

MS21 O3

Crystal structure of RbWOP₂O₇ a new diphosphate W(V) isotopic with KWOP₂O₇ *D. Mezaoui^a, S. Belkhiri^a, R. Belhouas^a, A. Leclaire^b, H. Rebbah^a.* ^a *Laboratoire des Sciences des Matériaux, Faculté de Chimie, USTHB, BP 32 El-Alia, 16111 Bab-Ezzouar, Alger, Algérie.* ^b *Laboratoire de Cristallographie et Sciences des Matériaux, CRISMAT, ENSICAEN, Campus II,6, Boulevard du Maréchal Juin, 14050 Caen Cedex, France.*

Keywords: W(v)diphosphate, tungstyl ion, mixed framework

Crystal structure of new diphosphate of W(V) RbWOP₂O₇ isotopic with KWOP₂O₇.

A new W(V) diphosphate RbWOP₂O₇ [1]isotypic to the KWOP₂O₇ [2] has been synthesized. It crystallises in space group P2₁/n with:

$$a=5.0988(1)\text{\AA} \quad b=11.9183(1)\text{\AA}$$

$$c=11.6910(1)\text{\AA} \quad \beta=90.632(2)^\circ$$

This structure is characterized by mixed framework of corner sharing P₂O₇ groups and WO₆ octahedra forms large tunnels where the Rb⁺ ions are located. This study shows that this structure is similar to that with potassium ion.

[1]: D.Mezaoui, S. Belkhiri, R. Belhouas, A. Leclaire, H.Rebbah, *J. Soc. Chem.*, 2006, 16(2), 163.

[2]:A. Leclaire, J. Chardon, B. Raveau, *J. Mater. Chem.*, 2001, 11, 846.

MS21 O4

Structural disorder in the Al_(1-x)Ga_xPO₄ solid solution at high temperature. *O. Cambon^a, J. Haines^a, D.A. Keen^b, M.G. Tucker^b, L. Chapon^b,* ^a*Institut Charles Gerhardt, UMR-CNRS-UM2 5253, PMOF, Place E.Bataillon, 34095 Montpellier, France.* ^b*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX, United Kingdom.*
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Keywords: Phosphates, total neutron scattering, structural disorder.

α -Quartz is the most commonly used piezoelectric material. Piezoelectric properties are limited in principle by the α - β phase transition at 846 K, however, piezoelectric measurements show that the properties of α -quartz resonators start to degrade at temperatures above 573 K. This degradation can be linked to increasing structural disorder found by neutron total scattering measurements. Structure-property relationships have been developed for α -quartz homeotypes in order to identify new materials such as AlPO₄ and GaPO₄ with better intrinsic properties. The thermal stability of the α -quartz form and the piezoelectric response were found to be a function of the structural distortion of a material with respect to the β -quartz structure type. Analysis by reverse Monte Carlo modelling of our recent total scattering experiments on quartz and GaPO₄ show that the degree of disorder in the instantaneous structure increases well before the phase transition, implying a rapid decrease of the piezoelectric properties.

New materials can also be obtained based on solid solutions between existing α -quartz homeotypes. Such an approach can in principle enable materials with tunable piezoelectric properties to be obtained by varying the chemical composition as in the case of the AlPO₄-GaPO₄ system in which the structural distortion varies linearly as a function of composition. Three representative compositions in the Al_(1-x)Ga_xPO₄ solid solution ($x = 0.14, 0.20, 0.63$) were investigated on the GEM diffractometer at the ISIS spallation neutron source. Total neutron scattering data were obtained from room temperature up to 873 K in the α -quartz-type phases and in the β -quartz-type phase at 1018 K for $x = 0.14$. Rietveld refinement does not support a domain-type model for the latter. In the present study the influence of the existing static Al/Ga disorder on thermally induced disorder is investigated, which can be correlated to their piezoelectric properties at high temperature. This thermally induced disorder is found to be most pronounced for the samples with high Al content, for which α - β transitions are observed.