| | | |
|---|---|---|
| ESRF | **Experiment title:**<br>$(K_4Li_4)Al_8Ge_8O_{32}\cdot 8H_2O$: an $Li^+$-exchanged potassium aluminogermanate with the zeolite gismondine (GIS) topology | **Experiment number**:<br>CH 1346 |
| **Beamline**:<br>ID11 | **Date of experiment**:<br>from: 22/02/2002 to: 27/02/2002 | **Date of report**:<br>25/02/2004 |
| **Shifts:** | **Local contact(s)**:<br>Gavin Vaughan | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

***Aaron J. Celestian, Stony Brook University, Geosciences**

**John B. Parise, Stony Brook University, Geosciences and Chemistry**

**Akhilesh Tripathi, Stony Brook University, Chemistry**

**Report:**

The title compound, lithium potassium dialuminium digermanium octaoxide dihydrate, (K,Li)-(Al,Ge)-GIS (GIS is gismondine), is the result of a 50% $Li^+$ exchange into the K-(Al,Ge)-GIS structure. The (K,Li)-(Al,Ge)-GIS structure was determined from a 4×4×2µm octahedral single crystal at the ESRF synchrotron X-ray source. The ion exchange results in a symmetry transformation from *I*2/*a* for K-(Al,Ge)-GIS to *C*2/*c* for (K,Li)-(Al,Ge)-GIS. The structural change is due to disordering of $K^+$ ions with $Li^+$ ions along the [001] channel and ordering of water molecules in the [101] channels. The distance between sites partially occupied by $K^+$ ions increases from 2.19(3)Å in K-(Al,Ge)-GIS to 2.94(3)Å in (K,Li)-(Al,Ge)-GIS. The $Li^+$ ions occupy positions along the twofold axis at the intersection of the eight-membered-ring channels in a twofold coordination with water molecules. For the four closest framework $O^{2-}$ anions, the Li···O distances are 3.87(4)Å.

Celestian, A. J., Parise, J. B., Tripathi, A., Kvick, Å. & Vaughan, G. M. B. (2003). *ACTA C.* **C59** i74-i76.