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Effect of hydrostatic pressure up to 6 GPa on the crystal structures of ammonium and sodium hexafluorosilicates, $(NH_4)_2SiF_6$ and Na_2SiF_6; a phase transition in $(NH_4)_2SiF_6$ at 0.2-0.3 GPa.

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Keywords: polymorphism, high pressure phase transformations, powder diffraction

An *in situ* X-ray powder diffraction study has shown that cubic modification of $(NH_4)_2SiF_6$ (cryptohalite) at 0.2-0.3 GPa transforms irreversibly into a trigonal polymorph with cell parameters a = 5.78 Å and c = 4.78 Å, presumably - the previously known bararite, space group P-3m1. The choice of a pressure-transmitting liquid (methanol/ethanol/water mixture or poly(chlortrifluorethylene) 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 $(NH_4)_2SiF_6$ was measured up to 6 GPa and compared with that in the trigonal Na_2SiF_6. The pressure-induced changes in the packing of $(SiF_6)^{2-}$ anions were analyzed, the changes in the IR-spectra of $(SiF_6)^{2-}$ ions induced by increasing pressure and on decompression were measured and compared for trigonal $(NH_4)_2SiF_6$ and Na_2SiF_6.
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Low temperature phase transition in $BaCuSi_2O_6$

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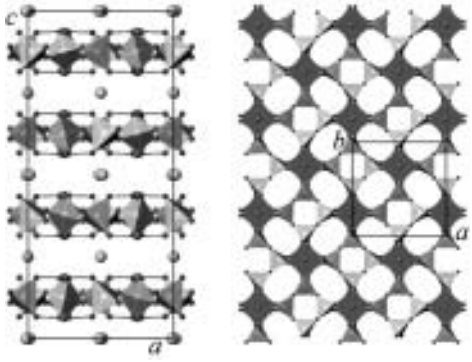
Keywords: spin gap, phase transitions, $BaCuSi_2O_6$

$BaCuSi_2O_6$ is a quasi two-dimensional spin gap compound crystallizing in a tetragonal layered structure [1,2]. The Cu^{2+} ions within the $Cu_2Si_4O_{12}$-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. $BaCuSi_2O_6$ has a spin-singlet dimerized quantum ground state with a spin gap D = 32 K [3]. It was already observed that $BaCuSi_2O_6$ 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 $BaCuSi_2O_6$. Left: Projection of the structure onto the (***a***,***c***) plane. Right: Projection of a $Cu_2Si_4O_{12}$-layer onto the (***a***,***b***) plane [2].

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