Crystals of $\beta$-barium borate ($\beta$-BaB$_2$O$_4$) are new nonlinear optical materials and are of great practical interest. They exhibit a strong nonlinearity of optical properties and a high conversion coefficient in a wide spectral range, indicating that these crystals hold promise in applications as laser frequency converters. The $\beta$-BaB$_2$O$_4$ crystals are low-temperature modifications of Ba$_2$O$_3$ and possess a trigonal crystal structure (space group $R3c$) with lattice parameters $a = 8.380$ Å, $a = 96.65^\circ$ (in hexagonal axes $a = b = 12.519$ Å and $c = 12.723$ Å (Ref. 4)). A high-temperature form of barium borate ($\alpha$-BaB$_2$O$_4$), crystallizing into a trigonal crystal structure (space group $R3c$) with lattice parameters in hexagonal axes $a = b = 7.235$ Å, $c = 39.192$ Å, also exists. The $\alpha$-BaB$_2$O$_4$ crystals possess a centrosymmetric crystal structure, while $\beta$-BaB$_2$O$_4$ crystals are noncentrosymmetric and are of greatest practical interest as nonlinear optical materials. The optical properties of $\beta$-BaB$_2$O$_4$ which characterize these crystals as laser radiation converters have been studied quite well, while investigations of the dynamic characteristics of these crystals are only beginning. The results of an investigation of the thermal expansion of $\beta$-BaB$_2$O$_4$ in a wide range of temperatures above room temperature are presented in Ref. 6, and it is shown there that these crystals exhibit a strong thermal expansion anisotropy.

It was of great interest to investigate the crystallographic parameters and thermal expansion of $\beta$-BaB$_2$O$_4$ crystals at low temperatures, especially since such information is lacking in the literature. The $\beta$-BaB$_2$O$_4$ crystals were flux-grown on a seed crystal from the surface of a Na$_2$O–B$_2$O$_3$-BaO flux following the technology presented in Ref. 7. Synthesis was conducted in a furnace with a vertical arrangement of SiC heaters. The temperature was monitored with a platinum–constantan thermocouple. This system made it possible to maintain the temperature to within 0.1 K in the experimental temperature range. Before each profile of the diffraction reflection intensity was recorded, the sample was held for ~20 min at a fixed temperature. The parameters $a$ and $c$ were measured with a temperature step of 20 K.

The temperature dependences of the experimental values of the $\beta$-BaB$_2$O$_4$ lattice parameters $a$ and $c$ in the temperature range 80–300 K and $a$ and $c$ in the temperature range 80–190 K were approximated by a quartic polynomial with coefficients

\[
L_0 = 12.539, \quad A = -1.390 \times 10^{-5}, \quad B = 9.375 \times 10^{-8}, \quad C = -3.281 \times 10^{-10}, \quad D = 4.984 \times 10^{-13}.
\]

The curves of the temperature dependence of the lattice parameters $a = f(T)$ and $c = f(T)$ as well as the cell volume $V = f(T)$ were approximated by a quartic polynomial with coefficients $L_0 = 12.539$, \( A = -1.390 \times 10^{-5} \), $B = 9.375 \times 10^{-8}$, \( C = -3.281 \times 10^{-10} \), and $D = 4.984 \times 10^{-13}$.
coefficients: For \( c = f(T) \) \( L_0 = 12.624 \), \( A = 1.226 \times 10^{-5} \), \( B = 9.899 \times 10^{-8} \), \( C = -1.411 \times 10^{-10} \) and for \( V = f(T) \) \( L_0 = 1716.170 \), \( A = 1.894 \times 10^{-3} \), \( B = 2.198 \times 10^{-10} \), and \( C = 6.012 \times 10^{-11} \). As one can see from Figs. 1 and 2, the analytical expression employed describe well the temperature dependences of the experimental values of the lattice parameters \( a \) and \( c \) (solid lines) and the volume \( V \) (dots). The thermal expansion coefficients as functions of temperature were determined from the equation

\[
\alpha = \frac{dL/dT}{L_0} = A + 2BT + 3CT^2 + 4DT^3.
\]

(1)

Hence the temperature dependences of the linear thermal expansion coefficients \( \alpha_a \) and \( \alpha_c \) of crystal \( \beta\text{-BaB}_2\text{O}_4 \) in the temperature range 80–300 K along the crystallographic axes and the volume coefficient \( \alpha_V \) can be represented in the form of the following expressions:

\[
\alpha_a = -1.390 \times 10^{-5} + 1.875 \times 10^{-7}T - 9.843 \times 10^{-10}T^2 + 1.994 \times 10^{-12}T^3,
\]

\[
\alpha_c = 1.226 \times 10^{-5} + 1.980 \times 10^{-7}T - 4.233 \times 10^{-10}T^2,
\]

\[
\alpha_V = 1.894 \times 10^{-5} + 4.396 \times 10^{-10}T + 1.804 \times 10^{-10}T^2.
\]

(2)

As follows from the experimental results presented (Fig. 1), the \( \beta\text{-BaB}_2\text{O}_4 \) lattice parameter \( c \) increases smoothly and practically linearly with increasing temperature in the investigated temperature range. The temperature dependence \( a = f(T) \) is more complicated. As the temperature increases, \( a \) at first decreases somewhat and then increases beginning at \( T \sim 190 \) K. However, it should be noted that in this temperature range the parameter \( a \) varies not in hundredths of an angstrom, as in the case of the parameter \( c \), but rather in thousands of an angstrom. On account of the substantial increase in the parameter \( c \) with temperature, the \( \beta\text{-BaB}_2\text{O}_4 \) unit cell volume also increases continuously (Fig. 2).

Figure 3 displays the temperature dependences of the thermal expansion coefficients \( \alpha_a \) and \( \alpha_c \) in crystallographic directions perpendicular and parallel, respectively, to the hexagonal axis \( c \) and the volume coefficient \( \alpha_V \). It follows