Accepted Manuscript

Synthesis, structure, UV–Vis–NIR, infrared and Raman spectroscopy, and force-field investigation for A_2GaSbO_7 (A^{3+} = Y, Dy, Gd) pyrochlores

S. Nandi, Y.M. Jana, S. Sarkar, R. Jana, G.D. Mukherjee, H.C. Gupta

PII: S0925-8388(18)33123-2

DOI: 10.1016/j.jallcom.2018.08.235

Reference: JALCOM 47323

To appear in: *Journal of Alloys and Compounds*

Received Date: 23 March 2018

Revised Date: 8 August 2018

Accepted Date: 24 August 2018

Please cite this article as: S. Nandi, Y.M. Jana, S. Sarkar, R. Jana, G.D. Mukherjee, H.C. Gupta, Synthesis, structure, UV–Vis–NIR, infrared and Raman spectroscopy, and force-field investigation for A_2GaSbO_7 (A^{3+} = Y, Dy, Gd) pyrochlores, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.08.235.

Synthesis, structure, UV-Vis-NIR, Infrared and Raman spectroscopy, and force-field investigation for A_2GaSbO_7 (A^{3+} = Y, Dy, Gd) pyrochlores

S. Nandi [a], Y.M. Jana [a,1], S. Sarkar [b], R. Jana [c], G.D. Mukherjee [c], H.C. Gupta [d]

[a] *Department of Physics, University of Kalyani, Kalyani 741235, Nadia, W.B., India*
[b] *Department of Chemistry, University of Kalyani, Kalyani 741235, Nadia, W.B., India*
[c] *Department of Physical Sciences, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, P.O. – BCKV Campus Main Office, Nadia, 741252, W.B., India*
[d] *Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi, 110016, India*

ABSTRACT

Three mixed pyrochlores, A_2GaSbO_7 (A^{3+} = Y, Dy, Gd) were synthesized using the solid-state reaction technique and characterized systematically through powder X-ray diffraction and its Rietveld analysis, SEM-EDAX, UV-Visible absorption spectra, Fourier-transform infrared and Raman spectroscopy. Scherrer analysis of the XRD pattern and SEM-image were used to estimate size of the nano-structured particles of the polycrystalline samples to be ~ 40–50 nm. From the UV-Vis absorbance data, absorption band edge and optical band gap were determined, and found to be ~ 350 ± 8 nm and 2–2.5 eV, respectively, for these compounds. Four F_{1u} bands were only observed in the infrared spectra within the phonon wave numbers range of 400–800 cm^{-1} for these samples. The highest wave number infrared mode arises due to the interaction between bending and stretching of A–O and B–O bonds. A mode-splitting caused by the mass-difference of M-site ions was found in the other three infrared modes. The Raman spectra of these compounds exhibit six Raman modes, e.g., A_{1g}, E_g, and $4F_{2g}$, within the experimental range of 50–1000 cm^{-1}, with few extra bands in the higher (>700 cm^{-1}) and lower (< 200 cm^{-1}) wave numbers range. A normal coordinate analysis using a generalized valence force-field model has been performed to assign and evaluate the vibration modes in these compounds. Five stretching and four bending force constants were considered to construct the force-field matrix. Comparison of the calculated phonon wave numbers with experimental values obtained in infrared and Raman excitation zones describes excellent agreement for all these isomorphous compounds.

Keywords: Pyrochlore oxides A_2GaSbO_7; X-ray Rietveld analysis; UV-Vis-NIR; FT-IR and Raman spectra; Force-field

[1] *Corresponding author*: *e-mail*- yatramohan@yahoo.com, ymjana@klyuniv.ac.in