Poster Presentation

MS01.P24

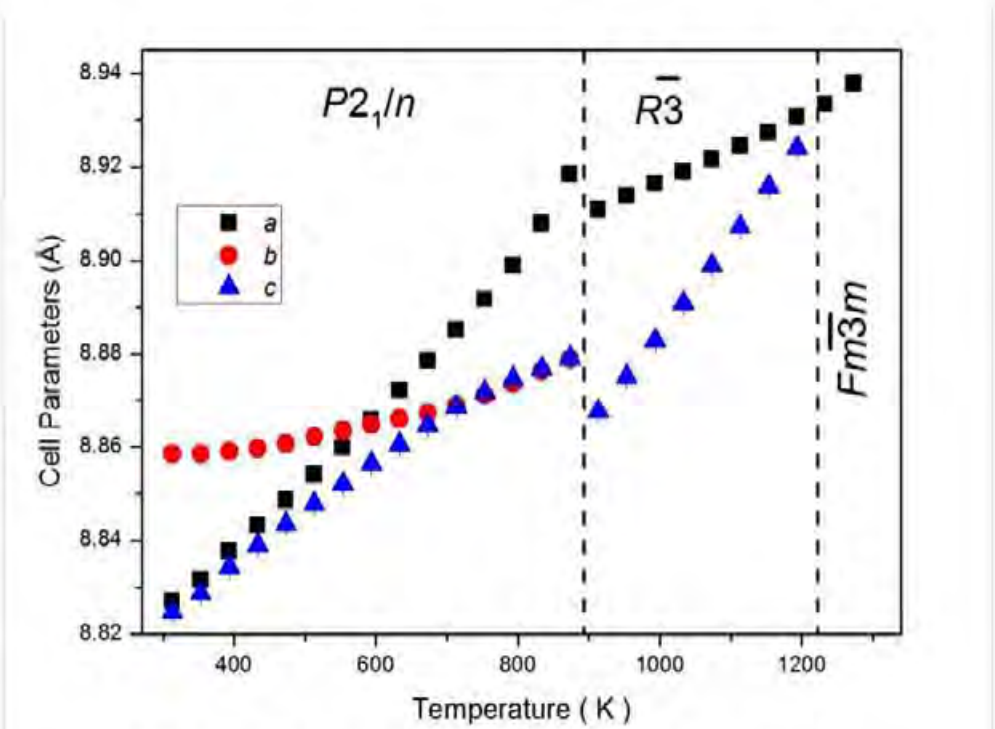
Investigation of thermally induced phase transitions in uranium perovskites

E. Reynolds[1], B. Kennedy[1]

[1]*The University of Sydney, Chemistry, Sydney, Australia*

The physical properties of inorganic solids are intimately related to their crystal structures and there is increasing awareness of the potential importance of metastable structures that exist over a limited temperature and/or pressure range. For the renaissance of nuclear energy to continue it is vital to improve the efficiency and safety of the nuclear fuel process. In order to do this, a comprehensive knowledge of the fundamental chemical, structural, and thermodynamic properties of uranium compounds is required. Compounds of the type A2BUO6 (A = Ba, Sr; B = Ba, Sr, Ca) have been prepared and characterised using neutron and X-Ray diffraction techniques as well as X-ray absorption spectroscopy. For the first time the high temperature behaviour of these complex oxides has been investigated, and as illustrated by Ba2SrUO6, heating such oxides can induce a sequence of phase transitions with the structure of Ba2SrUO6 changing from monoclinic in P21/n at room temperature to cubic in Fm-3m above 1200 K. [1] The compounds Ba2CaUO6 and BaSrCaUO6 were also found to undergo a series of thermally induced phase transitions from the P21/n monoclinic structure. In order to elucidate the structural changes involved in each system, a combination of diffraction techniques was required. We also utilised symmetry-mode analysis in which the structures are refined in terms of the fundamental tilting modes. This elegant way of tracking phase transitions provided vital insight when comparing and contrasting the thermal behaviour of these complex uranium oxides.

[1] *E. Reynolds, B.J. Kennedy, G.J. Thorogood et al, Journal of Nuclear Materials, 2012, 433, 37-40*



Reduced unit cell parameters for Ba_2SrUO_6 versus temperature.

Keywords: Perovskite