$K_2Ta_4O_{11}$ ("Kalitantite"): wide band gap semiconductor synthesized in molybdate flux medium

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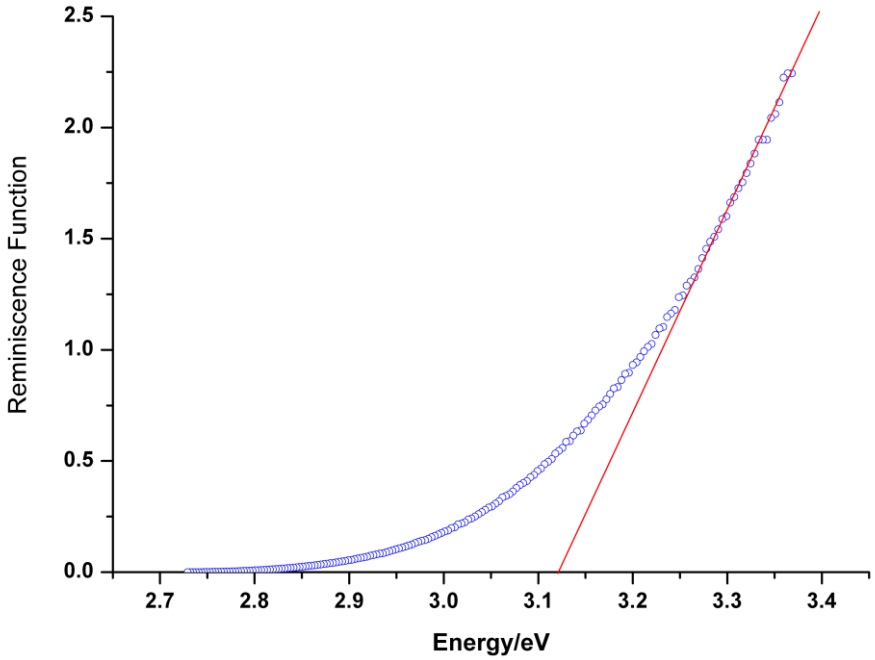
Supporting Information



Fig, S1. Kubelka-Munk processed UV-Vis diffuse electron spectra (blue open circles) for $K_2Ta_4O_{14}$. The onset of absorption edge is highlighted (solid red line) by extrapolation of linear segment of experimental curve[1].

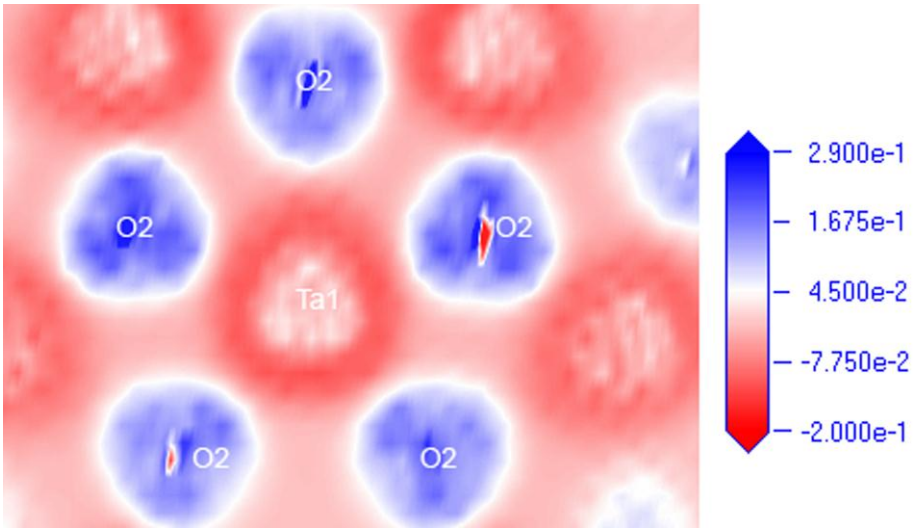


Fig. S2. Isosection (0.02 e×pm^{-6}) of difference electronic map in vicinity of Ta1 (30×30 pm^2).

Supporting information S3. Calculation of Voronoi-Dirichlet polyhedra (a) and results of topological analysis (b)**.**

A

############
2:K2 O11 Ta4
Author(s): Babaryk Artem A.,Inorganic,Faculty,Taras,Volodymyrska,01601
Journal: ? Year: 0 Volume: ? Number: ? Pages: ?-?
############
Central atom:Ta1 CN:6 0.000 0.000 0.500 Rsd:1.230
Atom:1.982 < r < 1.982 <r>=1.982 Top: 1.685 < R < 1.728 <R>=1.717
CN=6:0:0 NV=8 V=7.796/10.383 S=23.594 Cpac=0.523 Ccov=2.774
G3=0.083363846
Face distribution: {4/6 }
Vertex distribution: {3/8 }

	Atom	x	y	z	Dist.	SSeg.	VSeg.	SAng.	NV	Type
1	O	1	0.272	0.235	0.468	1.982	16.67	16.67	16.67	4	-
2	O	1	-0.272	-0.235	0.532	1.982	16.67	16.67	16.67	4	-
3	O	1	-0.037	-0.272	0.468	1.982	16.67	16.67	16.67	4	-
4	O	1	0.037	0.272	0.532	1.982	16.67	16.67	16.67	4	-
5	O	1	-0.235	0.037	0.468	1.982	16.67	16.67	16.67	4	-
6	O	1	0.235	-0.037	0.532	1.982	16.67	16.67	16.67	4	-

Central atom:Ta2 CN:7 0.333 0.300 0.417 Rsd:1.232
D(CP):0.194 (0.3333 0.2693 0.4167)
Atom:1.946 < r < 2.428 <r>=2.063 Top: 1.572 < R < 1.773 <R>=1.640
CN=7:0:0 NV=10 V=7.831/13.448 S=23.100 Cpac=0.493 Ccov=2.981
G3=0.082730807
Face distribution: {4/5 5/2 }
Vertex distribution: {3/10 }

	Atom	x	y	z	Dist.	SSeg.	VSeg.	SAng.	NV	Type
1	O	1	0.395	0.296	0.365	1.946	17.42	16.67	17.22	5	-
2	O	1	0.272	0.235	0.468	1.946	17.42	16.67	17.22	5	-
3	O	3	0.087	0.420	0.417	2.030	15.30	15.27	15.04	4	-
4	O	3	0.580	0.667	0.417	2.030	15.30	15.27	15.04	4	-
5	O	2	0.000	0.000	0.406	2.032	13.14	13.13	13.86	4	-
6	O	2	0.667	0.333	0.427	2.032	13.14	13.13	13.86	4	-
7	O	3	0.333	-0.087	0.417	2.428	8.26	9.86	7.75	4	-

B

############
2:K2 O11 Ta4
Author(s): Babaryk Artem A.,Inorganic,Faculty,Taras,Volodymyrska,01601
Journal: Silicon Year: 0 Volume: ? Number: ? Pages: ?-?
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Topology for K1

Atom K1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ta 2	1.0330	0.3333	0.5833	(1 0 1)	3.618A	1
Ta 2	0.6667	0.6997	0.5833	(1 1 1)	3.618A	1
Ta 2	0.3003	-0.0330	0.5833	(0 0 1)	3.618A	1
Common edge with					R(A-A)	
Ta 1	1.0000	0.0000	0.5000	(1 0 0)	3.632A	2
Ta 1	1.0000	1.0000	0.5000	(1 1 0)	3.632A	2
Ta 1	0.0000	0.0000	0.5000	(0 0 0)	3.632A	2
K 1	1.3333	0.6667	0.4925	(2 1 1)	3.664A	2
K 1	0.3333	0.6667	0.4925	(1 1 1)	3.664A	2
K 1	0.3333	-0.3333	0.4925	(1 0 1)	3.664A	2
Ta 2	0.9670	0.6667	0.4167	(1 1 0)	3.898A	2
Ta 2	0.6997	0.0330	0.4167	(1 0 0)	3.898A	2
Ta 2	0.3333	0.3003	0.4167	(0 0 0)	3.898A	2

Topology for Ta1

Atom Ta1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ta 2	-0.0330	-0.3333	0.4167	(0 0 0)	3.663A	1
Ta 2	0.3333	0.3003	0.4167	(0 0 0)	3.663A	1
Ta 2	-0.3003	0.0330	0.4167	(0 0 0)	3.663A	1
Ta 2	0.3003	-0.0330	0.5833	(0 0 1)	3.663A	1
Ta 2	0.0330	0.3333	0.5833	(0 0 1)	3.663A	1
Ta 2	-0.3333	-0.3003	0.5833	(0 0 1)	3.663A	1
Common edge with					R(A-A)	
K 1	0.6667	0.3333	0.5075	(0 0 0)	3.632A	2
K 1	-0.3333	0.3333	0.5075	(-1 0 0)	3.632A	2
K 1	-0.3333	-0.6667	0.5075	(-1-1 0)	3.632A	2
K 1	0.3333	-0.3333	0.4925	(1 0 1)	3.632A	2
K 1	0.3333	0.6667	0.4925	(1 1 1)	3.632A	2
K 1	-0.6667	-0.3333	0.4925	(0 0 1)	3.632A	2

Topology for Ta2

Atom Ta2 links by bridge ligands and has

Common vertex with					R(A-A)	f
K 1	0.3333	0.6667	0.3408	(0 1-1)	3.618A	1
K 1	0.3333	0.6667	0.4925	(1 1 1)	3.618A	1
Ta 1	0.6667	0.3333	0.3333	(0 0-1)	3.663A	1
Ta 1	0.0000	0.0000	0.5000	(0 0 0)	3.663A	1
Ta 2	-0.0330	0.6667	0.4167	(0 1 0)	3.981A	1
Ta 2	0.6997	1.0330	0.4167	(1 1 0)	3.981A	1
Common edge with					R(A-A)	
Ta 2	-0.0330	-0.3333	0.4167	(0 0 0)	3.456A	2
Ta 2	-0.3003	0.0330	0.4167	(0 0 0)	3.456A	2
Ta 2	0.9670	0.6667	0.4167	(1 1 0)	3.456A	2
Ta 2	0.6997	0.0330	0.4167	(1 0 0)	3.456A	2
K 1	-0.0000	-0.0000	0.3258	(-1-1 0)	3.898A	2
K 1	0.6667	0.3333	0.5075	(0 0 0)	3.898A	2

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Ta4K2O11

Coordination sequences

K1: 1 2 3 4 5 6 7 8 9 10
Num 12 44 96 170 264 380 516 674 852 1052
Cum 13 57 153 323 587 967 1483 2157 3009 4061

Ta1: 1 2 3 4 5 6 7 8 9 10
Num 12 44 96 170 264 380 516 674 852 1052
Cum 13 57 153 323 587 967 1483 2157 3009 4061

Ta2: 1 2 3 4 5 6 7 8 9 10
Num 12 42 96 170 264 378 516 674 852 1050
Cum 13 55 151 321 585 963 1479 2153 3005 4055

TD10=4058

Vertex symbols for selected sublattice

K1 Point symbol:{3^24.4^36.5^6}
Extended point
symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5(4).5(4).5(4).5(4).5(4).5(4)]

Ta1 Point symbol:{3^24.4^36.5^6}
Extended point
symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5(4).5(4).5(4).5(4).5(4).5(4)]

Ta2 Point symbol:{3^24.4^33.5^9}
Extended point
symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5(4).5(4).5(4).5(7).5(7).5(7).5(7).5(7).5(7)]

Point symbol for net: {3^24.4^33.5^9}{3^24.4^36.5^6}
12,12-c net with stoichiometry (12-c)(12-c); 2-nodal net

Topological type: tcj/hc (topos&RCSR.ttd) {3^24.4^33.5^9}{3^24.4^36.5^6} - VS
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.*]
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.*] (63707 types in 10 databases)

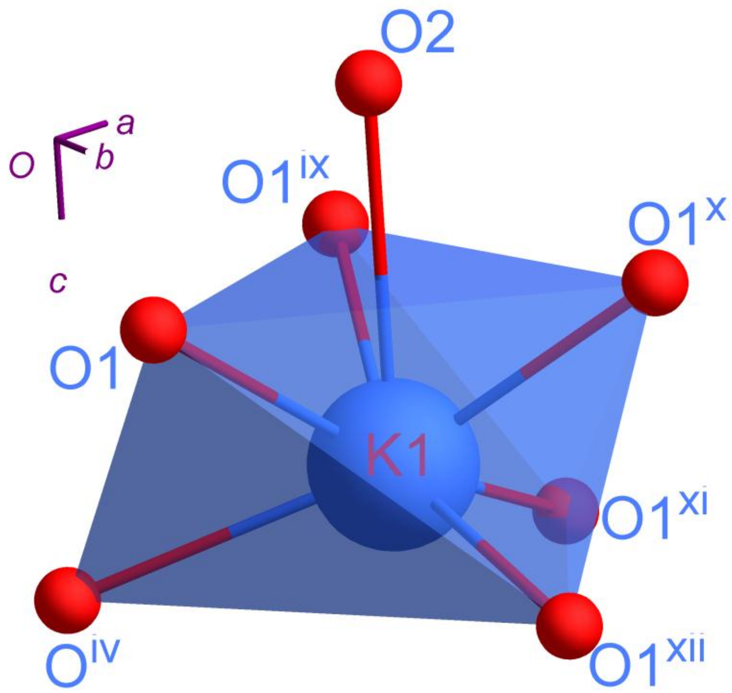
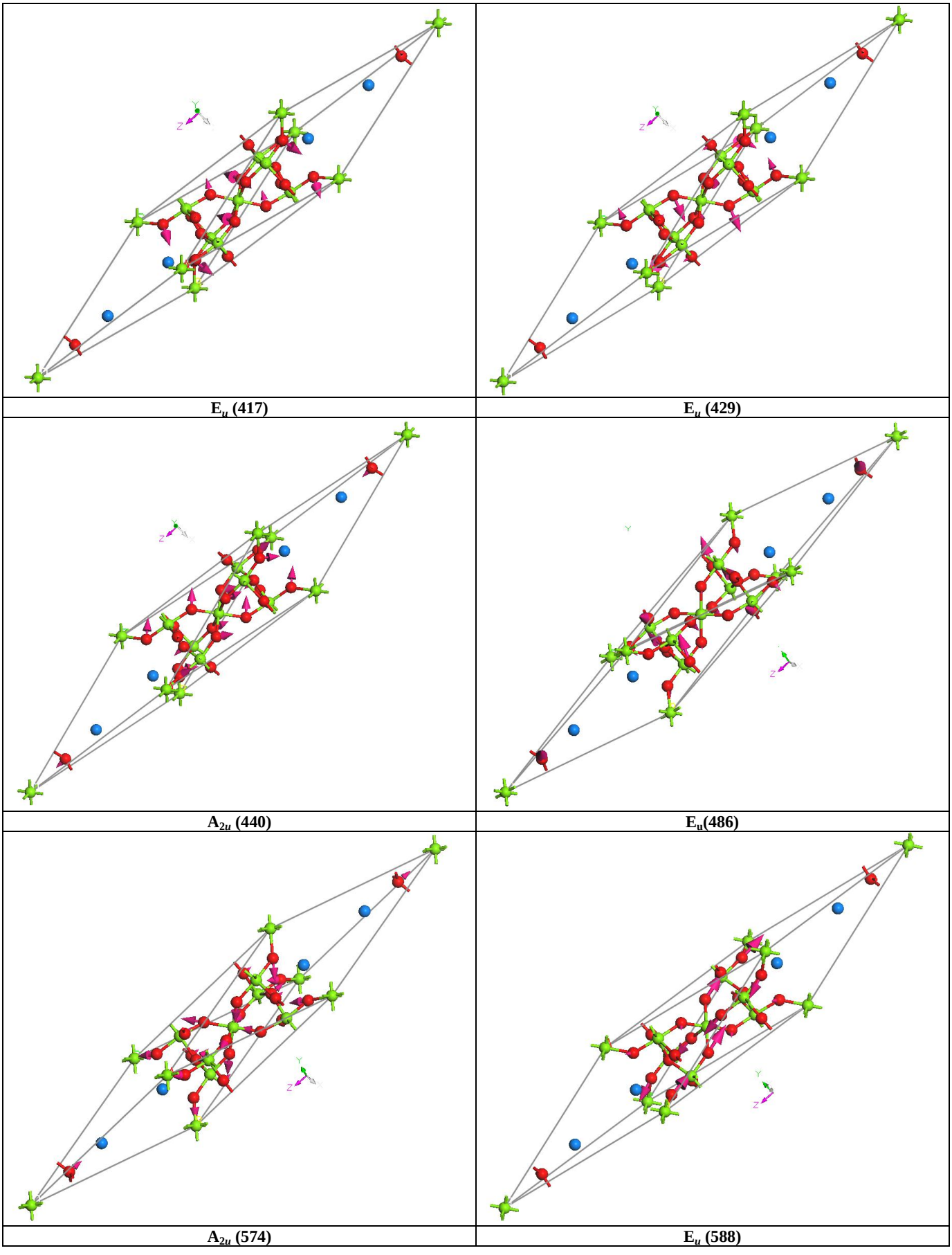


Fig. S3. Coordination polyhedron of K1 is view in the best projection.

Fig. S4. Visualization of calculated vibrational modes (trigonal cell setting was adopted to facilitate calculations, tantalum atoms are light blue, oxygens are red, potassium atoms are violet. Directions of displacement are shown by green arrows. Numbers in parentheses are calculated wavenumbers).

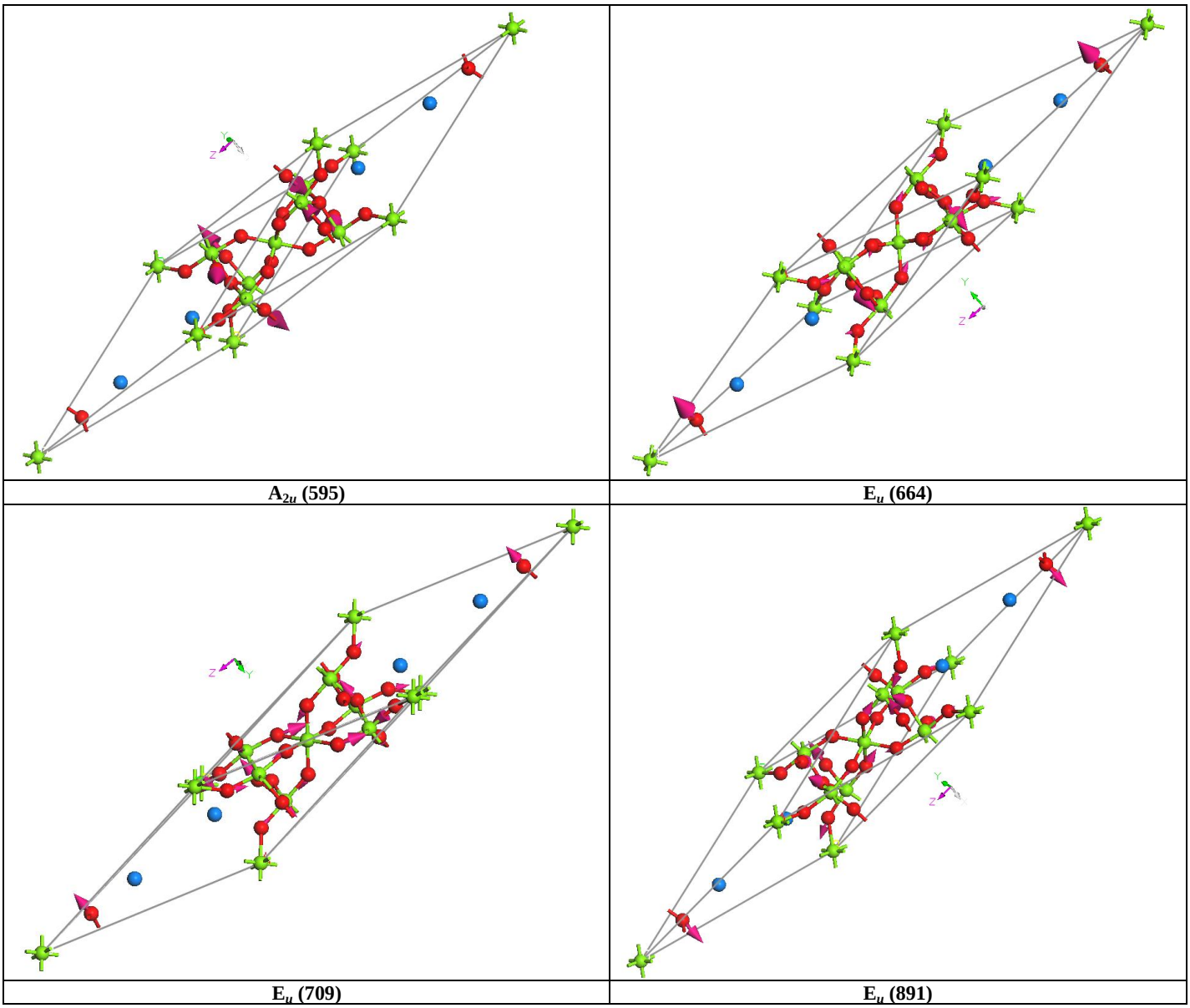


E_u (417) | **E_u (429)**

A_{2u} (440) | **E_u(486)**

A_{2u} (574) | **E_u (588)**

Figure S4. (Continue).



A_{2u} (595)	**E_u (664)**
E_u (709)	**E_u (891)**