**Origin of high pressure phase transition in the Ln2Ti2O7 (Ln = La, Nd, Pr) Carpy- Galy phases.**

**A.G. Asadov1,2,3, D.P. Kozlenko1, A.I. Mammadov2, R.Z. Mehdiyeva2, S.E. Kichanov1, E.V. Lukin1**

*1 Frank Laboratory of Neutron Physics, JINR, 141980 Dubna, Russia.*

*2 Institute of Physics, Azerbaijan National Academy of Sciences, Baku AZ-1143, Azerbaijan.*

*3 Khazar University, AZ1096, Baku, Azerbaijan.*

**Corresponding Author:** asifasadov@jinr.ru; +79773820587

**Abstract**

 The investigation of the layered perovskite-like compound Ln2Ti2O7 (Ln = La, Nd, Pr) involved a comprehensive examination of its structural and vibrational characteristics employing X-ray diffraction and Raman spectroscopy under pressures reaching 30 GPa. The findings suggest the occurrence of a gradual structural phase transition from the initial ferroelectric monoclinic P21 phase to the paraelectric monoclinic P21/m phase at approximately $P\_{Nd\_{2}Ti\_{2}O\_{7}}$=19.0 Gpa, $P\_{La\_{2}Ti\_{2}O\_{7}}$=16.7 Gpa and $P\_{Pr\_{2}Ti\_{2}O\_{7}}$=13.8 GPa. This pressure-induced transition manifested anomalies in unit cell compression and alterations in the pressure-dependent behavior of vibrational modes [1]. The monoclinic crystal structure of P21 symmetry, as predicted by group theory, presented 132 Raman-active modes. A discernible increase in observed mode wavenumbers was noted at pressures below the phase transition pressure, with anomalies in the pressure behavior of specific vibrational modes near the transition pressure being linked to changes in pressure coefficients [2]. Noteworthy alterations were observed in certain vibrational modes, such as the disappearance of some and the appearance of new modes post-transition, signifying a distortion in the TiO6 octahedra [3]. These anomalies, occurring in proximity to specific pressures, indicate the continuous nature of the phase transition. Furthermore, anomalies in the pressure behavior of lattice parameters were observed at approximately around 14.0 GPa -19.0 GPa, signifying a structural phase transformation. The anisotropic nature of lattice compression was evident, with the c-axis in the monoclinic phases displaying the highest compressibility. The average compressibility of the "c" parameter was approximately three times greater than that of the "a" and "b" parameters. Even post-structural phase transition, a pronounced compression anisotropy persisted. Additionally, a marked increase in the monoclinic angle “*β”* in the vicinity of the transition pressure was documented.

**References:**

1. M. Nanot, F. Queyroux, J.C. Gilles, A. Carpy, J. Galy, Phases multiples dans les systèmes Ca2Nb2O7-NaNbO3 et La2Ti2O7CaTiO3: Les séries homologues de formule AnBnO3n+2, J Solid State Chem. 11 (1974) 272–284. [https://doi.org/10.1016/S0022-4596(74)80032-0](https://doi.org/10.1016/S0022-4596%2874%2980032-0).
2. A.G. Asadov, D.P. Kozlenko, A. Mammadov, R. Mehdiyeva, S.E. Kichanov, E.V. Lukin, O.N. Lis, A.V. Rutkauskas, A structural phase transition in La2Ti2O7 at high pressure, Physica B: Condensed Matter, 655 (2023) 414753, <https://doi.org/10.1016/j.physb.2023.414753>
3. R.J. Angel, J. Zhao, N.L. Ross, General rules for predicting phase transitions in perovskites due to octahedral tilting, Phys Rev Lett. 95 (2005). <https://doi.org/10.1103/PhysRevLett.95.025503>.