

Combining modern structural tools to solve a tough lithium- tantalum-oxide problem; MicroED, laboratory and synchrotron X- ray, and DFT.

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Li-containing garnets show promise as candidates in multiple roles (anode, cathode, or electrolyte) in Li-ion batteries. We encountered “Li₈Ta₂O₉” as an impurity in a series of solid-state electrolytes such as Li₅Pr₃Ta₂O₁₂. A pattern in the Powder Diffraction File matched the impurity peaks well, but the structure was unknown and the pattern unindexed. We synthesized the material successfully along with other materials such as “Li₁₀Ta₂O₁₀” (also with unknown crystal structure), but were unable to find a suitable unit cell that gave satisfactory fit to the peaks. MicroED analysis revealed a recurring small body-centered orthorhombic cell among the crystallite grains, along with other unit cells belonging to related materials existing as impurities in the mixture. We determined that the major phase of “Li₈Ta₂O₉” is actually Li₂Ta₂O₆. We identified at least two other materials via MicroED, and will report on these discoveries also.

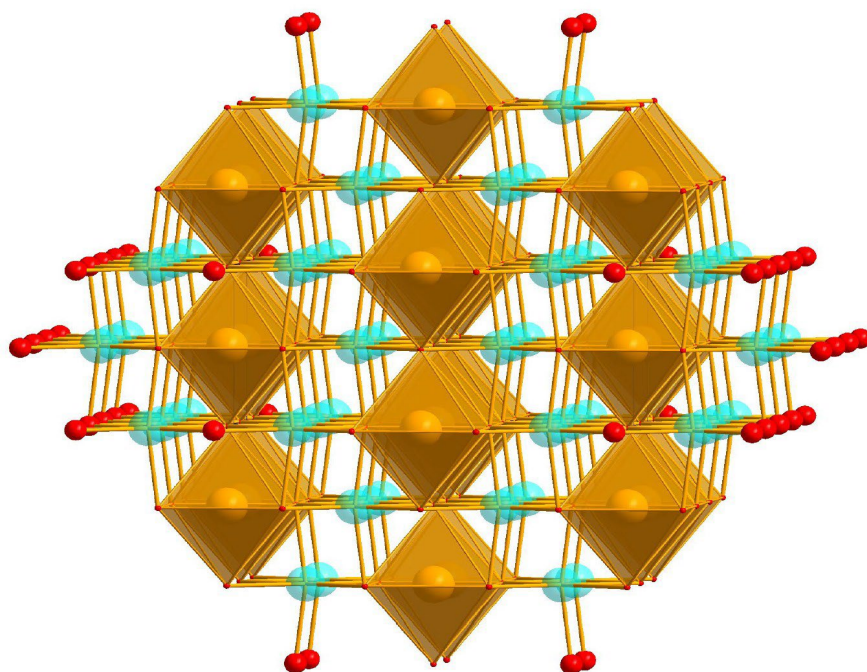


Figure 1