

was heated under dynamic vacuum; at 130°C deuterium is released and LiMgAlD_6 is formed: $\text{LiMg(AlD}_4)_3 \rightarrow \text{LiMgAlD}_6 + 2\text{Al} + 3\text{D}_2$. At 180°C LiMgAlD_6 decomposes: $\text{LiMgAlD}_6 \rightarrow \text{LiD} + \text{MgD}_2 + \text{Al} + 3/2\text{D}_2$. The first reaction is endothermic; the second exothermic, indicating that $\text{LiMg(AlD}_4)_3$ is not thermodynamic stable. $\text{LiMg(AlD}_4)_3$ crystallizes in the monoclinic space group $P2_1/c$ with cell parameters: $a = 8.37 \text{ \AA}$, $b = 8.74 \text{ \AA}$, $c = 14.30 \text{ \AA}$ and $\beta = 124.83^\circ$. The structure consists of isolated AlD_4 tetrahedra that are connected by octahedral Mg and Li atoms. LiMgAlD_6 crystallizes in the trigonal space group $P321$ with cell parameters: $a = 7.98 \text{ \AA}$ and $c = 4.38 \text{ \AA}$. The structure consists of isolated AlD_6 octahedra tied together by hexa-coordinated Li and Mg atoms. A small amount of TiCl_3 was added to $\text{LiMg(AlD}_4)_3$ and mixed using the ball milling technique. The effect of addition of TiCl_3 was also studied for LiMgAlD_6 .

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MS17 P11

Structural phase transitions in $\text{Sr}_2\text{ScReO}_6$

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In double perovskites A_2MReO_6 , where A – an alkaline-earth ion and M – a non-magnetic two – or three-valence cation such as Zn^{2+} , Mg^{2+} or Sc^{3+} , only the Re ion is relevant to the unusual magnetism in these compounds [1, 2]. Structural thermal behaviour of these compounds, which can be connected with magnetic and transport properties, is not yet investigated. In our work, high-temperature structure investigations of $\text{Sr}_2\text{ScReO}_6$ were performed at beamline B2 (HASYLAB DESY, Germany) in Debye-Scherrer mode using the on-site readable image-plate detector OBI and a STOE furnace. All diffraction patterns have been analyzed by using the software package WinPLOTR [3]. Two phase transitions with a change of symmetry of the crystal structure from monoclinic (S.G. $P2_1/n$) to tetragonal (S.G. $P4/mnc$) and then to cubic (Fm-3m) have been detected at elevated temperatures. These phase transitions were also proved by DSC measurements. Low-temperature investigations of $\text{Sr}_2\text{ScReO}_6$ are in progress.

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X-ray Induced Water Order-Disorder Transition in Hydrated Cesium Cobalt Oxide Hwo-Shuenn Sheu^a, Wei-Ju Shih^a, Horng-Yi Tang^b, Nien-Tsu Sun^b, ^aNational Synchrotron Radiation Research Center, Hsinchu, Taiwan ^b Department of Applied Chemistry, National Chi Nan

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Metal cobalt oxides, A_xCoO_2 (A= Li, Na, K, Rb, Cs), with layered structure have been attracting wide attention for the past two decades. Li_xCoO_2 is one of the most important intercalation compounds for secondary lithium ion batteries. Na_xCoO_2 is recognized to be a potential candidate for thermal electric power materials and non-cuprites superconductors. A_xCoO_2 compounds have a layered structure, with the CoO_2 layers consisting of CoO_6 octahedra sharing common edges and forming a triangular Co–O sublattice. Open and polarizable framework structure makes the compounds adaptable by chemical modification. The superconductivity of hydrated $\text{Na}_{0.35}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$ oxide was found and immediately targeted by research scientists owing to its unusual bilayer-hydrate (BLH) structure. In the coupling strength of CoO_2 layers might be varied by the replacement of different ionic size alkalis resulting in the change of c-axis lattice constant. The influence of coupling strength between CoO_2 layers on superconductivity, therefore, can be possibly studied when the process of controlling the interlayer spacing is developed. The bilayer-hydrate of $\text{Cs}_{0.2}\text{CoO}_2 \cdot 0.63\text{H}_2\text{O}$ with a greatest interlayer spacing $d_{10.0(2)} \text{ \AA}$ among alkali cobalt oxides has been grown in crystal form. Magnetic susceptibility measurement of $\text{Cs}_{0.2}\text{CoO}_2 \cdot 0.63\text{H}_2\text{O}$ displays a paramagnetic behavior down to 1.9 K. We find that X-ray powder diffraction patterns of $\text{Cs}_{0.2}\text{CoO}_2 \cdot 0.63\text{H}_2\text{O}$ changed according to various X-ray dosages during the XRD measurement. The water ordering in $\text{Cs}_{0.2}\text{CoO}_2 \cdot 0.63\text{H}_2\text{O}$ is sensitive to X-ray irradiation. The relative diffraction intensity vary is strongly dependent on the amount of water contain and the location at interfacial position. We will report the X-ray dosage dependent crystal structure of $\text{Cs}_{0.2}\text{CoO}_2 \cdot 0.63\text{H}_2\text{O}$ in the meeting.

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Investigation of $\text{K}_x\text{Na}_{1-x}\text{NbO}_3$ (KNN) near the Morphotropic Phase Boundaries N. Zhang & A.M. Glazer, Department of Physics, University of Oxford, UK. D. Baker & P.A. Thomas, Department of Physics, University of Warwick, UK.

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PZT is commonly regarded as the leading piezoelectric material for a wide range of applications, and one which all others must be assessed against. However, there are growing concerns over the toxicity and environmental issues of lead-based substances, which is why attention has turned to other lead-free piezoelectric materials, one of which is Sodium Potassium Niobate (KNN).

The newer lead-free materials are united with PZT in that they exhibit a region in their phase diagrams where there appears to be a sudden change in crystal structure. This region has been termed the Morphotropic Phase Boundary (MPB) and appears to coincide with the maximum piezo-response of these materials. Of particular interest in $\text{K}_x\text{Na}_{1-x}\text{NbO}_3$ (KNN) is the presence of three morphotropic phase boundaries (MPB) that occur at $x \sim 0.18$, $x \sim 0.35$, and $x \sim 0.48$ [1].