

Poster Presentations

[MS18-P01] Crystal structure features of Mn- and Sr-rich eudialyte from Sushina Hill, India.

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Eudialyte (zirconosilicate of sodium, calcium and iron) is the most important mineral of alkaline rocks and is a main concentrator of Zr, Hf, REE, etc. So far the finds of this mineral were limited by several massifs in Russia, Canada, Greenland and Brasil.

In this work Mn- and Sr-rich eudialyte from Sushina Hill (India) was studied by X-ray single crystal diffraction (diffractometer Xcalibur Oxford Diffraction with CCD detector). The experiment was bad quality because of rather blocked crystal and contained about 27% of rather strong reflections, which don't agree with *R*-lattice. Hence, we initially refined the crystal structure in space group *P3m*. However, refinement of the structure was impossible because of insufficient amount of reflections and strong correlations of atomic displacement parameters between pseudosymmetric atoms. The further structural study was carried out in the "traditional" space group *R3m*. The final *R*-value is 4.7% for 2008 independent reflections with $|F_{\text{obs}}| > 3\sigma(F)$. The main structural features of the mineral are reflected in its crystal chemical formula (*Z*=3) which rather well corresponds to the average empirical formula: $[\text{Na}_{11.81} \text{Sr}_{0.96} \text{REE}_{0.24} \text{Y}_{0.2} \text{K}_{0.2} \square_{1.59}] [\text{Ca}_{4.5} \text{Mn}_{1.2} \text{REE}_{0.3}] [\text{Mn}^{\text{V}}_{1.53} \text{Mn}^{\text{V}}_{1.47}] [\text{Si}^{\text{IV}}_{0.58} (\text{Ti}_{0.165} \text{Zr}_{0.165})^{\text{VI}} \text{Zr}^{\text{VI}}_{0.09}] [\text{Nb}^{\text{VI}}_{0.49} \text{Si}^{\text{IV}}_{0.32} \text{Al}^{\text{IV}}_{0.19}] [\text{Zr}_{2.985} \text{Hf}_{0.015}] [\text{Si}_{24} \text{O}_{72}] \text{OH}_{4.17} \text{C}_{10.67} (\text{OH}, \text{H}_2\text{O})_{0.5}$, where brackets denote the composition of the key structural sites and Roman numerals designate the coordination number of the cations. The idealized formula is

(*Z*=3): $(\text{Na}, \square, \text{Sr})_{15} (\text{Ca}, \text{Mn})_6 \text{Mn}_3 (\text{Si}, \text{Nb})_2 \text{Zr}_3 [\text{Si}_{24} \text{O}_{72}] (\text{OH}, \text{Cl}, \text{H}_2\text{O})_{5.5}$. The main distinctive feature of Mn, Sr-rich eudialyte is the high degree of cation ordering. It is reflected in split of all extraframework sites. The *M3* and *M4* sites are split into three subsites with *M3a-M3b* and *M3b-M3c* distances of 0.36(2) Å and 1.30(1) Å, respectively, and *M4a-M4b* and *M4b-M4c* distances of 1.11(3) Å and 0.56(2) Å. These subsites are predominantly occupied by silicon and niobium atoms with statistically domination of silicon in *M3* and niobium in *M4* microregion. This cation distribution is in a good correspondence with acentric character of crystal structure. The Na atoms occupy *N1-N5* sites with admixture of Sr, REE or vacancy. Each site is split into two (*N1, N3, N5*) or three (*N2, N4*) subsites. The distances *N1a-N1b, N3a-N3b, N5a-N5b* are 0.51(1) Å, 0.69(3) Å, 2.10(2) Å, respectively and *N2a-N2b-N2c* and *N4a-N4b-N4c* distances of 0.33(3) Å, 0.6(1) Å and 0.24(1), Å 0.51(1) Å. *N4* site is characterized of a rather high content of strontium atoms, but it is not enough for domination Sr over Na. Thus inspite of high content of Mn and Sr studied eudialyte is not a new mineral. However, the data about crystal structure features are useful for geochemical reconstructions of the region. This work was financially supported by Federal Programm of Leading Scientific Schools (project no. NSh-2883.2012.5).

Keywords: X-ray analysis; mineral; silicate