Supplementary Material (ESI) for Dalton Transactions

A series of new phases in the Alkali metal-Nb^{V}/Ta^{V}-Se^{IV}/Te^{IV}-O systems

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Supporting information

Topological analysis performed on TOPOS40 program.

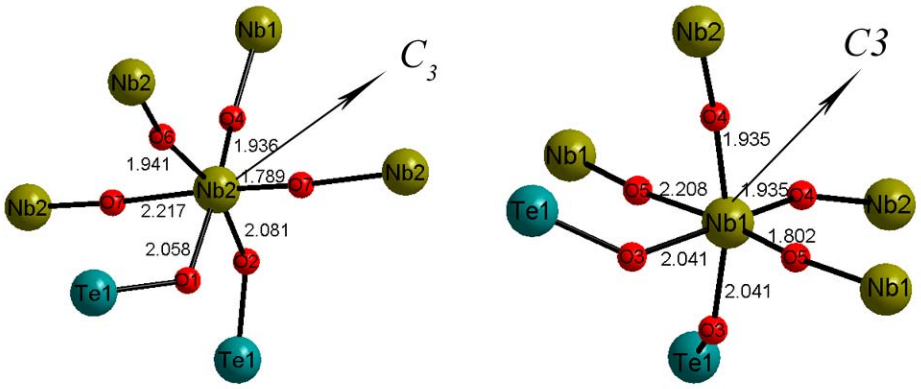
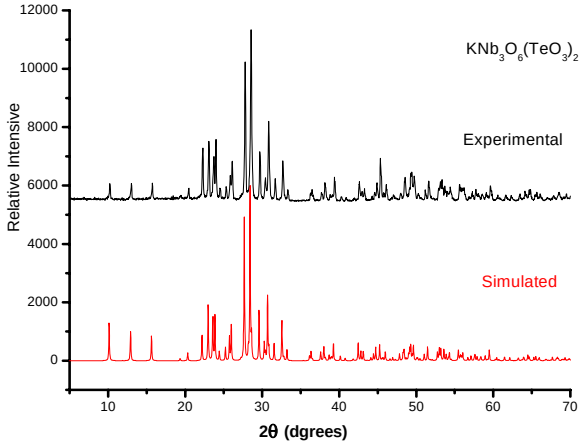
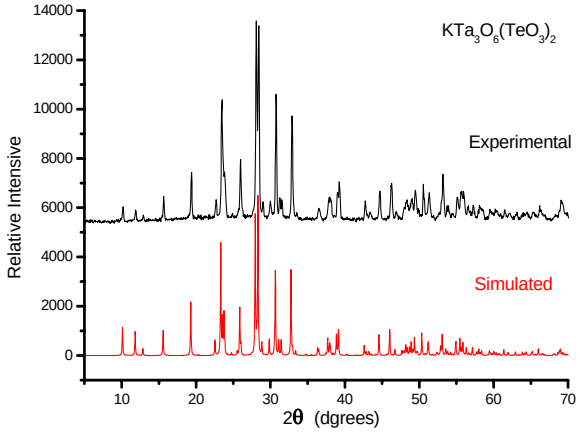


Figure S1. The coordinate environment of Nb(1) and Nb(2) ions in $KNb_3O_6(TeO_3)_2$.



(a)



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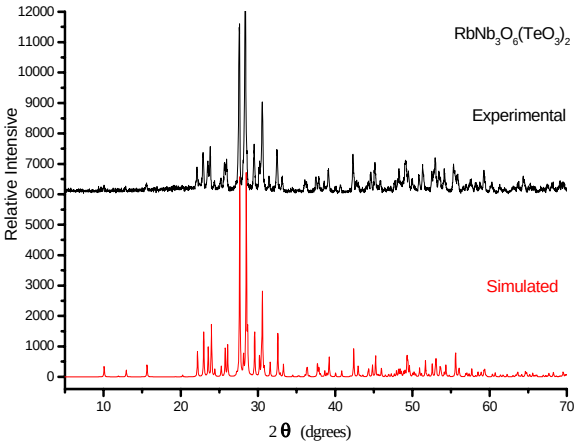

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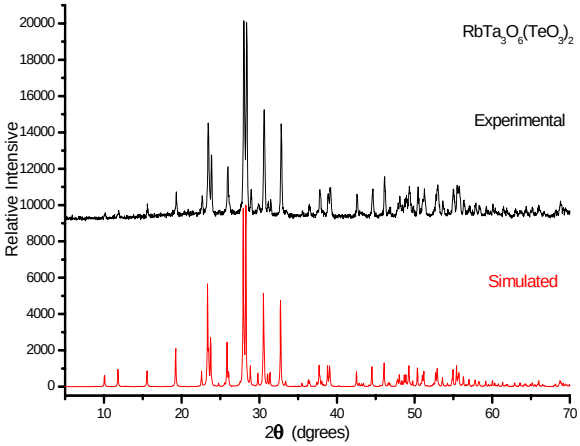

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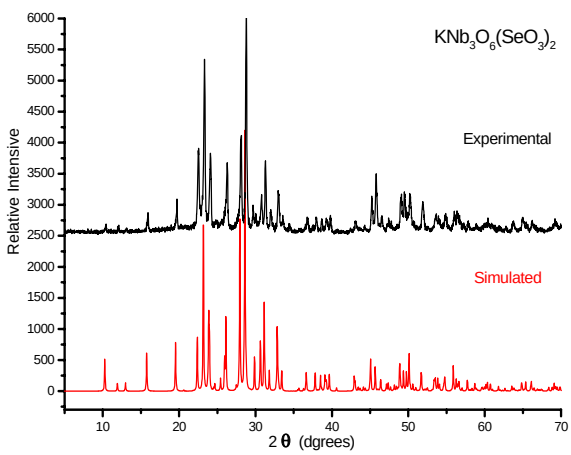

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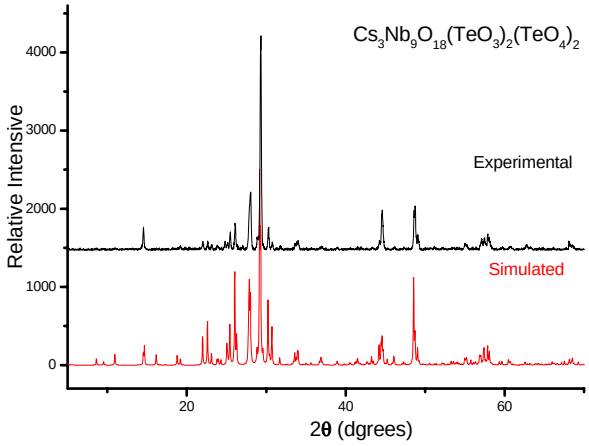
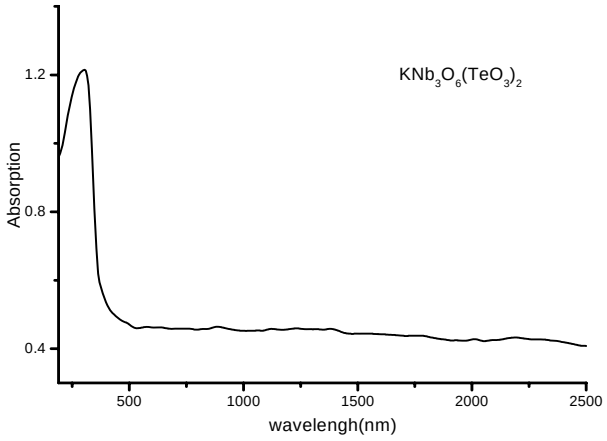
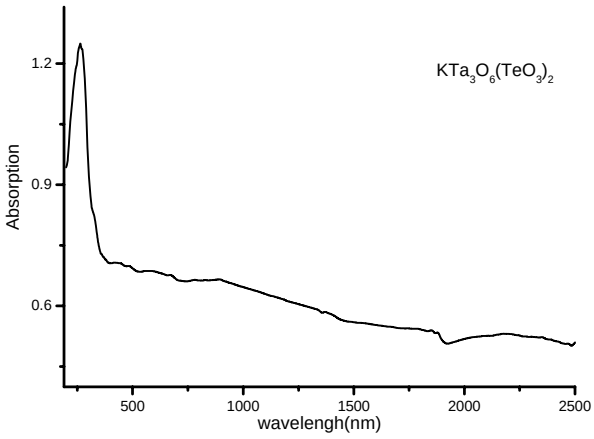


(f)

Figure S2. Simulated and experimental X-ray powder diffraction patterns for **1-6** (a-f)



(a)



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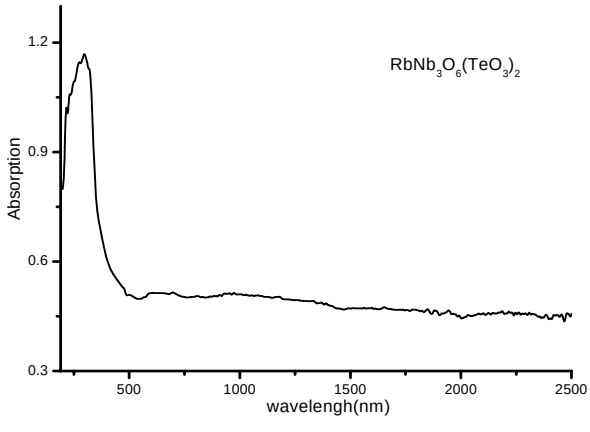

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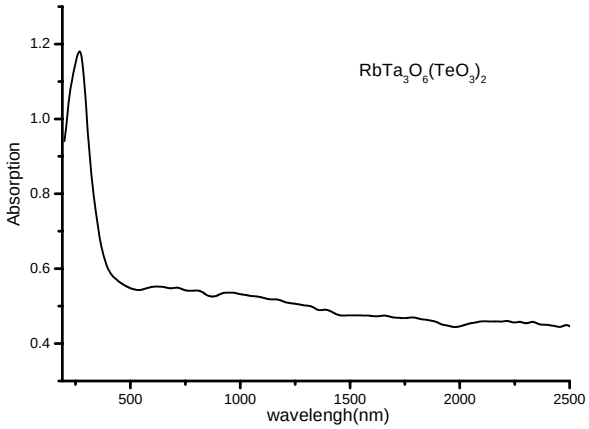

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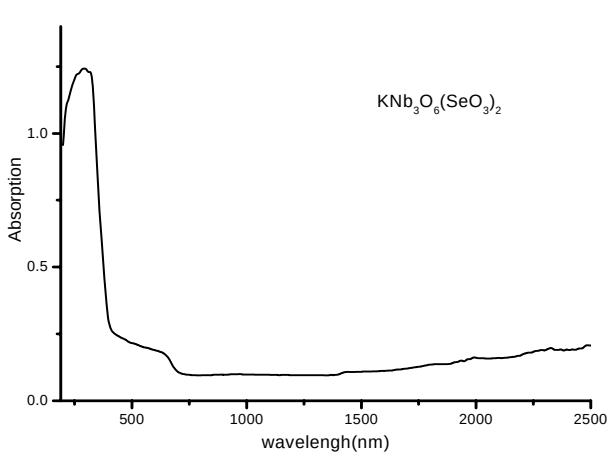

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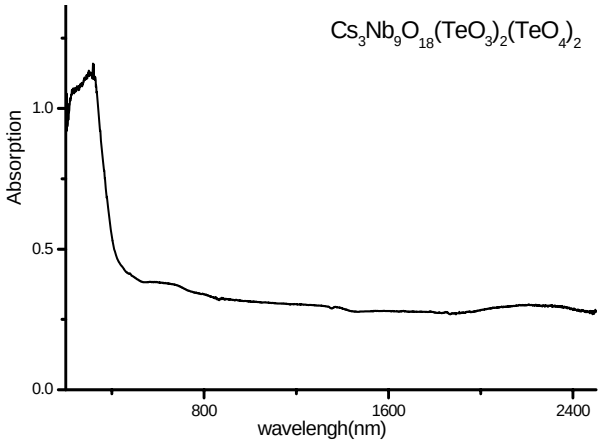
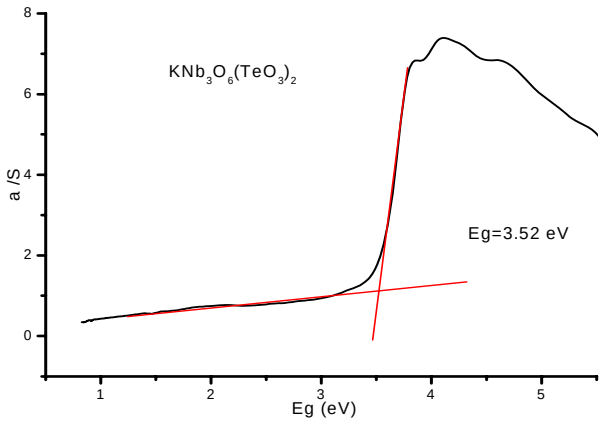
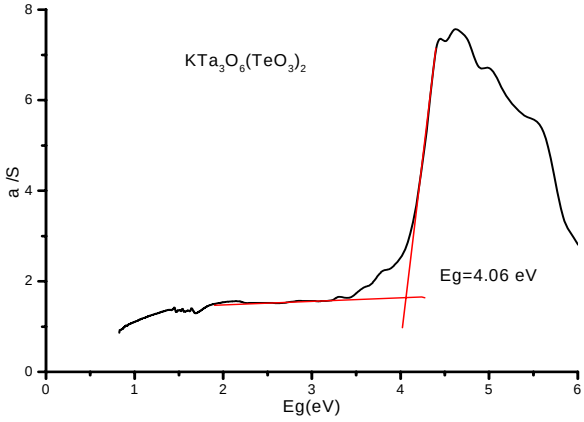


(f)

Figure S3. UV absorption spectra of **1-6** (a-f)



(a)



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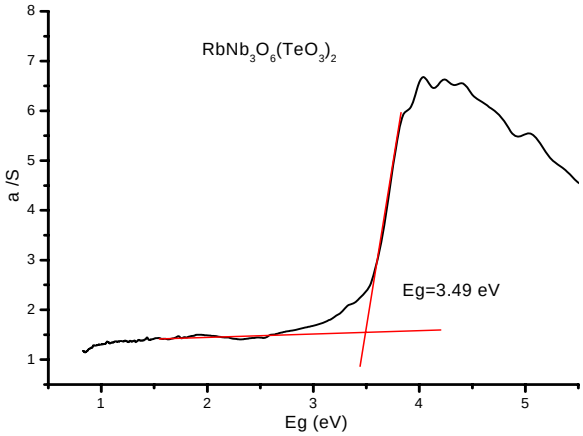

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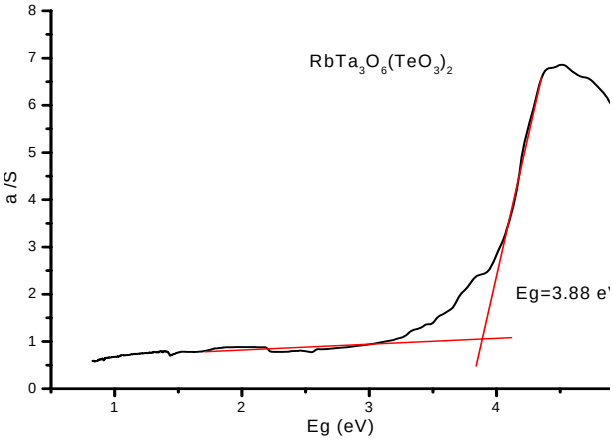

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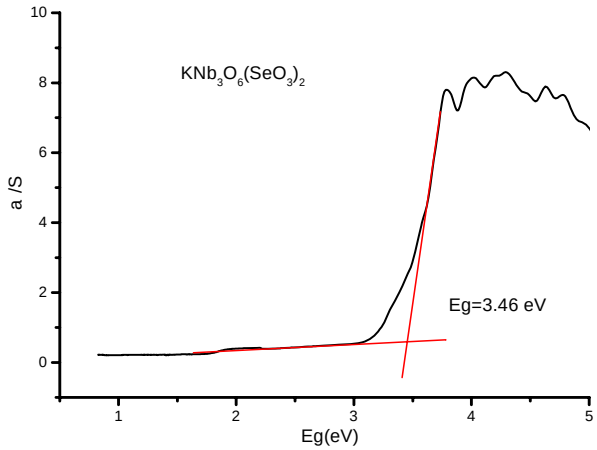

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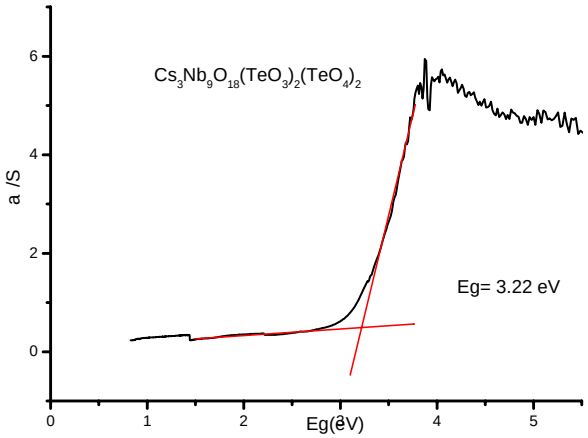
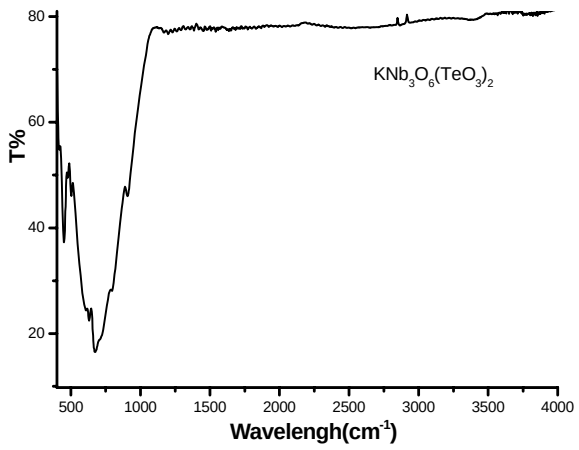
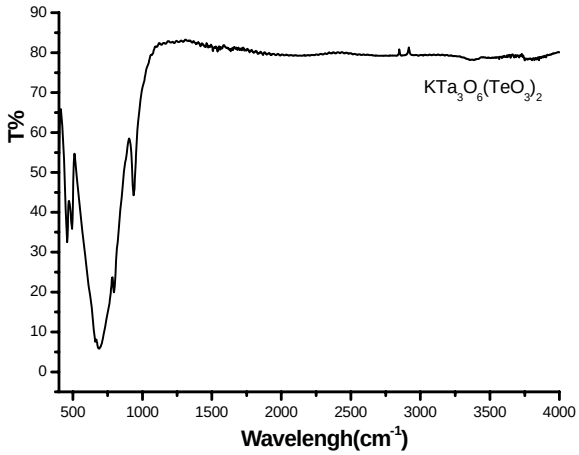


(f)

Figure S4. Optical diffuse reflectance spectra for**1-6** (a-f).



(a)



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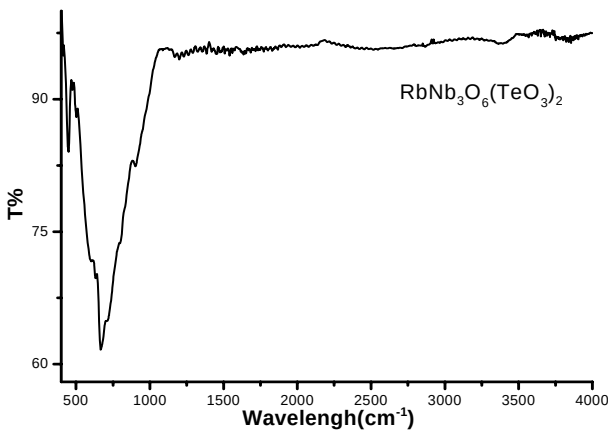

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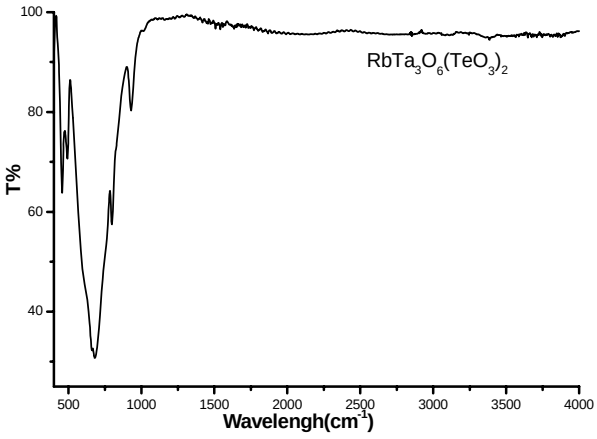

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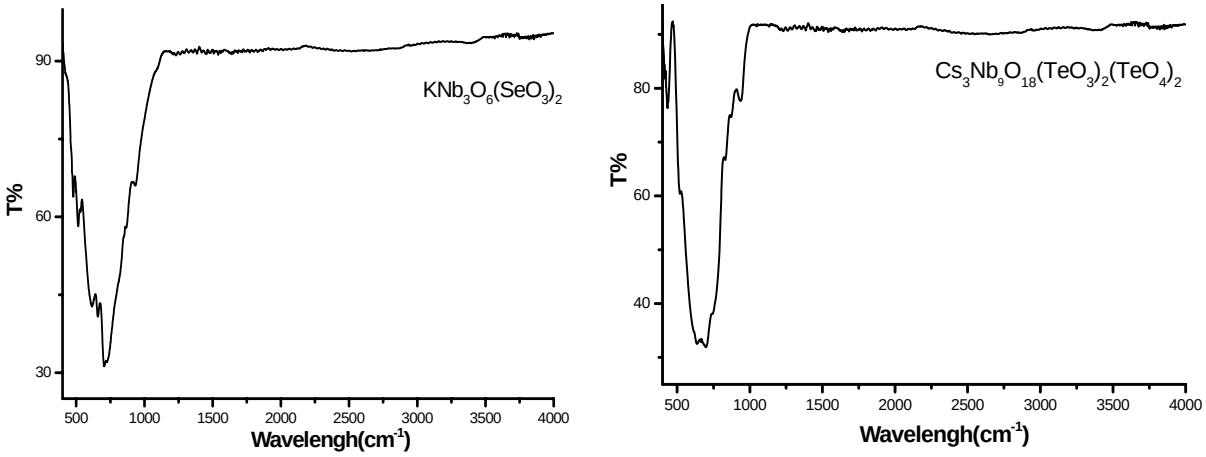

(e) (f)

Figure S5. The infrared spectra of **1-6** (a-f).

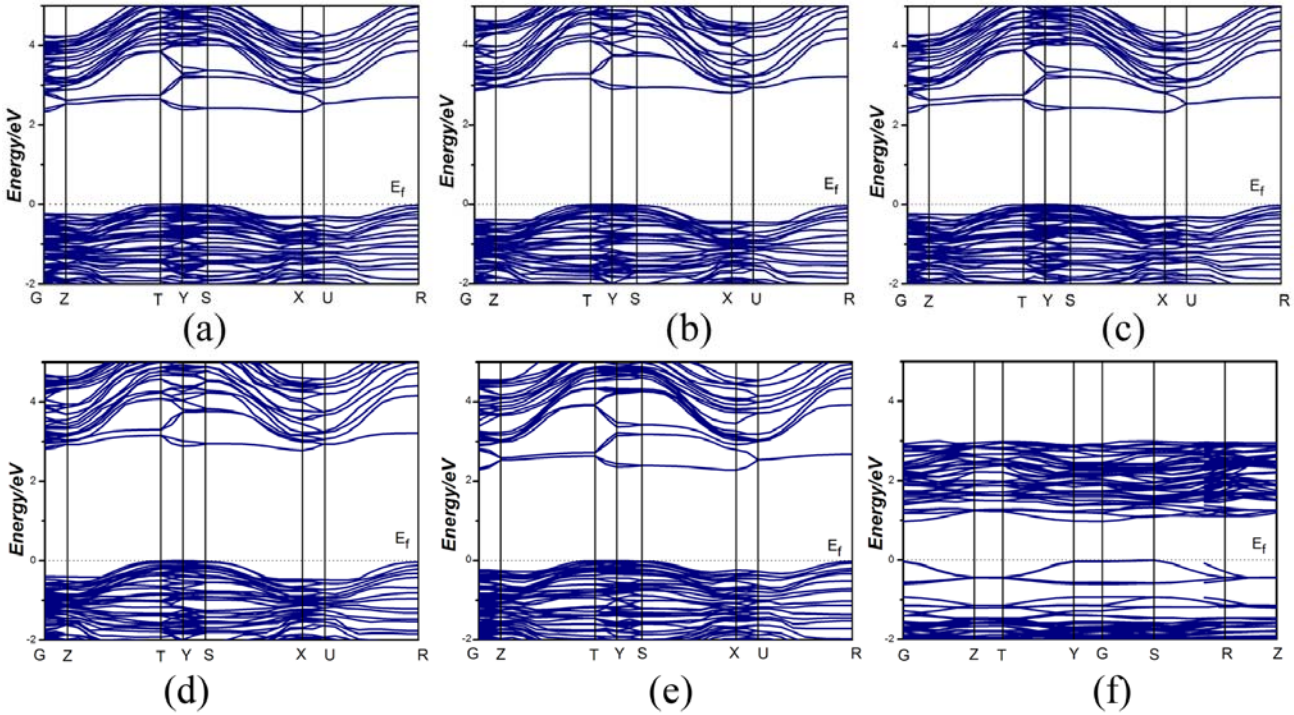

Figure S6. Band structures for the crystals for **1-6** (a-f) (bands are shown between -2 and 5 eV for clarity, and the Fermi level is set at 0 eV).

Topological analysis performed on TOPOS40 program

###############

1: K Nb3 O12 Te2

###############

Topology for Nb1

Atom Nb1 links by bridge ligands and has

Common vertex with					R(A-A)	
Te 1	0.6136	0.5863	0.4027	(0 0 0)	3.551A	1
Te 1	0.6136	0.5863	0.0973	(0 0 0)	3.551A	1
Nb 2	0.2311	0.8500	0.4303	(1 0 0)	3.809A	1
Nb 2	0.2311	0.8500	0.0697	(1 0 0)	3.809A	1
Nb 1	1.2335	0.7061	0.2500	(1 0 0)	4.005A	1
Nb 1	-0.7665	0.7061	0.2500	(-1 0 0)	4.005A	1

Topology for Nb2

Atom Nb2 links by bridge ligands and has

Common vertex with					R(A-A)	
Te 1	0.3864	0.4137	-0.0973	(1 1 0)	3.428A	1
Te 1	0.6136	0.5863	0.0973	(0 0 0)	3.609A	1
Nb 1	0.7665	0.2061	0.2500	(1-1 0)	3.809A	1
Nb 2	0.7689	0.1500	-0.0697	(0 0 0)	3.848A	1
Nb 2	-0.2311	0.3500	0.0697	(-1 0 0)	4.005A	1
Nb 2	1.7689	0.3500	0.0697	(1 0 0)	4.005A	1

Topology for Te1

Atom Te1 links by bridge ligands and has

Common vertex with					R(A-A)	
Nb 2	0.2311	0.6500	-0.0697	(1 1 0)	3.428A	1
Nb 1	0.2335	0.7061	0.2500	(0 0 0)	3.551A	1
Nb 2	0.7689	0.3500	0.0697	(0 0 0)	3.609A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Te2Nb3

Coordination sequences

Nb1:	1	2	3	4	5	6	7	8	9	10
Num	6	18	36	60	94	136	184	240	302	372
Cum	7	25	61	121	215	351	535	775	1077	1449

Nb2: 1 2 3 4 5 6 7 8 9 10

Num 6 17 35 62 96 135 183 240 302 372

Cum 7 24 59 121 217 352 535 775 1077 1449

Te1: 1 2 3 4 5 6 7 8 9 10

Num 3 13 34 60 92 134 183 237 302 373

Cum 4 17 51 111 203 337 520 757 1059 1432

TD10=1442

Vertex symbols for selected sublattice

Nb1 Point (Schlafli) symbol:{4^6.6^7.8^2}

Extended point symbol:[4.4.4.4.4.4.6.6(2).6(3).6(4).6(4).6(4).6(4).8(11).8(11)]

Nb2 Point (Schlafli) symbol:{4^7.6^8}

Extended point symbol:[4.4.4.4.4.4.4.6.6.6.6(2).6(3).6(3).6(5).6(5)]

Te1 Point (Schlafli) symbol:{4^2.6}

Extended point symbol:[4.4.6(4)]

Point (Schlafli) symbol for net: {4^2.6}2{4^6.6^7.8^2}{4^7.6^8}2

3,6,6-c net with stoichiometry (3-c)2(6-c)3; 3-nodal net

New topology, please, contact the authors (66909 types in 9 databases)