1987 Fiscal Year Final Research Report Summary

Structures of minerals with OH attached to Si and their properties.

Research Project

Project/Area Number

61540589

Research Category

Grant-in-Aid for General Scientific Research (C)

Allocation Type

Single-year Grants

Research Field

鉱物学(含岩石・鉱床学)

Research Institution

Kanazawa University

Principal Investigator

MATSUMOTO Takeo Dept.Earth Sciences, Faculty of Science, Kanazawa University, Professor, 理学部, 教授 (20019467)

Co-Investigator(Kenkyū-buntansha)

OKUNO Masayuki Dept.Earth Sciences, Faculty of Science, Kanazawa University, Research associate, 理学部, 助手 (40183032)
KIHARA Kuniaki Dept.Earth Sciences, Faculty of Science, Kanazawa University, Associate professo, 理学部, 助教授 (70019503)

Project Period (FY)

1986 – 1987

Keywords

Pumpellyite / Vesuvianite / Hydroxides / Crystallographic orbits / Lattice energy / Plane groups / Anharmonic thermal vibration / 結晶エネルギー計算

Research Abstract

1. Refinement of the crystal structure of Al-rich pumpellyite from Sanbagawa, Gunma Prefecture, Japan, was carried out by a least squares method with X-ray single-crystal counter-collected data. The positions of hydrogen atoms have been determined based on the difference Fourier maps, and are consistent with the results deduced from bond-valence calculations. This crystal has the following characters: the double tetrahedral unit [Si_2O_6(OH)] characteristically has a hydroxide group directly attached to Si atom; one of two kinds of octahedral sites is occupied by an aluminum ion in preference to the others; the other octahedral site if occupied by both divalent and trivalent ions , and the electric charge of the latter site is compensted by the amount of hydrogen atoms. We could not find Fe and Mn single pumpellyite crystals.
2. Refinement of the crystal structure of P/nnc-vesuvianite from Nakatatsu mine, Fukui Prefecture, Japan,was done using X-ray single - crystal diffraction data. From bond-valence calculations, the proton donor atoms are both O (11) and O (10). The B-sites(square pyramid) are half occupied by Fe atoms

3. Other studies related to this project.
3(1) Crystal structure refinements tridymite and Ag_3AsSe_3. structural change of orthorhombic-I tridymite with temperature and high-order thermal motion tensor analyses of high temperature tridymite have been carried out using X-ray single -crystal diffraction data. The crystal structure of Ag_3AsSe_3 has been refined based on high-order thermal motion tensors.
3(2) The structural and elastic properties of high-pressure phases of MgSiO_3 are investigated with a computational model based on energy minimization in collaboration with Masanori Matsui, Kanazawa Medical University.
3(3) The crystallographic orbits have been studied in collaboration with Wondratschek, Germany. The non-characteristic orbits of the plane have been derived.

Research Products (12 results)

All Other

All Publications (12 results)

[Publications] A.Yoshiasa and T.Matsumoto: Mineralogical Journal. 13. 1-12 (1986)

[Publications] A.Yoshiasa and T.Matsumoto: American Mineralogist. 70. 1011-1019 (1985)

[Publications] K.Kihara;T.Matsumoto and M.Imamura: Zeitschrift fiir Kristallographie. 177. 27-38 (1986)

[Publications] K.Kihara and T.Matsumoto: Zeitschrift fiir Kristallographie. 177. 211-217 (1986)

[Publications] M.Matsui;M.Akaogi and T.Matsumoto: Physics and Chemistry of Minerals. 14. 101-106 (1987)

[Publications] Takeo Matsumoto and Hans Wondratschek: Zeitschrift fiir Kristallographie. 17G. 7-30 (1987)

[Publications] Aira YOSHIASA and Takeo MATSUMOTO: "The crystal structure of vesuvianite from Nakatatsu mine: reinvestigation of the cation site-populations and of the hydroxyl groups." Mineralogical Journal. 13. 1-12 (1986)

[Publications] Akira YOSHIASA and Takeo MATSUMOTO: "Crystal structure refinement and crystal chemistry of pumpellyite." American Mineralogist. 70. 1011-1019 (1985)

[Publications] Kuniaki KIHARA, Takeo MATSUMOTO and Moritaka IMAMURA: "Structural change of orthorhombic-I tridymite with temperature: A study based on second-order thermal-vibrational parameters. High-order thermal tensor analyses of tridymite." Zeitschrift fur Kristallographie. 177. 27-52 (1986)

[Publications] Kuniaki KIHARA and Takeo MATSUMOTO: "Refinement of Ag_3AsSe_3 based on high-order thermal-motion tensors." Zeitschrift fur Kristallographie. 177. 211-217 (1986)

[Publications] Masanori MATSUI, Masaki AKAOGI and Takeo MATSKUMOTO: "Computational model of the structural and elastic properties of ilmenite and perovskite phases of MgSiO_3." Physics and Chemistry of Minerals. 14. 101-106 (1986)

[Publications] Takeo MATSUMOTO and Hans Wondratschek: "The non-characteristic G-orbits of the plane groups G." Zeitschrift fur Kristallographie. 179. 7-30 (1987)

URL: https://kaken.nii.ac.jp/report/KAKENHI-PROJECT-61540589/615405891987kenkyu_seika_hokoku_

Published: 1989-03-29