Speeds of Sound, Densities, and Isentropic Compressibilities of 1-Iodohexane at Temperatures from (293.15 to 413.15) K and Pressures up to 200 MPa

Vyacheslav V. Melent'ev, Mikhail F. Bolotnikov,* and Yurij A. Neruchev

Department of General Physics, Laboratory of Molecular Acoustics, Kursk State University, Kursk, Radishcheva 33, Russia

Experimental speeds of sound and densities are presented for the liquid phase of 1-iodohexane. The measurements were carried out along nine isotherms from (293.15 to 413.15) K at pressures from the saturation condition up to 200 MPa. The speed of sound was measured by a pulse-phase echo ultrasonic device at a frequency of (1 to 5) MHz with an uncertainty of ±0.2%. The density was measured by an acoustic piezometer with an uncertainty of ±0.3%. The experimental results have been used to calculate the isentropic compressibility, κ_S .

Introduction

A knowledge of the thermophysical properties of organic liquids at high temperatures and pressures is of particular importance in chemical technology. In recent years, interest in measuring the speed of sound in organic liquids has considerably increased.[1,2] In contrast to the *n*-alkanes, which have been studied by tje acoustic method in a single-phase area,[3−8] their halogen-substituted analogues are less well understood.

In this article, we present speed of sound and density experimental data for 1-iodohexane in the range of temperature from (293.15 to 413.15) K at high pressure. In our earlier work,[9] we studied the speed of sound and density of 1-iodohexane at the saturation line from (293.15 to 373.15) K. To the best of our knowledge, the speed of sound and density of 1-iodohexane under high pressure have not been studied.

Experimental Section

The speed of sound was measured using a pulse-phase echo ultrasonic device[10] at a frequency of 1−5 MHz with an uncertainty of ±0.2%. For simultaneous measurements of the speed of sound and density, an acoustic piezometer method has been developed.[11] This method allows us to measure the speed of sound and density of a liquid at pressures up to 600 MPa in the temperature range from (223.15 to 523.15) K. The density was measured by an acoustic piezometer with an uncertainty of ±0.3%. The density at atmospheric pressure P_0 was measured with an Ostwald−Sprengel-type pycnometer with a capacity of approximately 50 cm^3. The uncertainty of the density measurements at atmospheric pressure was estimated to be $\pm 3 \times 10^{-5}$ g·cm^{-3}. The acoustic piezometer was thermostated with a temperature stability of ±0.01 K. The temperature was measured with a platinum resistance thermometer with an uncertainty of 0.01 K. The pressure was measured by dead-weight pressure gauge MP-2500 with a relative uncertainty of 0.02%. 1-Iodohexane used in this study (mole fraction >0.99) was supplied by Sigma-Aldrich Ltd and was used without further purification.

Results and Discussion

The experimental results of the speed of sound, u, and density, ρ, in the liquid phase of 1-iodohexane at various temperatures, T, and pressures, P, are listed in Tables 1 and 2 and are plotted as a function of temperature and pressure in Figures 1 to 4. The data presented in Tables 1 and 2 have been fitted by the following cubic polynomial for each isotherm

$$Y = A_0 + A_1 P/\text{MPa} + A_2(P/\text{MPa})^2 + A_3(P/\text{MPa})^3 + A_4(P/\text{MPa})^4 \quad (1)$$

where Y is u/(m·s^{-1}) or ρ/(kg·m^{-3}), P is pressure, and A_0, A_1, A_2, A_3, and A_4 are the adjustable parameters. All of the measured data were used in the fitting process. The values of coefficients A_i were calculated by a least-squares method. The standard deviation σ(Y) of u and ρ is defined by

$$\sigma(Y) = \left[\frac{\sum_{i=1}^{n}(Y_{\text{obsd}} - Y_{\text{calcd}})^2}{n - p}\right]^{1/2}$$

where Y_{obsd} and Y_{calcd} are the observed and calculated quantities as defined earlier, n is the total number of experimental points, and p is the number of estimated parameters. The values of parameters A_i of eq 1 and standard deviation $\sigma(Y)$ are given in Tables 3 and 4 at temperatures from (293.15 to 413.15) K, respectively. As can be seen from Figures 1 and 2, the speed of sound and density for 1-iodohexane monotonically increase with the growth of pressure along the isotherms. Changes in the speed of sound and density values both with temperature and with pressure have nonlinear character along the pronounced isotherms. Also, the maximal change in the speed of sound and density values with the change in

* To whom correspondence should be addressed. E-mail: bolotnikov@mail.ru.

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Table 1. Speed of Sound, u, in the Liquid Phase for 1-Iodohexane at Various Temperatures, T, and Pressures, P

	T/K								T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15	P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
	u/m·s^{-1}								u/m·s^{-1}						
0.1	1045.5	989.2	934.2	880.5	828.0	776.7	725.6	98.2	1318.0	1277.7	1237.7	1200.6	1166.9	1133.9	1101.0
5.00	1064.5	1008.1	954.9	901.4	849.1	802.4	753.2	108.0	1339.6	1300.0	1260.6	1224.1	1190.8	1159.1	1126.6
9.91	1082.0	1026.8	974.8	922.9	872.1	827.2	779.8	117.8	1361.6	1321.6	1282.9	1246.8	1213.8	1183.3	1152.7
19.72	1113.9	1061.9	1012.2	963.3	915.3	873.1	828.6	127.6	1383.8	1342.6	1304.5	1268.9	1236.0	1206.4	1177.1
29.53	1144.3	1094.5	1046.7	1000.4	955.2	914.8	872.6	137.4	1403.0	1363.0	1325.5	1290.4	1257.4	1228.7	1200.6
39.34	1172.4	1124.9	1078.7	1034.7	992.0	959.9	912.5	147.2	1422.2	1382.7	1345.8	1311.4	1278.2	1249.0	1223.2
49.15	1198.8	1153.5	1108.8	1066.6	1026.1	988.0	949.2	157.1	1441.0	1401.6	1365.3	1331.8	1298.6	1267.9	1244.7
58.96	1224.5	1180.6	1137.0	1096.4	1057.9	1020.6	983.3	166.9	1458.3	1419.6	1383.9	1351.7	1318.3	1292.2	1266.0
68.77	1248.5	1206.3	1163.8	1124.4	1087.6	1051.2	1015.2	176.7	1473.8	1436.5	1401.5	1370.8	1337.6	1307.3	1283.2
78.58	1272.5	1231.0	1189.4	1151.0	1115.5	1080.1	1045.3	186.5	1486.4	1452.0	1417.7	1389.1	1356.4	1327.4	1298.6
88.39	1295.5	1254.8	1214.0	1176.3	1141.9	1107.6	1073.9	196.3	1498.6	1466.0	1432.3	1406.5	1374.6	1342.7	1314.1

Table 2. Density, ρ, in the Liquid Phase for 1-Iodohexane at Various Temperatures, T, and Pressures, P

	T/K								T/K						
P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15	P/MPa	293.15	313.15	333.15	353.15	373.15	393.15	413.15
	ρ/kg·m^{-3}								ρ/kg·m^{-3}						
0.1	1437.2	1410.4	1383.6	1356.7	1329.7	1302.0	1274.0	98.2	1519.2	1503.2	1482.2	1466.3	1446.8	1432.1	1416.0
5.00	1443.5	1418.1	1391.0	1365.6	1339.0	1314.3	1286.3	108.0	1525.9	1509.9	1490.0	1474.0	1455.1	1440.7	1425.0
9.91	1448.0	1423.2	1397.0	1372.3	1346.1	1321.2	1295.7	117.8	1532.0	1516.4	1496.6	1481.2	1462.8	1448.7	1433.5
19.72	1457.8	1434.5	1408.8	1386.1	1361.1	1338.3	1314.7	127.6	1538.0	1522.6	1503.8	1488.1	1470.0	1456.4	1441.6
29.53	1466.8	1445.0	1420.0	1398.7	1375.0	1353.7	1331.7	137.4	1544.4	1528.5	1510.0	1494.7	1477.1	1463.7	1449.2
39.34	1475.0	1454.8	1430.8	1410.4	1386.4	1367.6	1346.9	147.2	1550.1	1534.3	1516.4	1501.1	1483.8	1470.6	1456.5
49.15	1483.5	1464.0	1440.1	1421.3	1398.1	1380.5	1360.8	157.1	1556.0	1539.8	1522.5	1507.1	1490.8	1477.3	1463.4
58.96	1491.0	1472.7	1449.1	1431.4	1409.0	1392.3	1373.6	166.9	1561.1	1545.1	1528.5	1513.0	1497.0	1483.7	1470.1
68.77	1498.5	1480.9	1457.5	1440.9	1418.3	1403.3	1385.4	176.7	1566.5	1550.3	1534.5	1518.6	1503.1	1489.8	1476.4
78.58	1505.3	1488.7	1466.2	1449.9	1429.2	1413.5	1396.3	186.5	1571.3	1555.2	1539.6	1524.0	1509.3	1495.7	1482.5
88.39	1512.4	1496.1	1474.3	1458.3	1438.0	1423.1	1406.5	196.3	1576.0	1560.1	1544.9	1529.3	1515.6	1501.3	1488.4

Table 3. Values of the Parameters of Equation 1 and Standard Deviation for Speed of Sound from (293.15 to 413.15) K

T/K	A_0	A_1	A_2	A_3	A_4	σ/m·s^{-1}
293.15	1045.762	3.76916	−0.01754	9.92487×10^{-5}	-2.44094×10^{-7}	1.37
313.15	988.583	4.02753	−0.01716	7.88822×10^{-5}	-1.67488×10^{-7}	0.26
333.15	933.768	4.32697	−0.01955	8.94602×10^{-5}	-1.84662×10^{-7}	0.19
353.15	879.265	4.64504	−0.02082	8.43977×10^{-5}	-1.48557×10^{-7}	0.77
373.15	826.101	4.91029	−0.02024	6.57654×10^{-5}	-8.94239×10^{-8}	1.41
393.15	775.884	5.49162	−0.02906	1.28388×10^{-4}	-2.44298×10^{-7}	5.99
413.15	725.027	5.82896	−0.03270	1.57983×10^{-4}	-3.30470×10^{-7}	1.30

Table 4. Values of the Parameters of Equation 1 and Standard Deviation for Density from (293.15 to 413.15) K

T/K	A_0	A_1	A_2	A_3	A_4	σ/kg·m^{-3}
293.15	1437.56	1.09718	-4.215×10^{-3}	1.92×10^{-5}	-4.1×10^{-8}	0.80
313.15	1410.96	1.28084	-4.785×10^{-3}	1.56×10^{-5}	-2.5×10^{-8}	0.62
333.15	1383.95	1.35739	-5.282×10^{-3}	2.04×10^{-5}	-3.7×10^{-8}	1.18
353.15	1357.17	1.58735	-6.795×10^{-3}	2.35×10^{-5}	-3.7×10^{-8}	0.67
373.15	1330.29	1.66629	-6.713×10^{-3}	2.13×10^{-5}	-3.0×10^{-8}	1.67
393.15	1302.97	1.96799	-9.485×10^{-3}	3.43×10^{-5}	-5.5×10^{-8}	1.13
413.15	1274.45	2.24389	-0.012×10^{-3}	4.62×10^{-5}	-7.7×10^{-8}	1.01

pressure and temperature occurs in the range of small pressures and high temperatures.

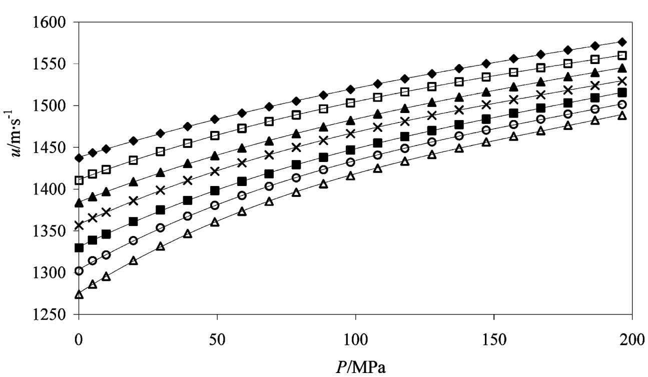

Figure 1. Speed of sound in the liquid phase of 1-iodohexane as a function of pressure: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

Isentropic compressibilities κ_S of 1-iodohexane were calculated from the Laplace equation

$$\kappa_S = \frac{1}{\rho u^2} \tag{3}$$

where u is the sound velocity and ρ is the density. The values of isentropic compressibilities κ_S for 1-iodohexane as a function of pressure at constant temperature are plotted in Figure 3. The uncertainty in the calculated isentropic compressibilities κ_S is 1%. The isentropic compressibility carries more information on the intensity of intermolecular interactions in liquids. It is well known that a larger intensity of intermolecular interaction corresponds to a lower isentropic compressibility. As was shown in previous work,[9] the isentropic compressibility of haloalkanes on the saturation line is less than the isentropic compressibility of the n-corresponding alkanes. From Figure 3, it follows that along isotherms with an increase in

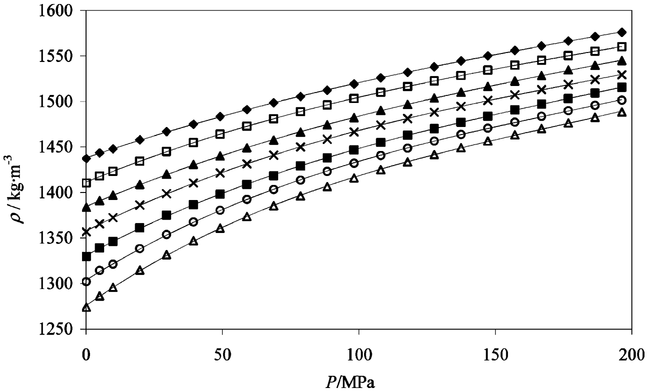

Figure 2. Density in the liquid phase of 1-iodohexane as a function of pressure: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

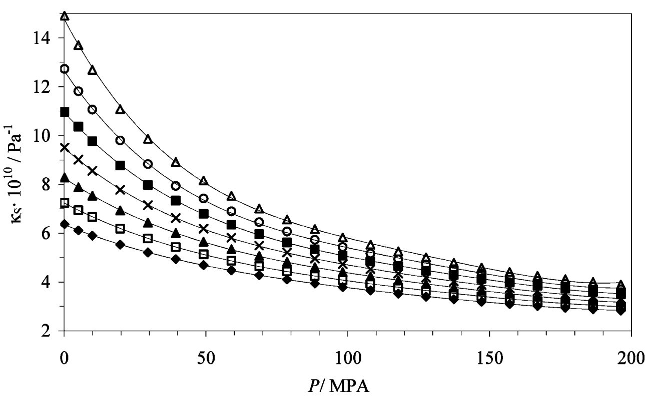

Figure 3. Pressure dependence, P, of isentropic compressibilities, κ_S, in the liquid phase of 1-iodohexane: ◆, 293.15 K; □, 313.15 K; ▲, 333.15 K; ×, 353.15 K; ■, 373.15 K; ○, 393.15 K; △, 413.15 K.

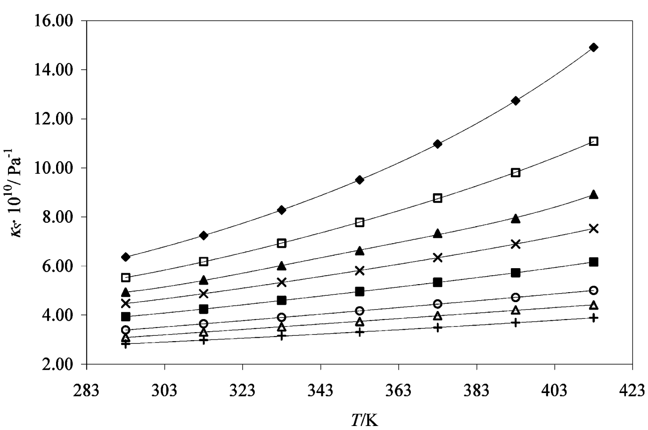

Figure 4. Temperature dependence, T, of isentropic compressibilities, κ_S, in the liquid phase of 1-iodohexane: ◆, 0.1 MPa; □, 19.72 MPa; ▲, 39.34 MPa; ×, 58.96 MPa; ■, 88.39 MPa; ○, 127.6 MPa; △, 157.1 MPa; +, 196.3 MPa.

pressure the intensity of intermolecular interaction increases for 1-iodohexane. From Figure 4, it follows that along isobars with an increase in temperature the intensity of intermolecular interaction for 1-iodohexane decreases.

In refs 12 and 13, a linear relationship was observed between u^3 and P

$$u^3 = {u_0}^3 + K(P - P_0) \tag{4}$$

where u is the speed of sound at some pressure P, u_0 is the speed of sound at atmospheric pressure P_0, and K is a pressure-independent constant. The values of coefficients u_0 and K for 1-iodohexane were calculated by the least-squares method and are presented in Table 5. In the same Table, the values of the standard deviation σ defined by the relation

Table 5. Values of the Parameters of Equation 4 and Standard Deviation σ

T/K	u_0/m·s^{-1}	K/m^4·kg^{-1}·s^{-1}	σ/m^3·s^{-3}
293.15	1050.4	11.531	5.3×10^7
313.15	993.9	11.221	3.3×10^7
333.15	938.3	10.897	2.4×10^7
353.15	881.2	10.691	1.3×10^7
373.15	828.8	10.344	1.8×10^7
393.15	780.1	10.993	2.6×10^7
413.15	722.6	9.793	3.2×10^7

Table 6. Values of the Parameters of Equation 6 and Standard Deviation σ

T/K	u_0/m·s^{-1}	K_0/m^4·kg^{-1}·s^{-1}	K_1/m^5·kg^{-2}·s	σ/m^3·s^{-3}
293.15	1044.7	12.125	-3.003×10^{-9}	5.8×10^7
313.15	988.6	11.715	-2.497×10^{-9}	2.3×10^7
333.15	934.3	11.228	-1.674×10^{-9}	1.9×10^7
353.15	881.6	10.665	0.134×10^{-9}	1.3×10^7
373.15	825.3	10.567	-1.129×10^{-9}	1.2×10^7
393.15	775.6	10.259	-1.296×10^{-9}	2.1×10^7
413.15	719.1	9.962	-0.854×10^{-9}	3.5×10^7

$$\sigma = \left[\frac{\sum_{i=1}^{n}(u_{\text{obsd}}^3 - u_{\text{calcd}}^3)^2}{n - p}\right]^{1/2}$$

are presented, where u_{obss} and u_{calcd} are the observed and calculated quantities as defined earlier, n is the total number of experimental points, and p is the number of parameters. However, as was shown later[14] parameter K shows a slight linear increase with increasing pressure at temperatures greater than 333 K

$$K = K_0[1 + \alpha(P - P_0)] \tag{5}$$

where K_0 and α are new constants. A new relationship between u^3 and P can be obtained by combining eqs 4 and 5:

$$u^3 = u_0^3 + K_0(P - P_0) + K_1(P - P_0)^2 \tag{6}$$

The values of parameters u_0, K_0, $K_1 = K_0\alpha$, and standard deviation σ for 1-iodohexane determined by the least-squares method are listed in Table 6. Deviations, calculated from eqs 4 and 6, of the values of the speed of sound at P_0 from experimental values for 1-iodohexane as a function of temperature are presented in Figure 5. As can be seen

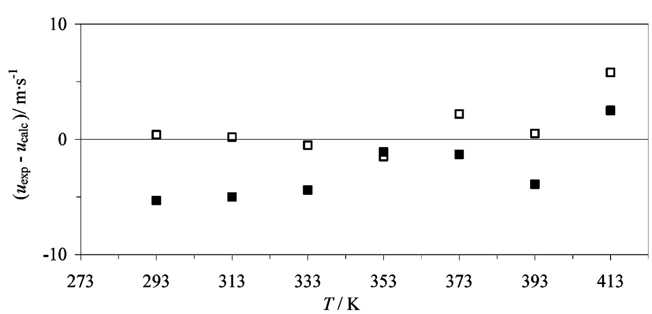

Figure 5. Deviations of calculated values of the speed of sound at P_0 from experimental values for 1-iodohexane as a function of temperature: □, eq 6; ■, eq 4.

from Figure 5, the speed of sound values calculated from eq 6 are preferred to those calculated from eq 4.

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