Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of the average structure of $K_8Nb_7P_7O_{39}$.

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Nb^1	0.77440 (4)	0.11937 (3)	0.070615 (19)	0.00819 (11)	
Nb^2	0.98212 (4)	0.73136 (3)	0.30766 (2)	0.00864 (12)	
Nb^3	0.88437 (4)	0.23012 (3)	0.30595 (2)	0.00898 (12)	
Nb^4	0.47911 (4)	1.10697 (3)	0.31043 (2)	0.00854 (12)	
Nb^5	1.38231 (4)	0.60709 (3)	0.30969 (2)	0.01040 (12)	
Nb^6	1.16398 (4)	0.19558 (3)	0.01483 (2)	0.00897 (12)	
Nb^7	1.29228 (4)	0.50993 (3)	0.07820 (2)	0.01189 (12)	
K^1	0.50693 (11)	0.32371 (8)	0.18916 (6)	0.0198 (3)	
K^2	0.24869 (15)	0.24917 (9)	0.49368 (6)	0.0306 (4)	
K^3	0.74701 (13)	0.91212 (11)	0.18076 (6)	0.0295 (4)	
K^4	0.97960 (15)	0.41130 (9)	0.17534 (7)	0.0298 (4)	
K^5	0.26232 (15)	0.82295 (9)	0.17160 (8)	0.0366 (4)	
P^1	0.62053 (12)	0.84906 (9)	0.33361 (7)	0.0132 (3)	
P^2	1.10802 (12)	0.00474 (9)	0.32137 (7)	0.0152 (3)	
P^3	0.59834 (11)	−0.04022 (8)	−0.10333 (6)	0.0083 (3)	
P^4	0.76412 (12)	0.50742 (9)	0.33212 (7)	0.0138 (3)	
P^5	1.07298 (13)	0.36514 (9)	−0.09748 (6)	0.0122 (3)	
P^6	1.25752 (12)	0.34431 (9)	0.32084 (7)	0.0123 (3)	
P^7	0.53895 (11)	0.31438 (8)	0.00688 (6)	0.0079 (3)	
O^1	1.3727 (3)	0.2491 (2)	0.29307 (18)	0.0160 (10)	
O^2	1.0906 (4)	0.5899 (3)	0.08726 (19)	0.0225 (11)	
O^3	0.4910 (3)	0.4305 (2)	0.05789 (16)	0.0117 (9)	
O^4	0.2596 (4)	1.0267 (3)	0.2919 (3)	0.0357 (15)	
O^5	0.8347 (3)	0.1780 (2)	0.17016 (17)	0.0132 (9)	
O^6	1.2814 (4)	0.3884 (3)	0.4053 (2)	0.0254 (12)	
O^7	0.6857 (3)	0.0705 (2)	−0.04996 (16)	0.0115 (9)	
O^8	0.9749 (3)	0.0717 (3)	0.28697 (18)	0.0175 (10)	
O^9	0.5608 (3)	0.0639 (3)	0.08201 (18)	0.0171 (10)	
O^{10}	0.7866 (3)	0.3791 (2)	0.29006 (17)	0.0145 (9)	
O^{11}	1.2889 (3)	0.4415 (2)	0.28266 (17)	0.0144 (9)	
O^{12}	1.0918 (4)	0.3426 (3)	−0.17959 (18)	0.0239 (11)	
O^{13}	0.6090 (3)	0.3413 (2)	−0.05798 (16)	0.0120 (9)	
O^{14}	1.1750 (3)	0.6595 (3)	0.2873 (2)	0.0199 (11)	
O^{15}	0.6744 (3)	0.1640 (2)	0.29107 (19)	0.0172 (10)	
O^{16}	0.9346 (4)	0.2730 (3)	0.40406 (19)	0.0240 (11)	
O^{17}	1.3588 (4)	0.5573 (3)	0.17793 (17)	0.0164 (9)	
O^{18}	1.0736 (3)	0.2463 (2)	−0.07838 (16)	0.0143 (9)	

O^{19}	0.5673 (3)	0.9460 (2)	0.29647 (18)	0.0160 (9)	
O^{20}	0.8818 (4)	0.5772 (3)	0.3039 (2)	0.0243 (12)	
O^{21}	0.9745 (3)	0.1785 (2)	0.04426 (17)	0.0138 (9)	
O^{22}	0.7919 (4)	0.5336 (3)	0.4167 (2)	0.0259 (11)	
O^{23}	0.5106 (4)	1.1501 (3)	0.40988 (19)	0.0298 (13)	
O^{24}	1.2025 (3)	0.3583 (2)	0.07441 (16)	0.0108 (8)	
O^{25}	0.8366 (3)	−0.0378 (2)	0.05439 (15)	0.0112 (8)	
O^{26}	0.7599 (3)	0.7960 (3)	0.29660 (19)	0.0191 (10)	
O^{27}	0.5949 (3)	0.5331 (3)	0.2975 (2)	0.0228 (11)	
O^{28}	0.5706 (4)	−0.0328 (3)	−0.18420 (17)	0.0175 (10)	
O^{29}	0.6695 (3)	0.2711 (2)	0.05942 (16)	0.0130 (9)	
O^{30}	0.3950 (3)	0.2286 (2)	−0.02315 (17)	0.0132 (9)	
O^{31}	1.4800 (4)	0.7565 (3)	0.3034 (2)	0.0316 (14)	
O^{32}	1.1990 (4)	0.4529 (2)	−0.04390 (17)	0.0158 (9)	
O^{33}	1.1331 (5)	0.0339 (3)	0.4053 (2)	0.0328 (13)	
O^{34}	1.3025 (3)	0.1473 (2)	0.09709 (16)	0.0122 (9)	
O^{35}	0.6560 (4)	0.8896 (3)	0.4181 (2)	0.0282 (12)	
O^{36}	1.4092 (5)	0.6416 (3)	0.4087 (2)	0.0318 (13)	
O^{37}	1.0871 (3)	0.2950 (3)	0.2837 (2)	0.0210 (11)	
O^{38}	1.0546 (3)	0.8737 (2)	0.28033 (18)	0.0167 (10)	
O^{39}	1.0291 (4)	0.7810 (3)	0.40641 (19)	0.0270 (12)	
K^{6}	0	0	0.5	0.0785 (16)	0.7312
K^{7}	0.1802 (4)	−0.0795 (3)	0.52932 (18)	0.0165 (10)	0.2688
K^{8}	0.6377 (2)	0.0977 (2)	0.53762 (11)	0.0530 (8)	0.7312
K^{9}	0.5	0.5	0.5	0.139 (3)	0.7609
K^{10}	0.6646 (9)	0.3950 (4)	0.4741 (3)	0.055 (2)	0.2391
K^{11}	0.8820 (2)	0.4220 (2)	0.53503 (11)	0.0553 (8)	0.7609
K^{12}	−0.3652 (3)	−0.3851 (3)	0.16563 (17)	0.0078 (9)	0.254

Table S2. Atomic displacement parameters (Å^2) of the average structure of $K_8Nb_7P_7O_{39}$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nb^{1}	0.00765 (17)	0.00901 (18)	0.00790 (18)	0.00142 (13)	0.00173 (13)	0.00216 (13)
Nb^{2}	0.00798 (18)	0.00667 (18)	0.01250 (19)	0.00100 (12)	0.00266 (13)	0.00420 (13)
Nb^{3}	0.00659 (18)	0.00753 (18)	0.01436 (19)	0.00076 (12)	0.00241 (13)	0.00529 (14)
Nb^{4}	0.00711 (18)	0.00701 (18)	0.01328 (19)	0.00120 (12)	0.00343 (13)	0.00481 (13)
Nb^{5}	0.00948 (18)	0.00679 (18)	0.0170 (2)	0.00147 (13)	0.00625 (14)	0.00452 (14)
Nb^{6}	0.00733 (17)	0.00936 (18)	0.01247 (19)	0.00178 (12)	0.00263 (13)	0.00621 (13)
Nb^{7}	0.0200 (2)	0.00792 (18)	0.01097 (19)	0.00612 (14)	0.00792 (14)	0.00465 (14)
K^{1}	0.0203 (5)	0.0198 (5)	0.0170 (4)	−0.0004 (4)	0.0033 (4)	0.0015 (4)
K^{2}	0.0537 (7)	0.0158 (5)	0.0223 (5)	0.0047 (4)	0.0030 (5)	0.0075 (4)
K^{3}	0.0312 (6)	0.0433 (6)	0.0193 (5)	0.0139 (5)	0.0103 (4)	0.0135 (5)
K^{4}	0.0431 (6)	0.0201 (5)	0.0339 (6)	0.0052 (4)	0.0183 (5)	0.0135 (4)
K^{5}	0.0392 (7)	0.0182 (5)	0.0516 (8)	−0.0063 (4)	0.0281 (6)	−0.0032 (5)

P^{1}	0.0097 (5)	0.0104 (5)	0.0247 (6)	0.0030 (4)	0.0062 (4)	0.0114 (4)
P^{2}	0.0086 (4)	0.0077 (5)	0.0315 (6)	0.0005 (3)	0.0015 (4)	0.0105 (4)
P^{3}	0.0082 (4)	0.0078 (4)	0.0092 (4)	0.0005 (3)	0.0006 (3)	0.0035 (3)
P^{4}	0.0098 (5)	0.0065 (4)	0.0254 (6)	0.0010 (3)	0.0047 (4)	0.0041 (4)
P^{5}	0.0194 (5)	0.0097 (5)	0.0080 (5)	0.0066 (4)	0.0025 (4)	0.0030 (4)
P^{6}	0.0097 (4)	0.0086 (4)	0.0234 (6)	0.0021 (3)	0.0072 (4)	0.0097 (4)
P^{7}	0.0079 (4)	0.0061 (4)	0.0114 (5)	0.0013 (3)	0.0038 (3)	0.0039 (3)
O^{1}	0.0112 (13)	0.0126 (14)	0.0288 (17)	0.0037 (11)	0.0067 (12)	0.0110 (12)
O^{2}	0.0186 (15)	0.0159 (15)	0.0307 (18)	0.0088 (12)	0.0046 (13)	0.0028 (13)
O^{3}	0.0100 (13)	0.0076 (12)	0.0184 (14)	0.0022 (10)	0.0075 (11)	0.0020 (11)
O^{4}	0.0123 (15)	0.0245 (18)	0.078 (3)	0.0020 (13)	0.0184 (17)	0.0208 (19)
O^{5}	0.0129 (13)	0.0150 (14)	0.0119 (13)	0.0020 (11)	0.0012 (11)	0.0046 (11)
O^{6}	0.0339 (19)	0.0209 (16)	0.0258 (18)	0.0047 (14)	0.0160 (15)	0.0077 (14)
O^{7}	0.0154 (13)	0.0090 (13)	0.0109 (13)	−0.0006 (10)	0.0003 (11)	0.0056 (10)
O^{8}	0.0163 (14)	0.0136 (14)	0.0256 (16)	0.0077 (11)	0.0046 (12)	0.0099 (12)
O^{9}	0.0095 (13)	0.0170 (14)	0.0241 (16)	0.0002 (11)	0.0046 (12)	0.0039 (12)
O^{10}	0.0120 (13)	0.0116 (13)	0.0208 (15)	0.0021 (10)	0.0041 (11)	0.0055 (11)
O^{11}	0.0176 (14)	0.0053 (12)	0.0247 (16)	0.0014 (10)	0.0079 (12)	0.0088 (11)
O^{12}	0.047 (2)	0.0151 (15)	0.0100 (14)	0.0041 (14)	0.0051 (14)	0.0043 (12)
O^{13}	0.0132 (13)	0.0081 (12)	0.0178 (14)	−0.0002 (10)	0.0061 (11)	0.0067 (11)
O^{14}	0.0097 (14)	0.0161 (15)	0.0388 (19)	0.0065 (11)	0.0119 (13)	0.0113 (13)
O^{15}	0.0064 (13)	0.0144 (14)	0.0332 (17)	−0.0012 (10)	0.0071 (12)	0.0088 (13)
O^{16}	0.0280 (18)	0.0253 (17)	0.0154 (16)	−0.0006 (14)	−0.0009 (13)	0.0033 (13)
O^{17}	0.0221 (15)	0.0148 (14)	0.0130 (14)	0.0012 (12)	0.0074 (12)	0.0024 (11)
O^{18}	0.0180 (14)	0.0109 (13)	0.0145 (14)	0.0033 (11)	−0.0029 (11)	0.0076 (11)
O^{19}	0.0176 (14)	0.0104 (13)	0.0210 (15)	0.0065 (11)	0.0036 (12)	0.0059 (12)
O^{20}	0.0165 (15)	0.0123 (14)	0.048 (2)	−0.0005 (12)	0.0111 (15)	0.0112 (14)
O^{21}	0.0072 (13)	0.0168 (14)	0.0177 (14)	−0.0028 (10)	0.0069 (11)	0.0026 (11)
O^{22}	0.0287 (18)	0.0178 (16)	0.0260 (18)	−0.0019 (13)	0.0050 (14)	−0.0020 (13)
O^{23}	0.041 (2)	0.038 (2)	0.0142 (16)	0.0175 (17)	0.0088 (15)	0.0111 (15)
O^{24}	0.0155 (13)	0.0070 (12)	0.0128 (13)	0.0019 (10)	0.0083 (11)	0.0039 (10)
O^{25}	0.0146 (13)	0.0089 (12)	0.0114 (13)	0.0008 (10)	0.0031 (11)	0.0045 (10)
O^{26}	0.0086 (13)	0.0207 (15)	0.0314 (18)	0.0058 (11)	0.0084 (12)	0.0099 (13)
O^{27}	0.0083 (13)	0.0161 (15)	0.042 (2)	0.0066 (11)	0.0057 (13)	0.0047 (14)
O^{28}	0.0239 (16)	0.0167 (15)	0.0108 (14)	0.0004 (12)	−0.0014 (12)	0.0050 (12)
O^{29}	0.0146 (13)	0.0117 (13)	0.0135 (14)	0.0015 (11)	0.0013 (11)	0.0053 (11)
O^{30}	0.0105 (13)	0.0087 (13)	0.0195 (15)	0.0003 (10)	0.0054 (11)	0.0011 (11)
O^{31}	0.0183 (16)	0.0097 (15)	0.073 (3)	−0.0009 (12)	0.0160 (17)	0.0170 (17)
O^{32}	0.0236 (15)	0.0109 (13)	0.0135 (14)	−0.0037 (11)	0.0029 (12)	0.0049 (11)
O^{33}	0.048 (2)	0.0163 (16)	0.0272 (19)	−0.0041 (15)	−0.0149 (16)	0.0083 (14)
O^{34}	0.0115 (13)	0.0111 (13)	0.0141 (14)	0.0029 (10)	−0.0001 (11)	0.0052 (11)
O^{35}	0.0324 (19)	0.0343 (19)	0.0276 (19)	0.0111 (15)	0.0099 (15)	0.0218 (16)
O^{36}	0.044 (2)	0.0278 (19)	0.0182 (17)	0.0075 (16)	0.0031 (16)	−0.0009 (14)

O^{37}	0.0106 (14)	0.0212 (16)	0.0371 (19)	−0.0008 (12)	0.0080 (13)	0.0156 (14)
O^{38}	0.0165 (14)	0.0095 (13)	0.0265 (17)	−0.0033 (11)	0.0063 (12)	0.0075 (12)
O^{39}	0.035 (2)	0.0275 (18)	0.0147 (16)	0.0089 (15)	−0.0033 (14)	0.0045 (14)
K^{6}	0.123 (3)	0.0406 (15)	0.082 (2)	−0.0152 (17)	0.088 (2)	−0.0064 (16)
K^{7}	0.0188 (16)	0.0136 (15)	0.0122 (14)	−0.0111 (12)	−0.0086 (12)	0.0027 (12)
K^{8}	0.0503 (11)	0.0786 (15)	0.0301 (9)	0.0418 (11)	0.0074 (8)	0.0143 (9)
K^{9}	0.126 (4)	0.128 (4)	0.151 (4)	−0.099 (3)	−0.118 (3)	0.109 (4)
K^{10}	0.121 (6)	0.019 (2)	0.034 (3)	−0.024 (3)	0.050 (3)	0.000 (2)
K^{11}	0.0597 (12)	0.0755 (14)	0.0351 (10)	0.0403 (11)	0.0177 (9)	0.0162 (9)
K^{12}	0.0002 (12)	0.0124 (14)	0.0062 (13)	−0.0073 (10)	0.0006 (10)	−0.0047 (11)

Table S3. Geometric parameters (Å) of the average structure of $K_8Nb_7P_7O_{39}$.

Nb^{1}—O^{5}	1.767 (3)	P^{6}—O^{37}	1.544 (3)
Nb^{1}—O^{7}	2.144 (3)	P^{7}—O^{3}	1.555 (3)
Nb^{1}—O^{9}	2.005 (3)	P^{7}—O^{13}	1.542 (3)
Nb^{1}—O^{21}	2.031 (3)	P^{7}—O^{29}	1.549 (3)
Nb^{1}—O^{25}	1.917 (3)	P^{7}—O^{30}	1.519 (3)
Nb^{1}—O^{29}	2.076 (3)	K^{1}—O^{1ix}	2.737 (4)
Nb^{2}—O^{12ii}	2.267 (3)	K^{1}—O^{3}	3.028 (3)
Nb^{2}—O^{14}	1.914 (3)	K^{1}—O^{5}	3.340 (3)
Nb^{2}—O^{20}	2.002 (3)	K^{1}—O^{9}	3.276 (3)
Nb^{2}—O^{26}	2.056 (3)	K^{1}—O^{10}	2.727 (3)
Nb^{2}—O^{38}	2.028 (3)	K^{1}—O^{11ix}	2.873 (3)
Nb^{2}—O^{39}	1.728 (3)	K^{1}—O^{15}	3.224 (3)
Nb^{3}—O^{5}	2.374 (3)	K^{1}—O^{17ix}	3.118 (3)
Nb^{3}—O^{8}	2.010 (3)	K^{1}—O^{24ix}	3.180 (3)
Nb^{3}—O^{10}	2.044 (3)	K^{1}—O^{27}	2.742 (3)
Nb^{3}—O^{15}	1.900 (3)	K^{1}—O^{29}	2.898 (3)
Nb^{3}—O^{16}	1.720 (3)	K^{1}—O^{34ix}	2.710 (2)
Nb^{3}—O^{37}	2.047 (3)	K^{2}—O^{6ix}	2.684 (4)
Nb^{4}—O^{1iii}	2.010 (3)	K^{2}—O^{16ix}	2.975 (3)
Nb^{4}—O^{4}	2.040 (3)	K^{2}—O^{22x}	2.726 (3)
Nb^{4}—O^{15i}	1.932 (3)	K^{2}—O^{23xi}	3.017 (4)
Nb^{4}—O^{19}	2.035 (3)	K^{2}—O^{33ix}	2.704 (3)
Nb^{4}—O^{23}	1.733 (3)	K^{2}—O^{35x}	2.680 (4)
Nb^{4}—O^{28iv}	2.223 (3)	K^{2}—O^{36xii}	3.224 (4)
Nb^{5}—O^{11}	2.028 (3)	K^{2}—O^{39x}	3.335 (4)
Nb^{5}—O^{14}	1.909 (3)	K^{3}—O^{5i}	3.326 (3)
Nb^{5}—O^{17}	2.314 (3)	K^{3}—O^{8i}	2.803 (3)
Nb^{5}—O^{27v}	2.057 (3)	K^{3}—O^{9i}	3.177 (3)
Nb^{5}—O^{31}	2.014 (3)	K^{3}—O^{12ii}	3.344 (3)
Nb^{5}—O^{36}	1.729 (3)	K^{3}—O^{15i}	3.274 (3)
Nb^{6}—O^{18}	2.018 (3)	K^{3}—O^{18ii}	2.932 (3)

Nb^{6}—O^{21}	1.829 (3)	K^{3}—O^{19}	2.786 (3)
Nb^{6}—O^{24}	1.944 (2)	K^{3}—O^{25i}	2.796 (3)
Nb^{6}—O^{25vi}	1.960 (2)	K^{3}—O^{26}	2.853 (4)
Nb^{6}—O^{30v}	2.281 (3)	K^{3}—O^{28iv}	3.099 (3)
Nb^{6}—O^{34}	1.990 (3)	K^{3}—O^{30iv}	2.975 (3)
Nb^{7}—O^{2}	1.991 (3)	K^{3}—O^{38}	3.064 (3)
Nb^{7}—O^{3v}	1.995 (3)	K^{4}—O^{2}	3.248 (4)
Nb^{7}—O^{13ii}	2.111 (3)	K^{4}—O^{5}	3.018 (3)
Nb^{7}—O^{17}	1.769 (3)	K^{4}—O^{10}	3.007 (3)
Nb^{7}—O^{24}	1.943 (3)	K^{4}—O^{11}	2.983 (3)
Nb^{7}—O^{32}	2.176 (3)	K^{4}—O^{12ii}	2.996 (3)
P^{1}—O^{19}	1.547 (3)	K^{4}—O^{14}	3.342 (3)
P^{1}—O^{26}	1.536 (3)	K^{4}—O^{20}	2.893 (3)
P^{1}—O^{31ix}	1.537 (3)	K^{4}—O^{21}	3.137 (3)
P^{1}—O^{35}	1.479 (3)	K^{4}—O^{24}	2.853 (3)
P^{2}—O^{4xiii}	1.537 (4)	K^{4}—O^{29}	3.228 (3)
P^{2}—O^{8}	1.556 (3)	K^{4}—O^{37}	2.782 (4)
P^{2}—O^{33}	1.480 (4)	K^{5}—O^{2ix}	3.014 (3)
P^{2}—O^{38xi}	1.561 (3)	K^{5}—O^{4}	2.805 (4)
P^{3}—O^{7}	1.518 (2)	K^{5}—O^{7iv}	2.972 (3)
P^{3}—O^{9viii}	1.531 (3)	K^{5}—O^{13iv}	2.838 (3)
P^{3}—O^{28}	1.505 (3)	K^{5}—O^{17ix}	3.320 (3)
P^{3}—O^{34vi}	1.560 (3)	K^{5}—O^{18iv}	3.077 (3)
P^{4}—O^{10}	1.551 (3)	K^{5}—O^{19}	3.210 (3)
P^{4}—O^{20}	1.554 (4)	K^{5}—O^{28iv}	2.808 (3)
P^{4}—O^{22}	1.481 (4)	K^{5}—O^{31ix}	3.101 (4)
P^{4}—O^{27}	1.549 (3)	K^{5}—O^{38ix}	2.860 (3)
P^{5}—O^{2ii}	1.530 (3)	*K^{6}—K^{7}*	*1.900 (3)*
P^{5}—O^{12}	1.506 (3)	*K^{6}—K^{7xi}*	*1.900 (3)*
P^{5}—O^{18}	1.557 (3)	*K^{7}—K^{8xii}*	*2.131 (4)*
P^{5}—O^{32}	1.517 (3)	*K^{9}—K^{10}*	*1.929 (7)*
P^{6}—O^{1}	1.561 (3)	*K^{9}—K^{10xiii}*	*1.929 (7)*
P^{6}—O^{6}	1.479 (3)	*K^{10}—K^{11}*	*1.979 (7)*
P^{6}—O^{11}	1.560 (3)		
Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) *x*−1, *y*+1, *z*; (iii) *x*, *y*+1, *z*; (iv) −*x*+1, −*y*+1, −*z*; (v) *x*+1, *y*, *z*; (vi) −*x*+2, −*y*, −*z*; (vii) *x*−1, *y*, *z*; (viii) *x*+1, *y*−1, *z*; (ix) *x*, *y*−1, *z*; (x) −*x*+1, −*y*, −*z*; (xi) −*x*, −*y*, −*z*+1; (xii) −*x*+1, −*y*, −*z*+1; (xiii) −*x*+1, −*y*+1, −*z*+1; (xiv) −*x*+2, −*y*+1, −*z*+1.			

Table S4. Interatomic Distances (Å) of K—O bonds(including K^{6}, K^{7}, K^{8}, K^{9}, K^{10}, K^{11} and K^{12} atoms) influenced by Strong Modulation in compound $K_8Nb_7P_7O_{39}$.

distance	average	minimum	maximum
K^{6}-O^{33}(i)	2.437(5)	2.552(6)	2.557(7)

K^{6}-O^{33}(v)	2.437(5)	2.250(6)	2.552(6)
K^{6}-O^{35}(vi)	3.093(5)	2.916(5)	3.511(5)
K^{6}-O^{35}(ii)	3.096(5)	2.916(5)	3.509(5)
K^{6}-O^{39}(vi)	2.747(4)	2.715(5)	2.794(5)
K^{6}-O^{39}(ii)	2.746(4)	2.715(5)	2.793(5)
K^{7}-O^{16}(v)	3.118(9)	3.041(10)	3.157(10)
K^{7}-O^{23}(ii)	2.927(8)	2.807(9)	3.010(9)
K^{7}-O^{33}(i)	2.846(9)	2.788(10)	2.935(10)
K^{7}-O^{33}(v)	2.917(8)	2.886(10)	2.993(10)
K^{7}-O^{35}(ii)	2.640(7)	2.591(8)	2.656(8)
K^{7}-O^{39}(vi)	2.605(6)	2.536(8)	2.641(8)
K^{8}-O^{23}(iii)	2.686(5)	2.675(6)	2.721(6)
K^{8}-O^{31}(iv)	3.361(5)	3.152(5)	3.506(5)
K^{8}-O^{33}(vii)	2.777(5)	2.736(5)	2.878(5)
K^{8}-O^{35}(iii)	2.801(4)	2.706(5)	3.059(5)
K^{8}-O^{35}(ii)	2.744(5)	2.662(6)	2.978(6)
K^{8}-O^{36}(iv)	3.036(5)	2.904(5)	3.230(5)
K^{8}-O^{39}(iv)	3.033(5)	2.922(5)	3.369(5)
K^{9}-O^{6}(i)	2.489(4)	2.367(5)	2.564(5)
K^{9}-O^{6}(iv)	2.489(4)	2.368(5)	2.564(5)
K^{9}-O^{22}	3.206(6)	2.953(7)	3.599(7)
K^{9}-O^{22}(ii)	3.202(6)	2.952(7)	3.596(7)
K^{9}-O^{36}(i)	2.734(6)	2.678(7)	2.826(7)
K^{9}-O^{36}(iv)	2.734(6)	2.678(7)	2.823(7)
K^{10}-O^{6}(i)	3.425(18)	2.521(19)	4.609(19)
K^{10}-O^{6}(iv)	2.751(12)	2.693(13)	2.842(13)
K^{10}-O^{16}	2.993(17)	2.646(19)	3.571(19)
K^{10}-O^{22}	2.683(17)	2.607(19)	2.837(19)
K^{10}-O^{23}(iii)	3.128(14)	2.910(15)	3.616(15)

K^{10}-O^{36}(iv)	2.663(18)	2.631(19)	2.771(19)
K^{11}-O^{6}(iv)	2.734(5)	2.671(6)	2.797(6)
K^{11}-O^{16}	2.707(5)	2.671(5)	2.738(5)
K^{11}-O^{20}(iv)	3.335(5)	3.224(6)	3.438(6)
K^{11}-O^{22}	2.798(6)	2.731(6)	2.988(6)
K^{11}-O^{22}(iv)	2.720(5)	2.657(6)	2.916(6)
K^{11}-O^{36}(iv)	3.027(6)	2.877(7)	3.447(7)
K^{11}-O^{39}(iv)	3.007(6)	2.915(6)	3.202(6)
K^{12}-O^{3}(vi)	2.658(6)	2.616(7)	2.677(7)
K^{12}-O^{12}(viii)	2.498(7)	2.432(8)	2.533(8)
K^{12}-O^{13}(ix)	2.807(7)	2.745(8)	2.872(8)
K^{12}-O^{17}(x)	2.606(7)	2.554(8)	2.628(8)
K^{12}-O^{20}(vi)	3.079(7)	3.059(8)	3.130(8)
K^{12}-O^{26}(vi)	2.721(6)	2.690(7)	2.789(7)
K^{12}-O^{27}(vi)	2.825(8)	2.801(9)	2.891(9)
K^{12}-O^{31}(x)	3.020(7)	2.982(8)	3.103(8)
K^{12}-O^{32}(viii)	2.797(7)	2.716(8)	2.871(8)
Symmetry codes: (i) x-1,y,z; (ii) -x+1,-y+1,-z+1; (iii) x,y-1,z; (iv) -x+2,-y+1,-z+1; (v) -x+1,-y,-z+1; (vi) x-1,y-1,z; (vii) -x+2,-y,-z+1; (viii) -x+1,-y,-z; (ix) -x,-y,-z; (x) x-2,y-1,z. x, y			

Table S5. Bond valence sums (BVS) influenced by structural modulation in compound $K_8Nb_7P_7O_{39}$.

Atoms	Average	Minimum	Maximum
Nb^{1}	5.1218(4)	5.075(7)	5.163(7)
Nb^{2}	5.1965(7)	5.081(7)	5.269(7)
Nb^{3}	5.1406(7)	5.119(7)	5.161(7)
Nb^{4}	5.1156(7)	5.090(7)	5.142(7)
Nb^{5}	5.0977(7)	5.033(7)	5.152(7)
Nb^{6}	4.9558(4)	4.905(7)	5.012(7)

Nb^{7}	5.0595(4)	5.032(7)	5.101(7)
K^{1}	1.37368(2)	1.325(7)	1.423(7)
K^{2}	1.10501(3)	1.076(7)	1.130(7)
K^{3}	1.139674(1)	1.083(7)	1.191(7)
K^{4}	1.024644(1)	0.983(7)	1.071(7)
K^{5}	1.040286(1)	1.007(7)	1.081(7)
K^{6}	1.38105(11)	1.163(7)	1.807(7)
K^{7}	0.96013(7)	0.910(7)	1.031(7)
K^{8}	0.99011(3)	0.848(7)	1.090(7)
K^{9}	1.23032(6)	1.124(7)	1.422(7)
K^{10}	0.9688(3)	0.884(7)	1.106(7)
K^{11}	1.00621(3)	0.858(7)	1.079(7)
K^{12}	1.68253(13)	1.650(7)	1.762(7)
P^{1}	5.0870(7)	5.015(7)	5.176(7)
P^{2}	4.9886(9)	4.927(7)	5.043(7)
P^{3}	5.1019(7)	5.046(7)	5.166(7)
P^{4}	5.0418(9)	4.990(7)	5.092(7)
P^{5}	5.0870(7)	5.015(7)	5.176(7)
P^{6}	5.0079(9)	4.988(7)	5.027(7)
P^{7}	4.9077(6)	4.877(7)	4.934(7)

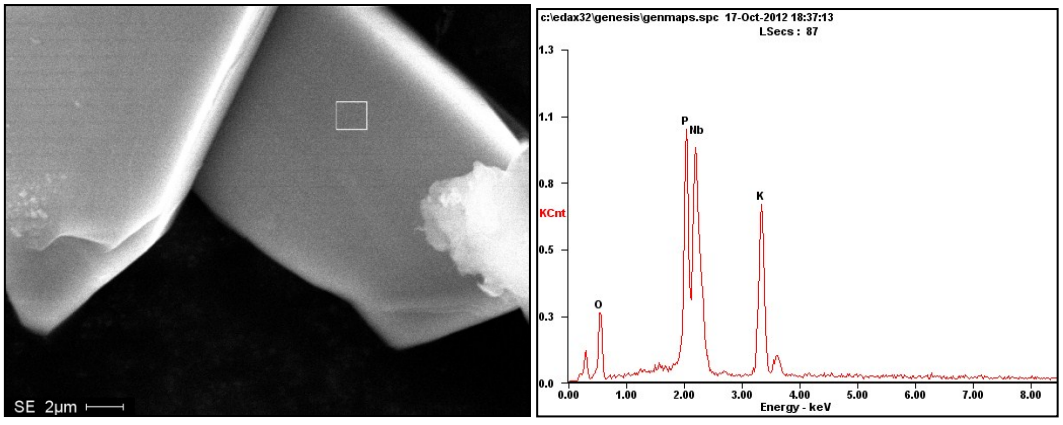

Figure S1. EDS analysis for compound $K_8Nb_7P_7O_{39}$.

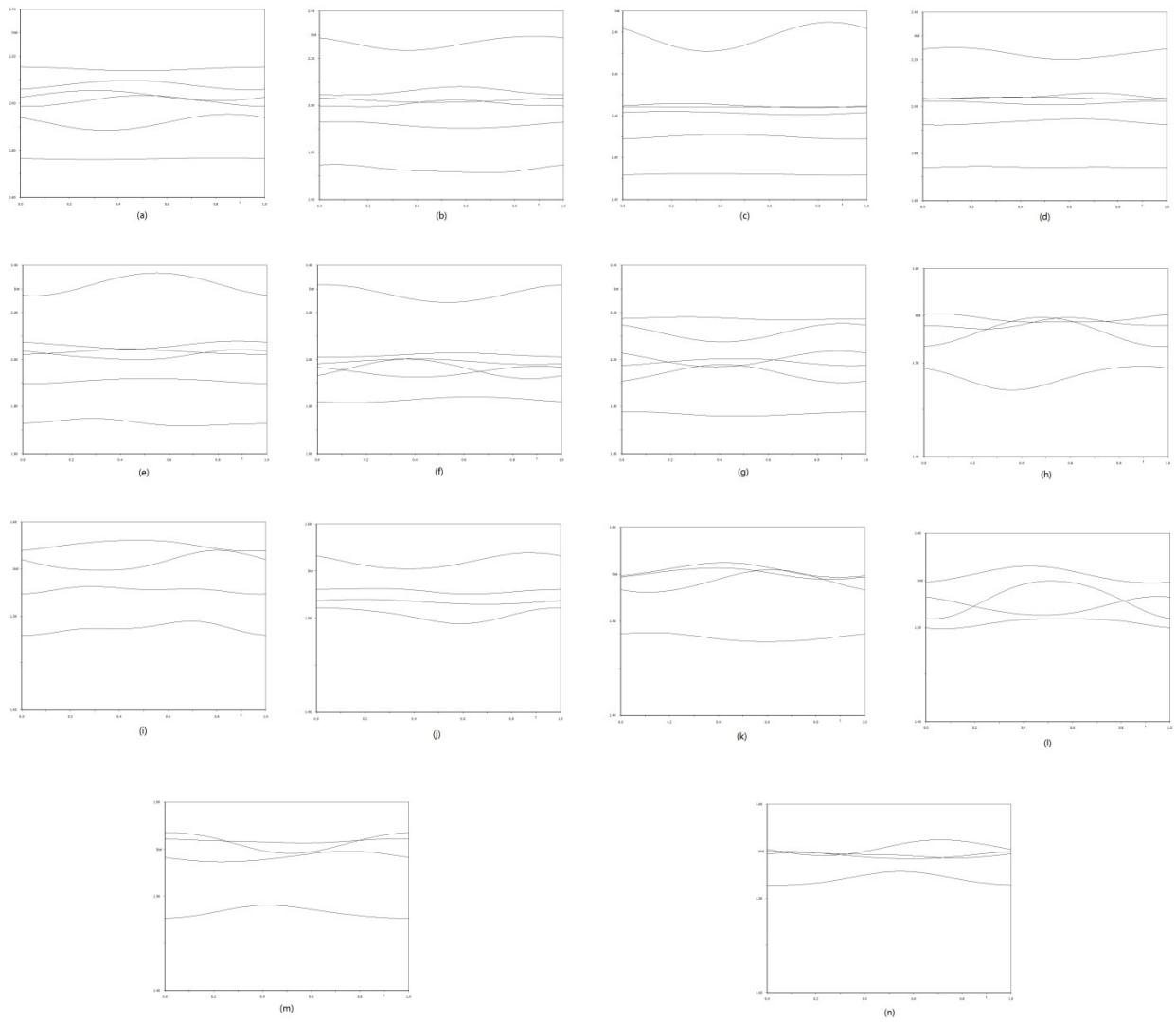

Figure S2. Evolution of Nb−O distances and P−O distances versus the internal parameter t for (a) Nb^1, (b) Nb^2, (c) Nb^3, (d) Nb^4, (e) Nb^5, (f) Nb^6, (g) Nb^7, (h) P^1, (i) P^2, (j) P^3, (k) P^4, (l) P^5, (m) P^6 and (n) P^7 atomic positions.

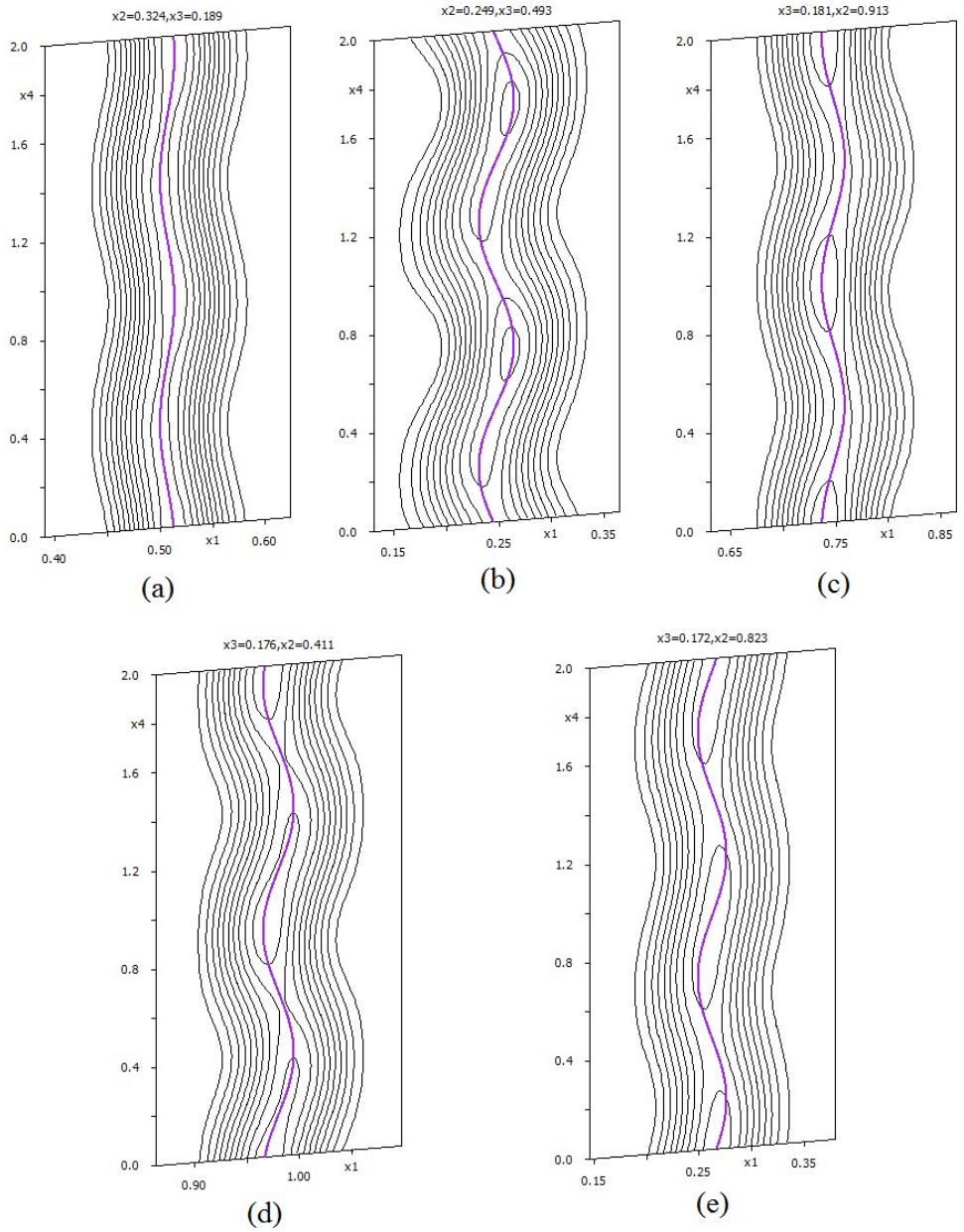

Figure S3. x_1–x_4 section through the superspace electron density at the position of the K^1(a), K^2(b), K^3(c), K^4(d) and K^5(e) atoms.

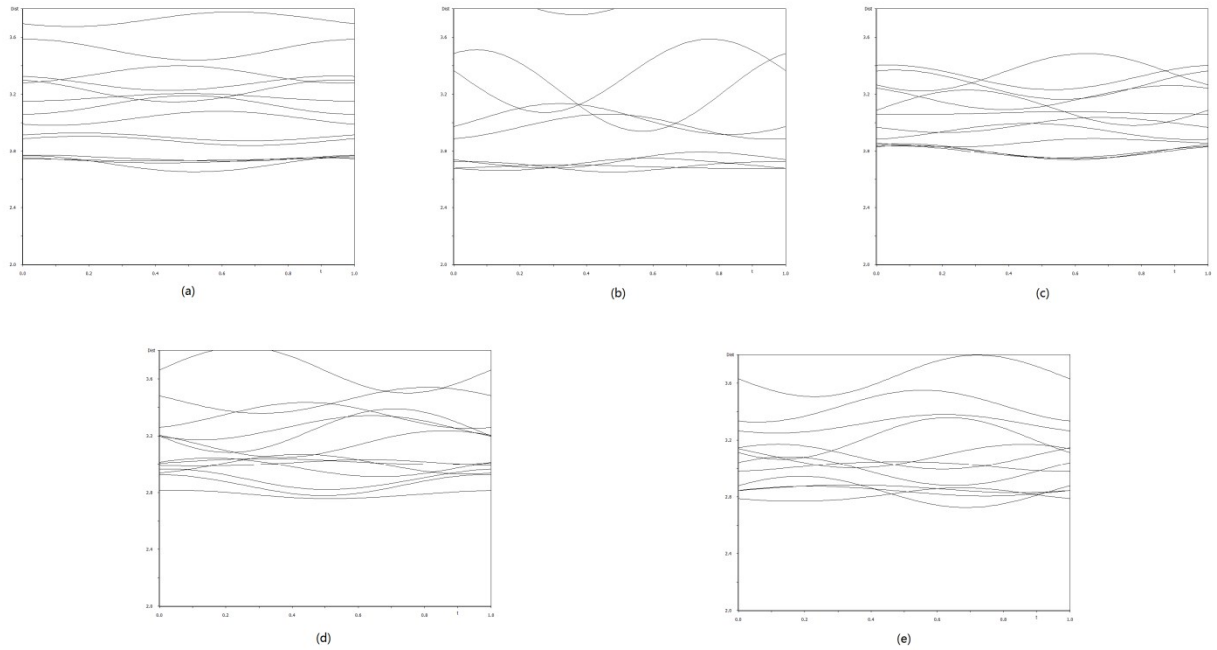

Figure S4. Evolution of K−O distances versus the internal parameter t for (a) K^1, (b) K^2, (c) K^3, (d) K^5 and (e) K^5 atoms.