Densities, isobaric thermal expansion coefficients and isothermal compressibilities of linear alkylbenzene

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Abstract

We report the measurements of the densities of linear alkylbenzene at three temperatures over 4 to 23 °C with pressures up to 10 MPa. The measurements have been analysed to yield the isobaric thermal expansion coefficients and, so far for the first time, isothermal compressibilities of linear alkylbenzene. Relevance of results for current generation (i.e., Daya Bay) and next generation (i.e., JUNO) large liquid scintillator neutrino detectors are discussed.

Keywords: neutrino oscillation, neutrino mixing, density, isobaric thermal expansion coefficient, isothermal compressibility, Daya Bay, JUNO

1. Introduction

Linear alkylbenzene (LAB), with a formula of C₆H₅CₙH₂n₊₁ (n = 10–13), is the solvent of a liquid scintillator (LS) in large LS detectors, such as Daya Bay [1–5], RENO [6], and JUNO (formerly called Daya Bay II) [7–9]. It has been reported that LAB would be the preferred solvent for a large-volume detector because of its high transparency [10]. The precision measurement for the density of LAB is important to determine the target mass of the detector and then the total number of free protons (hydrogen nuclei). The uncertainty of the number of protons comes from the target mass and the hydrogen fraction in the target. Daya Bay (and RENO and Double Chooze) determines θ₁₃ by relative measurements with near and far detectors at different baselines. Therefore, the uncertainty from the hydrogen fraction will cancel out. The uncertainty from the target mass will impact the θ₁₃ measurement directly. Very careful target mass measurements were conducted in Daya Bay, with a specialized 20-ton filling tank equipped with load cells and Coriolis flow meters, as described in [1]. The precision is 0.02%. The number of protons (and consequently the absolute efficiency) has negligible impact on the θ₁₃ measurement. But it is important in other studies such as measurement of the reactor neutrino flux (and consequently the so-called reactor anomaly phenomenon). It is also necessary to obtain the isobaric thermal expansion coefficient and isothermal compressibility of LAB to accurately describe the relations between the density of LAB with temperature and pressure. The JUNO detector will locate at 700 m underground. The rock temperature has measured to be 31 °C. The temperature of the underground hall and the big water pool that contains the LS detector will be controlled at 20 ± 1 °C during operation. The density of LAB changes with temperature which results in the expansion or shrink of the volume of the LS for a given mass. The detector will be filled 100% for uniform response. A overflow tank will accommodate the liquid due to thermal expansion. It is important to estimate the overflow volume of the central detector of JUNO by using the isobaric thermal expansion coefficient. The density of LAB also changes with pressure.
The largest pressure difference for LAB would be about 0.3 MPa for the central detector of JUNO whose diameter would be about 35 m. The isothermal compressibility of LAB, which had not been measured yet, is imperative for the calculation of the Rayleigh scattering lengths of LSs [10–14].

In this paper, we report the measurements for the densities of LAB from 4 to 23 °C and at pressures up to 10 MPa. We have derived the isobaric thermal expansion coefficients and the isothermal compressibilities of LAB from the data of densities.

2. Experimental method

The compressed liquid density of LAB was measured by the vibrating tube method and the whole measurement system was developed by the Thermodynamic Research Group in Xi’an Jiaotong University [15, 16]. The schematic diagram of the whole measurement system could be found in [15] and [16]. The measurement system contains a tube densimeter Anton Paar DMA-HPM (dimensions: 210 mm × 78 mm × 86 mm) with a measuring cell whose volume is about 2 ml where a U-shaped Hastelloy C-276 tube could be excited electronically to vibrate at the characteristic frequencies of liquid LAB at various temperatures and pressures. The evaluation unit mPDS 2000V3 connected to the tube densimeter could indicate the vibration period with seven significant digits. The tube densimeter was thermostated by an external thermostatic bath. The measuring cell was insulated from the environment. The temperature of the vibrating tube cell was measured using a 100 Ω platinum resistance thermometer which had been calibrated over the experimental temperature range against a 25 Ω reference thermometer certified by the National Institute of Metrology of China. The uncertainty of temperature measurement was estimated to be within ±0.02 °C. The pressure of measurement system was applied by a piston pump HIP 50-5.75-30 and measured by a high pressure transducer HBM P3MB. A data acquisition unit (Agilent 34970A) was employed for the transformation of the pressure transducer measurement signal. The uncertainty of pressure measurement was estimated to be within ±0.06 MPa. The density measurement system had been calibrated by water and vacuum over the entire temperature and pressure range with the method proposed by Lampreia and Nieto de Castro [17]. The uncertainty of density measurement for the LAB sample was estimated to be within ±0.4 kg m⁻³.

A vacuum test was applied to the entire system where the pressure had been lower than 10 Pa to ensure the precision and safety of measurements. The entire system had been firstly purged by acetone, and then blown dry three times using flowing nitrogen gas, and finally purged using the dry flowing nitrogen gas again after one or two days. The process of purge was repeated three times prior to the measurements. The sample of LAB was provided by the China Jinling Petrochemical Limited Corporation. The attenuation length of the LAB from the same batch is about 20 m [18]. It was purified by three freeze-pump-thaw cycles via liquid nitrogen prior to measurements. A vacuum was applied to the entire pipe circuit to remove air or nonvolatile gases, and then the LAB sample was loaded into the pipe circuit using corresponding valve operations. When the temperature for the vibrating tube stabilized, the vibration period of the U-tube could be determined from the change of pressure between the initial pressure and the maximum pressure.

3. Results

The compressed densities of LAB were measured at temperatures 4, 15, and 23 °C and at pressures 0.1, 0.3, 0.5, 2, 4, 6, 8, and 10 MPa. A total of 24 points were obtained, as listed in Table 1. The density of LAB decreases with temperature and increases with pressure.

| p [MPa] | 0.10 | 0.30 | 0.50 | 2.00 | 4.00 | 6.00 | 8.00 | 10.00 |
|---------|------|------|------|------|------|------|------|-------|
| T [°C]  | 4.00 | 869.0| 869.1| 869.2| 870.1| 871.4| 872.6| 873.7 | 874.9 |
| T [°C]  | 15.02| 860.7| 860.9| 861.0| 861.9| 863.2| 864.4| 865.7 | 866.9 |
| T [°C]  | 22.98| 854.5| 854.7| 854.8| 855.8| 857.1| 858.4| 849.6 | 860.9 |

The fitting curves of ρ(T) at eight pressures.
Table 2. The fitting parameters for density $\rho(T)$ of LAB.

| $p$ [MPa] | 0.10  | 0.30  | 0.50  | 2.00  | 4.00  | 6.00  | 8.00  | 10.00 |
|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| $\rho_0$ [kg m$^{-3}$] | 854.6 ± 0.1 | 854.7 ± 0.1 | 854.8 ± 0.1 | 855.8 ± 0.1 | 857.1 ± 0.1 | 858.4 ± 0.1 | 859.6 ± 0.1 | 860.9 ± 0.1 |
| $\beta_0$ [$10^{-4}$ °C$^{-1}$] | 8.894 ± 0.094 | 8.893 ± 0.099 | 8.879 ± 0.104 | 8.833 ± 0.092 | 8.756 ± 0.087 | 8.704 ± 0.098 | 8.629 ± 0.093 | 8.564 ± 0.084 |
3.1. Isobaric thermal expansion coefficients

The isobaric thermal expansion coefficient $\beta$ is defined as

$$\beta = -\frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_p = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p,$$  \hspace{0.5cm} (1)$$

where $V$ is the volume, $p$ is the pressure, $T$ is the temperature, and $\rho$ is the density. The isobaric thermal expansion coefficients could be derived from the empirical equation of state

$$\rho(T) = \rho_0 \left[ 1 - \beta_0(T - T_0) \right],$$  \hspace{0.5cm} (2)$$

where $T_0$ is 23 °C which is the operating temperature for Daya Bay antineutrino detectors, $\beta_0$ is the isobaric thermal expansion coefficient at $T_0$, and $\rho_0$ is the density at $T_0$. The fitting curves are shown in figure 1, the fitting parameters are listed in table 2 and $\beta_0$ is shown in figure 2. The relationship between isobaric thermal expansion coefficient and temperature at a given pressure could be derived by equations (1) and (2) which is

$$\beta(T) = \frac{\beta_0}{1 - \beta_0(T - T_0)}.$$

By using the parameters in table 2, $\beta(T)$ at 0.1 MPa with 1σ band is shown in figure 3.

3.2. Isothermal compressibility

The isothermal compressibility $\kappa$ is defined as

$$\kappa = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)_T,$$  \hspace{0.5cm} (4)$$

where $V$ is the volume, $p$ is the pressure, $T$ is the temperature, and $\rho$ is the density. The isothermal compressibilities at different temperatures could be derived from the empirical equation of state [20]

$$\rho(p) = \frac{\rho_0}{1 - \kappa_0(p - p_0) - \kappa_0'(p - p_0)^2},$$  \hspace{0.5cm} (5)$$

where $p_0$ is 0.101325 MPa, $\rho_0$ is the density at $p_0$, $\kappa_0$ is the isothermal compressibility at $p_0$, and $\kappa_0'$ equals to $\frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)|_{p=p_0}$. The fitting curves are shown in figure 4, the fitting parameters are listed in table 3, and $\kappa_0$ is shown in figure 5. It could be shown in figure 5 that the isothermal compressibility $\kappa_0$ increases with temperature. The relationship between the isothermal compressibility and pressure at a given temperature could be derived by equations (4) and (5) which is

$$\kappa(p) = \frac{\kappa_0 + 2\kappa_0'(p - p_0)}{1 - \kappa_0(p - p_0) - \kappa_0'(p - p_0)^2}.$$

Table 3. The fitting parameters of $\rho(p)$ for LAB.

| $T$ [K] | $\rho_0$ [$\text{kg m}^{-3}$] | $\kappa_0$ [10$^{-4}$ MPa$^{-1}$] | $\kappa_0'$ [10$^{-6}$ MPa$^{-2}$] |
|---------|-----------------|-----------------|-----------------|
| 4.00    | 868.974 ± 0.005 | 7.129 ± 0.035  | -3.391 ± 0.363  |
| 15.02   | 860.721 ± 0.003 | 7.478 ± 0.019  | -3.390 ± 0.194  |
| 22.98   | 854.533 ± 0.005 | 7.743 ± 0.035  | -3.258 ± 0.364  |
By using the parameters in table 3, $\kappa(p)$ at 22.98 °C with 1σ band is shown in figure 6. The isothermal compressibility $\kappa(p)$ decrease with pressure since the corresponding $\kappa'_0$ is negative.

4. Conclusions

We measured the densities of LAB at 4, 15, and 23 °C and at 0.1, 0.3, 0.5, 2, 4, 6, 8, and 10 MPa. The isobaric thermal expansion coefficients at eight pressures and the isothermal compressibilities at three temperatures were derived by fitting the empirical equations of state. The isobaric thermal expansion coefficient at 19 °C at 0.1 MPa is consistent with the one for the gadolinium-doped LS (Gd-LS) of Daya Bay within the margin of error [1]. The expansion and contraction of LAB caused by the temperature change per degree around 20 °C would be about 20 m$^3$ for the 35 m diameter central detector of JUNO. The density, isobaric thermal expansion coefficient, and isothermal compressibility of LAB change largely with temperature while they change insignificantly at the pressure difference of 0.3 MPa caused by the large scale of the central detector of JUNO.

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