American Mineralogist, Volume 95, pages 481–486, 2010

Reinvestigation of the crystal structure of the zeolite gobbinsite: A single-crystal X-ray diffraction study

G. Diego Gatta,[1,2,*] William D. Birch,[3] and Nicola Rotiroti[1,2]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Milano, via Botticelli 23, I-20133 Milano, Italy
[2]CNR-Istituto per la Dinamica dei Processi Ambientali, Milano, Italy
[3]Geosciences section, Museum Victoria, GPO Box 666, Melbourne, Victoria 3001, Australia

Abstract

The crystal structure of a natural Na-rich gobbinsite from Bundoora, a northern suburb of Melbourne, Victoria, Australia [$(Na_{4.97}K_{0.07}Ca_{0.48})_{\Sigma 5.52}(Al_{5.62}Si_{10.29})_{\Sigma 15.91}O_{32}\cdot 11.91H_2O$, $Z = 1$, $a = 10.1035(15)$, $b = 9.7819(10)$, $c = 10.1523(9)$ Å, and $V = 1003.37(20)$ Å^3, space group *Pmnb* (no. 62)], has been investigated by means of single-crystal X-ray diffraction, elemental CHN analysis, and electron microprobe analysis in the wavelength dispersive mode. For the first time, an anisotropic structural refinement has been performed on the basis of single-crystal X-ray diffraction data collected at 298 K, with: $R_1(F) = 0.0608$, 1362 unique reflections with $F_o > 4\sigma(F_o)$, and 114 refined parameters. The residuals in the final difference-Fourier maps are less than ±0.6 e^-/Å^3. Previous structure solutions based on powder diffraction data were performed in the space group $Pmn2_1$, with a significantly different description of the channels' content. In this study, the Si/Al distribution in the tetrahedral framework is found to be highly disordered. A complex configuration of the extra-framework population occurs, with two possible and mutually exclusive sites for cations (Na and Ca) and five independent sites partially occupied by water molecules (W1, W2, W2′, W3, and W3′). The coordination shell of the Na site is represented by a distorted polyhedron with coordination number CN = 6 (4 framework O atoms + 2 H_2O molecules), with at least five possible mutually exclusive configurations, whereas the coordination shell of the Ca site is represented by a distorted polyhedron with CN = 7 (5 framework O atoms + 2 H_2O molecules), with at least two possible mutually exclusive configurations.

Keywords: Zeolite, gobbinsite, Bundoora (Victoria), crystal structure, single-crystal X-ray diffraction