

determined isomekes for the almandine-quartz combination; and (2) the demonstration that extreme variations in composition of garnet cause only small variations in the trajectories of the isomekes. Referring to Equation (7), the minor effect of major compositional departures probably reflects the fact that the changes, respectively, in  $\alpha_g$  and  $\beta_g$  due to compositional variation at any  $P$  and  $T$  are small relative to  $(\alpha_q - \alpha_g)$  and  $(\beta_q - \beta_g)$  at the same  $P$  and  $T$ . This contrast in the properties of garnet and quartz, besides increasing sensitivity, thus becomes another asset of this pair of minerals for solid inclusion piezothermometry. The petrologist using the pair garnet-quartz will, for most occurrences, be working with garnets much closer to almandine than to the other garnets considered. It should therefore be justifiable for him to use isomekes derived for quartz and almandine-type garnet with only approximate determination that he is dealing with this type of garnet.

One additional conclusion from this work is the large difference between coefficients of thermal expansion of garnet, deduced below, and those obtained by X-ray diffraction on synthetic garnets (Skinner, 1956). Near 25°C and 1 bar, the data for one isomeke in Figure 4 very nearly parallel the temperature axis. Using the known properties of quartz referred to in Part I and the compressibility of almandine-type garnet (designated by  $a$ ),  $\beta_a = 0.189 \times 10^{-6} \text{bar}^{-1}$  (Soga, 1967), Equation (7) suggests that, near 25°C and 1 bar,

$$\alpha_{q||c} \approx \alpha_a \approx 7.56 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}.$$

Using this same equation, the compressibility of spinel ( $s$ ),  $\beta_s$  mentioned in Part I, our calculated value of  $\alpha_{s0} = 5.72 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$ , and the slope of an isomeke for the same garnet relative to spinel at its intercept with the temperature axis (60°C instead of 25°C), we obtain  $\alpha_{a0} = (7.58 \pm 0.14) \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$ . There is close agreement between our two independently determined values, which are ~39 percent larger than thermal expansions derived from the X-ray work of Skinner (1956) on synthetic almandine.

The differences between the previous data on thermal expansion for garnet and values inferred above account for the marked discordance between the calculated isomekes of Rosenfeld (1969) and those presented in this paper. Revised geological interpretations based upon the correct measurements are discussed below.

## Representation and Interpolation of Experimental Results

Were satisfactory equations of state for almandine and low quartz available, smoothing of experimental data and presentation of results would be easily accomplished utilizing these equations in the manner previously discussed. No such equations of state, valid throughout the pressure and temperature region of our experimentation, have been advanced. Much of the theoretical problem lies with changes in physical properties which are precursors to the low-high transition of quartz; some of these precursory phenomena are readily detected more than 75°C below the transition (Klement and Cohen, 1968).

Empirical methods were thus used to smooth and present the quartz-almandine data. The technique presented here yielded a relatively simple representation which, although suitable for geological applications, is not suitable for accurate equations of state.

The empirical equation is an excellent fit to the data for quartz  $\perp c$ -almandine and quartz 45° to  $c$ -almandine; the empirical equation fits the quartz  $||c$ -almandine data with less precision, although suitably for petrological purposes, to within 75° of the low-high transition. Progressive deviation of the empirical equation from the experimental data within ~75°C of the transition undoubtedly is an artifact of the mathematical form and simplicity of the equations.

The desired equation should generate isomekes as a function of temperature, pressure, and orientation of quartz. No single integrated equation was found to do this, although a differential equation was. The calculated quartz-almandine isomekes were thus obtained by numerical integration of

$$\frac{dP}{dT} = a_1 + a_2P + (a_3 + a_4P) \ln(T_\lambda - T) \quad (8)$$

where

$$a_1 = 56.391 + 13.323 \sin^2\theta - 23.646 \sin^4\theta \quad (9a)$$

$$a_2 = -9.241 \times 10^{-4} - 4.881 \times 10^{-3} \sin^2\theta + 7.718 \times 10^{-3} \sin^4\theta \quad (9b)$$

$$a_3 = -7.948 - 3.011 \sin^2\theta + 3.526 \sin^4\theta \quad (9c)$$

$$a_4 = 2.147 \times 10^{-4} + 7.634 \times 10^{-4} \sin^2\theta - 1.333 \times 10^{-3} \sin^4\theta \quad (9d)$$

and

$$T_{\lambda} = 573.2 + 0.02683P - 0.1435 \times 10^{-6}P^2 \quad (10)^e$$

$P$  is in bars and  $T$  in °C.

Briefly, coefficients in Equation (8) were obtained by numerical techniques as follows: The experimental data for one isomeke were ordered in ascending temperature or pressure, depending upon the slope of the isomeke. An arbitrary interval of 25°C was chosen, and data points which are separated by a distance greater than or equal to this arbitrary interval were selected by the computer starting from the lowest temperature or pressure. This ordered set was the basis of all succeeding calculations.

Next, the derivative of the isomeke,  $dP/dT_i$ , was found at each point  $T_i$  in succession by the Lagrangian interpolation polynomial of degree 2. Except at the end points,  $dP/dT_i$  was obtained using  $T_i$  and the adjacent higher and lower temperature points. The derivatives at the end points were found from the first three and last three points.

Each experimental determination of an isomeke was processed in this manner. All  $dP/dT$  values for isomekes involving a specific orientation of quartz were then grouped together and a smooth surface of the form of Equation (8) best fit by least squares analysis. For each of the three orientations of quartz utilized in the experiments, values of  $a_1$ ,  $a_2$ ,  $a_3$ , and  $a_4$  were found. Thus 12 coefficients were determined. Finally, a quadratic equation was fitted to each coefficient  $a$  as a function of the orientation of the quartz,  $\theta$ . These quadratics are given in Equations (9a-9d).

The isomekes for almandine together with any arbitrary orientation of quartz were then obtained by standard numerical integration techniques using Equation (8). These curves, spaced at intervals of 0.2 in  $\sin^2\theta$ , are given in Figure 8. Also, Figure 9 is a "fan" of isomekes emanating from  $P = 1$  bar and  $T = 25^\circ\text{C}$  at intervals of 0.1 in  $\sin^2\theta$  for petrographic convenience (see footnote 5; also cf Rosenfeld, 1969, p. 334-345).

A number of equations other than Equation (8) were examined to obtain a representation of all the data. Some utilized functions other than  $\ln(T_{\lambda} - T)$ ; others utilized additional terms. No consistently

better representation was found to fit *all* the data, although some may have yielded better representations in limited regions. Some equations with more coefficients may have fit the data just as well, but the simpler equation was chosen for presentation here. The  $\ln(T_{\lambda} - T)$  term allows presentation of an equation of simple form that approximates our data. This logarithmic term, however, has no particular theoretical basis and its behavior may cause deviations from a good fit to the quartz ||*c*-almandine data. Caution should be used in applying Equation 8 outside the region within which we have applied it.

### Geological Applications

Ideally one should be able to use solid inclusion piezothermometry alone to determine  $P - T$  conditions of metamorphism; the most precise such determinations would employ location of isomekes crossing at relatively high angles. For example, using thin sections of garnets with quartz inclusions in conjunction with Figure 8, such high-angle intersections would require finding conditions for elimination of birefringent halos around quartz grains having both low and high inclinations,  $\theta$ , of the *c* axis to the section normal. When applying solid inclusion piezothermometry to location of the  $\text{Al}_2\text{SiO}_5$  triple point, commercially available heating stages are suitable for determining such null conditions for quartz grains with low  $\theta$ . To obtain null conditions with quartz grains having high  $\theta$ , however, requires use of a high aperture window bomb. Thus, pending completion of such an optical high pressure device, we have not been able to investigate null conditions of halos for grains with values of  $\theta$  sufficiently far apart to give accurate "triangulation" in  $P - T$  space.

Instead of using piezobirefringent halos around quartz inclusions in garnet alone, we have thus been forced to combine their use with additional petrological data as was done by Rosenfeld (1969, p. 335-345) to infer pressures and temperatures of crystallization. In that paper isomekes were generated using the limited information on coefficients of compressibility and thermal expansion then available. For any particular temperature, the pressures implied in Figure 8 of that paper are higher than they would be using the isomekes of Figure 9 in this paper. The discrepancies, though not large ( $\sim 1.5$  kbar), result largely from coefficients of thermal expansion previously available for garnet, coefficients

<sup>e</sup> From preliminary work on the low-high quartz transition. More extensive work (Cohen, Klement, and Adams, 1974) suggests that the coefficient of the  $P^2$  term may be negligible and that slight alteration in the coefficient of the  $P$  term may be appropriate. Such modifications have no significant effect on our results.