Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Organic template-free synthesis of an open framework silicoaluminophoshate (SAPO) with high thermal stability and high ion conductivity

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Table s1. Atomic positions and Uiso parameters for both polymorphs Cs2(Al0.875Si0.125)4(P0.875Si0.125O4)4(HPO4).

Phase		**DFZ-64C-LT (20°C)**				**DFZ-64C-HT (570°C)**			
Atom	**Occ**	***x***	***y***	***z***	**U_{iso} (Å^2)**	***x***	***y***	***z***	**U_{iso} (Å^2)**
Al1	1	-0.9704(11)	-0.8894(2)	0.4787(6)	0.0141(14)	0.015(4)	0.1132(7)	0.4661(17)	0.026(5)
Al2	1	-0.5341(11)	0.0166(2)	0.0391(6)	0.0048(12)	-0.519(3)	0.0159(7)	0.0358(15)	0.007343
Al/Si3	0.5/0.5	-0.9700(12)	-0.1464(2)	0.1979(7)	0.0260(15)	0.034(3)	0.8539(7)	0.2093(14)	0.012(4)
Al4	1	-0.4851(12)	-0.2284(3)	0.7025(7)	0.0217(14)	-0.502(4)	-0.2312(7)	0.7139(15)	0.027(4)
Cs1	1	-0.0041(2)	-0.33486(5)	0.07600(14)	0.0293(4)	0.0034	0.1688	0.9234(3)	0.0566(13)
Cs2	1	-0.9932(2)	-0.06914(6)	0.69236(16)	0.0316(4)	0.0066(13)	-0.0692(2)	0.6957(4)	0.0532(13)
P1	1	-0.5357(10)	-0.3620(2)	0.7664(6)	0.0163(13)	-0.453(3)	-0.3594(7)	0.7651(13)	0.023(4)
P2	1	-0.4847(10)	-0.1331(2)	0.9887(5)	0.0116(13)	-0.492(4)	-0.1346(6)	-0.0153(14)	0.035(5)
P3	1	-0.5173(10)	-0.4423(2)	0.3351(6)	0.0125(11)	-0.480(3)	0.0608(5)	0.6628(12)	0.005(3)
P4	1	-1.0328(10)	-0.0072(2)	0.2460(6)	0.0190(15)	-0.011(3)	-0.0098(6)	0.2430(14)	0.013(4)
P/Si5	0.5/0.5	-0.9859(11)	-0.2412(2)	0.4893(7)	0.0237(15)	-1.032(3)	-0.2391(6)	0.4846(12)	0.016(4)
O1	1	-0.675(2)	-0.1632(4)	1.1184(12)	0.008(3)	-0.740(5)	-0.1688(12)	0.115(3)	0.005203
O2	1	-0.508(2)	-0.5060(4)	0.4433(13)	0.012(3)	-0.491(4)	-0.0070(9)	0.554(2)	0.005203
O3	1	-1.3234(19)	-0.0035(4)	0.2118(11)	0.004(3)	-0.313(5)	-0.0054(12)	0.209(2)	0.005203
O4	1	-1.038(2)	-0.3119(5)	0.4417(14)	0.043(4)	-0.968(5)	-0.3070(10)	0.436(2)	0.005203
O5	1	-0.5421(18)	-0.0667(5)	0.9776(10)	0.013(2)	-0.449(5)	-0.0689(12)	-0.029(2)	0.005203
O6	1	-0.698(2)	-0.2256(5)	0.5392(12)	0.012(3)	-0.828(4)	-0.2218(11)	0.596(3)	0.005203
O7	1	-0.7440(19)	-0.4092(4)	0.3891(12)	0.015(3)	-0.270(4)	0.0915(11)	0.605(3)	0.005203
O8	1	-0.954(2)	0.0263(4)	0.3994(13)	0.013(3)	0.030(5)	0.0264(10)	0.405(2)	0.005203
O9	1	-0.491(2)	-0.4027(4)	0.9275(14)	0.011(3)	-0.476(5)	-0.4067(10)	0.921(2)	0.005203
O10	1	-0.8046(18)	-0.3714(4)	0.7001(11)	0.008(3)	-0.198(5)	0.1307(11)	0.305(3)	0.005203
O11	1	-0.546(2)	-0.1630(4)	0.8213(13)	0.006(3)	-0.478(5)	-0.1603(10)	-0.179(3)	0.005203
O12	1	-0.337(2)	-0.3736(4)	0.6327(13)	0.018(3)	0.279(5)	0.1246(10)	0.347(2)	0.005203
O13	1	-0.2373(18)	-0.4190(4)	0.3426(11)	0.005(3)	0.242(4)	0.0879(10)	0.676(3)	0.005203
O14	1	-0.954(2)	-0.0762(6)	0.2975(13)	0.021(3)	0.001(7)	-0.0745(13)	0.303(3)	0.005203
O15	1	-0.205(2)	-0.1422(5)	1.0365(13)	0.029(4)	-0.323(5)	-0.1502(12)	0.069(3)	0.005203
O16	1	-0.578(2)	-0.4640(5)	0.1688(15)	0.022(3)	-0.432(5)	0.0417(11)	0.833(3)	0.005203
O17	1	-1.033(2)	-0.2007(4)	0.3347(13)	0.023(3)	-0.957(4)	-0.2042(10)	0.333(2)	0.005203
O18	1	-0.495(3)	-0.2939(5)	0.8276(15)	0.038(4)	-0.510(6)	-0.2911(10)	0.823(3)	0.005203
O19	1	-0.8653(19)	0.0126(5)	0.1005(12)	0.013(3)	0.147(4)	0.0091(11)	0.091(2)	0.005203
O20	1	-0.160(2)	-0.2186(5)	0.6368(12)	0.017(3)	-1.310(5)	-0.2219(11)	0.553(2)	0.005203
H1o2*	1	-0.5031	-0.5377	0.4971	0.014471	-0.496	-0.0391	0.5028	0.006244

** for both structures, the H atoms were added in apical geometric constrained positions and their positions were fixed during refinements.*

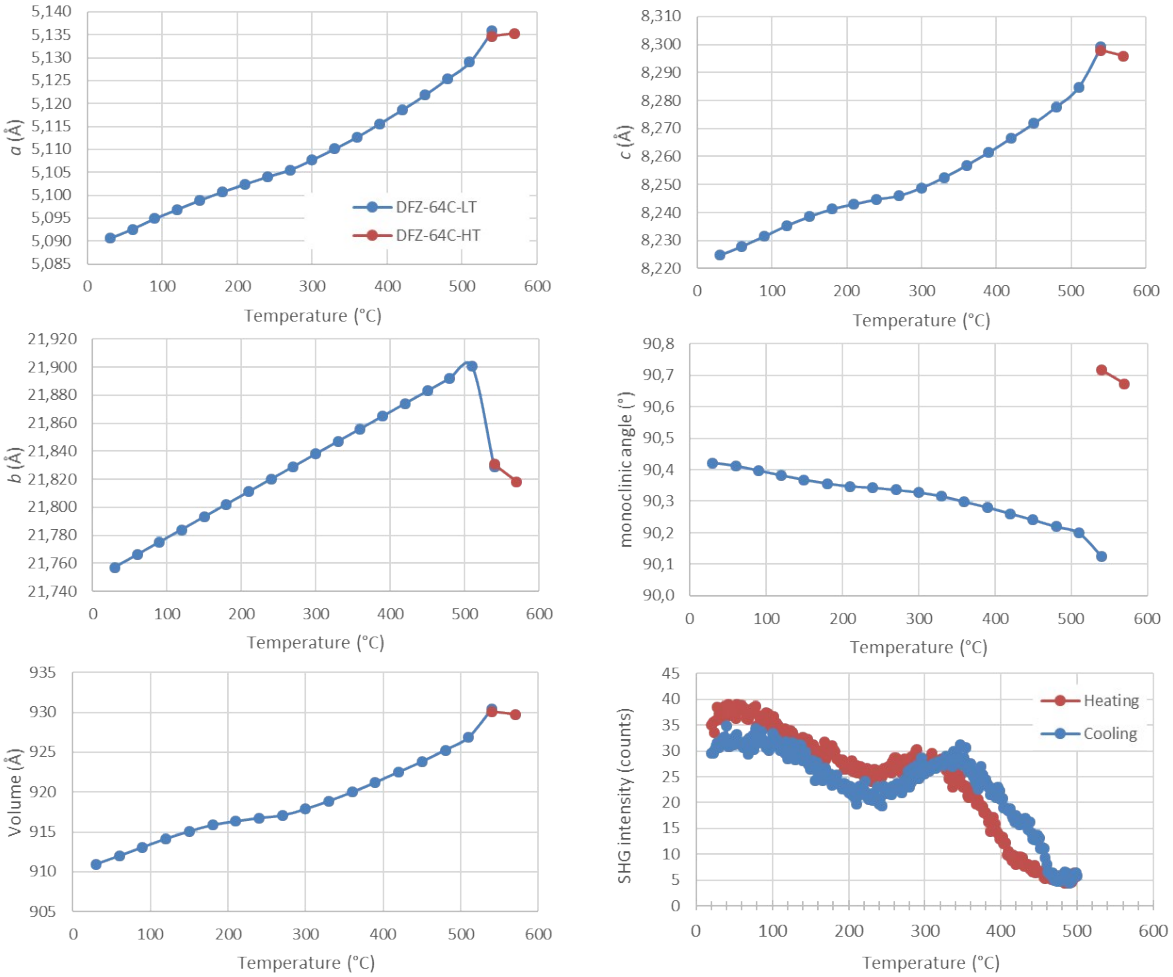

Figure s1. The variation of the unit-cell parameters and evolution of SHG intensity with the temperature of sample DFZ-64C

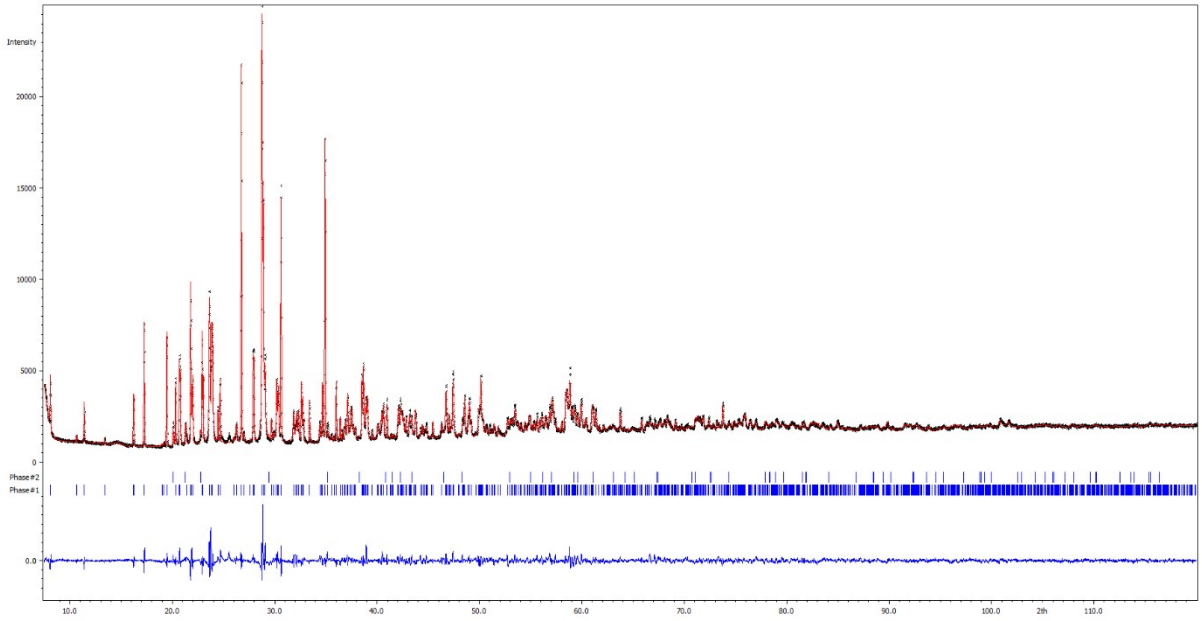

Figure s2. PXRD diagram of DFZ-64C-HT at 570°C (Cu–Kα1 radiation; 1.5406Å) with observed (dots), calculated (solid line), Bragg reflections (ticks), and difference profiles (bottom line) obtained after Rietveld refinements

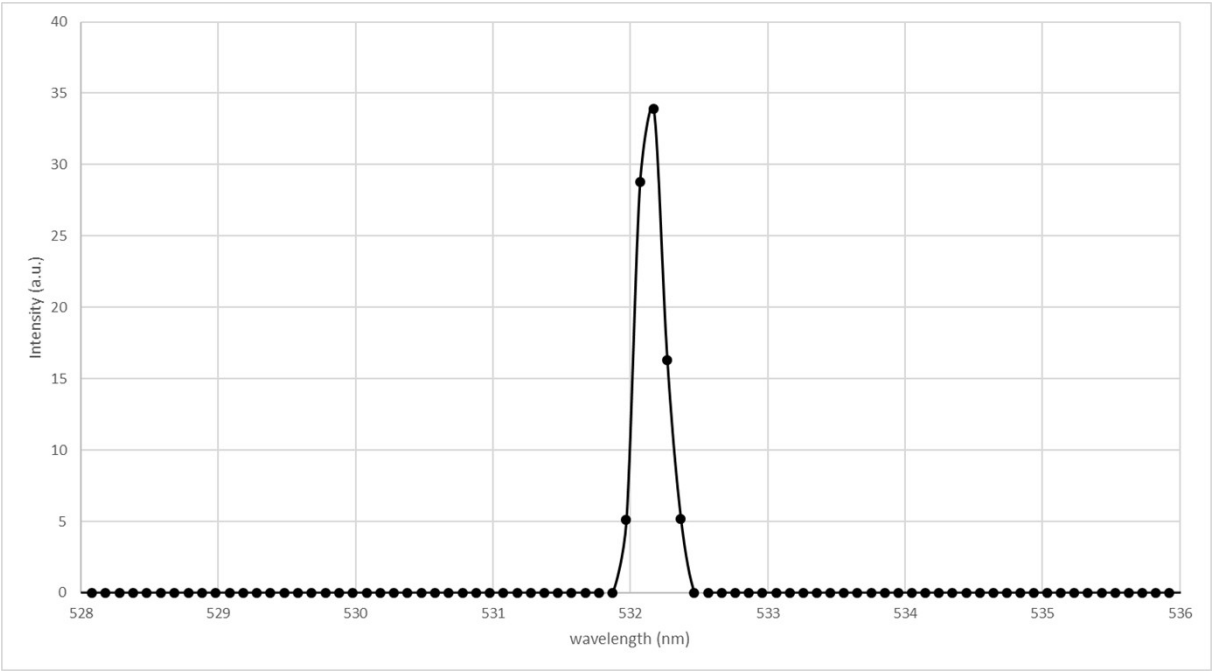

Figure s3. SHG response of DFZ-64C at 540°C

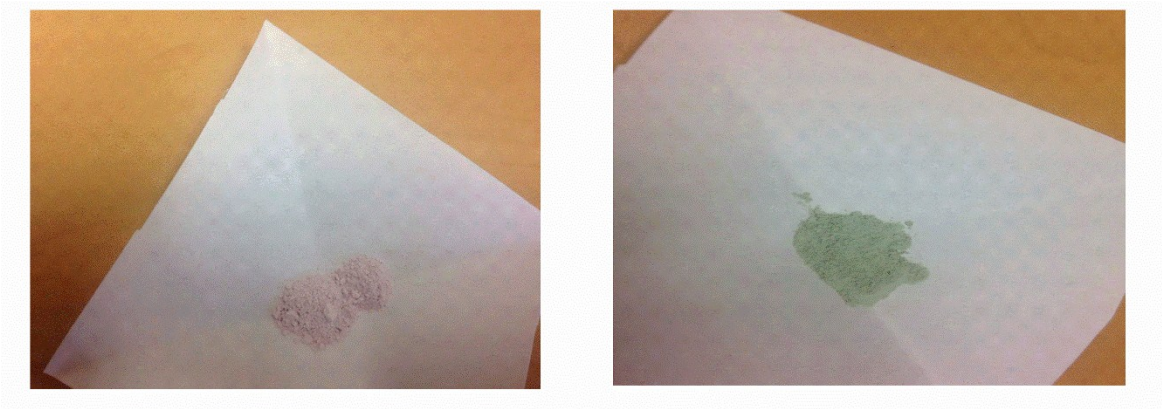

Figure s4 The pictures of sample DFZ-64C after Co^{2+} and Cu^{2+} exchange.