

# ***Pseudo-cubic crystal structure and phase transition in doped ye'elimite***

Ana Cuesta<sup>†</sup>, Ángeles G. De la Torre<sup>†</sup>, Enrique R. Losilla<sup>†</sup>, Isabel Santacruz<sup>†</sup>, Miguel A. G. Aranda<sup>\*† #</sup>

<sup>†</sup> Departamento de Química Inorgánica, Cristalografía y Mineralogía, Universidad de Málaga, 29071-Málaga, Spain.

<sup>#</sup> ALBA Synchrotron, Carretera BP 1413, Km. 3.3, E-08290 Cerdanyola, Barcelona, Spain

This supporting information includes:

**Table S1:** Final (refined) atomic parameters (coordinates and anisotropic displacement parameters) for doped ye'elimite at room temperature.

**Table S2:** Interatomic distances and angles for doped ye'elimite at room temperature.

**Figure S1:** Full thermodiffractometric study for doped ye'elimite with Si added as internal standard (starred peaks are those coming from the added standard).

**Figure S2.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimite mixed with silicon (internal standard) at 30 °C.

**Figure S3.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimite mixed with silicon (internal standard) at 100 °C.

**Figure S4.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimite mixed with silicon (internal standard) at 300 °C.

**Figure S5.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimite mixed with silicon (internal standard) at 500 °C.

**Figure S6.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimite mixed with silicon (internal standard) at 700 °C.

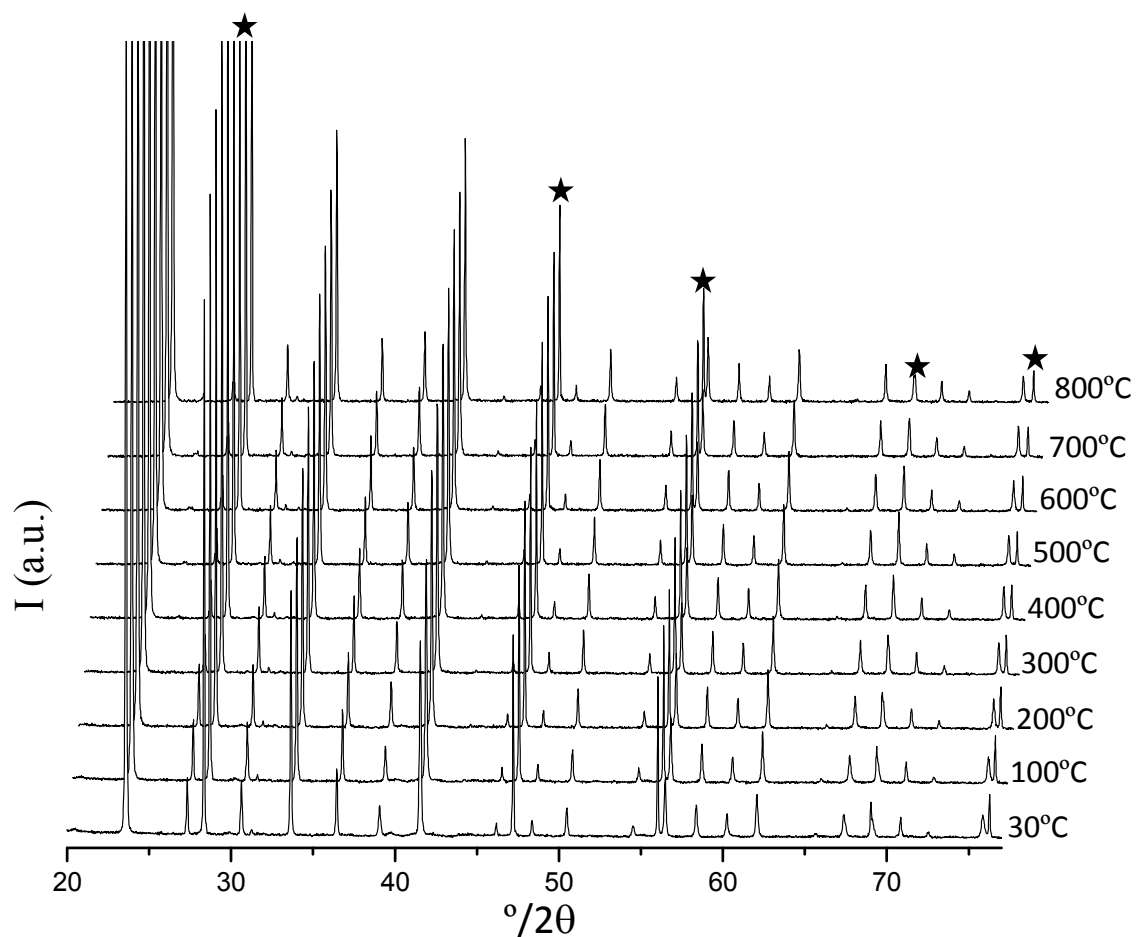
**Table S1:** Final (refined) atomic parameters (coordinates and anisotropic displacement parameters) for doped ye'elimite at room temperature.

Atom	Ca1	Al1	S1*	O1	O2*
Wyckoff position	8c	12d	2a	24g	24g
occupation factor	1	1	1	1	0.3333
x	0.2944(1)	0.2500	0.0000	0.3479(2)	0.1129(5)
y	0.2944 (1)	0.5000	0.0000	0.3479(2)	0.1129(5)
z	0.2944 (1)	0.0000	0.0000	0.0533(3)	0.0136(16)
u <sub>11</sub>	0.096(1)	0.007(1)	0.087(2)	0.028(1)	0.139(7)
u <sub>22</sub>	0.096(1)	0.015(1)		0.028(1)	
u <sub>33</sub>	0.096(1)	0.015(1)		0.034(2)	
u <sub>12</sub>	0.069(2)	0.000		0.009(1)	
u <sub>13</sub>	0.069(2)	0.000		0.007(1)	
u <sub>23</sub>	0.069(2)	0.000		0.007(1)	

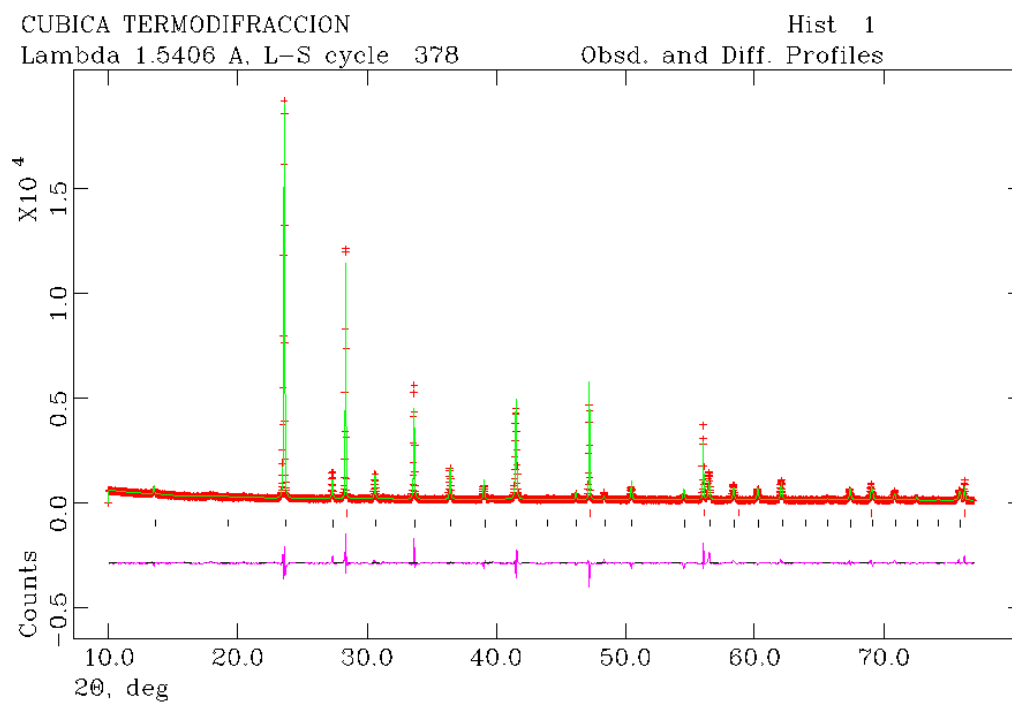
\*isotropic displacement parameters

**Table S2:** Selected interatomic distances (Å) and angles (°) for doped ye'elimite at room temperature.

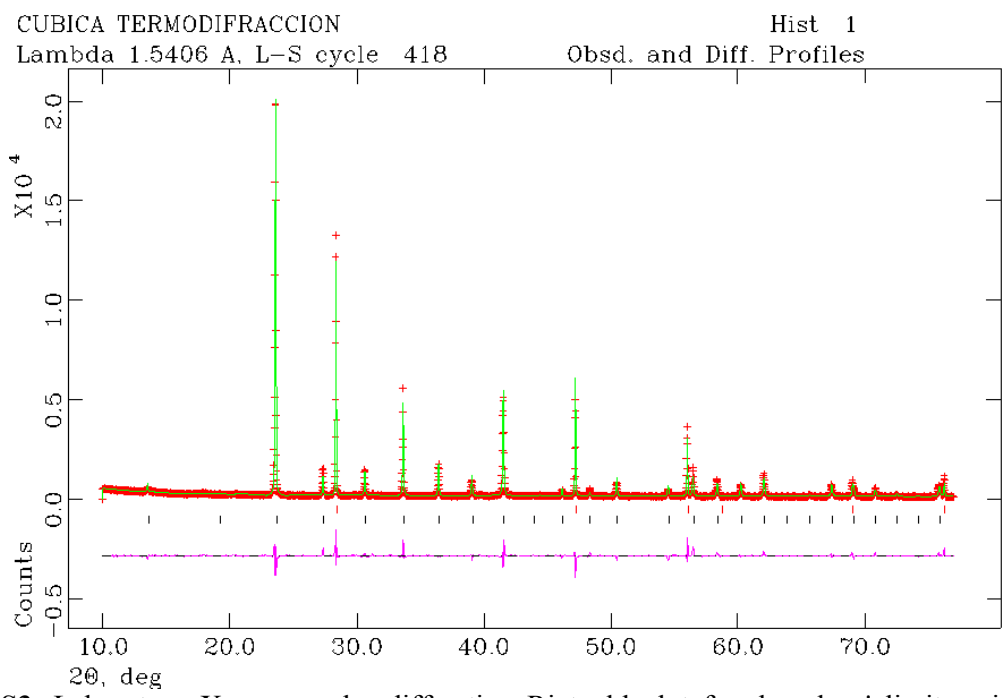
Ca-O	
Ca(1)-O(1)x3	2.324(3)
Ca(1)-O(1)x3	3.016(2)
Ca(1)-O(2)x3	2.350(14)
Al-O	
Al(1)-O(1) x4	1.734(1)
O(1)-Al(1)-O(1) x2	117.4 (2)
O(1)-Al(1)-O(1) x4	105.6(7)
S-O	
S(1)-O(2) x4	1.474(6)



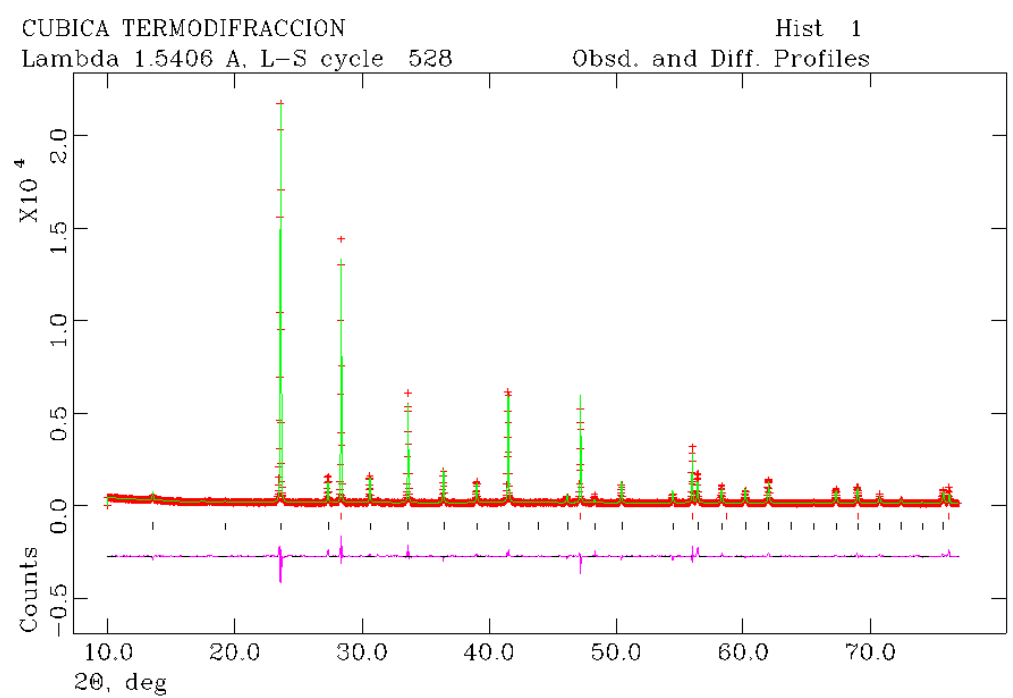
**Figure S1:** Full thermodiffractometric study for doped ye'elimitite with Si added as internal standard (starred peaks are those coming from the added standard).



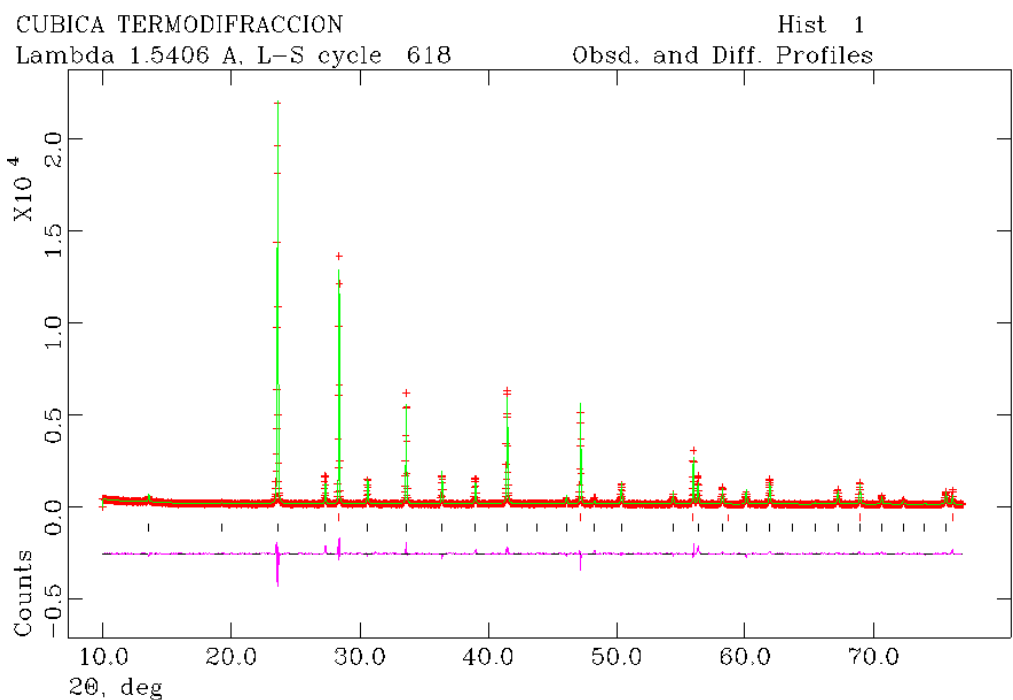
**Figure S2.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimitite mixed with silicon (internal standard) at 30 °C.



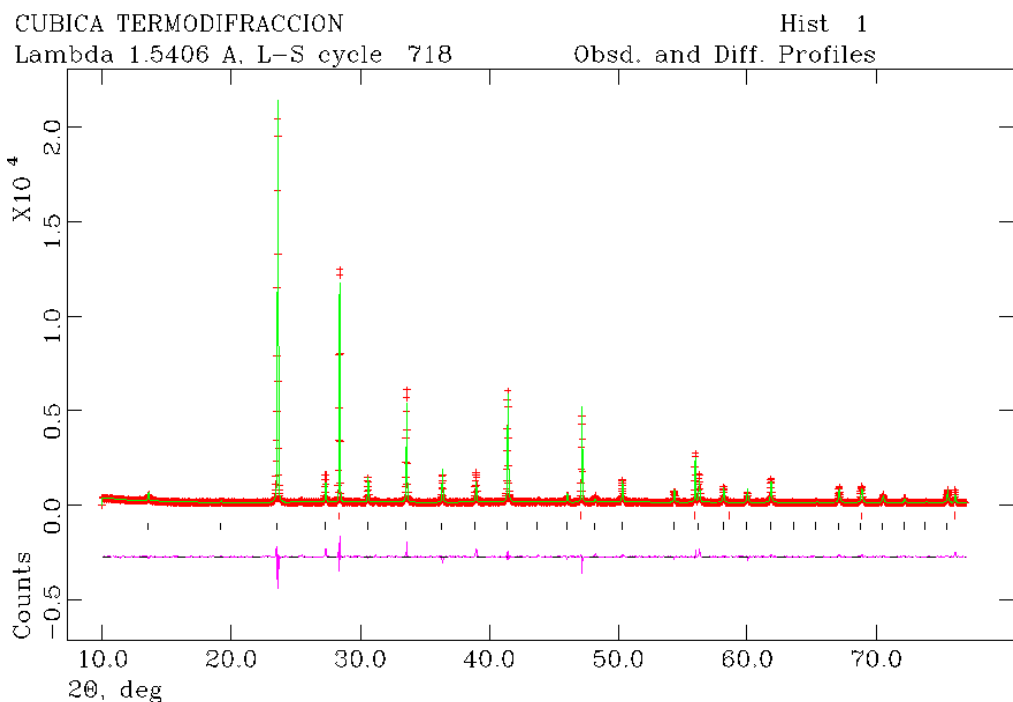
**Figure S3.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimitite mixed with silicon (internal standard) at 100 °C.



**Figure S4.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimitite mixed with silicon (internal standard) at 300 °C.



**Figure S5.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimitite mixed with silicon (internal standard) at 500 °C.



**Figure S6.** Laboratory X-ray powder diffraction Rietveld plot for doped ye'elimitite mixed with silicon (internal standard) at 700 °C.