

Infrared photoionization of neutral tantalum and tantalum oxide clusters

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Supporting Information

Supporting Information Figures:

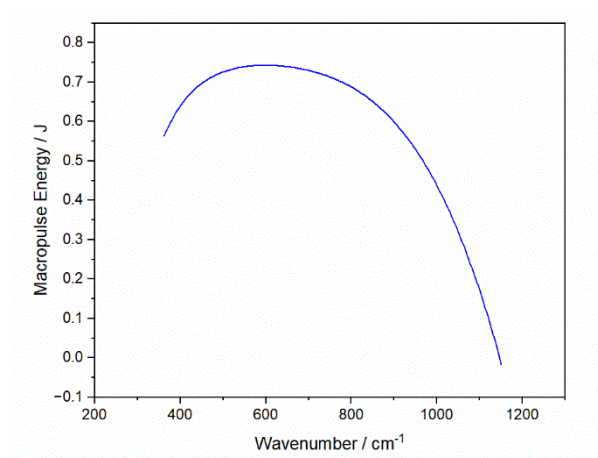


Figure S1: Example of the intracavity macropulse energy of FELICE as a function of photon energy. FELICE macropulse energy is determined by measuring the out-coupled energy which represents a fraction $f = \frac{0.128}{\lambda}$ of the intracavity energy.

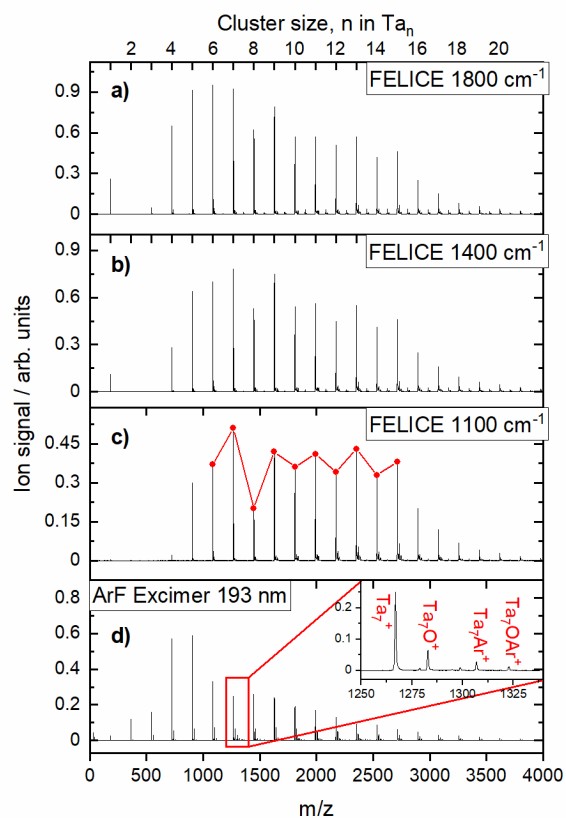


Figure S2: Time-of-flight mass spectra of neutral $Ta_nO_xAr_y$ produced by thermionic emission upon irradiation from FELICE at a) 1800 cm^{-1} , b) 1400 cm^{-1} , c) 1100 cm^{-1} and d) direct ionization by a 193 nm pulse (6.424 eV) from an ArF excimer laser. The red marks in panel c) illustrate the odd-even intensity alternation present.

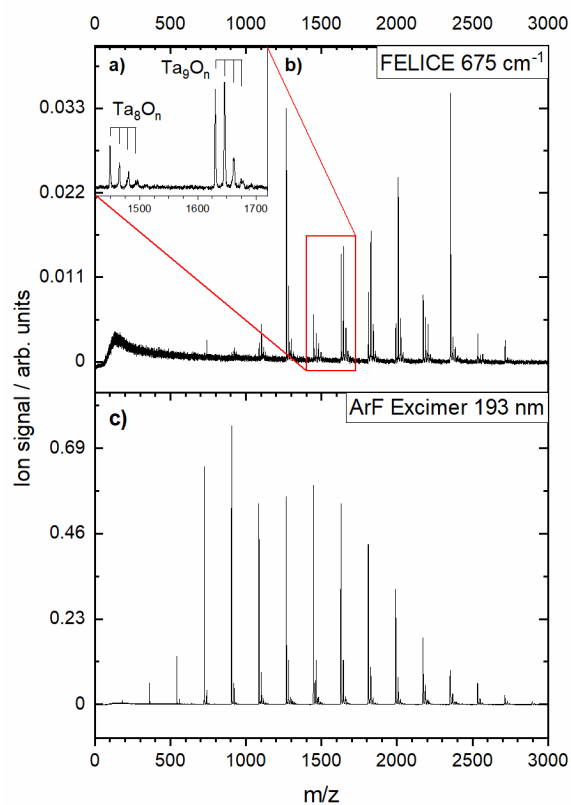


Figure S3: Mass spectra of the Ta_nO_m clusters from irradiation by b) FELICE at 675 cm⁻¹ (near the resonant absorption of oxide stretches) and c) the ArF excimer pulse. Panel a) shows the appearance of [Ta_{8,9}O₀₋₃]⁺ with relatively larger ion cross-sections for oxide species compared to pure Ta_n clusters.

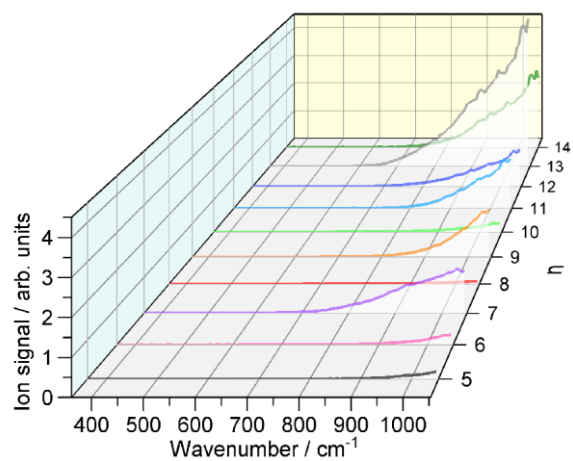


Figure S4: Photoionization spectra of the Ta_n clusters for n = 5-14. Each spectrum is measured in the Ta_n⁺ appearance channel relative to the ion cross-section on alternate ArF ionization pulses.

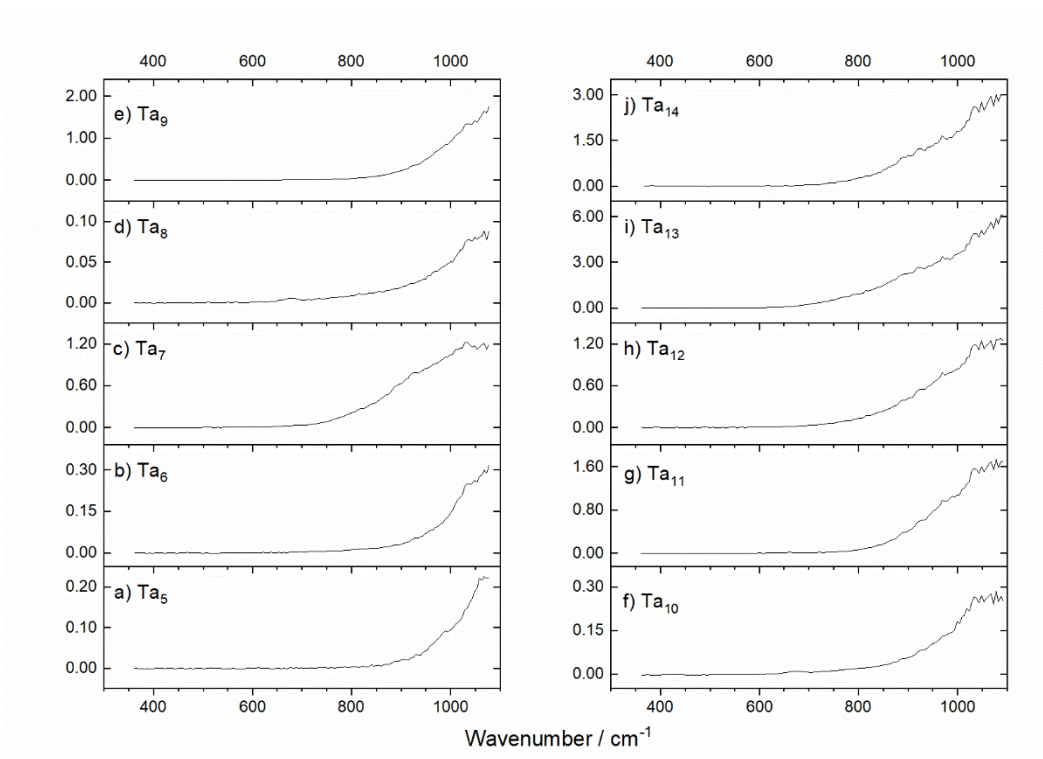


Figure S5: Photoionization spectra of the Ta_n clusters for $n = 5-14$ reproduced of Figure 3. Each spectrum is measured in the Ta_n^+ appearance channel relative to the ion cross-section on alternate ArF ionization pulses.

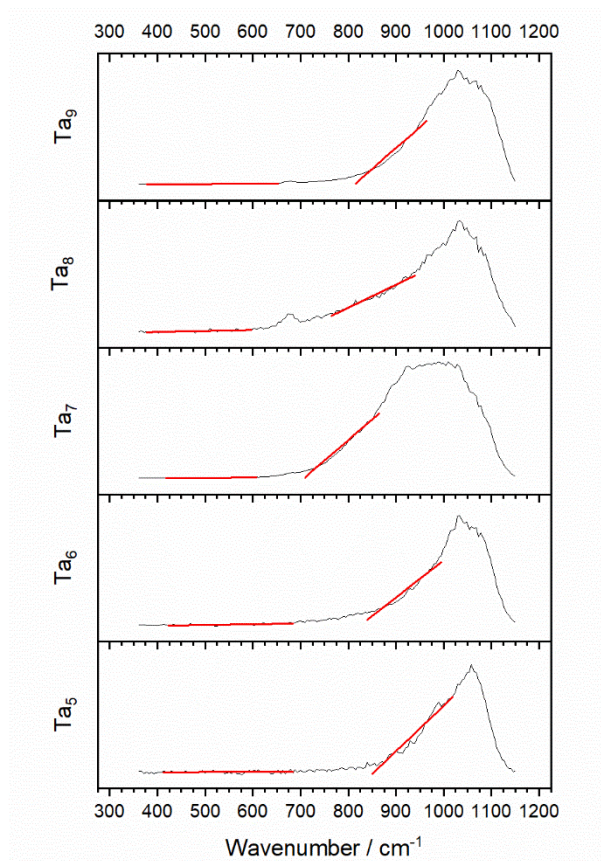


Figure S6: Example of the linear fitting of the baseline and rising edge of photoionization spectra of Ta₅₋₉. Intersection of the fitted lines is then used to determine the onset energy for photoionization. Ion signal reduction for photon energies >1050 cm⁻¹ is a result of normalization with FELICE macropulse energy.

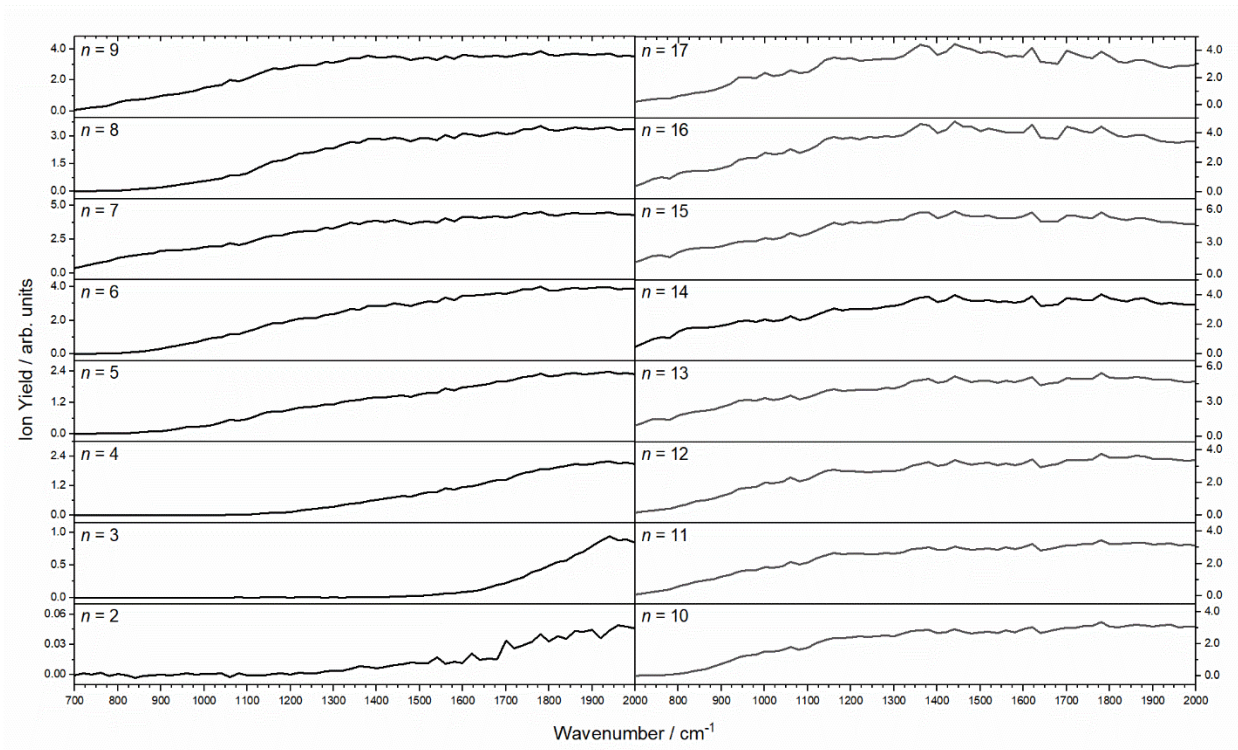


Figure S7: Photoionization spectra of the Ta_n clusters for $n = 2-17$ with photon energies between $700 - 2000 \text{ cm}^{-1}$. Each spectrum is measured in the Ta_n^+ appearance channel relative to the ion cross-section on alternate ArF ionization pulses.

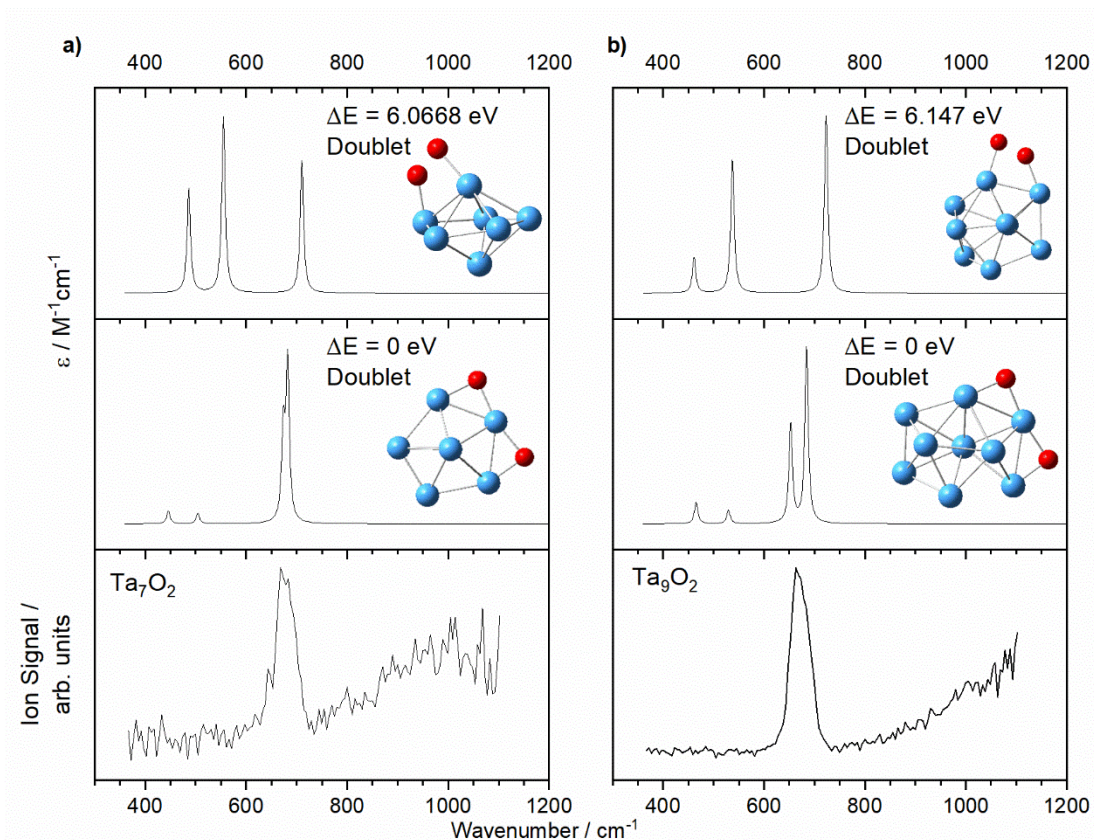


Figure S8: Comparison of experimental and simulated photoionisation spectra of $\text{Ta}_{7,9}\text{O}_2$, with both dioxide (Ta_nO_2) and oxygen bound ($\text{Ta}_n(\text{O}_2)$) clusters shown. Simulated spectra are generated from UB3P86/def2TZVP unscaled harmonic frequency calculations and convoluted with a Lorentz function ($\text{fwhm} = 8 \text{ cm}^{-1}$).

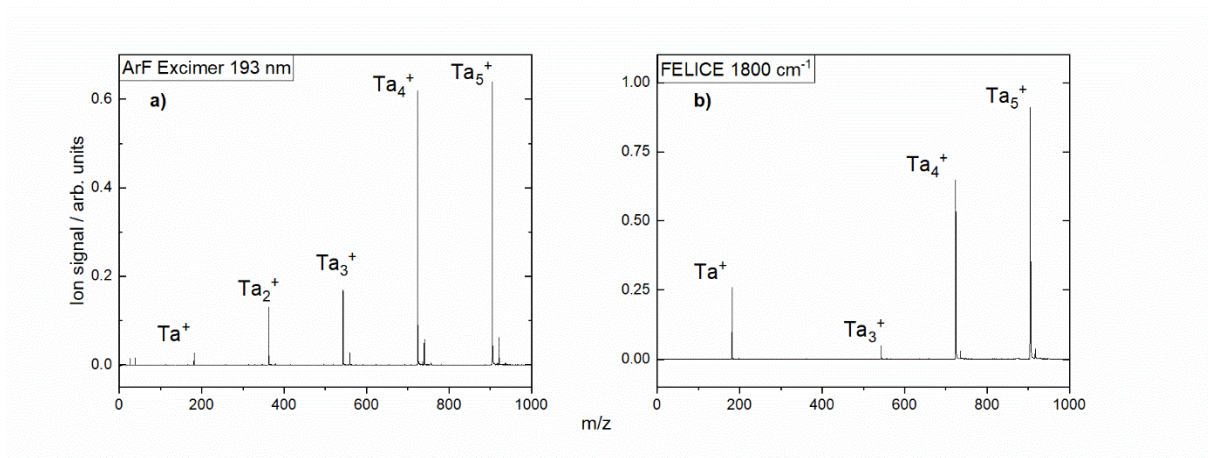


Figure S9: Mass spectra of $[Ta_{1-5}O_m]^+$ clusters produced by irradiation by an ArF excimer pulse (left) and FELICE at 1800 cm^{-1} (right).

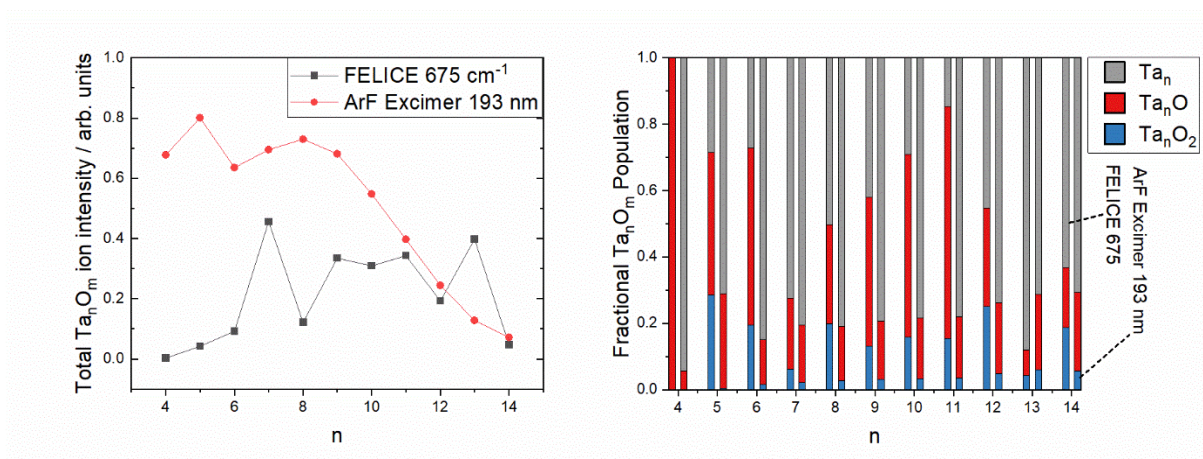


Figure S10: (left) Relative total ion intensities for $[Ta_nO_m]^+$ clusters ($n = 4-14$), upon irradiation of the neutral Ta_nO_m clusters by FELICE at 675 cm^{-1} (black) and an ArF excimer pulse (red). (right) Proportion of ions produced (Ta_n , Ta_nO and Ta_nO_2) for each $n = 4-14$ upon irradiation by FELICE at 675 cm^{-1} (left bar) and an ArF excimer pulse (right bar).

Supporting Information Tables:

Table S1: Calculated ionization energies for Ta_nO_{0-2} from UB3P86/def-TZVP calculations. All energies are in eV

n	Ta_n	2s+1	Ta_nO	2s+1	Ta_nO_2	2s+1
1			6.83	5		
2			6.70	3		
3			6.22	2		
4			5.83	1		
5			5.68	2		
6			5.74	1	6.21	1
7	5.37	2	5.58	2		
8	5.46	1	5.53	3	5.55	3
9	5.33	2	5.27	2	5.66	2
10	5.78	1	5.56	1		
11	5.18	4	4.97	4	5.42	2
12	4.23	3	4.81	1		
13	4.98	2	5.03	2		
14	4.64	3				

Table S2: Tabulated data for Ta₄ from UB3P86/def-TZVP calculations. Data includes the DFT energy, cartesian coordinates and harmonic frequencies.

Ta₄			
Multiplicity (2s+1)	1		
DFT Energy (E _h)	-229.1293651		
Cartesian Coordinates			
Element	X	Y	Z
Ta	1.43557	-0.59929	-0.04174
Ta	-0.02589	1.34006	-0.79075
Ta	-0.40999	0.26194	1.47818
Ta	-0.99968	-1.00272	-0.64569
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)		
141.5204	0		
141.5292	0		
200.5021	0.1565		
200.5054	0.1565		
200.519	0.1565		
278.6581	0		

Table S3: Tabulated data for Ta₇ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₇			
Multiplicity (2s+1)	2		
DFT Energy (E _h)	-401.1999446		
Ionisation Energy (eV)	5.37		
Cartesian Coordinates			
Element	X	Y	Z
Ta	-1.27461	-1.75180	-0.07706
Ta	-2.03871	0.64177	0.18076
Ta	2.01764	0.70513	0.18028
Ta	0.00035	-0.02179	1.62138
Ta	-0.03388	2.15943	-0.23495
Ta	0.00042	-0.02140	-1.59417
Ta	1.32879	-1.71134	-0.07624
Harmonic Frequencies			
Frequency (cm ⁻¹)		Intensity (km/mol)	
17.624		0.237	
59.05		1.5581	
82.0752		0.3744	
105.8612		0.7261	
122.2081		0.4571	
123.6816		0.0492	
129.3614		0.0069	
134.0881		0.2874	
157.0094		0.6482	
160.7115		0.0962	
181.4766		0.9374	
208.2935		0.0903	
217.5691		0.292	
222.4852		0.038	
232.4054		0.0418	

Table S4: Tabulated data for Ta₈ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₈			
Multiplicity (2s+1)	1		
DFT Energy (E _h)	-458.5517578		
Ionisation Energy (eV)	5.46		
Cartesian Coordinates			
Element	X	Y	Z
Ta	1.84991	0.00043	-1.28652
Ta	-0.66356	-0.00050	1.63328
Ta	-1.85254	1.50473	0.00025
Ta	0.66619	-1.94880	-0.00048
Ta	1.84990	-0.00041	1.28652
Ta	0.66616	1.94881	0.00049
Ta	-0.66353	0.00048	-1.63329
Ta	-1.85254	-1.50474	-0.00027
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)		
88.8485	0		
97.3902	0.0091		
109.385	0.7589		
110.802	0.015		
113.6844	0.8365		
133.6879	0.0294		
137.4256	0		
140.9879	1.6557		
143.4593	0.0776		
153.0401	0		
170.8878	0.0914		
184.312	2.1362		
185.097	0.2216		
191.7927	0.7417		
192.8527	0.2567		
212.9161	1.2343		
221.4282	0.0506		
236.9995	0.647		

Table S5: Tabulated data for Ta₉ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₉			
Multiplicity (2s+1)	2		
DFT Energy (E _h)	-515.8894215		
Ionisation Energy (eV)	5.33		
Cartesian Coordinates			
Element	X	Y	Z
Ta	2.15321	1.35087	-0.67144
Ta	1.40499	0.00002	1.43705
Ta	-0.00023	2.11564	0.59424
Ta	-1.40500	-0.00004	1.43705
Ta	2.15343	-1.35052	-0.67162
Ta	0.00022	-2.11564	0.59422
Ta	0.00000	0.00001	-1.37643
Ta	-2.15322	-1.35086	-0.67145
Ta	-2.15342	1.35054	-0.67162
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
47.8015	0	153.9571	0.0429
78.2658	0.7782	154.9387	0.1219
86.594	0	170.0711	0.2303
87.8634	1.7325	171.1167	0.7667
91.1624	0.1889	176.4427	0.2832
103.1686	0	195.6411	0.006
109.8662	0.0892	207.1328	0
124.1573	3.6055	214.9805	0.1082
130.1714	0.0029	215.6008	0.0296
131.3197	0.6677	237.3165	0.3135
148.3181	0.4971		

Table S6: Tabulated data for Ta₁₀ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₁₀			
Multiplicity (2s+1)	1		
DFT Energy (E _h)	-573.2794638		
Ionisation Energy (eV)	5.78		
Cartesian Coordinates			
Element	X	Y	Z
Ta	-1.07237	1.33125	-1.46622
Ta	-1.07077	1.46684	1.33137
Ta	-1.07352	-1.46646	-1.33034
Ta	-1.07172	-1.33067	1.46702
Ta	-2.69374	0.00066	0.00103
Ta	2.69381	-0.00048	-0.00109
Ta	1.07258	1.97806	-0.09529
Ta	1.07161	-1.97845	0.09439
Ta	1.07333	0.09453	1.97767
Ta	1.07079	-0.09527	-1.97855
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
80.704	0	175.1392	0
82.905	0.0042	175.2045	0
82.9086	0.0042	183.2652	0.9612
114.607	0	183.2772	0.9598
114.6149	0	187.3469	0.1146
118.6937	0	188.9609	0
118.7261	0	188.9773	0
121.8148	0	194.7206	0.2776
127.1544	0	194.7307	0.2775
127.1956	0	200.1234	0
156.5557	0	222.8378	0.344
156.5662	0	223.5997	0.0001

Table S7: Tabulated data for Ta₁₁ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₁₁			
Multiplicity (2s+1)	2		
DFT Energy (E _h)	-630.5996299		
Ionisation Energy (eV)	5.22		
Cartesian Coordinates			
Element	X	Y	Z
Ta	-2.41561	-0.00001	-1.51477
Ta	0.00000	0.00001	-1.57885
Ta	1.32842	2.15161	-0.31687
Ta	-1.32866	2.15150	-0.31682
Ta	2.18068	0.00012	1.10615
Ta	1.32865	-2.15150	-0.31684
Ta	2.41565	0.00008	-1.51476
Ta	-0.00006	1.36118	1.83176
Ta	-1.32845	-2.15161	-0.31688
Ta	-2.18068	-0.00012	1.10615
Ta	0.00007	-1.36122	1.83173
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
40.4825	0	161.2182	0.0029
63.8178	0.0296	168.4321	0.0904
70.9726	0.6322	168.8709	0.0071
85.6937	0	170.7458	0
90.4479	0.4196	177.7836	0.0745
92.4991	3.2338	181.6657	0.2278
95.6922	0.0008	192.3319	0.3254
100.2882	0	196.7214	0
118.9848	0.0261	198.8371	0.2219
123.8518	0.0405	199.056	0.0083
142.6135	0.1552	208.4555	0.0349
146.3122	0.341	209.5873	0.5987
147.5501	0.0036	234.751	1.0464
158.9082	0.3969		

Table S8: Tabulated data for Ta₁₂ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₁₂			
Multiplicity (2s+1)	3		
DFT Energy (E _h)	-687.9889473		
Ionisation Energy (eV)	4.23		
Cartesian Coordinates			
Element	X	Y	Z
Ta	-2.56429	0.026531	0.013254
Ta	2.564295	-0.02653	-0.01325
Ta	1.130225	-2.27001	0.207294
Ta	1.179231	1.94048	1.148762
Ta	1.162608	1.690248	-1.50521
Ta	-1.17923	-1.94048	-1.14876
Ta	-1.13023	2.27001	-0.20729
Ta	-1.15898	0.50671	-2.20765
Ta	-1.13215	0.911937	2.087731
Ta	-1.16261	-1.69025	1.505211
Ta	1.158983	-0.50671	2.207651
Ta	1.132146	-0.91194	-2.08773
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
49.7076	0	154.8099	0.0008
56.2512	0	160.3824	0.1699
74.2275	0	181.8495	0.2823
75.3432	0	181.881	0.2759
93.3352	0.0399	182.2507	0.0032
93.4707	0.0343	182.4941	0.0001
93.6287	0.0721	188.3238	0
102.7344	0	193.5519	0
103.0433	0.0001	194.0899	0
117.4229	0	195.3828	0
132.7909	0	196.4317	0
132.868	0	196.9576	0
141.2732	0	199.9856	0.1734
142.3362	0	200.0414	0.1769
154.5803	0.0005	206.1005	1.4617

Table S9: Tabulated data for Ta₁₃ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₁₃					
Multiplicity (2s+1)		2			
DFT Energy (E _h)		-745.3229929			
Ionisation Energy (eV)		4.98			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	-2.39492	-1.38676	-1.07597		
Ta	0.01441	0.14203	-0.77304		
Ta	-1.22476	-1.79650	1.34991		
Ta	2.36634	1.15064	-1.65019		
Ta	1.18355	2.51577	0.24650		
Ta	-1.37813	2.47678	0.32924		
Ta	-0.01535	0.65584	2.00652		
Ta	1.31150	-1.75840	1.36797		
Ta	2.62235	0.48373	0.92794		
Ta	-2.66019	0.36150	0.88094		
Ta	2.40571	-1.36236	-1.03217		
Ta	-2.24497	1.10749	-1.69141		
Ta	0.01446	-2.58977	-0.88624		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
42.7331	0.3578	123.8426	0.3129	175.7695	0.1057
55.8988	0.1355	126.3247	0.4337	179.6955	0.3928
67.9634	0.4314	128.7189	0.3708	182.4699	0.1451
71.3886	1.1829	130.9336	0.2688	191.626	0.9136
87.5237	1.0093	144.0385	0.0575	192.8867	0.0661
93.229	0.7682	149.0482	0.2733	196.3913	0.4089
98.1599	0.2667	152.6284	0.0409	202.1951	1.0014
100.5513	0.1861	155.5281	0.2548	209.5882	0.1931
103.9432	0.165	160.4069	0.5711	211.3533	0.7519
113.6388	0.8932	167.4281	1.3986	224.4453	0.1948
117.8186	2.0566	171.3587	1.4766	233.1307	0.1539

Table S10: Tabulated data for Ta₁₄ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies.

Ta₁₄					
Multiplicity (2s+1)		3			
DFT Energy (E _h)		-802.7005827			
Ionisation Energy (eV)		4.64			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	-2.85300	0.00609	-1.18307		
Ta	-2.24355	-1.30944	1.06645		
Ta	-1.39875	-2.19855	-1.32355		
Ta	-0.00004	-0.00001	-0.62796		
Ta	-2.23774	1.32005	1.06549		
Ta	-1.38728	2.20396	-1.32450		
Ta	1.38732	-2.20396	-1.32451		
Ta	1.39869	2.19861	-1.32353		
Ta	-0.00598	-2.64123	0.93303		
Ta	2.85289	-0.00614	-1.18318		
Ta	0.00607	2.64124	0.93307		
Ta	0.00002	0.00000	2.16037		
Ta	2.24360	1.30942	1.06636		
Ta	2.23776	-1.32004	1.06553		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
25.124	0	124.4375	0.0546	168.2413	0.0847
60.4514	0.0008	125.6926	0.105	175.3357	0.0113
63.8347	0	127.6038	0	175.7335	0.5973
72.9588	0.7845	134.7583	0.0004	177.7371	0.0002
73.1976	0.3901	135.3071	0.3666	186.2598	2.6824
84.3089	2.6259	137.909	2.581	186.9121	0.0862
85.8346	0	141.9833	0	194.5864	0.6083
87.289	0.0864	143.3906	0.2446	197.6914	0.0014
91.8491	0.5039	148.6634	0.0477	209.4383	0.0032
106.1418	0.3254	159.8498	0	209.4687	0.169
113.4399	0.0957	162.8366	0.0546	221.96	2.032
118.6903	0.6979	165.644	0.0435	227.4737	1.5189

Table S11: Tabulated data for Ta₆O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

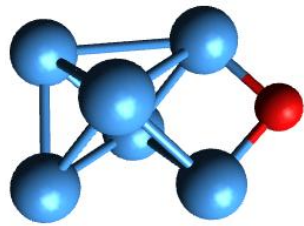
Ta₆O				
Multiplicity (2s+1)	1			
DFT Energy (E _h)	-419.3680692			
Ionisation Energy (eV)	5.74			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	-0.04829	-0.00012	1.54734	
Ta	-1.60163	1.31222	-0.00042	
Ta	1.49381	1.38495	0.00032	
Ta	-1.60096	-1.31288	0.00026	
Ta	-0.04784	-0.00025	-1.54740	
Ta	1.49519	-1.38407	-0.00018	
O	2.82624	0.00129	0.00070	
Harmonic Frequencies				
Frequency (cm ⁻¹)		Intensity (km/mol)		
67.9763		1.0559		
114.1588		0		
120.6845		0.0304		
136.1291		0.0882		
136.7359		0.3758		
155.9343		0		
160.8767		0.8229		
185.7838		0.1161		
191.0844		0.1379		
201.9358		0.2948		
234.7792		1.8079		
237.1645		0.5008		
254.3791		0.1941		
512.0273		0.0424		
681.2526		85.1156		

Table S12: Tabulated data for Ta₇O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

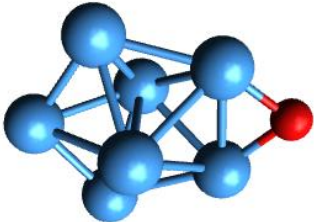
Ta₇O				
Multiplicity (2s+1)	2			
DFT Energy (E _h)	-476.7093234			
Ionisation Energy (eV)	5.58			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	-1.79515	1.26417	-0.01361	
Ta	0.79382	2.00941	0.04594	
Ta	0.78755	-2.01138	0.04341	
Ta	0.05478	-0.00186	1.57711	
Ta	2.27808	-0.00288	-0.06359	
Ta	0.03819	0.00229	-1.57543	
Ta	-1.79845	-1.26024	-0.01473	
O	-3.27420	0.00440	0.00820	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
34.0548	0.8158	168.3409	0.9685	
66.2804	0.0632	176.8291	0.0883	
100.853	0.0071	207.3645	1.5053	
108.221	0.1952	209.429	0.0055	
112.3641	0.0001	213.1234	1.8897	
116.8483	0.2778	231.6373	0.0099	
127.1503	0.219	243.3006	1.0309	
147.5849	0.2238	424.9677	5.2402	
156.9086	0.0174	694.8564	146.2425	

Table S13: Tabulated data for Ta₈O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

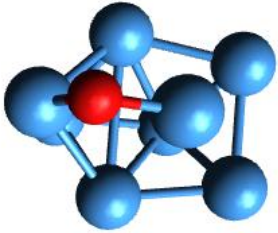
Ta₈O			
Multiplicity (2s+1)	3		
DFT Energy (E _h)	-534.0583008		
Ionisation Energy (eV)	5.53		
Cartesian Coordinates			
Element	X	Y	Z
Ta	1.90191	-0.35841	-1.25940
Ta	-0.56257	0.16169	1.64388
Ta	-1.46143	1.87693	-0.00104
Ta	0.15692	-2.06940	-0.00001
Ta	1.90125	-0.35828	1.26036
Ta	1.09706	1.81318	-0.00014
Ta	-0.56172	0.15976	-1.64418
Ta	-2.28672	-0.92570	0.00040
O	-1.68558	-2.73549	0.00126
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
62.87	0	175.6468	0.0056
94.9729	0.1068	182.1407	0.6405
112.6332	0.0094	184.0667	0.5655
114.12	1.2165	186.7295	0.4046
115.9314	0.0806	204.717	1.0326
118.1209	0.5014	219.199	0.6203
132.6451	1.0376	231.1106	0.4915
136.2571	0.0007	231.8242	0.7329
136.9881	0.0376	483.8218	12.6762
138.8361	0.0057	671.3756	129.7116
159.2773	0.2887		

Table S14: Tabulated data for Ta₉O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

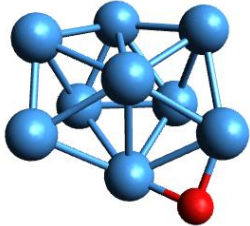
Ta₉O				
Multiplicity (2s+1)	2			
DFT Energy (E _h)	-591.406301			
Ionisation Energy (eV)	5.27			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	2.53478	0.93758	-0.65213	
Ta	1.41298	-0.21188	1.41691	
Ta	0.34382	2.11412	0.41462	
Ta	-1.30399	0.16289	1.51413	
Ta	1.84506	-1.75717	-0.60807	
Ta	-0.48230	-2.08096	0.55442	
Ta	0.03998	-0.00441	-1.32803	
Ta	-2.41658	-0.95507	-0.76122	
Ta	-2.19936	1.49274	-0.52118	
O	2.05872	2.75715	-0.26870	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
68.9541	0.8159	153.5211	0.1123	
72.1971	0.264	167.2466	0.0939	
77.5818	0.7569	168.8252	0.0246	
90.9436	0.6122	180.8967	0.3418	
93.7666	0.5649	188.875	1.5681	
109.0469	0.3838	202.3262	1.016	
117.3989	0.9527	214.7092	0.1817	
123.6145	0.4601	218.3081	0.6565	
131.2381	0.2376	224.6442	0.4205	
132.6675	0.8861	235.5494	0.5493	
146.6548	1.2282	477.7876	5.769	
148.5274	0.1099	667.4558	99.819	

Table S15: Tabulated data for Ta₁₀O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

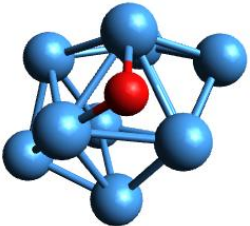
Ta₁₀O			
Multiplicity (2s+1)	1		
DFT Energy (E _h)	-648.7640727		
Ionisation Energy (eV)	5.56		
Cartesian Coordinates			
Element	X	Y	Z
Ta	1.18974	1.31052	1.39156
Ta	1.18801	1.31083	-1.39230
Ta	0.95881	-1.45286	1.44696
Ta	0.95726	-1.45315	-1.44749
Ta	2.71573	-0.21005	-0.00102
Ta	-2.73087	-0.01521	0.00079
Ta	-1.04764	1.99477	0.00018
Ta	-1.13349	-1.96202	0.00083
Ta	-1.09136	0.08090	-1.99044
Ta	-1.08964	0.08162	1.99099
O	0.76147	2.87119	-0.00063
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
73.2879	0.2193	175.0544	0.9894
93.5209	0.2478	179.1243	0.8336
95.783	0.1872	182.967	0.0953
107.4683	0.0309	189.1284	0.0178
113.1968	0.3567	190.1084	1.0402
116.1353	0.0145	195.7074	0.1113
123.708	1.0627	195.7911	0.0181
124.6774	0.0277	200.594	0.0532
125.8756	0.4368	214.6344	0.8366
129.1941	0.0005	225.2248	0.3644
149.6717	1.4816	249.5492	0.7665
155.9942	0.0168	366.15	3.4883
168.5066	0.6744	562.276	52.5523
171.7462	0.0789		

Table S16: Tabulated data for the second lowest conformer of Ta₁₀O from UB3P86/def-TZVP calculations. Data includes the DFT and relative energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

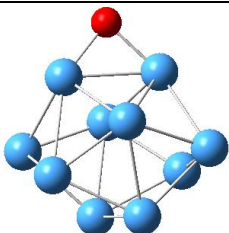
Ta₁₀O				
Multiplicity (2s+1)	1			
DFT Energy (E _h)	-648.7589735			
Relative Energy (eV)	0.1351			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	1.03642	0.99137	1.68288	
Ta	0.95545	1.84695	-1.01169	
Ta	1.09111	-1.70937	1.08051	
Ta	1.18753	-0.96063	-1.68511	
Ta	2.72114	-0.00545	0.05905	
Ta	-2.71631	-0.21208	-0.05396	
Ta	-1.18734	1.94831	0.54348	
Ta	-0.90551	-2.04929	-0.51721	
Ta	-1.03418	0.28014	-1.91274	
Ta	-1.10634	-0.48392	1.89220	
O	-0.38291	3.22988	-0.70626	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
43.3515	1.3087	169.1304	0.2224	
74.8055	0.1988	173.8545	0.1771	
91.0221	0.6273	180.1108	0.2084	
99.6675	1.0393	184.799	0.3134	
104.3884	0.2588	188.1893	0.4008	
106.7401	0.1258	188.7463	0.4362	
114.7842	0.1801	199.8591	0.3498	
116.0439	0.1331	203.0284	0.3214	
116.9764	0.2616	205.7854	0.866	
119.343	0.6058	215.0538	0.7276	
139.3229	0.3102	216.8024	0.1058	
152.3685	0.2407	443.8021	11.4284	
156.568	0.5207	651.2724	118.8337	
160.7805	0.0994			

Table S17: Tabulated data for Ta₁₁O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₁O					
Multiplicity (2s+1)		4			
DFT Energy (E _h)		-706.1190931			
Ionisation Energy (eV)		4.97			
Cartesian Coordinates					
Element	X		Y		Z
Ta	-2.76210		-0.12291		-1.37970
Ta	-0.07475		0.08012		-1.05462
Ta	1.23228		2.30946		-0.17551
Ta	-1.66965		2.05297		-0.12671
Ta	2.34281		0.05300		0.94180
Ta	1.67262		-1.98360		-0.64060
Ta	2.49769		0.45424		-1.62005
Ta	0.05422		1.16499		1.85890
Ta	-1.11237		-2.33213		-0.40816
Ta	-2.10863		-0.31553		1.15781
Ta	0.26928		-1.55233		1.60146
O	-3.11533		1.74940		-1.41103
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
45.9995	0.7977	121.091	0.1602	182.994	0.5948
64.7428	0.0885	127.7551	0.3089	188.342	1.7297
69.3658	0.2392	133.6712	0.017	192.6907	0.1312
80.9141	0.1039	141.4845	0.3093	198.985	0.1144
88.1843	0.1986	149.3722	0.5456	214.1394	0.5062
88.8532	0.4958	154.4215	0.0931	225.4491	0.3025
98.7665	0.3467	159.7132	0.2003	231.1606	0.1284
104.5949	0.4279	169.0345	0.9563	239.2346	0.2547
105.8723	0.9831	175.0313	0.4853	477.5922	3.3458
113.2769	0.1473	182.0836	0.2497	671.1772	117.9355

Table S18: Tabulated data for Ta₁₂O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₂O					
Multiplicity (2s+1)		1			
DFT Energy (E _h)		-763.5116517			
Ionisation Energy (eV)		4.81			
Cartesian Coordinates					
Element	X		Y		Z
Ta	2.05157		0.31275		1.50419
Ta	-1.98905		-0.32161		-1.54695
Ta	-0.46471		-2.37398		-0.78461
Ta	-0.46680		1.86627		-1.66330
Ta	-1.98894		1.50006		0.49711
Ta	0.52702		-1.87449		1.67034
Ta	0.52473		2.38431		0.78767
Ta	-0.46435		0.50721		2.44848
Ta	2.05018		1.14835		-1.02339
Ta	2.05139		-1.45859		-0.48337
Ta	0.52452		-0.50923		-2.45893
Ta	-1.98736		-1.18090		1.05261
O	-3.35978		-0.00133		0.00143
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
84.6627	0.0429	153.3886	0.1925	195.8839	1.0169
84.7149	0.0447	164.5971	1.4559	195.9594	1.0132
96.9734	0	165.2705	0.0396	199.5007	0.1059
104.9873	0.0797	165.3269	0.0392	200.1525	0.014
104.9934	0.0786	168.1034	0	200.253	0.0139
111.0762	0.0146	170.74	0.0075	209.1032	0.0261
111.1469	0.0148	175.1191	0	209.1657	0.163
116.6971	0.3735	178.9044	0.0494	209.2721	0.1885
118.0895	0.0057	185.3602	0.1014	284.0562	4.941
118.1594	0.0056	185.3811	0.0984	286.196	4.9645
153.3398	0.1954	189.8826	0.3653	546.0338	30.0596

Table S19: Tabulated data for Ta₁₃O from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₃O					
Multiplicity (2s+1)		2			
DFT Energy (E _h)		-820.8374425			
Ionisation Energy (eV)		5.03			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	-2.64711	1.24008	0.90702		
Ta	-0.01572	-0.07919	0.73987		
Ta	-1.37458	1.52246	-1.48116		
Ta	2.42488	-0.77759	1.77828		
Ta	1.48403	-2.42650	-0.02803		
Ta	-1.03105	-2.67854	-0.18901		
Ta	0.14737	-0.79939	-1.96659		
Ta	1.19959	1.74898	-1.44047		
Ta	2.71460	-0.36387	-0.86208		
Ta	-2.53032	-0.79938	-0.95585		
Ta	2.34228	1.61486	0.91562		
Ta	-2.20587	-1.22825	1.68603		
Ta	-0.29917	2.71362	0.70562		
O	-1.90664	2.85333	1.74063		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
41.8141	0.1062	123.0809	0.6793	181.7625	0.9045
57.1061	0.148	127.9901	0.1767	189.3168	0.423
61.5835	0.6868	136.9877	0.6992	191.7773	0.0027
76.5542	0.3568	143.5614	0.0066	195.1047	0.9811
87.8963	0.1561	147.6412	0.7157	202.1754	0.652
95.6663	0.1125	149.5637	0.0357	204.7274	2.3655
101.1187	0.1724	153.6853	0.7201	208.5791	0.3975
103.9419	0.3186	156.3064	0.2023	212.8762	0.287
110.1715	1.4783	160.6023	0.3418	221.8111	0.4044
112.6981	0.17	169.9713	0.9377	228.4634	0.0492
115.6957	0.1541	172.786	0.5076	483.6098	7.3201
121.4864	0.4883	175.4669	0.4321	648.9766	115.6435

Table S20: Tabulated data for Ta₆O₂ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

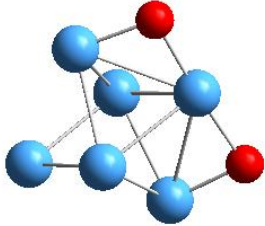
Ta₆O₂				
Multiplicity (2s+1)	1			
DFT Energy (E _h)	-494.890544			
Ionisation Energy (eV)	6.21			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	0.00113	-0.20556	-1.51946	
Ta	2.09201	0.12276	0.00010	
Ta	-0.00972	1.92846	0.00025	
Ta	0.01144	-2.17857	-0.00022	
Ta	0.00075	-0.20635	1.51935	
Ta	-2.09339	0.10166	-0.00014	
O	-2.00803	1.98628	0.00036	
O	1.98775	2.00679	0.00064	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
93.9328	0.0304	216.4624	0.8896	
100.8668	0.0181	217.7081	0	
113.7321	0.0474	226.0645	1.151	
127.1579	0.3856	234.1887	2.3829	
144.0653	0	251.7164	0.6473	
157.1138	0.0149	460.1183	18.3553	
177.6203	0.406	525.2916	1.3064	
178.4892	0.007	682.5331	92.5747	
185.8947	0.0207	691.9356	98.9001	

Table S21: Tabulated data for Ta₇O₂ from UB3P86/def-TZVP calculations. Data includes the DFT energy, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

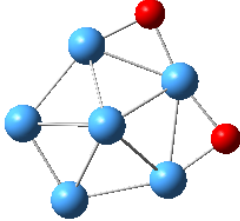
Ta₇O₂				
Multiplicity (2s+1)	2			
DFT Energy (E _h)	-552.233952			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	0.59482	-2.11109	-0.00032	
Ta	-1.94239	-1.20232	0.00005	
Ta	0.59897	2.11034	-0.00032	
Ta	-0.05144	0.00011	1.53416	
Ta	-1.94038	1.20539	-0.00013	
Ta	-0.05042	0.00001	-1.53423	
Ta	2.24257	-0.00195	0.00071	
O	2.49959	-1.96547	0.00024	
O	2.50338	1.96103	0.00056	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
73.44	0.4728	198.0612	0	
85.0803	0.0035	201.9748	0	
91.5226	0	217.9736	3.9635	
102.341	0.1633	222.6014	2.136	
108.8246	0	231.3636	0.5843	
123.3161	0.4191	247.2666	0.1539	
124.4694	0.012	445.7188	13.956	
137.8332	0.0961	504.1315	11.3619	
159.153	0.0873	673.4649	95.049	
164.4749	0.8587	682.0464	170.3239	
195.1851	0.3492			

Table S22: Tabulated data for Ta₇(O₂) from UB3P86/def-TZVP calculations. Data includes the DFT and relative energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

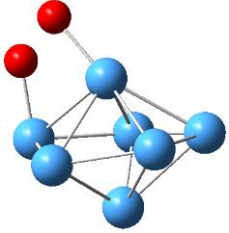
Ta₇(O₂)				
Multiplicity (2s+1)	2			
DFT Energy (E _h)	-552.009747704			
Relative Energy (eV)	6.0668			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	0.76133	-1.98623	-0.24628	
Ta	2.20463	0.17406	-0.28704	
Ta	-1.96530	1.08823	0.26205	
Ta	-0.32510	-0.07280	-1.62626	
Ta	0.34728	2.06946	-0.34359	
Ta	0.22743	0.06613	1.51488	
Ta	-1.72787	-1.38812	0.24156	
O	1.74903	0.18332	2.81997	
O	2.60911	0.26625	1.60281	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
35.0021	3.2027	188.6277	0.5988	
42.9359	2.1758	191.6082	0.3543	
71.7387	2.6792	206.9004	0.8761	
91.0128	0.0766	222.935	0.0213	
106.0902	0.1003	226.3864	1.2266	
119.91	0.0505	230.408	0.0261	
121.7965	0.1782	243.1992	6.9793	
127.9276	4.6393	486.2728	32.6311	
134.0713	1.434	554.9332	54.7175	
151.7334	0.2105	710.1452	41.1844	
176.1907	0.2851			

Table S23: Tabulated data for Ta₈O₂ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₈O₂			
Multiplicity (2s+1)	3		
DFT Energy (E _h)	-609.5697762		
Ionisation Energy (eV)	5.55		
Cartesian Coordinates			
Element	X	Y	Z
Ta	-2.28039	0.06734	-0.97151
Ta	0.94115	-0.28611	1.52934
Ta	1.98186	-1.40963	-0.40654
Ta	-0.72474	1.96400	0.28191
Ta	-1.59353	-0.43604	1.43300
Ta	-0.50284	-2.09130	-0.17656
Ta	0.31157	0.13958	-1.57663
Ta	2.03114	1.50872	-0.07978
O	0.94500	2.99836	0.32877
O	-2.44346	1.96042	-0.63189
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
44.3368	0.5611	174.0733	0.6443
64.089	0.6812	183.2346	0.116
79.1623	1.466	192.8367	1.0694
99.4014	0.6425	197.5967	0.333
110.9945	2.1269	205.3832	0.1572
115.8612	0.6123	221.8805	0.6908
132.3694	0.0721	236.2693	0.4748
132.6581	0.3236	242.6289	1.2586
136.3262	0.3618	490.9327	12.5211
146.2881	0.1764	537.0425	6.8327
157.5783	0.1562	662.5745	72.2285
167.545	0.9745	679.0513	109.6595

Table S24: Tabulated data for Ta₉O₂ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

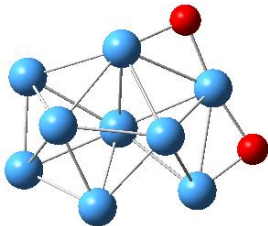
Ta₉O₂				
Multiplicity (2s+1)	2			
DFT Energy (E _h)	-666.9361318			
Ionisation Energy (eV)	5.66			
Cartesian Coordinates				
Element	X	Y	Z	
Ta	2.52939	1.06759	-0.55776	
Ta	1.28759	-0.18460	1.48258	
Ta	0.14719	2.10564	0.47687	
Ta	-1.51771	0.09377	1.47298	
Ta	2.11742	-1.61157	-0.54451	
Ta	-0.48931	-2.03972	0.58789	
Ta	0.05992	0.01614	-1.24499	
Ta	-2.41357	-1.06893	-0.88355	
Ta	-2.31018	1.36643	-0.65300	
O	1.80649	2.85274	-0.14873	
O	3.57045	-0.52368	-1.09697	
Harmonic Frequencies				
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	
57.9807	0.2225	167.9145	0.8254	
71.1568	0.3423	181.0357	0.7785	
71.7206	0.3348	192.0492	0.2331	
92.9358	0.8953	200.9696	0.3697	
96.1189	0.3987	206.3276	0.4519	
112.1938	0.4852	216.4875	1.3053	
114.5833	0.1508	221.3743	0.3312	
118.4847	0.2887	224.4016	0.3975	
131.0419	0.6365	236.6248	1.7392	
136.3218	0.3245	465.2111	18.5507	
143.4999	0.3679	529.2405	11.4475	
150.4802	0.4744	652.6597	84.3881	
154.1837	0.3985	684.1521	149.2384	
164.3493	0.4047			

Table S25: Tabulated data for Ta₉(O₂) from UB3P86/def-TZVP calculations. Data includes the DFT and relative energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

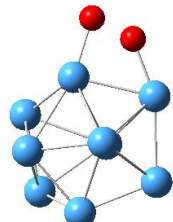
Ta₉O₂			
Multiplicity (2s+1)	2		
DFT Energy (E _h)	-666.70900379		
Relative Energy (eV)	6.147		
Cartesian Coordinates			
Element	X	Y	Z
Ta	2.57459	0.56721	-0.62812
Ta	1.33507	-0.43945	1.43780
Ta	0.59267	2.04419	0.38460
Ta	-1.27682	0.29169	1.52748
Ta	1.58608	-1.99529	-0.61174
Ta	-0.77066	-2.06169	0.55071
Ta	-0.03001	-0.08464	-1.37376
Ta	-2.53534	-0.70952	-0.73959
Ta	-1.96265	1.71721	-0.50958
O	2.69712	2.50516	-0.34387
O	1.74737	3.61119	-0.00100
Harmonic Frequencies			
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
48.0476	1.817	166.9257	0.0283
73.2709	0.9177	170.5878	0.0931
75.9597	0.4795	178.2454	0.0043
76.6782	0.4404	183.2284	1.1061
92.3671	0.7575	191.3435	1.065
94.0337	0.1272	201.7583	0.8667
111.5548	1.6475	212.3652	0.3306
114.6495	0.7636	214.8518	0.0601
120.0297	0.3637	232.0913	0.4373
129.1373	0.7158	255.556	0.7763
134.3537	0.2088	461.1447	15.9503
146.6095	0.4237	537.296	60.4584
152.7022	0.0424	722.9587	80.1354
155.9134	1.1135		

Table S26: Tabulated data for Ta₁₀O₂ from UB3P86/def-TZVP calculations. Data includes the DFT energy, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₀O₂					
Multiplicity (2s+1)		3			
DFT Energy (E _h)		-724.2974397			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	1.25525	-2.19862	0.03121		
Ta	-0.99608	-1.38210	-1.38659		
Ta	0.08147	0.00067	1.14191		
Ta	-2.63017	0.00107	0.20885		
Ta	-1.38968	-2.23725	1.02030		
Ta	1.26020	2.19691	0.03242		
Ta	1.31975	-0.00030	-1.55618		
Ta	-1.38792	2.24006	1.01878		
Ta	-0.99304	1.38301	-1.38647		
Ta	2.82172	-0.00282	0.69666		
O	3.00662	1.95602	0.81734		
O	3.00225	-1.96173	0.81704		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
51.2794	0	136.2081	0.1992	194.1667	0.4183
61.631	0.0941	141.9122	0.0942	206.4743	0.4773
85.0184	0.0764	146.8248	0.4527	209.8036	0.1063
88.1668	0.0781	148.3099	0.2215	218.0008	1.0593
93.5606	0.0638	155.0979	0.2933	228.305	0.0636
99.9699	0.3652	169.0741	0.0213	233.4882	0.3054
103.5764	0.011	174.567	0.274	447.877	16.8963
121.4059	0.1249	183.3056	0.0198	508.1589	10.1971
124.0542	0.1715	185.2361	0.7662	648.5392	65.7814
125.1085	0.4938	189.0432	0.2119	657.1716	157.7391

Table S27: Tabulated data for Ta₁₁O₂ from UB3P86/def-TZVP calculations. Data includes the DFT and ionization energies, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₁O₂					
Multiplicity (2s+1)		2			
DFT Energy (E _h)		-781.6513293			
Ionisation Energy (eV)		5.42			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	-2.80699	-0.42199	-1.26369		
Ta	-0.09233	0.07655	-0.97091		
Ta	0.86770	2.49337	-0.18496		
Ta	-1.88990	2.01792	-0.13827		
Ta	2.33120	0.36938	0.92885		
Ta	1.87944	-1.86629	-0.65349		
Ta	2.51219	0.53623	-1.57641		
Ta	-0.10881	1.09848	1.84494		
Ta	-0.81644	-2.47887	-0.52504		
Ta	-1.96604	-0.78311	1.15914		
Ta	0.55137	-1.57356	1.56688		
O	-3.44704	1.35430	-1.12134		
O	-0.76316	3.49938	-0.58546		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
54.3982	0.4677	132.5746	0.6667	193.1891	0.2612
65.731	0.5284	135.0713	0.4063	201.0772	1.1866
74.7339	2.0417	138.8137	0.4168	207.7324	0.3075
78.3392	0.1064	147.0683	0.3046	225.1728	0.3864
93.2245	1.0501	156.2309	1.0753	233.3348	0.5141
95.7831	0.247	158.5806	0.5987	233.8995	0.3462
101.3581	0.2541	170.134	0.9002	243.5295	0.6205
104.4805	0.4547	173.8967	0.5051	495.0481	10.5362
107.8506	0.2765	179.1934	0.0597	529.4134	3.4498
116.6251	0.1025	181.6954	0.5782	663.0041	44.8026
118.9855	0.2204	187.3435	0.16	669.4795	166.6155

Table S28: Tabulated data for Ta₁₂O₂ from UB3P86/def-TZVP calculations. Data includes the DFT energy, cartesian coordinates and harmonic frequencies. Oxide modes are highlighted in red.

Ta₁₂O₂					
Multiplicity (2s+1)		1			
DFT Energy (E _h)		-839.016674			
Cartesian Coordinates					
Element	X	Y	Z		
Ta	2.02421	0.92568	-1.27727		
Ta	-2.02453	-0.92548	1.27676		
Ta	-0.50502	1.02481	2.28882		
Ta	-0.50064	-2.49559	-0.25575		
Ta	-2.02482	-0.64686	-1.43808		
Ta	0.50059	2.49576	0.25609		
Ta	0.50499	-1.02541	-2.28845		
Ta	-0.50548	1.46862	-2.03254		
Ta	2.02777	-1.56573	-0.16073		
Ta	2.02496	0.64709	1.43761		
Ta	0.50550	-1.46854	2.03258		
Ta	-2.02753	1.56555	0.16107		
O	-3.39990	-0.00356	-0.00078		
O	3.39996	0.00430	-0.00009		
Harmonic Frequencies					
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
91.0631	0.0045	160.7785	0	199.0267	0
91.2174	0.0039	160.8653	0	202.0501	0.1016
107.7837	0.0001	164.5452	0.7038	202.1795	0.1033
109.5559	0	166.6501	0	205.6669	0.2684
109.6481	0	170.3323	0	211.6336	0
111.205	0.1871	173.493	1.2226	211.7254	0
111.2331	0.1882	178.8401	0	297.426	6.883
118.0551	0	188.8317	0	299.442	6.8769
119.4878	0	194.1984	0.0092	307.9085	0.0011
119.6694	0	194.286	0.0087	309.8459	0.0006
159.1452	0.0027	195.137	0	553.1211	102.8468
159.2106	0.0026	195.2124	0	556.5108	0.0367