High-pressure behavior of natural and synthetic triphylite

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The olivine-type mineral triphylite has attracted a lot of attention in recent years as a potential battery material [1]. In addition, the presence of $Fe^{2+}O_6$ octahedra in the structure implies the possibility of high-spin to low-spin (HS-LS) transition of Fe^{2+} upon sufficient compression, similar to other Fe^{2+}-bearing minerals as ferropericlase [2]. Indeed, a theoretical investigation has reported the possibility of a non-magnetic state close to ~50 GPa, accompanied by an electronic band gap closure (insulator-metal transition) [3]. Partly motivated by this possibility, we investigated the high-pressure structural, vibrational, and electronic behavior of synthetic and natural samples of the olivine-type lithiophilite-triphylite ($LiMnPO_4$-$LiFe^{2+}PO_4$) series. Our investigations revealed a structural transition close to ~65-70 GPa for all samples. The optical absorption studies showed a distinct color change accompayning the aforementioned transition (from colorless to blue), thus excluding a metallic state at that pressure. On the other hand, the predicted non-magnetic high-pressure state might indeed arise from a Fe^{2+}HS-LS transition, which may in turn trigger the pressure-induced structural and electronic changes.

[1] J. Wang and X. Sun, Energy Environ. Sci. 8, 1110 (2015) and refs. therein.

[2] J.-F. Lin, S. Speziale, Z. Mao, and H. Marquardt, Rev. Geophys. 51, 244 (2013) and refs. therein.

[3] H. Lin and Z. Zeng, IEEE Trans. Magn. **47**, 3817 (2011)