Journal of Physics and Chemistry of Solids 72 (2011) 988–993

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Cation mobility and structural changes on the water removal in zeolite-like zinc hexacyanometallates (II)

M. Avila [a], J. Rodríguez-Hernández [a,b], A.A. Lemus-Santana [a], E. Reguera [a,*]

[a] Center for Applied Science and Advanced Technology of IPN, México D.F., Mexico
[b] Institute of Materials Science and Technology, University of Havana, Havana, Cuba

ARTICLE INFO

Article history:
Received 1 July 2010
Received in revised form
8 March 2011
Accepted 19 May 2011
Available online 26 May 2011

Keywords:
A. Microporous Materials
B. Crystal Growth
C. X-ray diffraction
D. Crystal structure

ABSTRACT

The cation (A^+) mobility and structural changes on the water molecules removal in zeolite-like zinc hexacyanometallates series, $Zn_3A_2[Fe(CN)_6]_2 \cdot xH_2O$ with A=Na, K, Rb and Cs, were studied from X-ray diffraction data recorded for hydrated and anhydrous samples at room temperature and at 77 K. The crystal structure for the anhydrous phases were solved and refined and then compared with those corresponding to their hydrated form. On the water molecules removal the charge balancing cation (A^+) migrates to favor a stronger interaction with the N ends of the CN bridges where the framework negative charge is located. This cation–framework interaction model is supported by the recorded IR spectra for both hydrated and anhydrous samples. The new cation position induces distortion for both the cavity shape and their windows and also leads to cavity volume reduction. This is relevant for the properties of this family of solids as porous materials and their behavior in adsorption and separation processes, among them for hydrogen storage.