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SUPPLEMENTARY INFORMATIONS

Metastable ferroelectric phase and crossover in the $Ba_2NdFeNb_{4-x}Ta_xO_{15}$ TTB solid solution

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Table S1 Summary of crystallographic data for the structures of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$ (PXRD at RT, *P4/mbm*).

	x = 0	**x = 0.1**	**x = 0.3**	**x = 0.5**
a/Å	12.4753(1)	12.4768(1)	12.4768(1)	12.4774(1)
b/Å	12.4753(1)	12.4768(1)	12.4768(1)	12.4774(1)
c/Å	3.9271(1)	3.9256(1)	3.9247(1)	3.9247(1)
Volume/Å^3	611.19(1)	611.09(1)	610.95(1)	611.02(1)
Z, $\rho_{calculated}$/g.cm^{-3}	2, 5.984	2, 5.952	2, 6.049	2, 6.144
Θ range/°	7.016-129.992	8.008-130.000	8.008-130.000	7.008-139.992
Unique reflections	335	335	335	367
Parameters	35	38	43	35
R_p/R_{wp}	0.204/0.183	0.188/0.168	0.201/0.157	0.168/0.169
R_B/R_F	0.116/0.123	0.088/0.107	0.091/0.134	0.105/0.117

	x = 1	**x = 2**	**x = 3**	**x = 3.5**	**x = 4**
a/Å	12.4782(1)	12.4826(1)	12.4837(1)	12.4877(1)	12.4869(1)
b/Å	12.4782(1)	12.4826(1)	12.4837(1)	12.4877(1)	12.4869(1)
c/Å	3.9231(1)	3.9203(1)	3.9178(1)	3.9172(1)	3.9162(1)
Volume/Å^3	610.85(1)	610.85(1)	610.56(1)	610.84(1)	610.63(1)
Z, $\rho_{calculated}$/g.cm^{-3}	2, 6.436	2, 6.864	2, 7.346	2, 7.582	2, 7.824
Θ range/°	8.008-139.992	8.016-129.992	5.008-129.992	8.016-129.992	8.008-139.992
Unique reflections	370	336	336	336	375
Parameters	42	34	46	38	36
R_p/R_{wp}	0.180/0.178	0.216/0.177	0.204/0.171	0.190/0.180	0.206/0.208
R_B/R_F	0.115/0.126	0.121/0.171	0.136/0.197	0.117/0.145	0.153/0.185

Table S2 Selected inter-atomic distances (Å) and bond valence calculations of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$ (PXRD at RT, *P4/mbm*).

d_{ij} (Å)	x = 0	x = 0.1	x = 0.3	x = 0.5	x = 1	x = 2	x = 3	x = 3.5	x = 4
Ba(1)-O(1) x1	3.024(2)	3.012(7)	3.017(2)	3.015(1)	3.018(2)	3.017(2)	3.014(2)	3.016(2)	3.009(2)
Ba(1)-O(2) x 2	2.799(5)	2.772(5)	2.775(4)	2.781(4)	2.780(5)	2.757(5)	2.764(5)	2.759(5)	2.751(6)
Ba(1) -O(3) x 2	3.497(6)	3.284(5)	3.291(4)	3.282(5)	3.289(5)	3.273(7)	3.227(7)	3.226(7)	3.465(7)
Ba(1)'-O(3) x 2	3.331(6)	3.510(5)	3.521(5)	3.505(5)	3.509(5)	3.516(7)	3.484(7)	3.485(7)	3.220(6)
Ba(1)-O(4) x 2	2.789(5)	2.911(5)	2.777(5)	2.911(4)	2.784(5)	2.910(6)	2.911(6)	2.908(7)	2.758(6)
Ba(1)'-O(4) x 2	2.893(5)	2.777(4)	2.913(4)	2.779(4)	2.921(5)	2.768(5)	2.760(5)	2.758(5)	2.904(7)
Ba(1)-O(5) x 1	3.034(8)	3.112(5)	3.136(6)	3.126(5)	3.027(6)	3.108(7)	3.127(8)	3.147(8)	3.202(10)
Ba(1)'-O(5) x 1	3.172(7)	3.333(6)	3.324(5)	3.328(6)	3.209(5)	3.327(9)	3.300(9)	3.278(9)	3.400(8)
Ba(1)-O(5)' x 1	3.484(7)	3.293(6)	3.317(6)	3.306(6)	3.439(6)	3.304(9)	3.336(9)	3.356(9)	3.238(8)
Ba(1)'-O(5)' x 1	3.688(8)	3.611(6)	3.602(6)	3.604(5)	3.711(6)	3.626(7)	3.624(8)	3.602(8)	3.546(10)
< Ba-O >	3.135	3.125	3.130	3.126	3.131	3.122	3.113	3.111	3.106
Nd(1)-O(3) x 8	2.686(4)	2.704(4)	2.694(4)	2.705(4)	2.699(4)	2.704(5)	2.738(5)	2.738(5)	2.749(5)
Nd(1)-O(5) x 4	2.583(5)	2.634(5)	2.589(5)	2.612(5)	2.590(5)	2.621(7)	2.604(9)	2.614(8)	2.612(8)
< Nd(1)-O >	2.652	2.681	2.659	2.674	2.663	2.676	2.693	2.697	2.703
M(1)-O(1) x 2	1.964(1)	1.963(1)	1.962(1)	1.962(1)	1.962(1)	1.960(1)	1.959(1)	1.959(1)	1.958(1)
M(1)-O(4) x 4	2.069(6)	1.960(6)	1.949(6)	1.953(5)	2.020(6)	1.928(7)	1.924(7)	1.916(7)	1.949(9)
< M(1)-O >	2.034	1.961	1.953	1.956	2.001	1.939	1.936	1.930	1.952
M(2)-O(2) x 1	1.976(6)	1.988(6)	1.984(5)	1.980(5)	1.981(6)	1.992(8)	1.988(8)	1.990(8)	1.997(9)
M(2)-O(3) x 1	1.944(7)	1.999(6)	1.995(6)	1.988(6)	1.966(6)	2.008(9)	2.027(9)	2.032(9)	2.006(9)
M(2)-O(3)' x 1	2.062(7)	2.013(5)	2.021(5)	2.023(5)	2.042(6)	2.002(8)	1.977(8)	1.973(8)	1.993(8)
M(2)-O(4) x 1	1.809(6)	1.895(6)	1.905(6)	1.905(5)	1.844(6)	1.936(8)	1.945(8)	1.958(8)	1.928(9)
M(2)-O(5) x 2	1.987(1)	1.974(1)	1.978(1)	1.975(1)	1.983(1)	1.972(1)	1.972(9)	1.971(8)	1.970(1)
< M(2)-O >	1.961	1.974	1.977	1.974	1.967	1.980	1.980	1.983	1.977
O(1)-O(4)	2.852(5)	2.774(4)	2.766(4)	2.769(4)	2.816(4)	2.750(5)	2.745(5)	2.740(6)	2.763(6)
O(2)-O(3)	2.896(9)	2.891(8)	2.901(7)	2.890(7)	2.884(9)	2.892(11)	2.877(11)	2.879(11)	2.845(12)
O(2)-O(4)	2.849(9)	2.915(9)	2.913(7)	2.903(7)	2.871(9)	2.952(11)	2.950(11)	2.964(11)	2.962(12)
O(2)-O(5)	2.838(7)	2.862(6)	2.894(5)	2.875(5)	2.842(6)	2.872(7)	2.889(8)	2.896(8)	2.922(9)
O(3)-O(3)'	2.591(9)	2.629(9)	2.610(9)	2.633(9)	2.622(9)	2.635(12)	2.704(12)	2.706(12)	2.728(12)
O(3)-O(4)	2.663(9)	2.713(7)	2.737(7)	2.723(7)	2.682(9)	2.732(11)	2.683(11)	2.687(11)	2.659(12)
O(3)-O(5)	2.559(6)	2.667(5)	2.651(5)	2.655(5)	2.582(5)	2.668(7)	2.685(8)	2.7405(8)	2.712(8)
O(3)-O(5)'	2.810(7)	2.745(6)	2.717(6)	2.735(6)	2.790(6)	2.727(8)	2.693(8)	2.683(8)	2.674(8)
O(4)-O(4)	2.800(9)	2.657(8)	2.636(8)	2.645(7)	2.760(9)	2.595(11)	2.585(11)	2.566(12)	2.622(12)
O(4)-O(5)	2.876(7)	2.857(6)	2.875(6)	2.867(5)	2.889(6)	2.888(7)	2.890(8)	2.881(8)	2.833(9)
Atom, $v_{theo.}$	**$v_{exp.}$**								
Ba(1), *2*	2.04(2)	2.07(2)	2.05(2)	2.05(2)	2.06(2)	2.11(2)	2.13(2)	2.14(2)	2.15(2)
Nd(1), *3*	2.85(2)	2.63(2)	2.80(2)	2.68(2)	2.77(2)	2.66(2)	2.57(2)	2.54(2)	2.50(2)
M(1), *4.6*	4.00(2)	4.83(2)	4.94(2)	4.91(2)	4.37(2)	5.18(2)	5.25(2)	5.34(2)	5.04(2)
M(2), *4.6*	4.94(2)	4.69(2)	4.65(2)	4.69(2)	4.85(2)	4.64(2)	4.66(2)	4.64(2)	4.72(2)
O(1), *-2*	1.87(2)	1.89(2)	1.89(2)	1.89(2)	1.89(2)	1.91(2)	1.92(2)	1.93(2)	1.94(2)
O(2), *-2*	2.05(2)	2.04(2)	2.05(2)	2.06(2)	2.06(2)	2.06(2)	2.07(2)	2.08(2)	2.06(2)
O(3), *-2*	1.88(2)	1.84(2)	1.84(2)	1.84(2)	1.86(2)	1.85(2)	1.84(2)	1.84(2)	1.84(2)
O(4), *-2*	2.27(2)	2.22(2)	2.22(2)	2.22(2)	2.24(2)	2.22(2)	2.22(2)	2.22(2)	2.22(2)
O(5), *-2*	1.92(2)	1.91(2)	1.92(2)	1.92(2)	1.94(2)	1.94(2)	1.96(2)	1.95(2)	1.95(2)

Table S3 Summary of crystallographic data for the structures of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$ (NPD, *P4/mbm*).

	x = 0.3 T = 100 K	**x = 0.3 T = 400 K**	**x = 0.5 T = 300 K**	**x = 1 T = 300 K**	**x = 4 T = 300 K**
a/Å	12.4597(1)	12.4881(1)	12.4801(1)	12.4818(1)	12.4891(1)
b/Å	12.4597(1)	12.4881(1)	12.4801(1)	12.4818(1)	12.4891(1)
c/Å	3.9226(1)	3.9312(1)	3.9277(1)	3.9260(1)	3.9190(1)
Volume/Å^3	608.96(1)	613.08(1)	611.75(1)	611.65(1)	611.28(1)
Z, ρcalculated/g.cm^{-3}	2, 6.069	2, 6.028	2, 6.137	2, 6.428	2, 7.816
Θ range/°	4.580-129.530	4.580-121.030	4.610-121.110	4.610-121.110	4.610-121.110
Unique reflections	569	578	577	577	577
Parameters	93	98	110	104	106
R_p/R_{wp}	0.115/0.123	0.107/0.110	0.087/0.098	0.092/0.103	0.115/0.133
R_B/R_F	0.064/0.044	0.058/0.044	0.044/0.033	0.047/0.032	0.056/0.040

Table S4 Atomic positions, site occupancy and equivalent displacement parameters of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$.

	Atom, site	x	y	z	Site occupancy	B_{eq} (Å^2)
	Ba(1), *8i*	0.338(3)	0.823(3)	0	0.5	0.16(1)
	Nd(1), *2a*	0	0	0	1	0.37(1)
	Fe(1)/Nb(1)/Ta(1), *2c*	0	½	½	0.20/0.74/0.06	0.65(1)
x = 0.3	Fe(2)/Nb(2)/Ta(2), *8j*	0.2131(2)	0.0734(2)	½	0.20/0.74/0.06	0.27(1)
T = 100 K	O(1), *2d*	0	½	0	1	2.68(1)
	O(2), *4h*	0.2182(2)	0.7182(2)	½	1	0.54(1)
	O(3), *8j*	0.0615(3)	0.1309(4)	½	1	5.13(1)
	O(4), *8j*	0.1585(3)	0.4931(3)	½	1	1.45(1)
	O(5), *8i*	0.1940(3)	0.0771(6)	0	1	4.90(1)
	Ba(1), *8i*	0.339(2)	0.820(2)	0	0.5	0.79(1)
	Nd(1), *2a*	0	0	0	1	0.96(1)
	Fe(1)/Nb(1)/Ta(1), *2c*	0	½	½	0.20/0.74/0.06	1.04(1)
x = 0.3	Fe(2)/Nb(2)/Ta(2), *8j*	0.2134(2)	0.0735(2)	½	0.20/0.74/0.06	0.62(1)
T = 400 K	O(1), *2d*	0	½	0	1	3.32(1)
	O(2), *4h*	0.2184(2)	0.7184(2)	½	1	1.05(1)
	O(3), *8j*	0.0628(3)	0.1316(3)	½	1	4.42(1)
	O(4), *8j*	0.1577(2)	0.4934(2)	½	1	1.85(1)
	O(5), *8i*	0.1957(3)	0.0764(5)	0	1	4.50(1)
	Ba(1), *8i*	0.323(4)	0.8371(4)	0	0.5	0.87(1)
	Nd(1), *2a*	0	0	0	1	0.76(1)
	Fe(1)/Nb(1)/Ta(1), *2c*	0	½	½	0.20/0.70/0.10	0.88(1)
x = 0.5	Fe(2)/Nb(2)/Ta(2), *8j*	0.2133(1)	0.0736(2)	½	0.20/0.70/0.10	0.49(1)
T = 300 K	O(1), *2d*	0	½	0	1	3.40(1)
	O(2), *4h*	0.2181(2)	0.7181(2)	½	1	0.88(1)
	O(3), *8j*	0.0634(3)	0.1314(3)	½	1	4.42(1)
	O(4), *8j*	0.1579(2)	0.4934(2)	½	1	1.73(1)
	O(5), *8i*	0.1945(3)	0.0768(5)	0	1	4.42(1)
	Ba(1), *8i*	0.335(3)	0.825(3)	0	0.5	1.11(1)
	Nd(1), *2a*	0	0	0	1	0.62(1)
	Fe(1)/Nb(1)/Ta(1), *2c*	0	½	½	0.20/0.60/0.20	1.35(1)
x = 1	Fe(2)/Nb(2)/Ta(2), *8j*	0.2133(2)	0.0735(2)	½	0.20/0.60/0.20	0.42(1)
T = 300 K	O(1), *2d*	0	½	0	1	3.00(1)
	O(2), *4h*	0.2180(2)	0.7180(2)	½	1	0.91(1)
	O(3), *8j*	0.0624(3)	0.1312(3)	½	1	4.26(1)
	O(4), *8j*	0.1579(3)	0.4934(2)	½	1	1.74(1)
	O(5), *8i*	0.1939(3)	0.0787(5)	0	1	4.11(1)
	Ba(1), *8i*	0.342(9)	0.8190(8)	0	0.5	0.01(1)
	Nd(1), *2a*	0	0	0	1	0.70(1)
	Fe(1)/Ta(1), *2c*	0	½	½	0.20/0.80	0.79(1)
x = 4	Fe(2)/Ta(2), *8j*	0.2132(2)	0.0744(2)	½	0.20/0.80	0.23(1)
T = 300 K	O(1), *2d*	0	½	0	1	3.08(1)
	O(2), *4h*	0.2184(3)	0.7184(3)	½	1	1.03(1)
	O(3), *8j*	0.0619(4)	0.1331(4)	½	1	4.03(1)
	O(4), *8j*	0.1571(3)	0.4936(3)	½	1	1.50(1)
	O(5), *8i*	0.1950(4)	0.0746(7)	0	1	3.95(1)

Table S5 Anisotropic displacement parameters of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$. Negative U_{ij} values are non-physical.

	Atom	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
	Ba(1)	0.017(17)	-0.004(5)	-0.006(2)	-0.002(10)	0	0
	Nd(1)	0.006(1)	0.006(1)	0.003(2)	0	0	0
	M(1)	0.006(1)	0.006(1)	0.013(2)	-0.001(2)	0	0
x = 0.3	M(2)	0.008(1)	-0.001(1)	0.003(1)	-0.005(2)	0	0
T = 100 K	O(1)	0.049(4)	0.049(4)	0.004(4)	0.030(5)	0	0
	O(2)	-0.001(1)	-0.001(1)	0.022(3)	-0.001(2)	0	0
	O(3)	0.001(1)	0.067(4)	0.128(5)	0.020(2)	0	0
	O(4)	0.003(2)	0.007(2)	0.046(2)	-0.010(2)	0	0
	O(5)	0.037(3)	0.150(5)	0.001(2)	-0.063(4)	0	0
	Ba(1)	0.018(10)	0.011(7)	0.002(2)	-0.005(8)	0	0
	Nd(1)	0.016(1)	0.016(1)	0.005(2)	0	0	0
	M(1)	0.010(1)	0.010(1)	0.019(2)	0.001(2)	0	0
x = 0.3	M(2)	0.010(1)	0.003(1)	0.010(1)	-0.004(2)	0	0
T = 400 K	O(1)	0.058(4)	0.058(4)	0.011(3)	0.021(4)	0	0
	O(2)	0.007(1)	0.007(1)	0.027(3)	0.003(2)	0	0
	O(3)	0.007(2)	0.053(3)	0.106(4)	0.020(2)	0	0
	O(4)	0.004(2)	0.018(2)	0.047(2)	-0.012(2)	0	0
	O(5)	0.041(3)	0.127(4)	0.0033(16)	-0.048(3)	0	0
	Ba(1)	0.002(4)	0.031(20)	0.0002(20)	-0.010(10)	0	0
	Nd(1)	0.011(1)	0.011(1)	0.007(2)	0	0	0
	M(1)	0.010(1)	0.010(1)	0.013(2)	-0.003(2)	0	0
x = 0.5	M(2)	0.010(1)	0.003(1)	0.006(1)	-0.004(2)	0	0
T = 300 K	O(1)	0.061(4)	0.061(4)	0.008(3)	0.035(4)	0	0
	O(2)	0.005(1)	0.005(1)	0.023(2)	-0.001(2)	0	0
	O(3)	0.007(2)	0.053(3)	0.107(4)	0.011(2)	0	0
	O(4)	0.006(2)	0.010(2)	0.050(2)	-0.009(2)	0	0
	O(5)	0.038(2)	0.125(4)	0.005(2)	-0.050(3)	0	0
	Ba(1)	0.040(16)	0.000(4)	0.001(2)	-0.013(6)	0	0
	Nd(1)	0.009(1)	0.009(1)	0.006(2)	0	0	0
	M(1)	0.016(1)	0.016(1)	0.020(2)	-0.006(2)	0	0
x = 1	M(2)	0.007(1)	0.004(1)	0.005(1)	-0.001(2)	0	0
T = 300 K	O(1)	0.053(4)	0.053(4)	0.008(3)	0.035(4)	0	0
	O(2)	0.005(1)	0.005(2)	0.024(2)	-0.002(2)	0	0
	O(3)	0.006(2)	0.050(3)	0.106(4)	0.011(2)	0	0
	O(4)	0.005(2)	0.011(2)	0.051(2)	-0.010(2)	0	0
	O(5)	0.036(2)	0.117(4)	0.003(2)	-0.047(3)	0	0
	Ba(1)	0.004(7)	-0.010(4)	0.005(3)	0.005(5)	0	0
	Nd(1)	0.007(2)	0.007(2)	0.013(3)	0	0	0
	M(1)	0.008(2)	0.008(2)	0.015(3)	-0.014(3)	0	0
x = 4	M(2)	0.009(2)	0.001(2)	-0.001(1)	-0.003(2)	0	0
T = 300 K	O(1)	0.063(5)	0.063(5)	-0.010(4)	0.030(6)	0	0
	O(2)	0.009(2)	0.009(2)	0.021(3)	-0.005(3)	0	0
	O(3)	-0.001(3)	0.039(3)	0.114(6)	0.008(2)	0	0
	O(4)	0.001(2)	0.004(2)	0.050(3)	-0.014(2)	0	0
	O(5)	0.028(3)	0.110(6)	0.013(3)	-0.035(4)	0	0

Table S6 Selected inter-atomic distances (Å) and bond valence calculations of $Ba_2NdFeNb_{4-x}Ta_xO_{15}$ (NPD, *P4/mbm*). Maximum of the variation are estimated.

d_{ij} (Å)	x = 0.3 T = 100 K	x = 0.3 T = 400 K	x = 0.5 T = 300 K	x = 1 T = 300 K	x = 4 T = 300 K	Max Variation (%)
Ba(1)-O(1) x1	2.99(4)	3.01(2)	3.00(5)	3.00(4)	3.00(1)	0.67
Ba(1)-O(2) x 2	2.79(3)	2.79(2)	2.79(4)	2.79(3)	2.79(1)	0
Ba(1) -O(3) x 2	3.55(3)	3.56(2)	3.53(4)	3.51(3)	3.58(1)	2.00
Ba(1)'-O(3) x 2	3.34(3)	3.31(2)	3.33(4)	3.37(3)	3.27(1)	3.06
Ba(1)-O(4) x 2	2.76(3)	2.77(2)	2.78(4)	2.79(3)	2.74(1)	1.82
Ba(1)'-O(4) x 2	2.89(3)	2.92(2)	2.90(4)	2.88(3)	2.93(1)	1.74
Ba(1)-O(5) x 1	3.26(4)	3.29(3)	3.40(5)	3.21(4)	3.34(1)	5.91
Ba(1)'-O(5) x 1	3.64(4)	3.66(3)	3.63(5)	3.62(4)	3.68(1)	1.66
Ba(1)-O(5)' x 1	3.09(4)	3.08(3)	3.10(5)	3.10(4)	3.09(1)	0.65
Ba(1)'-O(5)' x 1	3.39(4)	3.35(3)	3.25(5)	3.45(4)	3.30(1)	6.15
< Ba-O >	3.135	3.139	3.136	3.137	3.135	0.13
Nd(1)-O(3) x 8	2.663(3)	2.679(3)	2.678(3)	2.672(3)	2.683(3)	0.75
Nd(1)-O(5) x 4	2.600(4)	2.624(4)	2.610(4)	2.612(4)	2.608(6)	0.92
< Nd(1)-O >	2.642	2.661	2.655	2.652	2.658	0.72
M(1)-O(1) x 2	1.961(1)	1.966(1)	1.964(1)	1.963(1)	1.960(1)	0.31
M(1)-O(4) x 4	1.977(4)	1.971(2)	1.972(2)	1.973(4)	1.964(4)	0.66
< M(1)-O >	1.972	1.969	1.969	1.970	1.963	0.46
M(2)-O(2) x 1	1.997(3)	2.000(3)	1.996(3)	1.997(3)	1.991(5)	0.45
M(2)-O(3) x 1	2.020(4)	2.016(4)	2.005(4)	2.017(4)	2.026(6)	1.05
M(2)-O(3)' x 1	1.968(5)	1.985(4)	1.992(4)	1.982(4)	1.975(6)	1.22
M(2)-O(4) x 1	1.887(4)	1.895(3)	1.893(3)	1.893(4)	1.908(5)	1.11
M(2)-O(5) x 2	1.976(1)	1.978(1)	1.978(1)	1.979(1)	1.973(1)	0.30
< M(2)-O >	1.971	1.975	1.974	1.975	1.974	0.20
O(1)-O(4)	2.785(3)	2.784(2)	2.783(2)	2.783(3)	2.774(3)	0.40
O(2)-O(3)	2.953(5)	2.940(5)	2.934(4)	2.947(5)	2.944(6)	0.65
O(2)-O(4)	2.902(4)	2.910(4)	2.903(3)	2.902(4)	2.910(5)	0.28
O(2)-O(5)	2.853(4)	2.856(4)	2.856(4)	2.844(4)	2.870(5)	0.91
O(3)-O(3)'	2.548(6)	2.575(5)	2.575(5)	2.565(5)	2.591(7)	1.69
O(3)-O(4)	2.711(6)	2.723(5)	2.723(4)	2.723(5)	2.712(6)	0.44
O(3)-O(5)	2.649(4)	2.663(4)	2.645(4)	2.641(4)	2.671(5)	1.14
O(3)-O(5)'	2.729(4)	2.743(4)	2.746(4)	2.751(4)	2.710(5)	1.51
O(4)-O(4)	2.671(5)	2.669(4)	2.670(4)	2.671(5)	2.662(5)	0.34
O(4)-O(5)	2.885(5)	2.879(4)	2.887(4)	2.900(4)	2.877(5)	0.80
Atom, $v_{theo.}$	**$v_{exp.}$**					
Ba(1), 2	2.07(2)	2.03(2)	2.03(2)	2.04(2)	2.08(2)	2.40
Nd(1), 3	2.91(2)	2.77(2)	2.81(2)	2.83(2)	2.79(2)	5.05
M(1), 4.6	4.70(2)	4.73(2)	4.73(2)	4.74(2)	4.90(2)	4.26
M(2), 4.6	4.74(2)	4.68(2)	4.70(2)	4.70(2)	4.77(2)	1.92
O(1), -2	-1.91(2)	-1.88(2)	-1.89(2)	-1.90(2)	-1.94(2)	3.20
O(2), -2	-1.98(2)	-1.97(2)	-1.99(2)	-1.99(2)	-2.03(2)	3.05
O(3), -2	-1.94(2)	-1.89(2)	-1.90(2)	-1.91(2)	-1.91(2)	2.65
O(4), -2	-2.23(2)	-2.20(2)	-2.21(2)	-2.22(2)	-2.23(2)	1.36
O(5), -2	-1.89(2)	-1.86(2)	-1.85(2)	-1.89(2)	-1.91(2)	3.24

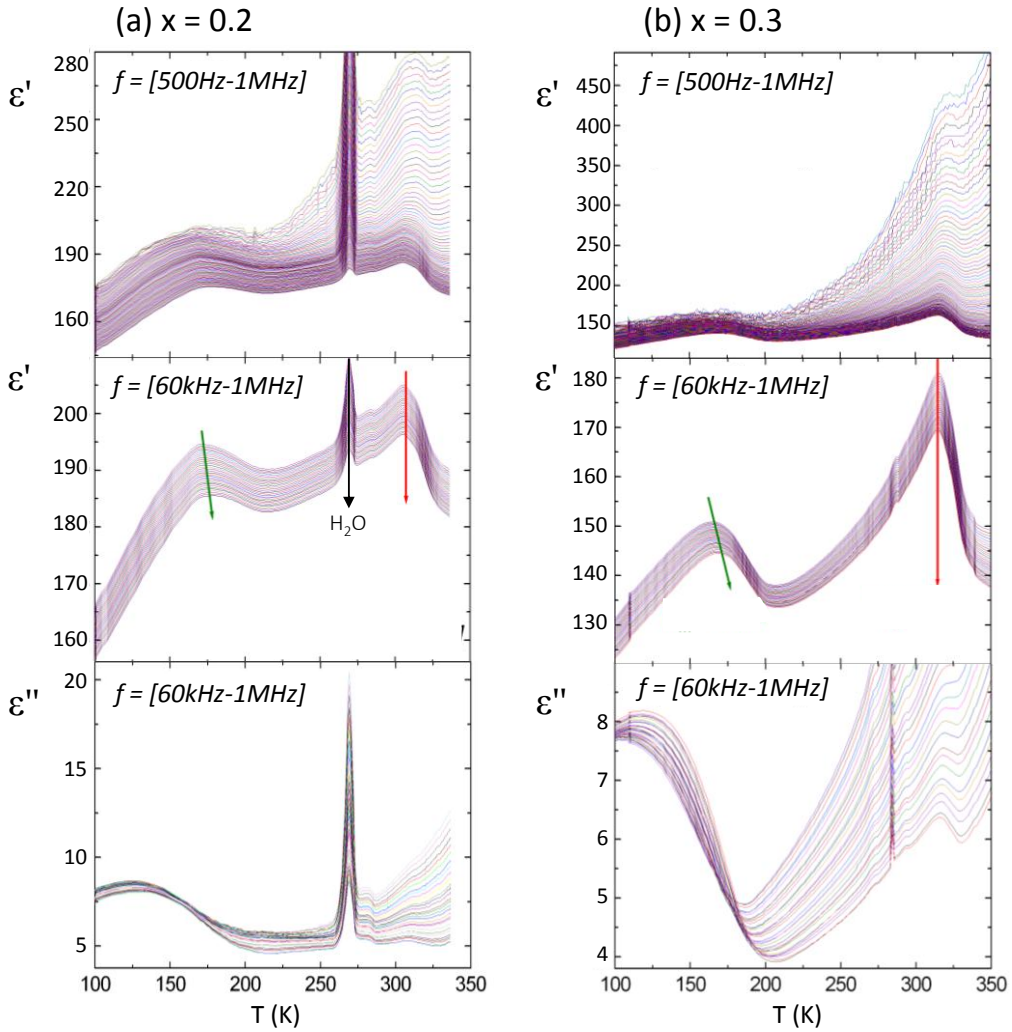

Fig. S1 Dielectric responses on heating of (a) x=0.2 and (b) 0.3 ceramics field-cooled at 10 kV.cm^{-1}.

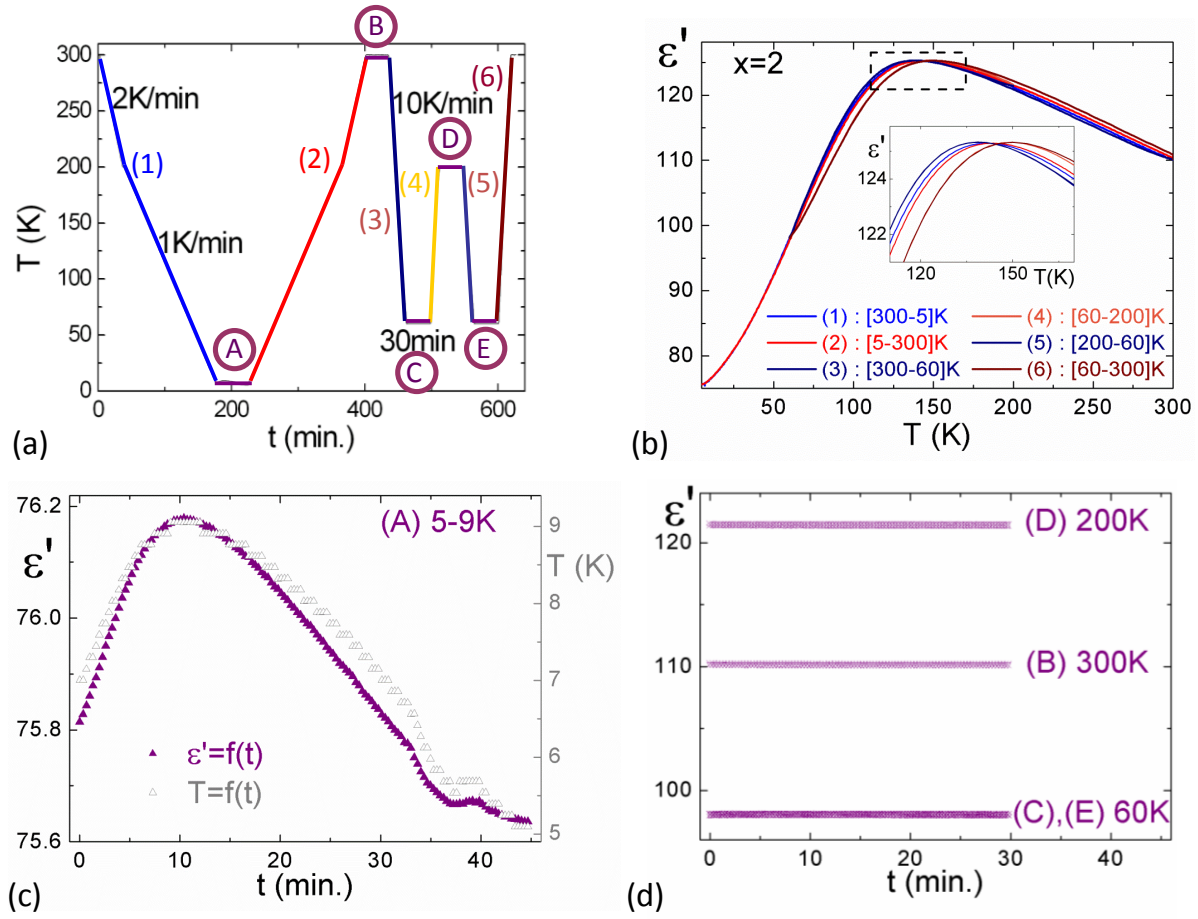

Fig. S2 (a) Thermal sequences applied on $Ba_2NdFeNb_2Ta_2O_{15}$ relaxor ceramics. (b) Temperature dependence of the dielectric permittivity on heating and on cooling, at f = 1 MHz. Time dependences of the dielectric permittivity (c) between 5 and 9 K, (d) at T = 60, 200 and 300 K.