m22.p10

Synthesis, Characterization and properties of alkali and earth-alkalisulfonates

H. Pöllmann, S. Stöber, Ch. Wagner, K. Merzweiler

University of Halle/Saale, Germany

Keywords: applied mineralogy, sulfones, layered structures

Stochiometric aqueous solutions of benzosulfonic acid and metalcarbonates were evaporated to crystallze different water-containing salts.
The crystals were characterized by X-ray, thermal, chemical and optical methods.
These layered materials can be used because of their ion-exchange ands intercalation properties, but also for controlling hydration beahviour of cements. A summary of lattice parameters of different phases is given in the table.

Compound	a_o[A°]	b_o [A°]	c_o[A°]
$LiC_6H_5SO_3$	17,1636	21,8470	14,1591
$NaC_6H_5SO_3$	29,8833	24,3355	10,2458
$KC_6H_5SO_3$	15,1770	28,8022	13,2028
$Mg(C_6H_5SO_3)_2$	30,4594	12,6911	14,2171
$Ca(C_6H_5SO_3)_2$	30,0150	20,4244	10,6854
$Sr(C_6H_5SO_3)_2$	31,3182	29,9525	10,1632
$Ba(C_6H_5SO_3)_2$	31,1896	30,1374	10,3097
$Ag(C_6H_5SO_3)_2$	5,1596	5,1979	15,2962
$Mn(C_6H_5SO_3)_2$*$6H_2O$	22,7596 /6,3312/7,0445		
Fe(C6H5SO3)2*2H2O22,586/16,3293			6,9989
Co(C6H5SO3)2*6H2O22,4279/6,3180			7,0068
Ni(C6H5SO3)2*6H2O22,3799/6,3016			6,9709
Zn(C6H5SO3)2*2H2O22,5006/6,3087			6,9890
Cu(C6H5SO3)2*6H2O22,5297/6,2980			7,0364
Compound	α [°]	β [°]	γ [°]
$LiC_6H_5SO_3$	90	96,741	90
$NaC_6H_5SO_3$	90	90	90
$KC_6H_5SO_3$	90	90	90
$Mg(C_6H_5SO_3)_2$	90	97,884	90
$Ca(C_6H_5SO_3)_2$	90	90	90
$Sr(C_6H_5SO_3)_2$	90	90	90
$Ba(C_6H_5SO_3)_2$	90	90	90
$Ag(C_6H_5SO_3)_2$	86,75	84,56	61,0
$Mn(C_6H_5SO_3)_2$*$6H_2O$90		93,564	90
Fe(C6H5SO3)2*2H2O90		93,608	90
Co(C6H5SO3)2*6H2O90		93,754	90
Ni(C6H5SO3)2*6H2O90		93,771	90
Zn(C6H5SO3)2*2H2O90		93,635	90
Cu(C6H5SO3)2*6H2O90		93,722	90

Tab. 1: Lattice parameters of *Benzolsulfonates*

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m22.p11

The Crystal Structure of Manganese modified Brownmillerite Solid Solutions

S. Stöber, H. Pöllmann

FB Geowissenschaften Mineralogie/Geochemie Von Seckendorffplatz 3 06120 Halle (Saale) Germany

Keywords: cements, neutron diffraction, perovskites

Brownmillerite originally describes the chemical composition Ca_2AlFeO_5 on the join $Ca_2Fe_2O_5$-$Ca_2Al_2O_5$ ($Ca_2Fe_{2-x}Al_xO_5$ x = 0,5) in different cement types. The main interest was focused on the solid solution series $Ca_2Fe_{2-x}Al_xO_5$ for their ability to react with water to hydration phases and form together with other hydration phases and quartz a 3-dimensional framework. With the addition of secondary manganese raw materials to cement its hydration properties were improved and Mn^{3+} is fixed in the Brownmillerite crystal structure.
The crystal structure of different solid solutions in the system $Ca_2Fe_{2-x}Al_xO_5$ with $0 \leqslant x \leqslant 1.33$ were recently investigated [1] and is best described as a 2-dimensional, oxygen deficient alternative of simple perovskite phases (e.g. $CaMnO_{3-d}$) [2]. The structure comprises alternating layers of cations sited in corner sharing octahedra and corner sharing tetrahedra, perpendicular [010]. However, the orthorhombic phases are not isostructural, because the space group Pnma for iron rich members changes into s. g. I2mb at approximately x = 0.6 for alumina rich phases. Recently, metric parameters of solid solutions $Ca_2(Fe_{1-y}Mn_y)_2AlO_5$ with $0 \leqslant y \leqslant 0.5$ were determined [3]. However, no structural data of these phases are available. Samples with the composition $Ca_2(Fe_yMn_y)_{2-2x}Al_{2x}O_5$ with y = 0,5; x = 0,042; 0,085; 0,25; 0,415; 0,585 were synthesized. Stochiometric oxide - concentrations were sintered at 1300°C for 96 h with several grinding steps in a tube furnace using Pt crucibles. The sinter products were quenched and analyzed by XRD. The Oxygen concentration was determined by Iodometric titration. The phase chemistry was determined by microprobe analysis. Structure refinements were performed at the BENSC Hahn-Meitner Institute Berlin. Neutron radiation was applied due to the fact, that Mn and Fe show strong electronic similarities: Mn (atomic number 25) and Fe (atomic number 26).

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