Accepted Manuscript

Structural and dielectric properties of a new cesium-rubidium dihydrogen arsenate: $Cs_{0.2}Rb_{0.8}H_2AsO_4$

Samia Chouchene, Khaled Jaouadi, Tahar Mhiri, Nabil Zouari

PII: S0925-8388(17)30597-2

DOI: 10.1016/j.jallcom.2017.02.159

Reference: JALCOM 40887

To appear in: *Journal of Alloys and Compounds*

Received Date: 31 December 2016

Revised Date: 13 February 2017

Accepted Date: 14 February 2017

Please cite this article as: S. Chouchene, K. Jaouadi, T. Mhiri, N. Zouari, Structural and dielectric properties of a new cesium-rubidium dihydrogen arsenate: $Cs_{0.2}Rb_{0.8}H_2AsO_4$, *Journal of Alloys and Compounds* (2017), doi: 10.1016/j.jallcom.2017.02.159.

Structural and dielectric properties of a new Cesium- Rubidium Dihydrogen Arsenate: $Cs_{0.2}Rb_{0.8}H_2AsO_4$

Samia CHOUCHENE*, Khaled JAOUADI, Tahar MHIRI, Nabil ZOUARI

Laboratoire physico-chimie de l'état solide, Faculté des Sciences de Sfax, 3038 Sfax, Tunisie

ABSTRACT

Ongoing studies of the CsH_2AsO_4-RbH_2AsO_4 system, aimed at developing novel proton conducting solids, resulted in the new compound $Cs_{0.2}Rb_{0.8}H_2AsO_4$ (CRDA). Single crystal X-ray diffraction (performed at room temperature) revealed $Cs_{0.2}Rb_{0.8}H_2AsO_4$ to crystallize in tetragonal space group I $\bar{4}$2d with lattice parameters a = 7.8090(1) Å and c= 7.5010(1) Å. It has a unit cell volume of 457.415(10) $Å^3$ and four formula units per cell. The title compound is isostructural with the tetragonal phases of CsH_2AsO_4 (CDA) and RbH_2AsO_4 (RDA). The main feature of this structure is the coexistence of two different cations (Cs^+ and Rb^+) in the same crystal. In this structure, the arsenic atom as well as the rubidium and cesium ions lie on points with site symmetry S_4, the oxygen atoms lies in general positions about the arsenic atoms, in a tetrahedral arrangement. The AsO_4 tetrahedra are connected by O-H…O hydrogen bonds laying essentially in the *a,b* plane. The infrared spectrum performed at room temperature in the frequency range 4000– 400 cm^{-1} confirms the presence of structural disorder in this material. A calorimetric study of the title compound shows two peaks, they are detected at 185 and 433 K. Samples were examined by impedance and modulus spectroscopy techniques. The first transition (185 K) is attributed to a ferroelectric–paraelectric type. A high temperature phase transition (433 K) leading to a superionic–protonic phase was found, characterised by an unusual high conductivity. The conductivity relaxation parameters associated with the high-disorder protonic conduction have been determined from analysis of the M''/M''_{max} spectrum measured in a wide temperature range. Transport properties in this material appear to be due to proton hopping mechanism.

Keywords: Inorganic materials; X-ray single crystal; Thermal behavior; ferroelectric–paraelectric transition; conductivity; proton hopping mechanism.