Methods for predicting isothermal and adiabatic compressibilities and velocity of sound—Table I

Parameter	Method	Reference
Isothermal compressibilty, α_T	Rao-Li	4
	Wada	12
Adiabatic compressibility, α_a	Rao	2
	Wada	12
Velocity of sound, u	Rao	3,5,8,9
	Rykov	6
	Surface tension	7

Predictive equations for isothermal and adiabatic compressibilities and velocity of sound—Table II

Parameter	Method	Equation
Isothermal compressibility, α_T	Rao-Li	$\alpha_T = [p^*Z(6 \ln Z - 11)\times (1.01325 \times 10^6)]^{-1}$ where $Z = \frac{82.06T}{p^*V}$.
	Wada	$\alpha_T = (M/\rho B)^7$ where B is a constant determined by the sum of the bond contributions given in Table III.
Adiabatic compressibility, α_a	Rao	$(1/\rho\alpha_a)^{1/2} = C(T_c - T)$ where C is a constant determined by one value of α_a and ρ.
	Wada	$\alpha_a = (M/\rho A)^7$ where A is a constant determined by the sum of the bond contributions given in Table III.
Velocity of sound, μ	Rao	$u = 0.032808(\beta\rho/M)^3$ where β is a constant determined by the sum of the structural contributions in Table IV.
	Rykov	$u = \left[\frac{c_p\lambda}{\alpha_T T(c_p - \alpha_T\lambda M)}\right]^{1/2} \times (3.2808)$ where c_p, λ and α_T are taken at absolute temperature T.
	Surface tension	$u = (355)\,(0.032808)\times \left[\frac{\sigma V^{2/3}}{MT_r}\right]^{1/2}$ where σ and V are taken at absolute temperature T.

Bond contributions for isothermal and adiabatic compressibilities (Wada's method)—Table III

Bond	Constant A	Constant B
C—C	−1.10	1.07
C—O	2.05	2.78
C—S	5.43	—
C—N	0.40	0.24
C—H	5.10	4.16
C—F	—	6.57
C—Cl	12.91	12.55
C—Br	15.54	15.33
C—I	19.65	—
O—H	4.64	5.07
N—H	5.57	5.00
C=C	5.68	6.36
C=O	9.93	9.08
C=S	16.83	—
C=N	7.60	—
N=O	8.17	8.28
C≡N	14.13	—
Ring	4.80	−0.43

Information regarding the velocity of sound is important in a variety of hydrodynamic calculations. Similarly, compressibility data can be useful for the extrapolation of saturated-liquid* densities to higher pressures.

Predictive Methods

The predictive methods evaluated here and their corresponding equations are listed in Tables I and II, respectively. Tables III and IV list the additive structural and bond contributions required in several of the procedures.

Results of Analysis, Recommendations

Table V summarizes the results of the statistical analysis of the methods evaluated. (The class symbols of Table V are defined in Part 8, Table IV *Chem. Eng.*, May 19, 1969, p. 194.) Our analysis of the methods for the three properties showed this:

Isothermal Compressibility—Clearly, large uncertainties exist in the Rao-Li and Wada methods for predicting this property. The problem is further complicated by the small number of samples. A choice between the two methods is largely based on simplicity, available data and general applicability. The Wada method is simpler, requires less data, but is also not as widely applicable as the Rao-Li method.

Adiabatic Compressibility—Here, Rao's technique is recommended (calculations made on 146 organics yielded 95% reliability limits of ±7%), but the method does require at least one known value of adiabatic compressibility. Wada's method, on the

* Liquids at their saturation pressure as opposed to compressed liquids (liquids at higher pressures).