

A new terrestrial Ti³⁺-rich oxide with a novel crystal structure

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The origin of titanium (III) oxides remains a subject of debate, particularly in light of the discovery of several such minerals as inclusions in corundum crystals. While minerals like tistarite, kaitianite, and jiansmuite have been unambiguously identified in extraterrestrial materials [1–3], their terrestrial counterparts [4,–6] often recovered from corundum xenocrysts—have sparked controversy regarding potential anthropogenic origins [7–9]. Here, we present a new Ti³⁺-bearing oxide with the ideal formula Zr₂Ti³⁺₇AlO₁₆, from a pegmatite in Jordanów Śląski (SW Poland), which represents the first finding of such a phase in situ within its unaltered geological setting.

This newly identified phase characterized by high levels of trivalent Ti³⁺, Zr, and Al, and its unique intergrowth with corundum. These features suggest its crystallization in a highly Si-depleted environment influenced by reductive fluids such as H₂, CH₄, or a combination of both, conditions typical of deep subduction zone levels at the upper mantle–lower crust interface. The crystallization environment and the associated fluid compositions are thought to occur under highly reducing conditions, similar to those proposed by Griffin et al. [10] for the formation of super-reduced oxide minerals, which are the result of interactions between mantle-derived fluids and basaltic magmas within the shallow lithosphere.

This phase represents a new type of crystal structure, not previously observed among minerals or synthetic compounds. Single-crystal synchrotron X-ray diffraction data indicate the tetragonal space group *I*4₁/*a*, with unit cell parameters *a* = 10.7053(3) Å and *c* = 9.6262(7) Å, *V* = 1103.19(10) Å³ and *Z* = 4. To enable detailed study of extremely small crystals (here 6.5 × 11 × 4 μm), we have developed a method for extracting microcrystals using Scanning Electron Microscopy-based techniques, optimized for direct use in X-ray diffraction analysis. This approach allows for the characterization of crystals that would otherwise be inaccessible, providing valuable insights into their structural properties and potential applications in planetary geology and extraterrestrial materials research. The phase is currently under evaluation by the IMA CNMNC as a potentially new mineral species.

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