American Mineralogist, Volume 97, pages 407–414, 2012

High-pressure behavior of space group *P*2/*n* omphacite

Francesco Pandolfo,[1,*] Fabrizio Nestola,[2] Fernando Cámara,[3] and M. Chiara Domeneghetti[1]

[1]Dipartimento di Scienze della Terra e dell'Ambiente, Università di Pavia, via Ferrata 1, I-27100 Pavia, Italy
[2]Dipartimento di Geoscienze, Università di Padova, via Gradenigo 6, I-35131 Padova, Italy
[3]Dipartimento di Scienze Mineralogiche e Petrologiche, Università degli Studi di Torino, via Valperga Caluso 25, I-10125 Torino, Italy

Abstract

A single-crystal X-ray diffraction (XRD) study, using a diamond-anvil cell at high pressure and room temperature, was performed on a crystal from a natural space group *P*2/*n* omphacite sample with composition very close to $Jd_{55}Di_{45}$ and with a high degree of order in cation distribution. Unit-cell parameters were determined at 13 different pressures up to about 7.5 GPa. A third-order Birch-Murnaghan equation of state (BM3-EoS) fitted to the *P*-*V* data yielded $V_0 = 421.43(4)$ Å^3, $K_{T0} = 122(1)$ GPa, and $K' = 5.1(3)$. The K_{T0} value for this sample lies between the data obtained for the two end-members jadeite and diopside, and describes a slight positive curvature trend.

During the same experiment, intensity data were collected and crystal structures were refined at 5 pressures up to 7.3 GPa. Both M1 and M2 polyhedra volumes showed a slight but significant change in slope at about 4 GPa. This behavior can likely be explained in terms of tilt angle variation of TA and TB tetrahedral, which also showed a change in slope with pressure, rather than in terms of bond length compression anomaly.

Keywords: Pyroxene, omphacite, high pressure, single-crystal XRD, crystal structures, diamond-anvil cell, equation of state