

Borosilicate Glass-Ceramics Containing Zirconolite and Powellite for RE- and Mo- Rich Nuclear Waste Immobilization

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Table S1. Structural Rietveld refinement results of the Nd-doped zirconolite phase for CTZ-40 sample.

Site	x	y	z	Mult	Occupancy	Uiso (Å ²)
CTZ-40: Ca _{0.78} Nd _{0.22} ZrTi _{1.78} Al _{0.22} O ₇ , space group C12/c1; Z=8; a=12.7909(1) Å, b=7.3946(4) Å, c=11.6172(1) Å; α=90.000(0) °, β=100.900(6) °, γ=90.000(0) °; V=1078.97(8) Å ³						
Ca(1)	0.3730	0.1230	0.4940	8	0.74	0.0268
Nd(1)	0.3810	0.1280	0.4939	8	0.22	0.0700
Zr(1)	0.3590	0.1250	0.4959	8	0.04	0.0220
Ca(2)	0.1212	0.1222	0.9744	8	0.04	0.0250
Zr(2)	0.1222	0.1222	0.9744	8	0.88	0.0240
Ti(1)	0.1232	0.1222	0.9744	8	0.08	0.0241
Zr(3)	0.2397	0.1120	0.7377	8	0.03	0.0190
Ti(2)	0.2497	0.1220	0.7467	8	0.97	0.0270
Zr(4)	0.04740	0.0560	0.2500	8	0.05	0.0250
Ti(3)	0.4740	0.0560	0.2500	8	0.23	0.0401
Al(1)	0.4770	0.0580	0.2600	8	0.22	0.0250
Ti(4)	0.0000	0.1270	0.2500	4	1.00	0.0341
O(1)	0.3110	0.1370	0.2750	8	1.00	0.0211
O(2)	0.4700	0.1440	0.1020	8	1.00	0.0199
O(3)	0.1960	0.0820	0.5740	8	1.00	0.0250
O(4)	0.4040	0.1750	0.7200	8	1.00	0.0220
O(5)	0.7030	0.1680	0.5910	8	1.00	0.0231
O(6)	0.0010	0.1110	0.4140	8	1.00	0.0180
O(7)	0.1190	0.0540	0.7870	8	1.00	0.0182