ELECTRONIC SUPPORTING INFORMATION FOR:

Ca $L_{2,3}$-edge near edge X-ray absorption fine structure of tricalcium aluminate, gypsum and calcium (sulfo)aluminate hydrates

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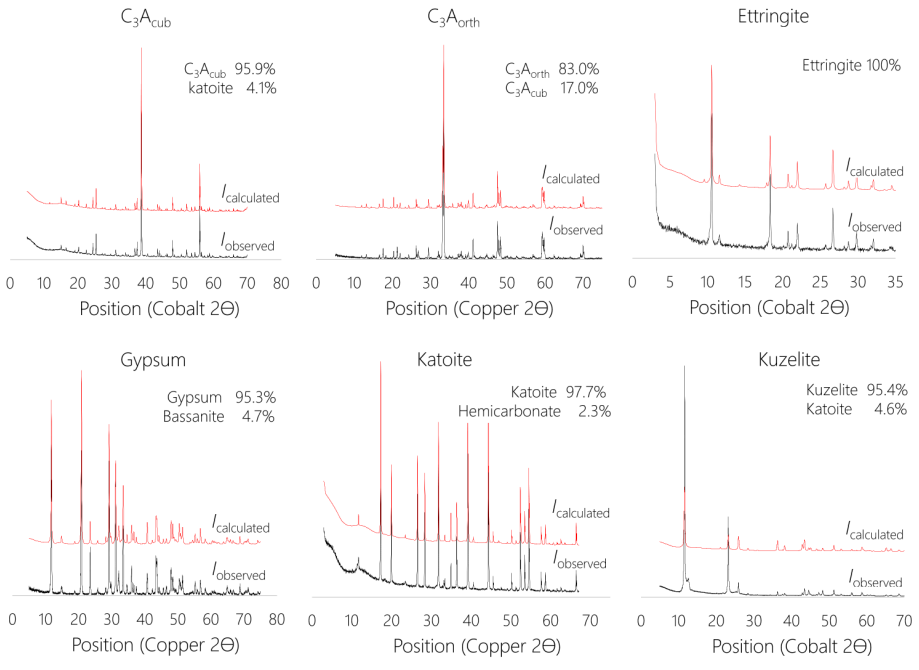
In the present work, C_3A_{cub}, C_3A_{orth}, ettringite and katoite were purchased from Mineral Research Processing (http://www.mineralresearchprocessing.fr/). Gypsum was purchased from Fisher Scientific (#S76764). Kuzelite were synthesized by stoichiometricly mixing C_3A_{cub}, gypsum and deionized water, and storing in seal plastic bottle for 17 days. The crystal structures and chemical compositions of were verified by powder X-ray diffraction performed with PANalytical X'Pert Pro diffractometer operating at 40 keV and 40 mA with a Cobalt anode for C_3A_{cub}, ettringite and kuzelite, and a Copper anode for C_3A_{orth}, gypsum and katoite. Sample purities were further verified by Rietveld refinement with software HighScorePlus and ICSD database (Supplementary Figure 1).

Thermogravimetric analysis (TGA) indicates total weight loss of 2.5% up until 1000 °C. X-ray fluorescence measurement of cubic C_3A and gypsum were performed with Philips PW2400 Wavelength-Dispersive XRF. The overall cation oxide impurity/CaO weight ratios are 0.02 in C_3A_{cub} and 0.003 in gypsum. C_3A_{orth} has atomic ratio of $Na_2O:CaO:Al_2O_3$ = 0.187:2.92:1, with 1.07 wt% impurities.

For reading convenience, Supplementary Table 1 lists peak positions of displayed spectra in Figure 3a in the paper. Ca in katoite, C_3A_{cub} and C_3A_{orth} are in cubic-like symmetry, while Ca in kuzelite, ettringite, gypsum are in octahedral-like symmetry.



SUPPLEMENTARY FIGURE 1. Powder XRD and Rietveld refinement of C_3A_{cub}, C_3A_{orth}, ettringite, gypsum, katoite and kuzelite.

SUPPLEMENTARY TABLE 1. Peak positions in the Ca $L_{2,3}$-edge NEXAFS spectra shown in Figure 3, eV

Symmetry	Mineral	1	a_1	2	a_2	b_{1o}	b_1	b_2	a_2-a_1	b_2-b_1
Cubic	katoite	346.85	347.43	348.24	349.13	–	351.17	352.38	1.70	1.21
	C3Acub	346.86	347.57	348.31	349.14	–	351.18	352.46	1.57	1.28
	C3Aorth	346.80	347.57	348.14	349.11	–	351.20	352.40	1.54	1.20
		1	2	a_1	a_2	b_{1o}	b_1	b_2	a_2-a_1	b_2-b_1
Octahedral	gypsum	347.00	347.56	348.21	349.06	350.82	351.43	352.33	0.85	0.90
	kuzelite	346.85	347.48	348.08	349.01	–	351.13	352.31	0.93	1.18
	ettringite	346.88	347.54	348.13	349.13	–	351.38	352.45	1.00	1.07

Note: Software aXis2000 allows peak position determination with sub-step size accuracy, with uncertainty of ~0.02 eV at the studied energy range.