The Crystal Structure of Chabasite-K

Polina Gavrilenko^a, Olga Yakubovish^a, Werner Massa^b, Igor Pekov^a, ^aGeological department, MSU, Russia. ^bPhilipp-Universitat, Marburg, Germany. E-mail: polinka_gav@mail.ru

The chabasite group contains four minerals: chabasite-Ca, chabasite-Na, chabasite-K, and chabasite-Sr. The crystal structure of the K representative in this group has not been investigated before.

The good isometric crystals of chabasite-K were found in late hydrothermalites of Khibiny alkaline massif, Kola Peninsula, Russia. The average result of electron-microprobe analyses is: Na₂O 2.62, K₂O 7.22, CaO 4.61, SrO 1.44, BaO 0.04, Al₂O₃ 18.75, SiO₂ 46.41, H₂O 19.35, total 100.44 wt.%. The crystal structure of chabasite-K (K_{1.33}Na_{1.02}Ca_{0.84})[Al₄Si₈O₂₄]12.17H₂O, hexagonal, space group $R \ 3c$, a=13.831(3), c=15.023(5)Å, V=2489.3(1) Å³, Z=3, has been determined using a pseudomerohedrically twinned crystal [Enraf Nonius CAD4, MoK_α, graphite monochromator, twin ratio 0.535(1) : 0.465(1), $wR_2=0.1177$ for all 6265 unique reflection, R=0.047 for 4745 observed reflection with $I > 1.96\sigma(I)$]. Because of a high mobility of cations within the big framework cavities the experimental data were received at low temperature T=193 K.

It has been established that K-bearing chabasite contains five independent sites of cations within the large cavities of Si,Al tetrahedral framework. Eight sites for water molecules were found in the structure. We compared the atoms' distribution in the framework cavities with similar data for chabasites of different composition and origin. Basing on the crystal chemical, mineralogical and geochemical data for zeolites of alkaline formation we assume that the number of cations in the chabasite-K from low-temperature hydrothermalites could be the result of a natural ion-exchange process.

Keywords: zeolite, chabasite-K, crystal structure