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Swinging symmetry, structural phase transitions and physical properties of RETGa3

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The compounds RETGa3 (RE = Rare Earths; T = Ni, Cu, Ag) were synthesized by various techniques. Preliminary X-ray diffraction (XRD) at room temperature suggests that compounds crystallize in the tetragonal system with either centrosymmetric space group I4/mmm (BaAl4 type) or non-centrosymmetricI4mm (BaNiSn3 type). A detailed single crystal XRD, neutron diffraction and synchrotron XRD on selected compounds confirmed the non-centrosymmetric BaNiSn3 structure type at room temperature with space group I4mm. Temperature dependent single crystal XRD and powder XRD and synchrotron beamline measurements show a structural transition between centro- and non-centro symmetry followed by a phase transition to the Rb5Hg19 type (I4/m space group) above 400 K and another transition to the Cu3Au structure type (Pm m) above 700 K. Combined single crystal X-ray and synchrotron powder X-ray studies of PrCuGa3 at high temperatures reveal structural transitions at higher temperatures, highlighting the closeness of the BaNiSn3 structure to other structure types not known to the RECuGa3 family. YbCuGa3 crystallizes in a new structure type in the monoclinic space group C2/m, which is the first monoclinic system in the RETX3 family. The crystal structure of all RETGa3 is composed of eight capped hexagonal prism cages [RE4T4Ga12] occupying one rare earth atom in each ring which are shared through the edge of T and Ga atoms along ab plane resulted in a three dimensional network. Resistivity and magnetization measurements demonstrate that all these compounds undergo magnetic ordering at temperatures between 1.8 and 80 K, apart from the Pr and La compounds: the former remains paramagnetic down to 0.3 K, while superconductivity has been observed in the La compound at T = 1 K. It is not clear if this is intrinsic or due to filamentary Ga present in the sample. The divalent nature of Eu in EuTGa3 and mixed valent Yb in YbTGa3 compounds were confirmed by magnetization measurements and X-ray absorption near edge spectroscopy (XANES), and is further supported by the crystal structure analysis. Temperature dependent single crystal XRD measurements on REAgGa3 suggests almost constant c parameter in all the compounds in the temperature range of 100-450 K, showing anisotropic zero thermal expansion in c direction. Electrical resistivity measurements reveal that all of the compounds from this series are metallic in nature. REAgGa3 materials show fermi liquid behavior at lower temp range.

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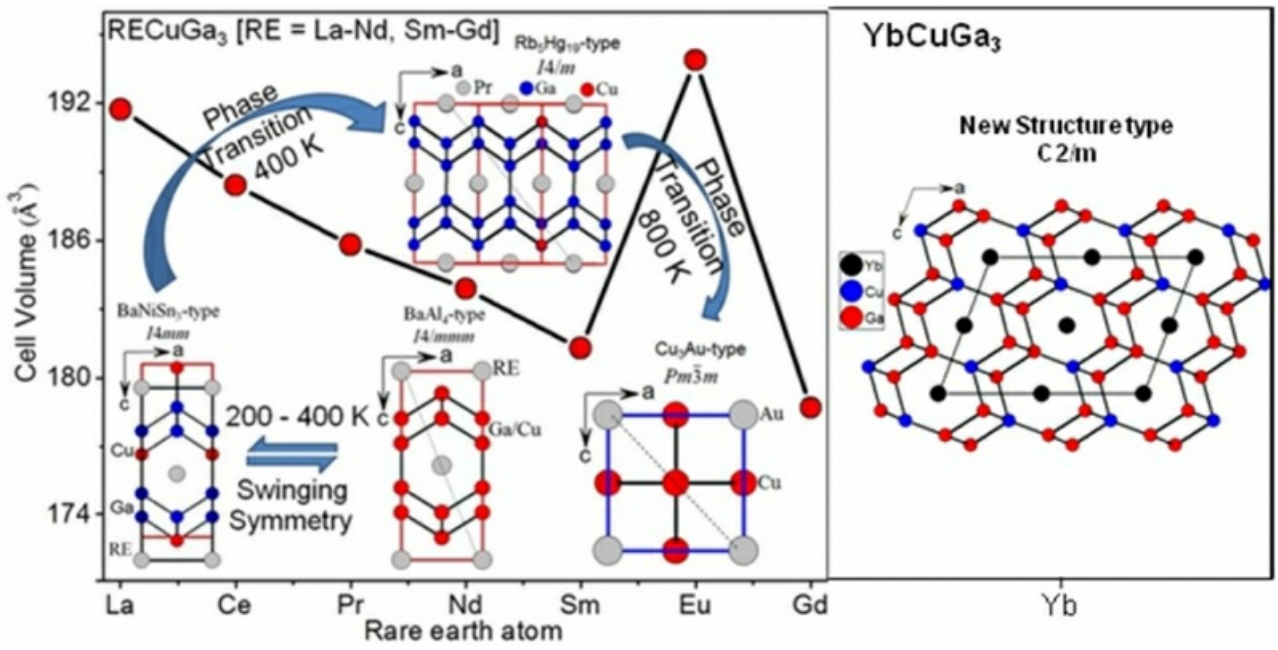
[2] Subbarao, U. et al. (2016)Inorg. Chem. 55, 666-75.



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