Supporting Information

Intra-octahedral distortion on lamellar potassium niobate $K_4Nb_6O_{17}$: a periodic DFT study of structural, electronic and vibrational properties

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1 Band Structure

Figure 1 shows the electronic band structure of $K_4Nb_6O_{17}$ at the B3LYP-D3 level.

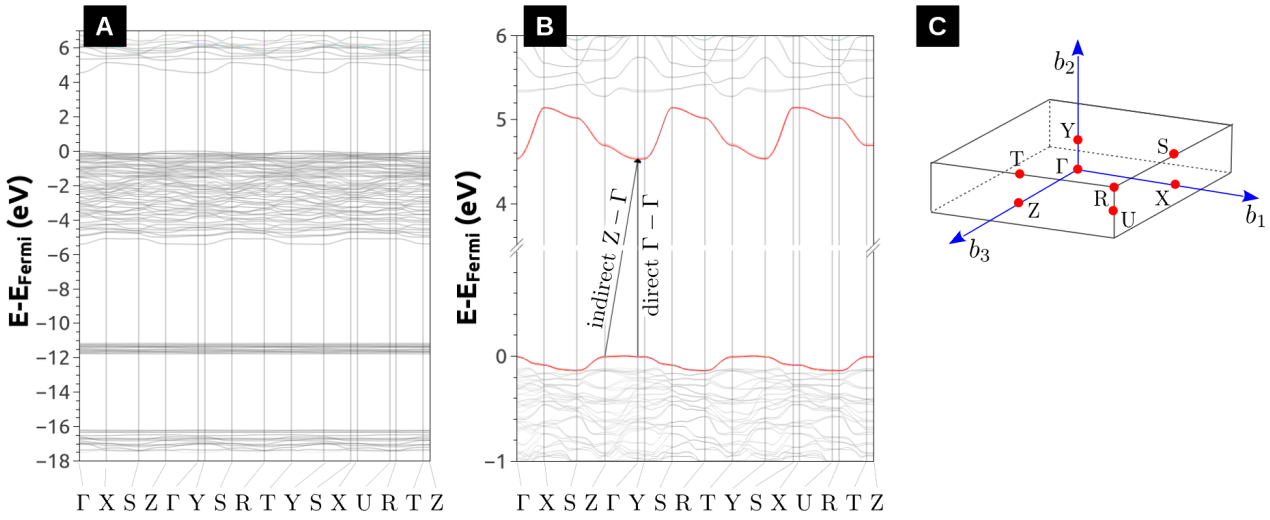

Figure 1: (a) Electronic band structure of $K_4Nb_6O_{17}$. (b) The top of valence band and the bottom of conduction band are shown in red. (c) The Brillouin zone for the orthorhombic cell with high-symmetry points.

2 Charge Density Isosurface

Figure 2 and 3 show the isosurface of electrostaic potential colored with the charge density and Hirshfeld-I charges at the B3LYP-D3 level.

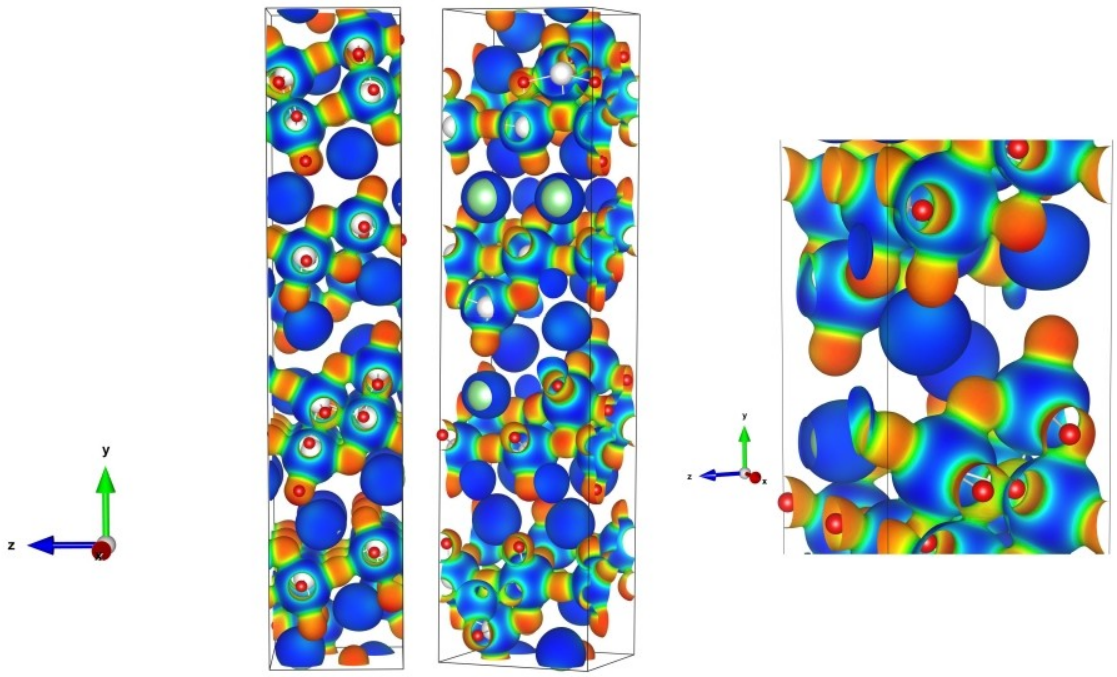

Figure 2: Charge density distribution on electrostatic 3D potential isosurface of $K_4Nb_6O_{17}$ unit cell. Red color denotes negative charge density (high values on oxygens), and blue regions denotes positive charges. Isosurfaces of 0.25 $|e| \cdot bohr^{-3}$.

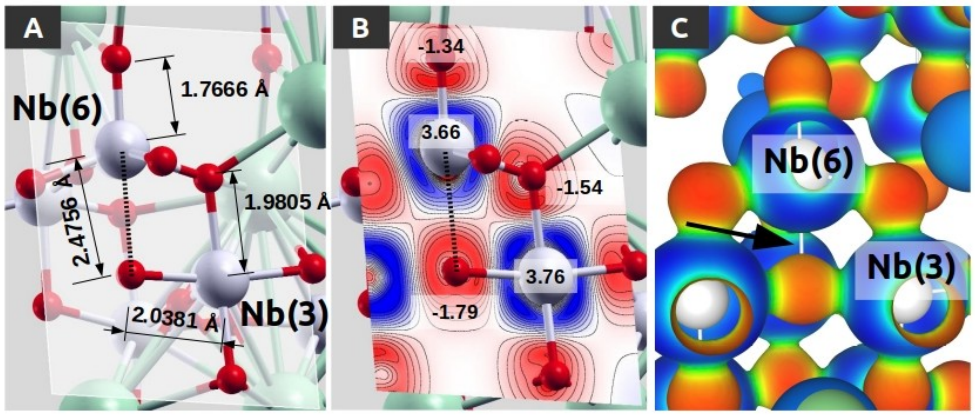

Figure 3: Highly distorted [Nb(6)O_6] polyhedron, focusing on shortest and longest Nb-O bond of $K_4Nb_6O_{17}$ structure. (a) Bond length. (b) Hirshfeld-I charges and charge density map (2D) (isolines 0.05 $|e| \cdot bohr^{-2}$). (c) Charge density surface (isosurface 0.25 $|e| \cdot bohr^{-3}$).

3 Equations for Mean Deviation of Lattice Parameters

The equations used to obtain the mean deviation of calculated lattice parameters ν_i from different DFT functionals (Table 1 of main text) were:

$$\overline{|\Delta|} = \frac{1}{N}\sum_{i=1}^{N}|\nu_i^{cal} - \nu_i^{exp}| \tag{1}$$

$$\overline{|\Delta|}\% = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{\nu_i^{cal} - \nu_i^{exp}}{\nu_i^{exp}}\right| \tag{2}$$

$$|\Delta_{max}| = max(|\nu_i^{cal} - \nu_i^{exp}|) \tag{3}$$

where N is the number of different lattice parameters.

4 Descriptors for Structural Distortion

4.1 Distortion Index

The distortion index (D) is defined in relation to bond length:

$$D = \frac{1}{n}\sum_{i=1}^{n}\frac{|d_i - \overline{d}|}{\overline{d}} \tag{4}$$

where d_i is the Nb-O distance, and $\overline{d}$ is the average of intra-polyhedra bond length.

4.2 Effective Coordination Number, ECoN

The effective coordination number (ECoN) is a number, not necesseraly an integer value, that denotes the amount of bonded atoms around the central cation. The weight ($0 < w_i < 1$) to ECoN accounts the distance of each atom (d_i) in relation to the mean distance of Nb and O on [NbO_6].

$$ECoN = \sum_i w_i = \sum_i exp\left[1 - \left(\frac{d_i}{d_{av}}\right)^6\right] \tag{5}$$

$$d_{av} = \frac{\sum_i d_i exp\left[1 - \left(\frac{d_i}{d_{min}}\right)^6\right]}{\sum_i exp\left[1 - \left(\frac{d_i}{d_{min}}\right)^6\right]} \tag{6}$$

where the shortest bond length is d_{min} and averaged bond length is d_{av}.

4.2.1 Quadratic Elongation, $< \lambda >$

The quadratic elongation ($< \lambda >$) is a dimensionless descriptor that measures the displacement (l_i) of the central atom toward the n vertices of a polyhedron with respect to a regular polyhedron with the same volume (length l_0), and is independent of the size of the polyhedron analyzed:

$$< \lambda >= \frac{1}{n}\sum_{i=1}^{n}\left(\frac{l_i}{l_0}\right)^2 \tag{7}$$

4.2.2 Internal bond angle variation, σ^2

Finally, the variation of the internal angles (ϕ) are calculated in comparison to the regular polyhedron of the same number of sides (m):

$$\sigma^2 = \frac{1}{m-1}\sum_{i=1}^{m}(\phi_i - \phi_0)^2 \tag{8}$$

5 Structural parameters from literature

Table 1: Structural descriptors for Nb polyhedra from experimental cif file [ref.6], where V[NbO_6] is the $[NbO_6]_d/Å^3$ volume, ECoN is the effective coordination number, d_{min} and d_{max} are the minima and maxima intraoctahedral Nb-O bond length, $\overline{d}_{(Nb-O)}/Å$ is the average bond length inside $[NbO_6]_d$, $<\lambda>$ is the quadratic elongation, D is the distortion index and σ^2 is the internal $\widehat{ONbO}$ bond angle variation.

Parameter	Nb(1)	Nb(3)	Nb(5)	Nb(6)
V[NbO_6]	9.999	10.385	10.095	11.094
ECoN	3.40	4.63	4.24	4.50
$d_{min}(Nb-O)$	1.697	1.790	1.776	1.828
$d_{max}(Nb-O)$	2.252	2.235	2.268	2.505
$\overline{d}_{(Nb-O)}$	1.996	2.004	1.998	2.069
$<\lambda>$	1.047	1.027	1.043	1.053
$D \times 10^{-2}$	6.9	5.2	6.6	7.2
σ^2	132.7	73.3	120.7	143.9

6 Atomic Charges

Table 2: Atomic net charge (q) as calculated by Mulliken (q_{Mul}) and Hirshfeld-I (q_{Hir}) methods for [NbO_6] polyhedral site at the B3LYP-D3 level. Two oxygen position (O_{ap} and O_{eq}) taking as reference the central Nb are displayed, with quantities given in $|e|$. [Nb(1)-O_6] ≈ [Nb(2)-O_6], [Nb(3)-O_6] ≈ [Nb(4)-O_6].

Atom	d(Nb-O)	q_{Hir}	q_{Mul}	Overlap
		[Nb(1)-O_6]		
Nb(1)	-	3.675	2.738	-
O_{ap} short	1.7815	-1.332	-1.086	0.150
O_{ap} long	2.3263	-1.656	-1.283	0.029
O_{eq}	1.9354	-1.541	-1.209	0.086
	1.9549	-1.587	-1.225	0.081
	2.0593	-1.696	-1.281	0.057
	2.1576	-1.525	-1.180	0.049
		[Nb(3)-O_6]		
Nb(3)	-	3.762	2.782	-
O_{ap} short	1.8451	-1.525	-1.086	0.114
O_{ap} long	2.2204	-1.656	-1.283	0.044
O_{eq}	1.9260	-1.561	-1.186	0.079
	1.9805	-1.549	-1.219	0.077
	2.0321	-1.541	-1.209	0.069
	2.0381	-1.790	-1.326	0.055
		[Nb(5)-O_6]		
Nb(5)	-	3.717	2.757	-
O_{ap} short	1.8210	-1.528	-1.142	0.117
O_{ap} long	2.3501	-1.790	-1.326	0.029
O_{eq}	1.9344	-1.562	-1.214	0.085
	1.9553	-1.656	-1.283	0.083
	1.9553	-1.656	-1.283	0.083
	2.1492	-1.696	-1.281	0.052
		[Nb(6)-O_6]		
Nb(6)	-	3.660	2.723	-
O_{ap} short	1.7666	-1.340	-1.071	0.158
O_{ap} long	2.4756	-1.790	-1.326	0.021
O_{eq}	1.9665	-1.562	-1.214	0.070
	1.9788	-1.549	-1.219	0.076
	1.9842	-1.549	-1.219	0.076
	2.0429	-1.528	-1.142	0.055

7 Vibrational Modes

Table 3: Vibrational frequencies on the Infrared and Raman at the B3LYP-D3 level, and its intensities.

Modes	Irrep	ν/cm^{-1}	Infrared Intensity		Raman Intensity	
			Activity	(km/mol)	Activity	(arb.units)
1	B1	0.0	A	0.0	A	0.0
2	B2	0.0	A	0.0	A	0.0
3	A1	0.0	A	0.0	A	0.0
4	B1	16.9	A	0.0	A	23.4
5	A1	22.2	A	3.9	A	29.6
6	B2	23.9	A	1.1	A	0.1
7	A2	26.1	I	0.0	A	0.0
8	B2	32.4	A	0.0	A	31.4
9	A2	33.5	I	0.0	A	13.0
10	B1	45.8	A	2.9	A	0.0
11	A2	48.7	I	0.0	A	0.0
12	A1	64.4	A	3.3	A	169.0
13	B2	69.3	A	0.0	A	155.3
14	A2	70.4	I	0.0	A	0.0
15	B1	70.6	A	0.2	A	111.2
16	A1	70.8	A	91.5	A	0.7
17	A2	74.6	I	0.0	A	0.2
18	B1	75.9	A	109.2	A	0.2
19	A1	78.4	A	25.5	A	214.4
20	A1	81.3	A	33.9	A	31.9
21	A1	82.0	A	731.9	A	11.2

22	A2	82.0	I	0.0	A	0.0
23	B1	82.9	A	0.0	A	235.0
24	B2	83.0	A	36.5	A	0.0
25	B2	83.2	A	14.3	A	0.0
26	B1	86.2	A	2.2	A	0.0
27	B2	87.0	A	60.4	A	0.0
28	A2	88.3	I	0.0	A	5.1
29	A2	93.0	I	0.0	A	0.0
30	B2	93.7	A	0.2	A	0.9
31	B1	94.6	A	0.2	A	42.9
32	A1	94.7	A	949.0	A	0.3
33	B2	95.3	A	290.0	A	0.0
34	A1	97.9	A	0.1	A	56.1
35	A1	99.4	A	210.3	A	0.1
36	B1	100.3	A	391.4	A	0.1
37	A2	101.3	I	0.0	A	0.1
38	B1	102.3	A	167.4	A	0.6
39	A2	102.4	I	0.0	A	1.2
40	B1	103.1	A	2.6	A	88.0
41	B2	104.4	A	0.0	A	128.4
42	B2	105.8	A	25.0	A	0.1
43	A1	106.1	A	0.0	A	174.6
44	A2	107.3	I	0.0	A	34.5
45	A2	107.8	I	0.0	A	0.2
46	B2	107.8	A	0.0	A	71.9
47	B2	110.1	A	80.6	A	0.0

48	A1	110.2	A	0.0	A	31.7
49	B1	110.3	A	3.2	A	0.0
50	A2	111.8	I	0.0	A	5.1
51	A1	116.9	A	76.4	A	1.2
52	B1	117.0	A	0.0	A	0.2
53	A1	118.2	A	0.1	A	59.0
54	B1	119.6	A	19.3	A	0.0
55	B2	120.1	A	24.6	A	0.0
56	A2	121.7	I	0.0	A	74.1
57	A2	125.3	I	0.0	A	1.0
58	A1	125.5	A	0.1	A	13.0
59	B1	126.7	A	18.2	A	0.0
60	A2	128.2	I	0.0	A	0.0
61	B2	128.4	A	0.0	A	124.7
62	A1	130.2	A	0.4	A	23.2
63	A1	130.6	A	2.5	A	0.8
64	B2	130.7	A	43.9	A	0.1
65	B1	131.1	A	176.9	A	2.8
66	B1	131.3	A	4.2	A	111.4
67	A2	133.4	I	0.0	A	0.0
68	B2	133.5	A	197.5	A	0.0
69	A1	134.4	A	411.2	A	0.1
70	B1	135.1	A	0.1	A	10.5
71	A2	135.3	I	0.0	A	0.3
72	B2	136.1	A	0.0	A	35.4
73	B2	142.3	A	0.0	A	301.1

74	A2	142.9	I	0.0	A	0.0
75	A1	144.2	A	39.6	A	0.0
76	B1	145.8	A	0.0	A	13.4
77	A1	146.6	A	2.6	A	209.4
78	B1	148.6	A	27.4	A	0.0
79	A2	148.9	I	0.0	A	16.4
80	A1	149.6	A	6.0	A	10.8
81	B2	149.9	A	15.1	A	0.0
82	B1	159.3	A	3.3	A	0.7
83	B1	159.5	A	0.0	A	55.8
84	B2	159.5	A	83.1	A	0.0
85	B2	160.0	A	0.0	A	2.5
86	A2	160.4	I	0.0	A	0.8
87	B1	163.1	A	7.9	A	0.0
88	B2	164.3	A	125.4	A	0.0
89	A1	164.7	A	0.0	A	74.0
90	A2	166.0	I	0.0	A	19.6
91	A1	166.7	A	112.0	A	0.1
92	A2	166.7	I	0.0	A	0.0
93	A1	167.6	A	0.0	A	37.9
94	B2	174.0	A	450.3	A	0.0
95	A2	174.0	I	0.0	A	49.8
96	B1	176.0	A	9.4	A	0.0
97	B1	179.4	A	0.1	A	239.6
98	A1	180.2	A	7252.1	A	1.2
99	B2	181.4	A	0.0	A	30.1

100	A2	182.0	I	0.0	A	0.0
101	B2	186.5	A	20.6	A	0.0
102	A1	188.2	A	2.7	A	250.0
103	B1	188.6	A	132.8	A	0.0
104	A2	189.6	I	0.0	A	11.8
105	A1	190.8	A	0.0	A	100.7
106	A2	194.8	I	0.0	A	4.2
107	B1	195.8	A	2603.0	A	0.0
108	A2	195.9	I	0.0	A	0.1
109	B1	197.2	A	74.3	A	0.0
110	B2	197.6	A	22.1	A	0.0
111	B2	199.3	A	0.0	A	200.7
112	A1	199.6	A	2158.8	A	0.4
113	B1	203.5	A	0.5	A	211.0
114	B2	205.2	A	0.0	A	79.7
115	A2	205.6	I	0.0	A	0.0
116	A1	207.2	A	1.5	A	321.6
117	B2	209.0	A	8.0	A	0.0
118	B1	209.5	A	1141.5	A	0.0
119	B2	211.8	A	36.8	A	0.0
120	A2	213.3	I	0.0	A	21.1
121	A1	214.0	A	5.4	A	244.2
122	A2	214.3	I	0.0	A	0.2
123	A1	216.7	A	9.2	A	367.3
124	B1	218.2	A	0.0	A	30.3
125	A1	218.9	A	1093.2	A	4.9

126	B1	219.5	A	2284.1	A	0.0
127	B2	220.3	A	0.0	A	78.3
128	A2	220.6	I	0.0	A	0.0
129	B2	221.4	A	40.7	A	0.1
130	A1	221.6	A	27.4	A	342.5
131	A1	222.7	A	3406.5	A	6.0
132	A2	223.8	I	0.0	A	26.4
133	B1	225.6	A	0.0	A	212.1
134	A2	226.3	I	0.0	A	32.4
135	A2	226.9	I	0.0	A	0.0
136	B1	231.3	A	171.1	A	0.0
137	B2	231.3	A	45.7	A	0.0
138	B2	234.0	A	0.0	A	514.2
139	A1	234.3	A	336.8	A	0.1
140	B1	238.5	A	0.0	A	243.8
141	A1	241.6	A	3.0	A	0.0
142	B1	244.1	A	0.0	A	1.6
143	A2	245.0	I	0.0	A	0.0
144	B2	245.9	A	0.0	A	28.0
145	B1	249.2	A	17.8	A	0.0
146	A1	251.0	A	32.9	A	53.0
147	A1	252.8	A	6018.1	A	12.9
148	A2	253.2	I	0.0	A	8.2
149	B1	253.4	A	26.0	A	0.0
150	A2	253.5	I	0.0	A	3.4
151	A1	254.2	A	428.9	A	131.4

152	B2	254.3	A	6.3	A	0.0
153	B1	256.2	A	0.0	A	50.3
154	B2	258.0	A	0.0	A	135.5
155	B2	266.8	A	23.7	A	0.0
156	A2	267.4	I	0.0	A	39.3
157	A2	269.7	I	0.0	A	0.0
158	A1	271.1	A	28.6	A	0.3
159	B2	271.1	A	0.0	A	9.0
160	B1	272.0	A	1.2	A	17.0
161	A1	273.8	A	0.0	A	67.7
162	A2	273.9	I	0.0	A	30.3
163	B1	274.6	A	990.1	A	0.0
164	B2	275.0	A	1.3	A	0.0
165	A2	277.2	I	0.0	A	0.0
166	B2	277.3	A	0.0	A	0.7
167	B1	278.4	A	1.9	A	94.5
168	A1	278.4	A	71.5	A	0.1
169	A1	279.1	A	1.6	A	624.0
170	B1	279.9	A	8142.4	A	0.0
171	B2	287.2	A	1.2	A	0.0
172	A2	287.6	I	0.0	A	40.9
173	A2	295.4	I	0.0	A	0.0
174	A1	297.5	A	0.0	A	0.0
175	B2	298.0	A	0.0	A	1.1
176	B1	300.2	A	0.0	A	40.7
177	A1	303.9	A	0.1	A	67.7

178	B1	306.2	A	3781.5	A	0.0
179	B2	306.6	A	169.9	A	0.0
180	A2	306.8	I	0.0	A	8.3
181	B1	316.5	A	16.2	A	0.0
182	A1	317.3	A	0.1	A	211.5
183	B2	317.8	A	31.9	A	0.0
184	A2	318.3	I	0.0	A	66.9
185	B2	320.8	A	60.5	A	0.0
186	B1	320.8	A	229.9	A	0.0
187	A1	322.8	A	0.4	A	112.0
188	A2	323.1	I	0.0	A	0.0
189	B2	323.7	A	0.0	A	0.8
190	A2	324.0	I	0.0	A	23.1
191	A1	324.4	A	0.1	A	0.1
192	B1	325.0	A	0.0	A	31.6
193	B1	330.3	A	1161.4	A	0.0
194	A1	330.7	A	0.0	A	52.7
195	B2	333.0	A	7.8	A	0.0
196	A2	333.2	I	0.0	A	10.6
197	A1	345.8	A	0.0	A	33.2
198	B1	346.3	A	277.2	A	0.0
199	A2	346.4	I	0.0	A	7.0
200	B2	346.7	A	31.3	A	0.0
201	B2	363.9	A	34.1	A	0.0
202	A2	364.1	I	0.0	A	0.2
203	A1	364.9	A	0.0	A	67.5

204	B1	365.1	A	288.9	A	0.0
205	A1	386.0	A	0.0	A	12.1
206	B1	386.2	A	157.4	A	0.0
207	A1	389.1	A	114.3	A	0.0
208	A2	390.8	I	0.0	A	0.0
209	B1	391.3	A	0.0	A	5.9
210	B2	392.9	A	0.0	A	0.6
211	B2	395.2	A	193.3	A	0.0
212	A2	395.4	I	0.0	A	2.5
213	B2	397.7	A	142.2	A	0.0
214	B1	399.1	A	69.3	A	0.0
215	A2	399.1	I	0.0	A	3.3
216	A1	399.5	A	0.0	A	55.5
217	B2	409.9	A	629.3	A	0.0
218	A1	412.4	A	41.5	A	1.3
219	A1	412.5	A	0.5	A	513.6
220	B1	412.6	A	35.8	A	0.1
221	B1	412.9	A	0.1	A	72.8
222	A2	413.2	I	0.0	A	0.0
223	B2	413.6	A	0.0	A	1.5
224	A2	414.9	I	0.0	A	41.6
225	A1	444.9	A	0.5	A	66.6
226	B1	445.0	A	22.3	A	0.0
227	B2	448.1	A	24.8	A	0.0
228	A2	448.1	I	0.0	A	1.4
229	A2	452.5	I	0.0	A	0.0

230	A1	453.4	A	6908.8	A	0.0
231	B2	455.8	A	0.0	A	13.3
232	B1	456.6	A	0.0	A	4.9
233	B2	470.9	A	1226.9	A	0.0
234	B1	472.5	A	144.5	A	0.0
235	A1	472.7	A	0.0	A	61.0
236	A2	476.1	I	0.0	A	13.4
237	B2	482.7	A	543.0	A	0.0
238	B1	487.5	A	290.5	A	0.0
239	A2	488.1	I	0.0	A	2.9
240	A1	488.1	A	0.6	A	62.6
241	A2	506.8	I	0.0	A	0.0
242	B2	507.2	A	0.0	A	0.0
243	A1	508.6	A	1826.6	A	0.0
244	B1	509.0	A	0.0	A	29.2
245	A1	517.8	A	15354.2	A	0.0
246	A2	518.4	I	0.0	A	0.0
247	B1	525.2	A	0.3	A	102.6
248	B2	525.8	A	0.1	A	17.4
249	B2	540.2	A	3105.1	A	0.3
250	A2	546.6	I	0.0	A	0.0
251	A1	547.2	A	10157.3	A	7.1
252	B2	547.2	A	7.7	A	167.8
253	B1	547.8	A	44.7	A	2.8
254	A1	549.9	A	168.0	A	321.7
255	B1	550.6	A	2543.5	A	0.0

256	A2	554.8	I	0.0	A	0.2
257	A1	560.2	A	3.0	A	594.4
258	A2	560.8	I	0.0	A	30.1
259	B1	568.0	A	876.1	A	0.0
260	B2	569.1	A	44.5	A	0.0
261	A1	570.3	A	0.6	A	88.2
262	B2	570.8	A	547.4	A	0.0
263	B1	572.2	A	3440.3	A	0.0
264	A2	574.2	I	0.0	A	3.5
265	A1	591.8	A	634.0	A	0.4
266	B1	593.1	A	0.0	A	20.4
267	A2	595.0	I	0.0	A	0.0
268	B2	595.8	A	1644.1	A	0.2
269	B2	596.3	A	89.7	A	5.0
270	A2	599.6	I	0.0	A	0.0
271	B2	599.7	A	3.0	A	0.3
272	A1	602.3	A	949.4	A	1.0
273	B1	602.5	A	0.6	A	11.7
274	A1	609.7	A	0.2	A	565.2
275	A2	609.9	I	0.0	A	29.1
276	B1	610.8	A	2137.3	A	0.0
277	A1	621.6	A	0.2	A	320.9
278	B1	623.5	A	15466.5	A	0.0
279	A2	632.1	I	0.0	A	46.6
280	B2	632.4	A	122.5	A	0.0
281	A2	636.9	I	0.0	A	0.0

282	A1	637.0	A	262.7	A	0.1
283	B1	638.4	A	0.8	A	32.4
284	B2	638.5	A	0.4	A	133.1
285	A1	668.3	A	0.2	A	625.3
286	B2	669.6	A	460.8	A	0.0
287	B1	669.8	A	2001.3	A	0.0
288	A2	670.6	I	0.0	A	75.8
289	A1	675.5	A	384.1	A	0.0
290	B1	675.8	A	0.1	A	39.6
291	A2	675.9	I	0.0	A	0.0
292	B2	676.2	A	0.3	A	32.0
293	B2	722.8	A	5307.6	A	0.0
294	A1	754.4	A	0.0	A	84.3
295	A2	754.4	I	0.0	A	7.6
296	B1	756.5	A	0.6	A	0.0
297	B1	806.7	A	0.0	A	0.3
298	A1	806.7	A	1443.4	A	0.0
299	B2	834.0	A	0.1	A	2.9
300	A2	834.0	I	0.0	A	0.0
301	B2	851.5	A	4074.1	A	0.0
302	A1	868.0	A	0.0	A	964.5
303	B1	868.1	A	2126.4	A	0.0
304	A2	868.3	I	0.0	A	77.9
305	B2	897.5	A	4469.6	A	0.0
306	A2	914.8	I	0.0	A	0.0
307	B2	914.9	A	0.8	A	6.8

308	A1	919.3	A	603.0	A	110.0
309	B1	919.4	A	39.4	A	0.1
310	B1	920.2	A	199.6	A	0.0
311	A1	920.4	A	94.4	A	1000.0
312	A1	921.3	A	112.6	A	28.9
313	B1	921.4	A	1.1	A	16.9
314	A2	921.6	I	0.0	A	0.0
315	B2	921.7	A	0.1	A	1.4
316	A1	926.2	A	0.0	A	638.2
317	A2	926.5	I	0.0	A	0.2
318	B1	943.3	A	2551.3	A	0.0
319	B2	944.5	A	11.8	A	0.0
320	A2	947.5	I	0.0	A	37.0
321	A1	950.8	A	0.0	A	77.2
322	A2	950.9	I	0.0	A	6.0
323	B2	970.9	A	421.8	A	0.0
324	B1	980.5	A	38.4	A	0.0

8 Coordinates of calculated $K_4Nb_6O_{17}$ unit cell

Table 4: Structural data of $K_4Nb_6O_{17}$ unit cell calculated at the B3LYP-D3 level.

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X	Y	Z
0.781855666519E+01	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00	0.324111644324E+02	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	0.650530671342E+01

ATOMS IN THE ASYMMETRIC UNIT 27 - ATOMS IN THE UNIT CELL: 108

ATOM	X/A	Y/B	Z/C
1 T NB	6.413648160130E-03	1.765233823406E-01	1.908034262838E-01
2 F NB	-4.935863518405E-01	-1.765233823406E-01	-1.908034262838E-01
3 F NB	-4.935863518405E-01	3.234766176594E-01	-3.091965737177E-01
4 F NB	6.413648160130E-03	-3.234766176594E-01	3.091965737147E-01
5 T NB	9.342215635856E-03	-1.765240329212E-01	-1.908015419020E-01
6 F NB	-4.906577843648E-01	1.765240329212E-01	1.908015419020E-01
7 F NB	-4.906577843648E-01	-3.234759670788E-01	3.091984580964E-01
8 F NB	9.342215635856E-03	3.234759670788E-01	-3.091984580995E-01
9 T NB	1.228541552380E-03	1.256555959783E-01	-2.486633579133E-01
10 F NB	-4.987714584483E-01	-1.256555959783E-01	2.486633579133E-01
11 F NB	-4.987714584483E-01	3.743444040217E-01	2.513366420851E-01
12 F NB	1.228541552380E-03	-3.743444040217E-01	-2.513366420882E-01
13 T NB	1.451298347027E-02	-1.256580347912E-01	2.486678889944E-01
14 F NB	-4.854870165304E-01	1.256580347912E-01	-2.486678889944E-01
15 F NB	-4.854870165304E-01	-3.743419652088E-01	-2.513321110071E-01
16 F NB	1.451298347027E-02	3.743419652088E-01	2.513321110040E-01
17 T NB	2.578836106634E-01	9.381138493390E-02	1.332153165826E-01

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18 F NB   -2.421163893372E-01 -9.381138493390E-02 -1.332153165826E-01
19 F NB   -2.421163893372E-01  4.061886150661E-01 -3.667846834189E-01
20 F NB    2.578836106634E-01 -4.061886150661E-01  3.667846834158E-01
21 T NB    2.578884829482E-01  4.616556790712E-02 -3.240124889831E-01
22 F NB   -2.421115170525E-01 -4.616556790712E-02  3.240124889831E-01
23 F NB   -2.421115170525E-01  4.538344320929E-01  1.759875110154E-01
24 F NB    2.578884829482E-01 -4.538344320929E-01 -1.759875110184E-01
25 T K     2.578570229634E-01  2.187800875334E-01 -3.674443898255E-01
26 F K    -2.421429770372E-01 -2.187800875334E-01  3.674443898255E-01
27 F K    -2.421429770372E-01  2.812199124666E-01  1.325556101729E-01
28 F K     2.578570229634E-01 -2.812199124666E-01 -1.325556101760E-01
29 T K    -2.421540887855E-01  2.166737437386E-01 -3.731026594541E-01
30 F K     2.578459112139E-01 -2.166737437386E-01  3.731026594541E-01
31 F K     2.578459112139E-01  2.833262562614E-01  1.268973405444E-01
32 F K    -2.421540887855E-01 -2.833262562614E-01 -1.268973405474E-01
33 T K    -2.421176703690E-01  8.614476016376E-02  3.276878113775E-01
34 F K     2.578823296304E-01 -8.614476016376E-02 -3.276878113775E-01
35 F K     2.578823296304E-01  4.138552398362E-01 -1.723121886240E-01
36 F K    -2.421176703690E-01 -4.138552398362E-01  1.723121886209E-01
37 T K    -2.421129047434E-01  2.169572340243E-02 -2.101428551475E-01
38 F K     2.578870952560E-01 -2.169572340243E-02  2.101428551475E-01
39 F K     2.578870952560E-01  4.783042765976E-01  2.898571448510E-01
40 F K    -2.421129047434E-01 -4.783042765976E-01 -2.898571448540E-01
41 T O     3.275617877284E-02  2.281445850716E-01  2.793646934058E-01
42 F O    -4.672438212278E-01 -2.281445850716E-01 -2.793646934058E-01
43 F O    -4.672438212278E-01  2.718554149284E-01 -2.206353065957E-01
44 F O     3.275617877284E-02 -2.718554149284E-01  2.206353065927E-01
45 T O     4.830052768448E-01  2.281444697713E-01  2.793751767393E-01
46 F O    -1.699472315584E-02 -2.281444697713E-01 -2.793751767393E-01
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47 F 0    -1.699472315584E-02  2.718555302287E-01 -2.206248232622E-01
48 F 0     4.830052768448E-01 -2.718555302287E-01  2.206248232592E-01
49 T 0     6.109690572274E-04  1.498383067148E-01  4.945770147313E-01
50 F 0    -4.993890309434E-01 -1.498383067148E-01 -4.945770147313E-01
51 F 0    -4.993890309434E-01  3.501616932852E-01 -5.422985270225E-03
52 F 0     6.109690572274E-04 -3.501616932852E-01  5.422985267198E-03
53 T 0    -4.848398219874E-01  1.498376118254E-01  4.945677793360E-01
54 F 0     1.516017801199E-02 -1.498376118254E-01 -4.945677793360E-01
55 F 0     1.516017801199E-02  3.501623881746E-01 -5.432220665527E-03
56 F 0    -4.848398219874E-01 -3.501623881746E-01  5.432220662499E-03
57 T 0     1.850964109717E-02  6.648820392592E-02 -3.218391139773E-01
58 F 0    -4.814903589035E-01 -6.648820392592E-02  3.218391139773E-01
59 F 0    -4.814903589035E-01  4.335117960741E-01  1.781608860212E-01
60 F 0     1.850964109717E-02 -4.335117960741E-01 -1.781608860242E-01
61 T 0     4.972683041527E-01  6.648841403467E-02 -3.218313616461E-01
62 F 0    -2.731695847895E-03 -6.648841403467E-02  3.218313616461E-01
63 F 0    -2.731695847895E-03  4.335115859653E-01  1.781686383524E-01
64 F 0     4.972683041527E-01 -4.335115859653E-01 -1.781686383554E-01
65 T 0     1.276970529845E-02  1.813266886861E-01 -1.056525316203E-01
66 F 0    -4.872302947022E-01 -1.813266886861E-01  1.056525316203E-01
67 F 0    -4.872302947022E-01  3.186733113139E-01  3.943474683782E-01
68 F 0     1.276970529845E-02 -3.186733113139E-01 -3.943474683812E-01
69 T 0    -4.969943088594E-01  1.813304460781E-01 -1.056577470388E-01
70 F 0     3.005691139961E-03 -1.813304460781E-01  1.056577470388E-01
71 F 0     3.005691139961E-03  3.186695539219E-01  3.943422529597E-01
72 F 0    -4.969943088594E-01 -3.186695539219E-01 -3.943422529628E-01
73 T 0     1.906089783968E-02  1.082965851999E-01  8.082659483336E-02
74 F 0    -4.809391021610E-01 -1.082965851999E-01 -8.082659483336E-02
75 F 0    -4.809391021610E-01  3.917034148001E-01 -4.191734051682E-01
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 76 F O     1.906089783968E-02 -3.917034148001E-01  4.191734051651E-01
 77 T O     4.967044180655E-01  1.082994357335E-01  8.082580663163E-02
 78 F O    -3.295581935087E-03 -1.082994357335E-01 -8.082580663163E-02
 79 F O    -3.295581935087E-03  3.917005642665E-01 -4.191741933699E-01
 80 F O     4.967044180655E-01 -3.917005642665E-01  4.191741933669E-01
 81 T O     2.578859756020E-01  1.187784500247E-01 -2.059604439812E-01
 82 F O    -2.421140243987E-01 -1.187784500247E-01  2.059604439812E-01
 83 F O    -2.421140243987E-01  3.812215499753E-01  2.940395560173E-01
 84 F O     2.578859756020E-01 -3.812215499753E-01 -2.940395560203E-01
 85 T O    -2.421177277641E-01  1.187485466855E-01 -2.181889590262E-01
 86 F O     2.578822722353E-01 -1.187485466855E-01  2.181889590262E-01
 87 F O     2.578822722353E-01  3.812514533145E-01  2.818110409723E-01
 88 F O    -2.421177277641E-01 -3.812514533145E-01 -2.818110409753E-01
 89 T O     2.578898031144E-01  4.270096052167E-02 -2.032175487445E-02
 90 F O    -2.421101968862E-01 -4.270096052167E-02  2.032175487445E-02
 91 F O    -2.421101968862E-01  4.572990394783E-01  4.796782451240E-01
 92 F O     2.578898031144E-01 -4.572990394783E-01 -4.796782451271E-01
 93 T O    -2.421203348312E-01  1.717425749826E-01  2.135402313228E-01
 94 F O     2.578796651681E-01 -1.717425749826E-01 -2.135402313228E-01
 95 F O     2.578796651681E-01  3.282574250174E-01 -2.864597686787E-01
 96 F O    -2.421203348312E-01 -3.282574250174E-01  2.864597686757E-01
 97 T O     2.578833191399E-01  1.581589353898E-01  2.129864737945E-01
 98 F O    -2.421166808607E-01 -1.581589353898E-01 -2.129864737945E-01
 99 F O    -2.421166808607E-01  3.418410646102E-01 -2.870135262070E-01
100 F O     2.578833191399E-01 -3.418410646102E-01  2.870135262040E-01
101 T O     2.578873115678E-01 -7.266795307648E-03 -3.776377462822E-01
102 F O    -2.421126884328E-01  7.266795307648E-03  3.776377462822E-01
103 F O    -2.421126884328E-01 -4.927332046924E-01  1.223622537163E-01
104 F O     2.578873115678E-01  4.927332046924E-01 -1.223622537193E-01
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105 T O     2.578985513938E-01  6.743342869883E-02  3.803692973295E-01
106 F O    -2.421014486069E-01 -6.743342869883E-02 -3.803692973295E-01
107 F O    -2.421014486069E-01  4.325665713012E-01 -1.196307026720E-01
108 F O     2.578985513938E-01 -4.325665713012E-01  1.196307026690E-01
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