American Mineralogist, Volume 97, pages 707–712, 2012

Crystal structure and thermal expansion of aragonite-group carbonates by single-crystal X-ray diffraction

Yu Ye,[1,*] Joseph R. Smyth,[2] and Paul Boni[2]

[1]Department of Physics, University of Colorado, Boulder, Colorado 80309, U.S.A.
[2]Department of Geological Sciences, University of Colorado, Boulder, Colorado 80309, U.S.A.

Abstract

Crystal structures of four aragonite-group carbonates—aragonite ($Ca_{0.997}Sr_{0.003}CO_3$), calcian strontianite ($Ca_{0.147}Sr_{0.853}CO_3$), cerussite ($Ca_{0.001}Pb_{0.999}CO_3$), and witherite ($Sr_{0.019}Ba_{0.981}CO_3$)—have been refined at ambient conditions, and thermal expansion has been measured over a range of temperatures from 143 to 586 K by single-crystal X-ray diffraction. Average linear thermal expansion coefficients $\alpha_0(V)$ are 58(2), 58.3(7), 64(2), and 57(2) ($\times 10^{-6}$ K^{-1}) for aragonite, strontianite, cerussite, and witherite, respectively, throughout the experimental temperature range. Aragonite, strontianite, and witherite have very similar $\alpha_0(V)$ values, whereas that of cerussite is significant larger, primarily due to the *c*-axis thermal expansion for cerussite being much larger than those of the other carbonates. There are no significant differences for $\alpha_0(a)$ values among the four carbonates, whereas $\alpha_0(b)$ values decrease in the order of aragonite > strontianite > cerussite ≈ witherite, and $\alpha_0(c)$ values increase in the order of aragonite < strontianite < witherite < cerussite. Crystal structures were refined for aragonite (184 to 527 K). <Ca-O> vs. *T* (K) is fitted linearly quite well, with a slope of $5.8(8) \times 10^{-6}$ (Å/K). Corrected for assumed rigid body motion, the CO_3 groups showed no significant change in C-O distances over the temperature range.

Keywords: Aragonite, strontianite, cerussite, witherite, thermal expansion, crystal structure