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Computation of acoustical parameters of pure liquids through simple C-program

S B Kalyana Raman[1]*, P Vasantharani and P Selvakumari

Department of Physics, Annamalai University,
Annamalainagar-608 002, Tamil Nadu, India

E-mail : pvrselvam@yahoo.co.in

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Abstract Experimentally determined ultrasonic velocity, density and viscosity have been used to compute various acoustical parameters such as adiabatic compressibility, free length, free volume, internal pressure, *etc*. These parameters provide valuable information about the various properties of liquids and liquid mixtures. This note presents a compact C-program to compute all the important acoustical parameters of pure liquids

Keywords Acoustical parameters, pure liquids, C-program

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Ultrasonic studies seem to be a complementary technique to spectroscopic [1, 2] and dielectric [3, 4] methods. The derived acoustical parameters from the experimentally measured values of ultrasonic velocity, density and viscosity provide a tool for understanding the molecular behaviour of liquid mixtures. The excess values of these parameters and their nonlinear variations observed in liquid mixtures reveal the nature of molecular interactions. To facilitate the computation of various acoustical parameters a compact C-program is developed and presented.

The definitions and formula of the most commonly used acoustical parameters of pure liquids are briefly presented as follows:

Adiabatic compressibility :

β (pascal^{-1}) is the fractional decrease of volume per unit increase of pressure, when no heat flows in or out [5] and is given by,

$$\beta = \frac{}{\rho U^2} \qquad (1)$$

where, ρ is density in kg m^{-3} and U is ultrasonic velocity in

Free length :

L_f (meters) is the distance between the surface of the neighbouring molecules [6] and is given by

$$L_f = K_T \beta^{1/2}, \qquad (2)$$

where K_T is temperature-dependent constant (for example, it has a value of 199.53×10^{-8} at 303 K).

Free Volume :

This is the free space between the molecules for movement, denoted as V_f(m^3 mol^{-1}) and is given by [7]

$$V_f = \left(\frac{M_{eff} U}{\eta K} \right)^{1/2} \qquad (3)$$

where M_{eff} is Molecular effective weight, η is viscosity in NS m^{-2} and K is temperature independent constant (it has a value of 4.28×10^9 for all liquids).

* Corresponding Author

[1] Physics Wing, Directorate of Distant Education, Annamalai University, Annamalainagar-608 002, Tamil Nadu, India

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Internal Pressure :

π_i (poise) is the cohesive force, which is a resultant of force of attraction and force of repulsion between the molecules [8]. It can be conveniently expressed as

$$\pi_i = bRT\left[\frac{K\eta}{U}\right]^{1/2}\left[\frac{\rho^{1/3}}{M^{1/6}}\right] \quad (4)$$

where b is cubic packing, R is universal gas constant and T is absolute temperature (b has a constant value of 2 for all liquids).

Molar available volume :

V_a ($m^3\ mol^{-1}$) is difference between the molar volume at $T(K)$ and at 0 (K). It is the direct measure of the compactness and strength of bonding between the molecules of the liquid. The available volume of liquid can be calculated from combined Jacobson and Schaaff's equation [9, 10].

$$V_a = V_T\left[1 - \frac{U}{U_\infty}\right] \quad (5)$$

where V_T is molar volume at T°K and U_∞ is 1600 m/sec.

Specific acoustic impedance :

This is denoted by Z ($kg\ m^{-2}\ s^{-1}$) and for a liquid, is related to the ultrasonic velocity as given below [11]

$$Z = \rho U \quad (6)$$

Relaxation time :

This (τ sec) describes the rate at which molecules return to their original positions after being displaced by force. The relaxation time is estimated from the following relation [12]

$$\tau = \frac{4}{3}\eta\beta. \quad (7)$$

Gibb's free energy :

This (ΔG in $kJ\ mol^{-1}$) can be estimated from the following relation [13]:

$$\Delta G = -2.303\, kT \log \frac{k\,T\,\tau}{h} \quad (8)$$

where k is Boltzmann constant, T is temperature in Kelvin and h is Plank's constant.

Attenuation of ultrasonic waves is a characteristic of the material and it is represented by the *absorption coefficient*, α / f^2 ($s^2\ m^{-1}$). The attenuation constant α is given by

$$\alpha = \frac{2\omega^2\eta}{3\rho U^3} \quad (9)$$

where, ω is $2\pi f$, f is frequency

These acoustical parameters can be very easily computed using the developed simple C-program given in the Appendix The variable names representing the acoustical parameters

Table 1. Values of density (ρ), viscosity (η), ultrasonic velocity (U) and acoustical parameters of pure liquids

T = 303 K, f = 3 MHz

Liquids	ρ kg m^{-3}	η 10^{-3} NSm^{-2}	U ms^{-1}	β $10^{-10}pa^{-1}$	L_f 10^{-10} m	V_f $10^{-7}m^3$ mol^{-1}	π_i 10^6 poise	V_a $10^{-6}m^3$ mol^{-1}	Z $10^{-6}kg\ m^{-2}$ s^{-1}	τ 10^{-12} S	ΔG^* 10^{20} kJ mol^{-1}	α / f^2 $10^{-15}S^2/m$
1-propanol	769 2	1.6459	1194 3	9 1145	0 6023	0 3251	862.83	19 808	0 9186	2.0002	1.0610	33.026
1-butanol	800.5	2 2141	1231.9	8 2317	0 5724	0 2990	792 17	21.302	0 9861	2.4300	1.1424	38.899
1-hexanol	811 3	5.5230	1288 1	7 4288	0 5438	0 2578	677 97	24 552	1 0450	3 4895	1.2938	53 421
1-heptanol	814 2	4 0221	1312 7	7 1275	0.5269	0 2637	619 10	25 627	1 0688	3.8222	1 3319	57.419
1-pentanol*	806 2	2 7639	1270 3	7 6868	0 5532	0 2912	715 39	22.531	1.0241	2 8327	1.2066	43 973
Triethylamine	718 9	0.3948	1098 5	11 5270	0.6774	5 3355	229.32	44 118	0.7897	0.6067	0.5619	10 893
Benzene	867 4	0 5683	1282 2	7 0124	0 5283	2 6422	390.38	17.886	1 1122	0.5313	0.5063	8 172
Hexane*	658.6	0.3001	1054 0	13.6680	0.7376	5 9471	232 20	44.655	0.6942	0 5468	0.5184	10 232
Acetic acid*	1046 7	1 2320	1175 0	6 9198	0 5248	0 4895	924.85	15.239	1.2299	1.1367	0.8245	19 076
Propionic acid*	980.7	0 9785	1199 3	7.0895	0 5312	0 9770	611.47	18 918	1.1761	0.9249	0 7382	15.208
Butyric acid*	946 3	1 4893	1188.9	7.4763	0.5455	0.6656	604 70	23.911	1.1250	1.4846	0.9362	24.624

*Ref [14], *Ref [15], *Ref [16], The remaining Ref [13]

and the other variable names used in the program are given below :

abs	:	Absorption coefficient,
ac	:	Adiabatic compressibility,
ai	:	Acoustic impedance,
av	:	Available volume,
fl	:	Free length,
fv	:	Free volume,
ip	:	Internal pressure,
n	:	Relaxation time,
m	:	Molecular weight,
d	:	Density,
el	:	Viscosity,
u	:	Velocity,
w	:	Angular frequency,
f	:	Frequency,
t	:	Temperature (K),
$ua = u_{\alpha}$	:	1600 m/sec, and
r	:	Universal gas constant.

Using the compact, simple, and easily readable C-program, the acoustical parameters of pure liquids are readily computed without any ambiguity. The program has been executed and the values of the various acoustical parameters obtained for some (eleven) pure liquids, are compared with the previously available literature values (Table 1).

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Appendix

C - Program :

```
/*COMPUTATION OF ACOUSTICAL PARAMETERS OF
  PURE LIQUIDS THROUGH SIMPLE C PROGRAM*/

#include<stdio.h>
#include<math.h>
void main()
{
char liquid[50];
int t=303,b=2,ua=1600;
float k=1.38054e-23,h=6.6256e-34,f=3e+6;
float m,d,e1,u,k1,k2,z1,z2,a1,a2,a3,w,r;
float ac,fl,fv,ip,av,ai,rt,gfe,abs;
double x,y;
clrscr();
printf("Enter the name of liquid:");
scanf("%s",liquid),
printf("Enter the value of m,d,e1,u\n");
scanf("%e%f%e%f",&m,&d,&e1,&u);
clrscr();
printf("\t\tACOUSTIC PARAMETERS OF: %s\n",liquid);
printf("\t\t**********************\n");
k1=199.53e-8;
k2=4.28e+9;
ac=(1/(d*u*u));
printf("\t\tAdia.compressibility =%6.4e\n",ac);
fl=k1*(sqrt(ac));
printf("\t\tFree length =%6.4e\n",fl);
x=(m*u)/(e1*k2);
y=1.5;
fv=pow(x,y);
printf("\t\tFree volume =%6.4e\n",fv);
x=(k2*e1)/u;
y=0.5;
z1=pow(x,y);
x=d;
```

```
y=0.6666;
a1=pow(x,y);
x=m;
y=1.1666;
a2=pow(x,y);
z2=a1/a2;
r=8.31;
ip=b*r*t*z1*z2;
printf("\t\tInternal pressure =%6.4e\n",ip);
av=m*(1-(u/ua))/d;
printf("\t\tAvailable volume =%6.4e\n",av);
ai=u*d;
printf("\t\tAcoustic Impedance =%6.4e\n",ai);
rt=(1.3333)*ac*e1;
printf("\t\tRelaxation time =%6.4e\n",rt);
gfe=(-2.303*k*t)*log10(h/(k*t*rt));
printf("\t\tGibbs free energy =%6.4e\n",gfe);
w=2*3.14*f;
abs=(2*w*w*e1)/(3*d*u*u*u*f*f);
printf("\t\tAbsorption coefficient=%6.4e\n",abs);
getch();
```