American Mineralogist, Volume 93, pages 177–186, 2008

The crystal structure of diopside at pressure to 10 GPa

Richard M. Thompson* and Robert T. Downs

Department of Geosciences, University of Arizona, Tucson, Arizona, 85721-0077, U.S.A.

Abstract

The crystal structure of diopside has been determined at various pressures to 10.16 GPa. The results to 5 GPa are consistent with Levien and Prewitt (1981). The crystal structures have been analyzed using the geometric pyroxene model of Thompson and Downs (2004), the anion packing algorithm of Thompson and Downs (2001), and a new algorithm that quantifies the distortion of observed pyroxenes from their geometric model equivalents. Diopside is shown to compress via three main mechanisms: isotropic scaling, kinking of the tetrahedral chains, and collapse of the M1 chain toward its axis. The kinking of the chains accounts for most of the anisotropy of compression observed in the **a-c** plane, and the collapse of the M1 chain explains the anisotropy seen in the **b-c** plane. Model behavior is shown to reproduce many of the observations of previous workers. Anion-anion interactions are shown to be important in the distortion of observed diopside from its geometric model equivalent.

Keywords: Diopside, crystal structure, high-pressure, model pyroxene