in a property prediction package, as computerization is straight forward. However, each individual must decide how well the equation meets his own particular computer design needs. Extension to mixtures is the topic of a future paper; however, past studies (*15*, *103*) have shown that the Chiu et al. and modified Rackett are quite suitable.

Table V gives a listing of the recommended Z_{RA}, the critical properties and number of data points used in obtaining Z_{RA}, the reduced temperature range of the data, and sources of the data for each compound in the data set. With the given input parameters, one can predict accurately the variation of the saturated liquid densities over the entire temperature range from the triple point to the critical point. It should be reemphasized, however, that to realize the accuracy of the recommended correlation these critical properties must be used.

Glossary

NP	number of data points
p_c	critical pressure, atm
R	universal gas constant, 82.06 (atm cm^3)/(g-mol K)
S	Joffe-Zudkevitch correlating parameter
T	temperature, K
T_c	critical temperature, K
T_r	reduced temperature, T/T_c
V_s	saturated liquid volume, cm^3/g
V_{scr}	scaling volume, cm^3/g
$V_{0.6}$	saturated liquid volume at a reduced temperature of 0.6, cm^3/g
Z_{RA}	constant of the modified Rackett equation

Greek Letters

α, β	constants of the Chiu et al. equation
ρ_r	reduced density
ρ_s	saturated liquid density, g/cm^3
ω	acentric factor
ψ	Joffe-Zudkevitch correlating parameter

Subscripts

Ref	reference point

Literature Cited

(1) Abraham, T., Bery, V., Kudchadker, A. P., *J. Chem. Eng. Data*, **16**, 355 (1971).
(2) Albright, L. F., Martin, J. J., *Ind. Eng. Chem.*, **44**, 188 (1952).
(3) Angus, S., Armstrong, B., de Reuck, K. M., "International Thermodynamic Tables of the Fluid State, Ethylene, 1972", Butterworths, London, 1972.
(4) American Petroleum Institute, "Technical Data Book—Petroleum Refining", 3rd American Petroleum Institute, Washington, D.C., 1977.
(5) API Research Project 44 Data, "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds", Carnegie Press, Pittsburgh, Pa., 1953.
(6) API Research Project 44 Data, "Selected Values of Properties of Hydrocarbons and Related Compounds", Texas A&M University, College Station, Texas, 1973.
(7) Arnold, E. W., *J. Chem. Eng. Data*, **10**, 88 (1965).
(8) Barron, R., "Cryogenic Systems", McGraw-Hill, New York, N.Y., 1966, p 634.
(9) Beattie, J. A., Marple, Jr., S., *J. Am. Chem. Soc.*, **72**, 1449 (1950).
(10) Benning, A. F., McHarness, R. C., *Ind. Eng. Chem.*, **32**, 814 (1940).
(11) Berman, W. A., West, E. D., *J. Chem. Eng. Data*, **12**, 197 (1967).
(12) Campbell, A. W., Chatterjer, R. M., *Can. J. Chem. Eng.*, **46**, 575 (1968).
(13) Carmichael, L. T., Sage, B. H., Lacey, W. N., *Ind. Eng. Chem.*, **45**, 2697 (1953).
(14) Carney, B. R., *Pet. Refiner*, **21**, (9), 84 (1942).
(15) Chiu, C. H., Hsi, C., Ruether, J. A., Lu, B. C-Y., *Can. J. Chem. Eng.*, **51**, 751 (1973).
(16) Chiu, C. H., Hsi, C., Ruether, J. A., Lu, B. C-Y., *J. Chem. Eng. Data*, **18**, 241 (1973).
(17) Coffin, C. C., Maass, O., *J. Am. Chem. Soc.*, **50**, 1427 (1926).
(18) Cook, D., *Trans. Faraday Soc.*, **49**, 716 (1953).
(19) Cosner, J. L., Gagliardo, J. E., Storvick, T. S., *J. Chem. Eng. Data*, **6**, 360 (1961).
(20) Costello, J. M., Bowden, S. T., *Recl. Trav. Chim. Pays-Bas*, **77**, 803 (1958).
(21) Costello, J. M., Bowden, S. T., *Recl. Trav. Chim. Pays-Bas*, **78**, 391 (1959).
(22) Couch, E. J., Kobe, K. A., *J. Chem. Eng. Data*, **6**, 229 (1961).
(23) Das, T. R., Eubank, P. T., *Adv. Cryog. Eng.*, **18**, 208 (1973).
(24) Das, T. R., Reed, C. O., Eubank, P. T., *J. Chem. Eng. Data*, **18**, 244 (1973).
(25) Das, T. R., Reed, C. O., Eubank, P. T., *J. Chem. Eng. Data*, **18**, 253 (1973).
(26) Date, K., *Rev. Phys. Chem. Jpn.*, **43**, 1 (1973).
(27) Davis, P., "Thermodynamic Functions of Gases", Vol. 1, F. Din, Ed., Butterworths, London, 1962, p 38.
(28) Dean, M. R., Legatski, T. W., *Ind. Eng. Chem., Anal. Ed.*, **16**, 7 (1944).
(29) Din, F., "Thermodynamic Functions of Gases", Vol. 2, Butterworths, London, 1962.
(30) Douslin, D. R., Harrison, R. H., Moore, R. T., *J. Chem. Thermodyn.*, **1**, 305 (1969).
(31) Douslin, D. R., Moore, R. T., Dawson, J. P., Waddington, G., *J. Am. Chem. Soc.*, **80**, 2031 (1958).
(32) Egloff, G., "Physical Constants of Hydrocarbons", Vol. I–VI, Reinhold, New York, N.Y., 1939–1953.
(33) Eubank, P. T., *Adv. Cryog. Eng.*, **17**, 270 (1972).
(34) Farrington, P. S., Sage, B. H., *Ind. Eng. Chem.*, **41**, 1734 (1949).
(35) Felsing, W. A., Watson, G. M., *J. Am. Chem. Soc.*, **64**, 1822 (1942).
(36) Fowler, R. D., Hamilton, J. M., Jr., Kasper, J. S., Weber, C. E., Burford, W. B., III, Anderson, H. C., *Ind. Eng. Chem.*, **39**, 375 (1947).
(37) Francis, A. W., *Ind. Eng. Chem.*, **49**, 1779 (1957).
(38) Glanville, J. W., Sage, B. H., *Ind. Eng. Chem.*, **41**, 1272 (1949).
(39) Goodwin, R. D., *Natl. Bur. Stand. (U.S.), Tech. Note*, **No. 653** (1974).
(40) Gornowski, E. J., Amick, E. H., Hixson, A. N., *Ind. Eng. Chem.*, **39**, 1348 (1947).
(41) Gunn, R. D., Yamada, T., *AIChE J.*, **17**, 1341 (1971).
(42) Gunn, R. D., Yamada, T., *J. Chem. Eng. Data*, **18**, 234 (1973).
(43) Haar, L., Gallagher, J. S., "Thermodynamic Properties For Ammonia", to be published by National Bureau of Standards.
(44) Hanson, G. H., *Trans. AIChE*, **42**, 959 (1946).
(45) Hanson, G. H., Kuist, B. B., Brown, G. G., *Ind. Eng. Chem.*, **36**, 1161 (1944).
(46) Hsu, C. C., McKetta, J. J., *J. Chem. Eng. Data*, **9**, 45 (1964).
(47) "International Critical Tables, III", McGraw-Hill, New York, N.Y., 1928.
(48) Isaac, R., Li, K., Canjar, L. N., *Ind. Eng. Chem.*, **46**, 199 (1954).
(49) Joffe, J., Zudkevitch, D., *AIChE Symp. Ser.*, **70** (No. 140), 22 (1974).
(50) Kang, T. L., Hirth, L. J., Kobe, K. A., McKetta, J. J., *J. Chem. Eng. Data*, **6**, 220 (1961).
(51) Kay, W. B., *Ind. Eng. Chem.*, **30**, 459 (1938).
(52) Kelso, E. A., Felsing, W. A., *Ind. Eng. Chem.*, **34**, 161 (1942).
(53) Khomutov, N. E., *Russ. J. Phys. Chem.*, **36**, 1342 (1962).
(54) Klosek, J., McKinley, C., "Proceedings of the First International Conference on LNG", Session No. 5, Chicago, Ill., 1968.
(55) Knobler, M., Pings, C. J., *J. Chem. Eng. Data*, **10**, 129 (1965).
(56) Kubicek, A. J., Eubank, P. T., *J. Chem. Eng. Data*, **17**, 232 (1972).
(57) Kudchadker, A. P., Ph.D. Thesis, Texas A&M University, College Station, Texas 1968.
(58) Kuloor, N. R., Newitt, D. M., Bateman, J. S., "Thermodynamic Functions of Gases", Vol. 2, F. Din, Ed., Butterworths, London, 1962, p 115.
(59) Kumagai, K., Toruimi, T., *J. Chem. Eng. Data*, **16**, 293 (1971).
(60) Leah, A. S., "Thermodynamic Functions of Gases", Vol. I, F. Din, Ed., Butterworths, London, 1962, p 135.
(61) Legatski, T. W., *Ind. Eng. Chem.*, **34**, 1240 (1942).
(62) Maass, O., Boomer, E. H., *J. Am. Chem. Soc.*, **44**, 1709 (1922).
(63) Malbrunot, P. F., Meunier, P. A., Scatena, G. M., Mears, W. H., Murphy, K. P., Sinka, J. V., *J. Chem. Eng. Data*, **13**, 16 (1968).
(64) Martin, J. J., *J. Chem. Eng. Data*, **5**, 335 (1960).
(65) Martin, J. J., *J. Chem. Eng. Data*, **7**, 68 (1962).
(66) Maxwell, J. B., "Data Book on Hydrocarbons", Van Nostrand, Princeton, N.J., 1950, p 136.
(67) McMicking, J. H., Ph.D. Thesis, Ohio State University, Columbus, Ohio, 1961.
(68) Montillon, G. H., Rohrbach, K. L., Badger, W. L., *Ind. Eng. Chem.*, **23**, 763 (1931).
(69) Morecroft, D. W., *J. Inst. Petrol.*, **44**, 433 (1958).
(70) Mousa, A. E., Kay, W. B., Kreglewski, A., *J. Chem. Thermodyn.*, **4**, 301 (1972).
(71) Newitt, D. M., Pai, M. U., Kuloor, N. R., "Thermodynamic Functions of Gases", Vol. 1, F. Din, Ed., Butterworths, London, 1962, p 102.
(72) Newton, R. H., *Ind. Eng. Chem.*, **27**, 302 (1935).
(73) Olds, R. H., Sage, B. H. Lacey, W. N., *Ind. Eng. Chem.*, **38**, 301 (1946).
(74) Organick, E. I., Studhalter, W. R., *Chem. Eng. Prog.*, **44**, 847 (1948).
(75) Othmer, D. F., Sze, A., "Liquid Densities at Saturation—Correlation and Prediction", paper presented at National Meeting of AIChE, Detroit, Mich., 1973.
(76) Perry, J. H., "Perry's Chemical Engineer's Handbook", 4th ed, McGraw-Hill, New York, N.Y., 1963, Chapter 3.
(77) Petro, A. J., Smyth, C. P., *J. Am. Chem. Soc.*, **80**, 74 (1958).
(78) Pohland, E., Mehl, W., *Z. Phys. Chem., Abt. A*, **164**, 48 (1933).
(79) Prengle, H. W., Felton, E. G., Pike, M. A., *J. Chem. Eng. Data*, **12**, 193 (1967).
(80) Quayle, O. R., Day, R. A., Brown, G. M., *J. Am. Chem. Soc.*, **66**, 938 (1944).
(81) Rackett, H. G., *J. Chem. Eng. Data*, **15**, 514 (1970).
(82) Reid, R. C., Smith, J. M., *Chem. Eng. Prog.*, **47**, 415 (1951).
(83) Riedel, L., *Chem.-Ing.-Tech.*, **26**, 259 (1954).
(84) Riedel, L., *Chem.-Ing.-Tech.*, **26**, 83 (1954).
(85) Roder, H. M., McCarty, R. D., Johnson, V. J., *Natl. Bur. Stand. (U.S.), Tech. Note*, **No. 361**, (1972).
(86) Rutenberg, O. L., Shakhova, S. F., *Russ. J. Phys. Chem.*, **47**, 27 (1973).
(87) Rykov, V. I., *Russ. J. Phys. Chem.*, **41**, 1173 (1967).
(88) Sage, B. H., Lacey, W. N., *Ind. Eng. Chem.*, **34**, 730 (1942).
(89) Sage, B. H., Lacey, W. N., "Some Properties of the Lighter Hydrocarbons, Hydrogen Sulfide, and Carbon Dioxide", American Petroleum Institute, New York, N.Y., 1955.
(90) Sage, B. H., Lacey, W. N., Schaafsma, J. G., *Ind. Eng. Chem.*, **27**, 48 (1935).
(91) Scott, R. B., "Cryogenic Engineering", Van Nostrand, Princeton, N.J., 1959, pp 269–319.

(92) Scott, R. B., Meyers, C. H., Rands, R. D., Brickwedde, F. G., Bekkedahl, N., *J. Res. Natl. Bur. Stand.*, **35,** 39 (1945).
(93) Selected Values of Properties of Chemical Compounds, Thermodynamic Research Center Data Project, TRC, Texas A&M University, College Station, Texas (loose-leaf data sheets: 9 to 9-1-d, 9-2 to 9-2-1-d, 10 to 10-1-d, 10-2 to 10-2-1-d) (1973).
(94) Selected Values of Properties of Chemical Compounds, [loose-leaf data sheets, 23-9-2-(10.011)-d] (1973).
(95) Selected Values of Properties of Chemical Compounds, [loose-leaf data sheets, 23-10-2-(10.011)-d] (1973).
(96) Selected Values of Properties of Chemical Compounds, [loose-leaf data sheets, 23-2-(1.101)-d] (1973).
(97) Shraiber, L. S., Pechenyuk, N. G., *Russ. J. Phys. Chem.*, **39,** 212 (1965).
(98) Silberberg, I. H., Lin, D. C-K., McKetta, J. J., *J. Chem. Eng. Data,* **15,** 483 (1970).
(99) Skaates, J. M., Kay, W. B., *Chem. Eng. Sci.*, **19,** 431 (1964).
(100) Smith, J. M., *Chem. Eng. Prog.*, **44,** 521 (1948).
(101) Spencer, C. F., to be submitted for publication.
(102) Spencer, C. F., Danner, R. P., *J. Chem. Eng. Data,* **17,** 236 (1972).
(103) Spencer, C. F., Danner, R. P., *J. Chem. Eng. Data,* **18,** 230 (1973).
(104) Spencer, C. F., Danner, R. P., Daubert, T. E., Documentation Report No. 6-72, American Petroleum Institute, Washington, D.C., 1973.
(105) Stauffer Chemical Co. Publication, "Carbon Disulfide", Dobbs FERRY= New York, N.Y., 1964.
(106) Stewart, D. E., Sage, B. H., Lacey, W. N., *Ind. Eng. Chem.*, **46,** 2529 (1954).
(107) Sugden, S., *J. Chem. Soc.*, **125,** 32 (1924).
(108) Swift, E., Jr., *J. Am. Chem. Soc.*, **64,** 115 (1942).
(109) Terry, M. J., Lynch, J. T., Bunclark, M., Mansell, K. R., Staveley, L. A. K., *J. Chem. Thermodyn.*, **1,** 413 (1969).
(110) Thermodynamic Research Center Data Book, "Component Physical Property Series", Vols. I–III, Washington University, 1970–1973.
(111) Thomas, W., Progress in International Research on Thermodynamic and Transport Properties, p 166, ASME, 1962.
(112) Timmermans, J., "Physical Constants of Pure Organic Compounds", Elsevier, New York, N.Y., 1950.
(113) Timmermans, J., "Physico-Chemical Constants of Pure Organic Compounds", Vol. 2, Elsevier, New York, N.Y., 1965.
(114) Timmermans, J., Hennaut-Roland, Mme., *J.Chim. Phys. Phys.-Chim. Biol.*, **27,** 401 (1930).
(115) Tonomura, T., *Sci. Rep. Tahoku Univ.*, **22,** 104 (1933).
(116) Tugarev, I. A., Avdus, Z. I., Nozdrew, V. F., *Zh. Fiz. Khim.*, **49,** 1256 (1975).
(117) Vaughan, W. E., Graves, N. R., *Ind. Eng. Chem.*, **32,** 1252 (1940).
(118) Vohra, S. P., Kang, T. L., Kobe, K. A., McKetta, J. J., *J. Chem. Eng. Data,* **7,** 150 (1962).
(119) Wackher, R. C., Linn, C. B., Grosse, A. V., *Ind. Eng. Chem.*, **37,** 464 (1945).
(120) Walters, C. J., Smith, J. M., *Chem. Eng. Prog.*, **48,** 337 (1952).
(121) Watson, K. M., *Ind. Eng. Chem.*, **35,** 396 (1943).
(122) Weber, J. H., *AIChE J.*, **2,** 514 (1956).
(123) Weinaug, C. F., Katz, D. L., *Ind. Eng. Chem.*, **35,** 239 (1943).
(124) Winkler, C. A., Maass, O., *Can. J. Res.*, **9,** 610 (1933).
(125) Wolfe, D. B., M.S. Thesis, Ohio State University, Columbus, Ohio, 1970.
(126) Woolrich, W. R., "Handbook of Refrigerating Engineering", 4th ed, Vol. I, AVI, Westport, Conn., 1965.
(127) Young, C. L., *Aust. J. Chem.*, **25,** 1625 (1972).
(128) Zander, M., Proceedings of the Fourth SYMPOSIUM ON Thermophysical Properties, p 114, ASME, 1968.
(129) Zordan, T. A., Henry, R. M., *J. Chem. Eng. Data,* **20,** 343 (1975).

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NEW COMPOUND SECTION

Synthesis of Some Local Anesthetics from 2-Aminonaphthothiazole

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Derivatives of 2-aminonaphthothiazole have been synthesized as potential local anesthetics by treating 2-aminonaphthothiazole with chloroacetyl chloride whereby chloroacetyl-2-aminonaphthothiazole is obtained. This is subsequently treated with various amines to afford morpholinoacetyl, piperidinoacetyl, dimethylaminoacetyl, *N,N*-dimethylanilino-*p*-aminoacetyl, *N,N*-diethylanilino-*p*-aminoacetyl, pyridine-2-aminoacetyl, pyrimidine-2-aminoacetyl, diphenylaminoacetyl, and piperazinoacetyl-2-aminonaphthothiazole.

Some derivatives of 2-aminobenzothiazole (*1, 2, 5*) and 2-aminothiazole (*3, 4*) are reported to possess considerable local anesthetic activity. It was thought worthwhile to prepare some new compounds from 2-aminonaphthothiazole which may exhibit local anesthetic activity. These compounds are synthesized by chloroacetylation of 2-aminonaphthothiazole with chloroacetyl chloride. The chloroacetylated product was then condensed with different amines. The bases, being liquid, were characterized through their solid derivatives.

Experimental Section

***2-Aminonaphthothiazole* (*6*).** It was prepared by oxidation of α-naphthylthiourea with bromine in chloroform medium. Naphthylthiourea (10 g) was suspended in chloroform (50 mL) and a solution of bromine (4 mL) in chloroform was added gradually with cooling and stirring of the reaction mixture. After allowing to stand overnight, the chloroform was evaporated and the residue was treated with a little sodium bisulfite solution to remove the unreacted bromine. The crude product was basified when a soft base crystallizable from aqueous ethanol, mp 190 °C, was obtained.

Preparation of Chloroacetyl-2-aminonaphthothiazole. The solution of about 2.82 g of chloroacetyl chloride in dry ether (20 cm^3) was gradually added to a solution of 2-aminonaphthothiazole (5 g) in dry ether (30 cm^3). The chloroacetyl-2-aminonaphthothiazole was separated immediately and filtered and res-

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