

## The World of Sodalite-type Structures

Fischer, Reinhard X<sup>1</sup> Baur, Werner H.<sup>2</sup>

<sup>1</sup>Universität Bremen, Fachbereich Geowissenschaften, Klagenfurter Straße, 28359 Bremen <sup>2</sup>Northwestern University, Department of Chemistry, 2145 Sheridan Road, Evanston, IL, 60208, USA

The mineral sodalite with the ideal composition  $\text{Na}_8[\text{Al}_6\text{Si}_6\text{O}_{24}]\text{Cl}_2$  is commonly assigned to the group of feldspathoids in the mineralogical literature. However, it is also classified as a zeolite-type material because it consists of a framework of  $\text{AlO}_4$  and  $\text{SiO}_4$  tetrahedra with clathrate-like pores as discussed by Depmeier (2005). So far, the solution of the framework structure has been attributed to Pauling (1930) but it has been shown recently by us (Baur & Fischer, 2008a) that it was Jaeger (1929) who first solved a SOD-type crystal structure with diffraction data on nosean, a natural sulfate analogue of sodalite.

Minerals and synthetic compounds with a SOD-type framework represent the most comprehensive family of zeolite-type compounds with the highest number of published crystal structures and the highest number of different space groups. Among these are aluminosilicates (e.g., sodalite, hatüyne, helvine, lazurite, nosean, tsaregodtsevite), beryllosilicates (e.g., danalite, genthelvite, tugtupite), chlorides, sulfides (e.g., tetrahedrite, binnite, freibergite, galkhaite, goldfieldite, tennantite), borates (rhodizite), synthetic phosphates, phosphides, nitrides and clathrate hydrates which have been shown by crystal structure analyses to adopt the SOD-type framework. More than 900 SOD-type crystal structures, which represent over 18% of the total number of published zeolite structures, are known and have been compiled by us (Baur & Fischer, 2008b) in the databank ZEOBASE.

We present here the complete symmetry relationships of SOD-type crystal structures comprising 27 space groups listed in a Bärnighausen (1980) tree together with the type and index of symmetry reduction. The complete information including descriptions of the framework structure, chemical compositions of all (>900) compounds, examples for all 27 different types with standardized coordinates, and additional information on properties will be published soon (Fischer & Baur, 2008).

### References

- Bärnighausen, H. (1980), Group-subgroup relations between space groups: a useful tool in crystal chemistry. *MATCH*, Nr. 9: 139-175.
- Baur, W.H., Fischer, R.X. (2008a) A historical note on the sodalite framework: the contribution of Frans Maurits Jaeger. *Microp. Mesop. Mater.*, in press.
- Baur, W.H., Fischer, R.X. (2008b) ZEOBASE, a databank of zeolite-type structures, Northwestern and Bremen Universities.
- Depmeier, W. (2005) The sodalite family. In: *Rev. Mineral. Geochem.* 57: 203-240.
- Fischer, R.X., Baur, W.H. (2008) Microporous and other framework materials with zeolite-type structures, *Landolt-Börnstein*, Group IV, Vol. 14E, in preparation.
- Jaeger, F.M. (1929) On the constitution and the structure of ultramarine. *Trans. Farad. Soc.* 25: 320-345.
- Pauling, L. (1930) The structure of sodalite and helvite. *Z. Kristallogr.* 74: 213-225.

Abs. No. **341**  
Meeting: **DMG 2008**  
submitted by: **Fischer, Reinhard X.**  
email: **rfischer@uni-bremen.de**  
date: **0000-00-00**  
Req. presentation: **Poster**  
Req. session: **S16**