Bi2WO6 shows temperature-dependent phase transitions. The room temperature orthorhombic phase (Pca21) undergoes phase transition to another orthorhombic phase with space group B2cb at 650°C and further a monoclinic phase (A2/m) at T > 950°C at above it [1]. In the present work, the monoclinic phase of Bi2WO6 has been stabilized by Eu & Tb substitution at the Bi position using a simple one step hydrothermal method for the first time. As synthesized nanomaterials are characterized by p-XRD, FE-SEM, DRS, TGA, & BET surface analysis measurements. Photocatalytic activity of as synthesized BiEuWO6 & BiTbWO6 nanoparticles was established for Congo-red dye degradation under visible light source. Rietveld refinement using GSAS-EXPGUI[2] suite has been carried out on these nanoparticles using combined synchrotron X-ray and spallation Neutron data obtained from Elettra, Trieste and ORNL, Oakridge respectively. Additionally, local structural analysis using atomic pair distribution function has been carried out on high Q data collected from NOMAD, ORNL by using PDFgui program [3].

Structures are refined in the A2/m space group using the BiNdWO6 model. The Tungsten octahedra are distorted and the oxygen were refined by a split atom model indicating that there is a disorder in the rare earth substituted analogue. Structural parameters obtained from Rietveld refinement were used as initial model to fit the local structure of BiEuWO6 and BiTbWO6 and a good fit is obtained for low r range 1.5 to 5Å. Positional disorder observed in average structure is also present in local structure. DFT calculations for band gap analysis and Raman studies were also carried out. As compared to Bi2WO6, the BiEuWO6 & BiTbWO6 nanoparticles showed superior Photocatalytic activity for the degradation of Congo red dye in the visible region. The detailed Crystal Structure-Local Structure implications on the Photocatalytic activity is discussed. Such studies are essential for the generation of new functional energy materials with improved properties.