SUPPLEMENTARY MATERIAL

Successive protonation of Lindqvist Hexaniobate, $[Nb_6O_{19}]^{8-}$: electronic properties and structural distortions

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S1: Supplementary Data

Table S1: Electronic energies (E) and their changes with respect to the most stable structure (ΔE) along each stage through the successive protonation of Hexaniobate (in Kcal/mol).

	E	ΔE
Nb6O19	**-1110926.70**	
Nb6O19Hb	**-1111259.57**	
Nb6O19He	-1111246.63	**12.94**
Nb6O19H2	E	ΔE
Nb6O19HbHb1	**-1111581.84**	**0.00**
Nb6O19HbHb2	-1111576.93	4.91
Nb6O19HbHb3	-1111581.64	0.20
Nb6O19HbHb4	-1111581.77	0.07
Nb6O19HbHb5	-1111581.65	0.19
Nb6O19HbHb6	-1111581.76	0.08
Nb6O19HbHb7	-1111581.24	0.60
Nb6O19HbHb8	-1111576.87	4.97
Nb6O19HbHb9	-1111579.22	2.62
Nb6O19HbHb10	-1111576.87	4.97
Nb6O19HbHb11	-1111578.52	3.31
Nb6O19HbHe1	-1111573.79	8.05
Nb6O19HbHe2	-1111572.00	9.84
Nb6O19HbHe3	-1111573.42	8.42
Nb6O19HbHe4	-1111573.47	8.37
Nb6O19HbHe5	-1111573.44	8.40
Nb6O19HbHe6	-1111572.06	9.77
Nb6O19H3	E	ΔE
Nb6O19Hb2Hb1	-1111889.32	5.18
Nb6O19Hb2Hb2	**-1111894.50**	**0.00**
Nb6O19Hb2Hb3	-1111894.31	0.19
Nb6O19Hb2Hb4	-1111889.31	5.19
Nb6O19Hb2Hb5	-1111894.37	0.13
Nb6O19Hb2Hb6	-1111894.32	0.18
Nb6O19Hb2Hb7	-1111894.29	0.20
Nb6O19Hb2Hb8	-1111889.31	5.19
Nb6O19Hb2Hb9	-1111887.67	6.82
Nb6O19Hb2Hb10	-1111894.36	0.14

Nb6O19Hb2He1	-1111889.99	4.50
Nb6O19Hb2He2	-1111888.25	6.25
Nb6O19Hb2He3	-1111889.79	4.70
Nb6O19Hb2He4	-1111888.25	6.25
Nb6O19Hb2He5	-1111888.39	6.10
Nb6O19Hb2He6	-1111888.57	5.93
Nb6O19H4	E	ΔE
Mn6O19Hb3Hb1	-1112192.17	4.11
Mn6O19Hb3Hb2	-1112191.97	4.31
Mn6O19Hb3Hb3	-1112193.38	2.90
Mn6O19Hb3Hb4	-1112193.13	3.15
Mn6O19Hb3Hb5	-1112194.70	1.58
Mn6O19Hb3Hb6	-1112193.20	3.08
Mn6O19Hb3Hb7	-1112193.92	2.36
Mn6O19Hb3Hb8	-1112196.00	0.28
Mn6O19Hb3Hb9	-1112194.37	1.91
Nb6O19Hb3He1	-1112194.53	1.75
Nb6O19Hb3He2	-1112192.85	3.43
Nb6O19Hb3He3	-1112194.60	1.68
Nb6O19Hb3He4	-1112195.13	1.15
Nb6O19Hb3He5	-1112194.68	1.60
Nb6O19Hb3He6	**-1112196.28**	**0.00**
Nb6O19H5	E	ΔE
Nb6O19Hb3HeHb1	-1112483.30	7.45
Nb6O19Hb3HeHb2	-1112484.60	6.13
Nb6O19Hb3HeHb3	-1112488.99	1.77
Nb6O19Hb3HeHb4	**-1112490.76**	**0.00**
Nb6O19Hb3HeHb5	-1112487.60	3.16
Nb6O19Hb3HeHb6	-1112488.45	2.30
Nb6O19Hb3HeHb7	-1112489.25	1.50
Nb6O19Hb3HeHb8	-1112488.54	2.21
Nb6O19Hb3HeHb9	-1112488.58	2.17
Nb6O19Hb3HeHe1	-1112485.32	5.43
Nb6O19Hb3HeHe2	-1112487.60	3.15
Nb6O19Hb3HeHe3	-1112488.37	2.39
Nb6O19Hb3HeHe4	-1112487.83	2.93
Nb6O19Hb3HeHe5	-1112488.04	2.71
Nb6O19H6	E	ΔE
Nb6O19Hb4HeHb1	-1112772.30	3.98
Nb6O19Hb4HeHb2	-1112767.16	9.11
Nb6O19Hb4HeHb3	-1112772.80	3.47
Nb6O19Hb4HeHb4	-1112772.87	3.41
Nb6O19Hb4HeHb5	-1112775.69	0.58
Nb6O19Hb4HeHb6	-1112774.52	1.75
Nb6O19Hb4HeHb7	-1112775.31	0.96
Nb6O19Hb4HeHb8	**-1112776.27**	**0.00**
Nb6O19Hb4HeHe1	-1112774.54	1.73
Nb6O19Hb4HeHe2	-1112773.68	2.59
Nb6O19Hb4HeHe3	-1112774.55	1.72
Nb6O19Hb4HeHe4	-1112775.21	1.06
Nb6O19Hb4HeHe5	-1112774.76	1.51
Nb6O19H7	E	ΔE
Nb6O19Hb5HeHb1	-1113048.54	5.86
Nb6O19Hb5HeHb2	-1113049.16	5.25
Nb6O19Hb5HeHb3	-1113050.11	4.29
Nb6O19Hb5HeHb4	-1113052.11	2.30
Nb6O19Hb5HeHb5	**-1113054.41**	**0.00**
Nb6O19Hb5HeHb6	-1113051.17	3.24

Nb6O19Hb5HeHb7	-1113053.33	1.08
Nb6O19Hb5HeHe1	-1113053.40	1.00
Nb6O19Hb5HeHe2	-1113051.99	2.42
Nb6O19Hb5HeHe3	-1113053.40	0.93
Nb6O19Hb5HeHe4	-1113052.53	1.88
Nb6O19Hb5HeHe5	-1113054.10	0.31

Nb6O19H8	E	ΔE
Nb6O19Hb6HeHb1	-1113318.86	5.41
Nb6O19Hb6HeHb2	-1113319.61	4.67
Nb6O19Hb6HeHb3	-1113322.38	1.90
Nb6O19Hb6HeHb4	-1113321.65	2.63
Nb6O19Hb6HeHb5	-1113321.74	2.54
Nb6O19Hb6HeHb6	-1113322.32	1.95
Nb6O19Hb5HeHe1	-1113322.44	1.84
Nb6O19Hb5HeHe2	-1113324.22	0.06
Nb6O19Hb5HeHe3	-1113322.79	1.49
Nb6O19Hb5HeHe4	**-1113324.27**	**0.00**
Nb6O19Hb5HeHe5	-1113323.52	0.75

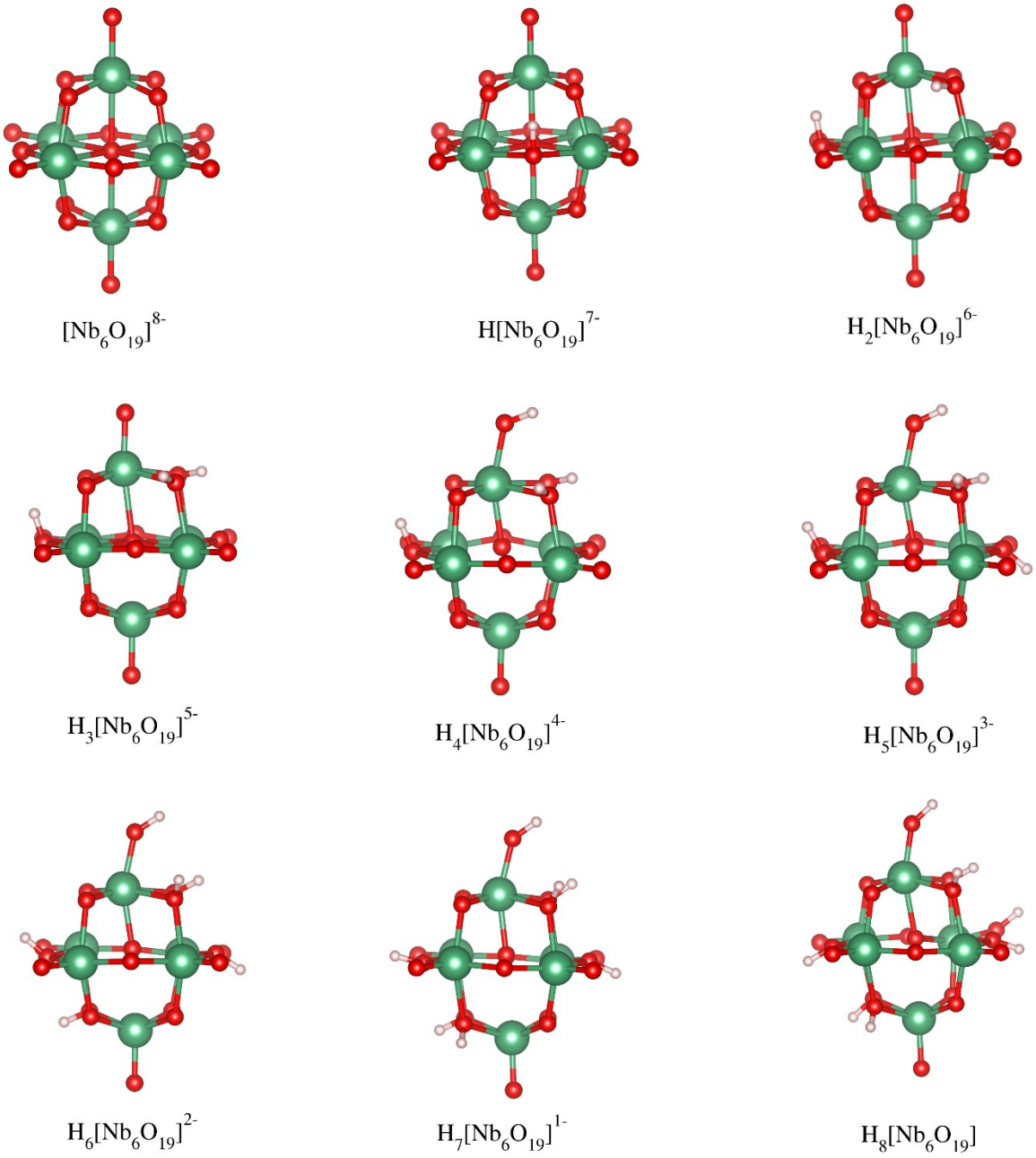

Figure S1: Equilibrium structures of $[Nb_6O_{19}]^{8-}$ and protonated species.

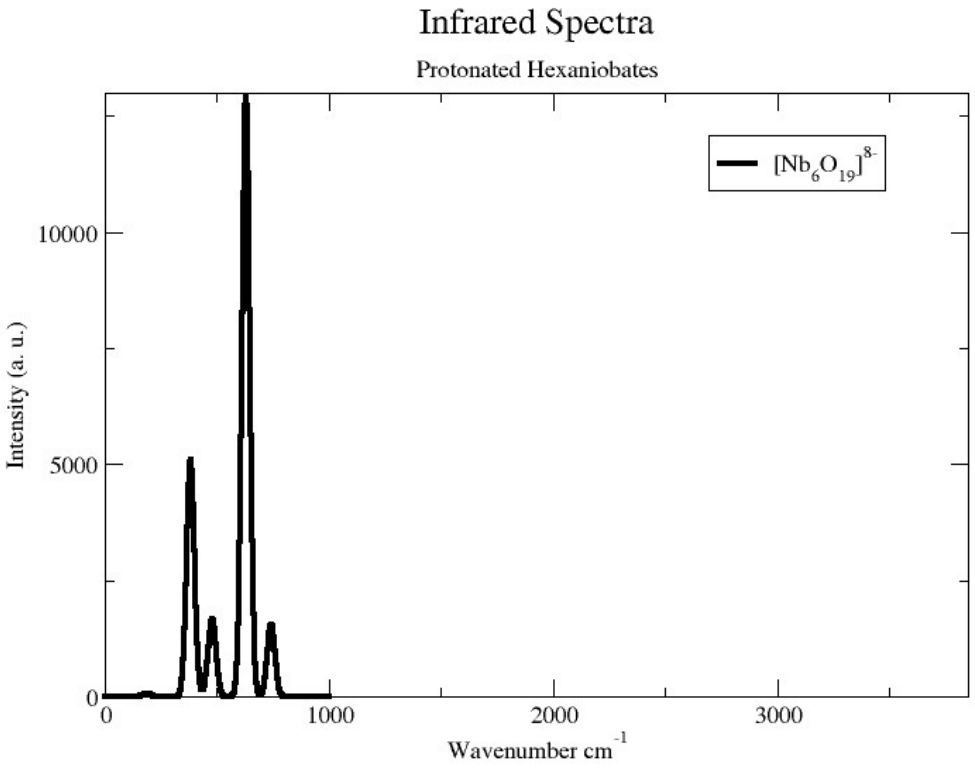

Figure S2: Infrared spectra of $[Nb_6O_{19}]^{8-}$ (in arbitrary units).

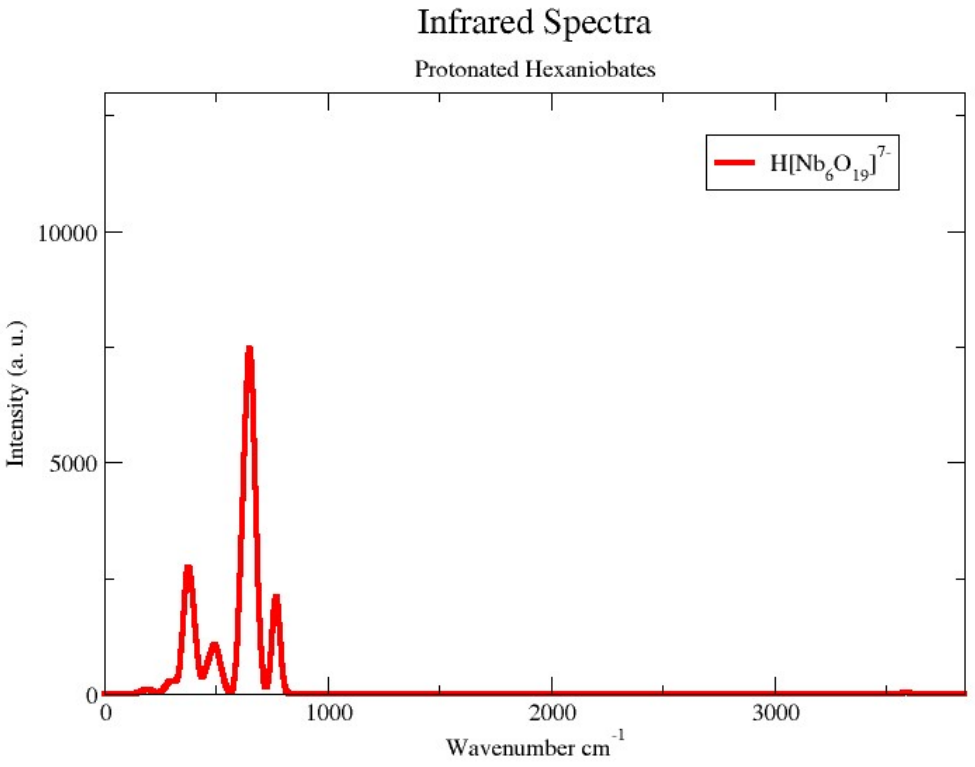

Figure S3: Infrared spectra of $H[Nb_6O_{19}]^{7-}$ (in arbitrary units).

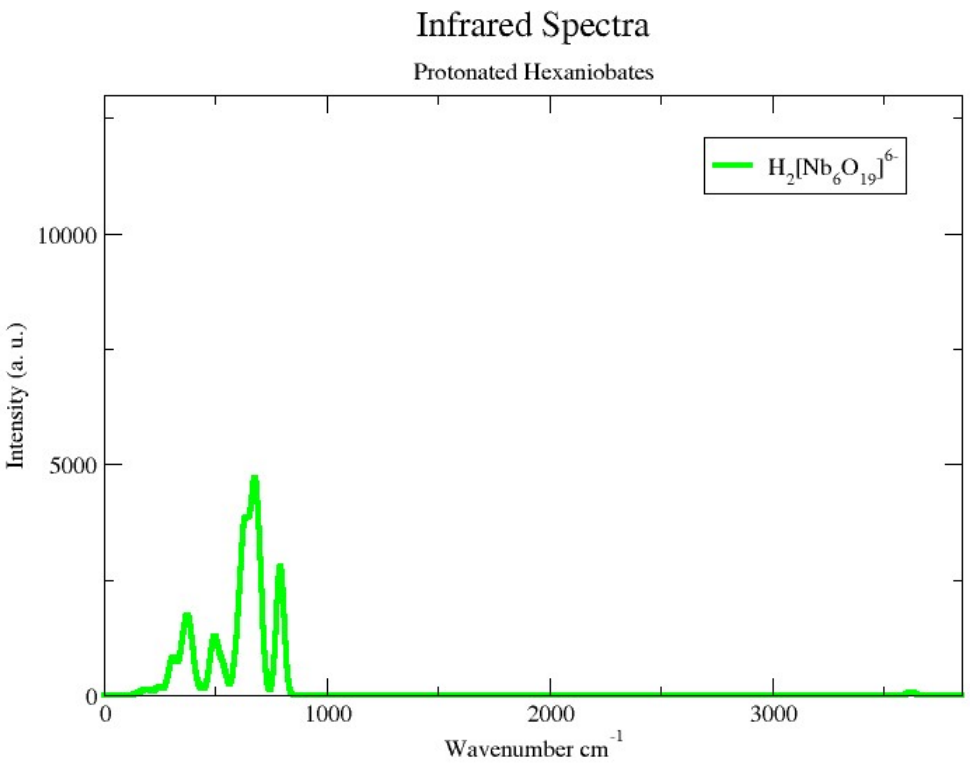

Figure S4: Infrared spectra of $H_2[Nb_6O_{19}]^{6-}$ (in arbitrary units).

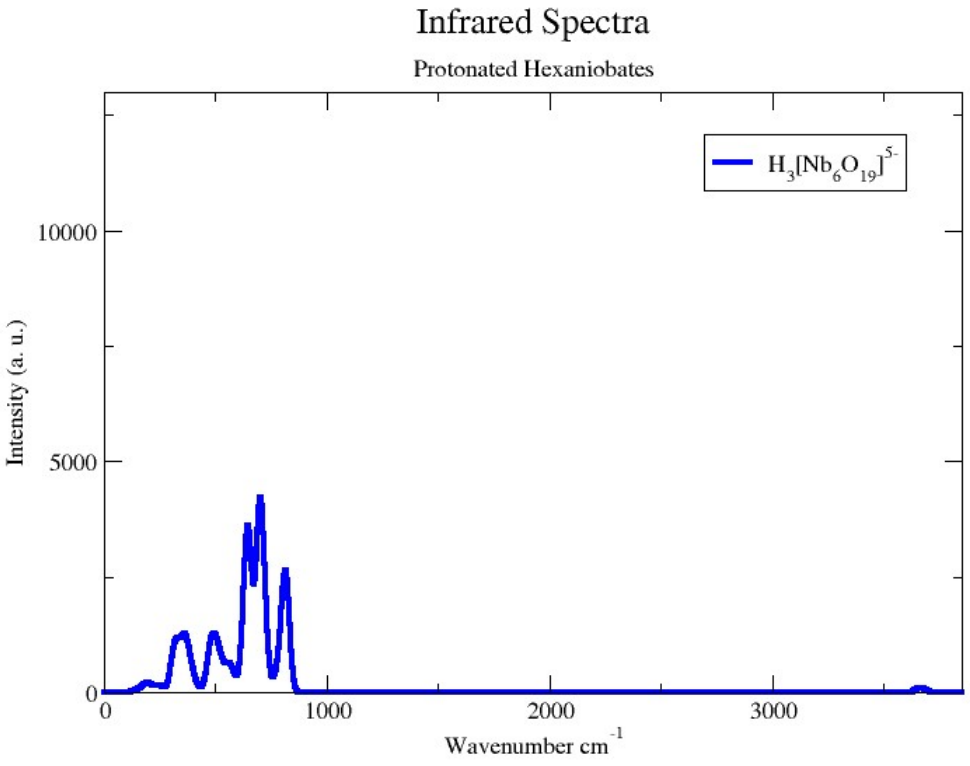

Figure S5: Infrared spectra of $H_3[Nb_6O_{19}]^{5-}$ (in arbitrary units).

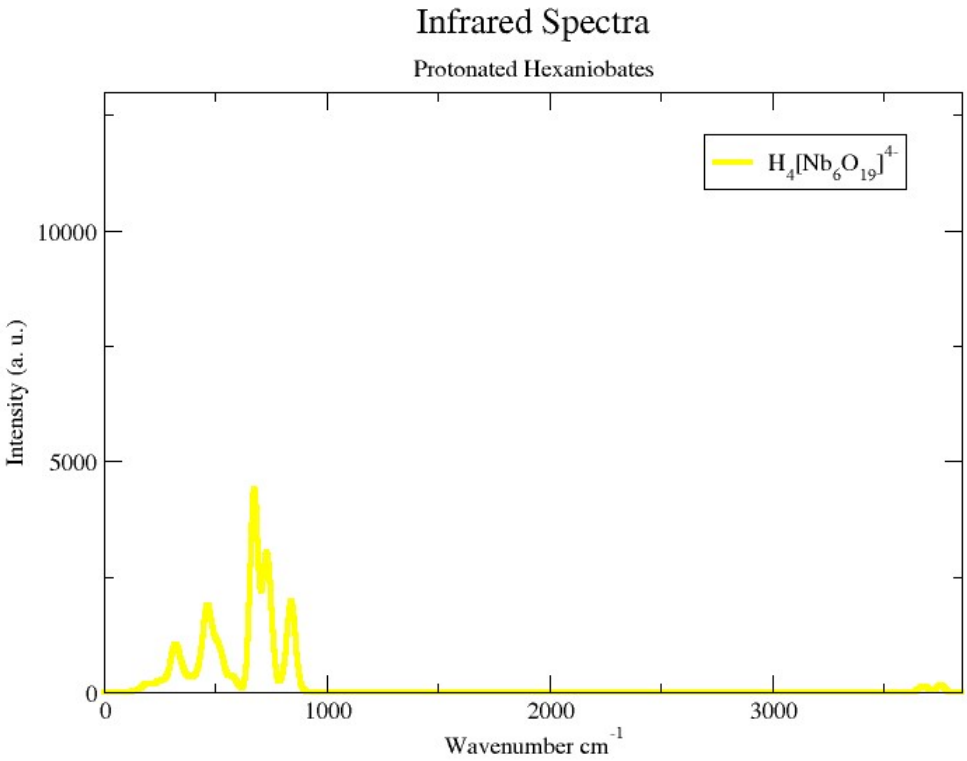

Figure S6: Infrared spectra of $H_4[Nb_6O_{19}]^{4-}$ (in arbitrary units).

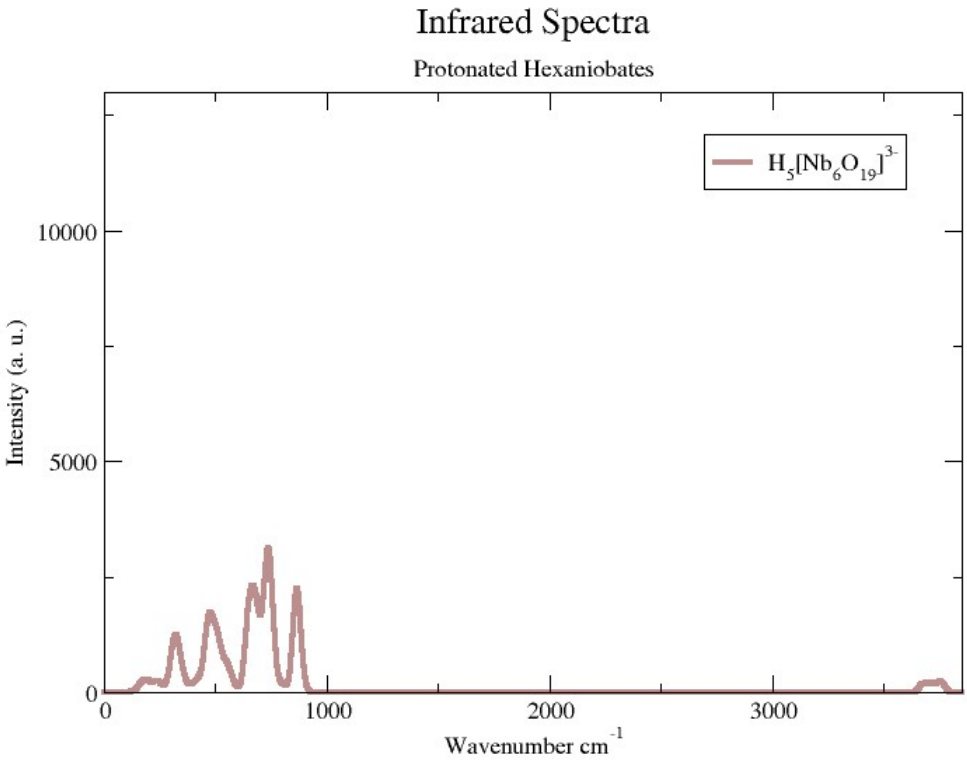

Figure S7: Infrared spectra of $H_5[Nb_6O_{19}]^{3-}$ (in arbitrary units).

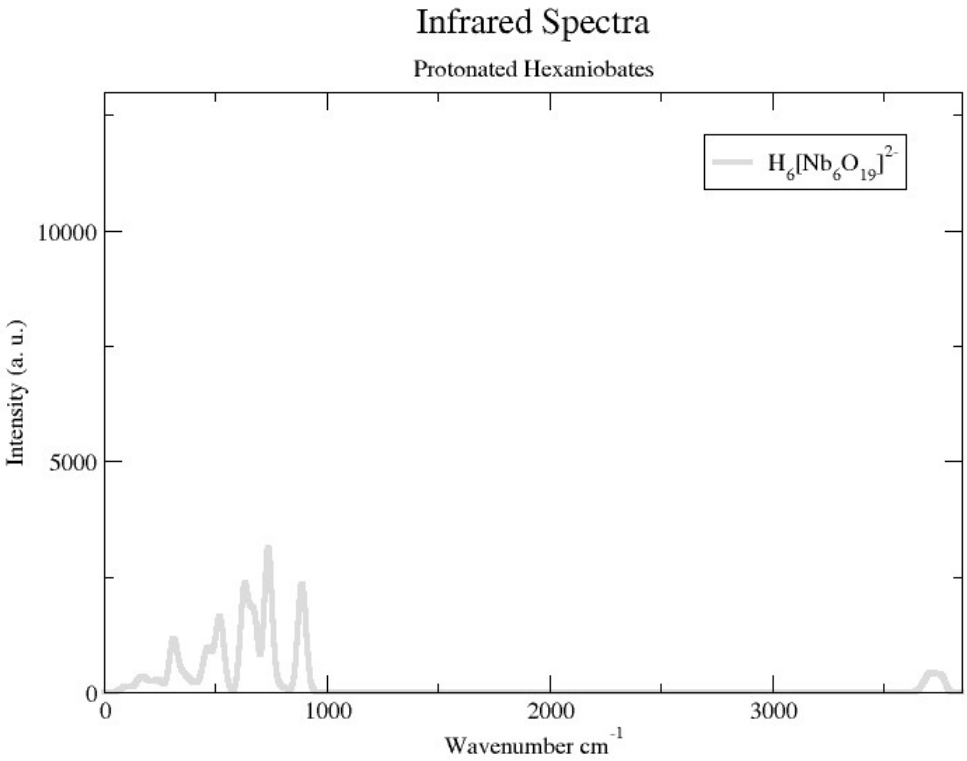

Figure S8: Infrared spectra of $H_6[Nb_6O_{19}]^{2-}$ (in arbitrary units).

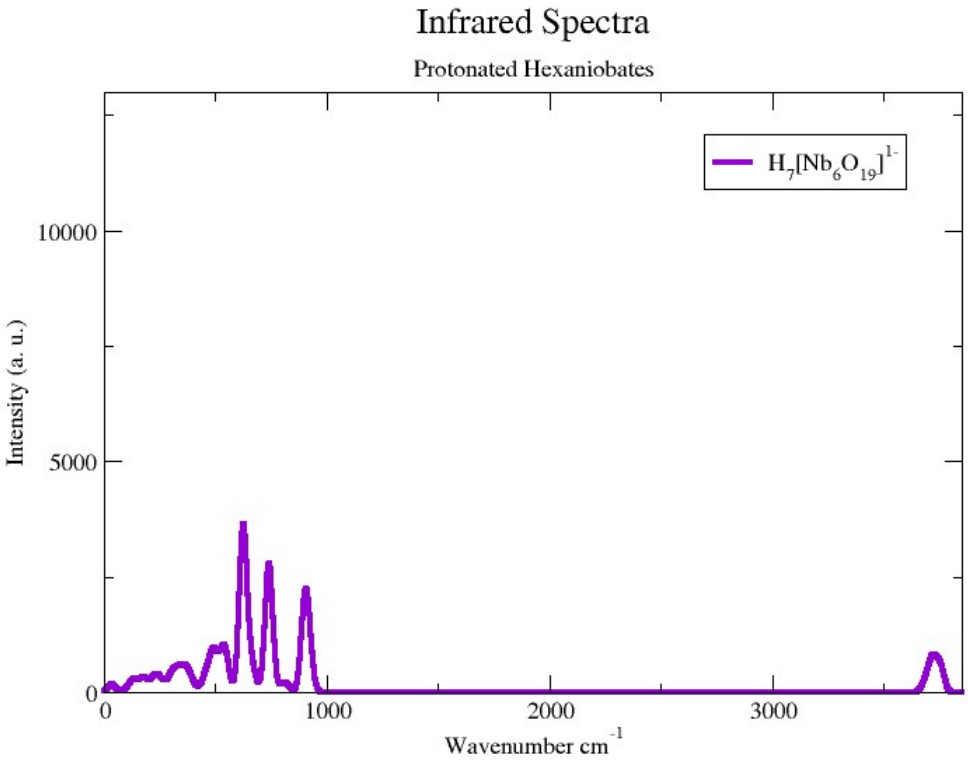

Figure S9: Infrared spectra of $H_7[Nb_6O_{19}]^{1-}$ (in arbitrary units).

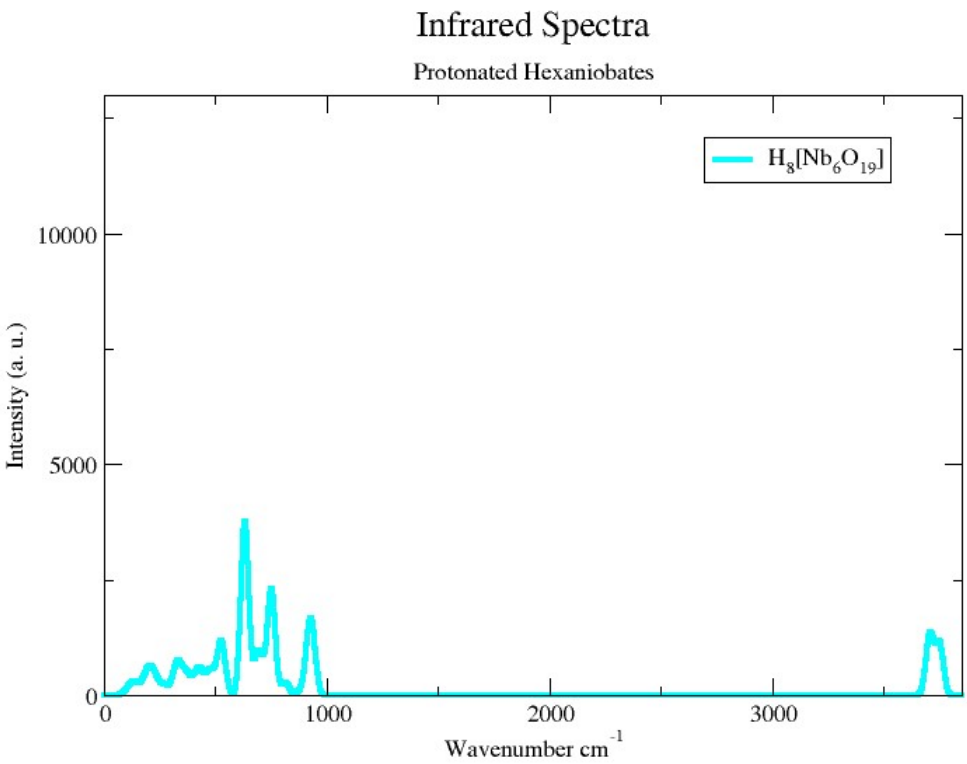

Figure S10: Infrared spectra of $H_8[Nb_6O_{19}]$ (in arbitrary units).

Table S2: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $[Nb_6O_{19}]^{8-}$, along with their respective variations due to excitation (Δq).

$[Nb_6O_{19}]^{8-}$	GS	ES_a	233 nm	ES_b	193 nm	ES_c	170.5 nm
	q (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)
Nb	2.80	2.72	-0.08	2.78	-0.02	2.79	-0.01
Nb	2.80	2.72	-0.08	2.78	-0.02	2.79	-0.01
Nb	2.81	2.72	-0.09	2.78	-0.02	2.79	-0.01
Nb	2.80	2.79	-0.02	2.78	-0.02	2.79	-0.01
Nb	2.80	2.79	-0.02	2.78	-0.02	2.79	-0.01
Nb	2.81	2.72	-0.09	2.78	-0.02	2.79	-0.01
O_i	-1.46	-1.47	0.00	-1.47	0.00	-1.46	0.00
O_e	-1.24	-1.26	-0.02	-1.39	-0.14	-1.21	0.04
O_e	-1.24	-1.26	-0.02	-1.39	-0.14	-1.21	0.04
O_b	-1.32	-1.28	0.04	-1.27	0.06	-1.34	-0.01
O_b	-1.32	-1.28	0.04	-1.26	0.06	-1.34	-0.01
O_b	-1.33	-1.30	0.03	-1.28	0.05	-1.33	-0.01
O_b	-1.33	-1.30	0.03	-1.28	0.05	-1.33	-0.01
O_b	-1.32	-1.28	0.04	-1.26	0.06	-1.34	-0.01
O_b	-1.32	-1.28	0.04	-1.27	0.06	-1.34	-0.01
O_e	-1.25	-1.27	-0.02	-1.30	-0.05	-1.23	0.02
O_b	-1.32	-1.29	0.04	-1.30	0.03	-1.34	-0.01
O_b	-1.32	-1.29	0.04	-1.30	0.03	-1.34	-0.01
O_e	-1.24	-1.24	0.00	-1.30	-0.05	-1.21	0.04
O_e	-1.24	-1.24	0.00	-1.30	-0.05	-1.21	0.04
O_b	-1.32	-1.29	0.04	-1.30	0.03	-1.34	-0.01
O_b	-1.32	-1.29	0.04	-1.30	0.03	-1.34	-0.01
O_e	-1.25	-1.27	-0.02	-1.30	-0.05	-1.23	0.02
O_b	-1.33	-1.28	0.05	-1.24	0.09	-1.33	-0.01
O_b	-1.33	-1.28	0.05	-1.24	0.09	-1.33	-0.01

Table S3: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H[Nb_6O_{19}]^{7-}$, along with their respective variations due to excitation (Δq).

$H[Nb_6O_{19}]^{7-}$	GS $q\ (e)$	ES_a $q\ (e)$	223 nm $\Delta q\ (e)$	ES_b $q\ (e)$	198 nm $\Delta q\ (e)$	ES_c $q\ (e)$	182 nm $\Delta q\ (e)$	ES_d $q\ (e)$	168 nm $\Delta q\ (e)$
Nb	2.79	2.75	-0.04	2.73	-0.06	2.73	-0.06	2.75	-0.03
Nb	2.77	2.67	-0.10	2.73	-0.04	2.70	-0.07	2.70	-0.07
Nb	2.79	2.75	-0.04	2.73	-0.06	2.73	-0.06	2.75	-0.04
Nb	2.81	2.75	-0.05	2.73	-0.07	2.75	-0.06	2.77	-0.04
Nb	2.81	2.75	-0.05	2.76	-0.05	2.76	-0.04	2.77	-0.04
Nb	2.77	2.67	-0.10	2.72	-0.04	2.70	-0.07	2.69	-0.08
O_i	-1.47	-1.43	0.04	-1.43	0.04	-1.42	0.05	-1.39	0.08
O_e	-1.19	-1.20	0.00	-1.20	-0.01	-1.20	-0.01	-1.20	0.00
O_e	-1.20	-1.21	-0.01	-1.19	0.01	-1.20	0.00	-1.21	-0.01
O_b	-1.30	-1.28	0.01	-1.27	0.02	-1.27	0.03	-1.27	0.02
O_b	-1.29	-1.28	0.00	-1.28	0.01	-1.23	0.06	-1.26	0.02
O_b	-1.30	-1.27	0.03	-1.27	0.03	-1.28	0.02	-1.28	0.02
O_b	-1.32	-1.26	0.06	-1.30	0.02	-1.29	0.03	-1.28	0.04
O_b	-1.29	-1.28	0.00	-1.28	0.01	-1.23	0.06	-1.26	0.02
O_b	-1.38	-1.36	0.02	-1.38	0.00	-1.35	0.03	-1.37	0.01
O_e	-1.19	-1.20	0.00	-1.20	-0.01	-1.20	-0.01	-1.20	-0.01
O_b	-1.30	-1.27	0.03	-1.27	0.03	-1.28	0.02	-1.28	0.02
O_b	-1.30	-1.27	0.03	-1.27	0.03	-1.28	0.02	-1.29	0.01
O_e	-1.20	-1.21	0.00	-1.21	-0.01	-1.20	0.00	-1.19	0.01
O_e	-1.20	-1.20	0.01	-1.21	0.00	-1.20	0.01	-1.20	0.00
O_b	-1.30	-1.25	0.05	-1.26	0.04	-1.28	0.02	-1.29	0.01
O_b	-1.32	-1.26	0.06	-1.30	0.02	-1.29	0.03	-1.28	0.04
O_e	-1.20	-1.21	-0.01	-1.19	0.01	-1.20	0.00	-1.22	-0.02
O_b	-1.30	-1.25	0.05	-1.26	0.04	-1.28	0.02	-1.29	0.01
O_b	-1.30	-1.28	0.02	-1.27	0.03	-1.28	0.02	-1.29	0.01
H_{b1}	0.63	0.62	0.00	0.63	0.00	0.63	0.00	0.63	0.00

Table S4: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_2[Nb_6O_{19}]^{6-}$, along with their respective variations due to excitation (Δq).

$H_2[Nb_6O_{19}]^{6-}$	GS	ES_a	242 nm	ES_b	217 nm	ES_c	195 nm	ES_d	172 nm
	q (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)
Nb	2.76	2.74	-0.02	2.75	-0.01	2.72	-0.04	2.69	-0.07
Nb	2.76	2.74	-0.02	2.75	-0.01	2.73	-0.03	2.69	-0.07
Nb	2.80	2.69	-0.11	2.66	-0.14	2.72	-0.07	2.75	-0.05
Nb	2.80	2.69	-0.11	2.64	-0.15	2.72	-0.08	2.74	-0.05
Nb	2.78	2.70	-0.07	2.77	-0.01	2.71	-0.07	2.75	-0.03
Nb	2.78	2.70	-0.07	2.77	-0.01	2.70	-0.07	2.75	-0.03
O_i	-1.47	-1.45	0.02	-1.44	0.03	-1.37	0.10	-1.39	0.08
O_e	-1.15	-1.15	0.00	-1.16	-0.01	-1.14	0.01	-1.16	-0.01
O_e	-1.15	-1.15	0.00	-1.16	-0.01	-1.15	0.00	-1.16	-0.01
O_b	-1.27	-1.25	0.02	-1.28	0.00	-1.27	0.01	-1.25	0.02
O_b	-1.26	-1.25	0.02	-1.27	0.00	-1.25	0.01	-1.24	0.02
O_b	-1.26	-1.25	0.02	-1.27	0.00	-1.25	0.01	-1.24	0.02
O_b	-1.28	-1.25	0.04	-1.28	0.00	-1.27	0.01	-1.26	0.02
O_b	-1.28	-1.24	0.04	-1.28	0.00	-1.27	0.01	-1.26	0.02
O_b	-1.36	-1.36	0.00	-1.36	0.00	-1.36	0.00	-1.35	0.01
O_e	-1.16	-1.16	0.00	-1.03	0.13	-1.14	0.01	-1.16	-0.01
O_b	-1.28	-1.22	0.06	-1.25	0.03	-1.27	0.01	-1.27	0.01
O_b	-1.28	-1.20	0.08	-1.26	0.02	-1.24	0.04	-1.26	0.02
O_e	-1.16	-1.16	0.00	-1.01	0.14	-1.14	0.02	-1.16	-0.01
O_e	-1.16	-1.17	0.00	-1.16	0.00	-1.15	0.01	-1.16	0.00
O_b	-1.28	-1.20	0.09	-1.26	0.02	-1.23	0.05	-1.26	0.02
O_b	-1.31	-1.27	0.03	-1.31	0.00	-1.28	0.02	-1.28	0.02
O_e	-1.16	-1.17	-0.01	-1.16	0.00	-1.15	0.01	-1.16	0.00
O_b	-1.27	-1.25	0.02	-1.28	0.00	-1.27	0.01	-1.25	0.03
O_b	-1.36	-1.36	0.00	-1.36	0.00	-1.36	0.00	-1.35	0.01
H_{b1}	0.63	0.62	0.00	0.63	0.00	0.63	0.00	0.63	0.00
H_{b2}	0.63	0.62	0.00	0.63	0.00	0.63	0.00	0.63	0.00

Table S5: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_3[Nb_6O_{19}]^{5-}$, along with their respective variations due to excitation (Δq).

$H_3[Nb_6O_{19}]^{5-}$	GS q (e)	ES_a q (e)	244 nm Δq (e)	ES_b q (e)	214 nm Δq (e)	ES_c q (e)	195 nm Δq (e)	ES_d q (e)	164 nm Δq (e)
Nb	2.77	2.67	-0.10	2.72	-0.04	2.74	-0.03	2.73	-0.04
Nb	2.77	2.75	-0.02	2.69	-0.08	2.72	-0.04	2.69	-0.08
Nb	2.79	2.75	-0.04	2.69	-0.09	2.66	-0.13	2.74	-0.05
Nb	2.76	2.74	-0.02	2.69	-0.08	2.68	-0.08	2.72	-0.04
Nb	2.77	2.68	-0.09	2.73	-0.04	2.69	-0.07	2.72	-0.04
Nb	2.76	2.64	-0.12	2.69	-0.06	2.75	-0.01	2.68	-0.08
O_i	-1.48	-1.48	0.00	-1.37	0.10	-1.43	0.05	-1.40	0.07
O_e	-1.11	-1.13	-0.02	-1.10	0.01	-1.10	0.01	-1.11	0.00
O_e	-1.12	-1.12	0.00	-1.10	0.02	-1.11	0.00	-1.13	-0.01
O_b	-1.25	-1.23	0.02	-1.22	0.03	-1.23	0.02	-1.24	0.01
O_b	-1.25	-1.24	0.01	-1.24	0.01	-1.22	0.03	-1.23	0.02
O_b	-1.25	-1.18	0.07	-1.22	0.03	-1.23	0.02	-1.22	0.03
O_b	-1.26	-1.19	0.06	-1.24	0.01	-1.23	0.03	-1.22	0.03
O_b	-1.25	-1.14	0.11	-1.25	0.01	-1.25	0.00	-1.23	0.03
O_b	-1.34	-1.33	0.01	-1.34	0.01	-1.34	0.00	-1.33	0.01
O_e	-1.11	-1.12	-0.01	-1.11	0.00	-1.06	0.05	-1.11	0.00
O_b	-1.25	-1.24	0.01	-1.21	0.04	-1.22	0.03	-1.22	0.02
O_b	-1.26	-1.24	0.02	-1.25	0.00	-1.20	0.05	-1.22	0.03
O_e	-1.12	-1.12	0.00	-1.10	0.02	-1.09	0.03	-1.11	0.01
O_e	-1.12	-1.13	-0.01	-1.10	0.01	-1.11	0.01	-1.10	0.02
O_b	-1.35	-1.34	0.00	-1.34	0.01	-1.35	0.00	-1.34	0.01
O_b	-1.26	-1.14	0.12	-1.25	0.01	-1.26	0.01	-1.22	0.04
O_e	-1.12	-1.14	-0.02	-1.09	0.03	-1.11	0.01	-1.14	-0.02
O_b	-1.27	-1.25	0.02	-1.22	0.04	-1.25	0.02	-1.24	0.02
O_b	-1.34	-1.34	0.01	-1.34	0.00	-1.34	0.00	-1.34	0.01
H_{b1}	0.63	0.63	0.00	0.63	0.00	0.63	0.00	0.62	0.00
H_{b2}	0.63	0.62	-0.01	0.63	0.00	0.63	0.00	0.63	0.00
H_{b3}	0.64	0.64	0.00	0.64	0.00	0.64	0.00	0.64	0.00

Table S6: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_4[Nb_6O_{19}]^{4-}$, along with their respective variations due to excitation (Δq).

$H_4[Nb_6O_{19}]^{4-}$	GS	ES_a	244 nm	ES_b	215 nm	ES_c	198 nm	ES_d	177 nm	ES_e	155 nm
	$q\ (e)$	$q\ (e)$	$\Delta q\ (e)$	$q\ (e)$	$\Delta q\ (e)$	$q\ (e)$	$\Delta q\ (e)$	$q\ (e)$	$\Delta q\ (e)$	$q\ (e)$	$\Delta q\ (e)$
Nb	2.74	2.66	-0.08	2.70	-0.04	2.67	-0.08	2.72	-0.02	2.71	-0.03
Nb	2.76	2.74	-0.02	2.70	-0.06	2.74	-0.03	2.75	-0.02	2.69	-0.08
Nb	2.77	2.61	-0.16	2.67	-0.10	2.66	-0.12	2.56	-0.22	2.72	-0.05
Nb	2.76	2.74	-0.02	2.72	-0.04	2.71	-0.05	2.75	-0.01	2.71	-0.06
Nb	2.75	2.67	-0.08	2.71	-0.03	2.71	-0.03	2.74	-0.01	2.70	-0.05
Nb	2.83	2.82	-0.02	2.71	-0.12	2.77	-0.06	2.79	-0.04	2.78	-0.05
O_i	-1.41	-1.41	0.00	-1.33	0.08	-1.37	0.03	-1.39	0.02	-1.35	0.06
O_e	-1.08	-1.08	-0.01	-1.07	0.00	-1.07	0.01	-1.09	-0.01	-1.06	0.01
O_e	-1.09	-1.09	0.00	-1.08	0.01	-1.07	0.01	-1.10	-0.01	-1.10	-0.01
O_b	-1.23	-1.11	0.12	-1.23	0.00	-1.16	0.07	-1.22	0.01	-1.20	0.03
O_b	-1.24	-1.22	0.02	-1.20	0.04	-1.20	0.04	-1.23	0.00	-1.21	0.03
O_b	-1.24	-1.20	0.04	-1.22	0.02	-1.22	0.02	-1.24	0.00	-1.21	0.03
O_b	-1.24	-1.20	0.05	-1.21	0.03	-1.24	0.00	-1.23	0.01	-1.21	0.03
O_b	-1.19	-1.19	0.01	-1.18	0.01	-1.16	0.03	-1.19	0.00	-1.18	0.01
O_b	-1.34	-1.33	0.00	-1.32	0.01	-1.33	0.01	-1.32	0.01	-1.33	0.01
O_e	-1.08	-1.07	0.01	-1.06	0.02	-1.05	0.03	-0.81	0.26	-1.08	0.00
O_b	-1.24	-1.22	0.01	-1.18	0.05	-1.20	0.04	-1.23	0.00	-1.22	0.02
O_b	-1.24	-1.11	0.13	-1.22	0.01	-1.20	0.04	-1.23	0.01	-1.22	0.02
O_e	-1.09	-1.09	0.00	-1.08	0.01	-1.08	0.00	-1.09	0.00	-1.08	0.01
O_e	-1.08	-1.09	-0.01	-1.08	0.01	-1.09	0.00	-1.08	0.00	-1.08	0.01
O_b	-1.34	-1.34	0.00	-1.31	0.03	-1.33	0.01	-1.34	0.01	-1.32	0.03
O_b	-1.21	-1.20	0.01	-1.18	0.03	-1.20	0.02	-1.21	0.00	-1.20	0.01
O_e	-1.28	-1.28	0.00	-1.28	0.00	-1.28	0.00	-1.28	0.00	-1.28	0.00
O_b	-1.25	-1.24	0.02	-1.23	0.03	-1.23	0.02	-1.25	0.00	-1.22	0.03
O_b	-1.34	-1.34	0.00	-1.34	0.00	-1.33	0.00	-1.34	0.00	-1.32	0.01
H_{b1}	0.63	0.63	0.00	0.63	0.00	0.63	0.00	0.63	0.00	0.63	0.00
H_{b2}	0.64	0.63	0.00	0.63	0.00	0.63	0.00	0.63	0.00	0.64	0.00
H_{b3}	0.64	0.64	0.00	0.65	0.00	0.64	0.00	0.64	0.00	0.65	0.00
H_{e1}	0.65	0.65	0.00	0.65	0.00	0.65	0.00	0.65	0.00	0.65	0.00

Table S7: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_5[Nb_6O_{19}]^{3-}$, along with their respective variations due to excitation (Δq).

$H_5[Nb_6O_{19}]^{3-}$	GS	ES_a	238 nm	ES_b	212 nm	ES_c	196 nm	ES_d	172 nm	ES_e	151 nm
	q (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)
Nb	2.75	2.70	-0.04	2.67	-0.08	2.68	-0.06	2.70	-0.04	2.70	-0.04
Nb	2.76	2.68	-0.08	2.71	-0.05	2.73	-0.03	2.71	-0.05	2.72	-0.05
Nb	2.78	2.70	-0.08	2.65	-0.13	2.72	-0.05	2.71	-0.07	2.73	-0.05
Nb	2.75	2.69	-0.06	2.73	-0.02	2.73	-0.02	2.68	-0.07	2.71	-0.04
Nb	2.75	2.70	-0.05	2.69	-0.06	2.68	-0.07	2.68	-0.07	2.68	-0.07
Nb	2.84	2.81	-0.03	2.81	-0.03	2.70	-0.14	2.77	-0.07	2.76	-0.08
O_i	-1.40	-1.41	0.00	-1.39	0.01	-1.35	0.05	-1.34	0.06	-1.37	0.04
O_e	-1.04	-1.03	0.00	-1.04	0.00	-1.04	0.00	-1.03	0.01	-1.03	0.01
O_e	-1.04	-1.02	0.02	-1.04	0.00	-1.03	0.01	-1.02	0.02	-1.03	0.01
O_b	-1.22	-1.20	0.01	-1.16	0.05	-1.17	0.04	-1.19	0.02	-1.20	0.02
O_b	-1.22	-1.13	0.09	-1.16	0.06	-1.20	0.02	-1.18	0.04	-1.20	0.02
O_b	-1.22	-1.18	0.04	-1.19	0.03	-1.20	0.02	-1.18	0.04	-1.19	0.03
O_b	-1.22	-1.18	0.04	-1.20	0.02	-1.19	0.03	-1.18	0.04	-1.19	0.03
O_b	-1.19	-1.16	0.02	-1.17	0.02	-1.16	0.03	-1.18	0.01	-1.19	0.00
O_b	-1.34	-1.33	0.01	-1.33	0.01	-1.30	0.04	-1.31	0.02	-1.31	0.02
O_e	-1.05	-1.05	-0.01	-1.05	0.00	-1.03	0.01	-1.05	0.00	-1.04	0.00
O_b	-1.22	-1.15	0.07	-1.14	0.08	-1.20	0.02	-1.19	0.03	-1.20	0.02
O_b	-1.22	-1.20	0.02	-1.19	0.03	-1.18	0.04	-1.20	0.02	-1.20	0.02
O_e	-1.05	-1.02	0.02	-1.04	0.00	-1.03	0.01	-1.05	0.00	-1.03	0.02
O_e	-1.04	-1.03	0.01	-1.05	-0.01	-1.04	0.00	-1.04	-0.01	-1.04	0.00
O_b	-1.34	-1.33	0.00	-1.33	0.01	-1.31	0.03	-1.33	0.01	-1.32	0.02
O_b	-1.20	-1.17	0.02	-1.17	0.03	-1.16	0.03	-1.19	0.01	-1.18	0.01
O_e	-1.26	-1.27	0.00	-1.26	0.00	-1.26	0.00	-1.25	0.01	-1.27	-0.01
O_b	-1.33	-1.32	0.01	-1.31	0.02	-1.33	0.00	-1.31	0.02	-1.31	0.02
O_b	-1.33	-1.33	0.00	-1.33	0.00	-1.31	0.02	-1.31	0.02	-1.29	0.04
H_{b1}	0.65	0.65	-0.01	0.65	0.00	0.65	0.00	0.65	0.00	0.65	0.00
H_{b2}	0.65	0.64	0.00	0.64	0.00	0.65	0.00	0.65	0.00	0.65	0.00
H_{b3}	0.66	0.65	0.00	0.66	0.00	0.66	0.00	0.65	0.00	0.66	0.00
H_{e1}	0.66	0.66	0.00	0.66	0.00	0.66	-0.01	0.66	0.00	0.66	-0.01
H_{b4}	0.65	0.65	-0.01	0.66	0.00	0.65	0.00	0.65	0.00	0.65	0.00

Table S8: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_6[Nb_6O_{19}]^{2-}$, along with their respective variations due to excitation (Δq).

$H_6[Nb_6O_{19}]^{2-}$	GS Charge	ES_a Charge	237 nm ΔV	ES_b Charge	220 nm ΔV	ES_c Charge	168.5 nm ΔV	ES_d Charge	149 nm ΔV
Nb	2.75	2.74	-0.01	2.72	-0.03	2.70	-0.05	2.70	-0.05
Nb	2.77	2.64	-0.13	2.71	-0.05	2.71	-0.06	2.73	-0.04
Nb	2.76	2.68	-0.08	2.67	-0.09	2.63	-0.13	2.70	-0.06
Nb	2.78	2.76	-0.01	2.74	-0.04	2.72	-0.05	2.69	-0.09
Nb	2.76	2.64	-0.12	2.69	-0.07	2.72	-0.03	2.72	-0.04
Nb	2.86	2.86	-0.01	2.77	-0.09	2.81	-0.05	2.81	-0.06
O_i	-1.40	-1.40	0.00	-1.34	0.05	-1.34	0.06	-1.35	0.05
O_e	-0.99	-0.99	0.00	-0.98	0.01	-0.98	0.01	-0.99	0.00
O_e	-1.00	-1.00	0.00	-1.00	0.00	-1.00	0.00	-0.99	0.01
O_b	-1.32	-1.31	0.01	-1.30	0.02	-1.27	0.04	-1.30	0.02
O_b	-1.20	-1.10	0.10	-1.16	0.04	-1.15	0.06	-1.19	0.02
O_b	-1.20	-1.18	0.01	-1.19	0.00	-1.17	0.03	-1.16	0.04
O_b	-1.20	-1.09	0.12	-1.16	0.04	-1.18	0.02	-1.17	0.03
O_b	-1.18	-1.18	0.00	-1.17	0.01	-1.16	0.02	-1.17	0.01
O_b	-1.34	-1.33	0.00	-1.33	0.01	-1.30	0.03	-1.32	0.02
O_e	-1.01	-1.00	0.01	-1.01	0.00	-1.02	0.00	-1.02	-0.01
O_b	-1.21	-1.20	0.01	-1.20	0.01	-1.17	0.04	-1.18	0.03
O_b	-1.21	-1.11	0.11	-1.13	0.09	-1.18	0.03	-1.19	0.03
O_e	-1.01	-1.01	0.00	-1.01	0.00	-1.00	0.01	-1.03	-0.02
O_e	-1.01	-1.03	-0.02	-1.00	0.01	-1.00	0.01	-0.98	0.03
O_b	-1.33	-1.33	0.00	-1.31	0.02	-1.31	0.02	-1.32	0.02
O_b	-1.17	-1.16	0.01	-1.12	0.05	-1.16	0.00	-1.15	0.02
O_e	-1.25	-1.25	0.00	-1.24	0.01	-1.25	0.00	-1.24	0.01
O_b	-1.33	-1.32	0.01	-1.32	0.00	-1.32	0.01	-1.30	0.03
O_b	-1.33	-1.33	0.00	-1.33	0.00	-1.32	0.01	-1.31	0.02
H_{b1}	0.67	0.67	-0.01	0.67	0.00	0.68	0.00	0.67	0.00
H_{b2}	0.66	0.66	0.00	0.66	0.00	0.66	0.00	0.66	0.00
H_{b3}	0.66	0.66	0.00	0.66	0.00	0.66	0.00	0.66	0.00
H_{e1}	0.68	0.68	0.00	0.68	0.00	0.68	0.00	0.68	0.00
H_{b4}	0.67	0.66	0.00	0.66	0.00	0.66	0.00	0.67	0.00
H_{b5}	0.66	0.66	0.00	0.66	0.00	0.67	0.00	0.66	0.00

Table S9: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_7[Nb_6O_{19}]^{1-}$, along with their respective variations due to excitation (Δq).

$H_7[Nb_6O_{19}]^{1-}$	GS Charge	ES_a Charge	237 nm ΔV	ES_b Charge	198 nm ΔV	ES_c Charge	172 nm ΔV	ES_d Charge	148 nm ΔV
Nb	2.76	2.71	-0.06	2.71	-0.05	2.70	-0.07	2.69	-0.07
Nb	2.78	2.71	-0.08	2.76	-0.02	2.73	-0.05	2.74	-0.04
Nb	2.75	2.74	-0.02	2.67	-0.08	2.68	-0.07	2.69	-0.07
Nb	2.78	2.69	-0.09	2.74	-0.04	2.70	-0.08	2.72	-0.06
Nb	2.77	2.66	-0.11	2.69	-0.07	2.72	-0.05	2.72	-0.05
Nb	2.88	2.86	-0.02	2.77	-0.11	2.82	-0.06	2.81	-0.07
O_i	-1.40	-1.40	0.00	-1.34	0.05	-1.36	0.04	-1.35	0.04
O_e	-0.96	-0.97	0.00	-0.95	0.01	-0.96	0.01	-0.98	-0.01
O_e	-0.97	-0.98	-0.01	-0.97	0.00	-0.97	0.01	-0.95	0.02
O_b	-1.32	-1.32	0.00	-1.30	0.02	-1.28	0.04	-1.29	0.03
O_b	-1.19	-1.16	0.03	-1.18	0.01	-1.17	0.02	-1.15	0.04
O_b	-1.18	-1.08	0.10	-1.17	0.01	-1.14	0.04	-1.16	0.02
O_b	-1.19	-1.05	0.14	-1.18	0.01	-1.16	0.03	-1.17	0.01
O_b	-1.16	-1.13	0.02	-1.14	0.02	-1.12	0.03	-1.14	0.01
O_b	-1.34	-1.33	0.00	-1.32	0.02	-1.33	0.01	-1.31	0.02
O_e	-0.97	-0.96	0.01	-0.93	0.04	-0.97	0.00	-0.96	0.01
O_b	-1.19	-1.13	0.06	-1.16	0.03	-1.16	0.03	-1.16	0.03
O_b	-1.33	-1.32	0.01	-1.30	0.03	-1.31	0.02	-1.29	0.03
O_e	-0.97	-0.98	-0.01	-0.96	0.01	-0.98	-0.01	-0.98	-0.01
O_e	-0.96	-0.98	-0.02	-0.94	0.02	-0.96	0.00	-0.95	0.01
O_b	-1.33	-1.32	0.00	-1.28	0.05	-1.30	0.03	-1.30	0.02
O_b	-1.16	-1.11	0.05	-1.14	0.02	-1.14	0.02	-1.14	0.02
O_e	-1.23	-1.23	0.00	-1.24	0.00	-1.23	0.01	-1.22	0.01
O_b	-1.33	-1.32	0.01	-1.32	0.01	-1.30	0.02	-1.30	0.03
O_b	-1.34	-1.33	0.01	-1.31	0.03	-1.32	0.02	-1.32	0.01
H_{b1}	0.69	0.68	0.00	0.69	0.00	0.69	0.00	0.69	0.00
H_{b2}	0.69	0.68	0.00	0.69	0.00	0.69	0.00	0.69	0.00
H_{b3}	0.68	0.67	0.00	0.68	0.00	0.68	0.00	0.67	0.00
H_{e1}	0.69	0.69	0.00	0.69	-0.01	0.69	0.00	0.69	0.00
H_{b4}	0.68	0.67	0.00	0.68	0.00	0.68	0.00	0.68	0.00
H_{b5}	0.67	0.67	0.00	0.67	0.00	0.68	0.00	0.68	0.00
H_{b6}	0.68	0.68	0.00	0.68	0.00	0.68	0.00	0.68	0.00

Table S10: Atomic charges (q) in the ground state (GS) and in excited states (ES) for $H_8[Nb_6O_{19}]$, along with their respective variations due to excitation (Δq).

$H_8[Nb_6O_{19}]$	GS	ES_a	241 nm	ES_b	198 nm	ES_c	168 nm	ES_d	148 nm
	q (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)	q (e)	Δq (e)
Nb	2.78	2.67	-0.11	2.74	-0.04	2.70	-0.07	2.72	-0.06
Nb	2.78	2.69	-0.10	2.75	-0.03	2.69	-0.10	2.74	-0.04
Nb	2.76	2.72	-0.05	2.69	-0.08	2.72	-0.05	2.70	-0.06
Nb	2.88	2.86	-0.03	2.82	-0.06	2.83	-0.05	2.82	-0.06
Nb	2.76	2.73	-0.04	2.67	-0.09	2.71	-0.05	2.71	-0.05
Nb	2.89	2.85	-0.04	2.84	-0.05	2.82	-0.07	2.82	-0.07
O_i	-1.39	-1.40	0.00	-1.35	0.04	-1.35	0.05	-1.37	0.03
O_e	-0.92	-0.94	-0.02	-0.89	0.03	-0.94	-0.01	-0.94	-0.01
O_e	-0.95	-0.97	-0.02	-0.94	0.01	-0.95	-0.01	-0.94	0.01
O_b	-1.33	-1.32	0.01	-1.28	0.04	-1.30	0.02	-1.30	0.03
O_b	-1.17	-1.07	0.10	-1.16	0.01	-1.13	0.05	-1.14	0.03
O_b	-1.14	-1.06	0.08	-1.13	0.01	-1.11	0.03	-1.12	0.02
O_b	-1.17	-1.08	0.09	-1.16	0.02	-1.12	0.06	-1.16	0.02
O_b	-1.14	-1.06	0.08	-1.13	0.01	-1.11	0.03	-1.11	0.03
O_b	-1.32	-1.32	0.01	-1.31	0.01	-1.29	0.03	-1.30	0.02
O_e	-0.93	-0.93	-0.01	-0.92	0.01	-0.93	0.00	-0.94	-0.01
O_b	-1.14	-1.12	0.02	-1.11	0.04	-1.12	0.02	-1.11	0.03
O_b	-1.32	-1.32	0.00	-1.32	0.01	-1.31	0.01	-1.29	0.03
O_e	-1.21	-1.21	0.00	-1.22	0.00	-1.21	0.00	-1.21	0.00
O_e	-0.93	-0.93	0.00	-0.91	0.02	-0.93	0.00	-0.93	0.00
O_b	-1.32	-1.32	0.00	-1.31	0.01	-1.30	0.01	-1.28	0.03
O_b	-1.14	-1.12	0.02	-1.11	0.03	-1.13	0.01	-1.10	0.04
O_e	-1.22	-1.22	0.00	-1.22	0.00	-1.21	0.00	-1.21	0.00
O_b	-1.33	-1.32	0.00	-1.32	0.01	-1.29	0.04	-1.31	0.02
O_b	-1.32	-1.32	0.00	-1.28	0.05	-1.30	0.03	-1.30	0.02
H_{b1}	0.69	0.68	0.00	0.69	0.00	0.69	0.00	0.69	0.00
H_{b2}	0.69	0.69	0.00	0.70	0.00	0.69	0.00	0.69	0.00
H_{b3}	0.68	0.68	0.00	0.68	0.00	0.68	0.00	0.68	0.00
H_{e1}	0.71	0.71	0.00	0.70	0.00	0.70	0.00	0.70	-0.01
H_{b4}	0.69	0.68	0.00	0.69	0.00	0.69	0.00	0.69	0.00
H_{b5}	0.70	0.69	0.00	0.70	0.00	0.70	0.00	0.70	0.00
H_{b6}	0.69	0.69	0.00	0.69	0.00	0.69	0.00	0.70	0.00
H_{e2}	0.71	0.71	0.00	0.70	0.00	0.71	0.00	0.70	0.00

Table S11: Standard deviation of the QTAIM charges obtained in each state (in *e*).

$[Nb_6O_{19}]^{8-}$	GS	ES_a	ES_b	ES_c		
Nb	0.0019	0.0354	0.0016	0.0013		
O_e	0.0026	0.0123	0.0462	0.0109		
O_b	0.0004	0.0058	0.0214	0.0027		
O_i	0.0000	0.0000	0.0000	0.0000		
H	0.0000	0.0000	0.0000	0.0000		
$H[Nb_6O_{19}]^{7-}$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0179	0.0420	0.0124	0.0274	0.0362	
O_e	0.0050	0.0074	0.0098	0.0026	0.0108	
O_b	0.0248	0.0284	0.0324	0.0308	0.0276	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0000	0.0000	0.0000	0.0000	0.0000	
$H_2[Nb_6O_{19}]^{6-}$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0166	0.0221	0.0566	0.0107	0.0272	
O_e	0.0060	0.0068	0.0728	0.0048	0.0031	
O_b	0.0332	0.0520	0.0368	0.0395	0.0382	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0002	0.0001	0.0001	0.0000	0.0002	
$H_3[Nb_6O_{19}]^{5-}$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0095	0.0466	0.0182	0.0331	0.0222	
O_e	0.0033	0.0087	0.0072	0.0212	0.0133	
O_b	0.0407	0.0701	0.0503	0.0521	0.0498	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0067	0.0080	0.0050	0.0065	0.0081	
$H_4[Nb_6O_{19}]^{4-}$	GS	ES_a	ES_b	ES_c	ES_d	ES_e
Nb	0.0324	0.0734	0.0187	0.0428	0.0831	0.0322
O_e	0.0801	0.0804	0.0847	0.0860	0.1497	0.0830
O_b	0.0509	0.0782	0.0569	0.0630	0.0497	0.0525
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H	0.0094	0.0096	0.0084	0.0084	0.0080	0.0097
$H_5[Nb_6O_{19}]^{3-}$	GS	ES_a	ES_b	ES_c	ES_d	ES_e
Nb	0.0357	0.0474	0.0564	0.0233	0.0333	0.0272
O_e	0.0905	0.0972	0.0890	0.0914	0.0876	0.0957
O_b	0.0608	0.0790	0.0767	0.0648	0.0646	0.0562
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H	0.0058	0.0075	0.0070	0.0039	0.0059	0.0030
$H_6[Nb_6O_{19}]^{2-}$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0413	0.0837	0.0356	0.0367	0.0583	
O_e	0.1000	0.1005	0.0998	0.1127	0.1024	
O_b	0.0697	0.0983	0.0838	0.0665	0.0730	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0074	0.0072	0.0061	0.0085	0.0076	
$H_7[Nb_6O_{19}]^{1-}$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0466	0.0714	0.0397	0.0490	0.0457	
O_e	0.1083	0.1044	0.1173	0.1066	0.1065	
O_b	0.0802	0.1154	0.0761	0.0842	0.0797	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0069	0.0068	0.0053	0.0055	0.0055	
$H_8[Nb_6O_{19}]$	GS	ES_a	ES_b	ES_c	ES_d	
Nb	0.0593	0.0806	0.0682	0.0640	0.0543	
O_e	0.1468	0.1410	0.1566	0.1437	0.1442	
O_b	0.0902	0.1230	0.0907	0.0940	0.0918	
O_i	0.0000	0.0000	0.0000	0.0000	0.0000	
H	0.0095	0.0100	0.0087	0.0081	0.0056	

Table S12: Cartesian Coordinates of Equilibrium Structures (in Å)

$[Nb_6O_{19}]^{8-}$

Atom	X	Y	Z
Nb	1.494539	-0.019094	-1.881086
Nb	-1.494539	0.019094	1.881086
Nb	-0.000606	-2.406098	0.023561
Nb	1.881073	0.014327	1.494479
Nb	-1.881073	-0.014327	-1.494479
Nb	0.000606	2.406098	-0.023561
O	0.000000	0.000000	0.000000
O	2.634894	-0.033891	-3.320169
O	-2.634894	0.033891	3.320169
O	1.224893	-1.992042	-1.532389
O	-1.223917	-1.962763	1.569136
O	2.782511	-0.001041	-0.320094
O	-2.782511	0.001041	0.320094
O	1.223917	1.962763	-1.569136
O	-1.224893	1.992042	1.532389
O	-0.002393	-4.242165	0.043168
O	1.552343	-1.965525	1.240963
O	-1.549141	-1.989268	-1.207858
O	3.320753	0.026476	2.634128
O	-3.320753	-0.026476	-2.634128
O	1.549141	1.989268	1.207858
O	-1.552343	1.965525	-1.240963
O	0.002393	4.242165	-0.043168
O	0.320041	0.024216	2.782817
O	-0.320041	-0.024216	-2.782817

$H[Nb_6O_{19}]^{7-}$

Atom	X	Y	Z
Nb	-1.687890	1.726150	-0.175397
Nb	1.847048	-1.603212	0.179590
Nb	1.690261	1.722246	-0.176901
Nb	0.000639	0.204944	2.361141
Nb	-0.000104	-0.278426	-2.350589
Nb	-1.850108	-1.601689	0.179138
O	0.002088	-0.033241	0.006238
O	-2.960979	3.020097	-0.294627
O	3.105553	-2.913004	0.311635
O	0.002362	2.796095	-0.271324
O	2.881849	0.023611	-0.004768
O	-1.407008	1.529478	1.812865
O	1.390557	-1.650680	-1.778899
O	-2.879952	0.028446	-0.004167
O	-0.003382	-2.926082	0.181366
O	2.965324	3.014399	-0.296391
O	1.409890	1.526646	1.811907
O	1.403758	1.154551	-2.076631
O	0.001938	0.362004	4.179136
O	-0.003031	-0.474067	-4.164809
O	-1.383868	-1.273878	2.068859
O	-1.393741	-1.648050	-1.778135
O	-3.113164	-2.906723	0.313338
O	1.383893	-1.277267	2.070050
O	-1.401050	1.156944	-2.074061
H	-0.001943	-3.044752	-0.788893

$H_2[Nb_6O_{19}]^{6-}$

Atom	X	Y	Z
Nb	-2.259240	-0.127314	0.991043
Nb	2.257509	-0.157294	-0.989010
Nb	0.680435	-1.662197	1.569512
Nb	-0.693472	-1.678569	-1.547456
Nb	0.909519	1.719569	1.431506
Nb	-0.895890	1.705964	-1.453863
O	0.000012	0.027750	-0.000197
O	-3.879412	-0.115706	1.785502
O	3.877604	-0.167144	-1.783549
O	-1.223950	-1.319213	2.158225
O	2.413722	-1.416204	0.468623
O	-2.423770	-1.405030	-0.449638
O	2.474703	1.426668	0.306771
O	-2.463822	1.440286	-0.325809
O	1.259818	1.496367	-2.123804
O	1.203708	-2.924293	2.753157
O	-0.009304	-2.727848	0.017592
O	1.172835	0.072353	2.491824
O	-1.224521	-2.951744	-2.715698
O	1.422796	3.015068	2.586545
O	-1.173282	0.047607	-2.492642
O	0.010596	2.792922	-0.018155
O	-1.398771	2.990009	-2.625837
O	1.213037	-1.356262	-2.140187
O	-1.248350	1.533748	2.102309
H	1.625351	2.242604	-1.612018
H	-1.607896	2.276207	1.580765

$H_3[Nb_6O_{19}]^{5-}$

Atom	X	Y	Z
Nb	-0.457264	2.109396	-1.132804
Nb	0.705320	-2.002893	1.190407
Nb	1.852101	-0.339737	-1.511336
Nb	1.502461	1.260953	1.433689
Nb	-1.344229	-1.451482	-1.406355
Nb	-2.046809	0.427980	1.268590
O	-0.054722	0.019119	0.038147
O	-0.900077	3.594049	-2.037621
O	1.104567	-3.478468	2.129865
O	1.030364	1.386278	-2.170177
O	2.031143	-1.912361	-0.223940
O	0.645243	2.730231	0.349961
O	-0.685374	-2.740426	-0.119892
O	-2.070804	1.999195	0.177087
O	-1.154793	-1.380402	2.254912
O	3.229796	-0.587630	-2.631387
O	2.697663	0.773392	-0.001052
O	0.349946	-1.315863	-2.400844
O	2.500740	2.197594	2.594808
O	-2.387819	-2.390559	-2.525444
O	-0.471980	1.279501	2.528733
O	-2.749218	-0.793631	-0.054707
O	-3.418393	0.629522	2.411138
O	1.518360	-0.562847	2.271207
O	-1.710830	0.618075	-2.202961
H	-1.800431	-2.078154	2.048319
H	-2.604723	0.808061	-1.864684
H	-0.300109	0.579028	3.183911

$H_4[Nb_6O_{19}]^{4-}$

Atom	X	Y	Z
Nb	1.984780	1.240579	-0.84025
Nb	-1.822802	-1.432909	0.856014
Nb	0.204702	-1.504844	-1.921230
Nb	1.591369	-1.439035	1.225655
Nb	-1.729583	1.257662	-1.237936
Nb	-0.139274	1.651311	1.557900
O	-0.018189	0.171103	0.171691
O	3.338731	2.200902	-1.487144
O	-3.154707	-2.431263	1.492859
O	1.656617	-0.101283	-2.182491
O	-1.295211	-2.269009	-0.824775
O	2.762988	0.018080	0.456010
O	-2.799441	0.019379	-0.210645
O	1.381773	2.454578	0.826382
O	-1.715648	0.179021	2.344315
O	0.359073	-2.587413	-3.323563
O	1.434387	-2.282133	-0.514842
O	-1.084718	-0.072082	-2.503160
O	2.722639	-2.450626	2.160804
O	-2.879971	2.245499	-2.176305
O	1.071405	0.154415	2.677847
O	-1.488563	2.437906	0.492634
O	-0.420323	2.583322	3.288091
O	-0.211625	-2.085166	1.797090
O	0.221821	2.271809	-1.692548
H	-2.551592	0.674188	2.315339
H	0.171490	3.132352	-1.239788
H	0.421414	-0.281689	3.257216
H	-0.746464	2.135537	4.082971

$H_5[Nb_6O_{19}]^{3-}$

Atom	X	Y	Z
Nb	-1.895808	-1.564738	-0.521320
Nb	1.860089	1.618673	0.434780
Nb	-0.119288	0.841188	-2.268276
Nb	-1.831445	1.607316	0.617995
Nb	1.838560	-1.542966	-0.702164
Nb	0.096522	-1.036325	2.004099
O	0.031995	-0.035297	0.243965
O	-3.145733	-2.744542	-0.936291
O	3.080013	2.846157	0.800529
O	-1.506060	-0.634632	-2.159516
O	1.293596	1.980580	-1.370363
O	-2.856952	-0.015876	0.257517
O	2.874088	0.013965	-0.068989
O	-1.371630	-2.070598	1.456741
O	1.499058	0.712045	2.353053
O	-0.207366	1.436742	-3.933043
O	-1.455471	1.961825	-1.235984
O	1.250827	-0.637315	-2.306948
O	-2.994934	2.854947	1.089731
O	3.037583	-2.724617	-1.248516
O	-1.265935	0.699641	2.493675
O	1.512532	-2.064945	1.302058
O	0.255905	-1.320539	3.943071
O	0.037239	2.647836	1.094794
O	-0.047044	-2.675388	-0.911996
H	2.292292	0.489364	2.865525
H	-0.009517	-3.418685	-0.284230
H	-0.688669	1.331913	2.957859
H	0.326488	-0.646713	4.635411
H	0.011849	3.555164	0.747875

$H_6[Nb_6O_{19}]^{2-}$

Atom	X	Y	Z
Nb	-2.321569	-0.529353	-0.934147
Nb	2.258036	0.525880	1.015088
Nb	0.738287	1.402872	-1.903358
Nb	-1.134319	2.015873	0.929469
Nb	1.156925	-1.925239	-1.046619
Nb	-0.628353	-1.440269	1.645392
O	-0.073975	-0.105041	0.224494
O	-3.808369	-0.971289	-1.755507
O	3.766442	0.941949	1.814070
O	-1.262758	0.590640	-2.410229
O	2.241972	1.556029	-0.649005
O	-2.652117	1.128030	0.004083
O	2.594970	-1.149139	0.062458
O	-2.313647	-1.618401	0.734574
O	1.214668	-0.582250	2.497886
O	1.163572	2.350571	-3.324305
O	-0.365357	2.592822	-0.747625
O	1.254117	-0.469292	-2.334175
O	-1.758946	3.479921	1.681031
O	1.864365	-3.312194	-1.869771
O	-1.391155	0.529397	2.449641
O	0.339160	-2.739068	0.703860
O	-0.927770	-2.206802	3.403721
O	0.864929	2.027422	1.761186
O	-0.942991	-2.022725	-1.706285
H	1.713418	-1.110518	3.140428
H	-1.317848	-2.916804	-1.629489
H	-0.959878	0.767504	3.286573
H	-0.830767	-1.880070	4.310517
H	1.241447	2.921398	1.816436
H	-1.132529	0.013471	-3.184078

$H_7[Nb_6O_{19}]^{1-}$

Atom	X	Y	Z
Nb	-1.933965	-1.049192	-1.246938
Nb	1.912747	1.012958	1.266007
Nb	0.201430	2.013123	-1.532680
Nb	-1.789428	1.318893	1.173367
Nb	1.779388	-1.352905	-1.171147
Nb	-0.190058	-1.859643	1.340982
O	-0.019160	-0.191597	0.168438
O	-3.148250	-1.754348	-2.288390
O	3.176246	1.738303	2.234369
O	-1.260934	0.648489	-2.375934
O	1.600109	2.270025	-0.210076
O	-2.836671	0.207159	-0.082803
O	2.817441	-0.250294	0.045217
O	-1.651523	-2.370846	0.227699
O	1.287018	-0.643889	2.406972
O	0.383482	3.351102	-2.642550
O	-1.215170	2.489445	-0.302488
O	1.444389	0.430889	-2.331333
O	-2.919956	2.277312	2.102573
O	2.946817	-2.230067	-2.131374
O	-1.578262	-0.450529	2.325552
O	1.218348	-2.603060	0.284836
O	-0.277586	-2.960304	2.913765
O	0.077510	1.806302	2.109850
O	-0.107076	-1.817816	-2.102637
H	1.786819	-0.979344	3.166921
H	-0.160781	-2.618381	-2.649667
H	-1.483909	-0.342079	3.285435
H	-0.242870	-2.859161	3.876951
H	0.132361	2.695401	2.497816
H	-0.970048	0.358339	-3.258865
H	2.259564	0.762410	-2.745295

$H_8[Nb_6O_{19}]$

Atom	X	Y	Z
Nb	2.122651	-0.034289	-1.426493
Nb	-2.086976	0.022714	1.427198
Nb	-1.131843	-1.915618	-1.266782
Nb	1.105071	-1.673159	1.228292
Nb	-1.163618	1.812831	-1.387828
Nb	1.079318	1.768984	1.119418
O	0.204339	0.003123	0.219754
O	3.371326	-0.063069	-2.637128
O	-3.503256	0.056431	2.441216
O	0.765235	-1.469517	-2.196784
O	-2.390774	-1.417165	0.106257
O	2.520969	-1.391467	-0.016999
O	-2.404157	1.367013	0.016516
O	2.499898	1.412301	-0.104112
O	-0.732071	1.427631	2.276704
O	-1.907284	-3.168785	-2.188921
O	0.036582	-2.769754	0.104510
O	-1.623361	-0.082334	-2.254260
O	1.772584	-2.791493	2.609916
O	-1.969208	3.009985	-2.356096
O	1.761006	0.094842	2.300263
O	0.001671	2.766407	-0.086397
O	1.676231	3.029122	2.406739
O	-0.710285	-1.285228	2.376874
O	0.746276	1.330778	-2.292183
H	-1.094046	2.186866	2.763804
H	0.784086	1.395742	-3.261956
H	1.507192	0.123339	3.238413
H	1.729935	3.155653	3.366705
H	-1.045496	-2.002045	2.940340
H	0.855141	-1.689086	-3.139672
H	-2.456489	-0.107304	-2.756598
H	1.900528	-2.790141	3.571636