Diffusion of C and O in calcite at 100 MPa

T.C. LABOTKA,[1,*] D.R. COLE,[2] AND L.R. RICIPUTI[2]

[1]Department of Geological Sciences, University of Tennessee, Knoxville, Tennessee 37996-1410, U.S.A.
[2]Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6110, U.S.A.

ABSTRACT

The diffusivities of C and O in calcite were determined in a pure CO_2 atmosphere at 100 MPa and temperatures ranging from 600 to 800 °C. The calcite crystals were preannealed and H_2O was excluded from the system to determine the self-diffusion coefficients. The CO_2 consisted of 99% ^{13}C and 90% ^{18}O. After heating for 7–147 d, diffusion profiles were measured with the use of secondary ion mass spectrometry. The results indicate that the diffusivity of C is $D_C = 7.77 \times 10^{-9} \exp(-166 \pm 16 \text{ kJ/mol}/RT)$ cm²/s and of O is $D_O = 7.5 \times 10^{-3} \exp(-242 \pm 39 \text{ kJ/mol}/RT)$ cm²/s. In comparison with other determinations of diffusivities in calcite, diffusion of O under the experimental conditions is consistent with vacancy migration in the intrinsic region, and diffusion of C seems to occur by diffusion of carbonate anions. Increased pressure appears to reduce the activation energy and the value of D_0, and the presence of H_2O greatly increases the diffusivity of O without appreciably changing the activation energy. Closure temperatures calculated for isotopic exchange by diffusion predict that C isotope compositions of calcite are preserved during cooling in most geologic environments, but that O isotope compositions in H_2O-rich environments are preserved only in rapidly cooling environments, such as contact metamorphic aureoles.