Supplementary:

Table S1. Phase contents determined by XRD and Rietveld refinement. E.s.d.s of the refinement are given in parentheses. Additional phase contents are ≤1.5 wt.%: Anhydrite and brownmillerite; ≤1 wt.%: Rondorfite, $CaCl_2$ and albite; ≤0.5 wt.%: microcline, $CaSiO_3Cl_2$ and ye'elimite.

Name	amorphous	β-C_2S	αH-C_2S	γ-C_2S	Quartz	$CaCO_3$	Lime	Elles-tadite mkl	Elles-tadite hex	Chlor-mayenite	Rusi-novite	Terne-site	Spurrite	Ranki-nit	Melilite	Bredigite	Mer-winite	Wollastonite	GoF	DW
HT[P]_800	20(1)	2.9(3)	7.3(3)	1.5(2)	8.33(9)	31.7(3)	0.10(3)	11.0(3)		0.8(1)			9.2(3)					2.8(2)	1.99	0.33
HT[P]_900	15.9(8)	3.4(2)	9.7(2)	1.8(1)	5.69(6)	11.5(1)		10.9(3)		2.29(7)	0.26(9)	0.29(8)	30.9(3)				1.7(2)	3.9(1)	1.45	0.54
HT[P]_950	17.8(8)	47.4(4)	2.6(2)	1.0(1)	2.89(4)		0.70(3)	10.6(2)		3.13(8)	0.4(1)		10.2(2)				1.2(1)	1.3(1)	1.49	0.51
HT[P]_1000	15.0(7)	63.8(5)		0.71(9)	2.12(4)		0.17(5)		9.9(1)	3.90(9)	0.7(1)	0.12(7)	0.5(1)		0.06(5)		0.5(1)	0.6(1)	1.67	0.46
HT[P]_1050	16.1(6)	55.2(4)		0.60(9)	1.38(5)		0.08(2)		9.8(1)	3.95(7)	0.29(9)	0.30(8)	0.5(1)		0.26(5)	7.3(1)	0.6(1)	2.0(1)	1.54	0.50
HT[P]_1100	29.3(5)	42.1(3)		0.67(8)	0.14(2)		0.15(3)		8.3(1)	0.56(6)	0.77(8)	0.21(7)	0.27(8)	7.8(1)	7.1(1)	1.0(1)		0.11(3)	1.52	0.58
HT[D2]_700	15.7(8)	4.1(2)	7.0(2)	0.50(9)	8.80(7)	21.0(2)	0.12(4)	26.7(3)		0.79(7)		0.38(9)	11.3(2)		0.13(5)		1.2(1)	0.68(9)	1.96	0.36
HT[D2]_800	8.6(7)	25.7(2)	2.7(2)	0.52(7)	6.80(6)	4.52(6)	0.22(5)	23.1(2)	5.3(2)	3.03(8)	1.8(1)	0.32(8)	15.0(2)		0.06(5)			0.25(8)	1.93	0.35
HT[D2]_900	12.3(8)	45.5(4)		0.36(6)	5.63(6)	0.08(4)	1.81(3)	13.6(3)	10.6(2)	3.59(8)	2.5(1)	1.2(1)			0.25(6)		0.14(8)	0.10(6)	2.00	0.32
HT[D2]_1000	14.6(9)	48.4(3)		0.30(6)	3.84(5)		2.45(4)		19.6(2)	2.63(7)	0.7(1)	4.6(1)			0.06(5)		0.40(8)	0.5(1)	1.73	0.44
HT[D2]_1100	12(1)	48.2(4)		0.6(1)	3.61(7)	0.17(7)	0.11(3)		18.4(2)	3.23(8)	0.9(1)	7.4(2)		0.6(2)	0.23(6)		0.4(1)	0.6(1)	1.62	0.51
HT[D2]_1200	16.7(8)	43.7(3)		0.7(1)	1.01(5)	0.04(3)	0.14(3)		17.3(2)	2.80(6)	0.07(6)	10.0(2)			1.1(1)	3.5(1)		1.1(1)	1.55	0.54

Table S2. Lattice parameters and site occupancies determined for ellestadite in sample mixtures D2 and P heated to 700-1200 °C. Cl_{calc}=chlorine content calculated from crystalline phase contents (ellestadite composition was considered in the calculation); Cl_{I-IC}=chlorine content determined by combustion-ion chromatography.

	Ellestadite monoclinic										Ellestadite hexagonal						Cl_{calc}	Cl_{C-IC}
Name	a	b	c	β	V	SOF S1 (S)	SOF S2 (S)	SOF Ca3 (Ca)	SOF O13 (Cl)	SOF Cl1 (Cl)	a	c	V	SOF Ca1 (Ca)	SOF Ca2 (Ca)	SOF Cl1 (Cl)		
HT[D2]_800	9.5690(8)	9.5372(7)	6.9201(3)	119.957(6)	547.16(7)	0.27(2)	0.34(2)	0.57(4)	0	0.16(5)							0.95	1.29
HT[D2]_900	9.5548(5)	9.5345(4)	6.9243(2)	120.043(4)	546.06(5)	0.41(2)	0.42(2)	0.65(3)	0.16(4)	0.16(5)	9.5927(6)	6.9008(7)	549.94(8)	1.0(2)	1.0(1)	0.48(5)	1.73	1.39
HT[D2]_950	9.5699(9)	9.551(1)	6.9085(4)	119.970(8)	547.01(9)	0.44(5)	0.47(5)	0.66(2)	0.18(4)	0.16(5)	9.6056(5)	6.8898(4)	550.54(6)	0.99(1)	0.993(7)	0.45(3)	1.46	1.40
HT[D2]_1000											9.6273(2)	6.8758(2)	551.90(2)	0.983(4)	0.992(2)	0.44(1)	1.56	1.35
HT[D2]_1050											9.6358(2)	6.8714(2)	552.52(3)	0.978(5)	0.996(3)	0.44(1)	1.46	1.29
HT[D2]_1100											9.6350(2)	6.8730(2)	552.56(3)	1.000(6)	0.987(3)	0.46(1)	1.45	1.21
HT[P]_700	9.579(2)	9.538(2)	6.913(1)	120.00(1)	547.0(2)	0	0.38(5)	0.6(1)	0	0							0.72	1.28
HT[P]_800	9.575(1)	9.552(2)	6.9122(6)	119.94(1)	547.8(2)	0	0.39(4)	0.49(8)	0	0							0.66	1.34
HT[P]_900	9.602(1)	9.564(2)	6.898(4)	119.95(1)	548.8(2)	1.00(4)	0.33(4)	0.57(7)	0	0.2(1)							0.71	1.40
HT[P]_1000											9.6432(3)	6.8674(3)	553.05(4)	1.000(9)	0.996(5)	0.49(2)	1.22	1.29
HT[P]_1100											9.6386(2)	6.8701(3)	552.74(3)	1.000(9)	0.994(4)	0.48(2)	1.20	1.09
HT[P]_1200											9.6226(3)	6.8873(3)	552.29(5)	0.99(1)	1.000(5)	0.48(2)	0.82	0.52