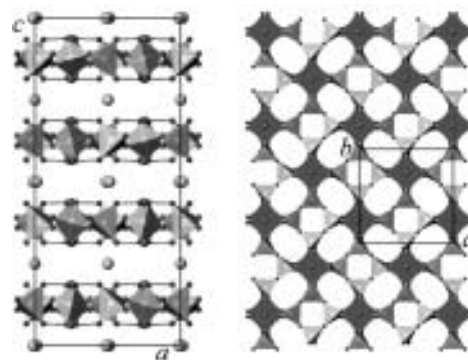


m19.p17**Effect of hydrostatic pressure up to 6 GPa on the crystal structures of ammonium and sodium hexafluorosilicates, $(\text{NH}_4)_2\text{SiF}_6$ and Na_2SiF_6 ; a phase transition in $(\text{NH}_4)_2\text{SiF}_6$ at 0.2-0.3 GPa.**Tatyana Shakhshneider^{a,b}, Elena Boldyreva^{a,b}, Heidrun Sowa, Hans Ahsbahs^c^{a,b}Institute of Solid State Chemistry and Mechanochemistry, SB RAS, and REC-008, Novosibirsk State University, Novosibirsk, Russia. ^cPhilipps-University Marburg/Lahn, Germany. E-mail: shah@solid.nsc.ru**Keywords: polymorphism, high pressure phase transformations, powder diffraction**

An *in situ* X-ray powder diffraction study has shown that cubic modification of $(\text{NH}_4)_2\text{SiF}_6$ (cryptoalite) at 0.2-0.3 GPa transforms irreversibly into a trigonal polymorph with cell parameters $a = 5.78 \text{ \AA}$ and $c = 4.78 \text{ \AA}$, presumably - the previously known bararite, space group P-3m1. The choice of a pressure-transmitting liquid (methanol/ethanol/water mixture or poly(chlorotrifluoroethylene) oil) has no effect on the transition. In malladrite, Na_2SiF_6 , no obvious phase transitions were observed, at least at pressures below 6 GPa, although some remarkable kinks in the $Dc/c(P)$ and $DV/V(P)$ were measured at about 3.5 GPa. The anisotropy of lattice strain in the high-pressure phase of $(\text{NH}_4)_2\text{SiF}_6$ was measured up to 6 GPa and compared with that in the trigonal Na_2SiF_6 . The pressure-induced changes in the packing of $(\text{SiF}_6)^{2-}$ anions were analyzed, the changes in the IR-spectra of $(\text{SiF}_6)^{2-}$ ions induced by increasing pressure and on decompression were measured and compared for trigonal $(\text{NH}_4)_2\text{SiF}_6$ and Na_2SiF_6 . Acknowledgments: Financial support has been obtained from DRL, Alexander von Humboldt Foundation and DLR.

[1] Boldyreva, E.; Shakhshneider, T.; Sowa, H.; Ahsbahs, H. *Z. Krist.*, submitted.**m19.p18****Low temperature phase transition in $\text{BaCuSi}_2\text{O}_6$** Karine Sparta^a, Michael Merz^a, Georg Roth^a, Raivo Stern^b, Radovan Cerny^c, Tsuyoshi Kimura^d^aInstitut für Kristallographie, RWTH Aachen, Germany. ^bNational Institute of Chemical Physics & Biophysics, Tallinn, Estonia. ^cLaboratoire de Cristallographie, Geneva, Switzerland. ^dLos Alamos National Laboratory, Los Alamos, USA. E-mail: sparta@xtal.rwth-aachen.de**Keywords: spin gap, phase transitions, $\text{BaCuSi}_2\text{O}_6$**

$\text{BaCuSi}_2\text{O}_6$ is a quasi two-dimensional spin gap compound crystallizing in a tetragonal layered structure [1,2]. The Cu^{2+} ions within the $\text{Cu}_2\text{Si}_4\text{O}_{12}$ -layers are arranged in a square lattice, forming quasi-isolated Cu-Cu dimers parallel to the c axis; the interlayer magnetic coupling is very weak. $\text{BaCuSi}_2\text{O}_6$ has a spin-singlet dimerized quantum ground state with a spin gap $D = 32 \text{ K}$ [3]. It was already observed that $\text{BaCuSi}_2\text{O}_6$ undergoes a first order structural phase transition at 610 K, from the space group $I4/mmm$ at high temperatures to the room temperature space group $I4_1/acd$ [2]. We present evidence for a new first order structural phase transition towards a slightly incommensurate phase below 100 K from powder and single crystal X-ray diffraction measurements.



Room temperature structure of $\text{BaCuSi}_2\text{O}_6$. Left: Projection of the structure onto the (a,c) plane. Right: Projection of a $\text{Cu}_2\text{Si}_4\text{O}_{12}$ -layer onto the (a,b) plane [2].

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