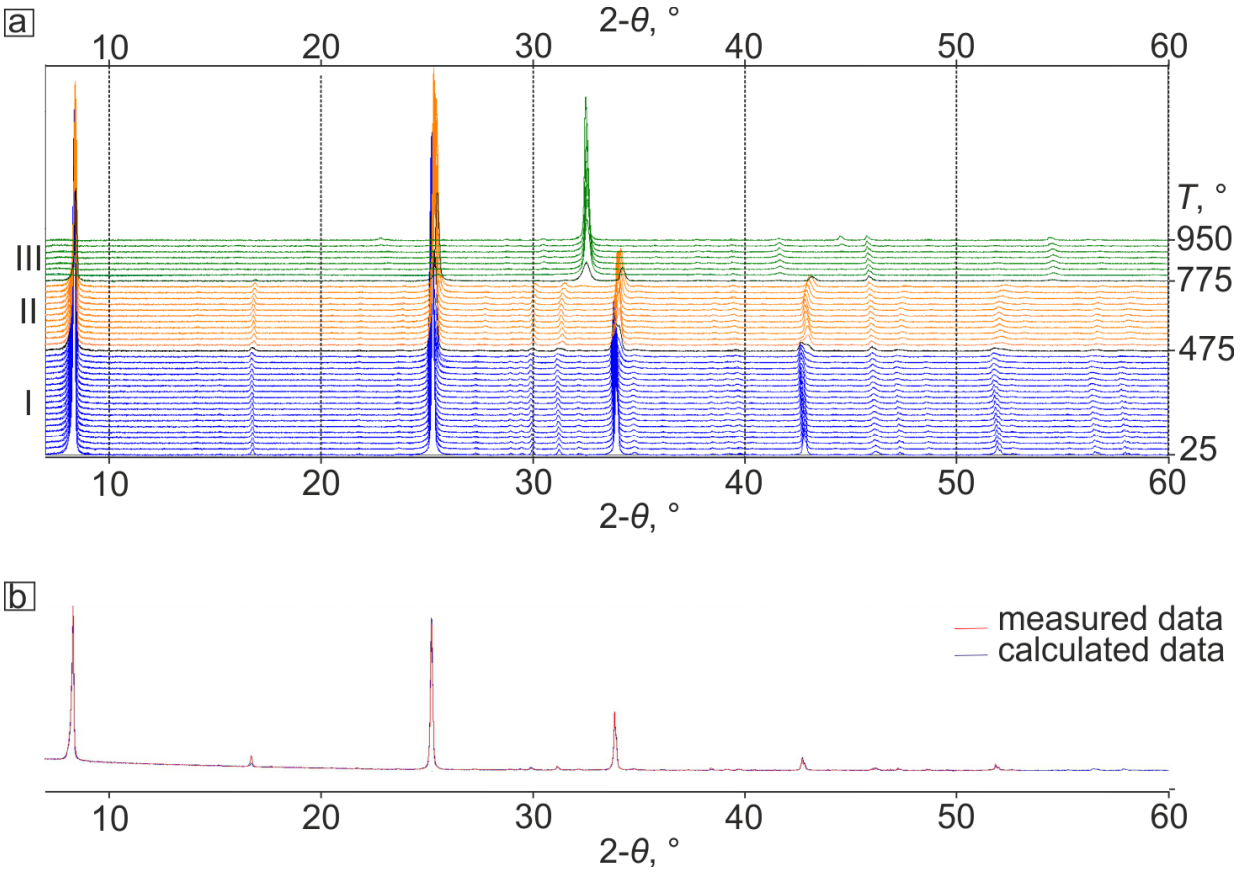


Figure S1. a) X-ray diffraction patterns for kupletskite in the temperature range from 25 to 950 °C: I) 25-475 °C kupletskite, II) 500-775 °C high-temperature modification of kupletskite, III) 800-950 °C products of kupletskite decomposition. b) X-ray diffraction pattern for kupletskite measured at 200 °C with fitting of the Rietveld refinement.

Table S1. Unit cell parameters refined for kupletskite and its high-temperature (HT) modification at different temperatures

T, °C	*a*, Å	*b*, Å	*c*, Å	*α*, °	*β*, °	*γ*, °	*V*, Å^3
Kupletskite							
25	5.3504(4)	11.9583(7)	11.7026(4)	113.280(4)	94.764(6)	102.553(8)	659.33(8)
50	5.3509(4)	11.9610(7)	11.7043(4)	113.274(4)	94.761(7)	102.564(8)	659.63(7)
75	5.3520(4)	11.9649(7)	11.7080(4)	113.283(4)	94.774(7)	102.541(8)	660.20(8)
100	5.3538(4)	11.9673(7)	11.7114(4)	113.285(4)	94.778(7)	102.531(8)	660.75(8)
125	5.3554(4)	11.9709(7)	11.7145(4)	113.287(4)	94.773(7)	102.529(8)	661.34(8)
150	5.3586(4)	11.9750(7)	11.7193(4)	113.287(4)	94.795(7)	102.520(8)	662.20(8)
175	5.3601(4)	11.9791(7)	11.7228(4)	113.287(4)	94.797(7)	102.522(8)	662.80(8)
200	5.3598(4)	11.9848(7)	11.7242(4)	113.286(4)	94.796(7)	102.518(8)	663.18(8)
225	5.3618(4)	11.9872(7)	11.7278(4)	113.287(4)	94.791(7)	102.518(8)	663.76(8)
250	5.3621(4)	11.9911(8)	11.7306(4)	113.287(4)	94.803(7)	102.508(8)	664.19(8)
275	5.3639(4)	11.9945(8)	11.7341(4)	113.284(4)	94.804(8)	102.510(9)	664.81(8)
300	5.3654(4)	11.9976(8)	11.7371(5)	113.287(4)	94.793(8)	102.510(9)	665.35(9)
325	5.3653(4)	11.9979(9)	11.7381(5)	113.277(5)	94.796(9)	102.51(1)	665.44(9)
350	5.3660(5)	12.000(1)	11.7407(6)	113.284(5)	94.80(1)	102.50(1)	665.8(1)
375	5.3655(5)	12.006(1)	11.7403(6)	113.284(6)	94.81(1)	102.51(1)	666.0(1)
400	5.3658(6)	12.012(1)	11.7411(7)	113.281(7)	94.81(1)	102.52(2)	666.3(1)
425	5.3654(7)	12.016(2)	11.7429(9)	113.286(9)	94.82(2)	102.52(2)	666.6(2)

450	5.3655(9)	12.014(3)	11.741(1)	113.29(1)	94.79(2)	102.54(2)	666.4(2)
Kupletskite HT modification							
550	5.3421(2)	11.7555(9)	11.6181(4)	112.633(4)	93.919(5)	103.568(5)	644.31(7)
575	5.3453(2)	11.7609(9)	11.6223(4)	112.639(5)	93.927(5)	103.533(5)	645.31(7)
600	5.3483(2)	11.7613(8)	11.6259(4)	112.641(4)	93.929(4)	103.514(4)	645.93(6)
625	5.3392(4)	11.7622(4)	11.6360(3)	112.780(3)	93.799(4)	103.392(2)	645.44(6)
650	5.3370(3)	11.7618(4)	11.6342(3)	112.774(3)	93.785(4)	103.393(2)	645.12(5)
675	5.3346(3)	11.7499(4)	11.6256(3)	112.733(3)	93.806(4)	103.413(2)	643.80(5)
700	5.3246(4)	11.7335(5)	11.6083(4)	112.743(4)	93.790(5)	103.414(3)	640.72(6)
725	5.3165(4)	11.7203(5)	11.5976(4)	112.745(4)	93.790(5)	103.452(3)	638.29(6)
750	5.3078(3)	11.7022(5)	11.5840(4)	112.742(4)	93.784(5)	103.456(3)	635.54(6)

Table S2. Unit-cell parameters refined for kupletskite-(Cs) and its HT modification at different temperatures

T, °C	*a*, Å	*b*, Å	*c*, Å	*α*, °	*β*, °	*γ*, °	*V*, Å^3
Kupletskite-(Cs)							
25	5.3953(8)	11.938(2)	11.8011(8)	113.123(7)	94.557(9)	103.16(1)	668.5(2)
50	5.3941(8)	11.946(2)	11.8085(8)	113.119(7)	94.579(8)	103.14(1)	669.2(2)
75	5.3954(8)	11.946(2)	11.8111(7)	113.114(7)	94.560(9)	103.16(1)	669.6(2)
100	5.3956(8)	11.944(2)	11.8130(8)	113.098(7)	94.545(9)	103.15(1)	669.7(2)
125	5.4002(7)	11.947(2)	11.8211(8)	113.097(7)	94.544(8)	103.16(1)	670.9(2)
150	5.4004(7)	11.949(2)	11.8238(7)	113.070(7)	94.531(8)	103.17(1)	671.4(2)
175	5.3991(7)	11.947(2)	11.8253(8)	113.071(7)	94.525(8)	103.18(1)	671.2(2)
200	5.3992(7)	11.954(2)	11.8337(8)	113.085(7)	94.525(8)	103.16(1)	672.0(2)
225	5.4013(8)	11.953(2)	11.8382(8)	113.086(7)	94.506(9)	103.15(1)	672.6(2)
250	5.4001(7)	11.956(2)	11.8435(7)	113.069(7)	94.507(9)	103.16(2)	672.9(2)
275	5.3983(8)	11.955(2)	11.8457(8)	113.074(8)	94.508(9)	103.15(1)	672.7(2)
300	5.3994(8)	11.950(2)	11.8503(8)	113.069(8)	94.525(9)	103.18(1)	672.7(2)
325	5.3953(7)	11.956(2)	11.8569(8)	113.058(7)	94.502(9)	103.20(1)	673.0(2)
350	5.3941(8)	11.957(2)	11.8644(8)	113.053(8)	94.512(9)	103.18(1)	673.4(2)
375	5.3959(8)	11.959(2)	11.8669(9)	113.023(8)	94.469(9)	103.23(1)	674.0(2)
400	5.3958(9)	11.956(2)	11.868(1)	113.01(1)	94.47(1)	103.22(2)	673.9(2)
425	5.399(1)	11.950(3)	11.868(1)	112.97(1)	94.48(3)	103.22(2)	674.2(3)
450	5.401(2)	11.946(3)	11.867(2)	112.96(2)	94.49(2)	103.23(3)	674.2(3)
Kupletskite-(Cs) HT modification							
550	5.346(1)	11.919(3)	11.850(1)	113.19(1)	93.58(1)	104.00(2)	662.9(2)
575	5.344(1)	11.906(2)	11.854(1)	113.180(9)	93.54(1)	104.06(2)	662.1(2)
600	5.3459(9)	11.906(2)	11.8589(9)	113.157(9)	93.49(1)	104.13(2)	662.5(2)
625	5.3419(9)	11.906(2)	11.8630(9)	113.166(9)	93.47(1)	104.12(2)	662.2(2)
650	5.3470(9)	11.900(2)	11.8636(9)	113.145(9)	93.48(1)	104.10(2)	662.8(2)
675	5.3462(9)	11.904(2)	11.8667(9)	113.134(9)	93.48(1)	104.09(2)	663.1(2)
700	5.347(1)	11.903(2)	11.867(1)	113.13(1)	93.48(1)	104.09(2)	663.3(2)
725	5.347(1)	11.906(3)	11.864(1)	113.11(1)	93.52(1)	104.04(2)	663.5(2)
750	5.346(1)	11.900(3)	11.860(1)	113.11(1)	93.60(1)	103.94(2)	663.0(3)
775	5.348(1)	11.893(3)	11.861(1)	113.07(1)	93.71(2)	103.82(2)	663.4(3)

Table S3. Coefficients of equations used for approximation of unit-cell parameters of kupletskite and its HT modification

	p_0	p_1*x*10^{-3}	$p_2*x^2*10^{-6}$	R^2
Kupletskite				
a	5.3466(6)	0.092(6)	-0.11(1)	0.98
b	11.953(1)	0.15(1)	-0.03(3)	0.99
c	11.696(1)	0.19(1)	-0.18(2)	0.99
α	113.279(3)	0.05(3)	-0.08(6)	0.17
β	94.754(6)	0.26(6)	-0.4(1)	0.78
γ	102.572(5)	-0.45(5)	0.8(1)	0.87
V	658.2(2)	31(2)	-27(3)	0.99
Kupletskite HT modification				
a	4.91(9)	1.5(3)	-1.3(2)	0.98
b	10.67(9)	3.6(3)	-3.0(2)	0.99
c	10.4(2)	3.9(5)	-3.1(4)	0.95
α	109(1)	10(4)	-7(3)	0.70
β	96(1)	-7(4)	5(3)	0.79
γ	109(1)	-15(3)	11(3)	0.84
V	461(14)	610(44)	-504(34)	0.99

Table S4. Coefficients of equations used for approximation of unit-cell parameters of kupletskite-(Cs) and its HT modification

	p_0	p_1*x*10^{-3}	$p_2*x^2*10^{-6}$	R^2
Kupletskite-(Cs)				
a	5.395(2)	0.03(2)	-0.06(4)	0.16
b	11.936(2)	0.12(2)	-0.20(5)	0.71
c	11.795(2)	0.22(2)	-0.10(5)	0.98
α	113.11(1)	0.1(1)	-0.8(2)	0.90
β	94.577(1)	-0.3(1)	0.2(2)	0.86
γ	103.16(1)	-0.1(1)	0.7(2)	0.80
V	668.0(2)	24(2)	-23(4)	0.98
Kupletskite-(Cs) HT modification				
a	5.38(5)	-0.1(2)	0.1(1)	0.37
b	12.0(1)	-0.3(4)	0.2(3)	0.63
c	11.47(4)	1.2(1)	-0.8(1)	0.94
α	113.2(3)	0.4(9)	-0.6(7)	0.95
β	99.4(5)	-18(2)	14(1)	0.96
γ	97.7(7)	20(2)	-16(2)	0.96
V	663(11)	-4(33)	6(25)	0.55

Table S5. The main characteristics of thermal expansion/contraction for kupletskite and its HT modification (angles are given in degrees, coefficients are × 10^6, $°C^{-1}$)

T, °C	α_{11}	α_{22}	α_{33}	$<\alpha_{11}a$	$<\alpha_{22}b$	$<\alpha_{33}c$	α_a	α_b	α_c	α_α	α_β	α_γ	α_V
Kupletskite													
25	19.4	11.2	14.4	39.2	26	31.6	16(1)	13(1)	15.2(8)	0.4(2)	2.6(6)	-4.0(4)	45(2)
50	18.2	11	13.7	41.2	28.6	33.6	15.1(9)	12.6(9)	14.4(7)	0.3(2)	2.4(5)	-3.6(4)	43(1)
75	17	10.8	13	43.7	32.4	36.4	14.1(8)	12.5(8)	13.6(6)	0.3(2)	2.2(5)	-3.2(3)	41(1)
100	15.9	10.5	12.4	47.1	38.3	40.2	13.0(7)	12.3(7)	12.8(5)	0.3(2)	2.1(4)	-2.8(3)	39(1)
125	14.9	10.1	11.8	51.8	46.3	44.6	12.0(6)	12.2(6)	12.1(4)	0.2(1)	1.9(3)	-2.4(2)	36.8(9)
150	9.5	13.9	11.3	40.6	44.3	47.2	11.0(5)	12.1(5)	11.3(4)	0.2(1)	1.7(3)	-2.1(2)	34.7(8)
175	8.9	13.1	10.7	39.9	35	45.9	10.0(4)	11.9(4)	10.5(3)	0.16(9)	1.5(2)	-1.7(2)	32.7(6)
200	8.1	12.5	10	38.3	25.4	41.4	9.0(3)	11.8(3)	9.8(2)	0.13(7)	1.3(2)	-1.3(1)	30.6(5)
225	7.2	12.1	9.3	35.5	18.2	35.6	7.9(3)	11.6(3)	9.0(2)	0.09(6)	1.1(2)	-0.9(1)	28.6(4)
250	6.3	11.8	8.4	31.9	14.3	29.9	6.9(3)	11.5(3)	8.2(2)	0.06(6)	1.0(2)	-0.5(1)	26.5(4)
275	5.3	11.6	7.5	28.2	12.7	24.6	5.9(3)	11.4(3)	7.5(2)	0.02(7)	0.8(2)	-0.2(1)	24.5(5)
300	4.3	11.5	6.7	24.9	12.2	20	4.9(4)	11.2(4)	6.7(3)	-0.01(9)	0.6(2)	0.2(2)	22.5(6)
325	3.2	11.3	5.8	22.3	12.2	16.3	3.8(5)	11.1(5)	6.0(4)	0.0(1)	0.4(3)	0.6(2)	20.4(8)
350	2.1	11.2	5	20.6	12.4	13.6	2.8(6)	10.9(6)	5.2(4)	-0.1(1)	0.2(3)	1.0(2)	18.4(9)
375	1	11.1	4.2	19.5	12.6	11.8	1.8(7)	10.8(7)	4.4(5)	-0.1(2)	0.0(4)	1.4(3)	16(1)
400	-0.1	11	3.4	18.9	12.9	10.8	0.8(8)	10.7(8)	3.7(6)	-0.2(2)	-0.2(5)	1.8(3)	14(1)
425	-1.3	11	2.6	18.7	13.1	10.3	-0.2(9)	10.5(9)	2.9(7)	-0.2(2)	-0.3(5)	2.1(4)	12(1)
Kupletskite HT modification													
550	56.5	-16	46.3	50.6	55.2	21.8	14(9)	28(4)	39(7)	18(6)	-19(7)	-27(5)	87(12)
575	37.7	-21.6	31.2	51	55.7	25.3	2(7)	15(3)	26(5)	15(5)	-17(6)	-22(4)	47(9)
600	19.5	-27.2	15.6	54.5	56.5	40.8	-10(5)	3(2)	12(4)	12(4)	-14(4)	-17(3)	8(6)
625	3.3	-33	-1.8	65.5	58.2	65.3	-22(3)	-10(1)	-1(3)	9(2)	-11(3)	-11(2)	-32(4)
650	-39.2	-19.9	-11.8	27.3	35.4	22.3	-34(2)	-23(1)	-15(2)	5(2)	-9(2)	-6(1)	-71(3)
675	-47.5	-36.4	-26.4	12.1	22.4	17.3	-47(3)	-36(1)	-28(3)	2(2)	-6(3)	0(2)	-110(4)
700	-62.1	-47.5	-40.3	28.3	16.5	18	-59(5)	-48(2)	-42(4)	-1(4)	-3(4)	5(3)	-150(6)
725	-80.2	-58.8	-50.5	37.8	32	44.1	-71(7)	-61(3)	-55(5)	-4(5)	-1(6)	11(4)	-189(9)

α - coeffecient of thermal expansion [α_{11}, α_{22}, α_{33}—eigenvalues (main values); α_a, α_b, α_c—values along crystallographic axes], $<\alpha_{11}a$—angle between axes α_{11} and *a*

Table S6. The main characteristics of thermal expansion/contraction for kupletskite-(Cs) and its HT modification (angles are given in degrees, coefficients are × 10^6, $°C^{-1}$)

T, °C	α_{11}	α_{22}	α_{33}	$<\alpha_{11}a$	$<\alpha_{22}b$	$<\alpha_{33}c$	α_a	α_b	α_c	α_α	α_β	α_γ	α_V
Kupletskite-(Cs)													
25	4.8	9.8	19.8	12.7	22.2	22.9	5(3)	9(2)	18(2)	0.2(9)	-3.1(9)	-1.0(1)	34(4)
50	4.3	8.8	19.5	10.1	19	23.2	5(3)	9(2)	18(2)	-0.2(8)	-3.0(8)	-0.7(9)	33(4)
75	3.9	7.8	19.2	7.8	15.1	23.5	4(2)	8(1)	17(1)	-0.5(7)	-2.9(7)	-0.4(8)	31(3)
100	3.4	6.8	19	7.9	10.3	23.8	4(2)	7(1)	17(1)	-0.9(6)	-2.8(6)	0.0(7)	29(3)
125	2.8	5.9	18.7	11.8	5.2	24.2	3(2)	6(1)	16(1)	-1.2(5)	-2.7(5)	0.3(6)	27(2)
150	2.2	5.1	18.4	17.9	5.6	24.5	3(1)	5.2(9)	15.9(9)	-1.6(5)	-2.6(4)	0.7(5)	26(2)
175	1.4	4.4	18.2	24.8	11.7	24.8	2(1)	4.3(7)	15.5(7)	-1.9(4)	-2.5(4)	1.0(4)	24(2)
200	0.5	3.7	17.9	31.2	18	25.2	1.4(1)	3.5(6)	15.0(6)	-2.3(3)	-2.4(3)	1.3(3)	22(1)
225	-0.4	3.2	17.7	36.6	23.4	25.6	0.9(8)	2.6(5)	14.6(5)	-2.6(2)	-2.3(2)	1.7(3)	20(1)
250	-1.4	2.6	17.5	40.9	27.7	25.9	0.4(8)	1.8(5)	14.1(5)	-3.0(2)	-2.2(2)	2.0(3)	19(1)
275	-2.4	2.1	17.3	44.3	31.2	26.3	-0.2(1)	0.9(6)	13.7(6)	-3.3(3)	-2.1(3)	2.3(3)	17(1)
300	-3.4	1.6	17.1	47	33.9	26.7	-1(1)	0.1(7)	13.3(7)	-3.7(4)	-2.0(4)	2.7(4)	15(2)
325	-4.5	1.1	16.9	49.2	36	27.1	-1(1)	-0.8(9)	12.8(8)	-4.1(4)	-1.9(4)	3.0(5)	14(2)
350	-5.5	0.6	16.7	50.9	37.8	27.5	-2(2)	-2(1)	12(1)	-4.4(5)	-1.8(5)	3.3(6)	12(2)
375	-6.6	0.1	16.6	52.3	39.3	27.8	-2(2)	-2(1)	12(1)	-4.8(6)	-1.7(6)	3.7(7)	10(3)
400	-7.7	-0.4	16.4	53.5	40.5	28.2	-3(2)	-3(1)	11(1)	-5.1(7)	-1.6(7)	4.0(8)	8(3)
425	-8.8	-0.8	16.2	54.5	41.6	28.6	-3(3)	-4(2)	11(2)	-5.5(8)	-1.5(8)	4.4(9)	7(4)
Kupletskite-(Cs) HT modification													
550	-37.7	4.8	37.8	55.2	48.4	32.7	-2(5)	-9(6)	20(2)	-3(1)	-30(3)	27(3)	5(8)
575	3.5	-28.2	30	44.5	47.4	31.7	-1(4)	-8(5)	16(2)	-3(1)	-22(2)	20(3)	5(7)
600	2	-18.7	22.5	38.7	43.7	30.8	0(3)	-8(4)	13(1)	-3.5(8)	-15(2)	12(2)	6(5)
625	0.6	-10	15.7	24.8	31.4	31.6	1(2)	-7(3)	9.0(8)	-3.8(6)	-7(1)	4(1)	6(3)
650	3.2	-6.7	10.3	26.9	10.8	39.5	2(1)	-6(2)	5.5(6)	-4.1(4)	0.6(9)	-3(1)	7(2)
675	12.2	-11	6.2	42.1	29.8	34.1	3(1)	-6(2)	1.9(6)	-4.3(4)	8.2(9)	-11(1)	7(2)
700	21.4	-17.6	4	44.6	38.3	44	4(2)	-5(3)	-1.6(8)	-4.6(6)	16(1)	-18(1)	8(3)
725	30.9	-25	2.3	46.3	43.3	48.9	5(3)	-4(4)	-5(1)	-4.9(8)	23(2)	-26(2)	8(5)
750	40.5	0.9	-32.8	47.2	61.8	47	6(4)	-3(5)	-9(2)	-5(1)	31(2)	-34(3)	9(7)

α - coeffecient of thermal expansion [α_{11}, α_{22}, α_{33}—eigenvalues (main values); α_a, α_b, α_c—values along crystallographic axes], $<\alpha_{11a}$—angle between axes α_{11} and *a*

Table S7. Atom coordinates, equivalent isotropic displacement parameters (Å²), site occupancies for kupletskite (K25), kupletskite-(Cs) (CsK25) and their high-temperature modifications (K650 and CsK650)

Atom	Sample	*x*	*y*	*z*	U_{eq}	Site occupancies	ref. s.s.
M(1)	K25	0.84984(8)	0.20616(4)	0.47959(4)	0.00965(13)	$Mn_{0.85}Mg_{0.15}$	23.1(2)
	K650	0.84559(9)	0.20156(4)	0.47807(5)	0.01251(15)	$Mn_{0.70}Mg_{0.30}$	21.1(2)
	CsK25	0.84949(13)	0.20469(6)	0.47688(7)	0.0104(2)	$Mn_{0.75}Mg_{0.25}$	21.8(2)
	CsK650	0.8448(2)	0.19955(10)	0.47546(11)	0.0130(4)	$Mn_{0.56}Mg_{0.44}$	19.3(3)
M(2)	K25	0.28024(7)	0.06737(3)	0.48852(4)	0.00973(9)	Mn	25
	K650	0.25273(8)	0.06311(4)	0.48638(4)	0.01299(13)	$Mn_{0.91}Mg_{0.09}$	23.8(2)
	CsK25	0.27836(12)	0.06658(6)	0.48667(6)	0.01193(15)	Mn	25
	CsK650	0.25085(17)	0.06276(8)	0.48559(8)	0.0147(3)	$Mn_{0.97}Mg_{0.03}$	24.6(3)
M(3)	K25	0.42295(7)	0.35272(4)	0.48576(4)	0.01013(12)	$Mn_{0.97}Mg_{0.03}$	24.6(2)
	K650	0.41897(8)	0.35978(4)	0.47721(4)	0.01329(12)	$Mn_{0.96}Mg_{0.04}$	24.5(2)
	CsK25	0.42068(12)	0.35082(6)	0.48239(7)	0.0117(2)	$Mn_{0.91}Mg_{0.09}$	23.8(2)
	CsK650	0.41597(16)	0.35822(8)	0.47448(8)	0.0138(3)	$Mn_{0.97}Mg_{0.03}$	24.6(3)
M(4)	K25	0	0.5000	0.5000	0.00931(17)	$Mn_{0.87}Mg_{0.13}$	23.3(2)
	K650	0	0.5000	0.5000	0.01040(16)	$Mn_{0.93}Mg_{0.07}$	24.1(2)
	CsK25	0	0.5000	0.5000	0.00889(18)	Mn	25
	CsK650	0	0.5000	0.5000	0.0120(4)	$Mn_{0.94}Mg_{0.06}$	24.2(4)
D	K25	0.08001(7)	0.08630(4)	0.19738(4)	0.00809(11)	$Ti_{0.91}Nb_{0.09}$	23.7(2)
	K650	0.08215(8)	0.08876(4)	0.19101(5)	0.01460(13)	$Ti_{0.91}Nb_{0.09}$	23.7(2)
	CsK25	0.07628(10)	0.08333(5)	0.19247(6)	0.01096(19)	$Ti_{0.66}Nb_{0.32}$	27.6(3)
	CsK650	0.07695(14)	0.08472(7)	0.18737(8)	0.0153(3)	$Ti_{0.61}Nb_{0.39}$	29.4(4)
Si(1)	K25	0.67866(13)	0.27210(6)	0.23134(7)	0.00764(13)	Si	14
	K650	0.69989(13)	0.27478(6)	0.22467(7)	0.00947(13)	Si	14
	CsK25	0.6795(2)	0.27278(10)	0.23364(11)	0.0096(2)	Si	14
	CsK650	0.6999(3)	0.27511(14)	0.22993(14)	0.0116(3)	Si	14
Si(2)	K25	0.81361(13)	0.54565(6)	0.25262(7)	0.00832(13)	Si	14
	K650	0.82286(14)	0.54815(6)	0.25054(7)	0.01014(13)	Si	14
	CsK25	0.8155(2)	0.54779(10)	0.25836(11)	0.0090(2)	Si	14
	CsK650	0.8233(3)	0.55051(14)	0.25920(14)	0.0117(3)	Si	14
Si(3)	K25	0.37986(13)	0.67465(6)	0.25523(7)	0.00843(13)	Si	14
	K650	0.39989(14)	0.68011(7)	0.25666(7)	0.01024(13)	Si	14
	CsK25	0.3808(2)	0.67667(10)	0.26071(11)	0.0086(2)	Si	14
	CsK650	0.4004(3)	0.68268(14)	0.26497(14)	0.0118(3)	Si	14
Si(4)	K25	0.50678(13)	0.93112(6)	0.23510(7)	0.00771(13)	Si	14
	K650	0.48561(14)	0.93410(6)	0.23607(7)	0.01021(13)	Si	14
	CsK25	0.5056(2)	0.93117(10)	0.23693(11)	0.0090(2)	Si	14
	CsK650	0.4824(3)	0.93386(14)	0.23923(15)	0.0126(3)	Si	14
A(1)	K25	0.1349(2)	0.26562(10)	0.99582(9)	0.0414(2)	$K_{0.95}$	18.1
	K650	0.17418(18)	0.27193(10)	0.98924(10)	0.0369(2)	$K_{0.95}$	18.1
	CsK25	0.15188(8)	0.29935(4)	0.99829(4)	0.02226(12)	$Cs_{0.76}$	41.8
	CsK650	0.17699(9)	0.30503(5)	0.99789(5)	0.01840(16)	$Cs_{0.76}$	41.8
A(2)	K25	0.0900(30)	0.1900(15)	0.9968(15)	0.026(3)	$K_{0.05}$	1.0
	K650	0.1350(30)	0.2058(16)	0.9906(16)	0.028(3)	$K_{0.05}$	1.0
	CsK25	0.1124(11)	0.2195(7)	0.9975(5)	0.0401(13)	$K_{0.24}$	4.6
	CsK650	0.1592(11)	0.2218(7)	0.9938(5)	0.0244(12)	$K_{0.24}$	4.6
B	K25	0.5000	0	0	0.0142(4)	$Na_{0.58}Ca_{0.42}$	14.8(3)
	K650	0.5000	0	0	0.0201(4)	$Na_{0.44}Ca_{0.56}$	16.0(3)
	CsK25	0.5000	0	0	0.0189(8)	$Na_{0.58}Ca_{0.42}$	14.8(4)

	CsK650	0.5000	0	0	0.0240(13)	$Na_{0.89}Ca_{0.11}$	12.0(6)
O(1)	K25	0.7267(4)	0.31958(17)	0.38404(17)	0.0108(3)	O	8
	K650	0.7327(4)	0.32435(18)	0.38041(18)	0.0136(3)	O	8
	CsK25	0.7280(5)	0.3185(3)	0.3839(3)	0.0113(6)	O	8
	CsK650	0.7302(8)	0.3236(4)	0.3823(4)	0.0160(8)	O	8
O(2)	K25	0.1483(4)	0.16007(18)	0.36829(18)	0.0113(3)	O	8
	K650	0.1654(4)	0.1716(2)	0.3725(2)	0.0215(4)	O	8
	CsK25	0.1454(5)	0.1578(3)	0.3665(3)	0.0115(6)	O	8
	CsK650	0.1610(8)	0.1713(4)	0.3715(4)	0.0223(9)	O	8
O(3)	K25	0.1289(4)	0.39326(18)	0.59453(18)	0.0107(3)	O	8
	K650	0.1279(4)	0.39470(18)	0.59428(18)	0.0128(3)	O	8
	CsK25	0.1272(5)	0.3906(2)	0.5912(3)	0.0103(6)	O	8
	CsK650	0.1267(8)	0.3911(4)	0.5892(4)	0.0143(8)	O	8
OH(4)	K25	0.2962(4)	0.46205(18)	0.39945(19)	0.0120(3)	O	8
	K650	0.2893(4)	0.4733(2)	0.4125(2)	0.0179(4)	O	8
	CsK25	0.2972(6)	0.4631(3)	0.4001(3)	0.0128(6)	O	8
	CsK650	0.2911(8)	0.4744(4)	0.4140(4)	0.0203(9)	O	8
H(4)	K25	0.2580(100)	0.4180(50)	0.3070(19)	0.058(17)	H	1
	CsK25	0.2620(150)	0.4220(60)	0.3116(19)	0.090(30)	H	1
OH(5)	K25	0.9915(4)	0.11711(19)	0.59345(19)	0.0133(3)	O	8
	K650	0.9912(4)	0.10628(19)	0.5821(2)	0.0155(4)	O	8
	CsK25	0.9912(6)	0.1181(3)	0.5920(3)	0.0142(6)	O	8
	CsK650	0.9878(8)	0.1054(4)	0.5773(4)	0.0167(8)	O	8
H(5)	K25	0.0210(110)	0.1580(60)	0.6844(19)	0.070(20)	H	1
	CsK25	0.0650(160)	0.1410(80)	0.6760(30)	0.120(30)	H	1
O(6)	K25	0.5556(4)	0.25790(17)	0.59119(17)	0.0105(3)	O	8
	K650	0.5337(4)	0.25091(19)	0.58716(19)	0.0144(3)	O	8
	CsK25	0.5565(5)	0.2566(2)	0.5882(3)	0.0097(6)	O	8
	CsK650	0.5319(8)	0.2472(4)	0.5813(4)	0.0146(8)	O	8
O(7)	K25	0.5722(4)	0.01400(18)	0.38764(18)	0.0110(3)	O	8
	K650	0.5414(4)	0.0128(2)	0.39140(19)	0.0166(4)	O	8
	CsK25	0.5735(5)	0.0136(3)	0.3874(3)	0.0114(6)	O	8
	CsK650	0.5388(8)	0.0147(4)	0.3914(4)	0.0166(8)	O	8
O(8)	K25	0.0736(4)	0.5905(2)	0.2007(2)	0.0183(4)	O	8
	K650	0.0935(4)	0.5930(2)	0.2028(2)	0.0205(4)	O	8
	CsK25	0.0769(5)	0.5918(3)	0.2058(3)	0.0139(6)	O	8
	CsK650	0.0938(8)	0.5943(4)	0.2113(4)	0.0170(8)	O	8
O(9)	K25	0.2476(4)	0.0403(2)	0.8283(2)	0.0262(5)	O	8
	K650	0.2677(4)	0.0177(2)	0.8225(2)	0.0196(4)	O	8
	CsK25	0.2501(6)	0.0412(3)	0.8275(3)	0.0198(7)	O	8
	CsK650	0.2744(7)	0.0193(4)	0.8217(4)	0.0168(8)	O	8
O(10)	K25	0.4282(4)	0.4151(2)	0.8010(2)	0.0176(4)	O	8
	K650	0.4062(4)	0.4066(2)	0.8021(2)	0.0181(4)	O	8
	CsK25	0.4259(5)	0.4120(3)	0.7946(3)	0.0133(6)	O	8
	CsK650	0.4063(8)	0.4049(4)	0.7933(4)	0.0153(8)	O	8
O(11)	K25	0.1274(5)	0.8084(3)	0.8317(2)	0.0260(5)	O	8
	K650	0.0799(4)	0.7904(2)	0.8323(2)	0.0171(4)	O	8
	CsK25	0.1249(6)	0.8063(3)	0.8295(3)	0.0191(7)	O	8
	CsK650	0.0792(8)	0.7879(4)	0.8268(4)	0.0185(9)	O	8
O(12)	K25	0.2644(5)	0.9566(2)	0.1692(2)	0.0262(5)	O	8
	K650	0.2265(4)	0.94802(19)	0.1718(2)	0.0181(4)	O	8

	CsK25	0.2619(6)	0.9557(3)	0.1730(3)	0.0199(7)	O	8
	CsK650	0.2211(8)	0.9452(4)	0.1759(4)	0.0180(9)	O	8
O(13)	K25	0.2671(5)	0.60787(19)	0.8079(2)	0.0205(4)	O	8
	K650	0.2765(4)	0.60556(18)	0.8151(2)	0.0168(4)	O	8
	CsK25	0.2669(6)	0.6055(3)	0.8030(3)	0.0148(6)	O	8
	CsK650	0.2766(8)	0.6035(4)	0.8065(4)	0.0156(8)	O	8
O(14)	K25	0.5722(5)	0.22135(19)	0.8034(2)	0.0212(4)	O	8
	K650	0.5539(4)	0.21753(19)	0.8052(2)	0.0179(4)	O	8
	CsK25	0.5713(6)	0.2218(3)	0.7993(3)	0.0149(6)	O	8
	CsK650	0.5554(8)	0.2175(4)	0.7985(4)	0.0153(8)	O	8
O(15)	K25	0.3834(4)	0.1895(2)	0.1664(2)	0.0255(5)	O	8
	K650	0.4110(4)	0.17778(19)	0.1579(2)	0.0159(4)	O	8
	CsK25	0.3853(6)	0.1909(3)	0.1697(3)	0.0185(7)	O	8
	CsK650	0.4126(7)	0.1760(4)	0.1625(4)	0.0161(8)	O	8
X^{P}_{D}	K25	0	0	0	0.0136(4)	$F^{(1)}$	9
	K650	0	0	0	0.0212(5)	$F^{(1)}$	9
	CsK25	0	0	0	0.0194(8)	$F^{(1)}$	9
	CsK650	0	0	0	0.0225(11)	$F^{(1)}$	9

(1) According to the results of electron-microprobe analysis, in the crystal structure of kupletskite X^{P}_{D} position is occupied by $F_{0.80}O_{0.20}$, and for kupletskite-(Cs) by $F_{0.65}O_{0.35}$, but since they are not distinguishable by single-crystal X-ray diffraction, only fluorine was used in the refinement.

Table S8. Anisotropic displacement parameters (Å²) for kupletskite (K25), kupletskite-(Cs) (CsK25) and their high-temperature modifications (K650 and CsK650)

Atom	Sample	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
M(1)	K25	0.0076(2)	0.00884(19)	0.0124(2)	0.00458(15)	0.00189(14)	0.00182(13)
	K650	0.0113(2)	0.0090(2)	0.0182(3)	0.00575(18)	0.00509(17)	0.00405(16)
	CsK25	0.0109(4)	0.0096(4)	0.0114(5)	0.0043(3)	0.0042(3)	0.0035(3)
	CsK650	0.0057(6)	0.0109(6)	0.0199(7)	0.0069(5)	0.0003(4)	-0.0019(4)
M(2)	K25	0.00747(16)	0.00923(17)	0.01272(18)	0.00501(13)	0.00227(12)	0.00199(12)
	K650	0.01174(19)	0.00967(19)	0.0175(2)	0.00430(15)	0.00594(15)	0.00448(14)
	CsK25	0.0111(3)	0.0113(3)	0.0141(4)	0.0053(3)	0.0048(3)	0.0038(2)
	CsK650	0.0068(5)	0.0125(4)	0.0203(5)	0.0049(4)	0.0027(3)	-0.0012(3)
M(3)	K25	0.00808(19)	0.00986(19)	0.0135(2)	0.00563(14)	0.00304(13)	0.00293(13)
	K650	0.01189(19)	0.01236(19)	0.0179(2)	0.00688(16)	0.00659(14)	0.00555(14)
	CsK25	0.0113(3)	0.0127(4)	0.0146(4)	0.0075(3)	0.0060(3)	0.0054(3)
	CsK650	0.0077(5)	0.0146(5)	0.0190(5)	0.0085(4)	0.0035(3)	0.0008(3)
M(4)	K25	0.0069(3)	0.0083(3)	0.0117(3)	0.0039(2)	0.00079(18)	0.00105(18)
	K650	0.0098(2)	0.0083(2)	0.0134(3)	0.0045(2)	0.00257(18)	0.00337(18)
	CsK25	0.0084(4)	0.0090(4)	0.0096(5)	0.0040(3)	0.0025(3)	0.0025(3)
	CsK650	0.0044(6)	0.0128(6)	0.0165(7)	0.0066(5)	-0.0004(4)	-0.0014(4)
D	K25	0.00502(17)	0.00827(17)	0.01064(19)	0.00398(14)	0.00106(12)	0.00144(12)
	K650	0.00989(19)	0.0129(2)	0.0257(3)	0.01112(18)	0.00632(16)	0.00566(14)
	CsK25	0.0072(3)	0.0106(3)	0.0180(4)	0.0080(3)	0.0042(2)	0.0036(2)
	CsK650	0.0040(4)	0.0140(4)	0.0310(5)	0.0139(3)	0.0035(3)	0.0003(3)
Si(1)	K25	0.0076(3)	0.0059(3)	0.0082(3)	0.0024(2)	0.0003(2)	0.0008(2)
	K650	0.0105(3)	0.0071(3)	0.0118(3)	0.0041(2)	0.0038(2)	0.0038(2)
	CsK25	0.0099(5)	0.0089(5)	0.0107(6)	0.0049(5)	0.0024(4)	0.0028(4)
	CsK650	0.0067(7)	0.0110(7)	0.0155(7)	0.0063(6)	0.0005(6)	-0.0011(5)
Si(2)	K25	0.0077(3)	0.0064(3)	0.0100(3)	0.0033(2)	0.0007(2)	0.0009(2)
	K650	0.0118(3)	0.0072(3)	0.0130(3)	0.0048(2)	0.0038(2)	0.0042(2)
	CsK25	0.0089(5)	0.0092(5)	0.0100(6)	0.0045(5)	0.0025(4)	0.0035(4)
	CsK650	0.0073(7)	0.0110(7)	0.0159(7)	0.0068(6)	0.0008(6)	-0.0005(5)
Si(3)	K25	0.0078(3)	0.0073(3)	0.0102(3)	0.0042(2)	0.0010(2)	0.0013(2)
	K650	0.0121(3)	0.0089(3)	0.0123(3)	0.0056(2)	0.0040(2)	0.0052(2)
	CsK25	0.0082(5)	0.0084(5)	0.0098(6)	0.0041(4)	0.0022(4)	0.0028(4)
	CsK650	0.0086(7)	0.0120(7)	0.0157(7)	0.0078(6)	0.0027(6)	0.0010(5)
Si(4)	K25	0.0074(3)	0.0073(3)	0.0083(3)	0.0035(2)	0.0009(2)	0.0014(2)
	K650	0.0115(3)	0.0072(3)	0.0128(3)	0.0048(2)	0.0033(2)	0.0030(2)
	CsK25	0.0102(5)	0.0077(5)	0.0097(6)	0.0041(4)	0.0023(4)	0.0026(4)
	CsK650	0.0085(7)	0.0107(7)	0.0174(8)	0.0071(6)	0.0012(6)	-0.0008(5)
A(1)	K25	0.0594(7)	0.0341(5)	0.0256(4)	0.0108(4)	0.0041(4)	0.0083(4)
	K650	0.0321(4)	0.0415(5)	0.0388(5)	0.0206(4)	0.0118(4)	0.0061(4)
	CsK25	0.0248(2)	0.0226(2)	0.0193(2)	0.00887(18)	0.00490(17)	0.00612(16)
	CsK650	0.0113(2)	0.0196(3)	0.0223(3)	0.0108(2)	0.00207(18)	-0.00167(18)
A(2)	CsK25	0.032(3)	0.058(4)	0.023(3)	0.007(3)	0.004(2)	0.016(3)
	CsK650	0.015(3)	0.042(4)	0.013(3)	0.005(2)	0.000(2)	0.014(3)
B	K25	0.0190(6)	0.0128(5)	0.0091(5)	0.0037(4)	0.0014(4)	0.0032(4)
	K650	0.0331(7)	0.0172(5)	0.0145(5)	0.0061(4)	0.0061(4)	0.0156(4)
	CsK25	0.0288(13)	0.0150(11)	0.0111(13)	0.0041(9)	0.0031(9)	0.0057(9)
	CsK650	0.042(2)	0.0180(18)	0.0141(18)	0.0067(13)	0.0004(14)	0.0145(15)
O(1)	K25	0.0096(7)	0.0112(8)	0.0087(8)	0.0028(6)	0.0008(6)	0.0009(6)

	K650	0.0164(8)	0.0122(8)	0.0113(8)	0.0040(7)	0.0033(7)	0.0040(6)
	CsK25	0.0109(13)	0.0125(13)	0.0098(16)	0.0041(12)	0.0026(12)	0.0030(11)
	CsK650	0.0129(19)	0.0186(19)	0.0157(19)	0.0085(16)	0.0018(15)	0.0014(16)
O(2)	K25	0.0107(8)	0.0112(8)	0.0103(8)	0.0034(6)	0.0010(6)	0.0024(6)
	K650	0.0214(10)	0.0263(11)	0.0156(9)	0.0046(8)	0.0046(8)	0.0113(9)
	CsK25	0.0133(14)	0.0121(13)	0.0070(15)	0.0016(12)	0.0010(11)	0.0044(11)
	CsK650	0.015(2)	0.029(2)	0.020(2)	0.0081(19)	0.0028(17)	0.0046(18)
O(3)	K25	0.0097(7)	0.0102(7)	0.0104(8)	0.0031(6)	0.0007(6)	0.0020(6)
	K650	0.0160(8)	0.0114(8)	0.0108(8)	0.0039(6)	0.0024(6)	0.0046(6)
	CsK25	0.0113(13)	0.0108(13)	0.0089(15)	0.0039(12)	0.0025(11)	0.0039(11)
	CsK650	0.0123(19)	0.0117(17)	0.0155(19)	0.0054(15)	0.0016(15)	-0.0014(15)
OH(4)	K25	0.0114(8)	0.0122(8)	0.0111(8)	0.0036(7)	0.0010(6)	0.0032(6)
	K650	0.0133(8)	0.0234(10)	0.0154(9)	0.0059(8)	0.0033(7)	0.0063(7)
	CsK25	0.0142(14)	0.0143(14)	0.0114(17)	0.0059(13)	0.0046(12)	0.0053(11)
	CsK650	0.013(2)	0.025(2)	0.022(2)	0.0112(18)	0.0031(17)	0.0017(17)
OH(5)	K25	0.0118(8)	0.0138(8)	0.0113(8)	0.0031(7)	0.0019(6)	0.0024(6)
	K650	0.0154(8)	0.0135(8)	0.0180(9)	0.0055(7)	0.0061(7)	0.0057(7)
	CsK25	0.0130(14)	0.0124(14)	0.0152(18)	0.0041(13)	0.0032(13)	0.0033(11)
	CsK650	0.0080(19)	0.0160(18)	0.024(2)	0.0082(17)	0.0008(16)	0.0002(15)
O(6)	K25	0.0120(8)	0.0100(7)	0.0085(7)	0.0028(6)	0.0015(6)	0.0033(6)
	K650	0.0164(8)	0.0150(8)	0.0120(8)	0.0055(7)	0.0031(7)	0.0051(7)
	CsK25	0.0106(13)	0.0110(13)	0.0076(15)	0.0031(11)	0.0029(11)	0.0042(11)
	CsK650	0.0097(19)	0.0179(19)	0.0131(19)	0.0042(16)	-0.0002(15)	0.0032(15)
O(7)	K25	0.0106(7)	0.0129(8)	0.0091(8)	0.0040(6)	0.0016(6)	0.0040(6)
	K650	0.0169(8)	0.0175(9)	0.0125(8)	0.0027(7)	0.0033(7)	0.0057(7)
	CsK25	0.0120(14)	0.0117(13)	0.0115(16)	0.0047(12)	0.0027(12)	0.0053(11)
	CsK650	0.0087(19)	0.0175(19)	0.019(2)	0.0066(17)	-0.0008(16)	-0.0003(15)
O(8)	K25	0.0112(8)	0.0237(10)	0.0142(9)	0.0065(8)	0.0008(7)	-0.00.8(7)
	K650	0.0169(9)	0.0228(10)	0.0192(10)	0.0085(8)	0.0059(8)	0.0011(8)
	CsK25	0.0114(14)	0.0159(14)	0.0130(16)	0.0061(12)	0.0036(12)	0.0011(11)
	CsK650	0.0096(19)	0.0161(19)	0.022(2)	0.0097(17)	0.0004(16)	-0.0031(15)
O(9)	K25	0.0191(10)	0.0271(11)	0.0148(10)	-0.0001(8)	0.0070(8)	-0.0113(8)
	K650	0.0143(8)	0.0216(10)	0.0265(11)	0.0146(9)	0.0078(8)	0.0030(7)
	CsK25	0.0155(16)	0.0204(16)	0.0156(18)	0.0035(14)	0.0057(13)	-0.0028(12)
	CsK650	0.0052(18)	0.0172(19)	0.026(2)	0.0117(17)	0.0025(16)	-0.0031(15)
O(10)	K25	0.0190(9)	0.0211(10)	0.0142(9)	0.0058(8)	0.0006(7)	0.0123(8)
	K650	0.0246(10)	0.0172(9)	0.0171(9)	0.0067(8)	0.0051(8)	0.0147(8)
	CsK25	0.0151(14)	0.0141(14)	0.0112(16)	0.0050(12)	0.0018(12)	0.0060(11)
	CsK650	0.0102(19)	0.0169(19)	0.019(2)	0.0095(16)	0.0016(15)	0.0021(15)
O(11)	K25	0.0399(14)	0.0367(13)	0.0140(10)	0.0103(9)	0.0099(9)	0.0331(11)
	K650	0.0186(9)	0.0172(9)	0.0217(10)	0.0095(8)	0.0083(8)	0.0124(7)
	CsK25	0.0262(17)	0.0240(16)	0.0161(18)	0.0107(14)	0.0089(14)	0.0179(13)
	CsK650	0.015(2)	0.0180(19)	0.027(2)	0.0131(18)	0.0060(18)	0.0069(16)
O(12)	K25	0.0330(12)	0.0298(12)	0.0144(10)	0.0017(9)	-0.0062(9)	0.0239(10)
	K650	0.0163(8)	0.0136(8)	0.0266(11)	0.0096(8)	0.0008(8)	0.0070(7)
	CsK25	0.0219(16)	0.0220(16)	0.0177(18)	0.0067(14)	0.0005(14)	0.0139(13)
	CsK650	0.0086(19)	0.0173(19)	0.028(2)	0.0124(18)	-0.0031(16)	0.0008(15)
O(13)	K25	0.0363(12)	0.0074(8)	0.0143(9)	0.0045(7)	0.0011(8)	0.0010(8)
	K650	0.0268(10)	0.0073(7)	0.0171(9)	0.0057(7)	0.0033(8)	0.0057(7)
	CsK25	0.0218(16)	0.0088(13)	0.0134(17)	0.0047(12)	0.0042(13)	0.0034(12)
	CsK650	0.015(2)	0.0103(17)	0.019(2)	0.0054(16)	0.0006(16)	0.0010(15)

O(14)	K25	0.0394(13)	0.0079(8)	0.0148(9)	0.0052(7)	0.0037(9)	0.0037(8)
	K650	0.0284(10)	0.0105(8)	0.0194(10)	0.0087(7)	0.0063(8)	0.0090(7)
	CsK25	0.0234(16)	0.0102(13)	0.0121(16)	0.0060(12)	0.0044(13)	0.0040(12)
	CsK650	0.014(2)	0.0099(17)	0.024(2)	0.0090(16)	0.0068(16)	0.0019(15)
O(15)	K25	0.0146(9)	0.0345(13)	0.0154(10)	0.0113(9)	-0.0038(7)	-0.0143(8)
	K650	0.0129(8)	0.0138(8)	0.0183(9)	0.0054(7)	0.0034(7)	0.0016(6)
	CsK25	0.0134(15)	0.0216(16)	0.0165(18)	0.0094(14)	0.0000(13)	-0.0041(12)
	CsK650	0.0082(18)	0.0147(18)	0.022(2)	0.0078(17)	0.0017(16)	-0.0024(15)
$X^{P}{}_{D}$	K25	0.0154(10)	0.0143(10)	0.0081(9)	0.0027(8)	0.0014(8)	0.0025(8)
	K650	0.0228(12)	0.0199(12)	0.0186(12)	0.0057(10)	0.0026(10)	0.0068(10)
	CsK25	0.0162(18)	0.0248(19)	0.019(2)	0.0102(17)	0.0049(16)	0.0072(15)
	CsK650	0.020(3)	0.024(3)	0.020(3)	0.007(2)	0.005(2)	0.003(2)

Table S9. Selected bond distances (Å) for for kupletskite (K25), kupletskite-(Cs) (CsK25) and their high-temperature modifications (K650 and CsK650)

Bond distance	K25	K650	CsK25	CsK650
M(1)-O(1)	2.236(2)	2.320(2)	2.223(3)	2.310(4)
M(1)-O(2)	2.1866(19)	2.177(2)	2.172(3)	2.154(4)
M(1)-O(3)	2.2046(19	2.227(2)	2.192(3)	2.205(4)
M(1)-OH(5)	2.192(2)	2.167(2)	2.190(3)	2.144(4)
M(1)-O(6)	2.1825(19)	2.207(2)	2.177(3)	2.191(4)
M(1)-O(7)	2.217(2)	2.213(2)	2.203(3)	2.179(4)
<*M*(1)-O>	**2.203**	**2.219**	**2.193**	**2.197**
M(2)-O(2)	2.265(2)	2.266(2)	2.262(3)	2.290(5)
M(2)-OH(5)	2.139(2)	1.8809(19)	2.136(3)	1.895(4)
M(2)-OH(5)	2.110(2)	1.922(2)	2.112(3)	1.865(4)
M(2)-O(6)	2.2056(19)	2.161(2)	2.206(3)	2.124(4)
M(2)-O(7)	2.1108(19)	2.022(2)	2.245(3)	2.010(4)
M(2)-O(7)	2.2241(19)	2.298(2)	2.115(3)	2.348(4)
<*M*(2)-O>	**2.176**	**2.092**	**2.179**	**2.089**
M(3)-O(1)	2.1232(19)	2.1076(19)	2.119(3)	2.085(4)
M(3)-O(2)	2.2415(19)	2.115(2)	2.244(3)	2.098(4)
M(3)-O(3)	2.1381(19)	2.1339(19)	2.136(3)	2.115(4)
M(3)-OH(4)	2.195(2)	2.008(2)	2.124(3)	1.997(5)
M(3)-OH(4)	2.126(2)	2.054(2)	2.210(3)	2.060(4)
M(3)-O(6)	2.1533(19)	2.285(2)	2.167(3)	2.295(4)
<*M*(3)-O>	**2.163**	**2.117**	**2.167**	**2.108**
M(4)-O(1) × 2	2.1453(18)	2.078(2)	2.152(3)	2.081(4)
M(4)-O(3) × 2	2.1716(19)	2.1437(19)	2.175(3)	2.146(4)
M(4)-OH(4) × 2	2.090(2)	1.920(2)	2.089(3)	1.921(4)
<*M*(4)-O>	**2.136**	**2.047**	**2.139**	**2.049**
D-O(2)	1.8076(19)	1.902(2)	1.855(3)	1.960(4)
D-O(9)	1.962(2)	1.930(2)	1.958(3)	1.934(4)
D-O(11)	1.965(2)	1.9408(19)	1.964(3)	1.946(4)
D-O(12)	1.962(2)	1.9527(19)	1.958(3)	1.949(4)
D-O(15)	1.966(2)	1.9500(19)	1.967(3)	1.945(4)
D-$X^{P}{}_{D}$	2.0877(4)	2.0017(6)	2.0509(7)	1.9927(12)
<*D*-φ>	**1.958**	**1.946**	**1.959**	**1.954**
Si(1)-O(1)	1.628(2)	1.642(2)	1.616(3)	1.634(4)
Si(1)-O(11)	1.610(2)	1.6013(19)	1.607(3)	1.588(4)
Si(1)-O(13)	1.643(2)	1.634(2)	1.646(3)	1.631(4)
Si(1)-O(15)	1.610(2)	1.601(2)	1.602(3)	1.602(4)
<Si(1)-O>	**1.623**	**1.620**	**1.618**	**1.614**
Si(2)-O(3)	1.617(2)	1.626(2)	1.604(3)	1.614(4)
Si(2)-O(8)	1.637(2)	1.615(2)	1.645(3)	1.615(4)
Si(2)-O(10)	1.641(2)	1.621(2)	1.644(3)	1.620(4)
Si(2)-O(13)	1.620(2)	1.608(2)	1.616(3)	1.602(4)
<Si(2)-O>	**1.629**	**1.618**	**1.627**	**1.613**
Si(3)-O(6)	1.625(2)	1.635(2)	1.610(3)	1.635(4)
Si(3)-O(8)	1.650(2)	1.627(2)	1.641(3)	1.629(4)
Si(3)-O(10)	1.649(2)	1.633(2)	1.643(3)	1.631(4)
Si(3)-O(14)	1.623(2)	1.611(2)	1.612(3)	1.605(4)
<Si(3)-O>	**1.637**	**1.627**	**1.627**	**1.625**
Si(4)-O(7)	1.627(2)	1.634(2)	1.617(3)	1.628(4)

Si(4)-O(9)	1.606(2)	1.596(2)	1.607(3)	1.600(4)
Si(4)-O(12)	1.612(2)	1.599(2)	1.603(3)	1.593(4)
Si(4)-O(14)	1.635(2)	1.628(2)	1.646(3)	1.623(4)
<Si(4)-O>	**1.620**	**1.614**	**1.618**	**1.611**
A(1)-O(8)	3.786(3)	3.606(4)	3.425(3)	3.495(4)
A(1)-O(9)	2.874(3)	3.075(3)	3.143(3)	3.393(4)
A(1)-O(10)	3.661(3)	3.283(2)	3.461(3)	3.415(4)
A(1)-O(10)	3.696(2)	3.648(3)	3.460(3)	3.243(4)
A(1)-O(11)	2.858(3)	2.767(2)	3.096(3)	2.945(4)
A(1)-O(12)	2.852(3)	2.789(2)	3.115(3)	3.005(4)
A(1)-O(13)	3.443(3)	3.201(2)	3.424(3)	3.246(4)
A(1)-O(13)	3.441(3)	3.588(3)	3.435(3)	3.507(4)
A(1)-O(14)	3.381(3)	3.026(2)	3.402(3)	3.213(4)
A(1)-O(14)	3.435(3)	3.577(3)	3.460(3)	3.591(5)
A(1)-O(15)	2.855(3)	2.949(2)	3.121(3)	3.253(4)
A(1)- X^{P}_{D}	3.1110(11)	3.1851(11)	3.4913(9)	3.5066(15)
<*A*(1)-φ>	**3.283**	**3.225**	**3.336**	**3.318**
A(2)-O(8)	4.30 (3)	4.17(3)	4.096(10)	4.181(11)
A(2)-O(9)	2.452(17)	2.621(17)	2.590(8)	2.701(8)
A(2)-O(10)	4.393(15)	3.203(19)	4.133(9)	4.083(8)
A(2)-O(10)	4.37(3)	4.243(15)	4.142(7)	3.862(10)
A(2)-O(11)	2.403(19)	2.396(19)	2.575(8)	2.550(9)
A(2)-O(12)	2.390(14)	2.384(14)	2.574(6)	2.528(6)
A(2)-O(13)	3.644(18)	3.748(18)	3.596(8)	3.795(8)
A(2)-O(13)	3.698(14)	3.400(14)	3.579(6)	3.318(7)
A(2)-O(14)	3.630(19)	3.203(19)	3.602(8)	3.202(8)
A(2)-O(14)	3.638(18)	3.709(19)	3.540(8)	3.802(9)
A(2)-O(15)	2.439(19)	2.52(3)	2.590(9)	2.626(10)
A(2)- X^{P}_{D}	2.23(2)	2.42(3)	2.566(9)	2.581(9)
<*A*(2)-φ>	**3.299**	**3.226**	**3.369**	**3.345**
B-O(9) × 2	2.596(3)	2.430(2)	2.617(3)	2.463(6)
B-O(11) × 2	2.626(3)	2.807(2)	2.657(3)	2.843(4)
B-O(12) × 2	2.595(3)	2.701(2)	2.656(3)	2.798(6)
B-O(15) × 2	2.589(3)	2.375(2)	2.616(3)	2.383(5)
B-X^{P}_{D} × 2	2.69878(10)	2.6616(2)	2.6952(5)	2.656(1)
<*B*-φ >	**2.621**	**2.595**	**2.648**	**2.629**