

## **Phase transitions in framework structures: geometrical aspects**

**M. Avdeev, S. Yakovlev, R. Piltz**

*Bragg Institute, Australian Nuclear Science and Technology Organisation, Menai, NSW, Australia*

It is known that evolution of crystal structures of framework materials with predominantly ionic bonding as a function of composition/temperature/pressure is usually driven by mismatch between the size of guest ions and voids they fill. The Inorganic Crystal Structure Database containing the large amount of accurate structural data accumulated over the last decades provides enough information for establishing quantitative relations between geometrical characteristics of such materials and structure type stability. We present the results of the analysis of structural data in terms of coordination polyhedra volumes for  $ABX_3$  compositions built of  $[BX_6]$  octahedra in order to rationalize phase transitions between  $CaIrO_3$ -type (post-perovskite phase), perovskite, and ilmenite modifications. As an example of application of the same approach to tetrahedral frameworks we also explore the family of "stuffed tridymites"  $AB_2X_4$ .