Na$_{11}$Ta$_8$P$_7$O$_{43}$: (Ta$_8$O$_{33}$) bi-capped triangular prisms connected by PO$_4$ groups resulting in phase-matched second harmonic response

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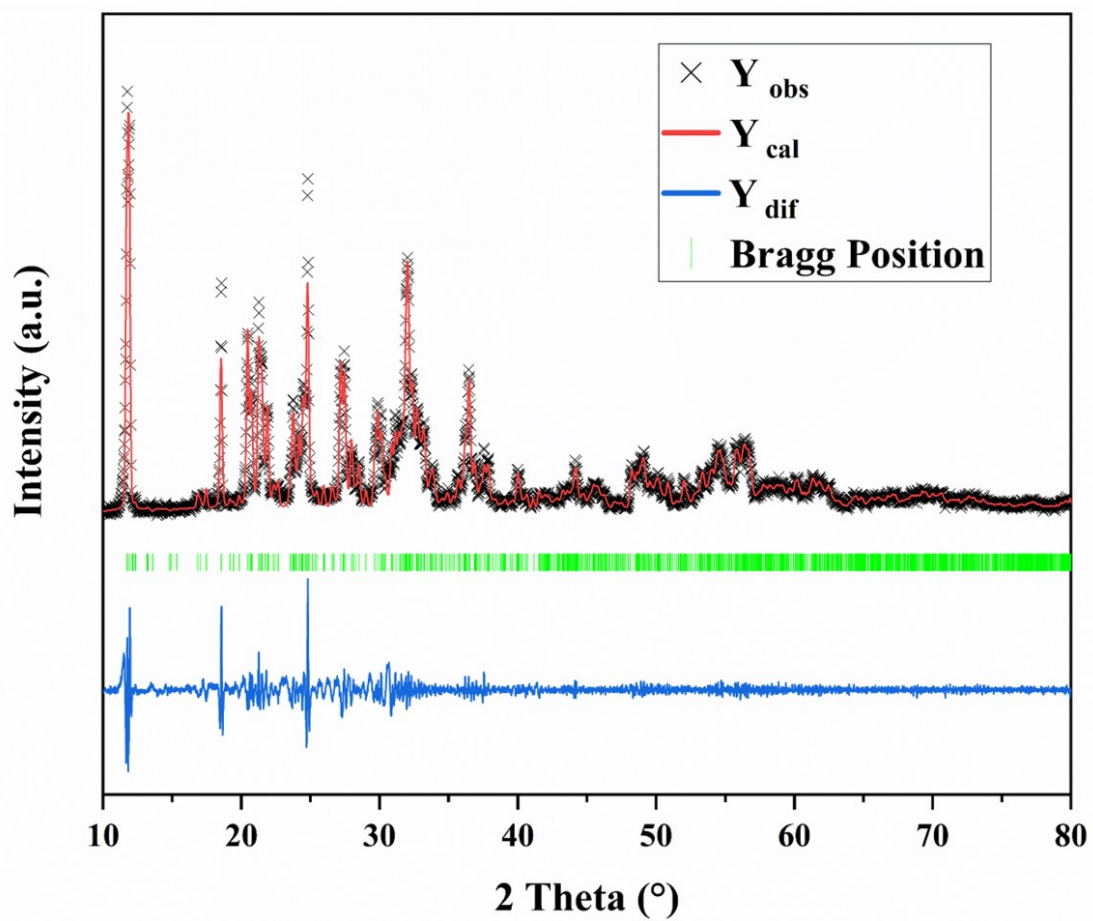
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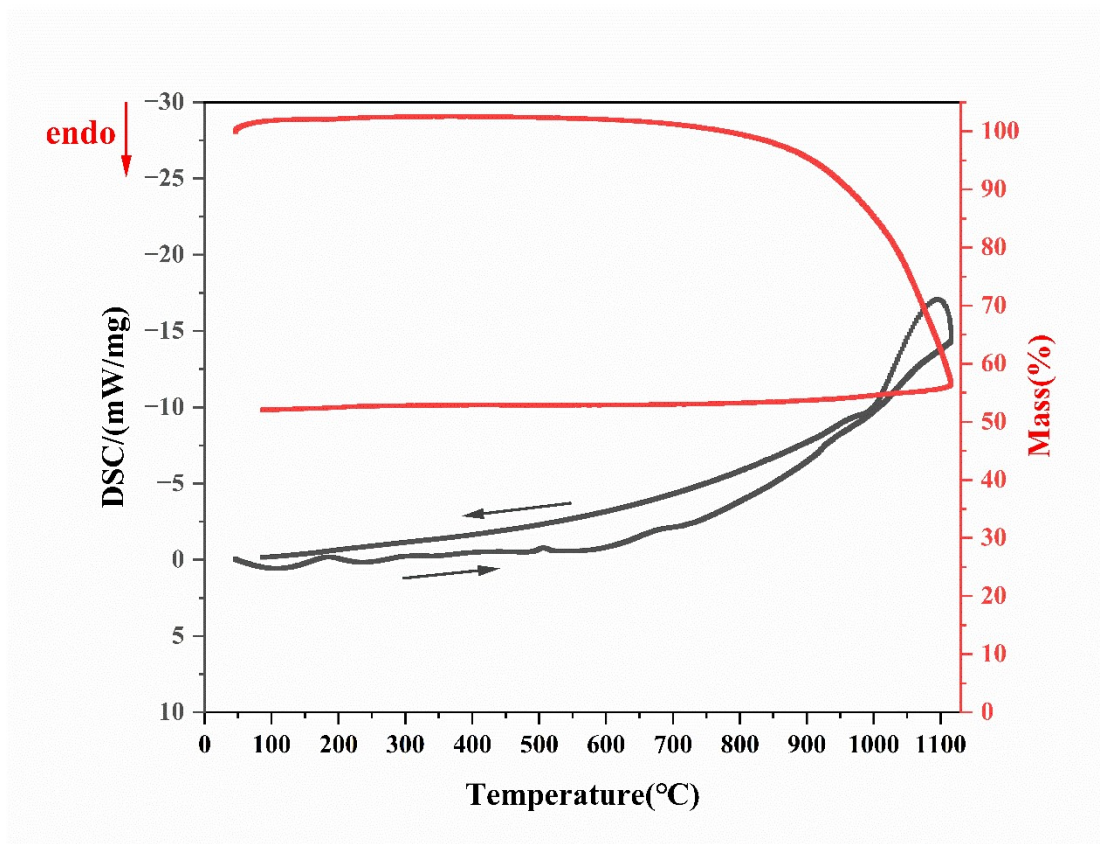
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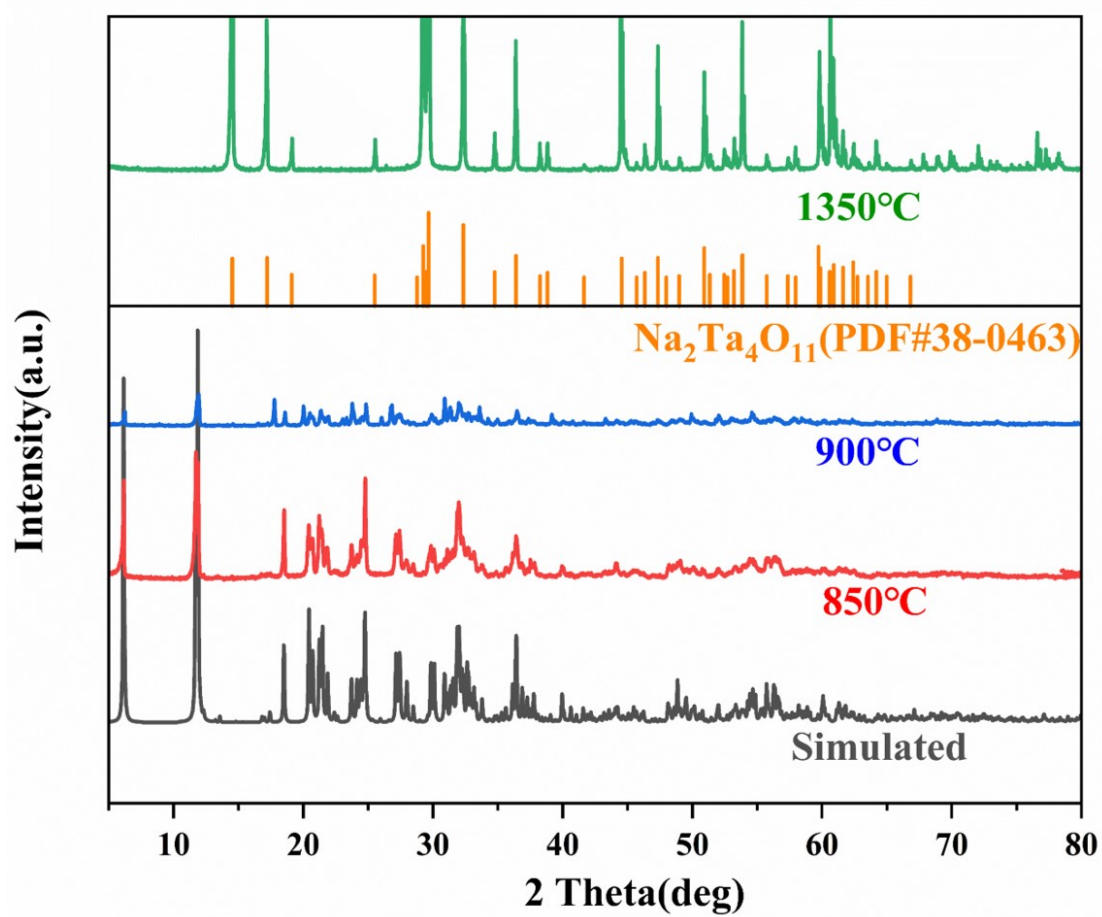
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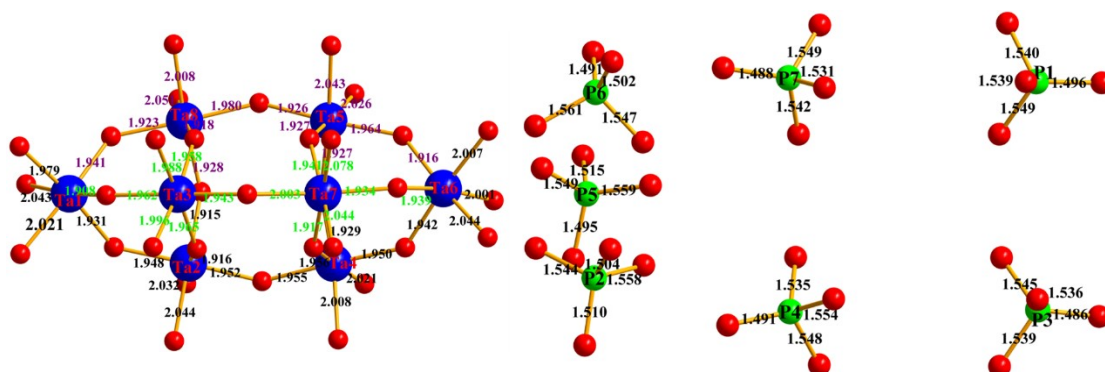
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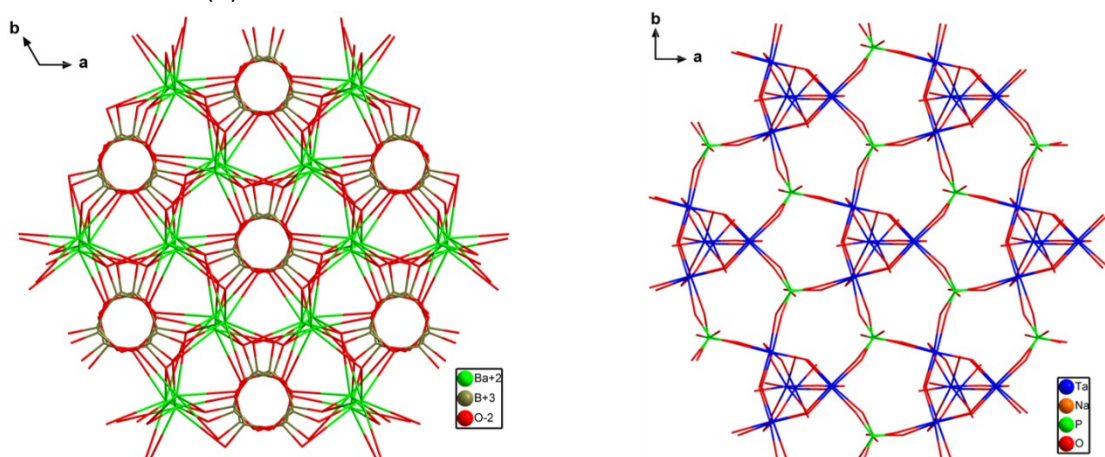
(b) ab plane structure of crystal BBO and NTPO.

(c) crystal structure of ab plane.

Figure S5. Calculated electronic band structure (a) and density of states (DOS) (b) of $Na_{11}Ta_8P_7O_{43}$.

$Eg = 5.55 \text{ eV}$

(a)

(b)

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($\mathring{A}^2$) for the compound $Na_{11}Ta_8P_7O_{43}$. Ueq is defined as one-third of the trace of the orthogonalised U_{ij} tensor.

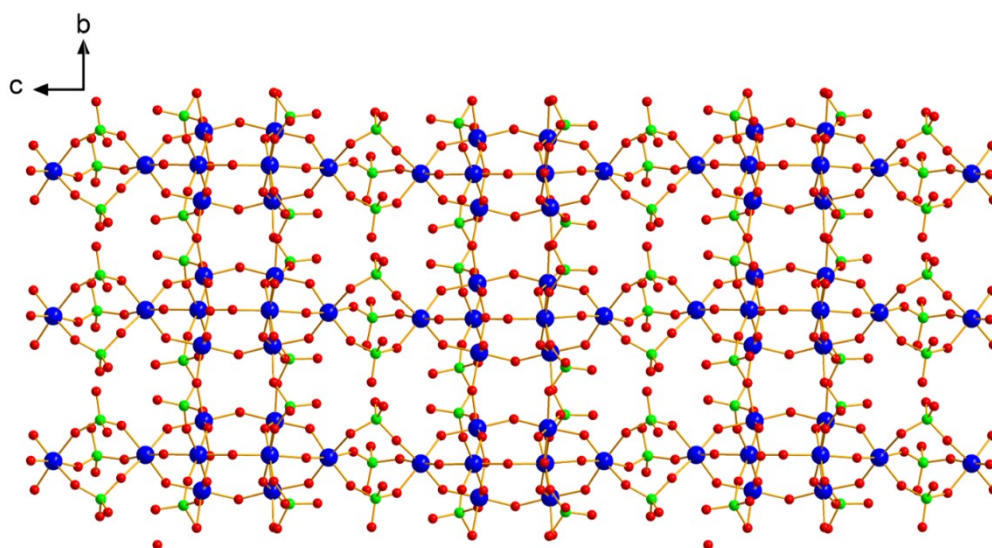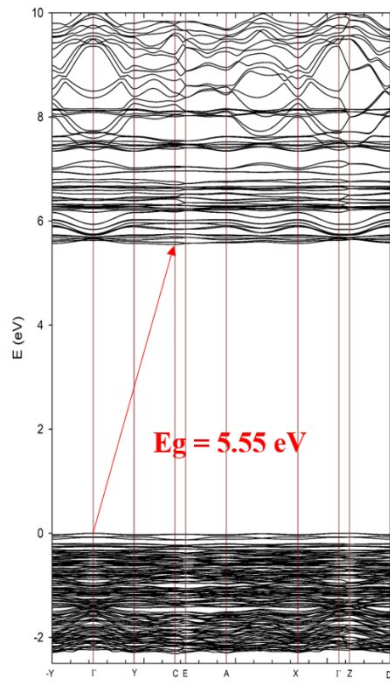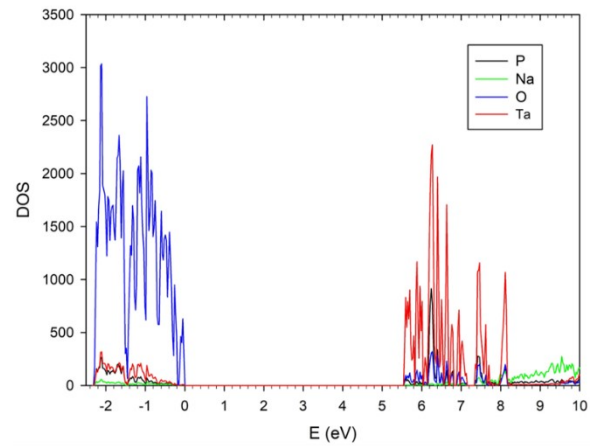| Atom	Wyck.	x	y	z	Ueq	BVS
Ta1	4a	0.66017(6)	0.98509(3)	0.64952(2)	0.0073(1)	5.0999
Ta2	4a	0.55559(5)	0.86818(3)	0.54351(2)	0.00553(10)	5.1124
Ta3	4a	0.42555(6)	0.48460(3)	0.55324(2)	0.00589(11)	5.0689
Ta4	4a	0.07281(5)	0.36817(3)	0.41444(2)	0.00575(10)	5.0656
Ta5	4a	0.07801(5)	0.60797(3)	0.41875(2)	0.00574(10)	5.0934
Ta6	4a	0.21058(6)	0.49395(3)	0.31696(2)	0.00684(10)	5.0574
Ta7	4a	0.44215(5)	0.48581(3)	0.42388(2)	0.00595(11)	4.9348
Ta8	4a	0.05839(5)	0.60781(3)	0.54694(2)	0.00598(10)	5.1083
Na1	4a	0.0846(8)	0.0295(4)	0.2911(2)	0.0284(14)	0.9788
Na2	4a	0.0301(8)	0.2792(4)	0.2989(2)	0.0295(14)	0.9484
Na3	4a	0.3922(11)	0.2797(4)	0.4862(3)	0.054(2)	0.8970
Na4	4a	0.7825(8)	0.4859(5)	0.4778(3)	0.0383(17)	1.0102
Na5	4a	0.9368(8)	0.6671(4)	0.6788(2)	0.0311(15)	0.9282
Na6	4a	0.1979(7)	0.8281(3)	0.7004(2)	0.0213(12)	1.1868
Na7	4a	0.0603(7)	0.0405(4)	0.6734(2)	0.0280(14)	0.8749
Na8	4a	0.0235(7)	0.2754(3)	0.6604(2)	0.0257(13)	1.0553
Na9	4a	0.3824(9)	0.6986(4)	0.4867(3)	0.0417(18)	0.9214
Na10	4a	0.9338(8)	0.6907(4)	0.3112(2)	0.0334(16)	0.8943
Na11	4a	0.1683(7)	0.8258(4)	0.2649(2)	0.0248(13)	1.1255
P1	4a	0.1876(4)	0.15375(18)	0.38806(11)	0.0066(6)	4.9840
P2	4a	0.3418(4)	0.63528(19)	0.23154(11)	0.0085(6)	5.0201
P3	4a	0.1838(4)	0.81812(18)	0.38680(11)	0.0072(6)	5.0392
P4	4a	0.1938(4)	0.81535(18)	0.57931(11)	0.0069(6)	4.9782
P5	4a	0.4035(4)	0.98846(18)	0.73743(12)	0.0095(6)	5.0105
P6	4a	0.8080(4)	0.13795(19)	0.73038(12)	0.0094(6)	5.0768
P7	4a	0.6835(4)	0.65923(18)	0.58052(11)	0.0068(6)	5.0251
O1	4a	0.2132(11)	0.6165(5)	0.1930(3)	0.0139(19)	2.1220
O2	4a	0.4933(11)	0.5930(6)	0.2190(3)	0.020(2)	1.9815
O3	4a	0.3505(12)	0.7341(5)	0.2389(3)	0.018(2)	1.9594
O4	4a	0.2904(12)	0.5914(6)	0.2769(3)	0.020(2)	2.1286
O5	4a	0.1130(11)	0.8082(6)	0.3391(3)	0.017(2)	1.8511
O6	4a	0.361(1)	0.8332(5)	0.3870(3)	0.0141(18)	2.0654
O7	4a	0.1147(10)	0.8948(5)	0.4149(3)	0.0141(19)	2.0642
O8	4a	0.1589(11)	0.7350(5)	0.4165(3)	0.0139(19)	2.0762
O9	4a	0.1118(11)	0.5831(5)	0.3529(3)	0.0129(18)	1.9443
O10	4a	0.3964(11)	0.4953(5)	0.3577(3)	0.0121(19)	1.9313
O11	4a	0.1279(10)	0.3944(5)	0.3508(3)	0.0070(16)	1.9494

O12	4a	0.0065(11)	0.4880(5)	0.4256(3)	0.0075(17)	2.0174
O13	4a	0.0186(10)	0.6383(5)	0.4806(3)	0.0118(18)	1.9658
O14	4a	0.1284(11)	0.2394(5)	0.4104(3)	0.018(2)	2.0923
O15	4a	0.3663(11)	0.1537(6)	0.3959(3)	0.018(2)	2.1370
O16	4a	0.122(1)	0.0764(5)	0.4167(3)	0.0122(18)	2.0235
O17	4a	0.1453(13)	0.1519(6)	0.3371(3)	0.026(2)	1.8680
O18	4a	0.2906(10)	0.3945(5)	0.4322(3)	0.0093(18)	1.9938
O19	4a	0.5088(11)	0.4843(5)	0.4914(3)	0.0105(18)	1.8774
O20	4a	0.2912(10)	0.5780(5)	0.4358(3)	0.0099(17)	2.0081
O21	4a	0.5809(11)	0.5763(5)	0.5728(3)	0.0147(18)	2.1086
O22	4a	0.8297(11)	0.6448(6)	0.5526(3)	0.0163(19)	2.0655
O23	4a	0.7119(12)	0.6737(6)	0.6313(3)	0.023(2)	1.8851
O24	4a	0.5948(10)	0.7368(5)	0.5562(3)	0.0138(19)	2.0689
O25	4a	0.7727(10)	0.8921(5)	0.5361(3)	0.0098(17)	1.9763
O26	4a	0.5205(10)	0.8377(5)	0.4780(3)	0.0103(18)	1.9516
O27	4a	0.5667(10)	0.8950(5)	0.6098(3)	0.0066(16)	1.9983
O28	4a	0.8490(11)	0.9826(5)	0.6166(3)	0.0100(18)	1.9552
O29	4a	0.4665(12)	0.0011(5)	0.6878(3)	0.017(2)	2.0735
O30	4a	0.7734(13)	0.0648(6)	0.6938(3)	0.022(2)	2.2208
O31	4a	0.9566(12)	0.1829(7)	0.7176(3)	0.026(2)	1.9990
O32	4a	0.6689(12)	0.1969(6)	0.7323(4)	0.024(2)	2.0355
O33	4a	0.8401(11)	0.0884(5)	0.7774(3)	0.0136(18)	2.0510
O34	4a	0.5298(11)	0.0261(6)	0.7720(3)	0.0158(19)	2.1026
O35	4a	0.2575(12)	0.0444(6)	0.7403(3)	0.022(2)	1.9356
O36	4a	0.3770(14)	0.8928(6)	0.7477(4)	0.034(3)	1.9424
O37	4a	0.2512(13)	0.7954(6)	0.6278(3)	0.024(2)	1.8229
O38	4a	0.0835(11)	0.8952(5)	0.5750(3)	0.0128(18)	2.0774
O39	4a	0.3266(10)	0.8340(5)	0.5454(3)	0.0149(19)	2.0749
O40	4a	0.1026(11)	0.7371(5)	0.5566(3)	0.0151(18)	2.0995
O41	4a	0.0733(10)	0.5818(5)	0.6124(3)	0.0089(16)	1.9380
O42	4a	0.994(1)	0.4884(5)	0.5325(3)	0.0085(17)	2.0889
O43	4a	0.2726(9)	0.5776(5)	0.5383(3)	0.0075(16)	1.9674

Table S2. Anisotropic displacement parameters (Å^2) for the compound $Na_{11}Ta_8P_7O_{43}$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ta1	0.0088(3)	0.0085(2)	0.0047(2)	0.00079(19)	0.00067(18)	-0.00015(18)
Ta2	0.0058(3)	0.0046(2)	0.0062(2)	-0.00068(19)	0.00036(18)	0.00010(18)
Ta3	0.0045(3)	0.0060(2)	0.0072(3)	0.00013(18)	0.00072(19)	0.00001(17)
Ta4	0.0060(3)	0.0046(2)	0.0067(3)	-0.00057(19)	0.00135(19)	-0.00012(17)
Ta5	0.0055(3)	0.0046(2)	0.0072(3)	0.00075(19)	0.00120(19)	-0.00026(17)
Ta6	0.0073(2)	0.0079(2)	0.0053(2)	-0.00029(18)	0.00088(18)	0.00018(17)
Ta7	0.0046(3)	0.0065(2)	0.0067(3)	-0.00010(18)	0.0004(2)	0.00030(17)
Ta8	0.0060(3)	0.0048(2)	0.0072(3)	0.00100(19)	0.00123(19)	0.00026(18)
Na1	0.022(3)	0.040(4)	0.023(3)	0.005(3)	-0.001(3)	-0.011(3)
Na2	0.032(4)	0.031(3)	0.026(3)	-0.010(3)	-0.006(3)	-0.001(2)
Na3	0.096(7)	0.025(3)	0.040(4)	0.037(4)	-0.005(4)	-0.002(3)
Na4	0.010(3)	0.075(5)	0.030(4)	-0.001(3)	-0.007(3)	0.001(3)
Na5	0.038(4)	0.026(3)	0.028(4)	0.009(3)	-0.011(3)	-0.007(2)
Na6	0.023(3)	0.020(3)	0.021(3)	0.002(2)	0.000(3)	-0.006(2)
Na7	0.022(3)	0.039(3)	0.023(3)	-0.001(3)	0.000(3)	0.004(2)
Na8	0.026(3)	0.024(3)	0.026(3)	-0.003(2)	-0.001(3)	0.013(2)
Na9	0.059(5)	0.026(3)	0.040(4)	-0.025(3)	-0.009(4)	0.001(3)
Na10	0.041(4)	0.036(4)	0.023(4)	-0.006(3)	-0.003(3)	-0.006(3)
Na11	0.024(3)	0.028(3)	0.023(3)	0.001(2)	0.002(3)	0.003(2)
P1	0.0034(15)	0.0056(13)	0.0108(16)	0.0017(10)	0.0012(12)	0.0006(10)
P2	0.0098(17)	0.0088(14)	0.0069(15)	-0.0013(10)	-0.0004(13)	0.0009(10)
P3	0.0073(16)	0.0072(14)	0.0071(16)	0.0014(10)	-0.0004(12)	-0.0004(10)
P4	0.0044(15)	0.0043(13)	0.0119(16)	0.0012(10)	-0.0011(12)	-0.001(1)
P5	0.0086(17)	0.0112(14)	0.0084(16)	-0.0015(11)	-0.0008(13)	0.0017(10)
P6	0.0105(17)	0.0071(14)	0.0105(16)	0.0006(10)	0.0009(12)	-0.0006(10)
P7	0.0061(16)	0.0060(13)	0.0082(16)	-0.0004(10)	0.0002(12)	0.0005(10)
O1	0.015(5)	0.013(4)	0.014(5)	0.000(3)	-0.001(4)	0.002(3)
O2	0.006(5)	0.032(5)	0.021(5)	0.002(4)	0.001(4)	-0.003(4)
O3	0.023(6)	0.014(4)	0.018(5)	-0.006(4)	-0.003(4)	0.005(3)
O4	0.030(6)	0.018(5)	0.011(5)	-0.005(4)	0.005(4)	0.007(3)
O5	0.017(5)	0.024(5)	0.010(5)	0.001(4)	-0.008(4)	-0.002(3)
O6	0.003(4)	0.019(4)	0.021(5)	-0.002(3)	0.001(4)	-0.001(3)
O7	0.010(5)	0.007(4)	0.025(5)	0.005(3)	0.002(4)	-0.006(3)
O8	0.018(5)	0.005(4)	0.018(5)	-0.004(3)	0.005(4)	-0.002(3)
O9	0.019(5)	0.015(4)	0.005(4)	0.000(3)	0.002(4)	-0.001(3)
O10	0.013(5)	0.007(4)	0.017(5)	-0.002(3)	-0.002(4)	0.001(3)
O11	0.0069(19)	0.0072(19)	0.0069(19)	-0.0006(12)	0.0010(12)	-0.0004(12)
O12	0.012(5)	0.005(4)	0.005(4)	-0.003(3)	0.001(3)	-0.002(3)
O13	0.012(5)	0.012(4)	0.012(5)	0.007(3)	-0.001(4)	0.000(3)
O14	0.018(2)	0.017(2)	0.019(2)	0.0000(13)	0.0018(13)	-0.0004(13)
O15	0.007(5)	0.021(5)	0.026(6)	0.005(3)	0.004(4)	0.014(4)

O16	0.009(5)	0.014(4)	0.014(5)	-0.008(3)	-0.003(4)	0.004(3)
O17	0.038(7)	0.030(5)	0.010(5)	-0.006(4)	-0.009(5)	0.002(4)
O18	0.006(4)	0.005(4)	0.017(5)	-0.003(3)	-0.002(4)	0.000(3)
O19	0.009(5)	0.014(4)	0.008(5)	0.002(3)	0.002(4)	0.006(3)
O20	0.013(5)	0.007(4)	0.010(4)	0.000(3)	-0.002(4)	-0.004(3)
O21	0.014(2)	0.014(2)	0.016(2)	-0.0008(12)	0.0004(13)	0.0004(12)
O22	0.010(5)	0.022(5)	0.017(5)	0.002(3)	0.005(4)	-0.001(3)
O23	0.022(6)	0.034(6)	0.013(5)	0.009(4)	-0.006(4)	-0.005(4)
O24	0.009(5)	0.006(4)	0.026(5)	0.002(3)	-0.002(4)	0.004(3)
O25	0.003(4)	0.015(4)	0.012(5)	-0.004(3)	-0.001(3)	-0.004(3)
O26	0.013(5)	0.009(4)	0.009(4)	0.000(3)	0.001(4)	0.000(3)
O27	0.009(4)	0.009(4)	0.002(4)	0.001(3)	0.002(3)	-0.001(3)
O28	0.020(5)	0.004(4)	0.006(4)	-0.003(3)	0.001(4)	0.001(3)
O29	0.016(5)	0.022(5)	0.013(5)	0.001(3)	0.002(4)	0.004(3)
O30	0.039(7)	0.017(5)	0.010(5)	-0.003(4)	-0.004(4)	-0.005(3)
O31	0.018(6)	0.041(6)	0.019(6)	-0.016(4)	-0.001(4)	0.017(4)
O32	0.020(6)	0.018(5)	0.036(6)	0.009(4)	0.016(5)	0.001(4)
O33	0.010(5)	0.025(5)	0.006(4)	-0.006(3)	-0.001(4)	0.006(3)
O34	0.016(5)	0.023(5)	0.008(5)	-0.002(3)	-0.001(4)	0.001(3)
O35	0.015(5)	0.027(5)	0.022(6)	0.007(4)	0.001(4)	-0.003(4)
O36	0.041(8)	0.022(5)	0.038(7)	-0.012(5)	-0.009(6)	0.015(4)
O37	0.034(6)	0.021(5)	0.018(6)	0.007(4)	-0.006(5)	0.004(4)
O38	0.014(5)	0.009(4)	0.016(5)	0.004(3)	0.002(4)	-0.002(3)
O39	0.005(5)	0.020(5)	0.020(5)	0.001(3)	0.002(4)	-0.001(3)
O40	0.015(2)	0.014(2)	0.016(2)	-0.0013(12)	0.0008(13)	-0.0004(12)
O41	0.009(2)	0.0088(19)	0.008(2)	0.0000(12)	0.0003(13)	-0.0009(12)
O42	0.006(5)	0.010(4)	0.010(5)	0.002(3)	0.000(4)	0.003(3)
O43	0.006(4)	0.006(4)	0.010(4)	0.001(3)	0.001(3)	-0.001(3)

Table S3. Selected bond lengths (Å) for the compound $Na_{11}Ta_8P_7O_{43}$.

Ta1— O1³	2.022(8)	P5—O35	1.515(10)
Ta1— O27	1.930(8)	P5—O36	1.495(9)
Ta1— O28	1.909(10)	P6—O30	1.547(9)
Ta1— O29	2.043(10)	P6—O31	1.502(10)
Ta1— O30	1.979(9)	P6—O32	1.491(10)
Ta1— O41⁴	1.942(8)	P6—O33	1.561(9)
Ta2— O24	2.045(8)	P7—O21	1.542(9)
Ta2— O25	1.916(8)	P7—O22	1.531(10)
Ta2— O26	1.952(9)	P7—O23	1.487(10)
Ta2— O27	1.949(8)	P7—O24	1.549(8)
Ta2— O39	2.033(9)	Na1—O2²	2.388(12)
Ta2— O42⁴	1.915(7)	Na1—O4²	2.705(12)
Ta3— O19	1.942(9)	Na1—O10²	2.606(12)
Ta3— O21	1.988(9)	Na1—O17	2.321(11)
Ta3— O25²	1.965(8)	Na1—O33⁸	2.767(11)
Ta3— O28²	1.961(9)	Na1—O35¹⁰	2.399(12)
Ta3— O38⁵	1.996(8)	Na2—O3²	2.366(11)
Ta3— O43	1.958(7)	Na2—O11	2.421(10)
Ta4— O6²	2.021(8)	Na2—O17	2.409(12)
Ta4— O11	1.950(8)	Na2—O32⁷	2.324(12)
Ta4— O12	1.929(7)	Na3—O13⁵	2.404(9)
Ta4— O14	2.008(8)	Na3—O22²	2.859(12)
Ta4— O18	1.956(8)	Na3—O25²	2.474(11)
Ta4— O26²	1.955(9)	Na3—O18	2.465(10)
Ta5— O8	2.043(8)	Na3—O40⁵	2.734(11)
Ta5— O9	1.966(9)	Na4—O7⁵	2.651(11)
Ta5— O12	1.927(7)	Na4—O12¹¹	2.485(12)
Ta5— O13	1.927(9)	Na4—O16⁴	2.581(11)
Ta5— O15¹	2.027(9)	Na4—O19	2.393(13)
Ta5— O20	1.927(8)	Na4—O42¹¹	2.352(11)
Ta6— O4	2.007(9)	Na5—O3³	2.423(11)
Ta6— O9	1.915(9)	Na5—O23	2.321(12)
Ta6— O10	1.940(9)	Na5—O29⁵	2.534(10)
Ta6— O11	1.941(8)	Na5—O32⁵	2.507(13)
Ta6— O33⁷	2.044(8)	Na5—O41¹¹	2.620(11)
Ta6— O34⁷	2.001(9)	Na6—O2¹⁴	2.204(11)
Ta7— O7⁵	2.043(8)	Na6—O32²	2.203(11)
Ta7— O10	1.933(9)	Na6—O36	2.234(12)
Ta7— O16⁴	2.078(8)	Na6—O37	2.212(12)
Ta7— O18	1.917(8)	Na7—O2³	2.486(11)

Ta7— O19	2.004(9)	Na7—O21[4]	2.959(11)
Ta7— O20	1.942(8)	Na7—O23[4]	2.709(13)
Ta8— O13	1.978(9)	Na7—O28	2.546(11)
Ta8— O22[6]	2.051(9)	Na7—O30	2.577(13)
Ta8— O40	2.008(8)	Na7—O31	2.669(13)
Ta8— O41	1.922(8)	Na7—O35[11]	2.510(12)
Ta8— O42	1.928(7)	Na8—O1[15]	2.463(10)
Ta8— O43	1.918(8)	Na8—O23[4]	2.404(12)
P1— O14	1.541(9)	Na8—O27[4]	2.358(9)
P1— O15	1.539(10)	Na8—O31	2.252(11)
P1— O16	1.549(8)	Na8—O37[4]	2.499(12)
P1— O17	1.495(10)	Na9—O8	2.781(12)
P2— O1	1.557(9)	Na9—O20	2.446(10)
P2— O2	1.504(10)	Na9—O24	2.712(11)
P2— O3	1.511(9)	Na9—O26	2.431(10)
P2— O4	1.545(9)	Na9—O39	2.710(11)
P3— O5	1.485(9)	Na9—O43	2.559(10)
P3— O6	1.535(9)	Na10—O5	2.461(11)
P3— O7	1.546(8)	Na10—O9	2.502(11)
P3— O8	1.539(9)	Na10—O15[1]	2.587(12)
P4— O37	1.491(10)	Na10—O17[1]	2.676(14)
P4— O38	1.535(8)	Na10—O36[7]	2.259(12)
P4— O39	1.554(10)	Na11—O31[17]	2.229(11)
P4— O40	1.548(9)	Na11—O35[18]	2.231(11)
P5— O29	1.559(11)	Na11—O3	2.238(11)
P5— O34	1.549(9)	Na11—O5	2.223(11)

[1]-1/2+X,1/2+Y,+Z; [2]-1/2+X,-1/2+Y,+Z; [3]1/2+X,3/2-Y,1/2+Z; [4]1/2+X,1/2+Y,+Z; [5]1/2+X,-1/2+Y,+Z; [6]-1+X,+Y,+Z; [7]-1/2+X,3/2-Y,-1/2+Z; [8]-1+X,1-Y,-1/2+Z; [9]+X,-1+Y,+Z; [10]+X,1-Y,-1/2+Z; [11]1+X,+Y,+Z; [12]1+X,1-Y,1/2+Z; [13]+X,1-Y,1/2+Z; [14]-1/2+X,3/2-Y,1/2+Z; [15]1+X,2-Y,1/2+Z; [16]+X,1+Y,+Z; [17]-1+X,2-Y,-1/2+Z; [18]+X,2-Y,-1/2+Z; [19]1/2+X,3/2-Y,-1/2+Z; [20]+X,2-Y,1/2+Z.

Appendix. The original calculation results for $Na_{11}Ta_8P_7O_{43}$.

CRYSTAL CALCULATION
(INPUT ACCORDING TO THE INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY)
CRYSTAL FAMILY   :   MONOCLINIC
CRYSTAL CLASS   (GROTH - 1921)   :   MONOCLINIC DOMATIC

SPACE GROUP (NONCENTROSYMMETRIC)   :   C C

LATTICE PARAMETERS   (ANGSTROMS AND DEGREES) - CONVENTIONAL CELL

A	B	C	ALPHA	BETA	GAMMA
8.57100	15.11440	28.77120	90.00000	92.30400	90.00000

INSULATING STATE
 TOP OF VALENCE BANDS -   BAND   674; K   1; EIG -2.2357695E-01 AU
 BOTTOM OF VIRTUAL BANDS - BAND   675; K   13; EIG -1.9634350E-02 AU
 INDIRECT ENERGY BAND GAP: 5.5496 eV
 BOTTOM OF VIRTUAL BANDS - BAND   675; K   1; EIG -1.6754668E-02 AU
TOTAL ATOMIC CHARGES:

10.4330342	10.4330342	10.4902562	10.4902562	10.4897239	10.4897239
10.4740400	10.4740400	10.4698870	10.4698870	10.4709497	10.4709497
10.4458154	10.4458154	10.4798867	10.4798867	13.6158961	13.6158961
13.4565222	13.4565222	13.6601651	13.6601651	13.6670453	13.6670453
13.4843968	13.4843968	13.4426413	13.4426413	13.6428962	13.6428962
10.2262282	10.2262282	10.2180444	10.2180444	10.2622165	10.2622165
10.2905420	10.2905420	10.2304782	10.2304782	10.1849337	10.1849337
10.2299345	10.2299345	10.2230198	10.2230198	10.2730637	10.2730637
10.2253413	10.2253413	10.1832399	10.1832399	9.0180385	9.0180385
8.9881214	8.9881214	8.8180853	8.8180853	8.8245894	8.8245894
9.0311041	9.0311041	8.9809902	8.9809902	8.7931456	8.7931456
8.9977935	8.9977935	8.8401193	8.8401193	9.0217200	9.0217200
8.8159025	8.8159025	8.7864413	8.7864413	8.7764007	8.7764007
8.9964762	8.9964762	8.9834296	8.9834296	8.8064730	8.8064730
8.8080132	8.8080132	8.9911823	8.9911823	8.9732522	8.9732522
8.8524855	8.8524855	8.7545477	8.7545477	9.0107909	9.0107909
8.7349299	8.7349299	8.9842335	8.9842335	8.9952826	8.9952826
8.8953392	8.8953392	9.0057446	9.0057446	8.8121554	8.8121554
8.8885177	8.8885177	8.9008971	8.9008971	8.8497164	8.8497164
8.9574969	8.9574969	8.7753670	8.7753670	8.9490968	8.9490968
8.9448509	8.9448509	8.9596634	8.9596634	8.8092194	8.8092194
8.8884978	8.8884978	8.8147944	8.8147944	8.9535964	8.9535964
8.8748391	8.8748391	8.9455848	8.9455848	8.9208762	8.9208762

TENSOR IN PRINCIPAL AXES SYSTEM

AA   2.835543E+00 BB   2.846642E+00 CC   3.043057E+00

REFRACTIVE INDICES

AA   1.683907E+00 BB   1.687200E+00 CC   1.744436E+00

OPTICALLY ANISOTROPIC - BIAXIAL CRYSTAL

ACUTE ANGLE BETWEEN OPTIC AXES (DEGREES)

2V=   27.66862

BIAXIAL POSITIVE: 2V ANGLE BISECTED BY THE LARGEST REFRACTIVE INDEX (CC)

FIRST HYPERPOLARIZABILITY (BETA) AND SECOND ELECTRIC SUSCEPTIBILITY (CHI(2))
 TENSORS (INDEPENDENT COMPONENTS)

COMPONENT	BETA		CHI(2)	d(MKS)	d(cgs)
XXX	-1.2924E+03	(-1.2924E+03)	-6.4624E-01	-6.2837E-01	-1.4991E-02
XXY	-8.8801E-14	(-6.9421E-05)	-4.4402E-17	-4.3174E-17	-1.0300E-18
XXZ	-1.5157E+02	(-1.5157E+02)	-7.5788E-02	-7.3692E-02	-1.7581E-03
XYY	1.5956E+03	(1.5956E+03)	7.9780E-01	7.7574E-01	1.8507E-02
XYZ	-2.0234E-14	(-5.2047E-04)	-1.0118E-17	-9.8377E-18	-2.3470E-19
XZZ	-1.7183E+02	(-1.7183E+02)	-8.5918E-02	-8.3542E-02	-1.9930E-03
YYY	3.3086E-13	(-7.1099E-04)	1.6543E-16	1.6086E-16	3.8375E-18
YYZ	1.9743E+02	(1.9743E+02)	9.8718E-02	9.5988E-02	2.2900E-03
YZZ	-6.8558E-15	(-1.5352E-03)	-3.4280E-18	-3.3332E-18	-7.9519E-20
ZZZ	5.7506E+01	(5.7506E+01)	2.8754E-02	2.7959E-02	6.6700E-04