

The Role of Local Structure in the Optical Properties of Hexagonal $\text{YMn}_{1-x}\text{Ga}_x\text{O}_3$ and Isostructural Compounds

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$\text{YMn}_{1-x}\text{Ga}_x\text{O}_3$ forms in a hexagonal structure over the entire composition range. The Mn^{+3} and Ga^{+3} ions are surrounded by 5 oxygen atoms in a trigonal bipyramid arrangement. As with similar isostructural solid solutions, this series of samples exhibits a remarkable color variation with composition from YMnO_3 which is bluish black, to the bright purple of the samples with small amounts of Mn, to white for YGaO_3 . The color is due to the Mn-O5 chromophore which has an axial distortion of the axial oxygens of the trigonal bipyramid unit. We have prepared samples over the entire composition range using sol-gel methods and by applying different thermal treatments for each composition in order to obtain phase pure samples of hexagonal phase material and eliminate the $\text{Y}_3\text{Ga}_5\text{O}_{12}$ garnet phase in the Ga-rich compositions. We will report the results of Rietveld refinement of the powder x-ray diffraction data for the series, the fitting of the x-ray absorption spectroscopy data (XANES and EXAFS) for both Mn and Ga K-edges, and Raman spectroscopy.

These data will be compared with our recently published results on the structurally identical $\text{YMn}_{1-x}\text{In}_x\text{O}_3$ solid solution [1] and other oxide systems where the local structure is critical to determining the physical properties.

[1] "Evolution of the local structure within chromophoric Mn-O₅ trigonal bipyramids in $\text{YMn}_{1-x}\text{In}_x\text{O}_3$ with composition," S. Mukherjee, H. Ganegoda, A. Kumar, S. Pal, C.U. Segre, and D.D. Sarma, *Inorg. Chem.* **57**, 9012-9019 (2018).