

The modular structure of dovyrenite, $\text{Ca}_6\text{Zr}[\text{Si}_2\text{O}_7]_2(\text{OH})_4$: Alternate stacking of tobermorite and rosenbuschite-like units

MILEN KADIYSKI,^{1,*} THOMAS ARMBRUSTER,¹ EVGENY V. GALUSKIN,² NIKOLAY N. PERTSEV,³
ALEKSANDER E. ZADOV,⁴ IRINA O. GALUSKINA,² ROMAN WRZALIK,⁵ PIOTR DZIERZANOWSKI,⁶ AND
EVGENY V. KISLOV⁷

¹Mineralogical Crystallography, Institute of Geological Sciences, University of Bern, Freiestr. 3, CH-3012 Bern, Switzerland

²Faculty of Earth Sciences, Department of Geochemistry, Mineralogy and Petrography, University of Silesia, Bedzinska 60, 41-200 Sosnowiec, Poland

³Institute of Geology of Ore Deposits, Geochemistry, Mineralogy and Petrography (IGEM) RAS, Staromonetny 35, Moscow, Russia

⁴Sci.-Research Center “NEOCHEM,” Altuf’evskoye Highway 43, Moscow, Russia

⁵Institute of Geochemistry, Mineralogy and Petrology, Warsaw University, al. Zwirki i Wigury 93, 02-089 Warszawa, Poland

⁶Institute of Geology, Siberian Branch, RAS, Sakhyanova Str. 6,670042 Ulan-Ude, Russia

⁷Institute of Physics, University of Silesia, Uniwersytecka 12, 41-200 Katowice, Poland

ABSTRACT

The average structure, space group *Pnmm* [subcell: $A = 5.666(16)$, $B = 18.844(5)$, $C = 3.728(11)$ Å, $V = 398.0(2)$ Å³, $Z = 1$], of the new mineral dovyrenite $\text{Ca}_6\text{Zr}[\text{Si}_2\text{O}_7]_2(\text{OH})_4$ has been refined from single-crystal X-ray data to $R = 7.97\%$. The modular structure of dovyrenite is built by alternate stacking of Ca-polyhedral layers characteristic of the tobermorite structure and octahedral layers with attached disilicate groups known from the rosenbuschite group of minerals. No indications of ordered polytypes were detected for the potential OD-structure. Either the small crystal size producing only weak diffraction intensities did not allow detecting diffuse diffraction features (or “super-structure” reflections) or the structure is built by disordered stacks of OD layers. Nevertheless, the resolved average structure allowed unraveling the possible order patterns within the rosenbuschite-like octahedral layers. The key for understanding the polytypic character of this structure is the short periodicity of the tobermorite-like Ca polyhedral layer of only 3.73 Å along *c*, whereas the periodicity of the attached rosenbuschite-like octahedral layer is doubled. In dovyrenite Ca occurs in sixfold-, sevenfold-, and eightfold-coordination. The octahedral Ca site is only half occupied and may reveal additional vacancies, which must be charge balanced by disordered OH-groups replacing O. A corresponding modular structure with the same subunits but different composition and without octahedral vacancies exists for rinkite $(\text{Ti,Nb,Al,Zr})(\text{Na,Ca})_3(\text{Ca,Ce})_4[\text{Si}_2\text{O}_7]_2(\text{O,F})_4$, which has hitherto been considered as heterophyllosilicate.

Keywords: Dovyrenite, zirconosilicates, single-crystal X-ray diffraction, structure solution, modular structure, tobermorite, rinkite, heterophyllosilicate