Thermal expansion and structural stability of $In_2Mo_3O_{12}$ studied by high-resolution X-ray powder diffraction

F. F. Ferreira[1], B. A. Marinkovic[2], M. Ari[2], P. M. Jardim[2], F. Rizzo[2], R. R. de Avillez[2]
[1]*CCNH, Universidade Federal do ABC, Santo André, SP, Brazil*
[2]*PUC-Rio, RJ, Brazil*

The possibility of controlling the coefficient of thermal expansion in pure and composite materials has been the principal driving force in the search for crystal phases with unusually low, zero, or even negative thermal expansion (NTE) [1]. In accordance to some recent findings, $In_2Mo_3O_{12}$ compound is an outstanding catalyst for the production of olefin from paraffin [paraffin = olefin + hydrogen] through dehydrogenation (DH) followed with selective hydrogen combustion (SHC) in a process which is not thermodynamically restricted [2]. A detailed understanding of thermal expansion properties of $A_2M_3O_{12}$ family is fundamental for eventual future applications of these phases in composites, substrates for high-precision optical applications and/or Fiber Bragg gratings. However, several issues essential for application of this family in practical purposes are not well understood. The present work reports our findings on the thermal expansion and structure stability of $In_2Mo_3O_{12}$, a member of $A_2M_3O_{12}$ family not previously characterized for these properties as far as the authors are aware of [3] in the temperature range below room temperature. For this end, *in situ* high-resolution x-ray powder diffraction (HRXRPD) measurements were performed at the X-ray Powder Diffraction (D10B-XPD) beamline of the Brazilian Synchrotron Light Laboratory (LNLS, Campinas, SP, Brazil) using X-rays of λ = 1.2388 Å wavelength. The powdered sample was loaded in a closed-cycle He cryostat and the temperature was varied from 20 K up to 450 K. Our previous results [3] indicated that a phase transition between 593 K and 643 K took place evolving from monoclinic to orthorhombic as confirmed through LeBail and Rietveld refinements of X-ray diffraction patterns. Recent measurements revealed that from 20 K up to 450 K no phase transition occurred and all three unit-cell axes (*a*, *b* and *c*) demonstrated normal, positive, thermal expansion in the investigated temperature range, the same behavior presented for measurements performed at high temperatures.

Keywords: Negative thermal expansion, X-ray powder diffraction.

Work supported by CNPq (proc. 490925/2008-1).

[1] B. A. Marinkovic, M. Ari, R. R. de Avillez, F. Rizzo, F. F. Ferreira, K. J. Miller, M. B. Johnson, M. A. White, Chem. Mater. **21**, 2886 (2009).
[2] J. G. Tsikoyiannis, D. L. Stern, R. K. Grasselli, J. Catal. **184**, 77 (1999).
[3] B. A. Marinkovic, M. Ari, P. M. Jardim, R. R. de Avillez, F. Rizzo, F. F. Ferreira, Thermochim. Acta **499**, 48 (2010).
e-mail: fabio.furlan@ufabc.edu.br, Centro de Ciências Naturais e Humanas (CCNH), Universidade Federal do ABC (UFABC), Rua Santa Adélia, 166, Bairro Bangu, CEP: 09210-170, Santo André, SP, Brazil.