Supporting Information for

"Screening Surface Structure of MXenes by High-Throughput Computation and Vibrational Spectroscopic Confirmation"

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Supplementary summary

List of structures

From page **S14** on we provide crystal structure data about multi-component MXenes, reported in the following order according to their chemical formula. Below we list all MXenes with the corresponding section number, linking to the page dedicated to this material.

Benchmark calculations

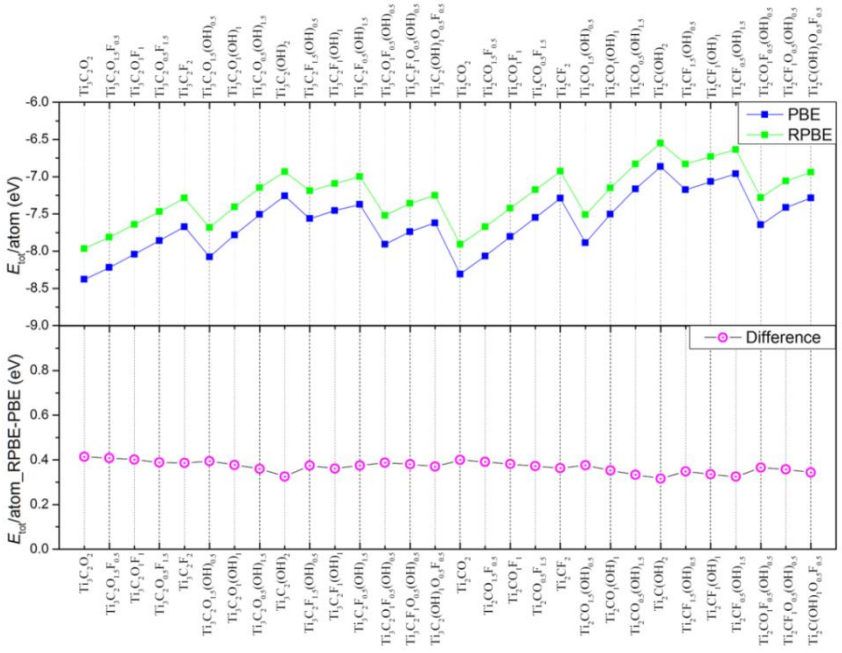

Figure S1. Calculated total energy of $Ti_3C_2T_x$ and Ti_2CT_x MXenes with respect to atoms using PBE and RPBE functionals and their difference.

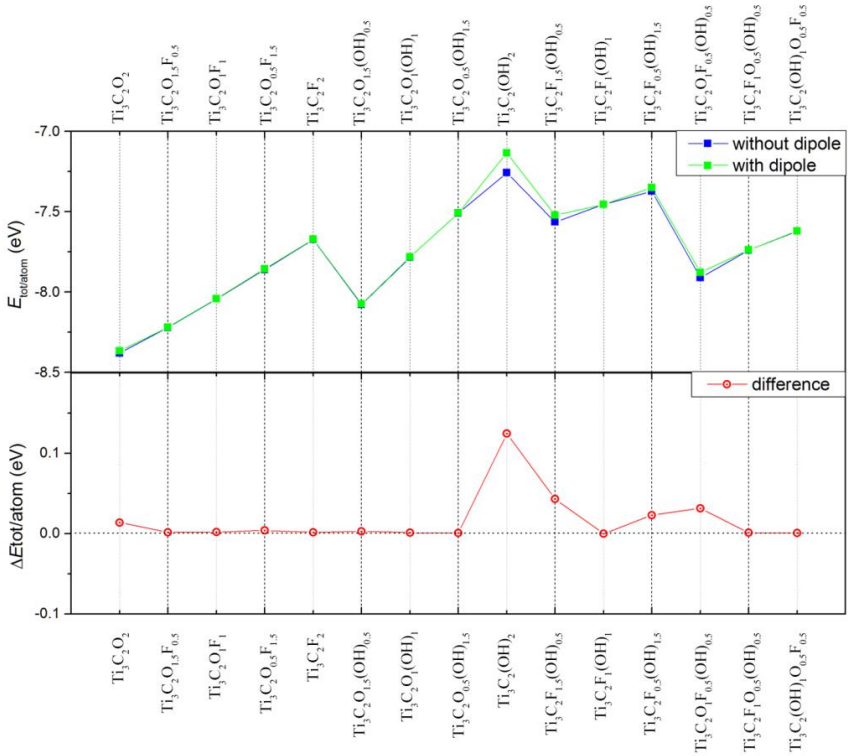

Figure S2. Benchmark calculations of dipole in MXenes. Note that the dipole corrections do not change the order of E_{tot}/atom.

Ground-state surface structure screening

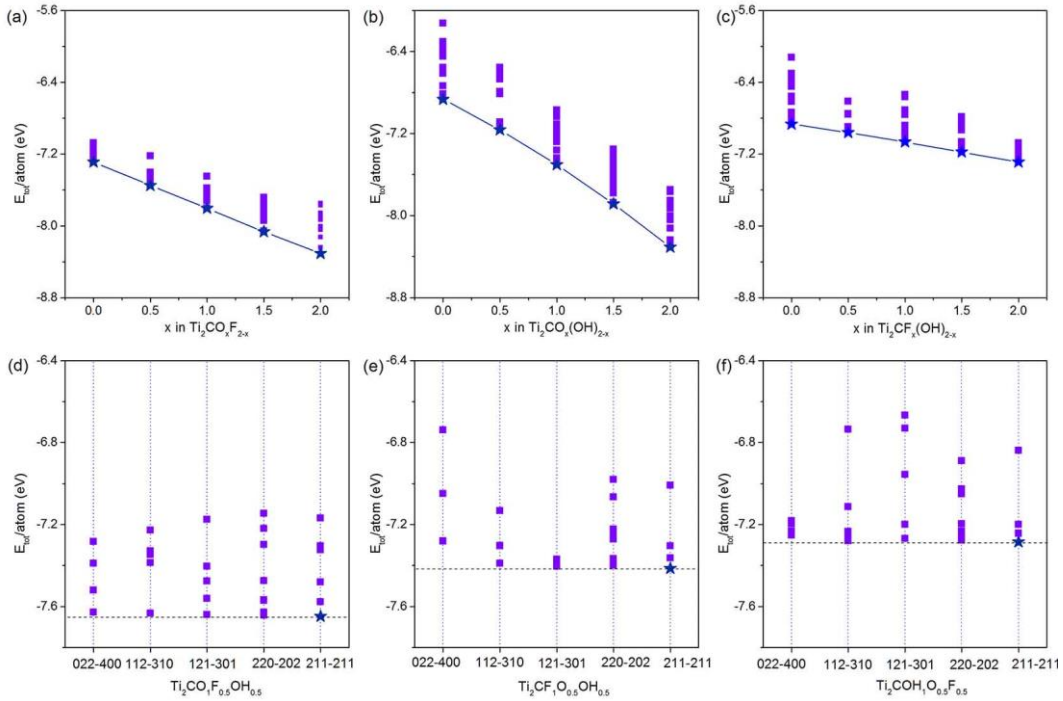

Figure S3. Energetic distributions of randomly generated structures for termination-mixed functionalized Ti_2CT_x MXenes.

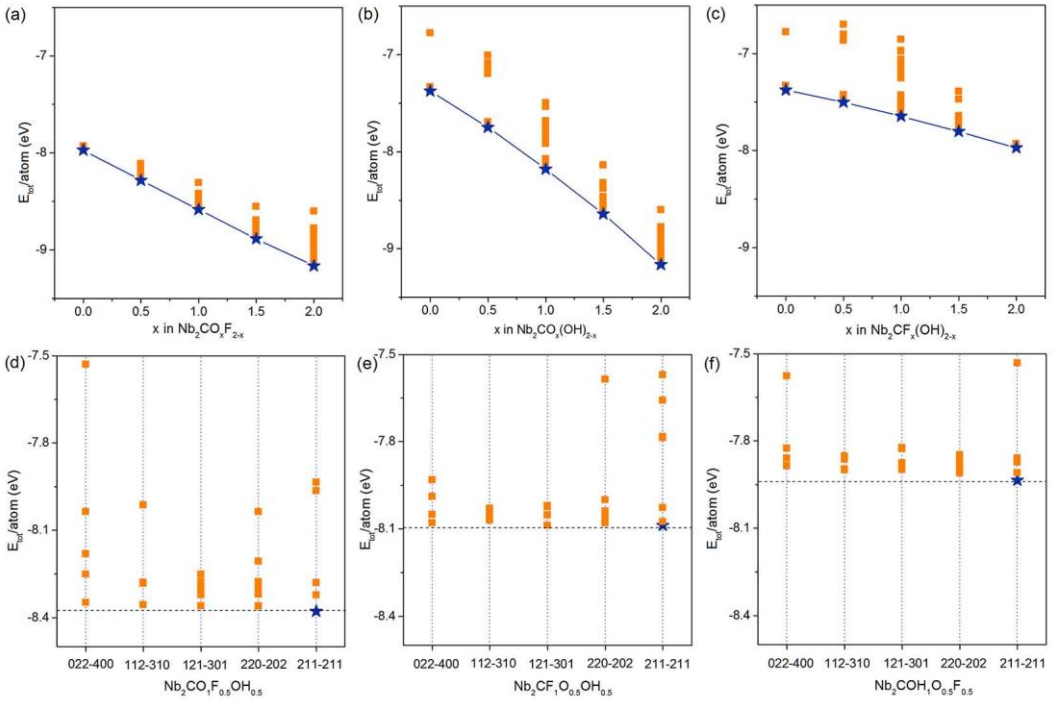

Figure S4. Energetic distributions of randomly generated structures for termination-mixed functionalized Nb_2CT_x MXenes.

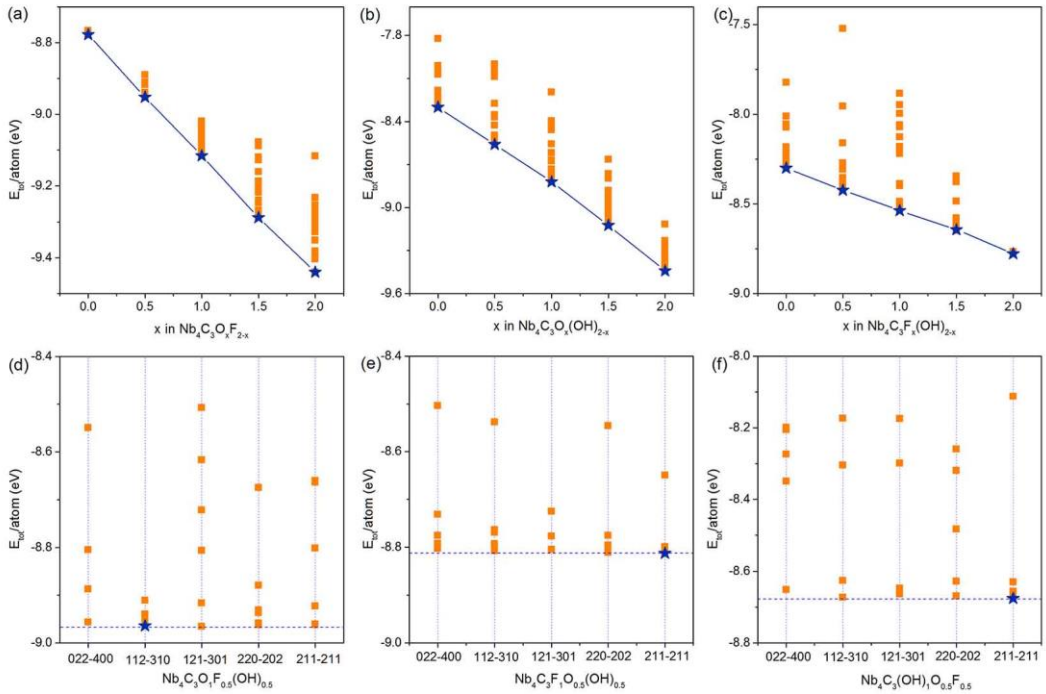

Figure S5. Energetic distributions of randomly generated structures for termination-mixed functionalized $Nb_4C_3T_x$ MXenes.

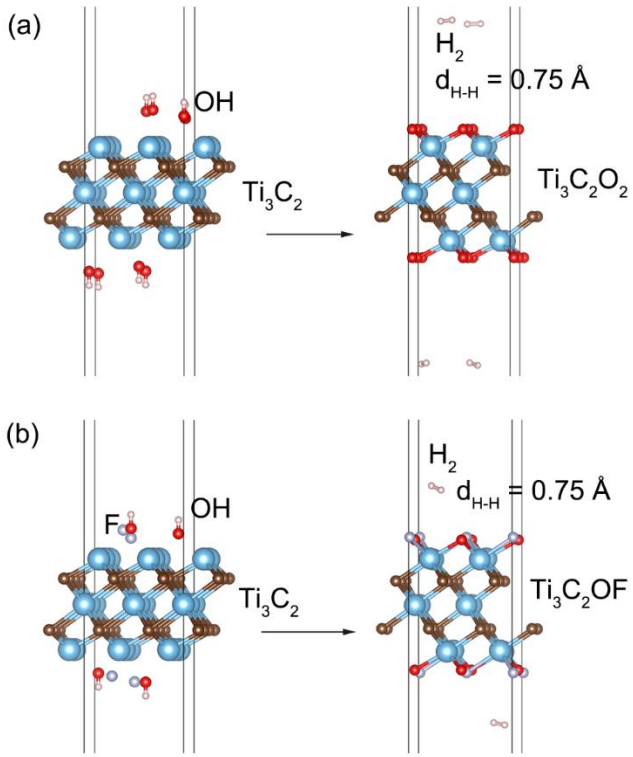

Figure S6. Schematic of dehydrogenation observed during the global surface structure search. (a) $Ti_3C_2+2OH \rightarrow Ti_3C_2O_2+H_2$, (b) $2Ti_3C_2+2F+2OH \rightarrow 2Ti_3C_2OF+H_2$.

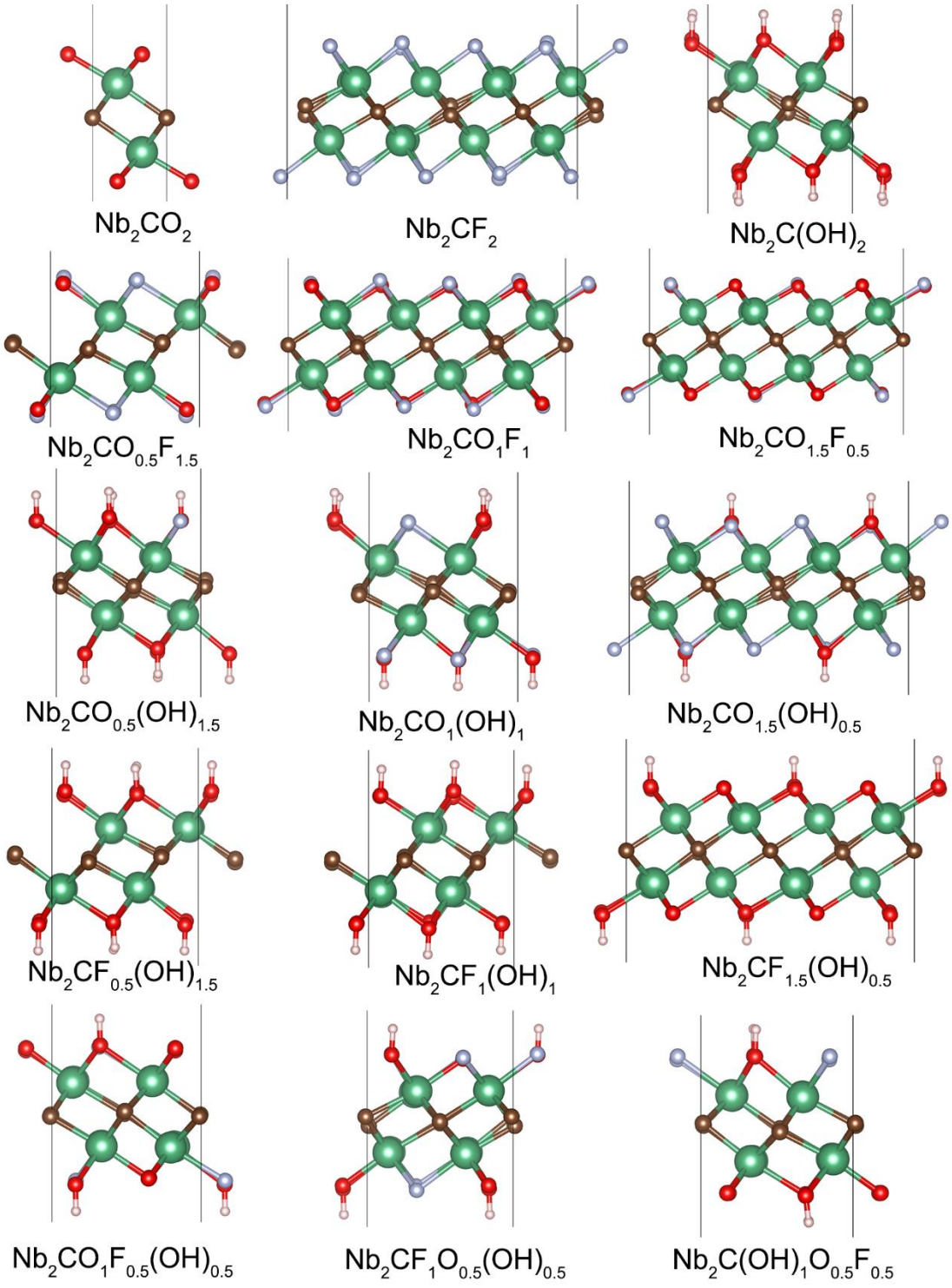

Figure S7. Screened low-energy structures of Nb_2CT_x. It is noteworthy that dramatic structure changes occur in the substrate during structural relaxation of F and OH containing Nb_2CT_x structures.

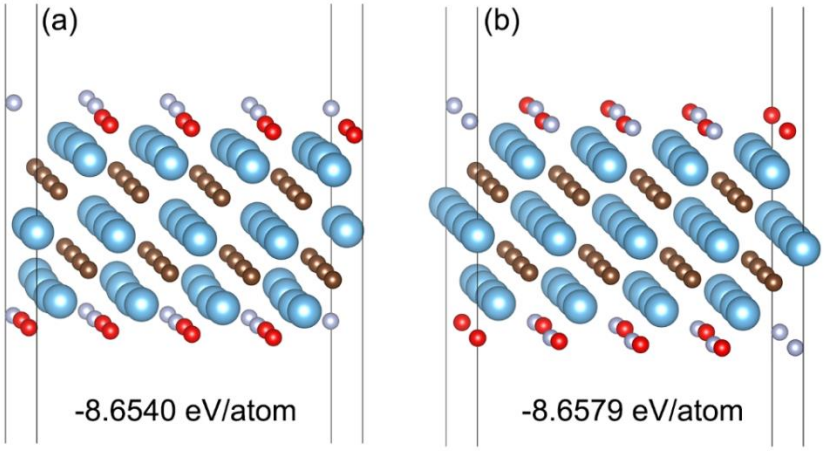

Figure S8. Optimized $Ti_{48}C_{32}O_{16}F_{16}$ structures and free energies. (a) non-mixed in-plane distribution pattern and (b) mixed in-plane distribution pattern. The identical terminations tend to repulse each other, resulting higher free energy.

The bubble size is determined by:

$$R_B = \frac{(E-E_{min})}{(E_{max}-E_{min})} \times (R_{max} - R_{min}) + R_{min}$$

where R_B the bubble radius, E the absolute value of free energy, E_{min} the minimum absolute value of free energy, E_{max} the maximum absolute value of free energy, R_{min} the minimum radius and R_{max} the maximum radius. The E_{min}= 6.86 eV corresponding to $Ti_2C(OH)_2$, E_{max}= 9.44 eV corresponding to $Nb_4C_3O_2$. In this plot, the smallest bubble radius and biggest bubble radius are set to 0.06 and 0.27 inch, respectively. The bubble radius at any other E can be obtained by the above formula. In this way, the relative stability between different systems can also be compared: the stability increases with the thickness.

Table S1 Bubble sizes used in Figure 4

	E_{min} (eV)	R_{min} (inch)	E_{max} (eV)	R_{max} (inch)
Ti_2CT_x	6.86	0.06	8.31	0.18
$Ti_3C_2T_x$	7.26	0.09	8.38	0.18
$Nb_4C_3T_x$	8.30	0.18	9.44	0.27

Phonon calculations

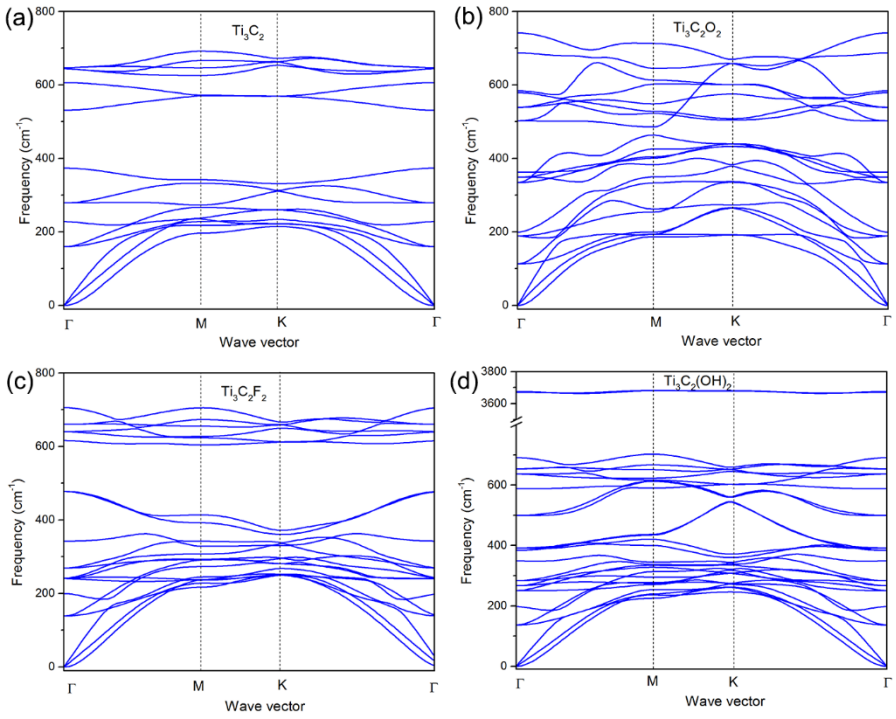

Figure S9. Phonon dispersions of (a)Ti_3C_2, (b)$Ti_3C_2O_2$, (c)$Ti_3C_2F_2$, and (d)$Ti_3C_2(OH)_2$. Note that no negative frequency in the whole first Brillouin zone indicates that all the $Ti_3C_2T_2$ (T = O, F and OH) MXenes are dynamically stable.

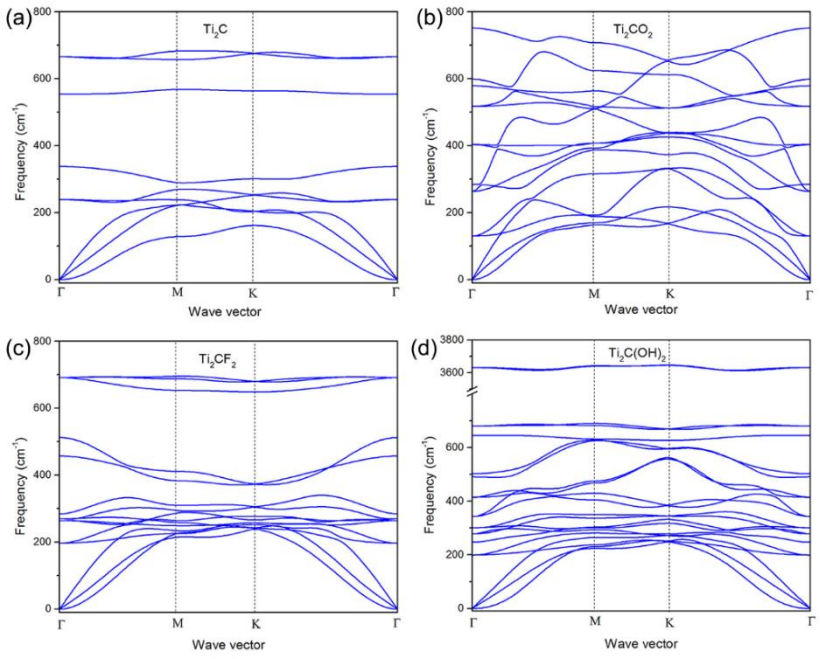

Figure S10. Phonon dispersions of (a)Ti_2C, (b)Ti_2CO_2, (c)Ti_2CF_2, and (d)$Ti_2C(OH)_2$.

Note that no negative frequency in the whole first Brillouin zone indicates that all the Ti_2CT_2 (T = O, F and OH) MXenes are dynamically stable.

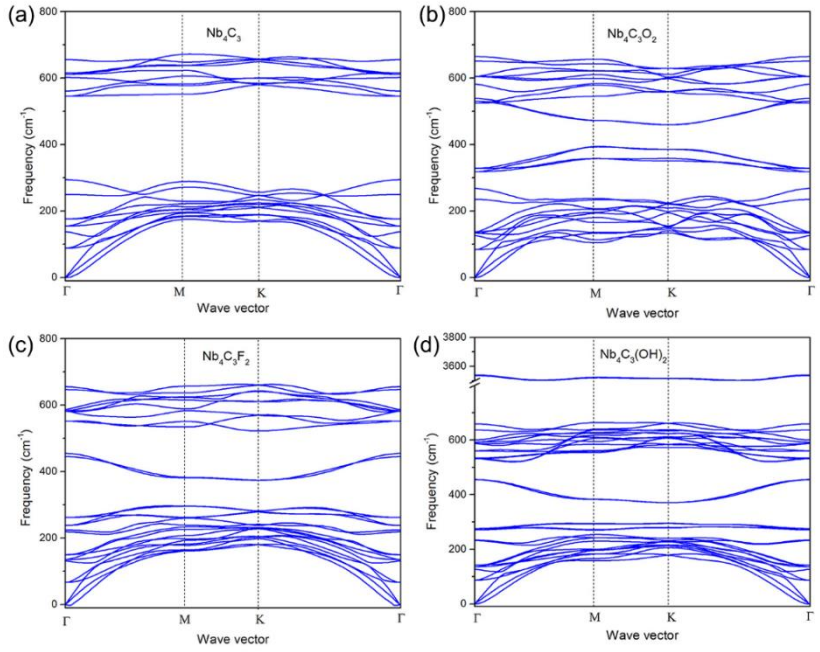

Figure S11. Phonon dispersions of (a)Nb_4C_3, (b)$Nb_4C_3O_2$, (c) $Nb_4C_3F_2$, and (d)$Nb_4C_3(OH)_2$. Note that no negative frequency in the whole first Brillouin zone indicates that all the $Nb_4C_3T_2$ (T = O, F and OH) MXenes are dynamically stable.

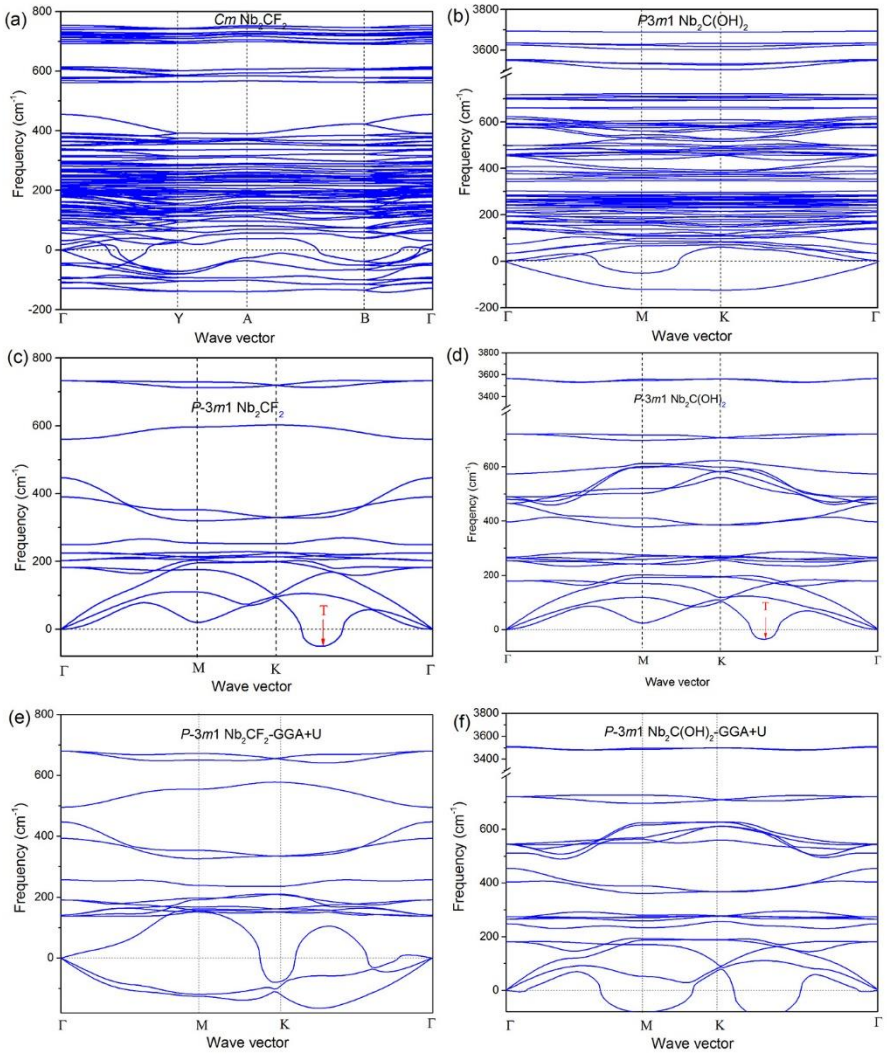

Figure S12. Phonon dispersions of (a) *Cm* Nb_2CF_2, (b) *P*3*m*1 $Nb_2C(OH)_2$, (c) $P\bar{3}m1$ Nb_2CF_2, (d) $P\bar{3}m1$ $Nb_2C(OH)_2$ by standard GGA and (e) $P\bar{3}m1$ Nb_2CF_2, (f) $P\bar{3}m1$ $Nb_2C(OH)_2$ by GGA+U. Both *Cm* and $P\bar{3}m1$ Nb_2CF_2, *P*3*m*1 and $P\bar{3}m1$ $Nb_2C(OH)_2$ are dynamically unstable.

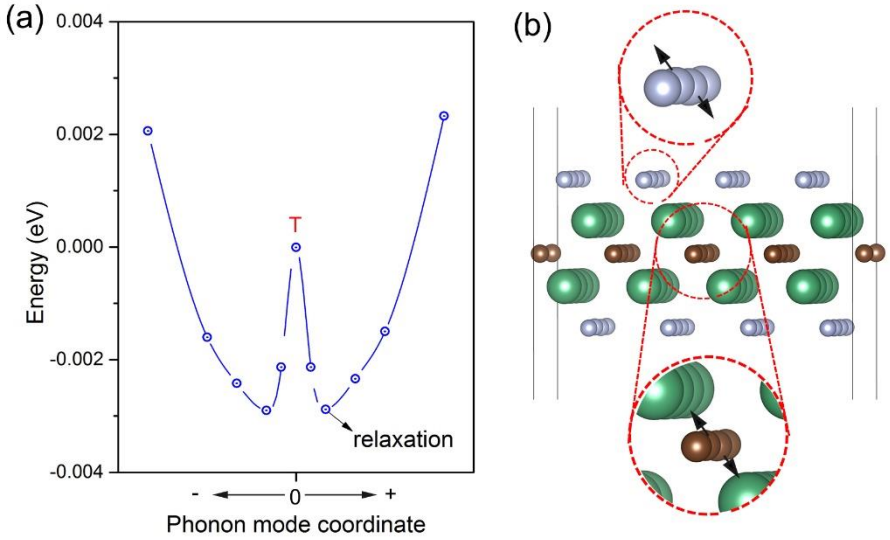

Figure S13. Origin of the imaginary mode of Nb_2CF_2 at T point. (a) Potential energy as a function of the phonon displacement along the mode. (b) The relaxed structure of the potential energy minimum. The anharmonic double-well potentials along the modes labeled T, and this is also found in SnSe (Ref. 1).

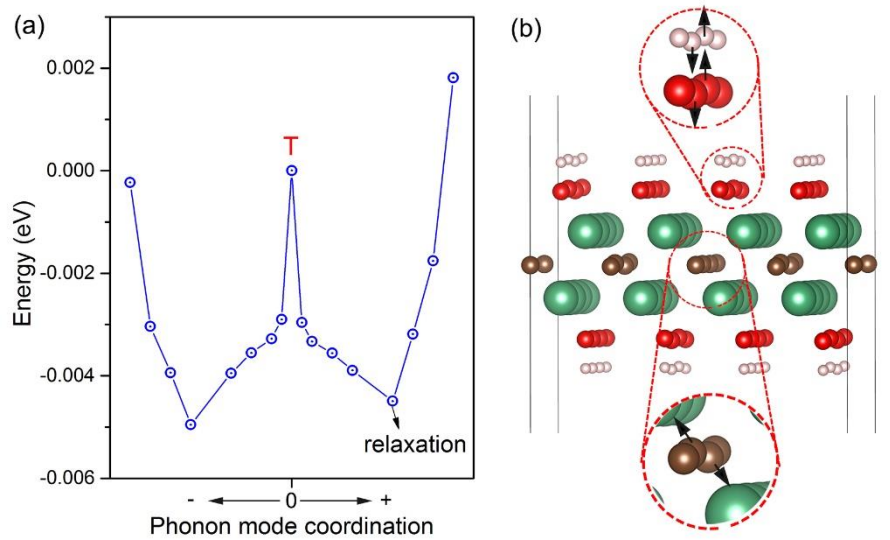

Figure S14. Origin of the imaginary mode of $Nb_2C(OH)_2$ at T point. (a) Potential energy as a function of the phonon displacement along the mode. (b) The relaxed structure of the potential energy minimum.

(1) Skelton, J. M.; Burton, L. A.; Parker, S. C.; Walsh, A.; Kim, C. E.; Soon, A.; Buckeridge, J.; Sokol, A. A.; Catlow, C. R.; Togo, A.; Tanaka, I. Anharmonicity in the High-Temperature *Cmcm* Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Phys. Rev. Lett.* **2016** *117*, 075502.

Assignment of Raman active vibration modes

The Raman active vibration modes of $Ti_3C_2T_2$, Ti_2CT_2, Nb_2CT_2 and $Nb_4C_3T_2$ monosheets are assigned to three kinds: external modes of M-C_3T_3 octahedron, internal modes of M-C_3T_3 octahedron, and internal modes of OH group.

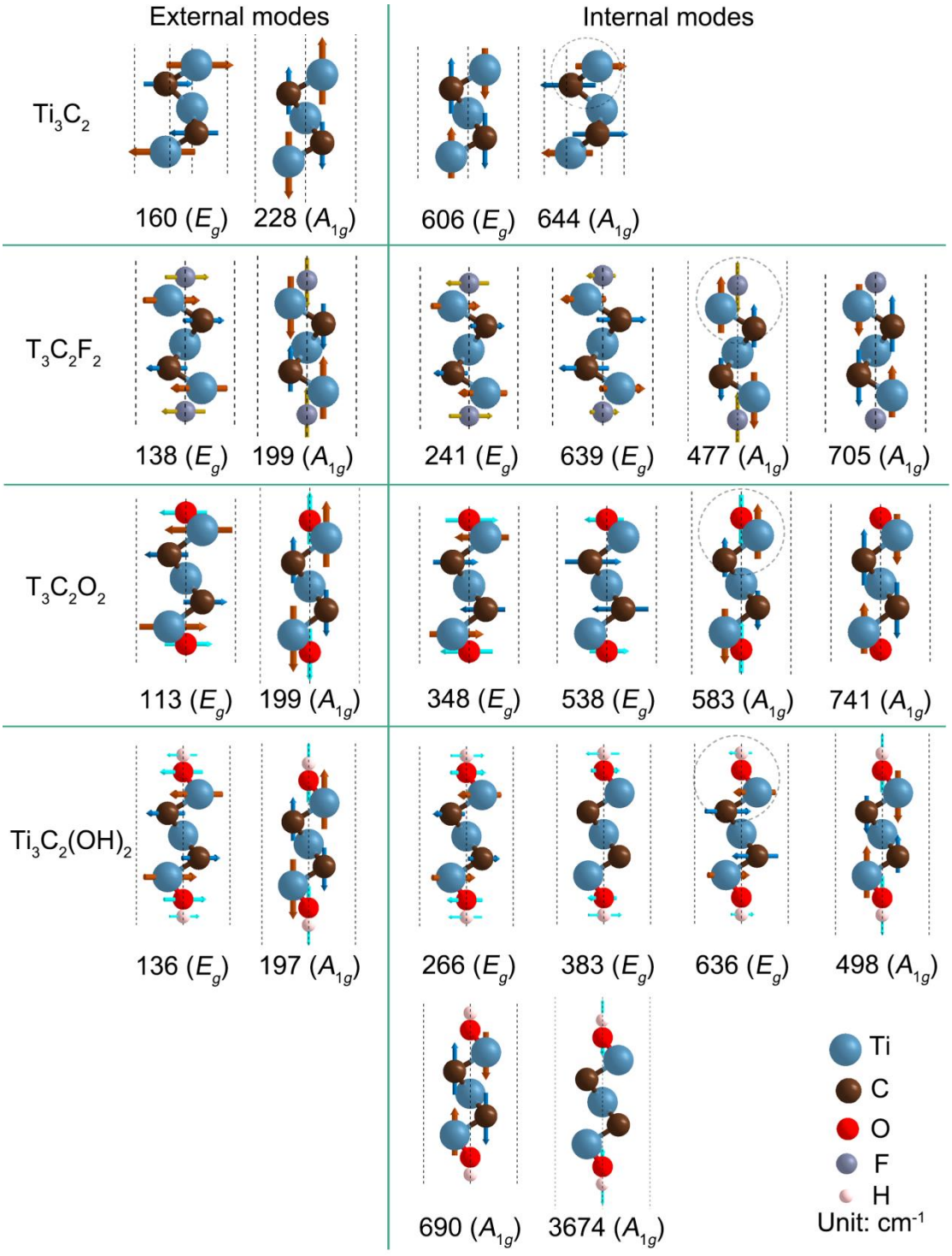

Figure S15. Raman active vibration modes of $Ti_3C_2T_2$.

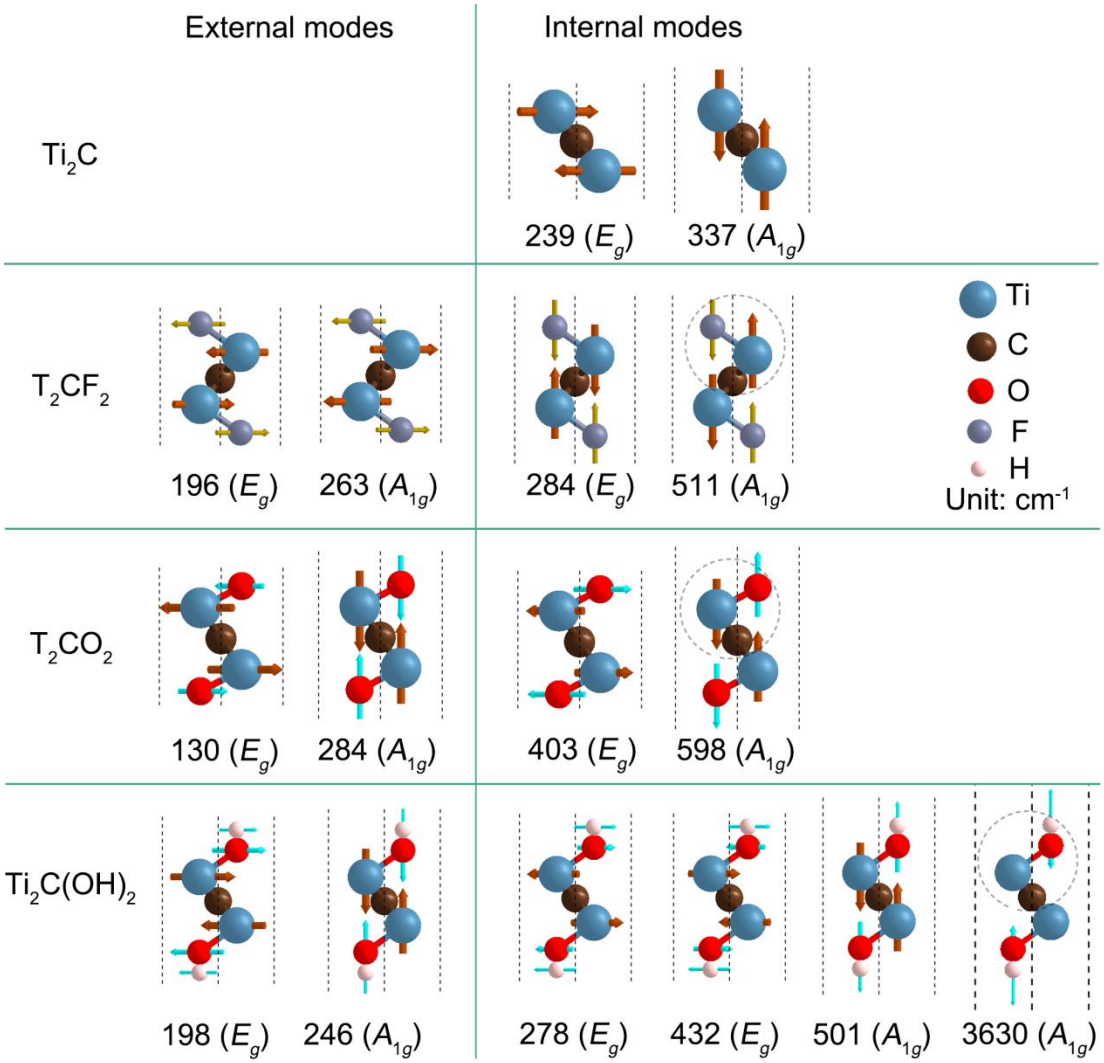

Fig. S16 Raman active vibration modes of Ti_2CT_2.

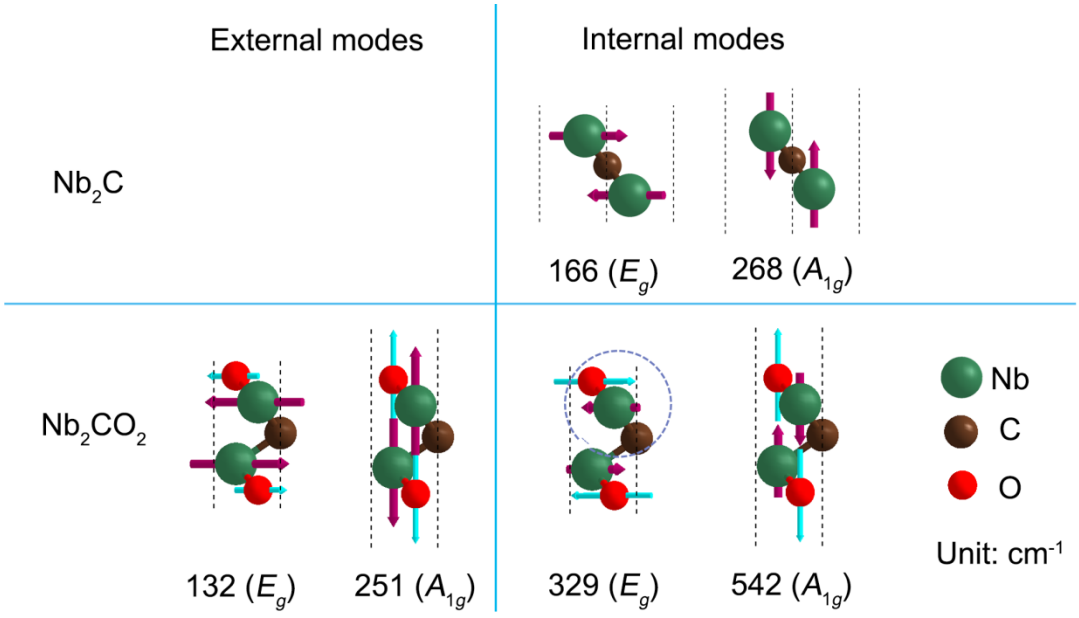

Figure S17. Raman active vibration modes of Nb_2CT_2.

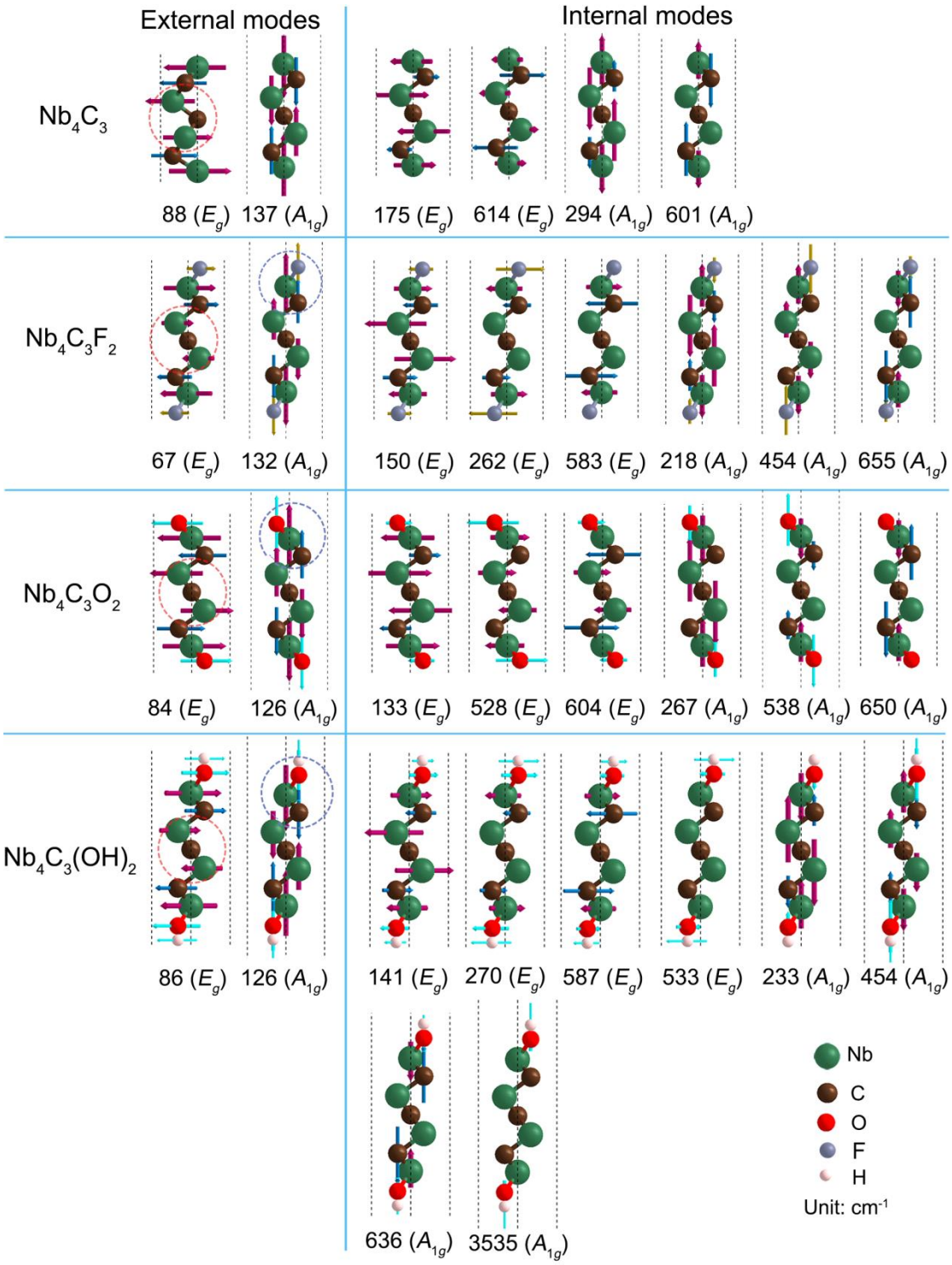

Figure S18. Raman active vibration modes of $Nb_4C_3T_2$.

Crystal structures

1 $Ti_3C_2O_2$

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.0418999195	0.0000000000	0.0000000000
a_2	-1.5209499598	2.6343626061	0.0000000000
a_3	0.0000000000	0.0000000000	22.3178997040

	Fraction coordination		
Ti	0.000000000	0.000000000	0.500000000
Ti	0.333330005	0.666670024	0.384160012
Ti	0.666670024	0.333330005	0.615840018
C	0.666670024	0.333330005	0.443109989
C	0.333330005	0.666670024	0.556890011
O	0.000000000	0.000000000	0.343059987
O	0.000000000	0.000000000	0.656939983

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2 $Ti_3C_2O_{1.5}F_{0.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.0836000443	0.0000000000	0.0000000000
a_2	-3.0418000221	5.2685521848	0.0000000000
a_3	0.0000000000	0.0000000000	22.4335994720

	Fraction coordination		
Ti	0.000000000	0.500000000	0.500000000
Ti	0.000000000	0.000000000	0.500000000
Ti	0.500000000	0.500000000	0.500000000
Ti	0.500000000	0.000000000	0.500000000
Ti	0.173199996	0.826799989	0.611559987
Ti	0.173199996	0.346390009	0.611559987
Ti	0.653609991	0.826799989	0.611559987
Ti	0.666670024	0.333330005	0.614730000
Ti	0.333330005	0.666670024	0.385270000
Ti	0.346390009	0.173199996	0.388440013
Ti	0.826799989	0.653609991	0.388440013
Ti	0.826799989	0.173199996	0.388440013
C	0.333330005	0.666670024	0.556200027
C	0.333499998	0.166749999	0.556789994
C	0.833249986	0.666499972	0.556789994
C	0.833249986	0.166749999	0.556789994
C	0.166749999	0.833249986	0.443210006

C	0.166749999	0.333499998	0.443210006
C	0.666499972	0.833249986	0.443210006
C	0.666670024	0.333330005	0.443800002
O	0.499430001	0.500569999	0.655809999
O	0.499430001	0.998870015	0.655809999
O	0.001130000	0.500569999	0.655809999
O	0.500569999	0.001130000	0.344190001
O	0.500569999	0.499430001	0.344190001
O	0.998870015	0.499430001	0.344190001
F	0.000000000	0.000000000	0.662109971
F	0.000000000	0.000000000	0.337889999

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3 Ti_3C_2OF

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	21.9305992126	0.0000000000	0.0000000000
a_2	0.0000000000	3.0539999008	0.0000000000
a_3	0.0000000000	0.0000000000	5.2845997810

	Fraction coordination		
Ti	0.500000000	0.000000000	0.000000000
Ti	0.500000000	0.500000000	0.500000000
Ti	0.388639987	0.500000000	0.176899999
Ti	0.386099994	0.000000000	0.649699986
Ti	0.611360013	0.500000000	0.823099971
Ti	0.613900006	0.000000000	0.350300014
C	0.441390008	0.500000000	0.834429979
C	0.442099988	0.000000000	0.331160009
C	0.558610022	0.500000000	0.165570006
C	0.557900012	0.000000000	0.668839991
O	0.340970010	0.500000000	0.496890008
O	0.659030020	0.500000000	0.503109992
F	0.334439993	0.000000000	0.000600000
F	0.665560007	0.000000000	0.999400020

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4 $Ti_3C_2O_{0.5}F_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1265401840	0.0000000000	0.0000000000
a_2	-3.0632698820	5.3051272773	0.0000000000
a_3	0.0000000000	0.0000000000	22.2315006256

	Fraction coordination		
Ti	0.958800018	0.971930027	0.500810027

Ti	0.958779991	0.471920013	0.500810027
Ti	0.458819985	0.971939981	0.500800014
Ti	0.458790004	0.471940011	0.500810027
Ti	0.118790001	0.292039990	0.609979987
Ti	0.118809998	0.811689973	0.609969974
Ti	0.625450015	0.305180013	0.608139992
Ti	0.638520002	0.811730027	0.609960020
Ti	0.279009998	0.132110000	0.391620010
Ti	0.292169988	0.638750017	0.393469989
Ti	0.798789978	0.132100001	0.391640007
Ti	0.798690021	0.651769996	0.391649991
C	0.293430001	0.139200002	0.558189988
C	0.292089999	0.638540030	0.559679985
C	0.791440010	0.139210001	0.558189988
C	0.791480005	0.637269974	0.558179975
C	0.126120001	0.306639999	0.443430007
C	0.126149997	0.804669976	0.443430007
C	0.625469983	0.305319995	0.441940010
C	0.624159992	0.804690003	0.443459988
O	0.958739996	0.971819997	0.657440007
O	0.958859980	0.972100019	0.344159991
F	0.461019993	0.976390004	0.663649976
F	0.954289973	0.469630003	0.663649976
F	0.461050004	0.469509989	0.663649976
F	0.456499994	0.967549980	0.337929994
F	0.456629992	0.474500000	0.337960005
F	0.963549972	0.474480003	0.337969989

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5 $Ti_3C_2F_2$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.0752000809	0.0000000000	0.0000000000
a_2	-1.5376000404	2.6632013918	0.0000000000
a_3	0.0000000000	0.0000000000	22.0603008270

		Fraction coordination	
Ti	0.000000000	0.000000000	0.500000000
Ti	0.333330005	0.666670024	0.393559992
Ti	0.666670024	0.333330005	0.606440008
C	0.666670024	0.333330005	0.442319989
C	0.333330005	0.666670024	0.557680011
F	0.000000000	0.000000000	0.336800009
F	0.000000000	0.000000000	0.663200021

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6 $Ti_3C_2O_{1.5}(OH)_{0.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.0820999146	0.0000000000	0.0000000000
a_2	-3.0410077319	5.2674277266	0.0000000000
a_3	0.0000000000	0.0000000000	22.2176990509
		Fraction coordination	
Ti	0.984790027	0.015790001	0.499909997
Ti	0.984809995	0.515739977	0.499900013
Ti	0.484770000	0.015740000	0.499900013
Ti	0.484730005	0.515720010	0.499909997
Ti	0.157000005	0.360199988	0.612489998
Ti	0.157069996	0.843360007	0.612519979
Ti	0.651289999	0.348870009	0.615660012
Ti	0.640070021	0.843339980	0.612479985
Ti	0.329369992	0.188150004	0.387340009
Ti	0.318230003	0.682650030	0.384119987
Ti	0.812709987	0.188160002	0.387340009
Ti	0.812579989	0.671299994	0.387349993
C	0.316769987	0.181700006	0.557280004
C	0.318040013	0.682319999	0.556420028
C	0.818679988	0.181700006	0.557269990
C	0.818710029	0.683610022	0.557269990
C	0.150869995	0.347920001	0.442559987
C	0.150920004	0.849770010	0.442559987
C	0.651480019	0.349110007	0.443430007
C	0.652679980	0.849770010	0.442559987
O	0.484149992	0.516240001	0.657989979
O	0.985750020	0.516229987	0.657980025
O	0.484129995	0.014560000	0.657970011
O	0.984579980	0.015750000	0.664150000
O	0.983619988	0.515280008	0.341850013
O	0.485529989	0.017109999	0.341859996
O	0.485500008	0.515399992	0.341859996
O	0.984860003	0.015610000	0.335709989
H	0.984080017	0.016030001	0.707930028
H	0.984889984	0.015350000	0.291960001

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7 $Ti_3C_2O(OH)$

	x (Å)	*y* (Å)	*z* (Å)
a_1	22.3367004395	0.0000000000	0.0000000000
a_2	0.0000000000	3.0569999218	0.0000000000
a_3	0.0000000000	0.0000000000	5.2902002335

		Fraction coordination	
Ti	0.500000000	0.000000000	0.000000000
Ti	0.500000000	0.500000000	0.500000000
Ti	0.388460010	0.500000000	0.150680006
Ti	0.390920013	0.000000000	0.676110029
Ti	0.611540020	0.500000000	0.849319994
Ti	0.609080017	0.000000000	0.323890001
C	0.443379998	0.500000000	0.832750022
C	0.442629993	0.000000000	0.335060000
C	0.556620002	0.500000000	0.167250007
C	0.557370007	0.000000000	0.664940000
O	0.342729986	0.000000000	0.998310030
O	0.336650014	0.500000000	0.502460003
O	0.657270014	0.000000000	0.001690000
O	0.663349986	0.500000000	0.497539997
H	0.293240011	0.500000000	0.513040006
H	0.706759989	0.500000000	0.486959994

---

8 $Ti_3C_2O_{0.5}(OH)_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1466898918	0.0000000000	0.0000000000
a_2	-3.0733390155	5.3233086459	0.0000000000
a_3	0.0000000000	0.0000000000	22.1910991669

		Fraction coordination	
Ti	0.000420000	0.250459999	0.500000000
Ti	0.000530000	0.750280023	0.500000000
Ti	0.500509977	0.250380009	0.500039995
Ti	0.500429988	0.750270009	0.499969989
Ti	0.167239994	0.583609998	0.607209980
Ti	0.179700002	0.089869998	0.608959973
Ti	0.660889983	0.571070015	0.608919978
Ti	0.660870016	0.089840002	0.608900011
Ti	0.340050012	0.410730004	0.391130000
Ti	0.340090007	0.929679990	0.391110003
Ti	0.821139991	0.410809994	0.391020000
Ti	0.833779991	0.917100012	0.392780006
C	0.333330005	0.417420000	0.557330012
C	0.333350003	0.916109979	0.557319999
C	0.834580004	0.417369992	0.557259977
C	0.833819985	0.916960001	0.558430016
C	0.167150006	0.583710015	0.441570014
C	0.166329995	0.083300002	0.442730010

C	0.667620003	0.584550023	0.442680001
C	0.667599976	0.083310001	0.442680001
O	0.497649997	0.748929977	0.664110005
O	0.001670000	0.748740017	0.664269984
O	0.500500023	0.250270009	0.658529997
O	0.001770000	0.253060013	0.664229989
O	0.500339985	0.250380009	0.341520011
O	0.999210000	0.752030015	0.335740000
O	0.503329992	0.752040029	0.335839987
O	0.999629974	0.247569993	0.335770011
H	0.002710000	0.746100008	0.707989991
H	0.490900010	0.746320009	0.707790017
H	0.004080000	0.258489996	0.707939982
H	0.998019993	0.754899979	0.292030007
H	0.510909975	0.756780028	0.292160004
H	0.000670000	0.242359996	0.292070001

---

9 $Ti_3C_2(OH)_2$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.0896999836	0.0000000000	0.0000000000
a_2	-1.5448499918	2.6757586759	0.0000000000
a_3	0.0000000000	0.0000000000	22.1053009033

	Fraction coordination		
Ti	0.000000000	0.000000000	0.500000000
Ti	0.333333343	0.666666687	0.606800020
Ti	0.666666627	0.333333313	0.393199980
C	0.666666687	0.333333343	0.557929993
C	0.333333313	0.666666627	0.442070007
O	0.000000000	0.000000000	0.664730012
O	0.000000000	0.000000000	0.335269988
H	0.000000000	0.000000000	0.708720028
H	0.000000000	0.000000000	0.291279972

---

10 $Ti_3C_2F_{1.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1548099518	0.0000000000	0.0000000000
a_2	-3.0774173911	5.3306071834	0.0000000000
a_3	0.0000000000	0.0000000000	20.9519004822

	Fraction coordination		
Ti	0.016080000	0.020640001	0.497860014
Ti	0.016130000	0.520680010	0.497839987

Ti	0.516030014	0.020690000	0.497830003
Ti	0.516089976	0.520690024	0.497850001
Ti	0.181280002	0.350829989	0.610549986
Ti	0.181299999	0.855669975	0.610589981
Ti	0.683019996	0.354200006	0.610130012
Ti	0.685920000	0.855690002	0.610689998
Ti	0.346130013	0.185699999	0.385049999
Ti	0.349280000	0.687219977	0.385560006
Ti	0.850899994	0.185629994	0.385100007
Ti	0.850860000	0.690349996	0.385080010
C	0.350529999	0.187840000	0.559059978
C	0.349680007	0.687539995	0.559660017
C	0.848909974	0.187700003	0.559090018
C	0.849039972	0.686580002	0.559130013
C	0.183109999	0.354799986	0.436619997
C	0.183070004	0.853479981	0.436580002
C	0.682579994	0.353909999	0.436019987
C	0.681739986	0.853470027	0.436610013
F	0.515680015	0.520229995	0.671339989
F	0.016700000	0.521000028	0.671310008
F	0.517000020	0.020479999	0.671299994
F	0.516120017	0.520110011	0.324369997
F	0.015370000	0.520079970	0.324369997
F	0.516059995	0.020660000	0.324369997
O	0.018080000	0.021860000	0.671010017
O	0.015550000	0.020400001	0.324690014
H	0.023460001	0.025970001	0.717410028
H	0.014200000	0.020350000	0.278250009

---

11 $Ti_3C_2F(OH)$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1718101501	0.0000000000	0.0000000000
a_2	-3.0858909939	5.3306292612	0.0000000000
a_3	0.0000000000	0.0000000000	22.2098007202

		Fraction coordination	
Ti	0.045150001	0.991410017	0.498879999
Ti	0.045139998	0.491360009	0.498879999
Ti	0.545189977	0.991490006	0.498879999
Ti	0.545159996	0.491349995	0.498879999
Ti	0.210460007	0.321920007	0.604820013
Ti	0.213129997	0.827180028	0.605210006
Ti	0.710460007	0.321909994	0.604839981
Ti	0.713069975	0.827180028	0.605210006

Ti	0.377110004	0.155579999	0.392500013
Ti	0.379929990	0.660969973	0.392969996
Ti	0.877200007	0.155560002	0.392509997
Ti	0.879920006	0.660950005	0.392910004
C	0.378910005	0.158790007	0.556519985
C	0.378170013	0.657310009	0.556879997
C	0.878870010	0.158790007	0.556519985
C	0.878139973	0.657270014	0.556900024
C	0.212109998	0.325349987	0.440869987
C	0.211439997	0.824119985	0.441280007
C	0.712140024	0.325450003	0.440829992
C	0.711520016	0.824100018	0.441289991
F	0.544550002	0.490240008	0.663510025
F	0.044650000	0.490249991	0.663519979
F	0.045680001	0.492839992	0.334239990
F	0.545499980	0.492850006	0.334239990
O	0.544659972	0.989809990	0.662419975
O	0.044860002	0.990159988	0.662400007
O	0.545440018	0.991840005	0.335339993
O	0.045770001	0.992699981	0.335330009
H	0.545239985	0.989170015	0.706139982
H	0.046379998	0.991219997	0.706130028
H	0.544120014	0.986760020	0.291619986
H	0.046119999	0.991819978	0.291570008

---

12 $Ti_3C_2F_{0.5}(OH)_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1762199402	0.0000000000	0.0000000000
a_2	-3.0881097788	5.3486594136	0.0000000000
a_3	0.0000000000	0.0000000000	22.3619995117

Fraction coordination

Ti	0.000230000	0.998369992	0.500909984
Ti	0.000230000	0.498420000	0.500919998
Ti	0.500249982	0.998399973	0.500909984
Ti	0.500240028	0.498409986	0.500919998
Ti	0.167970002	0.334010005	0.606000006
Ti	0.168080002	0.830460012	0.606060028
Ti	0.666769981	0.331580013	0.606419981
Ti	0.664470017	0.830479980	0.606100023
Ti	0.336050004	0.166400000	0.395770013
Ti	0.333669990	0.665170014	0.395410001
Ti	0.832449973	0.166419998	0.395760000
Ti	0.832499981	0.662810028	0.395779997

C	0.332870007	0.164560005	0.558269978
C	0.333570004	0.665069997	0.557959974
C	0.833769977	0.164550006	0.558279991
C	0.833800018	0.665610015	0.558319986
C	0.166630000	0.331200004	0.443529993
C	0.166649997	0.832170010	0.443540007
C	0.666989982	0.331829995	0.443879992
C	0.667630017	0.832210004	0.443529993
F	0.000580000	0.998669982	0.665239990
F	0.000370000	0.998549998	0.336569995
O	0.499689996	0.998130023	0.663550019
O	0.000120000	0.497539997	0.663500011
O	0.499949992	0.497770011	0.663510025
O	0.000520000	0.498840004	0.338290006
O	0.500270009	0.498780012	0.338299990
O	0.500180006	0.998470008	0.338290006
H	0.496360004	0.995660007	0.706950009
H	0.001010000	0.493900001	0.706900001
H	0.498609990	0.494940013	0.706920028
H	0.999989986	0.499619991	0.294880003
H	0.500230014	0.499590009	0.294889987
H	0.500159979	0.999740005	0.294880003

---

13 $Ti_3C_2OF_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1011600494	0.0000000000	0.0000000000
a_2	-3.0505980248	5.2913918747	0.0000000000
a_3	0.0000000000	0.0000000000	22.3908996582

		Fraction coordination	
Ti	0.978439987	0.972320020	0.499749988
Ti	0.978470027	0.472350001	0.499760002
Ti	0.478439987	0.972289979	0.499749988
Ti	0.478469998	0.472369999	0.499749988
Ti	0.153830007	0.296750009	0.611050010
Ti	0.141680002	0.811399996	0.608789980
Ti	0.639519989	0.309249997	0.608789980
Ti	0.652949989	0.797479987	0.611220002
Ti	0.303920001	0.147220001	0.388280004
Ti	0.317339987	0.635330021	0.390700012
Ti	0.815379977	0.133350000	0.390700012
Ti	0.803120017	0.648069978	0.388399988
C	0.312669992	0.138129994	0.556410015
C	0.311260015	0.639460027	0.557099998

C	0.811349988	0.139530003	0.557120025
C	0.812849998	0.637910008	0.556360006
C	0.144069999	0.306769997	0.443159997
C	0.145530000	0.805100024	0.442389995
C	0.645690024	0.305260003	0.442389995
C	0.644270003	0.806559980	0.443080008
O	0.980769992	0.971870005	0.656140029
O	0.477939993	0.972280025	0.662639976
O	0.479020000	0.470149994	0.656109989
O	0.478740007	0.972029984	0.337000012
O	0.477919996	0.474539995	0.343369991
O	0.976199985	0.972809970	0.343369991
H	0.473630011	0.974810004	0.706099987
H	0.482710004	0.968559980	0.293570012
F	0.977829993	0.473179996	0.662750006
F	0.979460001	0.471249998	0.336670011

---

14 $Ti_3C_2FO_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1288700104	0.0000000000	0.0000000000
a_2	-3.0644694962	5.3073908778	0.0000000000
a_3	0.0000000000	0.0000000000	22.1994991302

		Fraction coordination	
Ti	0.973439991	0.969219983	0.499170005
Ti	0.973490000	0.469220012	0.499159992
Ti	0.473500013	0.969269991	0.499159992
Ti	0.473540008	0.469330013	0.499170005
Ti	0.139149994	0.303810000	0.606549978
Ti	0.152520001	0.807919979	0.608349979
Ti	0.635029972	0.290459991	0.608430028
Ti	0.633340001	0.809790015	0.608219981
Ti	0.313659996	0.128950000	0.390150011
Ti	0.311960012	0.648199975	0.389869988
Ti	0.794439971	0.130720004	0.389899999
Ti	0.807959974	0.634800017	0.391799986
C	0.306190014	0.136899993	0.556620002
C	0.306690007	0.635140002	0.556540012
C	0.807799995	0.136299998	0.556569993
C	0.806640029	0.636240005	0.557950020
C	0.140310004	0.302379996	0.440349996
C	0.139249995	0.802240014	0.441790015
C	0.640380025	0.303409994	0.441799998
C	0.640799999	0.801819980	0.441680014

O	0.971580029	0.470670015	0.335500002
O	0.474070013	0.968829989	0.656629980
O	0.975390017	0.469049990	0.662710011
O	0.472950011	0.969789982	0.341699988
H	0.980690002	0.469309986	0.706489980
H	0.966329992	0.474339992	0.291770011
F	0.976289988	0.974489987	0.663139999
F	0.468780011	0.466659993	0.663139999
F	0.971040010	0.964349985	0.335209996
F	0.478069991	0.471399993	0.335209996

---

15 $Ti_3C_2(OH)O_{0.5}F_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1347899437	0.0000000000	0.0000000000
a_2	-3.0674128732	5.3146635448	0.0000000000
a_3	0.0000000000	0.0000000000	22.4228992462

		Fraction coordination	
Ti	0.007880000	0.984009981	0.503210008
Ti	0.007890000	0.483929992	0.503210008
Ti	0.507910013	0.984030008	0.503210008
Ti	0.507929981	0.484030008	0.503210008
Ti	0.188109994	0.325010002	0.611159980
Ti	0.175760001	0.816280007	0.609430015
Ti	0.669009984	0.323410004	0.611270010
Ti	0.667280018	0.804310024	0.611039996
Ti	0.348600000	0.163849995	0.395289987
Ti	0.346969992	0.644819975	0.395190001
Ti	0.840020001	0.151629999	0.397049993
Ti	0.827859998	0.643130004	0.395310014
C	0.340490013	0.149670005	0.560079992
C	0.340979993	0.651019990	0.559909999
C	0.841549993	0.150610000	0.561169982
C	0.842490017	0.651570022	0.560010016
C	0.173460007	0.316450000	0.446399987
C	0.174309999	0.817460001	0.445149988
C	0.674799979	0.316989988	0.446520001
C	0.675329983	0.818359971	0.446410000
O	0.009120000	0.487520009	0.665509999
O	0.507489979	0.484829992	0.659600019
O	0.505320013	0.982649982	0.665419996
O	0.006360000	0.480630010	0.340990007
O	0.510869980	0.984939992	0.340990007
O	0.508369982	0.483220011	0.346839994

H	0.501230001	0.978550017	0.708710015
H	0.010520000	0.494940013	0.708769977
H	0.003050000	0.473369986	0.297719985
H	0.517639995	0.986769974	0.297719985
F	0.009960000	0.981970012	0.666360021
F	0.005410000	0.985979974	0.340039998

---

16 Ti_2CO_2

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.0355999470	0.0000000000	0.0000000000
a_2	-1.5177999735	2.6289066698	0.0000000000
a_3	0.0000000000	0.0000000000	17.6979007721

	Fraction coordination		
Ti	0.333330005	0.666670024	0.573119998
Ti	0.666670024	0.333330005	0.426880002
C	0.000000000	0.000000000	0.500000000
O	0.333330005	0.666670024	0.373620003
O	0.666670024	0.333330005	0.626380026

---

17 $Ti_2CO_{1.5}F_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	10.5059003830	0.0000000000	0.0000000000
a_2	0.0000000000	6.0592999458	0.0000000000
a_3	0.0000000000	0.0000000000	17.7558994293

	Fraction coordination		
Ti	0.830129981	0.239930004	0.429289997
Ti	0.589139998	0.000000000	0.430550009
Ti	0.830129981	0.760070026	0.429289997
Ti	0.582300007	0.500000000	0.426239997
Ti	0.910860002	0.500000000	0.569450021
Ti	0.669870019	0.260069996	0.570710003
Ti	0.917699993	0.000000000	0.573759973
Ti	0.669870019	0.739929974	0.570710003
Ti	0.330130011	0.739929974	0.429289997
Ti	0.089139998	0.500000000	0.430550009
Ti	0.330130011	0.260069996	0.429289997
Ti	0.082300000	0.000000000	0.426239997
Ti	0.410860002	0.000000000	0.569450021
Ti	0.169870004	0.760070026	0.570710003
Ti	0.417699993	0.500000000	0.573759973

Ti	0.169870004	0.239930004	0.570710003
C	0.750609994	0.500000000	0.499249995
C	0.000000000	0.748610020	0.500000000
C	0.749390006	0.000000000	0.500750005
C	0.000000000	0.251390010	0.500000000
C	0.250609994	0.000000000	0.499249995
C	0.500000000	0.248610005	0.500000000
C	0.249390006	0.500000000	0.500750005
C	0.500000000	0.751389980	0.500000000
O	0.832790017	0.251580000	0.626450002
O	0.832790017	0.748420000	0.626450002
O	0.583339989	0.500000000	0.626919985
O	0.916660011	0.000000000	0.373079985
O	0.667209983	0.248420000	0.373549998
O	0.667209983	0.751580000	0.373549998
O	0.332789987	0.751580000	0.626450002
O	0.332789987	0.248420000	0.626450002
O	0.083339997	0.000000000	0.626919985
O	0.416660011	0.500000000	0.373079985
O	0.167209998	0.748420000	0.373549998
O	0.167209998	0.251580000	0.373549998
F	0.583570004	0.000000000	0.634559989
F	0.916429996	0.500000000	0.365440011
F	0.083570004	0.500000000	0.634559989
F	0.416429996	0.000000000	0.365440011

---

18 Ti_2COF

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	18.0499992371	0.0000000000	0.0000000000
a_2	0.0000000000	3.0395998955	0.0000000000
a_3	0.0000000000	0.0000000000	5.2649998665

		Fraction coordination	
Ti	0.568300009	0.500000000	0.820439994
Ti	0.567830026	0.000000000	0.347869992
Ti	0.431699991	0.500000000	0.179560006
Ti	0.432170004	0.000000000	0.652130008
C	0.500000000	0.000000000	0.000000000
C	0.500000000	0.500000000	0.500000000
O	0.375519991	0.000000000	0.333249986
O	0.624480009	0.000000000	0.666750014
F	0.367370009	0.500000000	0.836539984
F	0.632629991	0.500000000	0.163460001

---

19 $Ti_2CO_{0.5}F_{1.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	10.5538997650	0.0000000000	0.0000000000
a_2	0.0000000000	6.0981998444	0.0000000000
a_3	0.0000000000	0.0000000000	17.7705001831
		Fraction coordination	
Ti	0.163499996	0.760879993	0.433070004
Ti	0.163499996	0.239120007	0.433070004
Ti	0.924269974	0.000000000	0.431829989
Ti	0.916989982	0.500000000	0.435119987
Ti	0.075730003	0.000000000	0.568170011
Ti	0.083010003	0.500000000	0.564880013
Ti	0.836499989	0.239120007	0.566929996
Ti	0.836499989	0.760879993	0.566929996
Ti	0.663500011	0.260879993	0.433070004
Ti	0.663500011	0.739120007	0.433070004
Ti	0.424270004	0.500000000	0.431829989
Ti	0.416990012	0.000000000	0.435119987
Ti	0.575730026	0.500000000	0.568170011
Ti	0.583010018	0.000000000	0.564880013
Ti	0.336499989	0.739120007	0.566929996
Ti	0.336499989	0.260879993	0.566929996
C	0.000000000	0.749400020	0.500000000
C	0.000000000	0.250600010	0.500000000
C	0.250209987	0.500000000	0.498380005
C	0.249789998	0.000000000	0.501619995
C	0.500000000	0.249400005	0.500000000
C	0.500000000	0.750599980	0.500000000
C	0.750209987	0.000000000	0.498380005
C	0.749790013	0.500000000	0.501619995
O	0.914879978	0.000000000	0.627120018
O	0.085120000	0.000000000	0.372880012
O	0.414880008	0.500000000	0.627120018
O	0.585120022	0.500000000	0.372880012
F	0.167610005	0.745909989	0.634509981
F	0.918280005	0.500000000	0.634019971
F	0.167610005	0.254090011	0.634509981
F	0.081720002	0.500000000	0.365979999
F	0.832390010	0.254090011	0.365489990
F	0.832390010	0.745909989	0.365489990
F	0.667609990	0.245910004	0.634509981
F	0.418280005	0.000000000	0.634019971
F	0.667609990	0.754090011	0.634509981

F	0.581719995	0.000000000	0.365979999
F	0.332390010	0.754090011	0.365489990
F	0.332390010	0.245910004	0.365489990

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20 Ti_2CF_2

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.0529999733	0.0000000000	0.0000000000
a_2	-1.5264999866	2.6439755346	0.0000000000
a_3	0.0000000000	0.0000000000	17.3679008484

	Fraction coordination		
Ti	0.666670024	0.333330005	0.564580023
Ti	0.333330005	0.666670024	0.435420007
C	0.000000000	0.000000000	0.500000000
F	0.666670024	0.333330005	0.360689998
F	0.333330005	0.666670024	0.639310002

---

21 $Ti_2CO_{1.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	10.4944000244	0.0000000000	0.0000000000
a_2	0.0000000000	6.0576000214	0.0000000000
a_3	0.0000000000	0.0000000000	17.9349994659

	Fraction coordination		
Ti	0.582319975	0.000000000	0.572719991
Ti	0.588469982	0.500000000	0.568880022
Ti	0.830190003	0.260069996	0.570029974
Ti	0.830190003	0.739929974	0.570029974
Ti	0.669809997	0.239930004	0.429969996
Ti	0.669809997	0.760070026	0.429969996
Ti	0.917680025	0.500000000	0.427280009
Ti	0.911530018	0.000000000	0.431120008
Ti	0.082319997	0.500000000	0.572719991
Ti	0.088469997	0.000000000	0.568880022
Ti	0.330190003	0.760070026	0.570029974
Ti	0.330190003	0.239930004	0.570029974
Ti	0.169809997	0.739929974	0.429969996
Ti	0.169809997	0.260069996	0.429969996
Ti	0.417679995	0.000000000	0.427280009
Ti	0.411529988	0.500000000	0.431120008
C	0.749970019	0.000000000	0.501100004
C	0.750029981	0.500000000	0.498899996
C	0.000000000	0.249699995	0.500000000

C	0.000000000	0.750299990	0.500000000
C	0.249970004	0.500000000	0.501100004
C	0.250030011	0.000000000	0.498899996
C	0.500000000	0.749700010	0.500000000
C	0.500000000	0.250299990	0.500000000
O	0.582740009	0.000000000	0.373349994
O	0.832660019	0.248999998	0.373910010
O	0.832660019	0.750999987	0.373910010
O	0.582719982	0.500000000	0.366180003
O	0.917259991	0.500000000	0.626649976
O	0.667339981	0.749000013	0.626089990
O	0.667339981	0.250999987	0.626089990
O	0.917280018	0.000000000	0.633819997
O	0.082740001	0.500000000	0.373349994
O	0.332659990	0.749000013	0.373910010
O	0.332659990	0.250999987	0.373910010
O	0.082719997	0.000000000	0.366180003
O	0.417259991	0.000000000	0.626649976
O	0.167339996	0.248999998	0.626089990
O	0.167339996	0.750999987	0.626089990
O	0.417279989	0.500000000	0.633819997
H	0.579930007	0.500000000	0.312000006
H	0.920069993	0.000000000	0.688000023
H	0.079930000	0.000000000	0.312000006
H	0.420069993	0.500000000	0.688000023

---

22 $Ti_2CO(OH)$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	18.1548995972	0.0000000000	0.0000000000
a_2	0.0000000000	3.0443000793	0.0000000000
a_3	0.0000000000	0.0000000000	5.2680997849

	Fraction coordination		
Ti	0.432529986	0.000000000	0.346179992
Ti	0.432319999	0.500000000	0.820559978
Ti	0.567680001	0.500000000	0.179440007
Ti	0.567470014	0.000000000	0.653819978
C	0.500000000	0.000000000	0.000000000
C	0.500000000	0.500000000	0.500000000
O	0.625349998	0.000000000	0.332949996
O	0.632830024	0.500000000	0.834609985
O	0.374650002	0.000000000	0.667050004
O	0.367170006	0.500000000	0.165390000
H	0.686299980	0.500000000	0.836579978

H	0.313699991	0.500000000	0.163420007

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23 $Ti_2CO_{0.5}(OH)_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	10.6077995300	0.0000000000	0.0000000000
a_2	0.0000000000	6.1303000450	0.0000000000
a_3	0.0000000000	0.0000000000	17.8054008484
		Fraction coordination	
Ti	0.423850000	0.000000000	0.432000011
Ti	0.416289985	0.500000000	0.435649991
Ti	0.163739994	0.261020005	0.433690012
Ti	0.163739994	0.738979995	0.433690012
Ti	0.336259991	0.238979995	0.566309988
Ti	0.336259991	0.761020005	0.566309988
Ti	0.076150000	0.500000000	0.568000019
Ti	0.083710000	0.000000000	0.564350009
Ti	0.923850000	0.500000000	0.432000011
Ti	0.916289985	0.000000000	0.435649991
Ti	0.663739979	0.761020005	0.433690012
Ti	0.663739979	0.238979995	0.433690012
Ti	0.836260021	0.738979995	0.566309988
Ti	0.836260021	0.261020005	0.566309988
Ti	0.576150000	0.000000000	0.568000019
Ti	0.583710015	0.500000000	0.564350009
C	0.250440001	0.000000000	0.498059988
C	0.249559999	0.500000000	0.501940012
C	0.000000000	0.250250012	0.500000000
C	0.000000000	0.749750018	0.500000000
C	0.750440001	0.500000000	0.498059988
C	0.749559999	0.000000000	0.501940012
C	0.500000000	0.750249982	0.500000000
C	0.500000000	0.249750003	0.500000000
O	0.414600015	0.000000000	0.629000008
O	0.166710004	0.246790007	0.635529995
O	0.417389989	0.500000000	0.634320021
O	0.166710004	0.753210008	0.635529995
O	0.085400000	0.500000000	0.370999992
O	0.082610004	0.000000000	0.365680009
O	0.333290011	0.746789992	0.364470005
O	0.333290011	0.253210008	0.364470005
O	0.914600015	0.500000000	0.629000008
O	0.666710019	0.746789992	0.635529995
O	0.917389989	0.000000000	0.634320021

O	0.666710019	0.253210008	0.635529995
O	0.585399985	0.000000000	0.370999992
O	0.582610011	0.500000000	0.365680009
O	0.833289981	0.246790007	0.364470005
O	0.833289981	0.753210008	0.364470005
H	0.170619994	0.239099994	0.689899981
H	0.421160012	0.500000000	0.688709974
H	0.170619994	0.760900021	0.689899981
H	0.078840002	0.000000000	0.311289996
H	0.329380006	0.739099979	0.310099989
H	0.329380006	0.260899991	0.310099989
H	0.670620024	0.739099979	0.689899981
H	0.921159983	0.000000000	0.688709974
H	0.670620024	0.260899991	0.689899981
H	0.578840017	0.500000000	0.311289996
H	0.829379976	0.239099994	0.310099989
H	0.829379976	0.760900021	0.310099989

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24 $Ti_2C(OH)_2$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.0782999992	0.0000000000	0.0000000000
a_2	-1.5391499996	2.6658859998	0.0000000000
a_3	0.0000000000	0.0000000000	17.5897998810

	Fraction coordination		
Ti	0.666666687	0.333333343	0.435140014
Ti	0.333333313	0.666666627	0.564859986
O	0.666666687	0.333333343	0.637369990
O	0.333333313	0.666666627	0.362630010
H	0.666666687	0.333333343	0.692659974
H	0.333333313	0.666666627	0.307340026
C	0.000000000	0.000000000	0.500000000

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25 $Ti_2CF_{1.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	10.5923995972	0.0000000000	0.0000000000
a_2	0.0000000000	6.1132001877	0.0000000000
a_3	0.0000000000	0.0000000000	17.6287994385

	Fraction coordination		
Ti	0.582199991	0.500000000	0.564970016
Ti	0.583069980	0.000000000	0.564329982
Ti	0.834370017	0.750980020	0.564859986

Ti	0.834370017	0.249019995	0.564859986
Ti	0.665629983	0.749019980	0.435140014
Ti	0.665629983	0.250979990	0.435140014
Ti	0.917800009	0.000000000	0.435030013
Ti	0.916930020	0.500000000	0.435669988
Ti	0.082199998	0.000000000	0.564970016
Ti	0.083070002	0.500000000	0.564329982
Ti	0.334369987	0.250979990	0.564859986
Ti	0.334369987	0.749019980	0.564859986
Ti	0.165629998	0.249019995	0.435140014
Ti	0.165629998	0.750980020	0.435140014
Ti	0.417800009	0.500000000	0.435030013
Ti	0.416929990	0.000000000	0.435669988
C	0.750280023	0.500000000	0.500329971
C	0.749719977	0.000000000	0.499669999
C	0.000000000	0.748910010	0.500000000
C	0.000000000	0.251089990	0.500000000
C	0.250279993	0.000000000	0.500329971
C	0.249720007	0.500000000	0.499669999
C	0.500000000	0.248909995	0.500000000
C	0.500000000	0.751089990	0.500000000
F	0.833260000	0.750190020	0.363070011
F	0.583909988	0.000000000	0.362690002
F	0.833260000	0.249809995	0.363070011
F	0.666740000	0.250189990	0.636929989
F	0.666740000	0.749809980	0.636929989
F	0.916090012	0.500000000	0.637310028
F	0.333260000	0.250189990	0.363070011
F	0.083910003	0.500000000	0.362690002
F	0.333260000	0.749809980	0.363070011
F	0.166740000	0.750190020	0.636929989
F	0.166740000	0.249809995	0.636929989
F	0.416090012	0.000000000	0.637310028
O	0.583949983	0.500000000	0.363709986
O	0.916050017	0.000000000	0.636290014
O	0.083949998	0.000000000	0.363709986
O	0.416049987	0.500000000	0.636290014
H	0.585699975	0.500000000	0.308569998
H	0.914300025	0.000000000	0.691429973
H	0.085699998	0.000000000	0.308569998
H	0.414299995	0.500000000	0.691429973

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26 $Ti_2CF(OH)$

	***x* (Å)**	***y* (Å)**	***z* (Å)**

a_1	10.6177997589	0.0000000000	0.0000000000
a_2	0.0000000000	6.1259999275	0.0000000000
a_3	0.0000000000	0.0000000000	17.4143009186

Fraction coordination

Ti	0.333840013	0.000750000	0.434720010
Ti	0.082350001	0.747420013	0.434269994
Ti	0.332509995	0.497970015	0.434460014
Ti	0.083300002	0.251249999	0.435039997
Ti	0.417650014	0.247419998	0.565729976
Ti	0.167490005	0.997969985	0.565540016
Ti	0.416700006	0.751250029	0.564960003
Ti	0.166160002	0.500750005	0.565280020
Ti	0.833840013	0.500750005	0.434720010
Ti	0.582350016	0.247419998	0.434269994
Ti	0.832509995	0.997969985	0.434460014
Ti	0.583299994	0.751250029	0.435039997
Ti	0.917649984	0.747420013	0.565729976
Ti	0.667490005	0.497970015	0.565540016
Ti	0.916700006	0.251249999	0.564960003
Ti	0.666159987	0.000750000	0.565280020
C	0.249550000	0.249320000	0.500230014
C	0.000000000	0.000260000	0.500000000
C	0.250449985	0.749319971	0.499769986
C	0.000000000	0.498650014	0.500000000
C	0.749549985	0.749319971	0.500230014
C	0.500000000	0.500259995	0.500000000
C	0.750450015	0.249320000	0.499769986
C	0.500000000	0.998650014	0.500000000
F	0.083260000	0.249660000	0.640070021
F	0.332670003	0.499419987	0.639630020
F	0.167329997	0.999419987	0.360370010
F	0.416740000	0.749660015	0.359930009
F	0.583260000	0.749660015	0.640070021
F	0.832669973	0.999419987	0.639630020
F	0.667330027	0.499419987	0.360370010
F	0.916740000	0.249660000	0.359930009
O	0.083310001	0.749029994	0.638320029
O	0.332729995	0.000150000	0.638509989
O	0.167270005	0.500150025	0.361490011
O	0.416689992	0.249029994	0.361680001
O	0.583310008	0.249029994	0.638320029
O	0.832729995	0.500150025	0.638509989
O	0.667270005	0.000150000	0.361490011

O	0.916689992	0.749029994	0.361680001
H	0.085689999	0.744970024	0.694010019
H	0.332610011	0.000240000	0.694329977
H	0.167390004	0.500240028	0.305669993
H	0.414310008	0.244969994	0.305990010
H	0.585690022	0.244969994	0.694010019
H	0.832610011	0.500240028	0.694329977
H	0.667389989	0.000240000	0.305669993
H	0.914309978	0.744970024	0.305990010

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27 $Ti_2CF_{0.5}(OH)_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	10.6515998840	0.0000000000	0.0000000000
a_2	0.0000000000	6.1441001892	0.0000000000
a_3	0.0000000000	0.0000000000	17.5753002167

		Fraction coordination	
Ti	0.333029985	0.748499990	0.435369998
Ti	0.084579997	0.500000000	0.435609996
Ti	0.333029985	0.251500010	0.435369998
Ti	0.083659999	0.000000000	0.434749991
Ti	0.415419996	0.000000000	0.564390004
Ti	0.166970000	0.751500010	0.564629972
Ti	0.416339993	0.500000000	0.565249979
Ti	0.166970000	0.248500004	0.564629972
Ti	0.833029985	0.248500004	0.435369998
Ti	0.584580004	0.000000000	0.435609996
Ti	0.833029985	0.751500010	0.435369998
Ti	0.583660007	0.500000000	0.434749991
Ti	0.915419996	0.500000000	0.564390004
Ti	0.666970015	0.251500010	0.564629972
Ti	0.916339993	0.000000000	0.565249979
Ti	0.666970015	0.748499990	0.564629972
C	0.250380009	0.000000000	0.499810010
C	0.000000000	0.749090016	0.500000000
C	0.249620005	0.500000000	0.500190020
C	0.000000000	0.250910014	0.500000000
C	0.750379980	0.500000000	0.499810010
C	0.500000000	0.249090001	0.500000000
C	0.749620020	0.000000000	0.500190020
C	0.500000000	0.750909984	0.500000000
F	0.083779998	0.500000000	0.639699996
F	0.416220009	0.000000000	0.360300004
F	0.583779991	0.000000000	0.639699996

F	0.916220009	0.500000000	0.360300004
O	0.333119988	0.749490023	0.637480021
O	0.083319999	0.000000000	0.637170017
O	0.333119988	0.250510007	0.637480021
O	0.416680008	0.500000000	0.362830013
O	0.166879997	0.249489993	0.362520009
O	0.166879997	0.750509977	0.362520009
O	0.833119988	0.249489993	0.637480021
O	0.583320022	0.500000000	0.637170017
O	0.833119988	0.750509977	0.637480021
O	0.916679978	0.000000000	0.362830013
O	0.666880012	0.749490023	0.362520009
O	0.666880012	0.250510007	0.362520009
H	0.330190003	0.748730004	0.692669988
H	0.084059998	0.000000000	0.692359984
H	0.330190003	0.251269996	0.692669988
H	0.415939987	0.500000000	0.307639986
H	0.169809997	0.248730004	0.307330012
H	0.169809997	0.751269996	0.307330012
H	0.830190003	0.248730004	0.692669988
H	0.584060013	0.500000000	0.692359984
H	0.830190003	0.751269996	0.692669988
H	0.915939987	0.000000000	0.307639986
H	0.669809997	0.748730004	0.307330012
H	0.669809997	0.251269996	0.307330012

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28 $Ti_2COF_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.0919699669	0.0000000000	0.0000000000
a_2	-3.0460021320	5.2649108358	0.0000000000
a_3	0.0000000000	0.0000000000	17.2684001923

	Fraction coordination		
Ti	0.340559989	0.163859993	0.429439992
Ti	0.358709991	0.653010011	0.428840011
Ti	0.859380007	0.153170004	0.427210003
Ti	0.846499979	0.666729987	0.431340009
Ti	0.173109993	0.310220003	0.573170006
Ti	0.185599998	0.836499989	0.568979979
Ti	0.673740029	0.310609996	0.571500003
Ti	0.691699982	0.839460015	0.570829988
C	0.016179999	0.992730021	0.500159979
C	0.016190000	0.493809998	0.500180006
C	0.516020000	0.994930029	0.498930007

C	0.516210020	0.494989991	0.501389980
O	0.850839972	0.662039995	0.638859987
O	0.349000007	0.157120004	0.630659997
O	0.848280013	0.163499996	0.631460011
O	0.181109995	0.826510012	0.361490011
O	0.683440030	0.823889971	0.369650006
O	0.184000000	0.331110001	0.368840009
H	0.855899990	0.667439997	0.695179999
H	0.174309999	0.823859990	0.305209994
F	0.350100011	0.663689971	0.640060008
F	0.682290018	0.329650015	0.360269994

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29 $Ti_2CFO_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1091299057	0.0000000000	0.0000000000
a_2	-3.0545657125	5.2728020115	0.0000000000
a_3	0.0000000000	0.0000000000	17.9134407043

	Fraction coordination		
Ti	0.299609989	0.130559996	0.431419998
Ti	0.296750009	0.650669992	0.433129996
Ti	0.802810013	0.145229995	0.435059994
Ti	0.817979991	0.649710000	0.432889998
Ti	0.144679993	0.304159999	0.565760016
Ti	0.145919994	0.826990008	0.566540003
Ti	0.624450028	0.304769993	0.565729976
Ti	0.639289975	0.814090014	0.563440025
C	0.971350014	0.978280008	0.499080002
C	0.972450018	0.479840010	0.500989974
C	0.471020013	0.977349997	0.499269992
C	0.470809996	0.477950007	0.497480005
O	0.803520024	0.143969998	0.632499993
O	0.305849999	0.147569999	0.626119971
O	0.642390013	0.312700003	0.365189999
O	0.136549994	0.807070017	0.372339994
H	0.797070026	0.135710001	0.686720014
H	0.655319989	0.315620005	0.311030000
F	0.308470011	0.643700004	0.633960009
F	0.799279988	0.643909991	0.633870006
F	0.640630007	0.816399992	0.365440011
F	0.134100005	0.313300014	0.364749998

---

30 $Ti_2C(OH)O_{0.5}F_{0.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.0995202065	0.0000000000	0.0000000000
a_2	-3.0497237327	5.3015193403	0.0000000000
a_3	0.0000000000	0.0000000000	18.2101993561
		Fraction coordination	
Ti	0.315290004	0.176909998	0.440079987
Ti	0.330229998	0.685790002	0.437860012
Ti	0.810630023	0.164260000	0.438080013
Ti	0.812120020	0.687520027	0.436800003
Ti	0.153349996	0.346720010	0.566020012
Ti	0.138180003	0.837819993	0.568379998
Ti	0.657939970	0.359549999	0.568159997
Ti	0.656430006	0.836090028	0.569350004
C	0.983699977	0.011980000	0.503449976
C	0.982890010	0.511680007	0.501399994
C	0.485570014	0.012020000	0.504840016
C	0.484869987	0.511569977	0.502680004
O	0.313730001	0.674759984	0.635320008
O	0.315329999	0.178519994	0.634339988
O	0.817879975	0.675750017	0.628639996
O	0.152989998	0.345519990	0.371800005
O	0.155080006	0.849020004	0.370829999
O	0.650749981	0.848259985	0.377629995
H	0.304049999	0.668609977	0.688589990
H	0.309419990	0.180710003	0.687569976
H	0.156979993	0.343750000	0.318529993
H	0.164829999	0.854900002	0.317570001
F	0.821120024	0.183300003	0.636439979
F	0.647520006	0.340400010	0.369650006

---

31 $Nb_4C_3O_2$

	x (Å)	*y* (Å)	*z* (Å)
a_1	3.152600050	0.0000000000	0.0000000000
a_2	-1.5763000250	2.7302317312	0.0000000000
a_3	0.0000000000	0.0000000000	26.899904364
		Fraction coordination	
Nb	0.666666687	0.333333373	0.549210012
Nb	0.333333313	0.666666627	0.450789988
Nb	0.000000000	0.000000000	0.643079996
Nb	0.000000000	0.000000000	0.356920004
C	0.666666687	0.333333373	0.682399988

C	0.333333313	0.666666627	0.317600012
C	0.333333373	0.666666746	0.596809983
O	0.666666627	0.333333254	0.403190017
O	0.000000000	0.000000000	0.500000000

---

32 $Nb_4C_3O_{1.5}F_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.3253297806	0.0000000000	0.0000000000
a_2	-3.1626653042	5.4763256590	0.0000000000
a_3	0.0000000000	0.0000000000	26.9828891754
		Fraction coordination	
Nb	0.323119998	0.149570003	0.549629986
Nb	0.319849998	0.646929979	0.549870014
Nb	0.819159985	0.149560004	0.549640000
Nb	0.819100022	0.645460010	0.549239993
Nb	0.154280007	0.316119999	0.450100005
Nb	0.150940001	0.813459992	0.450329989
Nb	0.655049980	0.317629993	0.450720012
Nb	0.654969990	0.813510001	0.450329989
Nb	0.987339973	0.981939971	0.642069995
Nb	0.962719977	0.469110012	0.641420007
Nb	0.497900009	0.002920000	0.641300023
Nb	0.499210000	0.469190001	0.641420007
Nb	0.976199985	0.960110009	0.358639985
Nb	0.974960029	0.493840009	0.358539999
Nb	0.486710012	0.981060028	0.357890010
Nb	0.511340022	0.493950009	0.358520001
C	0.154670000	0.316590011	0.597130001
C	0.154809996	0.813470006	0.597039998
C	0.653330028	0.313899994	0.594210029
C	0.651400030	0.813440025	0.597039998
C	0.319270015	0.149590001	0.402940005
C	0.319409996	0.646440029	0.402830005
C	0.822690010	0.149590001	0.402929991
C	0.820800006	0.649190009	0.405750006
C	0.987760007	0.982919991	0.500660002
C	0.989269972	0.481539994	0.499980003
C	0.486330003	0.980120003	0.499309987
C	0.484860003	0.481530011	0.499980003
O	0.821699977	0.146929994	0.682699978

O	0.318150014	0.146929994	0.682680011
O	0.821759999	0.650590003	0.682749987
O	0.652339995	0.312449992	0.317220002
O	0.155910000	0.816139996	0.317290008
O	0.652400017	0.816129982	0.317290008
F	0.319759995	0.646610022	0.685679972
F	0.154410005	0.316480011	0.314260006

---

33 Nb_4C_3OF

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.3279500008	0.0000000000	0.0000000000
a_2	-3.1639728889	5.4685706344	0.0000000000
a_3	0.0000000000	0.0000000000	26.6735992432
	Fraction coordination		
Nb	0.339309990	0.179289997	0.551140010
Nb	0.329430014	0.673629999	0.552479982
Nb	0.835129976	0.181299999	0.551079988
Nb	0.836250007	0.674090028	0.552100003
Nb	0.170809999	0.342680007	0.450729996
Nb	0.168550000	0.837509990	0.451700002
Nb	0.664349973	0.343109995	0.450379997
Nb	0.662490010	0.835560024	0.451750010
Nb	0.992410004	0.004190000	0.644159973
Nb	0.969739974	0.492729992	0.645200014
Nb	0.509609997	0.027990000	0.643180013
Nb	0.512269974	0.500060022	0.643360019
Nb	0.996940017	0.012470000	0.358669996
Nb	0.020930000	0.516460001	0.359459996
Nb	0.490280002	0.988879979	0.359679997
Nb	0.485749990	0.523930013	0.357639998
C	0.167539999	0.343300015	0.600600004
C	0.167510003	0.841709971	0.600470006
C	0.666869998	0.342130005	0.596130013
C	0.664080024	0.842100024	0.600570023
C	0.334450006	0.175040007	0.402399987
C	0.333400011	0.674740016	0.406679988
C	0.830619991	0.174529999	0.402289987
C	0.832840025	0.673340023	0.402220011
C	0.000300000	0.008350000	0.501439989
C	0.999170005	0.508650005	0.501309991

C	0.499430001	0.008370000	0.501429975
C	0.498910010	0.508120000	0.501529992
O	0.835889995	0.679629982	0.686940014
O	0.834869981	0.173580006	0.686640024
O	0.669929981	0.843150020	0.316260010
O	0.164969996	0.336760014	0.315899998
F	0.336659998	0.677579999	0.689000010
F	0.338519990	0.180810004	0.697109997
F	0.667739987	0.339599997	0.313800007
F	0.166740000	0.835240006	0.305729985

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34 $Nb_4C_3O_{0.5}F_{1.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.1974802017	0.0000000000	0.0000000000
a_2	-3.0987372873	5.3649132663	0.0000000000
a_3	0.0000000000	0.0000000000	27.7217006683
		Fraction coordination	
Nb	0.361550003	0.184949994	0.547439992
Nb	0.362300009	0.685329974	0.548009992
Nb	0.862439990	0.185059994	0.547590017
Nb	0.862429976	0.685620010	0.547590017
Nb	0.194729999	0.351819992	0.453000009
Nb	0.194769993	0.851239979	0.453009993
Nb	0.695630014	0.351940006	0.453159988
Nb	0.694869995	0.851540029	0.452580005
Nb	0.028000001	0.017560000	0.640770018
Nb	0.019029999	0.513100028	0.642080009
Nb	0.532329977	0.026170000	0.641910017
Nb	0.532310009	0.513220012	0.641919971
Nb	0.038100000	0.023680000	0.358530015
Nb	0.029139999	0.519230008	0.359820008
Nb	0.524820030	0.023550000	0.358680010
Nb	0.524850011	0.510640025	0.358700007
C	0.194839999	0.350030005	0.597090006
C	0.194820002	0.852530003	0.597079992
C	0.694670022	0.351209998	0.594389975
C	0.696200013	0.851949990	0.597270012
C	0.362459987	0.185609996	0.406210005
C	0.360920012	0.684840024	0.403340012
C	0.862330019	0.186790004	0.403499991

C	0.862349987	0.684300005	0.403510004
C	0.027880000	0.018069999	0.499570012
C	0.029260000	0.518779993	0.501039982
C	0.528569996	0.017400000	0.500299990
C	0.528590024	0.519450009	0.500299990
O	0.694090009	0.350639999	0.685419977
O	0.362930000	0.186100006	0.315180004
F	0.190439999	0.345470011	0.692210019
F	0.191479996	0.852519989	0.692200005
F	0.699490011	0.852829993	0.692189991
F	0.865899980	0.684289992	0.308389992
F	0.358260006	0.684050024	0.308420002
F	0.866119981	0.191249996	0.308389992

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35 $Nb_4C_3F_2$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.1001000404	0.0000000000	0.0000000000
a_2	-1.5500500202	2.6847653893	0.0000000000
a_3	0.0000000000	0.0000000000	27.0324001312
		Fraction coordination	
Nb	0.333330005	0.666670024	0.547689974
Nb	0.666670024	0.333330005	0.452309996
Nb	0.000000000	0.000000000	0.644240022
Nb	0.000000000	0.000000000	0.355760008
C	0.666670024	0.333330005	0.598919988
C	0.333330005	0.666670024	0.401080012
C	0.000000000	0.000000000	0.500000000
F	0.666670024	0.333330005	0.696959972
F	0.333330005	0.666670024	0.303039998

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36 $Nb_4C_3O_{1.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.3189301491	0.0000000000	0.0000000000
a_2	-3.1594452577	5.4722035972	0.0000000000
a_3	0.0000000000	0.0000000000	27.0869007111
		Fraction coordination	
Nb	0.304210007	0.157159999	0.547490001
Nb	0.304210007	0.662609994	0.547479987
Nb	0.806020021	0.160740003	0.547280014
Nb	0.809620023	0.662530005	0.547490001

Nb	0.136140004	0.325760007	0.448269993
Nb	0.139620006	0.827499986	0.448469996
Nb	0.641460001	0.325720012	0.448260009
Nb	0.641449988	0.831139982	0.448249996
Nb	0.983150005	0.983370006	0.638859987
Nb	0.983160019	0.515309989	0.638840020
Nb	0.451290011	0.983449996	0.638849974
Nb	0.472550005	0.494080007	0.639670014
Nb	0.962620020	0.004930000	0.356889993
Nb	0.962599993	0.473120004	0.356900007
Nb	0.494329989	0.004900000	0.356909990
Nb	0.473300010	0.494300008	0.356110007
C	0.138249993	0.326900005	0.594609976
C	0.139290005	0.827430010	0.591780007
C	0.639760017	0.326889992	0.594609976
C	0.639760017	0.828400016	0.594609976
C	0.305920005	0.159899995	0.401140004
C	0.305949986	0.661430001	0.401140004
C	0.806500018	0.160960004	0.403970003
C	0.807479978	0.661469996	0.401129991
C	0.972829998	0.994130015	0.497880012
C	0.972819984	0.494139999	0.497869998
C	0.472820014	0.994149983	0.497869998
C	0.472849995	0.494150013	0.497880012
O	0.803529978	0.659489989	0.680679977
O	0.307000011	0.659539998	0.680679977
O	0.306970000	0.162970006	0.680670023
O	0.805719972	0.160789996	0.683499992
O	0.638660014	0.825240016	0.315100014
O	0.142100006	0.328770012	0.315090001
O	0.638700008	0.328810006	0.315090001
O	0.140440002	0.827870011	0.312200010
H	0.805419981	0.161100000	0.719460011
H	0.142260000	0.828350008	0.276239991

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37 $Nb_4C_3O(OH)$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2114300728	0.0000000000	0.0000000000
a_2	-3.1057168476	5.3775691749	0.0000000000
a_3	0.0000000000	0.0000000000	27.2020492554

	Fraction coordination		
Nb	0.319260001	0.167630002	0.551509976
Nb	0.319370002	0.667630017	0.551320016
Nb	0.820969999	0.168620005	0.550339997
Nb	0.820840001	0.668309987	0.550639987
Nb	0.153500006	0.335319996	0.453640014
Nb	0.152960002	0.833970010	0.452960014
Nb	0.653900027	0.335599989	0.453940004
Nb	0.652909994	0.833840013	0.452769995
Nb	0.976920009	0.996389985	0.645569980
Nb	0.976750016	0.495829999	0.645529985
Nb	0.492879987	0.004120000	0.646229982
Nb	0.492790014	0.504159987	0.646260023
Nb	0.989400029	0.007340000	0.357950002
Nb	0.981060028	0.491389990	0.358729988
Nb	0.489430010	0.007540000	0.358119994
Nb	0.481649995	0.491600007	0.358729988
Nb	0.152960002	0.334520012	0.600679994
C	0.152850002	0.834020019	0.600629985
C	0.652760029	0.334250003	0.598039985
C	0.652480006	0.834079981	0.598100007
C	0.319240004	0.167140007	0.406170011
C	0.319359988	0.667420030	0.403670013
C	0.819729984	0.167400002	0.406239986
C	0.819949985	0.667670012	0.403589994
C	0.986699998	0.000660000	0.501730025
C	0.987290025	0.501969993	0.502139986
C	0.485240012	0.999930024	0.502129972
C	0.486009985	0.501380026	0.502569973
O	0.656099975	0.836049974	0.691030025
O	0.655200005	0.335170001	0.691030025
O	0.148359999	0.331440002	0.695500016
O	0.146190003	0.830940008	0.695379972
O	0.820559978	0.169790000	0.313239992
O	0.321379989	0.170780003	0.313259989
O	0.317649990	0.663590014	0.308950007
O	0.815150023	0.660539985	0.308699995
H	0.138170004	0.325190008	0.731239974
H	0.131219998	0.823780000	0.731050014
H	0.314159989	0.655730009	0.273180008
H	0.804700017	0.644050002	0.273079991

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38 $Nb_4C_3O_{0.5}(OH)_{1.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.21482	0	0.0000000000
a_2	-3.10741	5.384594	0.0000000000
a_3	0	0	27.2351207733
		Fraction coordination	
Nb	0.328979999	0.160249993	0.549969971
Nb	0.328660011	0.659979999	0.549600005
Nb	0.829400003	0.160779998	0.549610019
Nb	0.829280019	0.660090029	0.549449980
Nb	0.163399994	0.327450007	0.453110009
Nb	0.163760006	0.827690005	0.453460008
Nb	0.662919998	0.326880008	0.453480005
Nb	0.663160026	0.827700019	0.453640014
Nb	0.989369988	0.991259992	0.645179987
Nb	0.997780025	0.495420009	0.644020021
Nb	0.502219975	0.991169989	0.645330012
Nb	0.502269983	0.504260004	0.645160019
Nb	0.990300000	0.983420014	0.357890010
Nb	0.990140021	0.496360004	0.357719988
Nb	0.494639993	0.992129982	0.359030008
Nb	0.503139973	0.496479988	0.357890010
C	0.163169995	0.328110009	0.599789977
C	0.162640005	0.827170014	0.599600017
C	0.663980007	0.328599989	0.599590003
C	0.663619995	0.827650011	0.597259998
C	0.329279989	0.159600005	0.403290004
C	0.329710007	0.660409987	0.403459996
C	0.828350008	0.159020007	0.403459996
C	0.828790009	0.660030007	0.405820012
C	0.996869981	0.994530022	0.501540005
C	0.996590018	0.493640006	0.500890017
C	0.495860010	0.994149983	0.502170026
C	0.495519996	0.493209988	0.501540005
O	0.664390028	0.829039991	0.691439986
O	0.164230004	0.330590010	0.695420027
O	0.666930020	0.329890013	0.695330024
O	0.163289994	0.826990008	0.695349991
O	0.828100026	0.658710003	0.311639994

O	0.825730026	0.156460002	0.307669997
O	0.327879995	0.660489976	0.307709992
O	0.329409987	0.157639995	0.307660013
H	0.164309993	0.335839987	0.731159985
H	0.674610019	0.333050013	0.731050014
H	0.160500005	0.823180020	0.731090009
H	0.819119990	0.149509996	0.271950006
H	0.327329993	0.664449990	0.271959990
H	0.332890004	0.154290006	0.271899998

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39 $Nb_4C_3(OH)_2$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.1152000427	0.0000000000	0.0000000000
a_2	-1.5576000214	2.6978423749	0.0000000000
a_3	0.0000000000	0.0000000000	27.1252994537
		Fraction coordination	
Nb	0.333330005	0.666670024	0.451249987
Nb	0.666670024	0.333330005	0.548749983
Nb	0.000000000	0.000000000	0.356359988
Nb	0.000000000	0.000000000	0.643639982
C	0.666670024	0.333330005	0.401520014
C	0.333330005	0.666670024	0.598479986
C	0.000000000	0.000000000	0.500000000
O	0.666670024	0.333330005	0.304939985
O	0.333330005	0.666670024	0.695060015
H	0.666670024	0.333330005	0.268830001
H	0.333330005	0.666670024	0.731169999

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40 $Nb_4C_3F_{1.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2074899673	0.0000000000	0.0000000000
a_2	-3.1037450311	5.3757052254	0.0000000000
a_3	0.0000000000	0.0000000000	27.1922092438
		Fraction coordination	
Nb	0.355989993	0.197180003	0.550159991
Nb	0.355760008	0.697009981	0.550450027
Nb	0.856000006	0.197280005	0.550419986
Nb	0.856079996	0.697030008	0.550459981
Nb	0.189429998	0.364080012	0.455430001
Nb	0.189569995	0.864210010	0.455159992

Nb	0.689279974	0.363909990	0.455159992
Nb	0.689199984	0.864300013	0.455150008
Nb	0.022650000	0.032019999	0.646210015
Nb	0.022440000	0.531549990	0.645799994
Nb	0.522740006	0.031490002	0.646089971
Nb	0.522310019	0.531679988	0.646279991
Nb	0.022660000	0.029470000	0.359349996
Nb	0.022120001	0.529579997	0.359519988
Nb	0.522509992	0.029460000	0.359780014
Nb	0.522310019	0.529169977	0.359400004
C	0.188830003	0.364919990	0.601249993
C	0.188840002	0.863520026	0.601230025
C	0.690029979	0.364919990	0.601239979
C	0.689230025	0.864300013	0.600960016
C	0.356310010	0.196190000	0.404320002
C	0.356200010	0.697520018	0.404370010
C	0.855069995	0.196290001	0.404350013
C	0.855939984	0.696839988	0.404680014
C	0.022679999	0.030630000	0.502789974
C	0.022520000	0.530759990	0.502770007
C	0.522809982	0.030470001	0.502830029
C	0.522689998	0.530650020	0.502789974
F	0.188700005	0.365399987	0.699549973
F	0.688539982	0.364490002	0.699500024
F	0.189480007	0.866249979	0.699460030
F	0.355969995	0.196850002	0.306030005
F	0.355569988	0.695349991	0.306129992
F	0.855090022	0.195720002	0.306100011
O	0.689159989	0.866270006	0.696839988
O	0.855480015	0.695379972	0.308829993
H	0.688830018	0.869690001	0.732699990
H	0.855050027	0.693159997	0.272960007

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41 $Nb_4C_3F(OH)$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2170901299	0.0000000000	0.0000000000
a_2	-3.1085432767	5.3881075928	0.0000000000
a_3	0.0000000000	0.0000000000	27.2232093811
		Fraction coordination	
Nb	0.34921	0.16558	0.54602

Nb	0.34925	0.66561	0.54604
Nb	0.84961	0.1659	0.54657
Nb	0.84967	0.66591	0.54658
Nb	0.18391	0.33193	0.4501
Nb	0.184	0.83194	0.45011
Nb	0.68352	0.33152	0.44959
Nb	0.68351	0.83156	0.44958
Nb	0.01725	0.99965	0.64058
Nb	0.01726	0.49974	0.6406
Nb	0.51591	0.99905	0.64066
Nb	0.51595	0.49905	0.64071
Nb	0.0171	0.99853	0.35545
Nb	0.01712	0.49851	0.3554
Nb	0.51574	0.99791	0.35555
Nb	0.51567	0.49771	0.35557
C	0.1825	0.33203	0.59633
C	0.1825	0.83204	0.59632
C	0.68447	0.33318	0.59581
C	0.68446	0.83314	0.59581
C	0.35051	0.16534	0.39983
C	0.3506	0.66544	0.39983
C	0.84861	0.16434	0.40032
C	0.84858	0.66428	0.40032
C	0.01619	0.99854	0.49802
C	0.01622	0.49857	0.49804
C	0.51689	0.99888	0.49811
C	0.51687	0.49887	0.49809
F	0.17815	0.83257	0.69577
F	0.1792	0.33371	0.69574
F	0.35453	0.16362	0.30038
F	0.35319	0.66223	0.3004
O	0.68213	0.33288	0.69174
O	0.68211	0.83305	0.69174
O	0.85168	0.1655	0.3044
O	0.85015	0.66503	0.3044
H	0.68363	0.33537	0.72753
H	0.68312	0.83538	0.72753
H	0.85303	0.16664	0.26861
H	0.84694	0.66414	0.26861

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42 $Nb_4C_3F_{0.5}(OH)_{1.5}$

	x (Å)	*y* (Å)	*z* (Å)
a_1	6.2259998322	0.0000000000	0.0000000000
a_2	-3.1129966688	5.3923840948	0.0000000000
a_3	0.0000000000	0.0000000000	27.2422409058
		Fraction coordination	
Nb	0.321440011	0.141210005	0.550050020
Nb	0.321359992	0.640890002	0.550029993
Nb	0.821780026	0.141340002	0.550040007
Nb	0.821590006	0.641059995	0.550419986
Nb	0.154499993	0.307319999	0.453689992
Nb	0.154670000	0.807709992	0.453680009
Nb	0.654190004	0.307280004	0.453689992
Nb	0.654439986	0.807539999	0.453299999
Nb	0.988499999	0.974590003	0.644140005
Nb	0.988560021	0.474599987	0.644289970
Nb	0.488440007	0.974550009	0.644540012
Nb	0.488570005	0.474370003	0.644159973
Nb	0.987709999	0.974300027	0.359580010
Nb	0.987770021	0.474110007	0.359210014
Nb	0.487679988	0.974259973	0.359450012
Nb	0.487560004	0.474139988	0.359600008
C	0.155169994	0.307859987	0.599960029
C	0.154310003	0.807529986	0.599550009
C	0.655380011	0.308490008	0.599550009
C	0.655390024	0.807380021	0.599430025
C	0.320969999	0.140880004	0.403780013
C	0.321790010	0.641149998	0.404179990
C	0.820720017	0.140070006	0.404179990
C	0.820699990	0.641229987	0.404289991
C	0.987869978	0.974150002	0.501869977
C	0.987990022	0.474269986	0.501820028
C	0.488009989	0.974349976	0.501909971
C	0.488099992	0.474420011	0.501869977
F	0.154239997	0.308310002	0.699760020
F	0.321440011	0.140129998	0.303959996
O	0.656449974	0.307770014	0.695829988
O	0.654969990	0.807250023	0.695699990
O	0.155340001	0.809490025	0.695819974
O	0.820349991	0.640460014	0.308050007
O	0.821340024	0.141570002	0.307900012

O	0.320950001	0.640829980	0.307909995
H	0.661570013	0.308609992	0.731700003
H	0.654749990	0.805329978	0.731570005
H	0.155839995	0.812629998	0.731710017
H	0.818499982	0.639880002	0.272190005
H	0.821529984	0.143690005	0.272029996
H	0.321859986	0.641770005	0.272020012

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43 $Nb_4C_3OF_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2663002014	0.0000000000	0.0000000000
a_2	-3.1331676031	5.4254022666	0.0000000000
a_3	0.0000000000	0.0000000000	27.3124008179
		Fraction coordination	
Nb	0.326359987	0.155029997	0.547550023
Nb	0.326339990	0.654540002	0.547529995
Nb	0.826349974	0.154809996	0.547259986
Nb	0.825850010	0.654560030	0.547500014
Nb	0.159940004	0.321859986	0.450289994
Nb	0.160070002	0.822009981	0.450239986
Nb	0.659690022	0.321660012	0.450170010
Nb	0.659659982	0.822109997	0.450170010
Nb	0.997160017	0.996479988	0.641520023
Nb	0.997169971	0.483570009	0.641520023
Nb	0.492819995	0.987909973	0.640999973
Nb	0.483509988	0.483280003	0.641409993
Nb	0.986859977	0.976249993	0.359400004
Nb	0.987060010	0.494780004	0.359530002
Nb	0.493149996	0.988849998	0.358590007
Nb	0.505530000	0.494949996	0.359400004
C	0.160040006	0.321579993	0.593930006
C	0.160420001	0.821780026	0.596650004
C	0.659039974	0.321069986	0.597069979
C	0.659049988	0.821169972	0.597069979
C	0.325780004	0.155980006	0.403499991
C	0.325940013	0.654009998	0.403530002
C	0.827780008	0.155890003	0.403490007
C	0.826430023	0.655390024	0.404940009
C	0.992950022	0.988290012	0.500689983
C	0.992940009	0.488139987	0.500680029

C	0.493019998	0.988269985	0.499909997
C	0.493090004	0.488279998	0.500639975
O	0.163240001	0.822619975	0.690829992
O	0.159410000	0.321079999	0.685880005
O	0.159860000	0.322600007	0.312700003
O	0.659780025	0.321779996	0.317939997
O	0.659759998	0.822369993	0.317869991
O	0.159989998	0.822160006	0.317900002
H	0.173639998	0.826839983	0.726499975
H	0.160150006	0.324950010	0.277009994
F	0.653110027	0.310739994	0.693799973
F	0.652830005	0.824530005	0.693780005

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44 $Nb_4C_3FO_{0.5}(OH)_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2004098892	0.0000000000	0.0000000000
a_2	-3.1002011689	5.3687565857	0.0000000000
a_3	0.0000000000	0.0000000000	27.2940006256
		Fraction coordination	
Nb	0.359589994	0.169679999	0.547850013
Nb	0.359569997	0.669439971	0.547850013
Nb	0.858839989	0.169149995	0.547439992
Nb	0.858929992	0.669210017	0.547670007
Nb	0.192240000	0.335799992	0.451570004
Nb	0.192410007	0.835879982	0.451779991
Nb	0.691709995	0.335550010	0.451370001
Nb	0.691699982	0.835430026	0.451380014
Nb	0.029490000	0.998629987	0.643360019
Nb	0.029510001	0.511099994	0.643339992
Nb	0.516149998	0.998130023	0.643109977
Nb	0.524919987	0.502550006	0.642509997
Nb	0.021989999	0.006560000	0.355890006
Nb	0.021989999	0.493959993	0.355919987
Nb	0.535309970	0.006980000	0.356110007
Nb	0.526570022	0.502569973	0.356730014
C	0.192580000	0.336189985	0.597700000
C	0.192509994	0.836179972	0.595200002
C	0.691579998	0.335559994	0.597989976
C	0.691600025	0.835879982	0.597989976
C	0.359780014	0.169200003	0.401239991

C	0.359809995	0.669539988	0.401250005
C	0.858820021	0.168889999	0.404040009
C	0.858770013	0.668889999	0.401540011
C	0.025650000	0.002520000	0.499610007
C	0.025650000	0.502550006	0.499610007
C	0.525610030	0.002500000	0.499610007
C	0.525640011	0.502520025	0.499630004
O	0.194680005	0.337830007	0.692749977
O	0.192179993	0.836199999	0.688030005
O	0.857659996	0.667580009	0.306529999
O	0.859290004	0.168840006	0.311210006
H	0.203240007	0.342970014	0.728450000
H	0.851100028	0.663169980	0.270819992
F	0.688000023	0.339500010	0.695320010
F	0.688000023	0.828899980	0.695320010
F	0.363350004	0.176139995	0.303909987
F	0.363290012	0.665610015	0.303939998

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45 $Nb_4C_3(OH)O_{0.5}F_{0.5}$

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	6.2055201530	0.0000000000	0.0000000000
a_2	-3.1027451348	5.3785224723	0.0000000000
a_3	0.0000000000	0.0000000000	26.9937000275
		Fraction coordination	
Nb	0.320710003	0.159219995	0.549950004
Nb	0.321420014	0.659590006	0.549530029
Nb	0.820900023	0.158969998	0.549719989
Nb	0.820990026	0.659780025	0.549730003
Nb	0.155729994	0.326310009	0.452609986
Nb	0.155790001	0.827040017	0.452639997
Nb	0.655200005	0.326420009	0.452809989
Nb	0.655929983	0.826789975	0.452399999
Nb	0.988179982	0.993780017	0.645449996
Nb	0.979759991	0.489430010	0.646340013
Nb	0.492480010	0.002400000	0.646160007
Nb	0.492339998	0.489250004	0.646130025
Nb	0.988900006	0.992519975	0.356970012
Nb	0.997359991	0.496749997	0.356000006
Nb	0.484580010	0.983789980	0.356180012
Nb	0.484620005	0.496980011	0.356209993

C	0.154970005	0.326370001	0.600229979
C	0.155049995	0.827220023	0.600220025
C	0.654169977	0.326249987	0.597739995
C	0.654389977	0.826529980	0.600600004
C	0.322589993	0.159689993	0.401760012
C	0.322640002	0.659770012	0.404590011
C	0.821759999	0.158960000	0.402139992
C	0.821789980	0.659619987	0.402139992
C	0.988340020	0.993009984	0.501160026
C	0.988330007	0.493019998	0.501179993
C	0.488330007	0.992999971	0.501160026
C	0.488350004	0.493019998	0.501179993
O	0.153750002	0.325549990	0.696539998
O	0.152559996	0.827359974	0.696560025
O	0.654039979	0.326779991	0.692170024
O	0.824930012	0.158309996	0.305799991
O	0.824460030	0.661989987	0.305830002
O	0.322959989	0.659439981	0.310160011
H	0.151230007	0.321610004	0.732590020
H	0.146599993	0.828779995	0.732599974
H	0.832279980	0.155479997	0.269789994
H	0.830380023	0.669610023	0.269789994
F	0.662079990	0.830850005	0.699779987
F	0.314779997	0.155259997	0.302590013

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46 Nb_2CO_2

	***x* (Å)**	***y* (Å)**	***z* (Å)**
a_1	3.1324000359	0.0000000000	0.0000000000
a_2	-1.5662000179	2.7127380059	0.0000000000
a_3	0.0000000000	0.0000000000	17.1508007050
		Fraction coordination	
Nb	0.333330005	0.666670024	0.573419988
Nb	0.666670024	0.333330005	0.426580012
C	0.000000000	0.000000000	0.500000000
O	0.333330005	0.666670024	0.364369988
O	0.666670024	0.333330005	0.635630012
