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XIX International Meeting on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals

Dedicated to the memory of Academician E. S. Fedorov (1853 - 1919)

BOOK OF ABSTRACTS

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XIX INTERNATIONAL MEETING ON CRYSTAL CHEMISTRY, X-RAY DIFFRACTION AND SPECTROSCOPY OF MINERALS

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Сборник включает в себя тезисы докладов, представленных на XIX Международном совещании по кристаллохимии, рентгенографии и спектроскопии минералов, проходившем с 1 по 5 июля 2019 года в г. Апатиты (Кольский полуостров, Россия). В число основных тем докладов входят: теория и современные методы дифракционного и спектроскопического исследования минерального вещества и неорганических материалов; кристаллохимия неорганических соединений природного (минералы) и искусственного происхождения, включая материалы с интересными физико-химическими свойствами; неорганическое материаловедение (катодные материалы, протонные проводники, микропористые материалы и сорбенты, ионные проводники и т.д.); проблемы генезиса и свойств алмазов; описательная минералогия (новые минералы и новые находки минералов); прикладная минералогия (в связи с проблемами археологии и захоронения радиоактивных отходов); история кристаллографии.

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The crystal structure of a new microporous mineral kruijenite, $Ca_4Al_4(SO_4)F_2(OH)_{16}\cdot 2H_2O$

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The crystal structure of the new mineral kruijenite, ideally $Ca_4Al_4(SO_4)F_2(OH)_{16}\cdot 2H_2O$, found in a metasomatically altered calcic xenolith from tephra of the Feuerberg paleovolcano (Eifel paleovolcanic region, Rhineland-Palatinate, Germany) [Chukanov et al., 2019] is presented. Kruijenite is tetragonal, sp. gr. *P*4/*ncc*, a = 12.9299(4), c = 5.2791(3) Å, V = 882.57(6) Å^3, Z = 2. The structure of kruijenite (Fig. 1) is unique: the mineral represents a novel structure type. The structure is based on a microporous pseudo-framework built by $Al(OH)_6$ octahedra and $CaF_2(OH)_6$ eight-fold polyhedra. The Al-centred octahedra share edges to form zig-zag chains running along the *c* axis. The Ca-centred polyhedra share the F–F edge to form dimers; adjacent dimers are also connected *via* common edges thus building columns along [001]. Each column is connected with four octahedral chains of Al-centred octahedra. There are two crystallographically non-equivalent O sites and one F site which participate in the formation of the pseudo-framework. Both O atoms belong to OH-groups. All H sites of OH groups are located inside the wide channels (with approximate width of 7.4 Å) running along the *c* axis. These channels contain H_2O molecules and significantly distorted SO_4 tetrahedra. The SO_4 tetrahedra and H_2O molecules located in the channels are connected with the pseudo-framework *via* the system of H-bonds. The most interesting structural feature of kruijenite is a positively charged pseudo-framework hosting sulfate anions and H_2O molecules, which is an indication of possible anion-exchange properties (in particular, the ability to accumulate sulfate anions) of compounds belonging to this structure type. This assumption is confirmed by the absence in association with kruijenite of ettringite-group members which are in general very typical for hydrothermally altered calcic xenoliths in Eifel volcanic rocks.

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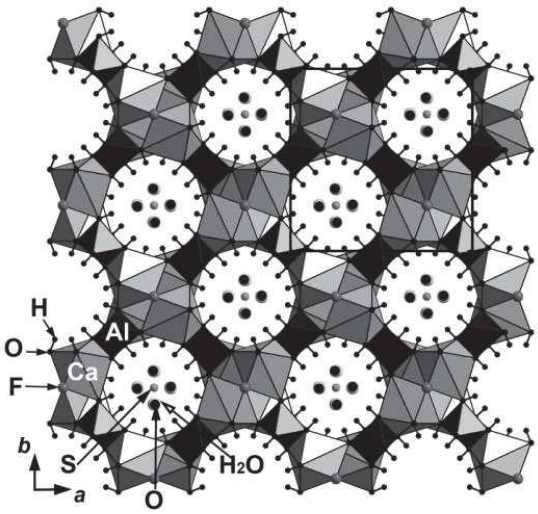

Fig. 1. The crystal structure of kruijenite projected along the *c* axis. The unit cell is outlined.