

Supplementary Material

Ermeloite, $\text{AlPO}_4 \cdot \text{H}_2\text{O}$ a new phosphate mineral with kieserite-type structure from Galicia, Spain

Guillermo. Z. Vérez,^{1*} Carlos J. Rodríguez Vázquez¹, Bruno Dacuña Mariño¹, Inés Fernández Cereijo¹, José González Del Tánago², Ramón Jiménez Martínez³, Ramiro Barreiro Pérez¹, Raquel Antón Segurado¹, Ezequiel Vázquez Fernández¹, Montse Gómez Dopazo¹, Aida González Pazos¹ and Oscar Lantes-Suárez¹.

¹Área de Infraestructuras de Investigación, Universidad de Santiago de Compostela. 15782 Galicia, Spain.

² Departamento de Mineralogía y Petrología, Facultad de Ciencias Geológicas, Universidad Complutense, 28040 Madrid, Spain.

³ Departamento de Recursos Geológicos para la Transición Ecológica, Instituto Geológico y Minero de España (CSIC), 28003 Madrid, Spain.

*Author for correspondence: Guillermo Z. Vérez, E-mail: g.zaragoza@usc.es

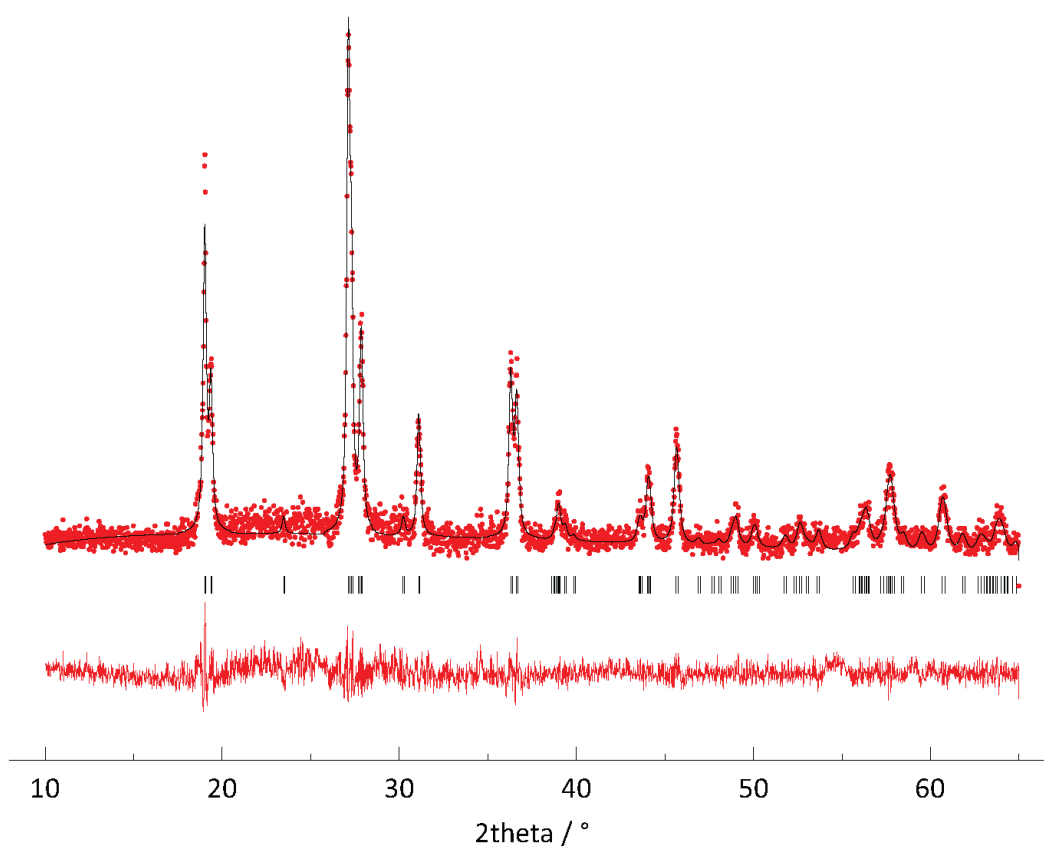


Fig S1. Graphical representation of the experimental powder diffraction data fitted by the Pawley method.

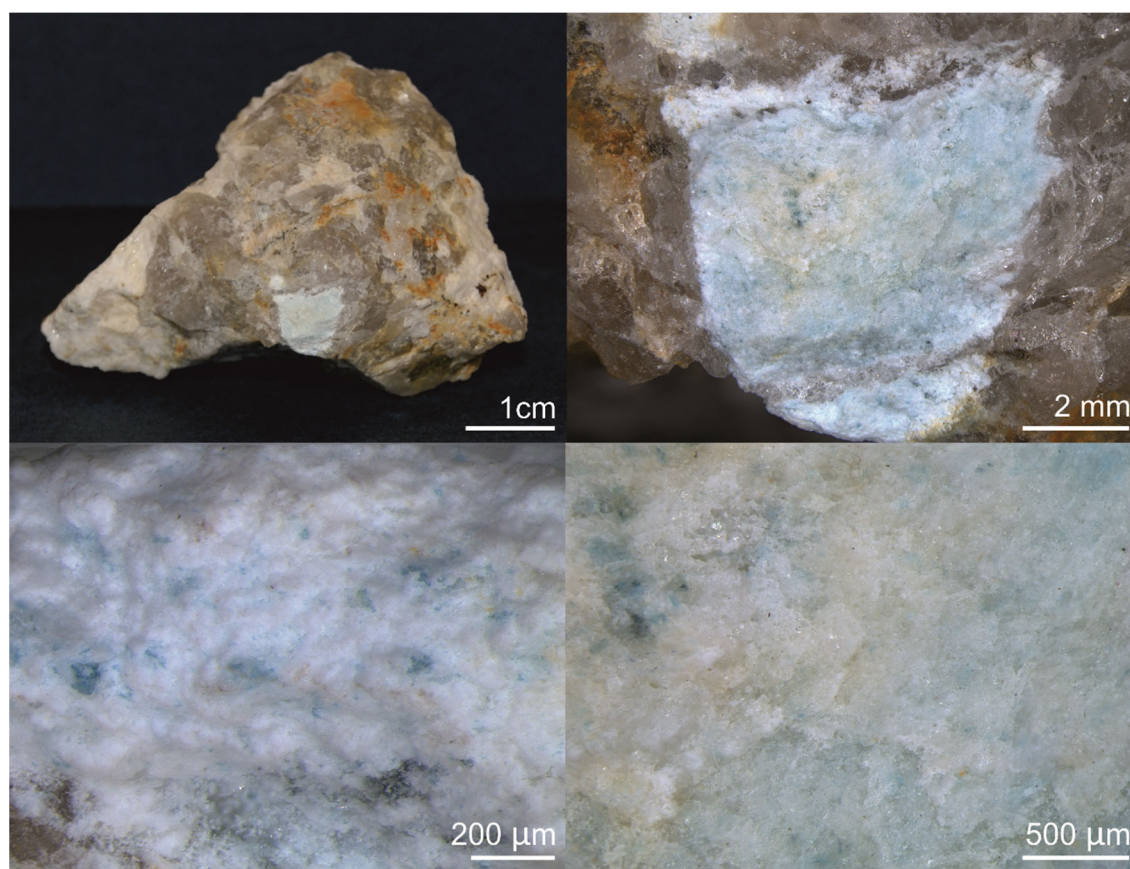


Fig S2. Mineral photographs.

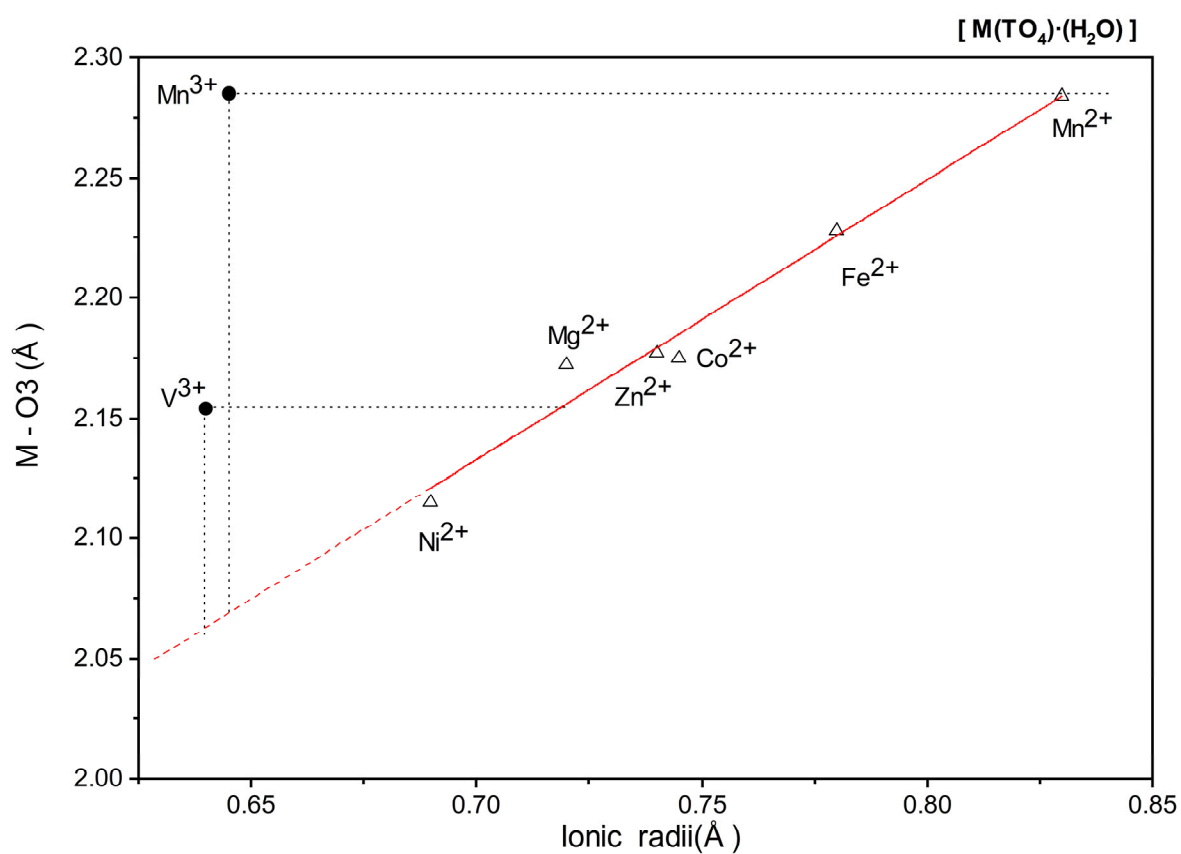


Fig S3. Relationship between ionic radii of cation and M-O3 bond length. Up triangles represent divalent cations in kieserite type compounds ($\text{M}^{2+}\text{SO}_4 \cdot \text{H}_2\text{O}$), line represents calculated regression and black circles represent trivalent cations ($\text{M}^{3+}\text{PO}_4 \cdot \text{H}_2\text{O}$).

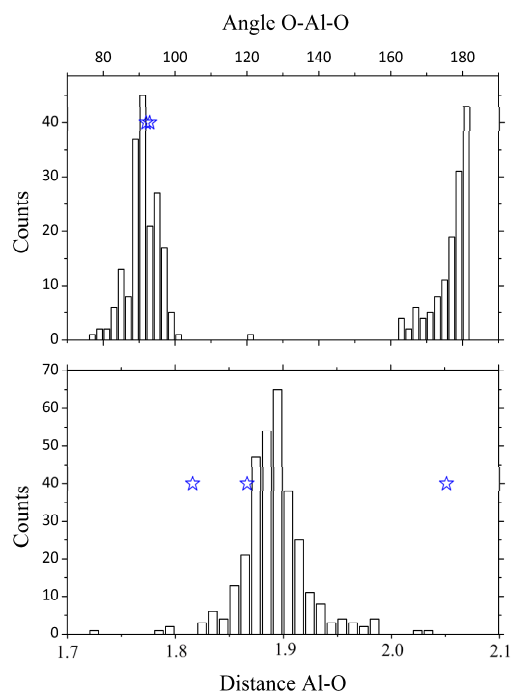


Fig S4. Bond distances and angles histograms for AlO_6 octahedral coordination. Stars represent the values for ermeloite and columns the CCDC data base entries.

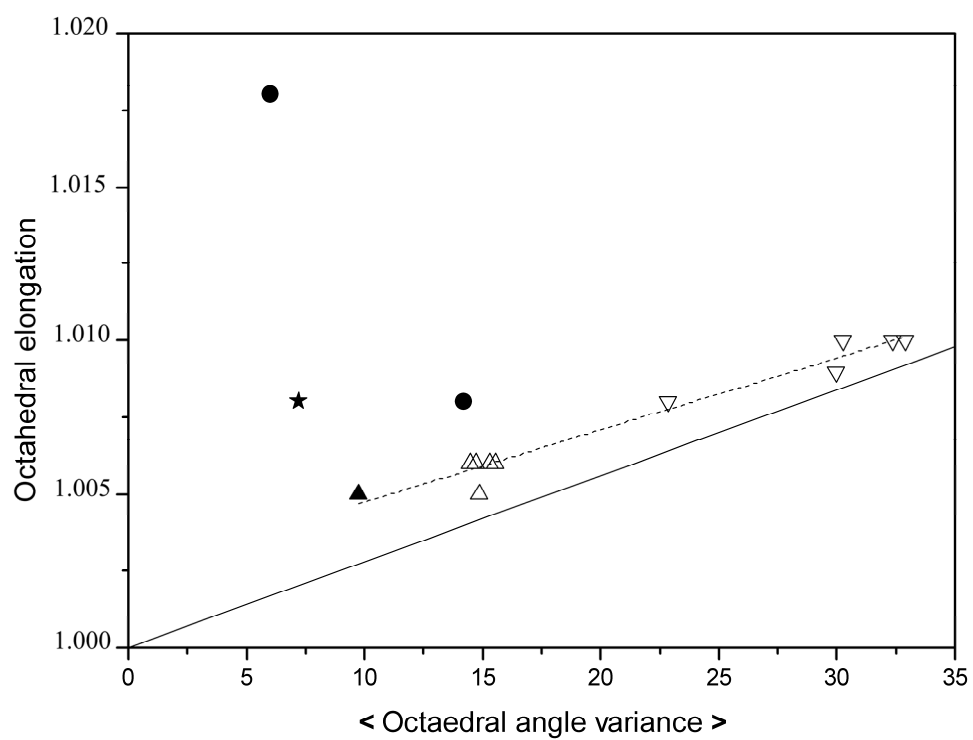


Fig S5. Octahedral angle variance Vs Octahedral elongation. Ermeloite (start) and $M^{3+}PO_4 \cdot H_2O$ (black circles). Up triangles ($M^{2+}SO_4 \cdot H_2O$), Up closed triangle (Kieserite (Mg^{2+})) down triangles ($M^{2+}SeO_4 \cdot H_2O$). Line represents calculated regression for Keith Robison data.

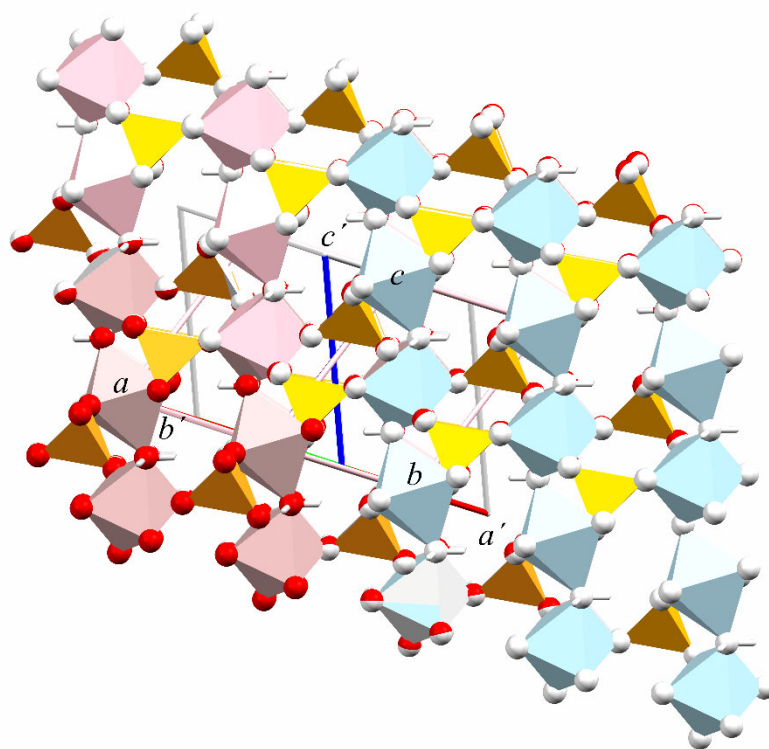


Fig. S6. Relationship between standard settings of ermeloite (pink octahedral), with the AlO_6 octahedral chains along $[101]$ (pink axis (a , b , c , β)) and the kieserite settings (colour axis (a' , b' , c' , β')), along $[001]$ (blue octahedral). Transformation matrix $(-1 \ 0 \ 0 \ 0 \ -1 \ 0 \ 1 \ 0 \ 1)$.