Supplementary Material (ESI) for Journal of Materials Chemistry

A New Family of Ferroelectric Materials: $Me_2Nb_4O_{11}$ (Me = Na and Ag)

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Electronic Supplementary Information

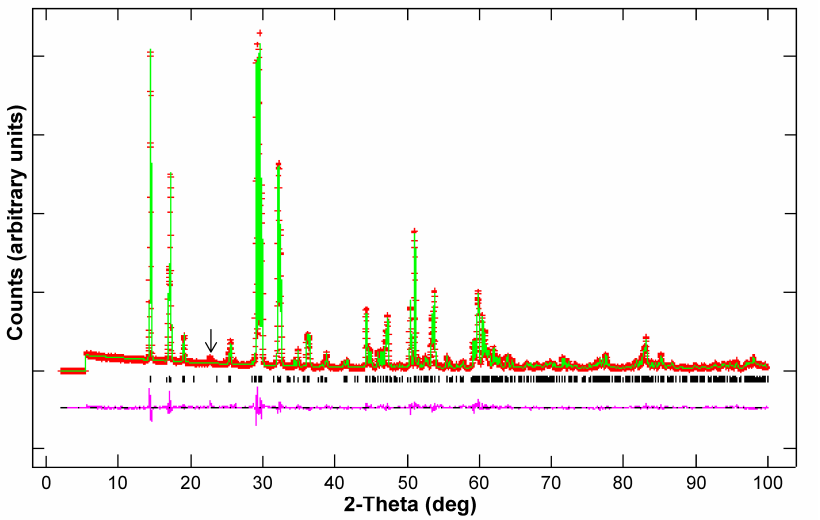

Figure 1-ESI. Experimental, calculated and difference XRD patterns for $Na_2Nb_4O_{11}$. The 2-theta range 0-5^o was excluded for refinement. Arrow shows secondary phase, $NaNb_3O_8$.

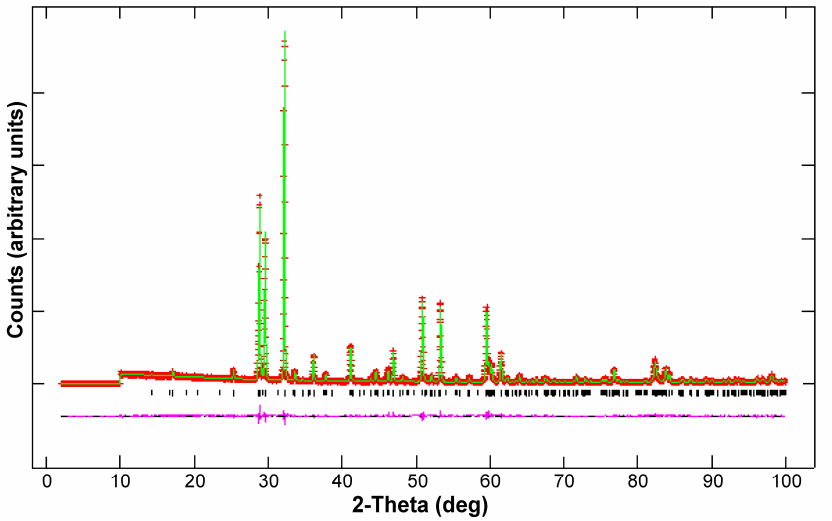

Figure 2-ESI. Experimental, calculated and difference XRD patterns for $Ag_2Nb_4O_{11}$. The 2-theta range 0-10^o was excluded for refinement.

Table I-ESI. Unit cell parameters, atomic positions and isotropic thermal parameters for $Na_2Nb_4O_{11}$. Space group C*c* (0,0,0; ½,½,0)+

Atom	Site	x	y	z	Site occupancy	100*U_{iso}
Nb(1)	4(a)	0.179(1)	0.5711(5)	0.247(1)	1	1.54(7)
Nb(2)	4(a)	0.8180(2)	0.5710(5)	0.2477(3)	1	1.34(7)
Nb(3)	4(a)	0.0022(4)	0.1181(4)	0.2548(3)	1	1.63(6)
Nb(4)	4(a)	0.2588(3)	0.261(1)	0.5015(4)	1	1.71(6)
Na(1)	4(a)	0.0911(4)	0.245(3)	1.0029(4)	1	1.19(2)
Na(2)	4(a)	0.9235(4)	0.253(3)	0.5082(4)	1	1.19(2)
O(1)	4(a)	0.2340(4)	0.537(3)	0.4043(4)	1	0.2(1)
O(2)	4(a)	0.7670(4)	0.495(3)	0.0929(4)	1	0.2(1)
O(3)	4(a)	0.1528(4)	0.591(3)	0.0829(4)	1	0.2(1)
O(4)	4(a)	0.8433(4)	0.601(3)	0.4049(5)	1	0.2(1)
O(5)	4(a)	0.0834(4)	0.147(3)	0.4159(4)	1	0.2(1)
O(6)	4(a)	0.9201(4)	0.131(3)	0.0965(4)	1	0.2(1)
O(7)	4(a)	0.1185(4)	0.858(3)	0.2511(5)	1	0.2(1)
O(8)	4(a)	0.8745(4)	0.887(3)	0.2493(4)	1	0.2(1)
O(9)	4(a)	0.1614(4)	0.245(3)	0.2134(4)	1	0.2(1)
O(10)	4(a)	0.8457(4)	0.256(3)	0.2819(4)	1	0.2(1)
O(11)	4(a)	0.0018(4)	0.496(2)	0.2461(5)	1	0.2(1)

a = 10.8427(1), b = 6.1664(6), c = 12.7524(1) Å and β = 106.176(1)°

χ^2 = 2.949, R_{wp} = 10.01%, R_p = 6.80%

Table II-ESI. Unit cell parameters, atomic positions and isotropic thermal parameters for $Ag_2Nb_4O_{11}$. Space group C*c* (0,0,0; ½,½,0)+

Atom	Site	x	y	z	Site occupancy	100*U_{iso}
Nb(1)	4(a)	0.181(1)	0.5660(7)	0.250(2)	1	0.86(7)
Nb(2)	4(a)	0.8179(2)	0.5720(8)	0.2496(4)	1	0.64(6)
Nb(3)	4(a)	0.001(4)	0.1182(4)	0.2543(5)	1	0.81(6)
Nb(4)	4(a)	0.2532(4)	0.259(1)	0.5034(6)	1	1.00(5)
Ag(1)	4(a)	0.0767(3)	0.2469(8)	0.9855(2)	1	1.44(5)
Ag(2)	4(a)	0.9205(3)	0.254(1)	0.5156(2)	1	2.81(6)
O(1)	4(a)	0.2284(4)	0.527(4)	0.4053(7)	1	0.09(9)
O(2)	4(a)	0.7695(4)	0.504(4)	0.0922(7)	1	0.09(9)
O(3)	4(a)	0.1580(4)	0.564(4)	0.0909(7)	1	0.09(9)
O(4)	4(a)	0.8412(4)	0.617(4)	0.4099(7)	1	0.09(9)
O(5)	4(a)	0.0838(4)	0.144(4)	0.4195(7)	1	0.09(9)
O(6)	4(a)	0.9213(4)	0.130(4)	0.1051(7)	1	0.09(9)
O(7)	4(a)	0.1259(4)	0.880(4)	0.2357(7)	1	0.09(9)
O(8)	4(a)	0.8764(4)	0.877(5)	0.2496(7)	1	0.09(9)
O(9)	4(a)	0.1599(4)	0.268(5)	0.2179(6)	1	0.09(9)
O(10)	4(a)	0.8366(4)	0.251(6)	0.2771(6)	1	0.09(9)
O(11)	4(a)	-0.0029(4)	0.496(3)	0.2382(7)	1	0.09(9)

a = 10.7642(1), b = 6.20097(5), c = 12.8582(1) Å and β = 106.183(2)°

χ^2 = 1.404, R_{wp} = 9.28%, R_p = 6.65%

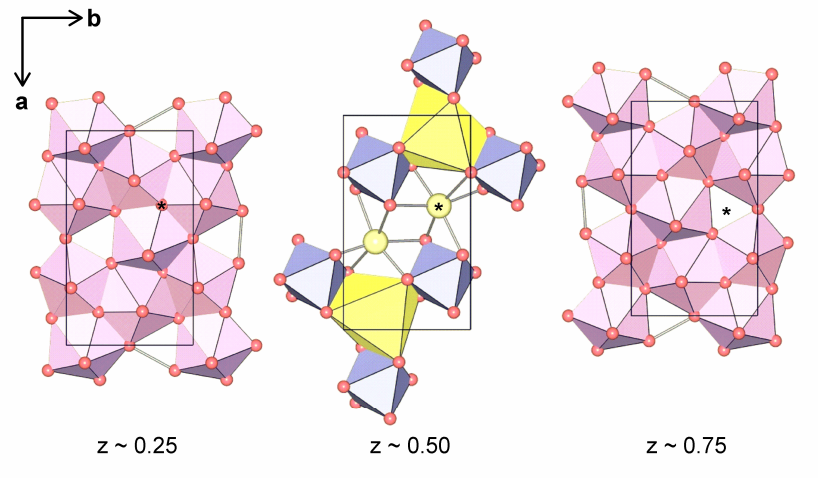

Figure 3-ESI. Crystal structure of the $Me_2Nb_4O_{11}$ family (Me = Na and Ag). The projections, perpendicular to the *ab* plane, show layers of pentagonal bipyramids alternating with layers of Me (yellow) and Nb (blue) octahedra. Asterisks show points in the same vertical.

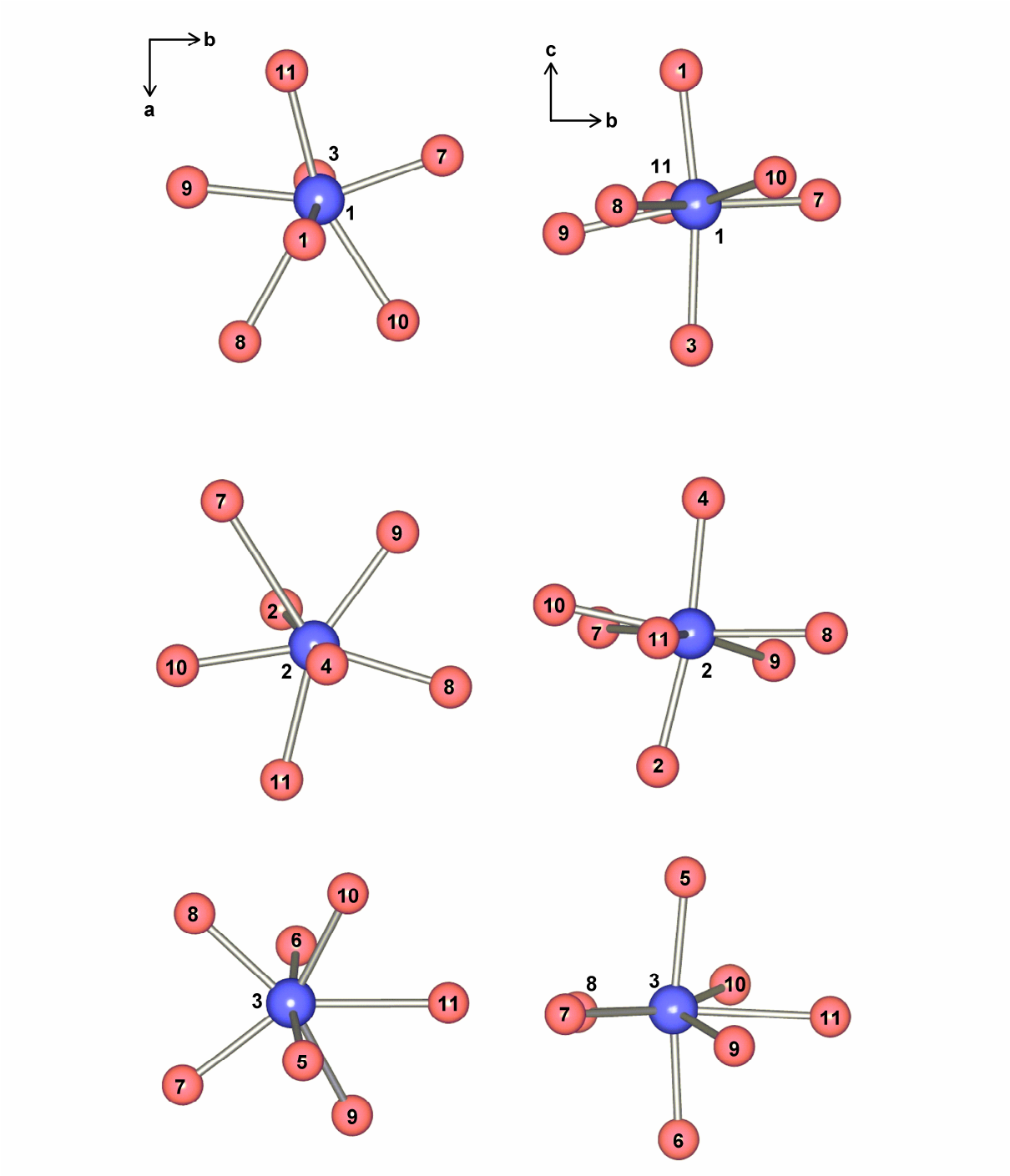

Figure 4-ESI. Projections of pentagonal bipyramids perpendicular to the *ab* and *bc* planes, left and right hand side; blue and red balls show niobium and oxygen atoms, respectively. Numbers refer to atom names in the space group *Cc* (0,0,0; ½,½,0)+.

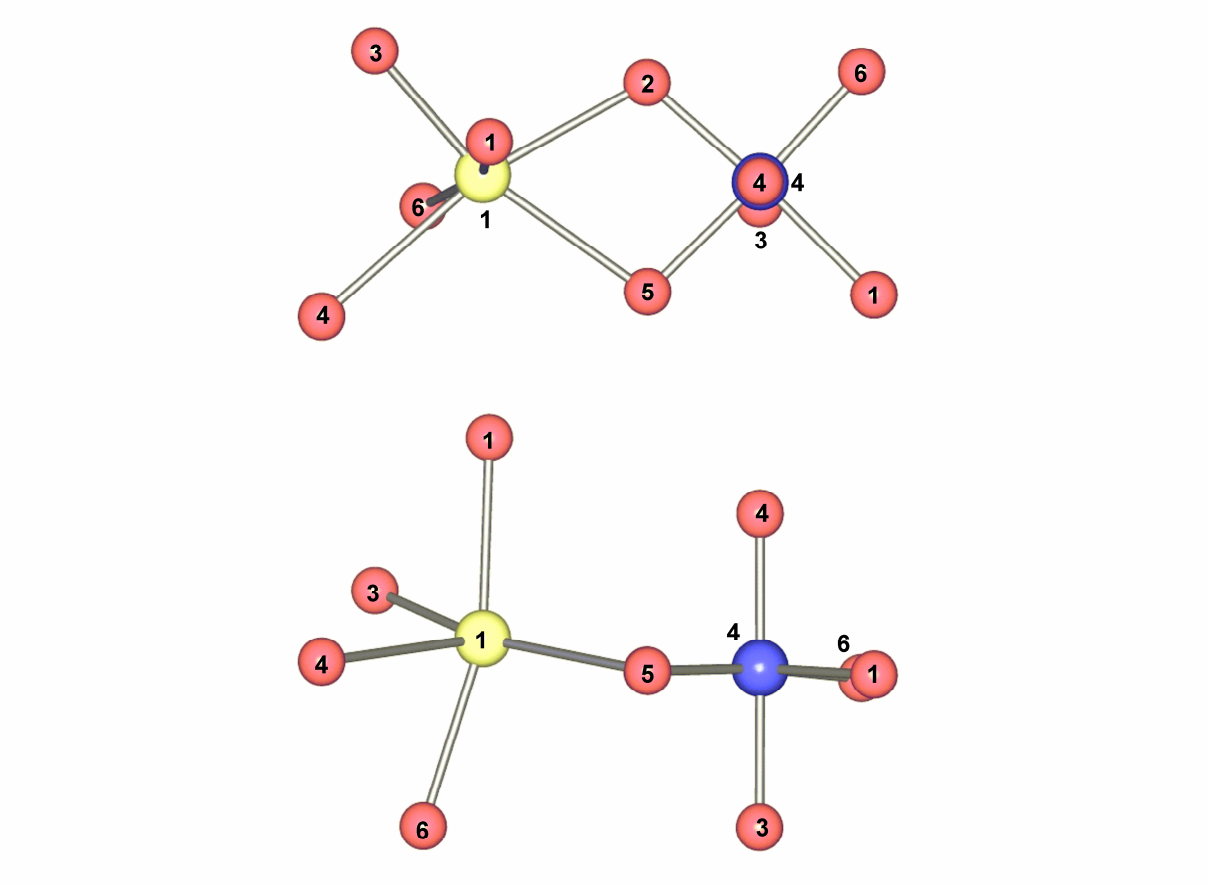

Figure 5-ESI. Projections of Me and Nb octahedra; yellow, blue and red balls show sodium/silver niobium and oxygen atoms, respectively. Numbers refer to atom names in the space group *Cc* (0,0,0; ½,½,0)+.