

# Unveil the Relative Stability and Proton Binding of Non-Classical Wells-Dawson Isomers of $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$ and $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ : A DFT Study

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**Table S1.** The Height ( $\text{W}_p$ - $\text{W}_p$  distance between two polar rings, Figure 1), cap radius (radius of three  $\text{W}_p$  ring), belt radius (radius of  $\text{W}_6$  in  $\text{W}_6\text{O}_6$  cycle) of  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ .

$\{\text{H}_2\text{SbW}_{18}\}$	Height (Å)	Cap radius (Å)	Belt radius (Å)
$\alpha$	9.851	1.908	3.447
$\beta$	9.872	1.906	3.449
$\gamma$	9.894	1.905	3.453
$\alpha^*$	9.811	1.902	3.480
$\beta^*$	9.862	1.912	3.482
$\gamma^*$	9.907	1.917	3.484

**Table S2.** The Height ( $W_p$ - $W_p$  distance between two polar rings, Figure 1), cap radius (radius of three  $W_p$  ring), belt radius (radius of  $W_6$  in  $W_6O_6$  cycle) of  $[(NaF_6)W_{18}O_{54}(OH)_2]^{7-}$ .

$\{H_2NaW_{18}\}$	Height (Å)	Cap radius (Å)	Belt radius (Å)
$\alpha$	9.825	1.916	3.514
$\beta$	9.851	1.916	3.522
$\gamma$	9.886	1.920	3.532
$\alpha^*$	9.813	1.907	3.542
$\beta^*$	9.860	1.924	3.542
$\gamma^*$	9.897	1.933	3.544

**Table S3.** The Height ( $W_p$ - $W_p$  distance between two polar rings, Figure 1), cap radius (radius of three  $W_p$  ring), belt radius (radius of  $W_6$  in  $W_6O_6$  cycle) of  $[(SiO_4)W_{18}O_{54}]^{8-}$ .

$\{P_2W_{18}\}$	Height (Å)	Cap radius (Å)	Belt radius (Å)
$\alpha$	9.860	1.927	3.476
$\beta$	9.885	1.925	3.481
$\gamma$	9.922	1.931	3.489
$\alpha^*$	9.845	1.915	3.499
$\beta^*$	9.891	1.936	3.499
$\gamma^*$	9.931	1.944	3.502

**Table S4.** Optimized distances ( $\text{\AA}$ ) of the six  $[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$  isomers at the level of PBEsol/TZP.

$\{\text{Si}_2\text{W}_{18}\}$	W-O <sub>a</sub>	W-O <sub>i</sub>	W-O <sub>b</sub>	Si-O <sub>i</sub>	W-O <sub>t</sub>
$\alpha$	2.298	2.235	1.899-1.940	1.638-1.679	1.734-1.735
$\beta$	2.298-2.306	2.239	1.899-1.945	1.640-1.681	1.734-1.735
$\gamma$	2.312	2.245	1.904-1.945	1.644-1.683	1.733-1.735
$\alpha^*$	2.299	2.269	1.902-1.943	1.645-1.690	1.734
$\beta^*$	2.299-2.336	2.253-2.268	1.900-1.945	1.6404-1.684	1.733-1.735
$\gamma^*$	2.327	2.259	1.902-1.946	1.645-1.680	1.732-1.735

**Table S5.** Angles of W-O<sub>eq</sub>-W (degree, O<sub>eq</sub> is oxygen atom at equatorial position), distances of W<sub>belt</sub>-W<sub>belt</sub> ( $\text{\AA}$ ) inside the same {W<sub>6</sub>O<sub>6</sub>} and between two {W<sub>6</sub>O<sub>6</sub>} of the belt for  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ . There are two kinds of W<sub>belt</sub>-W<sub>belt</sub> in  $\beta$  and  $\beta^*$  due to the nonequivalence of the two {SbW<sub>9</sub>} halves.

Anions	W-O <sub>eq</sub> -W	W <sub>belt</sub> -W <sub>belt</sub> (between)	W <sub>belt</sub> -W <sub>belt</sub> (inside)	W <sub>belt</sub> -W <sub>belt</sub> (inside)
$\alpha$	153.6	3.712	3.227/3.667(0.440)	-
$\beta$	153.3/154.6(153.9)	3.713/3.720(3.716)	3.214/3.685(0.471)	3.234/3.669(0.435)
$\gamma$	154.5	3.721	3.220/3.689(0.469)	-
$\alpha^*$	153.7	3.720	3.290/3.676(0.386)	-
$\beta^*$	155.6/155.9(155.8)	3.727/3.730(3.728)	3.274/3.673(0.399)	3.706/3.287(0.419)
$\gamma^*$	157.1	3.737	3.271/3.704(0.433)	-

**Table S6.** Angles of W-O<sub>eq</sub>-W (degree, O<sub>eq</sub> is oxygen atom at equatorial position), distances of W<sub>belt</sub>-W<sub>belt</sub> (Å) *inside* the same {W<sub>6</sub>O<sub>6</sub>} and *between* two {W<sub>6</sub>O<sub>6</sub>} of the belt for [(NaF<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>7-</sup>. There are two kinds of W<sub>belt</sub>-W<sub>belt</sub> in β and β\* due to the nonequivalence of the two {NaW<sub>9</sub>} halves. Difference is given in parenthesis.

Anions	W-O <sub>eq</sub> -W	W <sub>belt</sub> -W <sub>belt</sub>	W <sub>belt</sub> -W <sub>belt</sub>	W <sub>belt</sub> -W <sub>belt</sub>
		(between)	(inside)	(inside)
α	160.9	3.759	3.307/3.717(0.410)	
β	163.5	3.772	3.292/3.752(0.460)	3.717/3.316(0.401)
γ	167.4	3.788	3.303/3.755(0.452)	
α*	166.8	3.792	3.371/3.712(0.341)	
β*	169.2	3.796	3.347/3.707(0.360)	3.742/3.358(0.384)
γ*	174.1	3.805	3.338/3.746(0.408)	

**Table S7.** Angles of W-O<sub>eq</sub>-W (degree, O<sub>eq</sub> is oxygen atom at equatorial position), distances of W<sub>belt</sub>-W<sub>belt</sub> (Å) *inside* the same {W<sub>6</sub>O<sub>6</sub>} and *between* two {W<sub>6</sub>O<sub>6</sub>} of the belt for [(SiO<sub>4</sub>)W<sub>18</sub>O<sub>54</sub>]<sup>8-</sup>. There are two kinds of W<sub>belt</sub>-W<sub>belt</sub> in β and β\* due to the nonequivalence of the two {NaW<sub>9</sub>} halves. Difference is given in parenthesis.

Anions	W-O <sub>eq</sub> -W	W <sub>belt</sub> -W <sub>belt</sub>	W <sub>belt</sub> -W <sub>belt</sub>	W <sub>belt</sub> -W <sub>belt</sub>
		(between)	(inside)	(inside)
α	159.7	3.746	3.262/3.686(0.424)	
β	162.4	3.759	3.270/3.686(0.415)	3.243/3.717(0.474)
γ	166.8	3.778	3.254/3.720(0.466)	
α*	161.1	3.779	3.323/3.672(0.349)	
β*	167.1	3.780	3.298/3.674(0.385)	3.311/3.702(0.391)
γ*	171.8	3.793	3.289/3.710(0.421)	

**Table S8.** Torsion angles (degree) of the six oxo-ligands inside equatorial  $\{W_6O_6\}$  ring (chair conformation) for  $[(SbO_6)W_{18}O_{54}(OH)_2]^{9-}$ ,  $[(NaF_6)W_{18}O_{54}(OH)_2]^{7-}$  and  $[(SiO_4)_2W_{18}O_{54}]^{8-}$ .

Isomers	$\{H_2SbW_{18}\}$	$\{H_2NaW_{18}\}$	$\{Si_2W_{18}\}$
$\alpha$	41.2	38.7	37.6
$\beta$	33.1/39.8	26.0/36.0	24.5/34.7
$\gamma$	31.4	20.5	17.6
$\alpha^*$	19.5	15.8	12.8
$\beta^*$	3.1/23.6	7.8/22.2	12.1/22.1
$\gamma^*$	8.2	0.0	2.1

**Table S9.** Bonding energies (a.u.) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(IO_6)W_{18}O_{54}(OH)_2]^{7-}$  ( $\{H_2IW_{18}\}$ ),  $[(IO_6)W_{18}O_{54}(OH)_2H]^{6-}$  ( $\{H_3IW_{18}\}$ ),  $[(IO_6)W_{18}O_{54}(OH)_2H_2]^{5-}$  ( $\{H_4IW_{18}\}$ ) at PBEsol/TZP level. There are two kinds of arrangements for the third proton for  $\beta$  and  $\beta^*$  isomers. Only the most stable arrangements of  $\{H_4IW_{18}\}$  are provided.

Types	$\{H_2IW_{18}\}$	$\{H_3IW_{18}\}$	$\{H_4IW_{18}\}$
$\alpha$	-27.18466	-27.19810	-27.19226
$\beta$	-27.17911	-27.19144/-27.19034	-27.18497
$\gamma$	-27.17520	-27.18520	-27.17900
$\alpha^*$	-27.21920	-27.21997	-27.20256
$\beta^*$	-27.22363	-27.22720/-27.22414	-27.20600
$\gamma^*$	-27.22552	-27.22725	-27.20603

**Table S9-1.** Single-point energies (a.u.) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$  ( $\{\text{H}_3\text{IW}_{18}\}$ ),  $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{5-}$  ( $\{\text{H}_4\text{IW}_{18}\}$ ) at PBE0/TZP level. There are two kinds of arrangements for the third proton for  $\beta$  and  $\beta^*$  isomers. Only the most stable arrangements of  $\{\text{H}_4\text{IW}_{18}\}$  are provided.

Types	$\{\text{H}_3\text{IW}_{18}\}$	$\{\text{H}_4\text{IW}_{18}\}$
$\alpha$	-33.79384	-33.80809
$\beta$	-33.78791/-33.78790	-33.80185
$\gamma$	-33.78254	-33.79612
$\alpha^*$	-33.82810	-33.82769
$\beta^*$	-33.83619/-33.83285	-33.83142
$\gamma^*$	-33.83658	-33.83305

**Table S10.** Bonding energies (a.u.) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$  ( $\{\text{H}_2\text{TeW}_{18}\}$ ),  $[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{7-}$  ( $\{\text{H}_3\text{TeW}_{18}\}$ ),  $[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{6-}$  ( $\{\text{H}_4\text{TeW}_{18}\}$ ) . There are two kinds of arrangements for the third proton for  $\beta$  and  $\beta^*$  isomers. Only the most stable arrangements of  $\{\text{H}_4\text{TeW}_{18}\}$  are provided.

Types	$\{\text{H}_2\text{TeW}_{18}\}$	$\{\text{H}_3\text{TeW}_{18}\}$	$\{\text{H}_4\text{TeW}_{18}\}$
$\alpha$	-27.54957	-27.57573	-27.58847
$\beta$	-27.54034	-27.56728/-27.56547	-27.58271
$\gamma$	-27.53459	-27.56143	-27.57490
$\alpha^*$	-27.56719	-27.58553	-27.58953
$\beta^*$	-27.56821	-27.59191/-27.59020	-27.59440
$\gamma^*$	-27.56894	-27.59322	-27.59497

**Table S11.** Crystal data and refinement parameters for  $\gamma^*-[({\text{IO}}_6){\text{W}}_{18}{\text{O}}_{54}(\text{OH})_2{\text{H}}]^{7-}$ 

Compound $\gamma^*-[({\text{IO}}_6){\text{W}}_{18}{\text{O}}_{54}(\text{OH})_2{\text{H}}]^{7-}$			
Empirical formula	$\text{C}_{41.5}\text{H}_{37.8}\text{N}_{3.8}\text{O}_{3.8}\text{W}_{3.8}\text{I}_{3.8}$	$\rho_{\text{calc}}(\text{mg cm}^{-3})$	3.463
Formula weight	1824.48	$\mu(\text{mm}^{-1})$	15.768
Crystal system	trigonal	$F(000)$	14824.0
Space group	<b>R-3</b>	Crystal size (mm)	0.24×0.20×0.18
<i>a</i> (Å)	37.307(2)	Reflections	11631
<i>b</i> (Å)	37.307(2)	$R_{\text{int}}$	0.0541
<i>c</i> (Å)	13.0641(7)	$T_{\text{max}}/T_{\text{min}}$	1.000/0.157
$\alpha(^{\circ})$	90	Data/parameters	7155/445
$\beta(^{\circ})$	90	$R_1^{\text{a}}$	0.0754
$\gamma(^{\circ})$	120	$wR_2^{\text{b}}[I > 2(I)]$	0.1872
<i>V</i> (Å <sup>3</sup> )	15746.8(19)	$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}(\text{e}\text{\AA}^{-3})$	4.88/-4.55
<i>Z</i>	18		

$$^{\text{a}} R_1 = \sum ||\text{Fo}| - |\text{Fc}|| / \sum |\text{Fo}|, ^{\text{b}} wR_2 = [\sum w(\text{Fo}^2 - \text{Fc}^2)^2 / \sum w(\text{Fo}^2)^2]^{1/2}$$

**Synthesis:**  $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$  (20.0 g, 60.6 mmol) was dissolved in water (50 mL) and  $\text{H}_5\text{IO}_6$  (1.0 g, 4.4 mmol) in water (10 mL) was added. The pH was adjusted to 1.0 by the addition of 6m HCl followed by heating the solution to reflux for 1.5 h. After the solution was cooled to around 80°C,  $\text{NH}_4\text{Cl}$  (15 g) was added under stirring. As the solution cooled, a white powder formed and was removed by filtration, and light green crystals were isolated from the filtrate after a few hours. Collection of these crystals by soaking the solid using filtered mother liquid to remove further white powder, and recrystallization from a minimum amount of water, gave large crystals. The above experimental procedure and corresponding crystal data have been put into ESI.

**Table S12.** Bonding energies (a.u.) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$  ( $\{\text{H}_2\text{WW}_{18}\}$ ),  $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{7-}$  ( $\{\text{H}_3\text{WW}_{18}\}$ ),  $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{6-}$  ( $\{\text{H}_4\text{WW}_{18}\}$ ). There are two kinds of arrangements for the third proton for  $\beta$  and  $\beta^*$  isomers. Only the most stable arrangements of  $\{\text{H}_4\text{WW}_{18}\}$  are provided.

Type	$\{\text{H}_2\text{WW}_{18}\}$	$\{\text{H}_3\text{WW}_{18}\}$	$\{\text{H}_4\text{WW}_{18}\}$
s			
$\alpha$	-28.06994	-28.10574	-28.12485
$\beta$	-28.06184	-28.10025/-28.09654	-28.11243
$\gamma$	-28.05630	-28.09350	-28.10788
$\alpha^*$	-28.06595	-28.09366	-28.10604
$\beta^*$	-28.07092	-28.10120/-28.09772	-28.11338
$\gamma^*$	-28.07265	-28.10139	-28.11559

**Table S13.** Relative stability varies with heteroatom (X) and protons.

	Stability order	Anions
1	$\alpha > \beta > \gamma > \gamma^* > \beta^* > \alpha^*$	$[(\text{NaF}_6)\text{W}_{18}\text{O}_{56}\text{H}_2]^{7-}$ and $[(\text{XO}_4)\text{W}_{18}\text{O}_{54}]^{n-}$ ( $\text{X}=\text{P, As, Si, etc}$ )
2	$\gamma^* > \beta^* > \alpha^* > \alpha > \beta > \gamma$	$[(\text{IO}_6)\text{W}_{18}\text{O}_{56}\text{H}_2]^{7-}$ , $[(\text{IO}_6)\text{W}_{18}\text{O}_{56}\text{H}_3]^{6-}$ , $[(\text{IO}_6)\text{W}_{18}\text{O}_{56}\text{H}_4]^{5-}$ $[(\text{TeO}_6)\text{W}_{18}\text{O}_{56}\text{H}_2]^{8-}$ , $[(\text{TeO}_6)\text{W}_{18}\text{O}_{56}\text{H}_3]^{7-}$ , $[(\text{TeO}_6)\text{W}_{18}\text{O}_{56}\text{H}_4]^{6-}$
3	$\gamma^* > \beta^* > \alpha > \alpha^* > \beta > \gamma$	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{56}\text{H}_2]^{9-}$ , $[(\text{WO}_6)\text{W}_{18}\text{O}_{56}\text{H}_2]^{6-}$
4	$\gamma^* > \alpha > \beta^* > \alpha^* > \beta > \gamma$	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{56}\text{H}_4]^{7-}$
5	$\alpha > \gamma^* > \beta^* > \beta > \gamma > \alpha^*$	$[(\text{WO}_6)\text{W}_{18}\text{O}_{56}\text{H}_4]^{6-}$ and $[(\text{WO}_6)\text{W}_{18}\text{O}_{56}\text{H}_3]^{7-}$

**Table S14.** Mayer index of W-O<sub>a</sub>(apical), W-O<sub>i</sub> (interior) and Sb-O<sub>i</sub>/Na-F  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$  and  $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers.

$\{\text{H}_2\text{SbW}_{18}\}$	W-O <sub>a</sub>	W-O <sub>i</sub>	Sb-O <sub>i</sub>	$\{\text{H}_2\text{NaW}_{18}\}$	W-O <sub>a</sub>	W-O <sub>F</sub>	Na-F
$\alpha$	0.22	0.37-0.38	0.47	$\alpha$	0.20	0.17-0.18	0.00
$\beta$	0.22	0.38-0.40	0.46	$\beta$	0.20	0.19-0.20	0.00
$\gamma$	0.22	0.38-0.40	0.46	$\gamma$	0.22	0.20	0.00
$\alpha^*$	0.21-0.22	0.35-0.37	0.47	$\alpha^*$	0.21	0.19-0.20	0.00
$\beta^*$	0.21-0.22	0.36-0.37	0.47	$\beta^*$	0.21	0.19-0.20	0.00

$\gamma^*$	0.21-0.22	0.36-0.38	0.47	$\gamma^*$	0.22	0.20	0.00
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**Table S15.** Mayer index of W-O<sub>a</sub>(apical), W-O<sub>i</sub> (interior) for  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$  [(SiO<sub>4</sub>)<sub>2</sub>W<sub>18</sub>O<sub>54</sub>]<sup>8-</sup> isomers.

{Si <sub>2</sub> W <sub>18</sub> }	W-O <sub>a</sub>	W-O <sub>i</sub>
$\alpha$	0.20	0.24
$\beta$	0.20	0.24
$\gamma$	0.19	0.25
$\alpha^*$	0.20	0.24
$\beta^*$	0.19-0.20	0.25
$\gamma^*$	0.19	0.26

**Table 16.** Deformation energies (kcal/mol) of host (DE<sub>host</sub>), guest (DE<sub>guest</sub> or DE<sub>SbO<sub>6</sub></sub>), OH (DE<sub>OH</sub>) and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$  [(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>9-</sup> isomers.

Types	FIE	DE	DE <sub>host</sub>	DE <sub>SbO<sub>6</sub></sub>	DE <sub>OH</sub>
$\alpha/D_3$	-985.25	319.75	269.65	49.05	1.06
$\beta/C_3$	-986.76	320.90	270.80	49.05	1.05
$\gamma/D_3$	-989.14	332.64	281.38	50.21	1.05
$\alpha^*/S_6$	-970.46	301.17	298.34	1.98	0.85
$\beta^*/C_3$	-967.69	301.83	299.63	1.32	0.88
$\gamma^*/S_6$	-967.11	294.72	293.60	0.22	0.90

**Table 17.** Deformation energies (kcal/mol) of host ( $DE_{host}$ ), guest ( $DE_{guest}$  or  $DE_{NaF6}$ ), OH ( $DE_{OH}$ ) and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(NaF_6)W_{18}O_{54}(OH)_2]^{7-}$  isomers.

Types	FIE	DE	$DE_{host}$	$DE_{NaF6}$	$DE_{OH}$
$\alpha/D_{3h}$	-699.25	195.15	164.01	30.39	0.75
$\beta/C_{3v}$	-702.10	196.49	166.11	29.63	0.74
$\gamma/D_{3h}$	-704.18	206.16	176.34	29.07	0.74
$\alpha^*/D_{3d}$	-695.05	212.68	195.02	16.91	0.74
$\beta^*/C_{3v}$	-694.02	210.40	191.83	17.82	0.75
$\gamma^*/D_{3d}$	-693.67	200.52	182.23	17.53	0.75

**Table 18.** Deformation energies (kcal/mol) of host ( $DE_{host}$ ), guest ( $DE_{guest}$  or  $DE_{SiO4}$ ), and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(SiO_4)_2W_{18}O_{54}]^{8-}$  isomers.

Types	FIE	DE	$DE_{host}$	$DE_{SiO4}$
$\alpha/D_{3h}$	-761.96	222.48	216.39	6.09
$\beta/C_{3v}$	-762.64	222.13	216.58	5.55
$\gamma/D_{3h}$	-763.63	230.59	225.25	5.34
$\alpha^*/D_{3d}$	-769.49	249.72	245.81	3.90
$\beta^*/C_{3v}$	-768.33	246.66	240.79	5.88
$\gamma^*/D_{3d}$	-768.42	236.17	231.25	4.93

**Table 19.** Relative energies (kcal/mol) of the  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{SiO}_4)\text{W}_{18}\text{O}_{54}]^{8-}$  isomers at the GGA-PBESol/TZP level.

Types	$\Delta E_t$	$\Delta E_{\text{free}}$	$\Delta FIE$	$\Delta DE$	$\Delta E_{\text{host}}$	$\Delta E_{\text{guest}}$	$\Delta E_{\text{host}}$
$\alpha/D_{3h}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$\beta/C_{3v}$	4.12	5.59	-0.68	-0.35	5.78	-0.54	0.19
$\gamma/D_{3h}$	4.49	0.00	-1.67	8.11	8.86	-0.75	8.86
$\gamma^*/D_{3d}$	8.49	5.59	-6.46	13.69	20.45	-1.16	14.86
$\beta^*/C_{3v}$	10.47	0.00	-6.37	24.18	24.4	-0.21	24.40
$\alpha^*/D_{3d}$	17.63	5.59	-7.53	27.24	35.01	-2.19	29.42

**Table 20.** Relative energies (kcal/mol) of the  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$  isomers at the GGA-PBESol/TZP level.

Type s	$\Delta E_t (\Delta G)$	$\Delta FIE$	$\Delta E_{\text{free}}$	$\Delta DE (\Delta E_{\text{host}}/\Delta E_{\text{guest}})$	$\Delta E_{\text{host}}$
$\gamma^*/S_6$	0.00(0.00)	0.00	0.00	0.00(0.00/0.00)	0.00
$\beta^*/C_3$	0.93(0.84)	-0.58	-5.59	7.10(6.03/1.10)	0.44
$\alpha^*/S_6$	3.11(3.70)	-3.35	0.00	6.45(4.74/1.76)	4.74
$\alpha/D_3$	1.31(3.05)	-18.14	-5.59	25.03(-23.95/48.83)	-29.54
$\beta/C_3$	6.53(8.87)	-19.65	0.00	26.18(-22.80/48.83)	-22.80
$\gamma/D_3$	10.30(12.84)	-22.03	-5.59	37.92(-12.22/50.00)	-17.81

**Table 21.** Relative energies (kcal/mol) of the  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers at the GGA-PBEsol/TZP level.

Types	$\Delta E_t (\Delta G)$	$\Delta FIE$	$\Delta E_{\text{free}}$	$\Delta DE(\Delta E_{\text{host}}/\Delta E_{\text{guest}})$	$\Delta E_{\text{host}}$
Anions	$\Delta E_t (\Delta G)$	$\Delta FIE$	$\Delta E_{\text{free}}$	$\Delta DE(\Delta E_{\text{host}}/\Delta E_{\text{guest}})$	$\Delta E_{\text{host}}$
$\alpha/D_{3h}$	0.00(0.00)	0.00	0.00	0.00(0.00/0.00)	0.00
$\beta/C_{3v}$	4.08(3.09)	-2.85	5.59	1.34(2.10/-0.76)	7.69
$\gamma/D_{3h}$	6.09(6.84)	-4.93	0.00	11.01(12.33/-1.32)	12.33
$\alpha^*/D_{3d}$	28.78(29.03)	4.20	5.59	17.53(31.01/-13.48)	36.60
$\beta^*/C_{3v}$	20.48(19.30)	5.23	0.00	15.25(27.82/-12.57)	27.82
$\gamma^*/D_{3d}$	15.16(14.17)	5.58	5.59	5.37(18.22/-12.86)	23.81

**Table 22.** Deformation energies (kcal/mol) of host ( $DE_{\text{host}}$ ), guest ( $DE_{\text{guest}}$  or  $DE_{\text{TeO}_6}$ ), OH ( $DE_{\text{OH}}$ ) and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$  isomers.

Types	FIE	DE	$DE_{\text{host}}$	$DE_{\text{guest}}$	$DE_{\text{OH}}$
$\alpha$	-841.16	273.15	219.50	58.23	1.45
$\beta$	-834.91	282.74	215.86	55.77	1.52
$\gamma$	-835.30	239.00	223.70	57.34	1.70
$\alpha^*$	-810.90	273.15	228.01	1.87	1.30
$\beta^*$	-815.49	231.18	239.14	1.33	1.35
$\gamma^*$	-817.62	241.82	236.06	1.05	1.89

**Table 23.** Deformation energies (kcal/mol) of host ( $\text{DE}_{\text{host}}$ ), guest ( $\text{DE}_{\text{guest}}$  or  $\text{DE}_{\text{IO}_6}$ ), OH ( $\text{DE}_{\text{OH}}$ ) and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers.

Types	FIE	DE	$\text{DE}_{\text{host}}$	$\text{DE}_{\text{guest}}$	$\text{DE}_{\text{OH}}$
$\alpha$	-704.71	245.40	177.38	67.50	0.51
$\beta$	-700.50	239.07	171.72	65.87	1.48
$\gamma$	-697.62	244.24	177.28	65.41	1.55
$\alpha^*$	-669.09	178.55	171.02	6.57	0.96
$\beta^*$	-669.75	185.99	178.10	7.00	0.89
$\gamma^*$	-668.19	181.62	174.92	5.67	1.03

**Table 24.** Deformation energies (kcal/mol) of host ( $\text{DE}_{\text{host}}$ ), guest ( $\text{DE}_{\text{guest}}$  or  $\text{DE}_{\text{WO}_6}$ ), OH ( $\text{DE}_{\text{OH}}$ ) and sum of them (DE), host-guest fragment interaction (FIE) of  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{6-}$  isomers.

Types	FIE	DE	$\text{DE}_{\text{host}}$	$\text{DE}_{\text{WO}_6}$	$\text{DE}_{\text{OH}}$
$\alpha$	-851.72	289.08	258.91	29.05	1.12
$\beta$	-851.35	288.58	258.79	28.99	0.80
$\gamma$	-851.41	297.33	267.08	29.15	1.09
$\alpha^*$	-849.37	284.03	279.19	4.18	0.66
$\beta^*$	-850.73	287.48	281.28	5.75	0.45
$\gamma^*$	-850.21	280.66	275.46	4.34	0.85

**Table 25.** Percentages of several kinds of relative energies (kcal/mol) based on  $|\Delta FIE|/(|\Delta DE|+|FIE|+|\Delta E_{\text{free}}|)$ ,  $\Delta DE/(|\Delta DE|+|FIE|+|\Delta E_{\text{free}}|)$ , and  $|\Delta E_{\text{free}}|/(|\Delta DE|+|FIE|+|\Delta E_{\text{free}}|)$ , respectively. The “| |” denotes absolute value. The reference isomer is excluded due to its 0.0 kcal/mol.

Anions	$\Delta DE$	$\Delta FIE$	$\Delta E_{\text{free}}$
$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$	57.1%	12.4%	30.5%
$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$	50.8%	22.3%	26.9%
$[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$	57.6%	24.0%	15.3%

**Table 26.** Percentages of several kinds of relative energies (kcal/mol) based on  $|\Delta FIE|/(|\Delta FIE|+|\Delta E_{\text{host}}|+|\Delta E_{\text{guest}}|)$ ,  $|\Delta E_{\text{guest}}|/(|\Delta FIE|+|\Delta E_{\text{host}}|+|\Delta E_{\text{guest}}|)$ , and  $|\Delta E_{\text{host}}|/(|\Delta FIE|+|\Delta E_{\text{host}}|+|\Delta E_{\text{guest}}|)$ , respectively. The “| |” denotes absolute value. The reference isomer is excluded due to its 0.0 kcal/mol.

Anions	$\Delta FIE$	$\Delta E_{\text{guest}}$	$\Delta E_{\text{host}}$
$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$	25.2%	45.9%	28.9%
$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$	16.8%	19.3%	63.8%
$[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$	17.0%	4.8%	78.2%

**Table 27.** Block parameters of six  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^9$ -isomers.

Typ e	$\text{O}_t=\text{W}(\text{OH})_4$	$\text{O}_t=\text{W}(\text{OH})_5^-$	$\text{O}_t-\text{W}-$	$\text{O}_b-\text{W}-$	$\text{O}_b-\text{W}-$	$\text{W}-\text{O}_b-$	$\text{W}-\text{O}_i$	$\text{W}-$	$\text{W} \rightarrow \text{plane}$
	(a.u.)	(a.u.)	$\text{O}_b$	$\text{O}_b$	$\text{O}_p$	W	(Å)	$\text{O}_b$	(Å)
				(degree)	(degree)	(degree)		(Å)	
$\beta_1$	-2.35967	-2.90104	100.4	88.1	79.5	130.2	2.219	1.925	0.351
$\beta_2$	-2.34626	-2.89112	96.9	89.2	83.0	140.5	2.214	1.919	0.230
$\beta_3$	-2.34349	-2.88999	96.5	89.3	83.4	142.7	2.220	1.920	0.221
$\beta_4$	-2.35661	-2.89796	100.3	88.2	79.7	133.9	2.225	1.922	0.344
$\alpha_1^*$	-2.35827	-2.89827	100.7	88.0	79.2	133.1	2.222	1.923	0.360
$\alpha_2^*$	-2.33979	-2.88506	96.3	89.4	84.1	144.4	2.259	1.916	0.208
$\alpha_3^*$	-2.34101	-2.88819	95.9	89.5	84.6	143.5	2.231	1.917	0.194
$\alpha_4^*$	-2.35833	-2.89889	100.7	88.0	79.2	133.0	2.220	1.923	0.358
$\beta_1^*$	-2.35786	-2.89821	100.6	88.0	79.3	133.2	2.223	1.923	0.356
$\beta_2^*$	-2.34180	-2.88820	96.0	89.5	84.4	143.7	2.230	1.915	0.198
$\beta_3^*$	-2.33809	-2.88420	96.0	89.5	84.2	145.2	2.245	1.919	0.201
$\beta_4^*$	-2.35842	-2.89938	100.2	88.2	79.9	132.6	2.247	1.920	0.339
$\gamma_1^*$	-2.35803	-2.89907	100.2	88.2	79.8	132.1	2.243	1.921	0.341
$\gamma_2^*$	-2.34352	-2.88732	96.2	89.4	83.9	145.2	2.245	1.918	0.208
$\gamma_3^*$	-2.33855	-2.88400	96.1	89.4	83.9	145.3	2.244	1.918	0.206
$\gamma_4^*$	-2.35799	-2.89908	100.2	88.2	79.8	132.1	2.243	1.921	0.342

**Table 28.** Block parameters of six  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^9$ -isomers, and average data is provided for  $\beta$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$  isomers.

Typ e	$\text{O}_\text{l}=\text{W}(\text{OH})_4$	$\text{O}_\text{l}=\text{W}(\text{OH})_4\text{F}^-$	$\text{O}_\text{l}-\text{W}-$	$\text{O}_\text{b}-\text{W}-$	$\text{O}_\text{b}-\text{W}-$	$\text{W}-\text{O}_\text{b}-$	$\text{W}-\text{O}_\text{i}$	$\text{W}-$	$\text{W} \rightarrow \text{plane}$
	(a.u.)	(a.u.)	$\text{O}_\text{b}$	$\text{O}_\text{b}$	$\text{O}_\text{p}$	W	(Å)	$\text{O}_\text{b}$	(Å)
			(degree)	(degree)	(degree)	(degree)			(Å)
$\alpha_1$	-2.35724	-2.89854	100.3	88.2	79.7	133.9	2.225	1.921	0.344
$\alpha_2$	-2.34698	-2.89308	96.5	89.4	83.5	141.8	2.212	1.918	0.217
$\beta_1$	-2.35814	-2.89950	100.4	88.2	79.6	132.1	2.222	1.924	0.348
$\beta_2$	-2.34488	-2.89056	96.7	89.3	83.2	141.6	2.217	1.920	0.226
$\gamma_1$	-2.35925	-2.90066	100.4	88.1	79.5	130.4	2.222	1.925	0.351
$\gamma_2$	-2.34565	-2.89058	96.7	89.3	83.1	141.1	2.213	1.918	0.225
$\alpha_1^*$	-2.3583	-2.89858	100.7	88.0	79.2	133.1	2.221	1.923	0.359
$\alpha_2^*$	-2.34040	-2.88663	96.1	89.5	84.4	144.0	2.245	1.917	0.201
$\beta_1^*$	-2.35814	-2.89880	100.4	88.1	79.6	132.9	2.235	1.922	0.348
$\beta_2^*$	-2.33995	-2.88620	96.0	89.5	84.3	144.5	2.238	1.917	0.200
$\gamma_1^*$	-2.35801	-2.89908	100.2	88.2	79.8	132.1	2.243	1.921	0.342
$\gamma_2^*$	-2.34104	-2.88566	96.2	89.4	83.9	145.3	2.245	1.918	0.207

**Table 29.** Block parameters of  $\beta$  and  $\beta^*$   $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers.

Typ e	$\text{O}_t=\text{W}(\text{OH})_4$	$\text{O}_t=\text{W}(\text{OH})_5^-$	$\text{O}_t-\text{W}-$	$\text{O}_b-\text{W}-$	$\text{O}_b-\text{W}-$	$\text{W}-\text{O}_b-$	$\text{W}-\text{O}_i$	$\text{W}-\text{O}_b$	$\text{W} \rightarrow \text{plane}$
	(a.u.)	(a.u.)	$\text{O}_b$	$\text{O}_b$	$\text{O}_p$	W	(Å)	(Å)	(Å)
				(degree)	(degree)	(degree)			
$\beta_1$	-2.36053	-2.90007	100.3	88.2	79.8	134.8	2.246	1.922	0.343
$\beta_2$	-2.35108	-2.68999	99.3	88.6	80.9	147.0	2.231	1.915	0.308
$\beta_3$	-2.35097	-2.68953	99.6	88.5	80.4	146.5	2.227	1.916	0.319
$\beta_4$	-2.36332	-2.90305	100.2	88.2	79.9	131.9	2.252	1.923	0.341
$\beta_1^*$	-2.36097	-2.90069	100.3	88.2	79.7	134.1	2.246	1.923	0.344
$\beta_2^*$	-2.34775	-2.68649	99.1	88.6	81.4	149.0	2.248	1.913	0.299
$\beta_3^*$	-2.34759	-2.68495	98.9	88.7	81.4	149.9	2.262	1.914	0.295
$\beta_4^*$	-2.36069	-2.90023	99.6	88.4	80.8	133.8	2.280	1.921	0.319

**Table 30.** Block parameters of six  $[(\text{NaF}_6)_2\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers, and average data is provided for  $\beta$  and  $\beta^*$  isomers

	$\text{O}_\text{i}=\text{W}(\text{OH})_4$ Typ	$\text{O}_\text{i}=\text{W}(\text{OH})_4\text{F}^-$ or (a.u.)	$\text{O}_\text{i}-\text{W}-$ $\text{O}_\text{b}$ (a.u.)	$\text{O}_\text{b}-\text{W}-$ $\text{O}_\text{b}$ (degree)	$\text{O}_\text{b}-\text{W}-$ $\text{O}_\text{p}$ (degree)	$\text{W}-\text{O}_\text{b}-$ $\text{W}$ (degree)	$\text{W}-\text{O}_\text{i}$ (Å)	$\text{W}-\text{O}_\text{b}$ (Å)	$\text{W}\rightarrow\text{plane}$ (Å)
$\alpha_1$	-2.36027	-2.89985	100.3	88.2	79.9	135.0	2.247	1.921	0.343
$\alpha_2$	-2.35189	-2.69163	99.4	88.6	80.8	146.0	2.227	1.916	0.311
$\beta_1$	-2.36193	-2.90156	100.3	88.2	79.9	133.4	2.249	1.923	0.342
$\beta_2$	-2.35103	-2.68976	99.5	88.6	80.7	146.8	2.229	1.916	0.314
$\gamma_1$	-2.36286	-2.90266	100.1	88.2	80.0	132.3	2.256	1.923	0.337
$\gamma_2$	-2.35045	-2.68891	99.4	88.5	80.5	148.1	2.232	1.915	0.314
$\alpha_1^*$	-2.36097	-2.90039	100.5	88.1	79.5	133.7	2.243	1.924	0.350
$\alpha_2^*$	-2.34554	-2.68388	98.8	88.7	81.8	148.9	2.257	1.914	0.289
$\beta_1^*$	-2.36083	-2.90046	100.0	88.3	80.3	134.0	2.263	1.922	0.332
$\beta_2^*$	-2.34767	-2.68572	99.0	88.7	81.4	149.5	2.255	1.914	0.297
$\gamma_1^*$	-2.36162	-2.90119	99.7	88.4	80.6	133.4	2.274	1.922	0.322
$\gamma_2^*$	-2.34849	-2.68631	99.2	88.6	81.0	150.9	2.252	1.913	0.304

**Table 31.** Block parameters of  $\beta$  and  $\beta^*$   $[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$  isomers.

Typ	$O_t=\text{W}(\text{OH})_5^-$	$O_t-\text{W}-$	$O_b-\text{W}-$	$O_b-\text{W}-$	$\text{W}-O_b-$	$\text{W}-\text{O}_i$	$\text{W}-\text{O}_b$	$\text{W} \rightarrow \text{plane}$
	(a.u.)	$O_b$	$O_b$	$O_p$	$W$	(Å)	(Å)	(Å)
	e	(degree)	(degree)	(degree)	(degree)			
$\beta_1$	-2.90205914	100.4	88.1	79.7	131.5	2.306	1.919	0.345
$\beta_4$	-2.89963207	100.3	88.2	79.7	134.6	2.298	1.918	0.344
$\beta_3$	-2.89012975	97.7	89.0	82.4	145.2	2.239	1.917	0.257
$\beta_2$	-2.88956388	98.0	88.9	81.9	144.5	2.239	1.917	0.267
$\beta_1^*$	-2.89991024	100.3	88.2	79.7	134.0	2.299	1.919	0.344
$\beta_2^*$	-2.88719104	97.6	89.0	82.8	146.8	2.253	1.914	0.250
$\beta_3^*$	-2.88693776	97.4	89.1	82.8	147.2	2.269	1.915	0.246
$\beta_4^*$	-2.89874149	99.8	88.4	80.5	133.6	2.336	1.917	0.324

**Table 32.** Block parameters of six  $[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$  isomers, and average data is provided for  $\beta$  and  $\beta^*$  isomers

Typ	$\text{O}_i=\text{W}(\text{OH})_4\text{F}^-$ or	$\text{O}_i-\text{W}-\text{O}_b$	$\text{O}_b-\text{W}$	$\text{O}_b-\text{W}$	$\text{W}-\text{O}_b-$	$\text{W}-\text{O}_i$	$\text{W}-\text{O}_b$	$\text{W} \rightarrow \text{plane}$
	$\text{O}_i=\text{W}(\text{OH})_5^-$	(degree)	$\text{O}_b$	$\text{O}_p$	$\text{W}$	(Å)	(Å)	(Å)
	e	(a.u.)		(degree)	(degree)	(degree)		
$\alpha_1$	-2.89912773	100.3	88.2	79.8	134.8	2.298	1.917	0.344
$\alpha_2$	-2.89092161	97.8	89.0	82.3	144.3	2.235	1.917	0.260
$\beta_1$	-2.900845605	100.35	88.15	79.7	133.05	2.302	1.9185	0.3445
$\beta_2$	-2.889846815	97.85	88.95	82.15	144.85	2.239	1.917	0.262
$\gamma_1$	-2.90167354	100.2	88.2	79.9	132.0	2.311	1.919	0.340
$\gamma_2$	-2.88922828	97.9	89.0	82.1	146.3	2.245	1.915	0.263
$\alpha_1^*$	-2.90013429	100.4	88.1	79.6	133.4	2.299	1.919	0.346
$\alpha_2^*$	-2.88485028	97.3	89.1	83.2	146.9	2.269	1.914	0.239
$\beta_1^*$	-2.89932586	100.05	88.3	80.1	133.8	2.3175	1.918	0.334
$\beta_2^*$	-2.8870644	97.5	89.05	82.8	147	2.261	1.9145	0.248
$\gamma_1^*$	-2.90003917	99.9	88.3	80.3	133.0	2.327	1.918	0.329
$\gamma_2^*$	-2.88789680	97.6	89.0	82.5	148.3	2.259	1.914	0.254

**Table 33.** The first Reduction Potentials (in V) for two complexes

Isomers	$\alpha$	$\beta$	$\gamma$	$\alpha^*$	$\beta^*$	$\gamma^*$
{H <sub>2</sub> NaW <sub>18</sub> }	-0.79	-0.73	-0.66	-0.77	-0.72	-0.67
{H <sub>2</sub> SbW <sub>18</sub> }	-1.26	-1.25	-1.21	-1.31	-1.25	-1.18

**Table 34.** Energy levels of HOMO and LUMO (eV) for [(NaF<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>7-</sup>

Isomers	anion		cage	
	HOMO	LUMO	HOMO	LUMO
$\alpha$	-6.398	-3.968	-8.505	-6.034
$\beta$	-6.365	-4.034	-8.485	-6.097
$\gamma$	-6.316	-4.098	-8.420	-6.140
$\alpha^*$	-6.140	-3.992	-8.255	-6.051
$\beta^*$	-6.246	-4.037	-8.331	-6.065
$\gamma^*$	-6.274	-4.074	-8.374	-6.098

**Table 35.** Energy levels of HOMO and LUMO (eV) for  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ 

Isomers	anion		cage	
	HOMO	LUMO	HOMO	LUMO
$\alpha$	-5.349	-3.455	-8.565	-6.154
$\beta$	-5.331	-3.475	-8.573	-6.189
$\gamma$	-5.311	-3.491	-8.635	-6.222
$\alpha^*$	-5.504	-3.431	-8.449	-6.263
$\beta^*$	-5.475	-3.487	-8.499	-6.241
$\gamma^*$	-5.462	-3.519	-8.550	-6.229

**Table 36.** Inclusion energies (kcal/mol) of the third proton for a series of anions.

Isomers	$\{\text{NaW}_{18}\}$	$\{\text{IW}_{18}\}$	$\{\text{TeW}_{18}\}$	$\{\text{SbW}_{18}\}$	$\{\text{WW}_{18}\}$
$\alpha$	-21.94	-38.45	-46.43	-48.51	-52.48
$\beta$	-21.50	-37.76	-46.92	-50.31	-54.12
$\gamma$	-20.03	-36.29	-46.86	-47.95	-53.36
$\alpha^*$	-22.75	-30.50	-41.52	-50.90	-47.40
$\beta^*$	-23.50	-32.29	-44.89	-49.69	-49.08
$\gamma^*$	-21.65	-31.07	-45.25	-51.71	-48.05

**Table 37.** Inclusion energies (kcal/mol) of the fourth proton for a series of anions.

Isomers	{NaW <sub>18</sub> }	{IW <sub>18</sub> }	{TeW <sub>18</sub> }	{SbW <sub>18</sub> }	{WW <sub>18</sub> }
α	-15.17	-26.35	-38.01	-44.75	-42.01
β	-15.49	-25.95	-39.70	-46.42	-37.66
γ	-14.50	-26.12	-38.47	-44.87	-39.04
α*	-16.65	-19.09	-32.52	-42.68	-37.78
β*	-19.22	-16.68	-31.58	-42.46	-37.59
γ*	-18.49	-16.73	-31.11	-43.23	-38.93

**Table 38.** Total electronic energies (au) of α, β, γ, α\*, β\*, and γ\*[(NaF<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>7-</sup> isomers.

Types	{H <sub>2</sub> NaW <sub>18</sub> } <sup>7-</sup>	W <sub>18</sub> O <sub>54</sub>	[NaF <sub>6</sub> ] <sup>5-</sup>	2[OH] <sup>-</sup>
α/D <sub>3h</sub>	-27.12397935	-23.38731950	-1.64864348	-0.97368336
β/C <sub>3v</sub>	-27.11747940	-23.37506268	-1.64984392	-0.97369927
γ/D <sub>3h</sub>	-27.11427832	-23.36766705	-1.65073750	-0.97369924
α*/D <sub>3d</sub>	-27.07756817	-23.32898980	-1.67011945	-0.97369983
β*/C <sub>3v</sub>	-27.09133733	-23.34299275	-1.66867360	-0.97367760
γ*/D <sub>3d</sub>	-27.09981767	-23.34937039	-1.66913128	-0.97367982

(a) E<sub>host</sub>(free, eclipsed) = -23.70163 a.u., E<sub>host</sub>(free, staggered) = -23.69332 (b) E<sub>NaF6</sub>(free,

staggered) = -1.69707 a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u.

**Table 39.** Bonding energies (a.u.) of  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ , and molecule-fragments including  $\text{W}_{18}\text{O}_{54}$ ,  $\text{SbO}_6^{7-}$  and sum of two  $\text{OH}^-$

Type	$\{\text{H}_2\text{SbW}_{18}\}^{9-}$	$\text{W}_{18}\text{O}_{54}$	$\text{SbO}_6^{7-}$	$2[\text{OH}]^-$
s				
$a/D_3$	-27.80036	-23.21898	-2.03810	-0.97319
$\beta/C_3$	-27.79204	-23.20823	-2.03809	-0.97321
$\gamma/D_3$	-27.78602	-23.20028	-2.03624	-0.97321
$\alpha^*/S_6$	-27.79749	-23.16434	-2.11310	-0.97353
$\beta^*/C_3$	-27.80096	-23.17120	-2.11416	-0.97348
$\gamma^*/S_6$	-27.80244	-23.17190	-2.11591	-0.97344

(a)  $E_{\text{host}}(\text{free, eclipsed}) = -23.64869$  a.u.,  $E_{\text{host}}(\text{free, staggered}) = -23.63978$  (b)  $E_{\text{SbO}_6}(\text{free, staggered}) = -2.116261$  a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u

**Table 40.** Bonding energies (a.u.) of  $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$ , and molecule-fragments including  $\text{W}_{18}\text{O}_{54}$ ,  $\text{IO}_6^{5-}$  and sum of two  $\text{OH}^-$

Types	$[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$	$\text{W}_{18}\text{O}_{54}$	$\text{IO}_6^{5-}$	$2[\text{OH}]^-$
$a/D_{3h}$	-27.18465762	-23.36601109	-1.72155088	-0.97407075
$\beta/C_{3v}$	-27.17910765	-23.36612230	-1.72415234	-0.97252286
$\gamma/D_{3h}$	-27.17519826	-23.36617009	-1.72489492	-0.97241212
$\alpha^*/D_{3d}$	-27.21919720	-23.36103435	-1.82008622	-0.97324132
$\beta^*/C_{3v}$	-27.22362618	-23.36486327	-1.81797853	-0.97346352

$\gamma^*/D_{3d}$	-27.22551781	-23.36724645	-1.81864906	-0.97335647
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(a)  $E_{\text{host}}(\text{free, eclipsed}) = -23.70163$  a.u.,  $E_{\text{host}}(\text{free, staggered}) = -23.69332$  (b)  $E_{\text{TeO}_6}(\text{free, staggered}) = -1.82913$  a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u.

**Table 41.** Bonding energies (a.u.) of  $[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$ , and molecule-fragments including  $\text{W}_{18}\text{O}_{54}$ ,  $\text{TeO}_6^{6-}$  and sum of two  $\text{OH}^-$

Types	$[(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^8$	$\text{W}_{18}\text{O}_{54}$	$\text{TeO}_6^{6-}$	$2[\text{OH}]^-$
$a/D_{3h}$	-27.54957126	-23.29888786	-1.93764826	-0.97256388
$\beta/C_{3v}$	-27.54033712	-23.29578378	-1.94157996	-0.97245796
$\gamma/D_{3h}$	-27.53459134	-23.29220429	-1.93906869	-0.97217687
$\alpha^*/D_{3d}$	-27.56719125	-23.26359879	-2.02877266	-0.97186114
$\beta^*/C_{3v}$	-27.56821118	-23.26758959	-2.02832571	-0.97273600
$\gamma^*/D_{3d}$	-27.56894118	-23.27642803	-2.02746866	-0.97280080

(a)  $E_{\text{host}}(\text{free, eclipsed}) = -23.70163$  a.u.,  $E_{\text{host}}(\text{free, staggered}) = -23.69332$  (b)  $E_{\text{TeO}_6}(\text{free, staggered}) = -2.03045$  a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u.

**Table 42.** Bonding energies (a.u.) of  $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$ , and molecule-fragments including  $\text{W}_{18}\text{O}_{54}$ ,  $\text{IO}_6^{5-}$  and sum of two  $\text{OH}^-$

Types	$[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$	$\text{W}_{18}\text{O}_{54}$	$\text{WO}_6^{6-}$	$2[\text{OH}]^-$
$a/D_{3h}$	-28.06994118	-23.28903691	-2.45051355	-0.97309513
$\beta/C_{3v}$	-28.06184241	-23.28091036	-2.45061610	-0.97360532
$\gamma/D_{3h}$	-28.05629851	-23.27600427	-2.45035424	-0.97313925
$\alpha^*/D_{3d}$	-28.06595234	-23.24839660	-2.49015568	-0.97383512
$\beta^*/C_{3v}$	-28.07091924	-23.25338831	-2.48764794	-0.97415608

$\gamma^*/D_{3d}$	-28.07265266	-23.25434389	-2.48988912	-0.97351920
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(a)  $E_{\text{host}}(\text{free, eclipsed}) = -23.70163$  a.u.,  $E_{\text{host}}(\text{free, staggered}) = -23.69332$  (b)  $E_{\text{TeO}_6}(\text{free, staggered}) = -2.496811$  a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u.

**Table 43.** Bonding energies (a.u.) of  $[(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}]^{8-}$ , and molecule-fragments including  $\text{W}_{18}\text{O}_{54}$ ,  $\text{SiO}_4^{4-}$  (two kinds in  $\beta$  and  $\beta^*$ )

Types	anion	$\text{W}_{18}\text{O}_{54}$	$\text{SiO}_4^{4-}$	$\text{SiO}_4^{4-}$
$\alpha/D_{3h}$	-28.02531897	-23.30385707	-1.75360035	-1.75360035
$\beta/C_{3v}$	-28.01804375	-23.29463868	-1.75435324	-1.75370715
$\gamma/D_{3h}$	-28.01504794	-23.28973025	-1.75419892	-1.75419892
$\alpha^*/D_{3d}$	-27.98501144	-23.24805294	-1.75534536	-1.75534536
$\beta^*/C_{3v}$	-27.99693541	-23.26497038	-1.75403128	-1.75351541
$\gamma^*/D_{3d}$	-28.00488161	-23.27126739	-1.75452999	-1.75452999

(a)  $E_{\text{host}}(\text{free, eclipsed}) = -23.70163$  a.u.,  $E_{\text{host}}(\text{free, staggered}) = -23.69332$  a.u. (b)  $E_{\text{TeO}_6}(\text{free, staggered}) = -1.75845$  a.u. ;  $E_{\text{OH}}(\text{free}) = -0.48744$  a.u.

**Table 44.** Gibbs free energies (kcal/mol) of isomers at 298.15K.

Type	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$	$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$
S		
$\alpha$	-17369.36	-16954.79
$\beta$	-17363.54	-16951.70
$\gamma$	-17360.22	-16947.95
$\alpha^*$	-17368.71	-16925.76
$\beta^*$	-17371.57	-16935.49

$\gamma^*$	-17372.41	-16940.62
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**Table 45.** Bonding energies (a.u.) of  $[(\text{NaO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$

Type	$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$	$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$	$[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{5-}$
s			
$\alpha$	-27.12397935	-27.11117459	-27.08751186
$\beta$	-27.11747940	-27.10390339/-27.10076388	-27.08075183
$\gamma$	-27.11427832	-27.09836914	-27.07364796
$\alpha^*$	-27.07756817	-27.06599403	-27.04468862
$\beta^*$	-27.09133733	-27.08096348/-27.07935078	-27.06376853
$\gamma^*$	-27.09981767	-27.08649441	-27.06812288

**Table 46.** Bonding energies (a.u.) of  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$ ,

$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$  and  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{5-}$

Type	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$	$[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{5-}$
s			
$\alpha$	-27.80036	-27.82983	-27.85331
$\beta$	-27.79204	-27.82439/-27.82199	-27.85053
$\gamma$	-27.78602	-27.81460	-27.84071

$\alpha^*$	-27.79749	-27.83077	-27.85096
$\beta^*$	-27.80096	-27.83232/-27.83053	-27.85216
$\gamma^*$	-27.80244	-27.83702	-27.85808

**Table 47.** Bonding energies (a.u.) of single-reduced anions ( $2S+1=2$ )

Type	$\{\text{H}_2\text{NaW}_{18}\}-1e$	$\{\text{H}_2\text{SbW}_{18}\}-1e$
s		
$\alpha$	-27.25818386	-27.91704255
$\beta$	-27.25395629	-27.90932417
$\gamma$	-27.25328110	-27.90482943
$\alpha^*$	-27.21283670	-27.91239356
$\beta^*$	-27.22804532	-27.91819787
$\gamma^*$	-27.23847294	-27.92206997

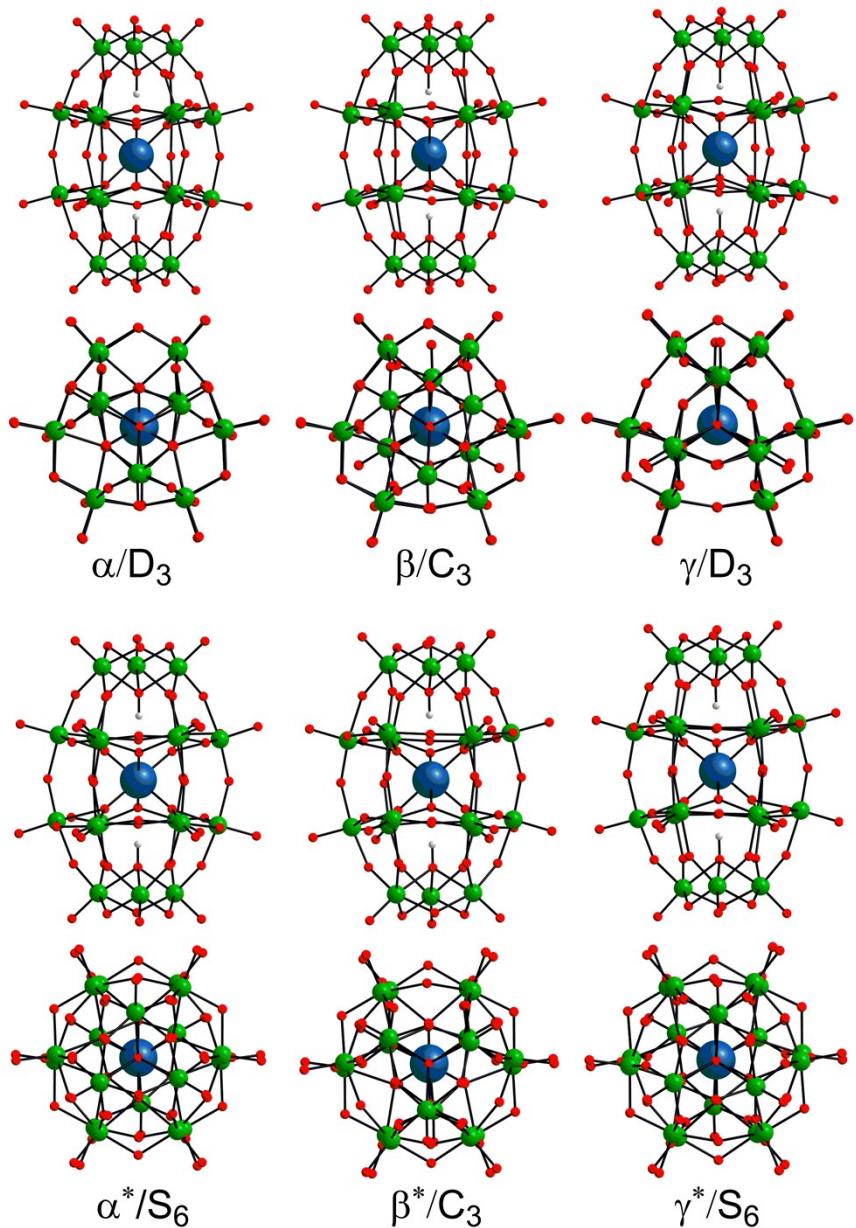
**Table 48.** The former five vibration frequencies ( $\text{cm}^{-1}$ ) of  $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$  isomers

Isomer	1	2	3	4	5
$\alpha$	14.156272	34.829279	45.401458	45.401458	55.894416

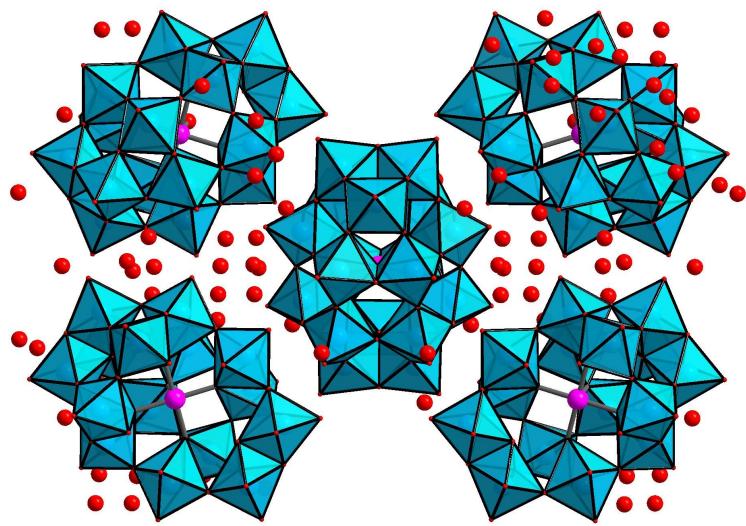
$\beta$	9.109342	34.323449	45.957741	45.957741	46.759157
$\gamma$	-10.626035	31.808844	45.865200	45.865200	48.951726
$\alpha^*$	-10.626035	31.808844	45.865200	45.865200	48.951726
$\beta^*$	-8.914722	29.973157	42.692197	42.692197	48.136222
$\gamma^*$	-14.27939	28.424140	42.457618	42.457618	44.054929

**Table 49.** The former five vibration frequencies ( $\text{cm}^{-1}$ ) of  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$  isomers

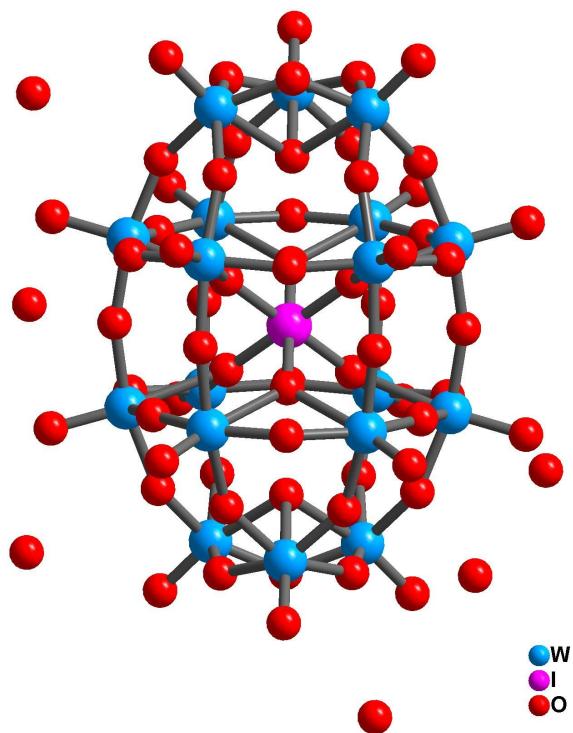
Isomer	1	2	3	4	5
$\alpha$	31.594042	38.768164	42.329133	42.329133	62.397831
$\beta$	36.608795	39.123680	44.343629	45.260447	49.135052
$\gamma$	34.769130	38.480473	38.480473	41.454570	56.217152
$\alpha^*$	28.738112	39.588835	42.586253	43.823873	45.187021
$\beta^*$	31.915810	38.003342	38.708647	39.041889	49.818214
$\gamma^*$	36.380223	36.949817	36.952860	38.468824	43.830148



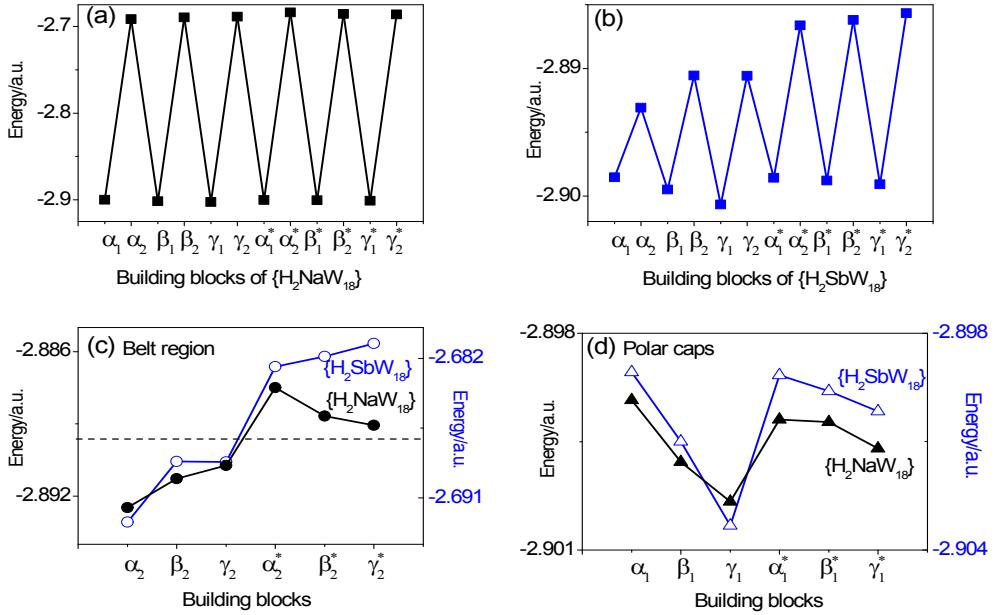
**Figure 1.** Ball-and-stick representations (top and side views) of the  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$   $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$  isomers.



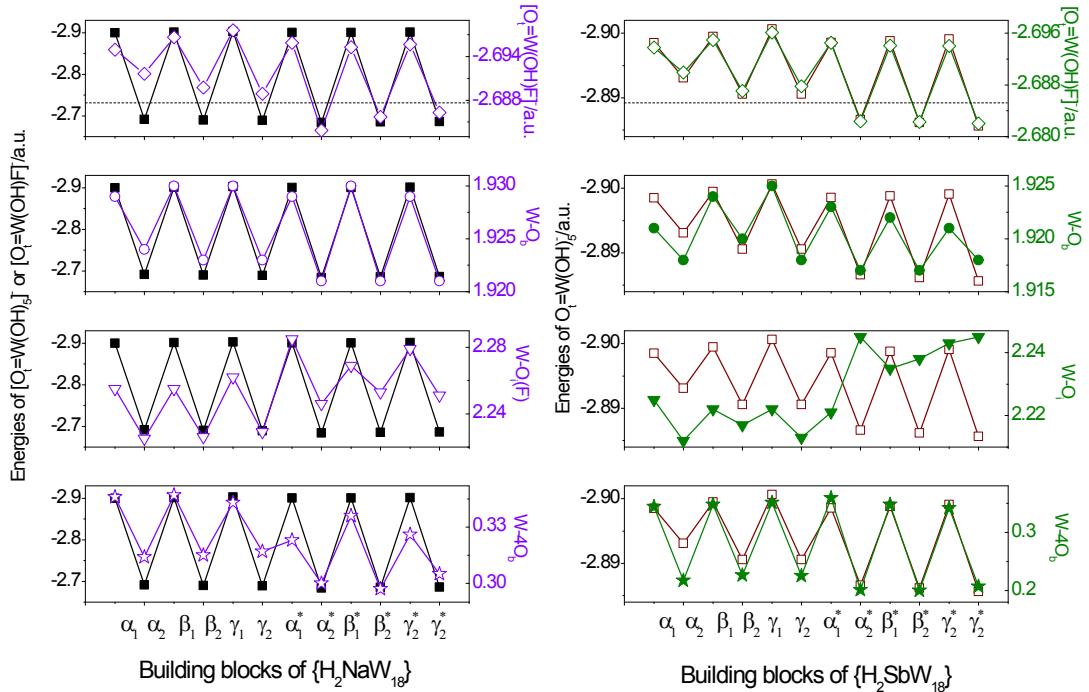
**Figure 2.** Polyhedron representations of  $\gamma^*$ - $[(\text{IO}_6)\text{W}_{18}\text{O}_{56}\text{H}_3]^{6-}$ .



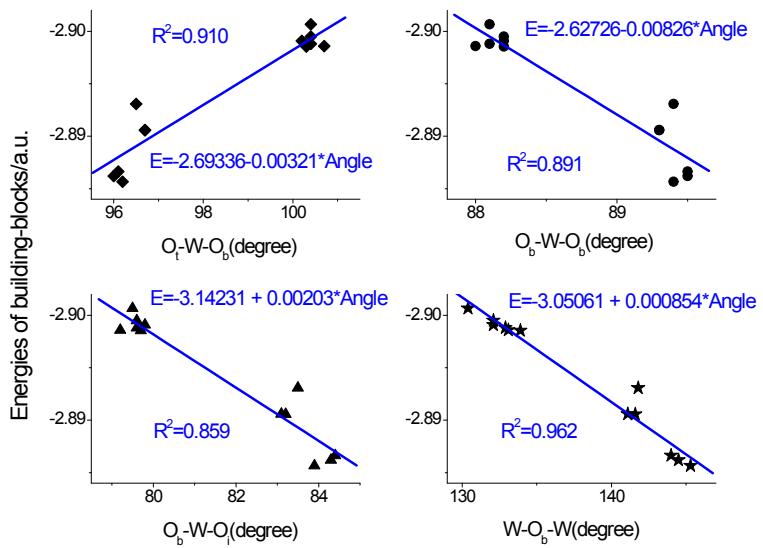
**Figure 3.** Ball-and-stick representations of  $\gamma^*$   $[(\text{IO}_6)\text{W}_{18}\text{O}_{56}\text{H}_3]^{6-}$ .



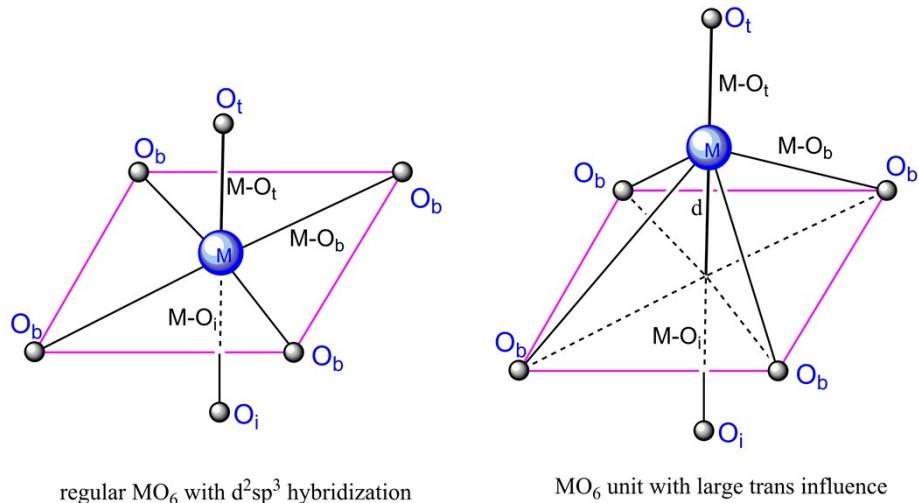
**Figure 4.** Building-block energies (a.u.) of two kinds of anions. Negative value denotes favorable energy.



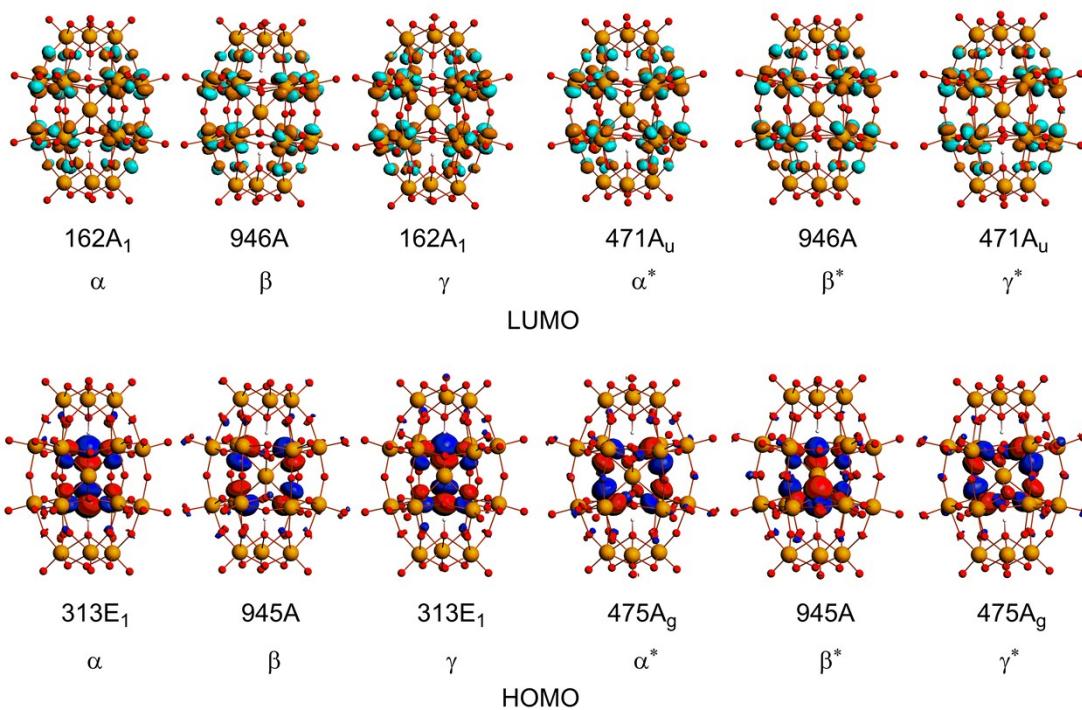
**Figure 5.** Dependences of building-block energies (a.u., absolute values) on four kinds of structural parameters of two species. Negative value denotes favorable energy.



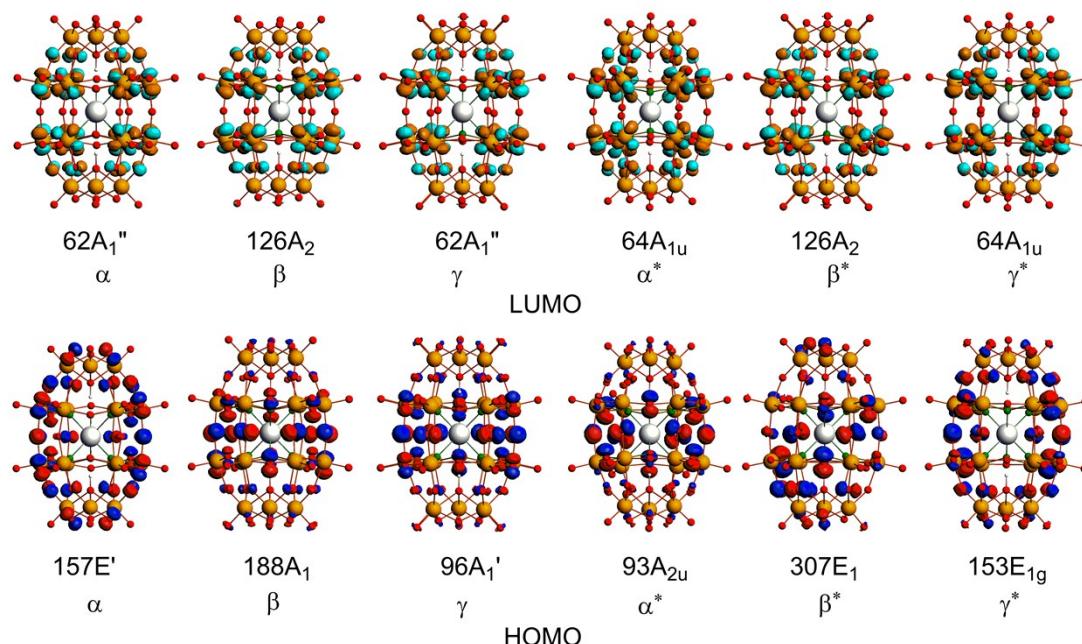
**Figure 6.** Dependences of building-block energies (a.u., absolute values) on four kinds of structural bond angles for  $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ . Negative value denotes favorable energy.



**Figure 7.** Model of building-block  $\{\text{MO}_6\}$  ( $\text{M}$  = metal) for Wells-Dawson anions. Three types of oxygen atoms: terminal ( $\text{O}_t$ ), interior ( $\text{O}_i$ ), bridging ( $\text{O}_b$ ).



**Figure 8.** Spatial representation of the frontier molecular orbitals of  $\alpha$ ,  $\beta$ ,  $\gamma$   $\alpha^*$ ,  $\beta^*$ ,  $\gamma^*$   $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{9-}$ .



**Figure 9.** Spatial representation of the frontier molecular orbitals of  $\alpha$ ,  $\beta$ ,  $\gamma$   $\alpha^*$ ,  $\beta^*$ ,  $\gamma^*$   $[(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{7-}$ .

**Coordinates of  $\alpha$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{7-}$**

W	0.958110	1.659495	4.912721	O	-4.588175	2.391871	-2.216219
W	-1.916219	0.000000	4.912721	O	0.222666	5.169411	-2.216219
W	0.958110	-1.659495	4.912721	O	4.365508	2.777541	-2.216219
W	0.958110	1.659495	-4.912721	O	1.554460	0.000000	5.713185
W	0.958110	-1.659495	-4.912721	O	2.393532	1.549777	3.662405
W	-1.916219	0.000000	-4.912721	O	-2.024865	-3.507170	2.167522
W	3.100453	-1.653463	-1.879786	O	4.049731	0.000000	2.167522
W	-2.982167	1.858340	-1.879786	O	-0.777230	-1.346202	5.713185
W	-0.118286	3.511802	-1.879786	O	0.145380	2.847748	3.662405
W	3.100453	1.653463	-1.879786	O	-2.024865	3.507170	2.167522
W	-2.982167	-1.858340	-1.879786	O	-0.777230	1.346202	5.713185
W	-0.118286	-3.511802	-1.879786	O	1.609775	-2.788213	1.504823
W	-2.982167	1.858340	1.879786	O	1.609775	2.788213	1.504823
W	3.100453	-1.653463	1.879786	O	-2.994529	2.174882	0.000000
W	3.100453	1.653463	1.879786	O	-2.538912	1.297971	3.662405
W	-0.118286	3.511802	1.879786	O	0.145380	-2.847748	3.662405
W	-0.118286	-3.511802	1.879786	O	-0.386239	-3.680779	0.000000
W	-2.982167	-1.858340	1.879786	O	2.393532	-1.549777	3.662405
O	-0.777230	1.346202	-5.713185	O	-2.538912	-1.297971	3.662405
O	0.145380	2.847748	-3.662405	O	-0.386239	3.680779	0.000000
O	-2.024865	-3.507170	-2.167522	O	-3.219551	0.000000	1.504823
O	-2.024865	3.507170	-2.167522	O	-4.588175	2.391871	2.216219
O	-0.777230	-1.346202	-5.713185	O	-3.195824	0.000000	6.079495
O	2.393532	1.549777	-3.662405	O	1.597912	2.767665	6.079495
O	4.049731	0.000000	-2.167522	O	1.597912	-2.767665	6.079495
O	1.554460	0.000000	-5.713185	O	-4.588175	-2.391871	2.216219
O	-3.219551	0.000000	-1.504823	O	0.222666	-5.169411	2.216219
O	1.609775	2.788213	-1.504823	O	4.365508	-2.777541	2.216219
O	3.380767	-1.505897	0.000000	O	4.365508	2.777541	2.216219
O	2.393532	-1.549777	-3.662405	O	0.222666	5.169411	2.216219
O	-2.538912	-1.297971	-3.662405	Na	0.000000	0.000000	0.000000
O	-2.994529	-2.174882	0.000000	H	0.000000	0.000000	2.750361
O	-2.538912	1.297971	-3.662405	H	0.000000	0.000000	-2.750361
O	0.145380	-2.847748	-3.662405	O	0.000000	0.000000	3.738013
O	3.380767	1.505897	0.000000	F	-0.827104	-1.432586	1.510124
O	1.609775	-2.788213	-1.504823	F	1.654208	0.000000	1.510124
O	4.365508	-2.777541	-2.216219	F	-0.827104	1.432586	1.510124
O	1.597912	-2.767665	-6.079495	O	0.000000	0.000000	-3.738013
O	1.597912	2.767665	-6.079495	F	-0.827104	-1.432586	-1.510124
O	-3.195824	0.000000	-6.079495	F	-0.827104	1.432586	-1.510124
O	0.222666	-5.169411	-2.216219	F	1.654208	0.000000	-1.510124

O	-4.588175	-2.391871	-2.216219				
<b>Coordinates of <math>\beta</math>-[<math>(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2</math>]<math>^{7-}</math></b>							
W	1.914768	0.000000	4.920087	O	4.594361	2.374748	-2.249190
W	-0.957384	1.658238	4.920087	O	4.594361	-2.374748	-2.249190
W	-0.957384	-1.658238	4.920087	O	-0.240588	-5.166207	-2.249190
W	0.958219	-1.659684	-4.930618	O	0.776170	-1.344365	5.725171
W	-1.916438	0.000000	-4.930618	O	2.529066	-1.304103	3.671569
W	0.958219	1.659684	-4.930618	O	-4.053341	0.000000	2.152769
W	0.116508	3.517043	1.890365	O	2.026671	-3.510297	2.152769
W	0.116508	-3.517043	1.890365	O	-1.552339	0.000000	5.725171
W	2.987595	-1.859420	1.890365	O	2.529066	1.304103	3.671569
W	2.987595	1.859420	1.890365	O	2.026671	3.510297	2.152769
W	-3.104102	-1.657623	1.890365	O	0.776170	1.344365	5.725171
W	-3.104102	1.657623	1.890365	O	-1.616616	-2.800062	1.538465
W	-3.116796	-1.646302	-1.881822	O	3.233233	0.000000	1.538465
W	2.984137	1.876073	-1.881822	O	3.036189	2.135499	0.005509
W	2.984137	-1.876073	-1.881822	O	-0.135147	2.842287	3.671569
W	0.132658	-3.522375	-1.881822	O	-2.393920	-1.538184	3.671569
W	0.132658	3.522375	-1.881822	O	-3.367491	1.561667	0.005509
W	-3.116796	1.646302	-1.881822	O	-0.135147	-2.842287	3.671569
O	1.553875	0.000000	-5.729108	O	-2.393920	1.538184	3.671569
O	2.406241	-1.540498	-3.688244	O	3.036189	-2.135499	0.005509
O	-1.600090	2.771437	-1.619575	O	-1.616616	2.800062	1.538465
O	3.200179	0.000000	-1.619575	O	-0.211915	5.173429	2.243814
O	-0.776938	1.345696	-5.729108	O	-1.599630	2.770640	6.081566
O	0.130990	-2.854115	-3.688244	O	3.199259	0.000000	6.081566
O	-1.600090	-2.771437	-1.619575	O	-1.599630	-2.770640	6.081566
O	-0.776938	-1.345696	-5.729108	O	-4.374363	2.770238	2.243814
O	2.054325	3.558195	-2.037891	O	-4.374363	-2.770238	2.243814
O	2.054325	-3.558195	-2.037891	O	-0.211915	-5.173429	2.243814
O	-3.367491	-1.561667	0.005509	O	4.586278	-2.403190	2.243814
O	-2.537231	-1.313617	-3.688244	O	4.586278	2.403190	2.243814
O	0.130990	2.854115	-3.688244	Na	0.000000	0.000000	0.004319
O	0.331302	3.697167	0.005509	H	0.000000	0.000000	2.755531
O	2.406241	1.540498	-3.688244	H	0.000000	0.000000	-2.759684
O	-2.537231	1.313617	-3.688244	O	0.000000	0.000000	3.743145
O	0.331302	-3.697167	0.005509	F	-1.660547	0.000000	1.507887
O	-4.108650	0.000000	-2.037891	F	0.830273	-1.438075	1.507887
O	-4.353772	-2.791459	-2.249190	F	0.830273	1.438075	1.507887
O	-3.192819	0.000000	-6.100087	O	0.000000	0.000000	-3.746952
O	1.596409	-2.765062	-6.100087	F	0.835108	1.446450	-1.485053
O	1.596409	2.765062	-6.100087	F	0.835108	-1.446450	-1.485053
O	-4.353772	2.791459	-2.249190	F	-1.670217	0.000000	-1.485053

O	-0.240588	5.166207	-2.249190	
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### Coordinates of $\gamma$ -[(NaF<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>7-</sup>

W	0.960017	-1.662798	4.942857	O	-0.221509	5.176934	-2.264483
W	0.960017	1.662798	4.942857	O	4.594111	2.396635	-2.264483
W	-1.920034	0.000000	4.942857	O	4.594111	-2.396635	-2.264483
W	0.960017	-1.662798	-4.942857	O	-0.221509	-5.176934	-2.264483
W	-1.920034	0.000000	-4.942857	O	-0.778347	-1.348136	5.733221
W	0.960017	1.662798	-4.942857	O	0.148433	-2.869731	3.703276
W	2.991025	1.877745	1.894332	O	-1.608814	2.786547	1.681320
W	0.130663	-3.529176	1.894332	O	-1.608814	-2.786547	1.681320
W	-3.121687	1.651431	1.894332	O	-0.778347	1.348136	5.733221
W	-3.121687	-1.651431	-1.894332	O	2.411044	-1.563412	3.703276
W	0.130663	3.529176	-1.894332	O	3.217628	0.000000	1.681320
W	2.991025	-1.877745	-1.894332	O	1.556693	0.000000	5.733221
W	-3.121687	-1.651431	1.894332	O	-4.110793	0.000000	2.008922
W	2.991025	-1.877745	1.894332	O	2.055396	-3.560051	2.008922
W	0.130663	3.529176	1.894332	O	3.071855	2.068549	0.000000
W	0.130663	-3.529176	-1.894332	O	2.411044	1.563412	3.703276
W	-3.121687	1.651431	-1.894332	O	-2.559476	1.306319	3.703276
W	2.991025	1.877745	-1.894332	O	-3.327344	1.626030	0.000000
O	1.556693	0.000000	-5.733221	O	-2.559476	-1.306319	3.703276
O	2.411044	-1.563412	-3.703276	O	0.148433	2.869731	3.703276
O	-1.608814	2.786547	-1.681320	O	3.071855	-2.068549	0.000000
O	3.217628	0.000000	-1.681320	O	2.055396	3.560051	2.008922
O	-0.778347	1.348136	-5.733221	O	4.594111	2.396635	2.264483
O	0.148433	-2.869731	-3.703276	O	1.592635	2.758526	6.124094
O	-1.608814	-2.786547	-1.681320	O	1.592635	-2.758526	6.124094
O	-0.778347	-1.348136	-5.733221	O	-3.185271	0.000000	6.124094
O	2.055396	3.560051	-2.008922	O	-0.221509	5.176934	2.264483
O	2.055396	-3.560051	-2.008922	O	-4.372602	2.780299	2.264483
O	-3.327344	-1.626030	0.000000	O	-4.372602	-2.780299	2.264483
O	-2.559476	-1.306319	-3.703276	O	-0.221509	-5.176934	2.264483
O	0.148433	2.869731	-3.703276	O	4.594111	-2.396635	2.264483
O	0.255489	3.694579	0.000000	Na	0.000000	0.000000	0.000000
O	2.411044	1.563412	-3.703276	H	0.000000	0.000000	2.767828
O	-2.559476	1.306319	-3.703276	H	0.000000	0.000000	-2.767828
O	0.255489	-3.694579	0.000000	O	0.000000	0.000000	3.755188
O	-4.110793	0.000000	-2.008922	F	-1.673418	0.000000	1.494814
O	-4.372602	-2.780299	-2.264483	F	0.836709	-1.449223	1.494814
O	-3.185271	0.000000	-6.124094	F	0.836709	1.449223	1.494814
O	1.592635	-2.758526	-6.124094	O	0.000000	0.000000	-3.755188
O	1.592635	2.758526	-6.124094	F	-1.673418	0.000000	-1.494814
O	-4.372602	2.780299	-2.264483	F	0.836709	1.449223	-1.494814
				F	0.836709	-1.449223	-1.494814

**Coordinates of  $\alpha^*-\text{[NaF}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{7-}$**

W	-1.855764	-3.017190	1.894635	O	2.713286	4.435527	2.312301
W	1.685081	3.115734	1.894635	O	-2.713286	4.435527	2.312301
W	-1.685081	3.115734	1.894635	O	-5.197922	0.132011	2.312301
W	-3.540845	-0.098544	1.894635	O	0.000000	-1.539443	-5.730695
W	3.540845	-0.098544	1.894635	O	-1.476890	-2.399614	-3.668120
W	1.855764	-3.017190	1.894635	O	3.512711	2.028065	-1.979760
W	-1.651294	0.953375	4.906288	O	0.000000	-4.056130	-1.979760
W	0.000000	-1.906750	4.906288	O	1.333197	0.769722	-5.730695
W	1.651294	0.953375	4.906288	O	-2.816572	-0.079218	-3.668120
W	-1.855764	3.017190	-1.894635	O	-3.512711	2.028065	-1.979760
W	1.685081	-3.115734	-1.894635	O	-1.333197	0.769722	-5.730695
W	-1.685081	-3.115734	-1.894635	O	2.904556	-1.676946	-1.713950
W	-3.540845	0.098544	-1.894635	O	-2.904556	-1.676946	-1.713950
W	3.540845	0.098544	-1.894635	O	1.874463	-3.246665	0.000000
W	1.855764	3.017190	-1.894635	O	-1.339681	2.478831	-3.668120
W	-1.651294	-0.953375	-4.906288	O	2.816572	-0.079218	-3.668120
W	0.000000	1.906750	-4.906288	O	3.748926	0.000000	0.000000
W	1.651294	-0.953375	-4.906288	O	1.476890	-2.399614	-3.668120
O	0.000000	1.539443	5.730695	O	1.339681	2.478831	-3.668120
O	-1.476890	2.399614	3.668120	O	-1.874463	3.246665	0.000000
O	3.512711	-2.028065	1.979760	O	0.000000	3.353892	-1.713950
O	0.000000	4.056130	1.979760	O	-2.484636	4.567538	-2.312301
O	1.333197	-0.769722	5.730695	O	0.000000	3.214396	-6.041210
O	-2.816572	0.079218	3.668120	O	-2.783749	-1.607198	-6.041210
O	-3.512711	-2.028065	1.979760	O	2.783749	-1.607198	-6.041210
O	-1.333197	-0.769722	5.730695	O	2.484636	4.567538	-2.312301
O	2.904556	1.676946	1.713950	O	5.197922	-0.132011	-2.312301
O	-2.904556	1.676946	1.713950	O	2.713286	-4.435527	-2.312301
O	-1.874463	-3.246665	0.000000	O	-2.713286	-4.435527	-2.312301
O	-1.339681	-2.478831	3.668120	O	-5.197922	-0.132011	-2.312301
O	2.816572	0.079218	3.668120	Na	0.000000	0.000000	0.000000
O	1.874463	3.246665	0.000000	H	0.000000	0.000000	-2.736461
O	1.476890	2.399614	3.668120	H	0.000000	0.000000	2.736461
O	1.339681	-2.478831	3.668120	O	0.000000	0.000000	-3.723586
O	-3.748926	0.000000	0.000000	O	0.000000	0.000000	3.723586
O	0.000000	-3.353892	1.713950	F	1.457967	0.841757	-1.441249
O	-2.484636	-4.567538	2.312301	F	0.000000	-1.683515	-1.441249
O	0.000000	-3.214396	6.041210	F	-1.457967	0.841757	-1.441249
O	-2.783749	1.607198	6.041210	F	1.457967	-0.841757	1.441249
O	2.783749	1.607198	6.041210	F	0.000000	1.683515	1.441249
O	2.484636	-4.567538	2.312301	F	-1.457967	-0.841757	1.441249
O	5.197922	0.132011	2.312301				

**Coordinates of  $\beta^*-\text{[NaF}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{7-}$**

W	0.955590	-1.655130	4.923841	O	4.584710	2.497622	-2.251879
W	0.955590	1.655130	4.923841	O	4.584710	-2.497622	-2.251879
W	-1.911179	0.000000	4.923841	O	-0.129351	-5.219286	-2.251879
W	0.968661	-1.677770	-4.936068	O	-0.772248	-1.337572	5.738286
W	-1.937322	0.000000	-4.936068	O	0.102920	-2.834810	3.684659
W	0.968661	1.677770	-4.936068	O	-2.027200	3.511214	2.053008
W	-3.130518	-1.679598	-1.887998	O	-2.027200	-3.511214	2.053008
W	3.019834	1.871309	-1.887998	O	-0.772248	1.337572	5.738286
W	3.019834	-1.871309	-1.887998	O	2.403558	-1.506536	3.684659
W	0.110684	-3.550907	-1.887998	O	4.054401	0.000000	2.053008
W	0.110684	3.550907	-1.887998	O	1.544495	0.000000	5.738286
W	-3.130518	1.679598	-1.887998	O	-3.328471	0.000000	1.672275
W	3.107429	1.673558	1.902983	O	1.664236	-2.882540	1.672275
W	-3.003058	-1.854333	1.902983	O	3.238259	1.734335	0.001820
W	-0.104370	-3.527891	1.902983	O	2.403558	1.506536	3.684659
W	3.107429	-1.673558	1.902983	O	-2.506477	1.328274	3.684659
W	-3.003058	1.854333	1.902983	O	-3.121108	1.937247	0.001820
W	-0.104370	3.527891	1.902983	O	-2.506477	-1.328274	3.684659
O	1.572728	0.000000	-5.687008	O	0.102920	2.834810	3.684659
O	2.430073	-1.669996	-3.709429	O	3.238259	-1.734335	0.001820
O	-1.655041	2.866615	-1.923970	O	1.664236	2.882540	1.672275
O	3.310082	0.000000	-1.923970	O	4.419411	2.731017	2.270090
O	-0.786364	1.362023	-5.687008	O	1.603000	2.776477	6.072922
O	0.231222	-2.939503	-3.709429	O	1.603000	-2.776477	6.072922
O	-1.655041	-2.866615	-1.923970	O	-3.205999	0.000000	6.072922
O	-0.786364	-1.362023	-5.687008	O	0.155425	5.192831	2.270090
O	2.041271	3.535585	-1.794070	O	-4.574836	2.461814	2.270090
O	2.041271	-3.535585	-1.794070	O	-4.574836	-2.461814	2.270090
O	-3.121108	-1.937247	0.001820	O	0.155425	-5.192831	2.270090
O	-2.661295	-1.269507	-3.709429	O	4.419411	-2.731017	2.270090
O	0.231222	2.939503	-3.709429	Na	0.000000	0.000000	-0.003370
O	-0.117151	3.671582	0.001820	H	0.000000	0.000000	2.754635
O	2.430073	1.669996	-3.709429	H	0.000000	0.000000	-2.744829
O	-2.661295	1.269507	-3.709429	O	0.000000	0.000000	3.742513
O	-0.117151	-3.671582	0.001820	F	-0.831849	1.440805	1.491821
O	-4.082542	0.000000	-1.794070	F	-0.831849	-1.440805	1.491821
O	-4.455359	-2.721664	-2.251879	F	1.663699	0.000000	1.491821
O	-3.148973	0.000000	-6.170885	O	0.000000	0.000000	-3.732565
O	1.574487	-2.727091	-6.170885	F	0.835642	1.447374	-1.479608
O	1.574487	2.727091	-6.170885	F	0.835642	-1.447374	-1.479608
O	-4.455359	2.721664	-2.251879	F	-1.671283	0.000000	-1.479608
O	-0.129351	5.219286	-2.251879				

**Coordinates of  $\gamma^*-\text{[(NaF}_6\text{)W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{7-}$**

W	0.000000	-1.933342	4.948717	O	-2.739970	4.433372	-2.246240
W	1.674324	0.966671	4.948717	O	2.739970	4.433372	-2.246240
W	-1.674324	0.966671	4.948717	O	5.209398	0.156198	-2.246240
W	1.674324	-0.966671	-4.948717	O	2.469427	-4.589570	-2.246240
W	-1.674324	-0.966671	-4.948717	O	-1.357566	-0.783791	5.710226
W	0.000000	1.933342	-4.948717	O	-1.280934	-2.637115	3.720238
W	3.542267	0.117864	1.899047	O	0.000000	3.290738	1.870928
W	-1.873207	3.008761	1.899047	O	-2.849863	-1.645369	1.870928
W	-1.669060	-3.126625	1.899047	O	0.000000	1.567582	5.710226
W	-1.873207	-3.008761	-1.899047	O	1.280934	-2.637115	3.720238
W	-1.669060	3.126625	-1.899047	O	2.849863	-1.645369	1.870928
W	3.542267	-0.117864	-1.899047	O	1.357566	-0.783791	5.710226
W	1.669060	-3.126625	1.899047	O	-3.546526	2.047588	1.870591
W	1.873207	3.008761	1.899047	O	0.000000	-4.095175	1.870591
W	-3.542267	0.117864	1.899047	O	3.639289	0.000000	0.000000
W	1.873207	-3.008761	-1.899047	O	2.924275	0.209236	3.720238
W	1.669060	3.126625	-1.899047	O	-1.643341	2.427879	3.720238
W	-3.542267	-0.117864	-1.899047	O	-1.819644	3.151716	0.000000
O	1.357566	0.783791	-5.710226	O	-2.924275	0.209236	3.720238
O	2.924275	-0.209236	-3.720238	O	1.643341	2.427879	3.720238
O	-2.849863	1.645369	-1.870928	O	1.819644	-3.151716	0.000000
O	2.849863	1.645369	-1.870928	O	3.546526	2.047588	1.870591
O	-1.357566	0.783791	-5.710226	O	5.209398	-0.156198	2.246240
O	1.643341	-2.427879	-3.720238	O	2.734439	1.578729	6.171442
O	0.000000	-3.290738	-1.870928	O	0.000000	-3.157459	6.171442
O	0.000000	-1.567582	-5.710226	O	-2.734439	1.578729	6.171442
O	0.000000	4.095175	-1.870591	O	2.469427	4.589570	2.246240
O	3.546526	-2.047588	-1.870591	O	-2.469427	4.589570	2.246240
O	-3.639289	0.000000	0.000000	O	-5.209398	-0.156198	2.246240
O	-1.643341	-2.427879	-3.720238	O	-2.739970	-4.433372	2.246240
O	-1.280934	2.637115	-3.720238	O	2.739970	-4.433372	2.246240
O	1.819644	3.151716	0.000000	Na	0.000000	0.000000	0.000000
O	1.280934	2.637115	-3.720238	H	0.000000	0.000000	2.763640
O	-2.924275	-0.209236	-3.720238	H	0.000000	0.000000	-2.763640
O	-1.819644	-3.151716	0.000000	O	0.000000	0.000000	3.751524
O	-3.546526	-2.047588	-1.870591	F	-1.444585	0.834031	1.501307
O	-2.469427	-4.589570	-2.246240	F	0.000000	-1.668063	1.501307
O	-2.734439	-1.578729	-6.171442	F	1.444585	0.834031	1.501307
O	2.734439	-1.578729	-6.171442	O	0.000000	0.000000	-3.751524
O	0.000000	3.157459	-6.171442	F	-1.444585	-0.834031	-1.501307
O	-5.209398	0.156198	-2.246240	F	0.000000	1.668063	-1.501307
				F	1.444585	-0.834031	-1.501307

**Coordinates of  $\alpha$ -[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{9-}$**

W	-1.046741	1.595722	-4.925633	O	0.388396	-3.793250	0.032461
W	1.905306	0.108643	-4.925633	O	3.090853	2.232986	0.032461
W	-0.858565	-1.704365	-4.925633	O	0.388396	3.793250	-0.032461
W	-0.858565	1.704365	4.925633	O	-3.479249	-1.560264	-0.032461
W	-1.046741	-1.595722	4.925633	O	3.090853	-2.232986	-0.032461
W	1.905306	-0.108643	4.925633	O	-3.479249	1.560264	0.032461
W	0.116903	3.468585	1.773329	O	-1.682632	-2.727480	6.086910
W	2.945431	-1.835533	1.773329	O	-1.520751	2.820941	6.086910
W	-3.062334	-1.633052	1.773329	O	3.203382	-0.093462	6.086910
W	0.116903	-3.468585	-1.773329	O	-1.558971	0.041192	5.754815
W	2.945431	1.835533	-1.773329	O	0.743812	-1.370705	5.754815
W	-3.062334	1.633052	-1.773329	O	0.815159	1.329513	5.754815
W	-3.029284	-1.588619	-1.936234	O	-2.339476	1.516414	3.690002
W	2.890426	-1.829127	-1.936234	O	-0.123082	2.821798	3.646520
W	0.138858	3.417746	-1.936234	O	-2.382207	-1.517491	3.646520
W	-3.029284	1.588619	1.936234	O	2.505290	-1.304306	3.646520
W	2.890426	1.829127	1.936234	O	2.482991	1.267839	3.690002
W	0.138858	-3.417746	1.936234	O	-0.143515	-2.784253	3.690002
O	3.203382	0.093462	-6.086910	O	-4.313498	-2.760316	2.229931
O	-1.682632	2.727480	-6.086910	O	-0.189029	-5.093475	2.289567
O	-1.520751	-2.820941	-6.086910	O	4.547253	-2.355441	2.229931
O	0.815159	-1.329513	-5.754815	O	4.505593	2.383034	2.289567
O	-1.558971	-0.041192	-5.754815	O	-0.233755	5.115757	2.229931
O	0.743812	1.370705	-5.754815	O	-4.316564	2.710441	2.289567
O	-2.339476	-1.516414	-3.690002	O	2.035912	-3.485324	2.186972
O	2.482991	-1.267839	-3.690002	O	2.000423	3.505814	2.186972
O	2.505290	1.304306	-3.646520	O	-4.036335	-0.020489	2.186972
O	-0.123082	-2.821798	-3.646520	O	3.237542	0.008887	1.468747
O	-2.382207	1.517491	-3.646520	O	-1.626467	2.799350	1.468747
O	-0.143515	2.784253	-3.690002	O	-1.611075	-2.808237	1.468747
O	4.547253	2.355441	-2.229931	O	0.000000	0.000000	3.778274
O	4.505593	-2.383034	-2.289567	O	0.000000	0.000000	-3.778274
O	-0.233755	-5.115757	-2.229931	O	0.808126	-1.391492	1.356351
O	-4.316564	-2.710441	-2.289567	O	0.801005	1.395603	1.356351
O	-4.313498	2.760316	-2.229931	O	-1.609130	-0.004111	1.356351
O	-0.189029	5.093475	-2.289567	O	0.801005	-1.395603	-1.356351
O	2.000423	-3.505814	-2.186972	O	-1.609130	0.004111	-1.356351
O	-4.036335	0.020489	-2.186972	O	0.808126	1.391492	-1.356351
O	2.035912	3.485324	-2.186972	Sb	0.000000	0.000000	0.000000
O	3.237542	-0.008887	-1.468747	H	0.000000	0.000000	2.780802
O	-1.626467	-2.799350	-1.468747	H	0.000000	0.000000	-2.780802
O	-1.611075	2.808237	-1.468747				

**Coordinates of  $\beta$ -[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{9-}$**

W	1.902671	0.047538	4.942029	O	-0.197647	3.824295	0.036653
W	-0.992725	1.624724	4.942743	O	-3.212833	-2.083064	0.036352
W	-0.911108	-1.671965	4.942654	O	3.539134	1.453008	-0.041771
W	-2.970802	-1.687164	1.943471	O	-3.026226	2.337515	-0.040481
W	0.024663	3.416012	1.943807	O	-0.511835	-3.791030	-0.040623
W	2.946277	-1.729498	1.943936	O	3.409865	-1.741408	0.036916
W	-0.300624	-3.467486	1.768402	O	-3.214596	0.141422	1.534176
W	3.153345	1.473684	1.767213	O	1.484171	-2.854785	1.533609
W	-2.852816	1.993756	1.768562	O	1.730122	2.713009	1.533041
W	0.915653	1.674357	-4.930013	O	-1.891806	3.621137	2.075587
W	0.991613	-1.630052	-4.929435	O	-2.190168	-3.449533	2.076165
W	-1.908022	-0.043575	-4.929820	O	4.081640	-0.172058	2.075658
W	-2.814231	1.944042	-1.951285	O	0.473424	5.053502	2.339661
W	3.091214	1.465559	-1.952078	O	-4.434473	2.541101	2.262784
W	-0.276321	-3.409593	-1.950830	O	-4.613164	-2.119294	2.338479
W	-3.022576	-1.715291	-1.768247	O	0.015853	-5.110859	2.262950
W	2.996942	-1.760221	-1.767664	O	4.140565	-2.936579	2.339324
W	0.026257	3.475561	-1.767848	O	4.418272	2.569168	2.262122
O	-3.206157	0.020026	-6.088890	O	2.388234	-1.389389	3.713236
O	1.586262	-2.787986	-6.087178	O	0.008356	2.762005	3.712239
O	1.620660	2.767781	-6.088212	O	-2.397440	-1.374567	3.712802
O	-0.765562	1.359722	-5.761709	O	-0.198873	-2.802824	3.662006
O	1.559603	-0.016790	-5.760904	O	-2.328400	1.572992	3.662094
O	-0.794649	-1.342873	-5.761040	O	2.525683	1.229475	3.660871
O	0.026500	-2.782007	-3.698184	O	0.760744	-1.355246	5.781911
O	2.320852	-1.607870	-3.646925	O	-1.554110	0.018487	5.781529
O	-2.552880	-1.206041	-3.647219	O	0.793604	1.337328	5.782151
O	0.231921	2.814225	-3.647296	O	-1.582320	2.799645	6.085261
O	2.396475	1.414223	-3.699630	O	3.215951	-0.028218	6.083830
O	-2.422085	1.369314	-3.699027	O	-1.633738	-2.771029	6.084390
O	-4.638621	-2.173461	-2.241479	O	-0.000681	-0.000243	3.794956
O	-4.398990	2.574141	-2.311827	O	-0.000205	0.000376	-3.781899
O	0.437807	5.104099	-2.240742	Sb	0.000584	-0.000038	-0.001581
O	4.428279	2.523974	-2.314808	H	-0.000220	0.000755	-2.784808
O	4.200997	-2.931504	-2.240721	H	-0.001095	-0.000309	2.797499
O	-0.029586	-5.096854	-2.313165	O	-0.742452	1.432856	-1.354967
O	-1.854428	3.587169	-2.177111	O	1.612997	-0.072759	-1.355230
O	4.033790	-0.187116	-2.177104	O	-0.868922	-1.360112	-1.354831
O	-2.178805	-3.400282	-2.177647	O	-0.864420	-1.361691	1.345177
O	1.743814	2.733782	-1.486394	O	1.612260	-0.068040	1.345101
O	1.495610	-2.876961	-1.485529	O	-0.746958	1.429543	1.345154
O	-3.237974	0.142926	-1.486389				

**Coordinates of  $\gamma$ -[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ]<sup>9-</sup>**

W	1.063573	1.580456	4.946797	O	-1.599381	2.796088	-1.555646
W	-1.900502	0.130853	4.946797	O	-3.472457	1.634208	-0.041197
W	0.836929	-1.711310	4.946797	O	0.320963	-3.824340	-0.041197
W	0.836929	1.711310	-4.946797	O	0.320963	3.824340	0.041197
W	1.063573	-1.580456	-4.946797	O	-3.472457	-1.634208	0.041197
W	-1.900502	-0.130853	-4.946797	O	3.151494	2.190132	-0.041197
W	2.936508	1.882351	1.768837	O	3.151494	-2.190132	0.041197
W	-3.098418	1.601915	1.768837	O	-1.599381	-2.796088	1.555646
W	0.161909	-3.484266	1.768837	O	3.221174	0.012940	1.555646
W	-3.098418	-1.601915	-1.768837	O	-1.621793	2.783148	1.555646
W	0.161909	3.484266	-1.768837	O	-4.088120	-0.007170	2.063470
W	2.936508	-1.882351	-1.768837	O	2.050269	-3.536830	2.063470
W	2.901908	-1.803145	1.951729	O	2.037850	3.544001	2.063470
W	0.110615	3.414698	1.951729	O	-4.320816	2.739833	2.273460
W	-3.012523	-1.611554	1.951729	O	-4.260613	-2.762160	2.349929
W	2.901908	1.803145	-1.951729	O	-0.212357	-5.111853	2.273460
W	-3.012523	1.611554	-1.951729	O	4.522407	-2.308720	2.349929
W	0.110615	-3.414698	-1.951729	O	4.533173	2.372019	2.273460
O	1.701841	-2.726953	-6.092226	O	-0.261794	5.070879	2.349929
O	1.510690	2.837314	-6.092226	O	2.392248	1.482698	3.664309
O	-3.212531	-0.110361	-6.092226	O	0.111882	2.764525	3.719678
O	-0.819087	1.322396	-5.784226	O	-2.480178	1.330399	3.664309
O	1.554772	0.048152	-5.784226	O	0.087930	-2.813097	3.664309
O	-0.735685	-1.370548	-5.784226	O	2.338207	-1.479155	3.719678
O	0.087930	2.813097	-3.664309	O	-2.450090	-1.285369	3.719678
O	2.392248	-1.482698	-3.664309	O	-0.819087	-1.322396	5.784226
O	-2.480178	-1.330399	-3.664309	O	1.554772	-0.048152	5.784226
O	2.338207	1.479155	-3.719678	O	-0.735685	1.370548	5.784226
O	-2.450090	1.285369	-3.719678	O	-3.212531	0.110361	6.092226
O	0.111882	-2.764525	-3.719678	O	1.701841	2.726953	6.092226
O	-0.261794	-5.070879	-2.349929	O	1.510690	-2.837314	6.092226
O	-4.320816	-2.739833	-2.273460	O	0.000000	0.000000	3.798578
O	-4.260613	2.762160	-2.349929	O	0.000000	0.000000	-3.798578
O	-0.212357	5.111853	-2.273460	Sb	0.000000	0.000000	0.000000
O	4.522407	2.308720	-2.349929	H	0.000000	0.000000	-2.801315
O	4.533173	-2.372019	-2.273460	H	0.000000	0.000000	2.801315
O	-4.088120	0.007170	-2.063470	O	-1.617931	0.003525	-1.345127
O	2.050269	3.536830	-2.063470	O	0.812018	1.399407	-1.345127
O	2.037850	-3.544001	-2.063470	O	0.805913	-1.402932	-1.345127
O	3.221174	-0.012940	-1.555646	O	-1.617931	-0.003525	1.345127
O	-1.621793	-2.783148	-1.555646	O	0.812018	-1.399407	1.345127
				O	0.805913	1.402932	1.345127

**Coordinates of  $\alpha^*-\text{[}(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^9-$**

W	1.689712	0.872860	4.905647	O	-2.507764	4.464173	-2.396083
W	-1.600950	1.026942	4.905774	O	2.416487	4.535071	-2.325756
W	-0.089164	-1.899493	4.905338	O	5.120875	-0.060587	-2.396060
W	0.089164	1.899493	-4.905338	O	1.325456	-0.792097	5.756788
W	1.600950	-1.026942	-4.905774	O	2.781756	0.086159	3.631304
W	-1.689712	-0.872860	-4.905647	O	-2.897089	1.633818	1.662063
W	1.859290	-2.912960	1.940802	O	0.033499	-3.325340	1.661469
W	3.502244	-0.070639	1.770251	O	-1.348575	-0.751738	5.757449
W	-3.453172	-0.153095	1.941083	O	1.419755	2.354562	3.681321
W	1.593850	3.066926	1.941072	O	2.864529	1.692386	1.661880
W	-1.812301	-2.996690	1.769865	O	0.023104	1.543896	5.757512
W	-1.689275	3.067577	1.770525	O	-3.494182	-2.070637	1.990076
W	1.689275	-3.067577	-1.770525	O	3.540655	-1.990200	1.989747
W	3.453172	0.153095	-1.941083	O	1.931673	3.394263	0.039734
W	-3.502244	0.070639	-1.770251	O	-1.465192	2.366232	3.631868
W	-1.593850	-3.066926	-1.941072	O	-1.316434	-2.451430	3.630988
W	-1.859290	2.912960	-1.940802	O	-3.906122	-0.024771	0.039789
W	1.812301	2.996690	-1.769865	O	1.329655	-2.406173	3.681104
O	-1.325456	0.792097	-5.756788	O	-2.749581	0.052110	3.681521
O	-1.329655	2.406173	-3.681104	O	3.906122	0.024771	-0.039789
O	-2.864529	-1.692386	-1.661880	O	-0.046422	4.060571	1.989385
O	-0.033499	3.325340	-1.661469	O	2.612157	4.404608	2.396221
O	-0.023104	-1.543896	-5.757512	O	-2.763247	1.666957	6.034248
O	1.316434	2.451430	-3.630988	O	2.825300	1.559617	6.033524
O	2.897089	-1.633818	-1.662063	O	-0.061301	-3.227025	6.032726
O	1.348575	0.751738	-5.757449	O	-2.720350	4.359081	2.325932
O	-3.540655	1.990200	-1.989747	O	-5.120875	0.060587	2.396060
O	3.494182	2.070637	-1.990076	O	-2.416487	-4.535071	2.325756
O	-1.931673	-3.394263	-0.039734	O	2.507764	-4.464173	2.396083
O	2.749581	-0.052110	-3.681521	O	5.136207	0.175820	2.326686
O	-1.419755	-2.354562	-3.681321	O	-0.000140	0.000388	3.753473
O	-1.973891	3.369280	-0.039370	O	0.000140	-0.000388	-3.753473
O	-2.781756	-0.086159	-3.631304	Sb	0.000000	0.000000	0.000000
O	1.465192	-2.366232	-3.631868	H	-0.000276	0.000773	2.761559
O	1.973891	-3.369280	0.039370	H	0.000276	-0.000773	-2.761559
O	0.046422	-4.060571	-1.989385	O	-1.444311	-0.854636	1.227813
O	2.720350	-4.359081	-2.325932	O	1.462908	-0.822562	1.227636
O	2.763247	-1.666957	-6.034248	O	-0.018170	1.677935	1.228170
O	0.061301	3.227025	-6.032726	O	0.018170	-1.677935	-1.228170
O	-2.825300	-1.559617	-6.033524	O	-1.462908	0.822562	-1.227636
O	-2.612157	-4.404608	-2.396221	O	1.444311	0.854636	-1.227813
O	-5.136207	-0.175820	-2.326686				

**Coordinates of  $\beta^*-\text{[NaF}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{9-}$**

W	1.694756	0.865880	4.922483	O	-2.460279	4.507438	-2.373526
W	-1.597351	1.034940	4.922819	O	2.465860	4.529914	-2.295511
W	-0.097578	-1.899912	4.922757	O	5.134267	-0.124267	-2.374699
W	1.593070	1.072920	-4.938626	O	1.325331	-0.797042	5.770362
W	0.132709	-1.915449	-4.939174	O	2.788471	0.091420	3.645550
W	-1.725253	0.843606	-4.938777	O	-2.881511	1.631166	1.639110
W	1.849408	-2.900850	1.953877	O	0.027384	-3.309811	1.638663
W	3.497661	-0.080167	1.780515	O	-1.353098	-0.748054	5.770855
W	-3.437949	-0.151675	1.954399	O	1.435953	2.349946	3.696312
W	1.587561	3.052453	1.953318	O	2.852981	1.678959	1.638399
W	-1.818173	-2.988728	1.780923	O	0.028291	1.546642	5.770678
W	-1.679702	3.068688	1.780898	O	-3.493276	-2.066776	2.043798
W	1.654606	-3.103133	-1.764211	O	3.535866	-1.991459	2.043771
W	3.466302	0.122810	-1.938892	O	1.852146	3.393624	0.040739
W	-3.515270	0.118707	-1.763729	O	-1.473234	2.369742	3.645923
W	-1.625787	-3.063120	-1.938456	O	-1.314870	-2.459792	3.645498
W	-1.839759	2.939318	-1.938194	O	-3.865365	-0.092903	0.040908
W	1.861010	2.983610	-1.763358	O	1.316800	-2.417649	3.696183
O	-0.060678	1.566102	-5.742206	O	-2.753620	0.068532	3.696886
O	1.554132	2.409082	-3.661046	O	3.876444	-0.054213	-0.033076
O	-2.855663	-1.655524	-1.807898	O	-0.043651	4.057414	2.043541
O	-0.005714	3.299158	-1.807486	O	2.629478	4.383928	2.375414
O	-1.325944	-0.835167	-5.742051	O	-2.755969	1.674198	6.054846
O	2.817811	0.204486	-3.712582	O	2.828051	1.551285	6.053350
O	2.861406	-1.645547	-1.808188	O	-0.070870	-3.222971	6.054884
O	1.386460	-0.729653	-5.742611	O	-2.732641	4.350871	2.316788
O	-3.550030	2.036562	-1.853562	O	-5.111957	0.084279	2.376168
O	3.539196	2.055016	-1.854591	O	-2.401965	-4.541860	2.316977
O	-1.984701	-3.330505	-0.032957	O	2.481685	-4.468781	2.376372
O	1.308952	-2.549957	-3.661686	O	5.134500	0.190622	2.316924
O	-2.863478	0.141006	-3.661381	O	-0.000116	0.000592	3.768963
O	-1.892442	3.382652	-0.032603	O	0.000087	0.000054	-3.770459
O	-1.585790	2.337246	-3.711511	Sb	-0.000102	-0.000164	-0.003801
O	-1.231569	-2.541736	-3.712219	H	-0.000233	0.000789	2.775906
O	2.012835	-3.300960	0.040536	H	0.000327	-0.000230	-2.777691
O	0.011025	-4.092063	-1.854563	O	-1.438990	-0.845737	1.248927
O	2.691975	-4.399709	-2.296611	O	1.451842	-0.822677	1.248779
O	0.134072	-3.183838	-6.132392	O	-0.013560	1.668720	1.249108
O	2.691384	1.708920	-6.131019	O	0.006755	-1.674268	-1.233559
O	-2.824322	1.477262	-6.131427	O	-1.453595	0.830698	-1.233219
O	-2.674425	-4.383871	-2.374165	O	1.446772	0.842041	-1.233262
O	-5.157143	-0.130399	-2.296546				

### Coordinates of $\gamma^*-\text{[}( \text{SbO}_6 )\text{W}_{18}\text{O}_{54}(\text{OH})_2 ]^{9-}$

W	1.728650	-0.828568	4.952941	O	-5.150533	-0.157932	-2.300946
W	-0.147678	1.911552	4.953674	O	-2.439161	4.501709	-2.373740
W	-1.582222	-1.083358	4.953291	O	2.438635	4.537156	-2.299775
W	1.582222	1.083358	-4.953291	O	5.118878	-0.139988	-2.375069
W	0.147678	-1.911552	-4.953674	O	0.065695	-1.563543	5.763942
W	-1.728650	0.828568	-4.952941	O	1.566386	-2.331722	3.727284
W	1.837318	-2.919957	1.959589	O	-2.849147	1.637343	1.773420
W	3.513689	-0.118824	1.766396	O	0.007435	-3.283401	1.772689
W	-3.448426	-0.129171	1.960645	O	-1.387168	0.724239	5.764454
W	1.611722	3.051212	1.960566	O	2.853075	-0.124594	3.670444
W	-1.860154	-2.981208	1.766166	O	2.842611	1.649541	1.773426
W	-1.652600	3.102341	1.766907	O	1.321033	0.838658	5.763980
W	1.652600	-3.102341	-1.766907	O	-3.537481	-2.059586	1.906423
W	3.448426	0.129171	-1.960645	O	3.553877	-2.032390	1.905792
W	-3.513689	0.118824	-1.766396	O	1.908747	3.349696	0.039290
W	-1.611722	-3.051212	-1.960566	O	1.236823	2.522925	3.728940
W	-1.837318	2.919957	-1.959589	O	-2.803682	-0.190192	3.728767
W	1.860154	2.981208	-1.766166	O	-3.856451	-0.022111	0.039206
O	-0.065695	1.563543	-5.763942	O	-1.535174	-2.408462	3.670559
O	1.535174	2.408462	-3.670559	O	-1.318424	2.533632	3.671017
O	-2.842611	-1.649541	-1.773426	O	3.856451	0.022111	-0.039206
O	-0.007435	3.283401	-1.772689	O	-0.015408	4.093710	1.906266
O	-1.321033	-0.838658	-5.763980	O	2.680003	4.363946	2.373984
O	2.803682	0.190192	-3.728767	O	-0.146105	3.189957	6.135964
O	2.849147	-1.637343	-1.773420	O	2.835121	-1.469632	6.134602
O	1.387168	-0.724239	-5.764454	O	-2.690277	-1.721893	6.135095
O	-3.553877	2.032390	-1.905792	O	-2.710818	4.381672	2.300229
O	3.537481	2.059586	-1.906423	O	-5.118878	0.139988	2.375069
O	-1.908747	-3.349696	-0.039290	O	-2.438635	-4.537156	2.299775
O	1.318424	-2.533632	-3.671017	O	2.439161	-4.501709	2.373740
O	-2.853075	0.124594	-3.670444	O	5.150533	0.157932	2.300946
O	-1.947126	3.328044	-0.038570	O	-0.000520	0.000252	3.786553
O	-1.566386	2.331722	-3.727284	O	0.000520	-0.000252	-3.786553
O	-1.236823	-2.522925	-3.728940	Sb	0.000000	0.000000	0.000000
O	1.947126	-3.328044	0.038570	H	-0.000788	0.000648	2.793001
O	0.015408	-4.093710	-1.906266	H	0.000788	-0.000648	-2.793001
O	2.710818	-4.381672	-2.300229	O	-1.443193	-0.837643	1.248279
O	0.146105	-3.189957	-6.135964	O	1.448624	-0.829324	1.247721
O	2.690277	1.721893	-6.135095	O	-0.004690	1.669236	1.248571
O	-2.835121	1.469632	-6.134602	O	0.004690	-1.669236	-1.248571
O	-2.680003	-4.363946	-2.373984	O	-1.448624	0.829324	-1.247721
				O	1.443193	0.837643	-1.248279

### Coordinates of $\alpha$ -[ $(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}$ ]<sup>8-</sup>

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Si	0.000000	0.000000	-1.997642	O	-0.157337	2.862451	-3.692470
O	0.000000	0.000000	-3.676517	O	-2.400287	-1.567484	-3.692470
O	-1.576225	0.000000	-1.549027	O	2.984487	-2.175869	0.000000
O	0.788113	1.365051	-1.549027	O	-1.632066	-2.826821	-1.518590
O	0.788113	-1.365051	-1.549027	O	-0.200780	-5.143144	-2.221626
Si	0.000000	0.000000	1.997642	O	-1.595600	-2.763660	-6.115596
O	0.000000	0.000000	3.676517	O	3.191200	0.000000	-6.115596
O	-1.576225	0.000000	1.549027	O	-1.595600	2.763660	-6.115596
O	0.788113	-1.365051	1.549027	O	-4.353704	-2.745453	-2.221626
O	0.788113	1.365051	1.549027	O	-4.353704	2.745453	-2.221626
W	0.122251	-3.474159	-1.872948	O	-0.200780	5.143144	-2.221626
W	0.122251	3.474159	-1.872948	O	4.554484	2.397692	-2.221626
W	2.947584	1.842952	-1.872948	O	4.554484	-2.397692	-2.221626
W	2.947584	-1.842952	-1.872948	O	0.774555	-1.341569	5.717649
W	-3.069835	1.631207	-1.872948	O	2.557624	-1.294967	3.692470
W	-3.069835	-1.631207	-1.872948	O	-4.043958	0.000000	2.173575
W	1.926688	0.000000	-4.929769	O	2.021979	-3.502170	2.173575
W	-0.963344	-1.668561	-4.929769	O	-1.549110	0.000000	5.717649
W	-0.963344	1.668561	-4.929769	O	2.557624	1.294967	3.692470
W	0.122251	3.474159	1.872948	O	2.021979	3.502170	2.173575
W	0.122251	-3.474159	1.872948	O	0.774555	1.341569	5.717649
W	2.947584	-1.842952	1.872948	O	-1.632066	-2.826821	1.518590
W	2.947584	1.842952	1.872948	O	3.264132	0.000000	1.518590
W	-3.069835	-1.631207	1.872948	O	0.392114	3.672576	0.000000
W	-3.069835	1.631207	1.872948	O	-0.157337	2.862451	3.692470
W	1.926688	0.000000	4.929769	O	-2.400287	-1.567484	3.692470
W	-0.963344	1.668561	4.929769	O	-3.376601	-1.496707	0.000000
W	-0.963344	-1.668561	4.929769	O	-0.157337	-2.862451	3.692470
O	0.774555	1.341569	-5.717649	O	-2.400287	1.567484	3.692470
O	2.557624	1.294967	-3.692470	O	2.984487	2.175869	0.000000
O	-4.043958	0.000000	-2.173575	O	-1.632066	2.826821	1.518590
O	2.021979	3.502170	-2.173575	O	-0.200780	5.143144	2.221626
O	-1.549110	0.000000	-5.717649	O	-1.595600	2.763660	6.115596
O	2.557624	-1.294967	-3.692470	O	3.191200	0.000000	6.115596
O	2.021979	-3.502170	-2.173575	O	-1.595600	-2.763660	6.115596
O	0.774555	-1.341569	-5.717649	O	-4.353704	2.745453	2.221626
O	-1.632066	2.826821	-1.518590	O	-4.353704	-2.745453	2.221626
O	3.264132	0.000000	-1.518590	O	-0.200780	-5.143144	2.221626
O	0.392114	-3.672576	0.000000	O	4.554484	-2.397692	2.221626
O	-0.157337	-2.862451	-3.692470	O	4.554484	2.397692	2.221626
O	-2.400287	1.567484	-3.692470				
O	-3.376601	1.496707	0.000000				

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## Coordinates of $\beta$ -[ $(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}$ ]<sup>8-</sup>

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Si	0.000000	0.000000	1.994127	O	-0.188734	5.146996	-2.244239
Si	0.000000	0.000000	-2.001985	O	4.551796	-2.410049	-2.244239
O	0.788287	1.365353	1.532200	O	4.558740	-2.370808	2.257884
O	0.000000	0.000000	3.677497	O	1.597331	-2.766658	6.126887
O	0.788911	1.366433	-1.553840	O	0.773598	-1.339911	-5.729033
O	0.788287	-1.365353	1.532200	O	2.550801	-1.300789	-3.702663
O	0.788911	-1.366433	-1.553840	O	2.023652	-3.505068	-2.156869
O	0.000000	0.000000	-3.682455	O	3.019823	-2.133593	-0.004839
O	-1.576574	0.000000	1.532200	O	2.050083	-3.550848	2.038170
O	-1.577821	0.000000	-1.553840	O	2.414092	-1.543495	3.720826
W	1.925362	0.000000	-4.937383	O	-1.596659	2.765494	-6.119791
W	2.952113	1.843014	-1.882873	O	-1.596659	-2.765494	-6.119791
W	2.945424	1.858386	1.876500	O	-4.363062	2.736947	-2.244239
W	0.962591	1.667257	4.947393	O	-0.188734	-5.146996	-2.244239
W	2.952113	-1.843014	-1.882873	O	-4.332550	2.762580	2.257884
W	2.945424	-1.858386	1.876500	O	-0.226190	-5.133388	2.257884
W	0.962591	-1.667257	4.947393	O	-3.194661	0.000000	6.126887
W	-0.962681	1.667412	-4.937383	O	-1.547196	0.000000	-5.729033
W	-0.962681	-1.667412	-4.937383	O	-2.401916	1.558664	-3.702663
W	-3.072153	1.635098	-1.882873	O	-0.148885	-2.859453	-3.702663
W	0.120040	-3.478111	-1.882873	O	-4.047304	0.000000	-2.156869
W	-3.082121	1.621620	1.876500	O	-1.639482	2.839667	-1.554688
W	0.136697	-3.480005	1.876500	O	-1.639482	-2.839667	-1.554688
W	-1.925182	0.000000	4.947393	O	-3.357657	1.548447	-0.004839
W	0.120040	3.478111	-1.882873	O	0.337834	-3.682039	-0.004839
W	-3.072153	-1.635098	-1.882873	O	-1.622110	2.809578	1.636253
W	0.136697	3.480005	1.876500	O	-1.622110	-2.809578	1.636253
W	-3.082121	-1.621620	1.876500	O	-4.100166	0.000000	2.038170
O	3.193317	0.000000	-6.119791	O	-2.543751	1.318917	3.720826
O	4.551796	2.410049	-2.244239	O	0.129660	-2.862412	3.720826
O	4.558740	2.370808	2.257884	O	-0.771934	1.337028	5.736742
O	1.597331	2.766658	6.126887	O	-0.771934	-1.337028	5.736742
O	0.773598	1.339911	-5.729033	O	-4.363062	-2.736947	-2.244239
O	2.550801	1.300789	-3.702663	O	-0.226190	5.133388	2.257884
O	2.023652	3.505068	-2.156869	O	-4.332550	-2.762580	2.257884
O	3.278964	0.000000	-1.554688	O	-0.148885	2.859453	-3.702663
O	3.019823	2.133593	-0.004839	O	-2.401916	-1.558664	-3.702663
O	3.244221	0.000000	1.636253	O	0.337834	3.682039	-0.004839
O	2.050083	3.550848	2.038170	O	-3.357657	-1.548447	-0.004839
O	2.414092	1.543495	3.720826	O	0.129660	2.862412	3.720826
O	1.543867	0.000000	5.736742	O	-2.543751	-1.318917	3.720826

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**Coordinates of  $\gamma$ -[ $(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}$ ]<sup>8-</sup>**

Si	0.000000	0.000000	2.007870	O	-4.356803	-2.747526	2.266860
Si	0.000000	0.000000	-2.007870	O	-0.773682	1.340056	5.739620
O	0.789255	-1.367029	1.548946	O	-0.773682	-1.340056	5.739620
O	-1.578510	0.000000	1.548946	O	2.420543	-1.571814	3.737877
O	0.000000	0.000000	3.690501	O	-2.571502	1.310344	3.737877
O	0.789255	1.367029	1.548946	O	0.150960	-2.882158	3.737877
O	0.000000	0.000000	-3.690501	O	0.150960	2.882158	3.737877
O	0.789255	1.367029	-1.548946	O	-2.571502	-1.310344	3.737877
O	0.789255	-1.367029	-1.548946	O	-1.632048	2.826790	1.712525
O	-1.578510	0.000000	-1.548946	O	-1.632048	-2.826790	1.712525
W	0.965332	-1.672005	-4.960980	O	2.051127	-3.552656	2.000321
W	-1.930665	0.000000	-4.960980	O	-4.102254	0.000000	2.000321
W	2.952531	-1.859882	-1.889075	O	3.054358	-2.052559	0.000000
W	-3.086970	1.627026	-1.889075	O	-3.304747	1.618872	0.000000
W	0.134440	-3.486908	-1.889075	O	0.250389	-3.671431	0.000000
W	0.134440	3.486908	-1.889075	O	0.250389	3.671431	0.000000
W	-3.086970	-1.627026	-1.889075	O	-3.304747	-1.618872	0.000000
W	0.965332	1.672005	-4.960980	O	1.592184	2.757743	-6.157127
W	2.952531	1.859882	-1.889075	O	4.557829	2.399339	-2.266860
W	0.965332	1.672005	4.960980	O	1.547363	0.000000	-5.739620
W	2.952531	1.859882	1.889075	O	2.420543	1.571814	-3.737877
W	0.965332	-1.672005	4.960980	O	3.264096	0.000000	-1.712525
W	-1.930665	0.000000	4.960980	O	2.051127	3.552656	-2.000321
W	2.952531	-1.859882	1.889075	O	1.592184	-2.757743	-6.157127
W	-3.086970	1.627026	1.889075	O	-3.184367	0.000000	-6.157127
W	0.134440	-3.486908	1.889075	O	4.557829	-2.399339	-2.266860
W	0.134440	3.486908	1.889075	O	-4.356803	2.747526	-2.266860
W	-3.086970	-1.627026	1.889075	O	-0.201026	-5.146865	-2.266860
O	1.592184	-2.757743	6.157127	O	-0.201026	5.146865	-2.266860
O	-3.184367	0.000000	6.157127	O	-4.356803	-2.747526	-2.266860
O	4.557829	-2.399339	2.266860	O	-0.773682	1.340056	5.739620
O	1.592184	2.757743	6.157127	O	-0.773682	-1.340056	-5.739620
O	4.557829	2.399339	2.266860	O	2.420543	-1.571814	-3.737877
O	1.547363	0.000000	5.739620	O	-2.571502	1.310344	-3.737877
O	2.420543	1.571814	3.737877	O	0.150960	-2.882158	-3.737877
O	3.264096	0.000000	1.712525	O	0.150960	2.882158	-3.737877
O	2.051127	3.552656	2.000321	O	-2.571502	-1.310344	-3.737877
O	3.054358	2.052559	0.000000	O	-1.632048	2.826790	-1.712525
O	-4.356803	2.747526	2.266860	O	-1.632048	-2.826790	-1.712525
O	-0.201026	-5.146865	2.266860	O	2.051127	-3.552656	-2.000321
O	-0.201026	5.146865	2.266860	O	-4.102254	0.000000	-2.000321

**Coordinates of  $\alpha^*$ -[ $(\text{SiO}_4)_2\text{W}_{18}\text{O}_{54}$ ]<sup>8-</sup>**

W	-3.497273	0.103010	1.886763	W	-1.663506	3.078307	-1.886530
W	3.497645	0.098515	1.886530	W	1.837846	-2.977223	-1.886763
W	1.837846	2.977223	1.886763	W	3.497645	-0.098515	-1.886530
W	-1.834139	2.979792	1.886530	W	-1.658908	0.957580	-4.922497
W	1.659428	-3.080232	1.886763	W	1.658743	0.957866	-4.922497
W	-1.663506	-3.078307	1.886530	W	0.000165	-1.915447	-4.922497
W	0.000165	1.915447	4.922497	O	2.775161	1.604302	-6.080875
W	-1.658908	-0.957580	4.922497	O	-2.776947	1.601209	-6.080875
W	1.658743	-0.957866	4.922497	O	0.001786	-3.205512	-6.080875
O	-2.776947	-1.601209	6.080875	O	-0.000346	1.533924	-5.735560
O	0.001786	3.205512	6.080875	O	-1.328245	-0.767261	-5.735560
O	2.775161	-1.604302	6.080875	O	1.328590	-0.766663	-5.735560
O	1.328590	0.766663	5.735560	O	1.498047	2.408208	-3.700876
O	-0.000346	-1.533924	5.735560	O	1.336546	-2.501451	-3.700876
O	-1.328245	0.767261	5.735560	O	-1.336173	-2.501924	-3.702074
O	1.336546	2.501451	3.700876	O	2.834816	0.093802	-3.702074
O	-1.336173	2.501924	3.702074	O	-1.498643	2.408122	-3.702074
O	-2.834593	-0.093243	3.700876	O	-2.834593	0.093243	-3.700876
O	1.498047	-2.408208	3.700876	O	2.670096	4.424453	-2.309505
O	2.834816	-0.093802	3.702074	O	5.166648	0.103813	-2.311528
O	-1.498643	-2.408122	3.702074	O	2.496640	-4.524598	-2.309505
O	-5.166737	-0.100145	2.309505	O	-2.493419	-4.526355	-2.311528
O	-2.673229	-4.422541	2.311528	O	-5.166737	0.100145	-2.309505
O	2.670096	-4.424453	2.309505	O	-2.673229	4.422541	-2.311528
O	5.166648	-0.103813	2.311528	O	3.504643	-2.021867	-1.956671
O	2.496640	4.524598	2.309505	O	-3.503310	-2.024176	-1.956671
O	-2.493419	4.526355	2.311528	O	-0.001333	4.046043	-1.956671
O	-0.001333	-4.046043	1.956671	O	0.000835	-3.389348	-1.734135
O	3.504643	2.021867	1.956671	O	-2.935679	1.693951	-1.734135
O	-3.503310	2.024176	1.956671	O	2.934844	1.695397	-1.734135
O	2.934844	-1.695397	1.734135	Si	0.000000	0.000000	1.960683
O	0.000835	3.389348	1.734135	O	0.000000	0.000000	3.650721
O	-2.935679	-1.693951	1.734135	O	-0.001690	-1.581527	1.507502
O	1.863498	3.227673	0.000000	O	1.370488	0.789300	1.507502
O	1.863498	-3.227673	0.000000	O	-1.368798	0.792227	1.507502
O	-1.865501	3.231142	0.000000	Si	0.000000	0.000000	-1.960683
O	-1.865501	-3.231142	0.000000	O	0.000000	0.000000	-3.650721
O	-3.726996	0.000000	0.000000	O	1.370488	-0.789300	-1.507502
O	3.731001	0.000000	0.000000	O	-1.368798	-0.792227	-1.507502
W	1.659428	3.080232	-1.886763	O	-0.001690	1.581527	-1.507502
W	-1.834139	-2.979792	-1.886530				
W	-3.497273	-0.103010	-1.886763				

**Coordinates of  $\beta^*$ -[(SiO<sub>4</sub>)<sub>2</sub>W<sub>18</sub>O<sub>54</sub>]<sup>8-</sup>**

W	0.960706	-1.663992	-4.940079	W	2.980364	-1.850893	1.879312
W	-1.921413	0.000000	-4.940079	W	-3.093102	-1.655625	1.879312
W	0.960706	1.663992	-4.940079	W	2.980364	1.850893	1.879312
W	3.073453	-1.648977	-1.894494	W	0.112738	3.506518	1.879312
W	-2.964782	-1.837200	-1.894494	W	0.112738	-3.506518	1.879312
W	3.073453	1.648977	-1.894494	W	-3.093102	1.655625	1.879312
W	-0.108671	3.486177	-1.894494	O	1.575047	-2.728061	6.200081
W	-0.108671	-3.486177	-1.894494	O	-3.150093	0.000000	6.200081
W	-2.964782	1.837200	-1.894494	O	1.575047	2.728061	6.200081
O	1.598793	2.769190	-6.112778	O	1.563748	0.000000	5.686773
O	1.598793	-2.769190	-6.112778	O	-0.781874	1.354245	5.686773
O	-3.197585	0.000000	-6.112778	O	-0.781874	-1.354245	5.686773
O	-0.769729	-1.333210	-5.741073	O	2.440013	1.681605	3.740298
O	1.539459	0.000000	-5.741073	O	2.440013	-1.681605	3.740298
O	-0.769729	1.333210	-5.741073	O	-2.676319	-1.272311	3.740298
O	2.410231	1.530465	-3.714697	O	0.236306	2.953916	3.740298
O	0.120306	-2.852554	-3.714697	O	0.236306	-2.953916	3.740298
O	-2.530537	1.322089	-3.714697	O	-2.676319	1.272311	3.740298
O	0.120306	2.852554	-3.714697	O	4.543299	2.505111	2.248987
O	2.410231	-1.530465	-3.714697	O	4.543299	-2.505111	2.248987
O	-2.530537	-1.322089	-3.714697	O	-4.441140	-2.682057	2.248987
O	4.402306	2.700146	-2.266394	O	-0.102159	5.187168	2.248987
O	0.137242	5.162582	-2.266394	O	-0.102159	-5.187168	2.248987
O	0.137242	-5.162582	-2.266394	O	-4.441140	2.682057	2.248987
O	-4.539548	2.462436	-2.266394	O	3.339106	0.000000	1.963419
O	4.402306	-2.700146	-2.266394	O	-1.669553	2.891751	1.963419
O	-4.539548	-2.462436	-2.266394	O	-1.669553	-2.891751	1.963419
O	-2.024575	3.506667	-2.056630	O	2.033836	3.522707	1.759089
O	-2.024575	-3.506667	-2.056630	O	2.033836	-3.522707	1.759089
O	4.049150	0.000000	-2.056630	O	-4.067671	0.000000	1.759089
O	1.677111	2.904842	-1.675894	Si	0.000000	0.000000	-1.994599
O	1.677111	-2.904842	-1.675894	O	0.000000	0.000000	-3.678174
O	-3.354222	0.000000	-1.675894	O	1.578187	0.000000	-1.545195
O	3.236097	-1.707816	-0.000506	O	-0.789093	1.366750	-1.545195
O	-3.097060	-1.948634	-0.000506	O	-0.789093	-1.366750	-1.545195
O	-0.139037	-3.656450	-0.000506	Si	0.000000	0.000000	1.986432
O	-3.097060	1.948634	-0.000506	O	0.000000	0.000000	3.666128
O	3.236097	1.707816	-0.000506	O	0.790685	-1.369507	1.531453
O	-0.139037	3.656450	-0.000506	O	-1.581370	0.000000	1.531453
W	0.975140	1.688993	4.951080	O	0.790685	1.369507	1.531453
W	0.975140	-1.688993	4.951080				
W	-1.950281	0.000000	4.951080				

### Coordinates of $\gamma^*-[{\rm SiO}_4]_2{\rm W}_{18}{\rm O}_{54}]^{8-}$

W	3.499690	0.121449	1.892356	W	0.000000	1.944394	-4.965572
W	1.644667	-3.091545	1.892356	W	1.644667	3.091545	-1.892356
W	-1.644667	-3.091545	1.892356	W	3.499690	-0.121449	-1.892356
W	-3.499690	0.121449	1.892356	W	1.855023	-2.970096	-1.892356
W	-1.855023	2.970096	1.892356	W	-1.855023	-2.970096	-1.892356
W	1.855023	2.970096	1.892356	W	-3.499690	-0.121449	-1.892356
W	1.683895	0.972197	4.965572	W	-1.644667	3.091545	-1.892356
W	0.000000	-1.944394	4.965572	O	-2.740161	-1.582033	-6.195420
W	-1.683895	0.972197	4.965572	O	2.740161	-1.582033	-6.195420
O	2.740161	1.582033	6.195420	O	0.000000	3.164065	-6.195420
O	0.000000	-3.164065	6.195420	O	0.000000	-1.557890	-5.715424
O	-2.740161	1.582033	6.195420	O	1.349172	0.778945	-5.715424
O	-1.349172	-0.778945	5.715424	O	-1.349172	0.778945	-5.715424
O	0.000000	1.557890	5.715424	O	2.932682	-0.207638	-3.751541
O	1.349172	-0.778945	5.715424	O	1.646161	-2.435958	-3.751541
O	2.932682	0.207638	3.751541	O	-1.646161	-2.435958	-3.751541
O	1.646161	2.435958	3.751541	O	-2.932682	-0.207638	-3.751541
O	-1.646161	2.435958	3.751541	O	-1.286521	2.643596	-3.751541
O	-2.932682	0.207638	3.751541	O	1.286521	2.643596	-3.751541
O	-1.286521	-2.643596	3.751541	O	2.706932	4.413812	-2.256420
O	1.286521	-2.643596	3.751541	O	5.175940	0.137366	-2.256420
O	5.175940	-0.137366	2.256420	O	2.469008	-4.551178	-2.256420
O	2.706932	-4.413812	2.256420	O	-2.469008	-4.551178	-2.256420
O	-2.706932	-4.413812	2.256420	O	-5.175940	0.137366	-2.256420
O	-5.175940	-0.137366	2.256420	O	-2.706932	4.413812	-2.256420
O	-2.469008	4.551178	2.256420	O	2.874033	1.659324	-1.891967
O	2.469008	4.551178	2.256420	O	3.538763	-2.043106	-1.857587
O	0.000000	3.318648	1.891967	O	0.000000	-3.318648	-1.891967
O	2.874033	-1.659324	1.891967	O	-3.538763	-2.043106	-1.857587
O	-2.874033	-1.659324	1.891967	O	-2.874033	1.659324	-1.891967
O	0.000000	-4.086212	1.857587	O	0.000000	4.086212	-1.857587
O	3.538763	2.043106	1.857587	Si	0.000000	0.000000	2.006497
O	-3.538763	2.043106	1.857587	O	0.000000	0.000000	3.686597
O	-1.817789	3.148502	0.000000	O	1.368726	0.790234	1.551788
O	1.817789	3.148502	0.000000	O	0.000000	-1.580469	1.551788
O	3.635577	0.000000	0.000000	O	-1.368726	0.790234	1.551788
O	1.817789	-3.148502	0.000000	Si	0.000000	0.000000	-2.006497
O	-1.817789	-3.148502	0.000000	O	0.000000	0.000000	-3.686597
O	-3.635577	0.000000	0.000000	O	-1.368726	-0.790234	-1.551788
W	-1.683895	-0.972197	-4.965572	O	1.368726	-0.790234	-1.551788
W	1.683895	-0.972197	-4.965572	O	0.000000	1.580469	-1.551788

**Coordinates of  $\alpha$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ]<sup>8-</sup> (single-reduced)**

W	0.960385	1.662609	4.911572	O	-4.593799	2.394726	-2.217549
W	-1.918876	-0.000360	4.911635	O	0.222964	5.174797	-2.217620
W	0.960329	-1.662987	4.912256	O	4.370119	2.781215	-2.217394
W	0.960609	1.663134	-4.911881	O	1.550525	-0.000082	5.722060
W	0.960308	-1.662851	-4.911139	O	2.401252	1.542585	3.680210
W	-1.919658	0.000759	-4.911824	O	-2.025284	-3.508276	2.174007
W	3.103360	-1.654149	-1.878740	O	4.049744	0.000231	2.174096
W	-2.984618	1.861274	-1.879418	O	-0.774955	-1.343284	5.722675
W	-0.119919	3.514708	-1.879401	O	0.135003	2.850502	3.680372
W	3.103851	1.653926	-1.879332	O	-2.025599	3.508129	2.173792
W	-2.984457	-1.861022	-1.879767	O	-0.774481	1.342491	5.722294
W	-0.120163	-3.514777	-1.878609	O	1.609466	-2.788187	1.530453
W	-2.984255	1.860762	1.879214	O	1.609127	2.787896	1.529317
W	3.103474	-1.654245	1.879551	O	-2.998660	2.170814	-0.000365
W	3.103437	1.654383	1.878867	O	-2.535073	1.308055	3.680087
W	-0.120130	3.514943	1.879218	O	0.134881	-2.850796	3.681145
W	-0.119482	-3.515105	1.879947	O	-0.381569	-3.682100	0.000533
W	-2.983933	-1.861110	1.879090	O	2.401479	-1.543014	3.680911
O	-0.774226	1.341951	-5.723774	O	-2.534314	-1.308433	3.679711
O	0.134491	2.850450	-3.681264	O	-0.381383	3.682328	-0.000291
O	-2.025526	-3.507988	-2.174873	O	-3.218820	-0.000123	1.529758
O	-2.025501	3.508287	-2.174799	O	-4.593421	2.394579	2.217169
O	-0.774543	-1.342251	-5.722598	O	-3.196345	-0.000638	6.088598
O	2.402017	1.543322	-3.681503	O	1.598943	2.768726	6.088700
O	4.049438	-0.000200	-2.174531	O	1.598527	-2.769016	6.089705
O	1.549718	-0.000040	-5.722146	O	-4.593061	-2.394862	2.217031
O	-3.219201	0.000098	-1.531069	O	0.222042	-5.175637	2.217646
O	1.608971	2.786986	-1.530092	O	4.370771	-2.780504	2.217002
O	3.379618	-1.511551	0.000295	O	4.370139	2.781262	2.216447
O	2.401645	-1.542699	-3.680744	O	0.221943	5.175404	2.216638
O	-2.536134	-1.308260	-3.681353	Na	-0.000506	-0.000010	-0.000229
O	-2.998495	-2.170945	-0.000536	H	0.001492	-0.001483	2.754515
O	-2.535898	1.309536	-3.681521	H	0.000733	0.001456	-2.754620
O	0.135123	-2.850317	-3.680009	O	0.000763	-0.000704	3.741886
O	3.380118	1.511749	-0.000316	F	-0.829134	-1.436421	1.511567
O	1.608359	-2.786412	-1.529007	F	1.658496	0.000034	1.511137
O	4.369237	-2.781820	-2.216865	F	-0.829698	1.436332	1.511305
O	1.598410	-2.768968	-6.088664	O	0.000198	0.000824	-3.741982
O	1.598588	2.768958	-6.089693	F	-0.830190	-1.435914	-1.511954
O	-3.196280	0.001266	-6.089644	F	-0.829932	1.436144	-1.512125
O	0.222776	-5.174918	-2.216315	F	1.658293	0.000340	-1.511623
O	-4.593667	-2.394478	-2.217972				

**Coordinates of  $\beta$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]$ <sup>8-</sup>(single-reduced)**

W	1.918547	-0.000234	4.918858	O	4.600577	2.375194	-2.248054
W	-0.960240	1.661706	4.919511	O	4.600571	-2.376477	-2.247825
W	-0.960031	-1.662069	4.919608	O	-0.242261	-5.172269	-2.246765
W	0.960546	-1.663971	-4.931376	O	0.772725	-1.339624	5.734521
W	-1.921385	-0.000128	-4.931339	O	2.526676	-1.314546	3.689831
W	0.960473	1.664005	-4.931139	O	-4.052917	0.000018	2.160607
W	0.118041	3.519355	1.890482	O	2.026819	-3.510363	2.161693
W	0.117787	-3.519340	1.890516	O	-1.547088	-0.000056	5.734585
W	2.989886	-1.861149	1.889697	O	2.526753	1.313723	3.689576
W	2.989843	1.861700	1.889998	O	2.027124	3.510967	2.161757
W	-3.106553	-1.658226	1.890245	O	0.772951	1.339959	5.733934
W	-3.106609	1.658334	1.889922	O	-1.615998	-2.799371	1.565135
W	-3.119991	-1.647074	-1.880921	O	3.233155	0.000157	1.565261
W	2.986047	1.878608	-1.880959	O	3.039804	2.129763	0.007262
W	2.986186	-1.878921	-1.881241	O	-0.126482	2.844938	3.689425
W	0.133908	-3.525222	-1.880974	O	-2.402103	-1.532185	3.690127
W	0.133867	3.525474	-1.881182	O	-3.363555	1.568132	0.007040
W	-3.120040	1.647260	-1.881346	O	-0.126282	-2.845977	3.690231
O	1.550766	-0.000003	-5.738285	O	-2.402522	1.532250	3.690133
O	2.410073	-1.543619	-3.705122	O	3.039619	-2.129414	0.007109
O	-1.598236	2.767981	-1.643611	O	-1.616027	2.799285	1.564809
O	3.195026	-0.000145	-1.644404	O	-0.212935	5.178509	2.244436
O	-0.776225	1.343906	-5.738673	O	-1.601429	2.771636	6.091622
O	0.130510	-2.857762	-3.704186	O	3.199207	-0.000350	6.092020
O	-1.598052	-2.767648	-1.643381	O	-1.601074	-2.771872	6.091887
O	-0.776534	-1.344613	-5.738660	O	-4.377509	2.775237	2.244131
O	2.054230	3.558605	-2.048135	O	-4.377377	-2.775274	2.244311
O	2.054281	-3.558850	-2.047957	O	-0.212908	-5.178647	2.244060
O	-3.363418	-1.568096	0.007256	O	4.592070	-2.404364	2.244471
O	-2.541026	-1.316295	-3.704651	O	4.592036	2.404757	2.244994
O	0.130016	2.858385	-3.704694	Na	0.000352	0.000096	0.003094
O	0.324342	3.695999	0.007429	H	-0.001172	0.000257	2.761020
O	2.409695	1.543075	-3.704840	H	-0.001207	-0.000418	-2.768658
O	-2.541033	1.315929	-3.704735	O	-0.000643	0.000072	3.748338
O	0.324598	-3.695745	0.007578	F	-1.664432	0.000119	1.509528
O	-4.108034	0.000072	-2.047570	F	0.832915	-1.441247	1.509701
O	-4.357327	-2.797382	-2.246850	F	0.833153	1.441591	1.509441
O	-3.191960	0.000032	-6.116051	O	-0.000327	-0.000221	-3.755653
O	1.595341	-2.763991	-6.116628	F	0.838240	1.451706	-1.486825
O	1.595402	2.764027	-6.116304	F	0.838490	-1.451535	-1.486850
O	-4.357362	2.797650	-2.247037	F	-1.676024	0.000182	-1.487109
O	-0.242132	5.172556	-2.246915				

### Coordinates of $\gamma$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$ (single-reduced)

W	0.962359	-1.666528	4.943648	O	-0.228281	5.181126	-2.261356
W	0.962306	1.666872	4.944183	O	4.600597	2.392274	-2.262041
W	-1.924166	0.000115	4.943515	O	4.600848	-2.392559	-2.261926
W	0.962624	-1.667145	-4.943967	O	-0.227791	-5.181192	-2.261787
W	-1.924372	-0.000087	-4.943609	O	-0.776980	-1.346737	5.742420
W	0.962701	1.666589	-4.943536	O	0.147167	-2.872526	3.718443
W	2.992077	1.879647	1.893448	O	-1.604236	2.779007	1.700172
W	0.131389	-3.530551	1.893202	O	-1.605229	-2.780018	1.699718
W	-3.123587	1.651705	1.893037	O	-0.777041	1.346601	5.742638
W	-3.123784	-1.651702	-1.893017	O	2.414150	-1.563898	3.718203
W	0.131260	3.531019	-1.892828	O	3.209994	0.000265	1.699821
W	2.991760	-1.879619	-1.893255	O	1.554818	0.000047	5.742369
W	-3.123831	-1.651961	1.893542	O	-4.110975	-0.000052	2.021755
W	2.991917	-1.879295	1.892891	O	2.055590	-3.560590	2.021892
W	0.131587	3.530811	1.893360	O	3.071781	2.064821	0.000013
W	0.131473	-3.531021	-1.893367	O	2.414194	1.564193	3.718628
W	-3.123822	1.651885	-1.893183	O	-2.561543	1.308803	3.718738
W	2.991608	1.879499	-1.892774	O	-3.322362	1.628509	-0.000332
O	1.554191	-0.000163	-5.743087	O	-2.561270	-1.308697	3.718523
O	2.414670	-1.564286	-3.719324	O	0.147280	2.872970	3.719063
O	-1.604852	2.779536	-1.700400	O	3.071248	-2.063752	-0.000262
O	3.208559	-0.000010	-1.700164	O	2.055711	3.560910	2.022272
O	-0.776949	1.346350	-5.743690	O	4.601247	2.392560	2.261729
O	0.147057	-2.872588	-3.719131	O	1.593083	2.758059	6.138844
O	-1.604975	-2.779626	-1.700321	O	1.593479	-2.758419	6.137524
O	-0.777152	-1.346672	-5.743679	O	-3.184589	0.000031	6.138370
O	2.055371	3.560519	-2.022869	O	-0.228862	5.180932	2.261569
O	2.055678	-3.560943	-2.022436	O	-4.372296	2.788452	2.261275
O	-3.323381	-1.628826	-0.000165	O	-4.373158	-2.788230	2.261840
O	-2.561039	-1.308642	-3.718928	O	-0.228283	-5.180881	2.260918
O	0.146734	2.872053	-3.718828	O	4.600736	-2.393616	2.260752
O	0.251387	3.691663	-0.000010	Na	-0.000106	0.000048	-0.000120
O	2.414074	1.563245	-3.718774	H	-0.000591	0.000336	2.775910
O	-2.561401	1.309298	-3.719475	H	-0.001160	-0.000946	-2.776412
O	0.251026	-3.691157	-0.000310	O	0.000103	0.000334	3.762983
O	-4.110697	-0.000008	-2.022430	F	-1.678724	-0.000508	1.496624
O	-4.371991	-2.789060	-2.262659	F	0.839550	-1.453550	1.496368
O	-3.185345	-0.000090	-6.138182	F	0.839941	1.453826	1.496449
O	1.593144	-2.758564	-6.138692	O	-0.000066	-0.000550	-3.763481
O	1.593740	2.758529	-6.137556	F	-1.678614	-0.000132	-1.497181
O	-4.372337	2.788940	-2.261669	F	0.839477	1.453850	-1.496345
				F	0.839494	-1.453786	-1.496881

**Coordinates of  $\alpha^*-\text{[NaF}_6\text{)W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$ (single-reduced)**

W	-1.654794	0.955523	4.906021	O	2.715826	4.439607	2.315079
W	0.000347	-1.910076	4.904956	O	-2.716552	4.439161	2.315751
W	1.655075	0.955815	4.905936	O	-5.203659	0.131086	2.316276
W	-1.654513	-0.955326	-4.905656	O	0.000033	-1.535420	-5.740469
W	0.000189	1.910932	-4.905718	O	-1.472458	-2.403765	-3.683836
W	1.655289	-0.955186	-4.906011	O	3.509901	2.026206	-1.995334
W	3.543802	-0.098235	1.892815	O	0.000143	-4.053398	-1.995066
W	-1.857030	-3.019955	1.892500	O	1.330298	0.768186	-5.740958
W	-1.687410	3.117523	1.892393	O	-2.816082	-0.074490	-3.682417
W	-1.856703	3.020204	-1.892668	O	-3.510312	2.026646	-1.996355
W	-1.687150	-3.118027	-1.892184	O	-1.330618	0.768224	-5.739648
W	3.544123	0.097664	-1.892766	O	2.896558	-1.672233	-1.725481
W	1.687011	3.117587	1.892646	O	-2.896351	-1.672528	-1.724485
W	-3.544322	-0.097983	1.893310	O	1.879295	-3.254967	-0.000424
W	1.856510	-3.020133	1.892198	O	-1.345421	2.477632	-3.684420
W	1.687469	-3.117765	-1.892969	O	2.818391	-0.074068	-3.684232
W	-3.543885	0.097789	-1.892018	O	3.758436	-0.000444	-0.000111
W	1.856597	3.019594	-1.892184	O	1.473218	-2.403369	-3.684238
O	0.000108	1.536244	5.739939	O	1.344088	2.475646	-3.682819
O	-1.473241	2.403455	3.683733	O	-1.879580	3.254764	-0.000183
O	3.510096	-2.026868	1.996067	O	-0.000199	3.343915	-1.725136
O	-0.000290	4.052668	1.994147	O	-2.486344	4.572394	-2.316023
O	1.330258	-0.767571	5.740195	O	0.001019	3.215091	-6.052927
O	-2.817709	0.074173	3.683964	O	-2.784059	-1.607175	-6.052792
O	-3.510391	-2.026616	1.995460	O	2.783138	-1.606967	-6.054654
O	-1.330272	-0.767714	5.740715	O	2.486210	4.571610	-2.315808
O	2.896722	1.672196	1.724766	O	5.203534	-0.131370	-2.315515
O	-2.897466	1.672470	1.725145	O	2.716470	-4.439387	-2.315929
O	-1.880092	-3.256513	-0.000079	O	-2.716575	-4.439215	-2.316527
O	-1.343795	-2.475173	3.682360	O	-5.203053	-0.131819	-2.315707
O	2.817095	0.074420	3.683103	Na	-0.000160	-0.000157	-0.000136
O	1.879072	3.254473	-0.000006	H	0.001144	-0.000507	-2.742672
O	1.473170	2.403553	3.683668	H	-0.000195	0.001502	2.742517
O	1.344918	-2.476348	3.683090	O	0.000538	0.000057	-3.729760
O	-3.759399	-0.000021	0.000266	F	1.462487	0.844010	-1.435215
O	-0.000129	-3.343696	1.724232	F	-0.000144	-1.688622	-1.436015
O	-2.486396	-4.571905	2.316650	F	-1.462962	0.844912	-1.434786
O	-0.001644	-3.213270	6.053513	O	0.000008	0.000685	3.729618
O	-2.784040	1.607627	6.053377	F	1.462643	-0.844697	1.434647
O	2.783951	1.607224	6.053810	F	-0.000359	1.687808	1.436226
O	2.485699	-4.572408	2.315466	F	-1.463421	-0.844559	1.434294
O	5.203235	0.131487	2.315262				

**Coordinates of  $\beta^*-\text{[}( \text{NaF}_6 )\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{8-}$ (single-reduced)**

W	0.957572	-1.658242	4.923367	O	4.587708	2.498509	-2.251681
W	0.957794	1.658754	4.923304	O	4.587548	-2.498921	-2.251261
W	-1.914257	0.000028	4.922738	O	-0.129893	-5.223368	-2.251937
W	0.970603	-1.680583	-4.936450	O	-0.769713	-1.334328	5.747880
W	-1.940236	0.000358	-4.936475	O	0.096442	-2.836358	3.700809
W	0.970264	1.680784	-4.936393	O	-2.025341	3.508091	2.063322
W	-3.130234	-1.681478	-1.886465	O	-2.025389	-3.508507	2.064371
W	3.020351	1.870214	-1.886043	O	-0.769537	1.333719	5.748020
W	3.020242	-1.870395	-1.885943	O	2.408754	-1.500959	3.700887
W	0.108573	-3.551741	-1.886504	O	4.050595	-0.000100	2.063368
W	0.108792	3.551658	-1.886760	O	1.540757	0.000079	5.747692
W	-3.130081	1.681301	-1.886469	O	-3.328052	-0.000157	1.692080
W	3.109166	1.675752	1.901501	O	1.665015	-2.884098	1.692382
W	-3.005528	-1.855056	1.901099	O	3.235761	1.738075	0.003252
W	-0.103548	-3.530631	1.901359	O	2.409510	1.501850	3.701444
W	3.109042	-1.675708	1.901461	O	-2.502863	1.334987	3.700493
W	-3.005411	1.854577	1.901148	O	-3.123999	1.935098	0.002876
W	-0.103523	3.530740	1.901520	O	-2.503588	-1.335510	3.700906
O	1.569196	-0.000088	-5.698653	O	0.096618	2.837240	3.701306
O	2.432851	-1.661029	-3.723565	O	3.236097	-1.738151	0.003391
O	-1.655147	2.866413	-1.928890	O	1.665239	2.884242	1.692844
O	3.308746	-0.000101	-1.928554	O	4.427478	2.730246	2.270279
O	-0.784009	1.358641	-5.700563	O	1.603404	2.776284	6.084852
O	0.221486	-2.938045	-3.724601	O	1.603731	-2.776168	6.084290
O	-1.655866	-2.867583	-1.929506	O	-3.205739	-0.000061	6.083546
O	-0.784076	-1.358941	-5.699768	O	0.149347	5.199867	2.270284
O	2.039631	3.533733	-1.813317	O	-4.577745	2.468066	2.271855
O	2.039363	-3.533827	-1.813141	O	-4.578059	-2.468325	2.271473
O	-3.123896	-1.935001	0.002893	O	0.150287	-5.199627	2.270334
O	-2.654435	-1.276913	-3.724568	O	4.426926	-2.730657	2.270877
O	0.221851	2.937337	-3.724041	Na	-0.000104	0.000032	-0.001476
O	-0.113130	3.671412	0.003297	H	0.001352	0.000207	2.760947
O	2.433053	1.660806	-3.723831	H	-0.001536	0.000126	-2.753380
O	-2.654476	1.277344	-3.724715	O	0.000644	0.000230	3.748863
O	-0.113694	-3.672020	0.002991	F	-0.832947	1.442928	1.490793
O	-4.079963	0.000026	-1.813968	F	-0.833213	-1.443386	1.490337
O	-4.457805	-2.724620	-2.253332	F	1.665740	0.000002	1.491479
O	-3.150251	0.000130	-6.180656	O	-0.000217	-0.000029	-3.741115
O	1.576876	-2.727635	-6.180476	F	0.836502	1.449182	-1.478218
O	1.576490	2.727864	-6.180426	F	0.836341	-1.449459	-1.478167
O	-4.457278	2.724967	-2.253213	F	-1.673375	-0.000426	-1.479126
O	-0.131087	5.223326	-2.250122				

### Coordinates of $\gamma^*-\text{[(NaF}_6\text{)W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$ (single-reduced)

W	-0.000083	-1.936105	4.948648	O	-2.741343	4.437532	-2.249445
W	1.676669	0.968167	4.948940	O	2.741976	4.437558	-2.248667
W	-1.677162	0.967979	4.948830	O	5.214029	0.155254	-2.249634
W	1.676773	-0.967624	-4.948874	O	2.473040	-4.591518	-2.249905
W	-1.676782	-0.968399	-4.948976	O	-1.354418	-0.781772	5.722766
W	-0.000696	1.936197	-4.948897	O	-1.287605	-2.629814	3.734185
W	3.543996	0.115478	1.897800	O	-0.000081	3.288574	1.876684
W	-1.873013	3.010115	1.896639	O	-2.848867	-1.644737	1.877397
W	-1.671478	-3.126828	1.897212	O	-0.000106	1.564108	5.722804
W	-1.872647	-3.010657	-1.897021	O	1.287636	-2.629763	3.734003
W	-1.670756	3.127415	-1.897323	O	2.849628	-1.645626	1.877570
W	3.544080	-0.115808	-1.897259	O	1.354879	-0.781989	5.722415
W	1.670894	-3.127309	1.897197	O	-3.544508	2.045856	1.887534
W	1.872654	3.009939	1.896196	O	-0.000365	-4.091828	1.887413
W	-3.544218	0.116299	1.898215	O	3.646064	0.000270	0.000112
W	1.873118	-3.009941	-1.896657	O	2.922186	0.199422	3.734709
W	1.671378	3.127351	-1.898124	O	-1.633860	2.429870	3.733887
W	-3.543007	-0.116018	-1.896568	O	-1.823458	3.156952	-0.000190
O	1.354206	0.782154	-5.723355	O	-2.922398	0.199831	3.734737
O	2.921693	-0.199349	-3.734365	O	1.633720	2.429229	3.733377
O	-2.848112	1.644863	-1.876989	O	1.823567	-3.157302	0.000195
O	2.850201	1.645623	-1.877416	O	3.544340	2.045451	1.886705
O	-1.355707	0.782176	-5.722840	O	5.214237	-0.155259	2.249128
O	1.633536	-2.429272	-3.733649	O	2.736407	1.579650	6.179615
O	0.000106	-3.288201	-1.876455	O	-0.000714	-3.159434	6.179583
O	-0.000040	-1.564208	-5.722548	O	-2.736369	1.579860	6.179729
O	0.000200	4.092452	-1.887507	O	2.473192	4.591466	2.248726
O	3.544668	-2.045621	-1.887279	O	-2.472808	4.591927	2.249695
O	-3.644308	-0.000384	0.000268	O	-5.214409	-0.155629	2.247322
O	-1.633678	-2.430505	-3.734172	O	-2.742010	-4.436635	2.250520
O	-1.288474	2.630506	-3.734540	O	2.740817	-4.437850	2.249707
O	1.823293	3.155979	-0.000504	Na	0.000030	0.000320	-0.000000
O	1.286732	2.629426	-3.733895	H	-0.000226	-0.000045	2.770178
O	-2.920866	-0.200445	-3.733592	H	-0.000115	0.000784	-2.770411
O	-1.823962	-3.157676	0.000156	O	-0.000136	0.000072	3.757968
O	-3.544116	-2.046078	-1.886896	F	-1.447575	0.835947	1.498642
O	-2.472441	-4.592473	-2.249527	F	-0.000186	-1.671756	1.498630
O	-2.735969	-1.580755	-6.179609	F	1.447923	0.835110	1.498562
O	2.735880	-1.579694	-6.179691	O	-0.000200	0.000187	-3.758211
O	-0.000200	3.159727	-6.179609	F	-1.447061	-0.836327	-1.498319
O	-5.213094	0.155240	-2.248398	F	0.000150	1.671923	-1.499233
				F	1.448100	-0.835522	-1.498071

**Coordinates of  $\alpha$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>10-</sup> (single-reduced)**

W	-0.972799	1.657832	-4.908797	O	0.380786	-3.793752	0.001103
W	1.907141	0.030007	-4.931654	O	3.083153	2.228384	0.008317
W	-0.942575	-1.655926	-4.908442	O	0.384174	3.791428	-0.001316
W	-0.938332	1.656703	4.908154	O	-3.486119	-1.594559	-0.007791
W	-0.969939	-1.658309	4.909487	O	3.078031	-2.228891	-0.010033
W	1.911556	-0.030441	4.927069	O	-3.486508	1.598361	0.009849
W	0.123709	3.446021	1.839945	O	-1.608928	-2.781254	6.086507
W	2.921197	-1.844548	1.833811	O	-1.576112	2.772929	6.092025
W	-3.070229	-1.614400	1.837991	O	3.223817	-0.031753	6.081133
W	0.119796	-3.446667	-1.841209	O	-1.527996	-0.005473	5.758951
W	2.922725	1.842250	-1.837707	O	0.788227	-1.365455	5.750683
W	-3.070090	1.616812	-1.835010	O	0.800204	1.330763	5.751285
W	-3.063858	-1.606600	-1.861241	O	-2.358017	1.508930	3.690012
W	2.912076	-1.827149	-1.875325	O	-0.097482	2.805046	3.684979
W	0.118427	3.443019	-1.858686	O	-2.368301	-1.524868	3.679238
W	-3.061394	1.610080	1.863474	O	2.498069	-1.296216	3.657122
W	2.916784	1.826903	1.871152	O	2.496842	1.276601	3.670582
W	0.116014	-3.444879	1.857989	O	-0.106660	-2.814978	3.685484
O	3.219302	0.027190	-6.085498	O	-4.335901	-2.739665	2.267124
O	-1.609288	2.782482	-6.085648	O	-0.211482	-5.115312	2.257595
O	-1.581918	-2.770884	-6.091738	O	4.535414	-2.374988	2.244019
O	0.797618	-1.334408	-5.749705	O	4.535321	2.360962	2.258567
O	-1.530023	0.006414	-5.759240	O	-0.205740	5.110156	2.264458
O	0.787236	1.365940	-5.750576	O	-4.330470	2.732235	2.290327
O	-2.360382	-1.506910	-3.688176	O	2.018963	-3.498216	2.182440
O	2.491571	-1.277352	-3.670797	O	2.021100	3.490718	2.191726
O	2.499970	1.293787	-3.659790	O	-4.048598	-0.003599	2.191853
O	-0.101610	-2.803444	-3.682990	O	3.231884	-0.004124	1.468953
O	-2.369944	1.527963	-3.678669	O	-1.623637	2.814229	1.510006
O	-0.105519	2.812107	-3.684474	O	-1.627369	-2.817638	1.499714
O	4.538590	2.369052	-2.245754	O	0.006414	-0.010970	3.772927
O	4.530468	-2.363218	-2.259236	O	0.003971	0.011315	-3.773672
O	-0.215892	-5.109770	-2.263838	O	0.788019	-1.395123	1.357245
O	-4.332076	-2.730467	-2.286795	O	0.792845	1.392503	1.356936
O	-4.334166	2.744463	-2.265255	O	-1.636780	-0.001884	1.347042
O	-0.209154	5.113674	-2.257765	O	0.790109	-1.392270	-1.357095
O	2.016961	-3.493591	-2.190884	O	-1.637739	0.005433	-1.346478
O	-4.049875	0.006911	-2.190238	O	0.789507	1.395180	-1.357014
O	2.022224	3.496732	-2.183492	Sb	-0.011568	0.000436	0.000126
O	3.227838	0.002325	-1.468444	H	0.038961	-0.022189	2.776980
O	-1.625091	-2.809647	-1.507437	H	0.037656	0.020196	-2.777759
O	-1.625111	2.817313	-1.498717				

### Coordinates of $\beta$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>10-</sup> (single-reduced)

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W	1.910678	-0.024046	4.930816	O	-0.176257	3.819068	0.013611
W	-0.928396	1.670020	4.939349	O	-3.223212	-2.063308	0.015962
W	-0.978911	-1.635548	4.934743	O	3.537916	1.469077	-0.026182
W	-2.988309	-1.719917	1.887937	O	-3.030997	2.324891	-0.020831
W	0.010362	3.446080	1.889647	O	-0.493815	-3.794969	-0.019704
W	2.984669	-1.730429	1.886415	O	3.401184	-1.767538	0.013886
W	-0.283484	-3.457566	1.820748	O	-3.220834	0.135969	1.576207
W	3.140904	1.481155	1.812180	O	1.493679	-2.855721	1.575895
W	-2.849853	1.975153	1.818229	O	1.729366	2.720748	1.565499
W	0.980710	1.635860	-4.923538	O	-1.895257	3.622684	2.079293
W	0.922914	-1.675994	-4.916296	O	-2.187242	-3.455313	2.085929
W	-1.915043	0.031494	-4.923259	O	4.088776	-0.165181	2.080081
W	-2.837244	1.948845	-1.893146	O	0.458776	5.080116	2.316046
W	3.111430	1.477218	-1.898036	O	-4.441730	2.535028	2.275914
W	-0.273244	-3.437176	-1.888227	O	-4.626323	-2.148378	2.321198
W	-3.010277	-1.721028	-1.822356	O	0.028747	-5.114593	2.281628
W	2.993105	-1.751191	-1.822045	O	4.174168	-2.933148	2.324196
W	0.019258	3.462845	-1.821988	O	4.417568	2.582257	2.275206
O	-3.213301	0.098622	-6.090050	O	2.405986	-1.398178	3.706841
O	1.512914	-2.828617	-6.090087	O	0.016032	2.783579	3.703176
O	1.684955	2.727985	-6.091750	O	-2.416042	-1.376188	3.707815
O	-0.737693	1.370193	-5.761620	O	-0.211548	-2.801147	3.692665
O	1.543705	-0.050841	-5.760905	O	-2.319258	1.590779	3.689730
O	-0.824192	-1.317117	-5.763124	O	2.530272	1.223319	3.683047
O	-0.003958	-2.797463	-3.695407	O	0.733335	-1.357938	5.778417
O	2.314374	-1.607909	-3.678151	O	-1.550356	0.054562	5.781529
O	-2.552957	-1.198484	-3.672869	O	0.818982	1.326503	5.777156
O	0.233717	2.805852	-3.673801	O	-1.521695	2.835553	6.099278
O	2.417135	1.398165	-3.695479	O	3.212989	-0.086633	6.095315
O	-2.421826	1.397180	-3.692232	O	-1.685468	-2.727730	6.102435
O	-4.636408	-2.188984	-2.260733	O	-0.001772	0.004097	3.793726
O	-4.421051	2.570495	-2.291150	O	-0.004645	-0.001196	-3.778680
O	0.424325	5.105468	-2.262388	Sb	0.002089	-0.002107	0.001908
O	4.438932	2.538922	-2.303804	H	-0.012577	0.005390	-2.782417
O	4.212459	-2.922047	-2.268102	H	-0.011645	0.013338	2.797422
O	-0.022610	-5.117652	-2.296204	O	-0.743038	1.431189	-1.353301
O	-1.864290	3.583639	-2.178923	O	1.621949	-0.076520	-1.352422
O	4.040300	-0.179857	-2.181528	O	-0.869589	-1.368315	-1.351070
O	-2.175111	-3.411205	-2.178766	O	-0.863527	-1.370465	1.344355
O	1.743182	2.739013	-1.517624	O	1.622957	-0.065428	1.339982
O	1.504731	-2.884542	-1.522872	O	-0.750305	1.428592	1.346571
O	-3.244246	0.136663	-1.514412				

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### Coordinates of $\gamma$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>]<sup>10-</sup> (single-reduced)

W	1.004381	1.627827	4.941332	O	-1.614789	2.798705	-1.603564
W	-1.909079	0.059211	4.943811	O	-3.452918	1.659966	-0.021802
W	0.904759	-1.680138	4.942915	O	0.290704	-3.814054	-0.019905
W	0.905308	1.680424	-4.942242	O	0.291690	3.814871	0.019010
W	1.004863	-1.628271	-4.942626	O	-3.450830	-1.657567	0.022489
W	-1.908477	-0.060331	-4.940877	O	3.161875	2.153940	-0.022478
W	2.937205	1.857839	1.820074	O	3.160862	-2.154677	0.022406
W	-3.073976	1.616107	1.819363	O	-1.615501	-2.796997	1.604248
W	0.138997	-3.468947	1.821818	O	3.234045	0.001658	1.613326
W	-3.076946	-1.614490	-1.817440	O	-1.614843	2.797977	1.602192
W	0.140019	3.471189	-1.822784	O	-4.093643	0.005912	2.064273
W	2.936310	-1.859948	-1.819658	O	2.041618	-3.546579	2.067491
W	2.918805	-1.842248	1.899696	O	2.051927	3.545541	2.064280
W	0.138759	3.448825	1.897088	O	-4.311391	2.759001	2.288454
W	-3.054101	-1.603755	1.901244	O	-4.300296	-2.748755	2.336782
W	2.917515	1.840568	-1.898612	O	-0.231090	-5.113337	2.285965
W	-3.053175	1.606205	-1.898571	O	4.532257	-2.352063	2.335429
W	0.135343	-3.447682	-1.897977	O	4.545561	2.361663	2.284740
O	1.642003	-2.760253	-6.112311	O	-0.230679	5.101215	2.328948
O	1.563628	2.799569	-6.112370	O	2.388685	1.501380	3.695416
O	-3.211859	-0.048442	-6.105619	O	0.110502	2.787330	3.712511
O	-0.794280	1.331579	-5.780560	O	-2.488352	1.319589	3.691082
O	1.550170	0.016170	-5.782898	O	0.099448	-2.813558	3.694037
O	-0.761213	-1.357780	-5.781028	O	2.354850	-1.490706	3.716034
O	0.099122	2.815255	-3.695306	O	-2.465536	-1.293350	3.712084
O	2.389491	-1.504308	-3.697010	O	-0.794944	-1.332684	5.782091
O	-2.488016	-1.320995	-3.690102	O	1.550221	-0.016451	5.782879
O	2.355138	1.491019	-3.716725	O	-0.761620	1.357814	5.779498
O	-2.463274	1.292619	-3.710180	O	-3.212628	0.049625	6.107604
O	0.110198	-2.787012	-3.713242	O	1.641919	2.758552	6.111757
O	-0.234151	-5.100024	-2.330870	O	1.563050	-2.799909	6.112085
O	-4.314528	-2.756821	-2.286586	O	0.001710	0.001940	3.798477
O	-4.298920	2.749741	-2.339947	O	0.002884	-0.003051	-3.798210
O	-0.231711	5.115215	-2.285770	Sb	0.000631	0.000275	-0.000158
O	4.531503	2.349814	-2.335317	H	0.003548	-0.004831	-2.801432
O	4.544511	-2.364437	-2.284122	H	0.001671	0.001034	2.801749
O	-4.094625	-0.004333	-2.064217	O	-1.622828	-0.005368	-1.345475
O	2.042157	3.546536	-2.068342	O	0.808238	1.406421	-1.345840
O	2.049709	-3.546457	-2.064397	O	0.816217	-1.403592	-1.346702
O	3.230992	-0.003350	-1.614317	O	-1.622793	0.007108	1.345532
O	-1.617295	-2.797714	-1.602496	O	0.807433	-1.405788	1.345105
				O	0.817872	1.403822	1.344765

**Coordinates of  $\alpha^*-\text{[}(SbO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{10-}$  (single-reduced)**

W	1.671768	0.915975	4.904772	O	-2.508020	4.479235	-2.382637
W	-1.628371	0.989273	4.901659	O	2.438529	4.524568	-2.332785
W	-0.042363	-1.903918	4.897117	O	5.139104	-0.072795	-2.383835
W	0.042545	1.903356	-4.898166	O	1.330850	-0.769903	5.762926
W	1.628085	-0.989133	-4.901403	O	2.783911	0.091952	3.657558
W	-1.672076	-0.915292	-4.904221	O	-2.903355	1.645740	1.682763
W	1.857840	-2.933604	1.898177	O	0.026110	-3.336325	1.687459
W	3.495680	-0.077928	1.806872	O	-1.333668	-0.761298	5.761861
W	-3.477057	-0.138299	1.901755	O	1.416638	2.370962	3.683812
W	1.617589	3.077922	1.906515	O	2.880710	1.695349	1.684897
W	-1.814535	-2.979601	1.801461	O	0.004768	1.543734	5.760189
W	-1.676008	3.063795	1.806936	O	-3.497861	-2.055533	2.005391
W	1.676431	-3.064470	-1.808841	O	3.531929	-1.993132	2.008694
W	3.475521	0.136820	-1.900774	O	1.923383	3.388187	0.027899
W	-3.494815	0.077757	-1.806255	O	-1.463879	2.366907	3.654665
W	-1.617506	-3.078673	-1.905232	O	-1.319971	-2.447400	3.657610
W	-1.857000	2.932875	-1.900234	O	-3.899928	-0.027480	0.026578
W	1.816717	2.980482	-1.801002	O	1.340729	-2.406089	3.682598
O	-1.333047	0.773017	-5.760598	O	-2.760250	0.047267	3.681733
O	-1.343077	2.405546	-3.680332	O	3.897023	0.028103	-0.026003
O	-2.880862	-1.693335	-1.682826	O	-0.034941	4.056301	2.002786
O	-0.026678	3.333092	-1.683256	O	2.631556	4.415932	2.383556
O	-0.006785	-1.541014	-5.760911	O	-2.785104	1.633441	6.041954
O	1.315182	2.448743	-3.654627	O	2.805402	1.599691	6.045074
O	2.906543	-1.648215	-1.686434	O	-0.018857	-3.225793	6.040066
O	1.332878	0.763869	-5.761415	O	-2.702793	4.375975	2.332356
O	-3.532745	1.995359	-2.005038	O	-5.140377	0.075525	2.384425
O	3.495962	2.056582	-2.007285	O	-2.441457	-4.521927	2.332181
O	-1.922743	-3.387201	-0.027896	O	2.510853	-4.478037	2.383280
O	2.758373	-0.047277	-3.683301	O	5.144660	0.156905	2.333251
O	-1.420809	-2.365949	-3.681531	O	0.001577	0.003775	3.755982
O	-1.970974	3.358556	-0.025385	O	-0.001259	-0.004138	-3.755986
O	-2.783813	-0.086941	-3.656099	Sb	0.000268	-0.000125	-0.000034
O	1.464117	-2.370249	-3.658811	H	0.006587	0.014305	2.764126
O	1.970653	-3.355931	0.025798	H	-0.003533	-0.016870	-2.764144
O	0.033882	-4.055043	-2.003893	O	-1.445662	-0.858849	1.227979
O	2.702047	-4.378726	-2.330497	O	1.464272	-0.821963	1.230949
O	2.780611	-1.632787	-6.046864	O	-0.018787	1.675203	1.233736
O	0.017776	3.227641	-6.038248	O	0.020067	-1.674202	-1.234853
O	-2.807179	-1.597845	-6.043869	O	-1.465520	0.822484	-1.228773
O	-2.632445	-4.415023	-2.384297	O	1.446264	0.857139	-1.228019
O	-5.143848	-0.154599	-2.333579				

**Coordinates of  $\beta^*-\text{[}(SbO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{10-}$  (single-reduced)**

W	1.678699	0.906908	4.919279	O	-2.486446	4.509619	-2.358136
W	-1.623417	0.999453	4.917092	O	2.455848	4.537804	-2.297451
W	-0.053136	-1.904770	4.914724	O	5.149552	-0.104408	-2.357886
W	1.624837	1.033846	-4.934750	O	1.331627	-0.777734	5.773101
W	0.084521	-1.923366	-4.936144	O	2.793166	0.094599	3.668630
W	-1.707667	0.890314	-4.932587	O	-2.892767	1.646082	1.661811
W	1.847736	-2.923391	1.914174	O	0.019794	-3.323287	1.661190
W	3.491359	-0.088977	1.814170	O	-1.338040	-0.758390	5.773594
W	-3.463340	-0.136983	1.916479	O	1.437587	2.363838	3.697548
W	1.612030	3.065217	1.918591	O	2.870696	1.680287	1.659345
W	-1.821904	-2.971793	1.809752	O	0.011987	1.544527	5.771447
W	-1.665954	3.062827	1.813973	O	-3.496378	-2.052284	2.062498
W	1.663339	-3.086631	-1.797588	O	3.527681	-1.997239	2.059729
W	3.482402	0.135815	-1.900700	O	1.843114	3.388792	0.033405
W	-3.504612	0.098922	-1.795790	O	-1.472630	2.372966	3.668611
W	-1.623884	-3.086780	-1.902928	O	-1.316299	-2.459345	3.668939
W	-1.861991	2.946310	-1.898361	O	-3.859634	-0.099315	0.033827
W	1.839692	2.982484	-1.794140	O	1.328411	-2.419493	3.696905
O	-0.033782	1.561778	-5.745616	O	-2.763240	0.064820	3.697852
O	1.565029	2.408799	-3.688321	O	3.863763	-0.060522	-0.021607
O	-2.860055	-1.666789	-1.829765	O	-0.030010	4.052129	2.056459
O	-0.012553	3.302261	-1.829096	O	2.649336	4.395955	2.366882
O	-1.333068	-0.811723	-5.745039	O	-2.774232	1.642931	6.063583
O	2.827018	0.189707	-3.710776	O	2.808810	1.586035	6.065208
O	2.869463	-1.643479	-1.825985	O	-0.030791	-3.222323	6.061985
O	1.374530	-0.751975	-5.746131	O	-2.710776	4.370166	2.314861
O	-3.551747	2.025704	-1.870167	O	-5.132959	0.095411	2.370149
O	3.531747	2.060710	-1.867297	O	-2.428992	-4.530103	2.316986
O	-1.982555	-3.314928	-0.024154	O	2.483834	-4.484808	2.369578
O	1.305547	-2.558777	-3.688270	O	5.144272	0.168391	2.317395
O	-2.869667	0.147323	-3.689724	O	0.001743	0.003233	3.769617
O	-1.879700	3.371046	-0.022820	O	0.001220	-0.001200	-3.772372
O	-1.578350	2.352527	-3.712508	Sb	-0.000607	-0.001750	-0.001555
O	-1.247507	-2.545970	-3.713899	H	0.004502	0.011334	2.776566
O	2.013032	-3.293128	0.032470	H	0.004685	-0.004628	-2.779828
O	0.019915	-4.090488	-1.868980	O	-1.439400	-0.849100	1.251338
O	2.703808	-4.397774	-2.298259	O	1.451942	-0.823167	1.252192
O	0.081160	-3.186050	-6.144000	O	-0.015651	1.664276	1.254957
O	2.721701	1.660988	-6.141463	O	0.014467	-1.676542	-1.236305
O	-2.797015	1.524426	-6.142437	O	-1.460499	0.822448	-1.234163
O	-2.662965	-4.412173	-2.359333	O	1.443808	0.848849	-1.234334
O	-5.160413	-0.143210	-2.297848				



**Coordinates of  $\gamma^*-[({\rm SbO}_6){\rm W}_{18}{\rm O}_{54}({\rm OH})_2]^{10-}$  (single-reduced)**

W	1.701426	-0.891058	4.941181	O	-5.150911	-0.173597	-2.302794
W	-0.080637	1.919612	4.946837	O	-2.472489	4.507338	-2.360097
W	-1.623349	-1.028472	4.943549	O	2.422421	4.540961	-2.305398
W	1.622597	1.028832	-4.941152	O	5.145365	-0.113902	-2.361054
W	0.081699	-1.920364	-4.948455	O	0.033767	-1.556662	5.762850
W	-1.702329	0.888951	-4.941260	O	1.557826	-2.346661	3.716417
W	1.867196	-2.934671	1.904621	O	-2.866424	1.633612	1.795141
W	3.497013	-0.096682	1.809462	O	0.020157	-3.291185	1.781399
W	-3.481540	-0.143719	1.910775	O	-1.369932	0.751493	5.764080
W	1.613428	3.086561	1.911353	O	2.851564	-0.127550	3.694852
W	-1.831993	-2.972454	1.805204	O	2.852143	1.669653	1.793655
W	-1.661389	3.077575	1.809336	O	1.333214	0.810883	5.761110
W	1.662821	-3.076911	-1.811303	O	-3.530408	-2.065426	1.923400
W	3.480230	0.144748	-1.908454	O	3.558206	-2.019571	1.925520
W	-3.496691	0.096063	-1.807980	O	1.907229	3.344770	0.029009
W	-1.611152	-3.086826	-1.912874	O	1.254356	2.530398	3.720319
W	-1.867751	2.934069	-1.905784	O	-2.819991	-0.176262	3.721763
W	1.831602	2.974349	-1.805558	O	-3.849473	-0.024704	0.028664
O	-0.035684	1.554833	-5.761731	O	-1.535543	-2.400316	3.692936
O	1.532772	2.403318	-3.694084	O	-1.310964	2.536438	3.695535
O	-2.848737	-1.668090	-1.792632	O	3.850048	0.025882	-0.027732
O	-0.021324	3.290043	-1.780750	O	-0.026371	4.092176	1.918441
O	-1.334110	-0.812900	-5.760393	O	2.669555	4.401433	2.361324
O	2.816524	0.177628	-3.720059	O	-0.079259	3.192898	6.143182
O	2.867672	-1.633621	-1.796718	O	2.803496	-1.528798	6.137076
O	1.369477	-0.752209	-5.764054	O	-2.725572	-1.667077	6.139089
O	-3.559672	2.019535	-1.923844	O	-2.718937	4.376891	2.306255
O	3.528633	2.067526	-1.923751	O	-5.147182	0.116627	2.361299
O	-1.906600	-3.341977	-0.029281	O	-2.424857	-4.538513	2.304733
O	1.310659	-2.539850	-3.697015	O	2.472080	-4.507684	2.359579
O	-2.852289	0.127484	-3.693842	O	5.151528	0.171431	2.303696
O	-1.953522	3.318549	-0.025182	O	-0.002254	0.003947	3.783979
O	-1.558897	2.345516	-3.715727	O	0.001565	-0.005782	-3.783601
O	-1.254578	-2.532101	-3.720985	Sb	0.000067	0.000287	-0.000054
O	1.952547	-3.316985	0.024979	H	-0.008059	0.009928	2.790773
O	0.027027	-4.092317	-1.916507	H	0.005476	-0.016349	-2.790425
O	2.720632	-4.376887	-2.305067	O	-1.436953	-0.849449	1.248535
O	0.079334	-3.193402	-6.145284	O	1.459629	-0.817855	1.245482
O	2.724111	1.665398	-6.138585	O	-0.018159	1.671281	1.249311
O	-2.804116	1.527349	-6.137034	O	0.019429	-1.669331	-1.251539
O	-2.669606	-4.400893	-2.360070	O	-1.459885	0.818459	-1.245235
				O	1.437777	0.850596	-1.247412

**Coordinates of  $\alpha$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{7-}$**

W	2.915461	1.959365	-1.844122	W	-3.155162	1.534030	1.877600
W	-3.013026	-1.796150	-1.877560	W	3.071419	-1.705543	1.843268
W	-3.155929	1.543239	-1.843279	W	0.247849	-3.496961	1.876974
W	-0.050632	3.506249	-1.876531	W	-0.999960	1.620097	4.902539
W	0.240271	-3.503412	-1.841918	W	-0.901692	-1.674780	4.901277
W	3.065114	-1.710816	-1.877707	W	1.902206	0.057555	4.903652
W	-1.038545	1.594345	-4.901690	O	-1.501067	-2.832705	6.043165
W	1.900997	0.102914	-4.904789	O	-1.700167	2.719430	6.044477
W	-0.858235	-1.697687	-4.901326	O	3.206443	0.115774	6.043935
O	3.206483	0.154878	-6.044016	O	-1.555847	-0.056111	5.718905
O	-1.732853	2.697003	-6.044389	O	0.829893	-1.320724	5.719326
O	-1.464719	-2.852411	-6.042703	O	0.731326	1.379711	5.719784
O	0.846440	-1.313140	-5.720158	O	-2.413654	1.412433	3.631302
O	-1.553043	-0.074661	-5.718743	O	-0.249350	2.797031	3.622562
O	0.717071	1.386426	-5.719728	O	-2.296634	-1.614369	3.622294
O	-2.286459	-1.610786	-3.632137	O	2.546896	-1.180812	3.621722
O	2.539792	-1.175249	-3.630772	O	2.430881	1.385200	3.630433
O	2.438071	1.390776	-3.621395	O	-0.014770	-2.796793	3.631609
O	-0.011509	-2.806065	-3.621406	O	-4.247050	-2.941991	2.263595
O	-2.424318	1.415049	-3.623488	O	0.027466	-5.161729	2.282902
O	-0.250581	2.786432	-3.632152	O	4.672286	-2.205977	2.258338
O	4.468291	2.593719	-2.258368	O	4.460099	2.604313	2.281960
O	4.666125	-2.216663	-2.282285	O	-0.424670	5.148298	2.257928
O	0.014574	-5.164907	-2.260130	O	-4.485605	2.557445	2.286458
O	-4.251132	-2.929651	-2.287056	O	2.138359	-3.354604	2.130661
O	-4.481511	2.569818	-2.263069	O	1.836034	3.527274	2.129422
O	-0.411373	5.146330	-2.281694	O	-3.977390	-0.174153	2.130044
O	2.129513	-3.359411	-2.129750	O	3.308694	0.144383	1.481404
O	-3.978304	-0.163803	-2.130944	O	-1.780949	2.794324	1.482750
O	1.845574	3.522588	-2.130183	O	-1.530265	-2.937900	1.482465
O	3.308580	0.135760	-1.480945	I	-0.006695	-0.001161	-0.000122
O	-1.537435	-2.934954	-1.482766	H	0.017126	0.005459	2.753872
O	-1.774129	2.798628	-1.484123	O	0.002568	0.001270	3.749923
O	0.511986	-3.773694	0.008552	O	0.818504	-1.283471	1.324919
O	3.009941	2.328079	0.008215	O	0.692374	1.351274	1.325474
O	0.191795	3.800981	-0.008567	O	-1.533043	-0.073451	1.321872
O	-3.394377	-1.744303	-0.008707	O	0.003760	0.000392	-3.750029
O	3.197413	-2.066106	-0.008539	O	0.804040	-1.289635	-1.325119
O	-3.527884	1.450953	0.008263	O	-1.534947	-0.057736	-1.322085
W	-3.014034	-1.806501	1.842266	O	0.705623	1.345490	-1.325663
W	2.907651	1.964369	1.877107	H	0.021291	0.001779	-2.754008
W	-0.059484	3.511239	1.842459				

**Coordinates of  $\beta$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{7-}$**

W	0.918173	-1.668417	-4.902717	O	-1.866405	3.543718	1.998106
W	-1.907235	0.018413	-4.913608	O	-2.142250	-3.403108	1.992382
W	0.968871	1.629112	-4.882430	O	4.052973	-0.132825	2.018553
W	-3.138862	-1.713231	-1.853394	O	0.408956	5.174941	2.373987
W	3.221718	1.565707	-1.924338	O	-4.467528	2.560749	2.274074
W	3.007428	-1.814304	-1.829278	O	-4.691802	-2.261466	2.340318
W	-0.243410	-3.541969	-1.909091	O	0.030096	-5.136181	2.275348
W	0.082587	3.493921	-1.796544	O	4.260673	-2.892319	2.351809
W	-2.933376	1.968820	-1.908657	O	4.465910	2.606848	2.284192
O	-3.210338	0.092694	-6.054307	O	2.397157	-1.375941	3.644820
O	1.516038	-2.821933	-6.051935	O	-0.006311	2.796189	3.674667
O	1.658604	2.731932	-6.025272	O	-2.425488	-1.392920	3.638906
O	-0.747675	1.363625	-5.709688	O	-0.204540	-2.781289	3.624271
O	1.542780	-0.046684	-5.711517	O	-2.319338	1.580567	3.644192
O	-0.831548	-1.338488	-5.731956	O	2.524648	1.239246	3.633616
O	0.013693	-2.806020	-3.643828	O	0.723643	-1.346528	5.714529
O	2.306594	-1.609852	-3.629176	O	-1.576754	0.047366	5.747384
O	-2.574874	-1.209046	-3.633461	O	0.801319	1.338267	5.749949
O	0.233191	2.787655	-3.603983	O	-1.552471	2.827622	6.071732
O	2.427704	1.415380	-3.641148	O	3.193179	-0.071028	6.035050
O	-2.432990	1.370002	-3.634254	O	-1.681428	-2.730935	6.027862
O	-4.721410	-2.248662	-2.283623	W	0.043424	3.546834	1.935835
O	-4.466338	2.644864	-2.314631	W	-0.216745	-3.484155	1.818937
O	0.400402	5.135298	-2.243058	W	3.040831	-1.756260	1.893200
O	4.557604	2.567884	-2.355340	W	3.170801	1.559115	1.817978
O	4.266112	-2.915699	-2.274852	W	-3.102767	-1.762829	1.895448
O	-0.059806	-5.201818	-2.342818	W	-2.915651	1.939269	1.836612
O	-1.828414	3.503087	-2.085130	W	1.890041	-0.003812	4.895457
O	3.986393	-0.163546	-2.113060	W	-0.939224	1.660514	4.944795
O	-2.135619	-3.337800	-2.098386	W	-0.984627	-1.618754	4.897464
O	1.832993	2.824433	-1.528946	I	0.038565	-0.019883	-0.002711
O	1.550228	-2.989617	-1.533868	H	-0.096939	-0.138744	-2.747512
O	-3.373946	0.135923	-1.541056	O	-0.020987	-0.029029	-3.739760
O	-0.118614	3.820180	0.046512	O	-0.616838	1.389707	-1.274736
O	-3.264664	-2.030138	0.006307	O	1.562052	-0.142905	-1.302586
O	3.540919	1.546312	-0.032899	O	-0.810749	-1.221586	-1.345596
O	-3.048636	2.241641	-0.020089	O	-0.729053	-1.354304	1.277865
O	-0.434760	-3.811485	-0.036923	O	1.594169	-0.020925	1.307005
O	3.404849	-1.792824	0.014610	O	-0.722427	1.253731	1.360795
O	-3.322602	0.100919	1.597913	O	-0.025748	0.035703	3.752326
O	1.567676	-2.918507	1.565231	H	-0.114836	0.171470	2.762266
O	1.762731	2.814119	1.597708				

**Coordinates of  $\gamma$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{7-}$**

W	1.002672	-1.629861	-4.948365	O	3.362504	-0.008053	1.655958
W	-1.890007	-0.073570	-4.903846	O	2.016052	3.457473	1.968615
W	0.921348	1.654787	-4.890282	O	-4.042957	-0.001202	1.982774
W	-3.102891	-1.679903	-1.809592	O	2.002202	-3.471132	1.958799
W	3.026183	1.872187	-1.887042	O	4.617599	2.429583	2.313451
W	3.055773	-1.844305	-1.873514	O	-0.168929	5.186368	2.373420
W	0.100051	-3.541213	-1.924385	O	-4.384549	2.737732	2.294093
W	0.072272	3.492119	-1.814752	O	-4.440818	-2.761015	2.395960
W	-3.164099	1.694980	-1.938128	O	-0.195592	-5.139235	2.275304
O	-3.185816	-0.063462	-6.053224	O	4.583971	-2.460296	2.334413
O	1.648397	-2.764106	-6.090146	O	0.105195	-2.792740	3.625137
O	1.573218	2.785350	-6.029673	O	2.367270	-1.489303	3.636519
O	1.575213	0.009798	-5.741851	O	2.403495	1.517190	3.660708
O	-0.752360	-1.375799	-5.748811	O	-2.489028	1.315576	3.632227
O	-0.778201	1.315551	-5.708954	O	-2.485176	-1.293022	3.660448
O	2.405142	-1.515925	-3.661285	O	0.134786	2.797914	3.672655
O	-2.488851	-1.317473	-3.632863	O	-0.753222	1.375831	5.748410
O	0.104032	2.791707	-3.624495	O	-0.776802	-1.315866	5.708500
O	0.137351	-2.798360	-3.672590	O	1.574812	-0.009002	5.742789
O	2.366311	1.489835	-3.636547	O	1.647650	2.764916	6.089520
O	-2.486654	1.291613	-3.661050	O	1.575933	-2.784235	6.029976
O	-4.441192	2.760319	-2.396181	O	-3.185951	0.061118	6.052244
O	-0.198288	5.138657	-2.275888	W	3.054901	1.845342	1.872696
O	4.582626	2.462355	-2.334937	W	-3.163157	-1.696116	1.938378
O	4.619008	-2.427858	-2.313172	W	0.073643	-3.491994	1.815803
O	-0.167001	-5.186324	-2.372208	W	3.027149	-1.871256	1.886435
O	-4.383063	-2.739819	-2.293185	W	-3.103681	1.679145	1.809632
O	2.000509	3.471700	-1.958298	W	0.098446	3.541486	1.924933
O	2.018226	-3.456948	-1.968304	W	0.923526	-1.654529	4.890193
O	-4.042784	-0.000365	-1.983217	W	1.002596	1.629959	4.948075
O	-1.670166	-2.911691	-1.648630	W	-1.888948	0.072375	4.904143
O	-1.713995	2.886308	-1.633408	I	-0.047210	-0.000025	0.000018
O	3.362459	0.009439	-1.655992	H	0.109158	-0.191891	-2.759924
O	3.206579	2.081673	-0.000901	O	0.024029	-0.041430	-3.750357
O	-3.459794	1.741031	-0.037629	O	0.675013	1.380015	-1.267125
O	3.207122	-2.080092	0.000680	O	0.753346	-1.236249	-1.357566
O	0.209780	3.816276	0.040669	O	-1.576365	-0.085357	-1.293846
O	0.212488	-3.814740	-0.040351	O	0.752617	1.236931	1.357243
O	-3.458265	-1.742287	0.037588	O	-1.576220	0.084534	1.293720
O	-1.672160	2.911931	1.648490	O	0.675610	-1.379507	1.267528
O	-1.713252	-2.888148	1.632795	O	0.024639	0.040960	3.750287
				H	0.109346	0.191231	2.759834

**Coordinates of  $\alpha^*-\text{[}(IO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{7-}$**

W	-1.628991	0.972808	-4.878394	O	-0.031913	-3.957434	1.937648
W	1.657746	0.918200	-4.877802	O	3.445943	1.947491	1.937360
W	-0.033230	-1.899753	-4.875914	O	-3.407263	2.006656	1.941349
W	1.755317	3.106266	-1.878655	O	-5.213352	-0.057113	2.370937
W	-1.865980	-3.049320	-1.854144	O	-2.727190	-4.439763	2.386874
W	-3.569792	-0.034970	-1.878471	O	2.657078	-4.489074	2.372560
W	-1.707529	3.138540	-1.859233	O	5.213777	-0.143925	2.380205
W	1.814894	-3.074321	-1.878142	O	2.558840	4.542989	2.369279
W	3.574998	-0.092730	-1.861029	O	-2.475752	4.583289	2.381860
O	2.806315	1.572735	-5.998032	O	1.343277	2.435065	3.605817
O	-2.768181	1.645338	-5.997126	O	-1.288817	2.457401	3.613003
O	-0.042021	-3.223734	-5.993833	O	-2.779044	-0.055404	3.609830
O	-1.351252	-0.759440	-5.710454	O	1.439376	-2.378400	3.606806
O	0.017570	1.542844	-5.710412	O	2.777982	-0.108442	3.613202
O	1.327364	-0.792450	-5.711101	O	-1.478453	-2.346202	3.615031
O	1.479721	2.343892	-3.613362	O	-0.016265	-1.541538	5.708556
O	1.291578	-2.456663	-3.612537	O	1.352176	0.759367	5.709244
O	-2.776405	0.107572	-3.614440	O	-1.327923	0.793663	5.712365
O	-1.437684	2.376606	-3.607337	O	-2.804778	-1.571966	5.999791
O	-1.341844	-2.435169	-3.604598	O	0.044871	3.223366	5.996366
O	2.781224	0.052720	-3.610563	O	2.769850	-1.644420	5.995191
O	5.216479	0.055394	-2.372145	W	-3.572016	0.091447	1.859017
O	2.478424	-4.584344	-2.384758	W	3.572849	0.032406	1.876197
O	-2.554919	-4.545376	-2.369062	W	1.868080	3.046596	1.858111
O	-5.211623	0.139622	-2.379964	W	-1.811275	3.072726	1.877948
O	-2.654165	4.487404	-2.371269	W	1.709950	-3.141359	1.858449
O	2.728008	4.438280	-2.385570	W	-1.753640	-3.107748	1.881822
O	0.033897	3.955316	-1.936025	W	0.033700	1.898477	4.879399
O	3.410756	-2.008613	-1.939700	W	-1.656691	-0.918180	4.878846
O	-3.443445	-1.949774	-1.936179	W	1.631012	-0.973605	4.875202
O	3.026827	1.709474	-1.680380	I	0.001733	-0.001686	0.000242
O	-0.029568	-3.470433	-1.670539	H	-0.001373	-0.009341	-2.723127
O	-2.998384	1.764280	-1.679895	O	-0.001277	-0.002891	-3.715639
O	2.002604	3.378447	-0.007006	O	1.358489	-0.797692	-1.174873
O	-1.999536	-3.383109	0.007881	O	-1.370543	-0.775092	-1.172505
O	-1.935056	3.414434	0.004438	O	0.012911	1.576559	-1.167803
O	1.937802	-3.420655	-0.004780	O	-0.010959	-1.581503	1.164806
O	3.928037	-0.038731	0.003567	O	1.372911	0.773415	1.172855
O	-3.923730	0.039859	-0.004125	O	-1.353176	0.794887	1.178783
O	2.998824	-1.765734	1.678448	O	0.000635	0.004140	3.715541
O	0.032668	3.471409	1.669566	H	-0.007334	0.022807	2.723216
O	-3.023464	-1.711228	1.678812				

**Coordinates of  $\beta^*-\text{[}(IO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{7-}$**

W	1.898211	0.026697	4.889288	O	1.758782	-2.957010	-1.819397
W	-0.929425	-1.653938	4.889431	O	1.681475	3.006149	-1.820749
W	-0.970572	1.636149	4.889309	O	-3.441855	-0.044896	-1.815428
W	-3.147156	1.687132	1.877618	O	-4.543884	-2.583292	-2.351293
W	0.112058	-3.565655	1.878016	O	4.509356	-2.640180	-2.350236
W	3.030895	1.883101	1.875457	O	0.030781	5.227976	-2.352569
W	-3.101709	-1.767995	1.875619	O	0.169565	-5.224135	-2.348026
W	3.080799	-1.798716	1.875092	O	4.438666	2.759280	-2.350906
W	0.016514	3.571444	1.873332	O	-4.609961	2.464175	-2.351919
O	-1.572888	-2.802390	6.015517	O	-0.128686	-2.841176	-3.636016
O	3.214934	0.045666	6.014919	O	2.521361	1.309208	-3.635801
O	-1.643559	2.767050	6.015494	O	-2.395865	1.528627	-3.634241
O	-1.548870	-0.016862	5.716523	O	-2.355075	-1.591514	-3.634936
O	0.790902	-1.327918	5.717862	O	2.555795	-1.242207	-3.636661
O	0.756644	1.354921	5.717104	O	-0.203350	2.835653	-3.637307
O	-2.384682	1.445794	3.621271	O	-1.564298	-0.021488	-5.697928
O	-2.345559	-1.503152	3.621016	O	0.798733	-1.344510	-5.698057
O	2.475655	-1.275300	3.620871	O	0.762010	1.364990	-5.698026
O	-0.134247	2.787673	3.620583	O	-1.559701	-2.781226	-6.074064
O	-0.059322	-2.784782	3.622993	O	3.184881	0.043249	-6.076259
O	2.440891	1.345022	3.620760	O	-1.633602	2.737742	-6.074641
O	-4.419628	-2.768871	2.364584	W	-0.028573	-3.579832	-1.862930
O	-4.492141	2.652638	2.364014	W	3.112461	1.767365	-1.865421
O	-0.051810	-5.213354	2.363739	W	-3.087685	1.814572	-1.862847
O	4.540338	2.563828	2.361314	W	3.158172	-1.682085	-1.865829
O	4.607585	-2.438051	2.362639	W	-0.122470	3.578747	-1.867895
O	-0.190797	5.214196	2.359313	W	1.910262	0.025780	-4.903322
O	2.023332	-3.399673	1.989602	W	-0.981096	1.642313	-4.902183
O	1.931569	3.455463	1.987568	W	-0.935230	-1.670168	-4.901002
O	-3.959471	-0.051396	1.986627	W	-3.038812	-1.893796	-1.864208
O	3.456451	0.047394	1.647124	I	-0.001806	0.001123	-0.000222
O	-1.690664	-3.017227	1.651184	H	0.006109	0.004412	2.730799
O	-1.771076	2.974875	1.648438	O	0.000076	0.003081	3.724090
O	-3.388160	-1.933923	0.004052	O	-1.572162	-0.019648	1.179747
O	-3.439032	1.845016	0.003988	O	0.800474	-1.346081	1.183613
O	3.363431	-1.968160	0.003212	O	0.763565	1.369755	1.183607
O	0.020542	3.899006	0.001515	O	-0.000554	-0.000542	-3.726272
O	0.123430	-3.894178	0.004869	O	-0.770304	-1.374111	-1.174696
O	3.309628	2.057830	0.002706	O	1.574242	0.021900	-1.174185
O	-2.041591	3.430600	-1.810676	O	-0.806319	1.355509	-1.174554
O	3.989249	0.053304	-1.808919	H	0.000189	-0.001163	-2.733614
O	-1.950654	-3.482122	-1.809452				



### Coordinates of $\gamma^*-[{\rm IO}_6]{\rm W}_{18}{\rm O}_{54}({\rm OH})_2]^{7-}$

W	-0.002974	-1.908360	-4.908019	O	-0.024381	-3.432854	1.777769
W	-1.647503	0.960549	-4.906307	O	0.029690	3.996740	1.853837
W	1.659713	0.949796	-4.905850	O	-3.473441	-1.970002	1.854650
W	-3.576642	0.104760	-1.868919	O	3.446381	-2.020525	1.857085
W	3.577239	0.049182	-1.875736	O	5.224716	0.083520	2.354078
W	1.699940	-3.150242	-1.867250	O	2.749263	4.441626	2.358436
W	-1.743940	-3.119832	-1.877741	O	-2.682911	4.484157	2.351179
W	1.880885	3.047090	-1.866061	O	-5.219060	0.163387	2.357163
W	-1.828442	3.072760	-1.875925	O	-2.539991	-4.562214	2.353390
O	-2.753425	1.611183	-6.069745	O	2.471208	-4.598206	2.360429
O	-0.013393	-3.191877	-6.071158	O	1.525469	-2.379343	3.640349
O	2.775111	1.584383	-6.069136	O	1.299825	2.515271	3.641203
O	1.351257	-0.787592	-5.708878	O	-1.267212	2.535195	3.637640
O	-1.353475	-0.773777	-5.708560	O	2.826477	-0.165454	3.637969
O	0.010901	1.559443	-5.709038	O	-1.557496	-2.360181	3.635755
O	-1.297619	-2.512650	-3.640947	O	-2.826406	-0.127946	3.639716
O	1.269338	-2.532986	-3.637454	O	2.755953	-1.608101	6.069772
O	2.828363	0.130666	-3.640146	O	-2.773572	-1.580672	6.068175
O	-1.521958	2.381453	-3.640141	O	0.013454	3.194549	6.071131
O	-2.824334	0.168289	-3.638215	O	1.355849	0.776571	5.709205
O	1.560726	2.363578	-3.636779	O	-0.008541	-1.557047	5.708092
O	-5.222142	-0.080743	-2.354857	O	-1.348963	0.790038	5.708617
O	-2.469335	4.599982	-2.360545	W	1.831100	-3.070489	1.876303
O	2.543929	4.564273	-2.352563	W	-1.698155	3.151750	1.868021
O	5.221019	-0.161298	-2.357149	W	-3.575486	-0.047100	1.874889
O	2.684311	-4.482857	-2.350629	W	-1.877912	-3.044842	1.866117
O	-2.747038	-4.439172	-2.358710	W	1.746071	3.122159	1.877946
O	-3.443397	2.022991	-1.857219	W	3.579181	-0.102254	1.868355
O	3.475877	1.972192	-1.854834	W	-1.657362	-0.946924	4.905227
O	-0.027527	-3.994165	-1.853758	W	1.650271	-0.957737	4.906042
O	-2.986132	-1.694651	-1.778890	W	0.005754	1.910723	4.908372
O	0.027329	3.436299	-1.778972	I	0.001119	0.001029	0.000167
O	2.962365	-1.738517	-1.778116	H	0.004087	-0.002236	-2.739655
O	3.893092	-0.026286	-0.001101	O	0.002963	-0.000820	-3.733136
O	1.970090	3.357389	0.002516	O	1.367227	0.775939	-1.179627
O	1.925278	-3.381418	0.002971	O	-0.010009	-1.569691	-1.179932
O	-1.921171	3.385165	-0.002862	O	-1.353515	0.795855	-1.179416
O	-3.891745	0.028057	0.000797	O	1.355963	-0.793379	1.179782
O	-1.968909	-3.355461	-0.002439	O	0.012364	1.571684	1.180905
O	2.988543	1.697250	1.779411	O	-1.365459	-0.773619	1.179068
O	-2.960014	1.740589	1.777154	O	-0.000217	0.003783	3.732925
				H	0.000071	0.007555	2.739452

### Coordinates of $\alpha$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\right]^{8-}$

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W	0.063090	-3.543023	1.643162	O	-4.343837	2.770101	-2.419947
W	-3.170219	1.629388	-1.860073	O	-1.799393	-1.332419	-5.127832
W	-1.611541	-0.869088	-3.466253	O	0.353154	-4.883741	-2.719099
W	0.021902	-3.579862	-1.622814	O	5.719287	1.694562	0.001199
W	-3.116092	1.575199	1.823656	O	4.345703	-0.087217	-1.507873
W	-1.612745	-0.827670	3.468692	O	0.817345	2.863561	3.471935
W	-3.693156	-3.347511	-1.654951	O	3.958876	-2.266299	0.004503
W	-3.639385	-3.329047	1.641366	O	4.500821	3.696115	1.349493
W	-5.174498	-0.915430	-0.013723	O	3.182600	1.815400	-2.795729
W	0.053479	3.502070	-1.827384	O	0.796272	2.854290	-3.470508
W	3.225400	-1.611962	1.648238	O	4.488917	3.676177	-1.349542
W	3.186763	-1.639728	-1.637466	O	2.139728	-0.602696	2.844175
W	1.534304	1.084878	-3.463099	O	2.124170	-0.608398	-2.829108
W	1.554717	1.091674	3.477258	O	-1.624415	2.655161	-2.209759
W	0.053553	3.510546	1.839193	O	1.813753	4.052728	-1.290970
W	4.691307	1.762009	-1.646511	O	3.203533	1.821808	2.803363
W	3.205102	4.213835	-0.004911	O	-0.166629	0.354310	3.800713
W	4.710217	1.795912	1.650073	O	4.363176	-0.072036	1.518936
O	-5.299209	-2.299206	-1.374006	O	1.821254	4.049763	1.279646
O	-3.022676	-2.000596	-2.809935	O	-0.185863	0.337863	-3.770422
O	-2.872122	0.619641	3.466662	O	-0.440362	3.583787	0.002864
O	-2.862829	0.602684	-3.436941	O	-0.450190	5.066096	-2.385167
O	-5.263613	-2.293447	1.330494	O	3.504136	5.925753	-0.009898
O	-1.863868	-3.888328	-1.516363	O	6.010098	1.811204	-2.776850
O	0.279617	-4.540689	0.012677	O	6.032854	1.841801	2.776268
O	-4.052211	-4.280866	-0.007484	O	-0.424288	5.085826	2.388833
O	-2.977960	2.060462	-0.016626	O	2.069903	1.035991	5.133786
O	-0.376599	-2.164529	-2.843800	O	4.247552	-2.479440	2.749893
O	1.858932	-2.941776	1.600372	O	4.218056	-2.495545	-2.741186
O	-1.844431	-3.878563	1.508333	O	2.038456	1.018996	-5.122686
O	-4.395227	0.252121	1.273633	Te	0.025109	0.005354	0.013038
O	-1.601848	2.668804	2.207884	H	2.365136	1.479375	0.053879
O	-4.415779	0.272362	-1.296067	H	-2.396005	-1.316323	-0.222764
O	-3.014162	-1.968963	2.790540	O	3.220894	1.991192	0.010157
O	1.831551	-2.950691	-1.578173	O	0.766797	1.381599	1.351663
O	-0.377286	-2.131872	2.839960	O	1.976005	-0.618708	0.003178
O	0.356714	-4.850406	2.752260	O	0.727081	1.383068	-1.349511
O	-4.288138	-4.479662	2.768048	O	-3.191113	-1.908434	-0.045893
O	-4.330747	-4.509145	-2.780906	O	-1.509797	0.009207	1.375645
O	-6.838015	-0.412475	-0.005195	O	-1.507115	-0.112724	-1.298151
O	-1.806661	-1.315807	5.124555	O	-0.253701	-2.042999	0.031584
O	-4.286266	2.726568	2.383444				

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### Coordinates of $\beta$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]^{8-}$

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W	-3.106569	-1.601729	-1.803471	O	-0.249036	5.134956	-2.316412
W	2.945510	1.881067	-1.801689	O	4.538180	2.389555	-2.268503
W	2.921597	-1.809562	-1.848049	O	4.524449	-2.329578	-2.261609
W	0.090528	-3.436093	-1.839147	O	-0.264686	-5.085535	-2.242853
W	0.110302	3.503397	-1.840059	O	0.792398	-1.362147	5.769341
W	-3.078835	1.661176	-1.833888	O	2.488066	-1.272636	3.666025
W	0.931360	-1.640541	-4.927145	O	-4.011106	-0.024368	2.174833
W	-1.909406	0.001531	-4.878167	O	1.957469	-3.418313	2.150177
W	0.956269	1.643673	-4.875499	O	-1.540157	-0.001694	5.746398
W	0.110901	3.472110	1.858758	O	2.526542	1.303987	3.680403
W	0.070030	-3.521968	1.895267	O	2.035637	3.478503	2.171094
W	2.947789	-1.789149	1.868895	O	0.787794	1.344096	5.745428
W	3.057283	1.892458	1.939004	O	-1.693308	-2.877285	1.560890
W	-3.153147	-1.707032	1.935790	O	3.329493	0.045069	1.541639
W	-3.057394	1.640214	1.865826	O	3.170751	2.213528	0.055539
W	1.904596	-0.004432	4.947565	O	-0.116200	2.808682	3.667625
W	-0.945238	1.655078	4.902630	O	-2.386096	-1.533590	3.688199
W	-0.946089	-1.647515	4.946722	O	-3.496496	1.661747	0.022085
O	1.549792	-0.004793	-5.735313	O	-0.143258	-2.810139	3.672469
O	2.344717	-1.470937	-3.645943	O	-2.357762	1.507588	3.667684
O	-1.638174	2.849483	-1.509224	O	3.069377	-2.141108	0.020255
O	3.241801	0.029497	-1.524804	O	-1.677335	2.911557	1.542237
O	-0.774028	1.332600	-5.706055	O	-0.142601	5.136858	2.308059
O	0.078666	-2.776622	-3.640237	O	-1.591862	2.771164	6.065905
O	-1.657674	-2.791003	-1.514076	O	3.208241	-0.014594	6.097368
O	-0.794263	-1.351906	-5.733611	O	-1.584027	-2.771965	6.107350
O	2.026059	3.546888	-2.020141	O	-4.370085	2.688563	2.322583
O	2.000457	-3.485869	-2.002943	O	-4.431958	-2.793077	2.354416
O	-3.494166	-1.639109	0.061998	O	-0.205949	-5.181005	2.299133
O	-2.476066	-1.292924	-3.613527	O	4.523091	-2.393155	2.269927
O	0.086842	2.792353	-3.634808	O	4.641959	2.449823	2.349614
O	0.320590	3.870922	0.011774	Te	-0.033932	0.074332	0.031705
O	2.360135	1.489480	-3.619804	H	0.123824	-0.193836	2.780151
O	-2.466715	1.326275	-3.631821	H	0.071052	-0.144514	-2.747142
O	0.303770	-3.743113	0.040879	O	0.022484	-0.030005	3.769624
O	-4.086810	0.028412	-2.005264	O	-1.593010	0.094117	1.327035
O	-4.348732	-2.723072	-2.262928	O	0.756726	-1.209879	1.382003
O	-3.221797	0.003721	-6.016456	O	0.709699	1.460309	1.319895
O	1.592441	-2.791380	-6.050081	O	0.004157	-0.018549	-3.738879
O	1.609240	2.773746	-6.022106	O	0.782627	1.411292	-1.295330
O	-4.315284	2.790136	-2.299493	O	0.732493	-1.290804	-1.328405
				O	-1.611520	0.040978	-1.295330

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### Coordinates of $\gamma$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ]<sup>8-</sup>

W	-0.141193	-3.471042	-1.843788	O	-4.532168	2.370800	-2.320531
W	-0.097571	3.578749	-1.893950	O	0.211782	5.220482	-2.339069
W	3.128183	1.722881	-1.828115	O	4.397143	2.810680	-2.270400
W	3.036311	-1.614524	-1.789348	O	4.318768	-2.697058	-2.240153
W	-2.951482	1.833259	-1.842628	O	0.807025	-1.348619	5.796194
W	-2.948458	-1.861130	-1.832415	O	2.512618	-1.299453	3.724989
W	1.911556	0.028469	-4.868236	O	-3.285568	0.014817	1.590806
W	-0.946454	-1.625954	-4.894400	O	1.657869	-2.881135	1.677205
W	-0.942080	1.663454	-4.926584	O	-1.508667	0.009701	5.740061
W	-0.141538	3.509186	1.849223	O	2.494726	1.307218	3.719428
W	-0.096632	-3.583177	1.899432	O	1.634949	2.871803	1.640137
W	3.116066	-1.692022	1.949226	O	0.804138	1.365511	5.792960
W	3.047460	1.649600	1.918860	O	-1.994631	-3.504049	2.048506
W	-2.941491	-1.818710	1.876022	O	4.023662	-0.007789	2.026551
W	-2.939757	1.863909	1.874072	O	-0.251600	3.848468	-0.014725
W	1.916155	0.009017	5.006379	O	-0.097360	2.817237	3.671772
W	-0.918853	1.663897	4.916303	O	-2.335947	-1.468333	3.675235
W	-0.917579	-1.642402	4.924770	O	-3.192097	-2.168089	0.022338
O	0.795116	1.374386	-5.723448	O	-0.085633	-2.809424	3.682788
O	2.488188	1.340786	-3.612656	O	-2.350014	1.492918	3.673179
O	-3.279464	-0.004598	-1.569104	O	3.398404	1.709242	0.032585
O	1.654865	2.904322	-1.607960	O	-2.047107	3.562820	2.047775
O	-1.544592	0.021068	-5.741366	O	0.185383	5.153586	2.305730
O	2.463130	-1.275386	-3.606381	O	-1.580489	2.783449	6.067029
O	1.629032	-2.851833	-1.559411	O	3.228383	0.012479	6.147541
O	0.788282	-1.312683	-5.701239	O	-1.583863	-2.760429	6.073841
O	-1.998740	3.513048	-1.996498	O	-4.532402	2.396097	2.327423
O	4.022933	0.041521	-1.947232	O	-4.519700	-2.366930	2.355586
O	-0.251767	-3.850358	0.046047	O	0.218143	-5.215788	2.374416
O	-0.104612	-2.790419	-3.643778	O	4.388580	-2.779712	2.384429
O	-2.343825	1.508588	-3.650763	O	4.327797	2.742042	2.341899
O	-3.174609	2.170754	0.006098	Te	-0.034978	0.002538	0.035499
O	-0.097778	2.835129	-3.658459	H	0.313718	0.012193	2.799316
O	-2.363001	-1.483661	-3.647344	H	-0.072019	0.155696	-2.742996
O	3.408608	-1.683503	0.076779	O	0.072843	0.007434	3.783152
O	-2.053372	-3.553602	-2.012817	O	-0.841325	-1.302506	1.315747
O	0.190585	-5.120253	-2.285958	O	1.458293	0.067344	1.425731
O	-1.587466	-2.751890	-6.050537	O	-0.834695	1.450307	1.311411
O	3.224830	0.021729	-6.004765	O	-0.007118	0.042699	-3.736522
O	-1.596566	2.795414	-6.071801	O	-0.831207	-1.440108	-1.294554
O	-4.539778	-2.381971	-2.305247	O	-0.800895	1.272133	-1.327613
				O	1.520078	-0.066087	-1.242556

**Coordinates of  $\alpha^*-\text{[TeO}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$**

W	3.523536	-0.093987	1.871596	O	-5.183348	0.110474	2.349338
W	-3.522220	-0.049538	1.892757	O	-2.453242	-4.541879	2.366742
W	-1.802438	-3.017508	1.867691	O	2.498614	-4.517883	2.440809
W	1.876785	-2.982201	1.932038	O	1.306964	0.776025	-5.682892
W	-1.712474	3.150681	1.925288	O	2.757414	-0.039713	-3.583068
W	1.664085	3.071523	1.810153	O	-3.421890	1.987108	-1.912453
W	-0.036585	-1.878322	4.923955	O	3.539704	2.047201	-1.970824
W	1.620272	0.963422	4.850410	O	-1.374420	0.794590	-5.726240
W	-1.663532	0.951835	4.930599	O	1.414945	-2.323434	-3.558832
W	-1.714689	-3.113722	-1.870377	O	-0.024173	-3.986590	-1.914779
W	1.883801	3.005703	-1.877566	O	-0.016770	-1.520454	-5.681962
W	3.535983	0.121746	-1.813788	O	0.036241	3.387509	-1.622467
W	1.663433	-3.039895	-1.759431	O	2.945272	-1.664653	-1.619502
W	-1.787579	3.001338	-1.806554	O	2.009985	3.430628	-0.013322
W	-3.531510	0.082062	-1.851719	O	-1.469283	-2.353618	-3.608303
W	1.632604	-0.936015	-4.798981	O	-1.317073	2.452666	-3.600072
W	-1.654798	-0.928827	-4.884166	O	-1.951704	3.363525	0.051858
W	-0.025629	1.904193	-4.873435	O	1.318182	2.438539	-3.611715
O	-1.381491	-0.771701	5.777868	O	-2.795593	-0.066051	-3.617504
O	-1.326322	-2.439686	3.651026	O	-1.956353	-3.345871	0.008125
O	-0.023992	4.024686	1.976454	O	-2.968345	-1.707604	-1.663817
O	-3.403813	-1.962232	1.950910	O	-2.714572	-4.439485	-2.350768
O	-0.024535	1.543823	5.733303	O	-2.803166	-1.600444	-6.002177
O	1.311186	-2.409611	3.659160	O	2.772740	-1.609878	-5.920437
O	3.530577	-2.023389	2.012788	O	-0.018871	3.233710	-5.994399
O	1.299093	-0.752670	5.729052	O	-5.189758	-0.095741	-2.310862
O	-2.975216	1.742023	1.723622	O	-2.442206	4.528586	-2.301442
O	0.026008	-3.375557	1.679733	O	2.504942	4.541468	-2.390010
O	3.996961	0.021197	0.026033	O	5.169056	-0.097085	-2.366278
O	2.750208	0.062142	3.635050	O	2.631128	-4.373848	-2.315681
O	-1.473726	2.379618	3.660748	Te	0.099934	0.023635	0.026790
O	-3.821518	0.018852	0.020887	H	-0.299565	0.175890	-2.707470
O	-2.800479	0.087585	3.667416	H	-0.330660	-0.160842	2.752986
O	1.414055	2.349682	3.610369	O	-0.067387	0.040832	-3.678642
O	1.994978	-3.398240	0.066206	O	-1.258915	0.786495	-1.250170
O	2.950553	1.698650	1.678986	O	1.535340	0.850571	-1.143133
O	5.161366	0.109561	2.417875	O	0.085241	-1.627659	-1.106854
O	2.763084	1.631219	5.972339	O	-0.079536	-0.018217	3.724015
O	-0.022635	-3.208373	6.043989	O	0.099904	1.679784	1.155463
O	-2.811333	1.621168	6.050921	O	-1.249659	-0.711979	1.310050
O	2.624719	4.409501	2.373519	O	1.537348	-0.810609	1.187770
O	-2.712559	4.476204	2.405747				

**Coordinates of  $\beta^*-\text{[TeO}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$**

W	-1.920861	0.010472	4.892734	O	-1.697570	2.975452	-1.835301
W	0.931949	1.653272	4.944320	O	-1.702587	-2.959614	-1.828718
W	0.930306	-1.631964	4.947284	O	3.370896	0.008752	-1.766084
W	3.091152	-1.651928	1.924802	O	-4.447173	2.705417	-2.339501
W	-0.088652	3.507963	1.900275	O	-0.136461	-5.250665	-2.326260
W	-2.962589	-1.825330	1.845952	O	4.480228	2.524401	-2.276063
W	3.089818	1.680085	1.917051	O	4.476846	-2.512627	-2.271290
W	-2.965540	1.845656	1.850374	O	-0.133174	5.270605	-2.326840
W	-0.083495	-3.486806	1.898892	O	-4.450650	-2.684900	-2.339106
O	-3.254778	0.011622	6.005067	O	0.152932	2.879526	-3.621088
O	1.581372	-2.779044	6.077880	O	-2.566392	-1.261695	-3.666187
O	1.583235	2.802477	6.073255	O	-2.568539	1.276499	-3.667394
O	1.532678	0.011460	5.786150	O	0.150872	-2.855686	-3.616001
O	-0.794718	1.345070	5.756569	O	2.337125	1.566691	-3.598009
O	-0.795526	-1.323389	5.759001	O	2.337060	-1.546531	-3.592425
O	0.074645	2.783511	3.668441	O	-0.803244	1.375526	-5.705245
O	-2.438953	-1.303489	3.637473	O	-0.801669	-1.357667	-5.700384
O	-2.440042	1.328996	3.638866	O	1.525504	0.010470	-5.639000
O	0.078863	-2.760869	3.669692	O	1.583731	2.760664	-6.040049
O	2.342916	1.479859	3.685826	O	-3.196391	0.007356	-6.129708
O	2.346407	-1.456244	3.690313	O	1.587259	-2.740050	-6.033887
O	0.150025	5.160283	2.369525	W	2.954396	1.846444	-1.788985
O	-4.513245	-2.444932	2.318418	W	0.084896	3.628541	-1.827835
O	4.392436	-2.687552	2.419690	W	-3.103857	-1.698828	-1.882046
O	4.386857	2.717616	2.419759	W	2.952773	-1.832991	-1.780089
O	-4.519165	2.462627	2.315864	W	-3.101714	1.718920	-1.878862
O	0.157852	-5.137771	2.371137	W	0.080519	-3.607672	-1.830180
O	-2.002317	3.495578	2.027964	W	-1.923619	0.009455	-4.944587
O	4.028428	0.014382	2.085554	W	0.932881	-1.652529	-4.850088
O	-1.997062	-3.473291	2.031125	W	0.928030	1.677078	-4.852982
O	1.682277	2.923950	1.653242	Te	0.045237	0.011114	0.027855
O	1.685494	-2.897442	1.654417	H	0.096280	0.008849	2.780570
O	-3.338830	0.010625	1.622180	O	0.006979	0.010597	3.769899
O	3.414511	1.870642	0.065157	O	1.616143	0.012534	1.309907
O	3.416351	-1.843919	0.068606	O	-0.077820	0.012041	-3.693853
O	-3.274660	2.016052	-0.012019	O	0.895578	1.427502	-1.105191
O	-0.097435	-3.896140	0.019762	O	-0.798706	1.422665	1.220919
O	-0.098945	3.916791	0.018060	O	-0.798453	-1.400256	1.221243
O	-3.277840	-1.994330	-0.011805	O	-1.474639	0.009946	-1.270320
O	1.990200	3.541119	-1.800749	O	0.895272	-1.408229	-1.101782
O	1.987947	-3.523346	-1.796605	H	-0.331931	0.012902	-2.718366
O	-3.979101	0.009817	-1.785447				



**Coordinates of  $\gamma^*-\text{[}(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{8-}$**

W	-1.898401	-3.061224	-1.927232	O	-2.705074	4.465289	-2.380080
W	1.729887	3.131448	-1.799592	O	2.745259	4.449456	-2.279294
W	3.459134	-0.143036	-1.851220	O	5.128615	0.038787	-2.288515
W	1.818986	-3.093520	-1.894659	O	2.434544	-4.638640	-2.372025
W	-1.699027	3.135329	-1.916026	O	-1.331536	-0.746314	5.688850
W	-3.504155	-0.091679	-1.813030	O	-1.302564	-2.491790	3.617230
W	1.643697	-0.989010	-4.935071	O	0.019523	3.350432	1.771283
W	-1.666300	-0.892333	-4.911031	O	-2.893780	-1.638790	1.703651
W	0.083905	1.927951	-4.911946	O	0.041580	1.574522	5.761640
W	3.479729	0.063606	1.875276	O	1.263848	-2.525298	3.633627
W	-3.488891	0.144388	1.889854	O	2.875680	-1.714779	1.757343
W	-1.686857	-3.077312	1.798039	O	1.359285	-0.812546	5.746175
W	1.630361	-3.138158	1.838890	O	-3.515728	2.073705	1.907404
W	-1.849137	3.017301	1.816080	O	-0.037189	-4.077964	1.880547
W	1.860136	3.017203	1.958149	O	3.773780	0.007924	0.010445
W	-0.030193	-1.908730	4.871855	O	2.838958	0.135915	3.695117
W	1.686181	0.907039	4.989590	O	-1.513558	2.396469	3.648053
W	-1.603270	1.013826	4.904288	O	-1.940347	3.384842	-0.020793
O	1.390215	0.771907	-5.729622	O	-2.787662	0.167306	3.662365
O	2.813593	-0.199152	-3.662880	O	1.582872	2.369646	3.719288
O	-2.933736	1.726443	-1.789760	O	1.893007	-3.401647	-0.024308
O	2.930010	1.682080	-1.808210	O	3.475838	1.995297	1.891741
O	-1.312833	0.818024	-5.713530	O	5.139067	-0.184916	2.316567
O	1.535240	-2.413796	-3.678291	O	2.806697	1.540348	6.158297
O	-0.036946	-3.420503	-1.814442	O	-0.048967	-3.194348	6.038639
O	-0.013697	-1.549832	-5.726438	O	-2.719266	1.647537	6.073523
O	0.018992	4.019560	-1.848440	O	2.474735	4.574573	2.394873
O	3.441486	-2.075223	-1.861251	O	-2.438157	4.566526	2.328755
O	-3.894362	0.067517	0.011306	O	-5.140955	-0.107490	2.366300
O	-1.556981	-2.356791	-3.672934	O	-2.739916	-4.363493	2.305984
O	-1.254789	2.546548	-3.671036	O	2.658244	-4.447861	2.321782
O	1.974412	3.309530	0.047077	Te	-0.036670	-0.006996	0.011365
O	1.305979	2.561527	-3.640421	H	0.288807	0.168038	2.765528
O	-2.800652	-0.119814	-3.637915	H	0.097463	0.018045	-2.749656
O	-1.967048	-3.395773	-0.055655	O	0.063106	0.037522	3.739969
O	-3.509244	-2.026455	-1.887914	O	-1.457560	0.837748	1.206916
O	-2.531197	-4.591815	-2.427940	O	-0.052060	-1.691272	1.152406
O	-2.782255	-1.516302	-6.085579	O	1.311817	0.705103	1.338551
O	2.751023	-1.629431	-6.110184	O	0.033126	0.012353	-3.743168
O	0.083512	3.200688	-6.093007	O	-1.460205	-0.770856	-1.174710
O	-5.148163	0.112111	-2.337991	O	0.003155	1.589278	-1.154761
				O	1.361191	-0.787343	-1.210433

**Coordinates of  $\alpha$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ] $^{8-}$**

W	2.862583	1.952496	-1.830607	W	-3.120079	1.492369	1.867937
W	-2.981814	-1.752524	-1.867916	W	3.018811	-1.703578	1.829965
W	-3.122983	1.502226	-1.830353	W	0.267386	-3.446512	1.868010
W	-0.026731	3.458334	-1.867411	W	-0.998552	1.620861	4.904986
W	0.260623	-3.455950	-1.829379	W	-0.903299	-1.673624	4.904875
W	3.008805	-1.706485	-1.867598	W	1.900730	0.055108	4.905012
W	-1.040331	1.593246	-4.905127	O	-1.505583	-2.837615	6.045710
W	1.899099	0.104271	-4.905801	O	-1.705043	2.723943	6.046280
W	-0.857826	-1.698017	-4.904531	O	3.210604	0.116379	6.045161
O	3.210636	0.154534	-6.044616	O	-1.553705	-0.055963	5.729598
O	-1.737803	2.701306	-6.047268	O	0.825941	-1.317430	5.731178
O	-1.468956	-2.856593	-6.046088	O	0.726985	1.373818	5.730796
O	0.842096	-1.308536	-5.730752	O	-2.405792	1.399763	3.640624
O	-1.550518	-0.074312	-5.729869	O	-0.242250	2.784194	3.630596
O	0.713391	1.382070	-5.730254	O	-2.289078	-1.601988	3.629891
O	-2.279441	-1.597436	-3.641242	O	2.529956	-1.181607	3.630130
O	2.521255	-1.176266	-3.639590	O	2.412168	1.384091	3.640070
O	2.421558	1.389448	-3.629576	O	-0.008266	-2.781589	3.640380
O	-0.005363	-2.793126	-3.630318	O	-4.194019	-2.936308	2.244195
O	-2.416306	1.403455	-3.631696	O	0.002943	-5.114107	2.265499
O	-0.243407	2.774022	-3.641940	O	4.639349	-2.164399	2.244887
O	4.438663	2.548543	-2.244365	O	4.427779	2.559280	2.266430
O	4.630432	-2.174731	-2.266217	O	-0.446262	5.100416	2.241725
O	-0.011063	-5.119011	-2.243091	O	-4.431603	2.555104	2.267263
O	-4.197435	-2.923764	-2.267504	O	2.155496	-3.380803	2.161122
O	-4.427765	2.568583	-2.244872	O	1.849154	3.556446	2.159689
O	-0.431733	5.097372	-2.265750	O	-4.005229	-0.176284	2.160013
O	2.145163	-3.387355	-2.160438	O	3.253727	0.141468	1.464581
O	-4.005795	-0.164371	-2.160977	O	-1.750066	2.747201	1.463979
O	1.860400	3.550443	-2.161457	O	-1.504424	-2.889328	1.463589
O	3.252918	0.133673	-1.463525	W	-0.001507	-0.000292	-0.000161
O	-1.510685	-2.885382	-1.464505	H	0.004502	0.001038	2.742989
O	-1.743695	2.751965	-1.465655	H	0.005614	0.001379	-2.742915
O	0.551645	-3.763126	0.009004	O	-0.000023	0.000560	3.741215
O	2.984271	2.357503	0.008712	O	0.000543	0.000271	-3.741094
O	0.231949	3.796520	-0.009392	O	0.817560	-1.282643	1.252583
O	-3.404955	-1.701645	-0.009448	O	0.699910	1.349425	1.251949
O	3.173963	-2.097811	-0.008584	O	-1.521757	-0.069090	1.250983
O	-3.534872	1.408124	0.008723	O	0.810516	-1.286093	-1.251516
W	-2.984544	-1.763329	1.828974	O	-1.522552	-0.060178	-1.251999
W	2.851579	1.954903	1.867796	O	0.706136	1.346564	-1.252672
W	-0.035495	3.466012	1.829627				

### Coordinates of $\beta$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2]$ <sup>8-</sup>

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W	0.926176	-1.661453	-4.908253	O	-1.888958	3.586667	2.062320
W	-1.901054	0.028147	-4.907975	O	-2.158487	-3.428538	2.061191
W	0.975391	1.633591	-4.907139	O	4.047962	-0.156795	2.059821
W	-3.017086	-1.717596	-1.820709	O	0.452873	5.075098	2.311324
W	3.109492	1.502102	-1.886378	O	-4.451767	2.521541	2.270848
W	2.995091	-1.753918	-1.819536	O	-4.621065	-2.147943	2.309916
W	-0.252329	-3.442087	-1.884221	O	0.046783	-5.117934	2.270356
W	0.022098	3.470566	-1.817593	O	4.170966	-2.932155	2.313475
W	-2.857484	1.940798	-1.885668	O	4.409940	2.596373	2.271704
O	-3.212298	0.086631	-6.046788	O	2.376830	-1.389660	3.656459
O	1.530301	-2.824970	-6.049183	O	0.014606	2.756118	3.660762
O	1.678204	2.739199	-6.048664	O	-2.394249	-1.368467	3.661113
O	-0.739333	1.365918	-5.735134	O	-0.185392	-2.775553	3.641071
O	1.552147	-0.043745	-5.734928	O	-2.310835	1.551345	3.643314
O	-0.815311	-1.324786	-5.735156	O	2.492653	1.226334	3.637184
O	0.016652	-2.779444	-3.650234	O	0.739554	-1.360803	5.750994
O	2.301584	-1.593402	-3.631513	O	-1.548112	0.040229	5.753938
O	-2.527837	-1.197375	-3.629880	O	0.810066	1.321380	5.753070
O	0.226620	2.787662	-3.630346	O	-1.540911	2.829488	6.042554
O	2.398932	1.404293	-3.651989	O	3.222279	-0.078867	6.035277
O	-2.412323	1.374054	-3.648813	O	-1.678814	-2.750384	6.041128
O	-4.632565	-2.186614	-2.247547	W	0.018726	3.451251	1.882466
O	-4.433529	2.544740	-2.285584	W	-0.264550	-3.472126	1.820488
O	0.420905	5.104309	-2.246411	W	2.983521	-1.744589	1.881821
O	4.421934	2.564260	-2.285977	W	3.139322	1.506131	1.817949
O	4.210800	-2.917108	-2.246523	W	-2.998427	-1.710562	1.880322
O	0.008534	-5.110907	-2.281380	W	-2.871188	1.966997	1.818870
O	-1.862434	3.551068	-2.151607	W	1.895703	-0.020210	4.915491
O	4.008731	-0.163601	-2.153532	W	-0.931193	1.654005	4.918071
O	-2.146052	-3.389220	-2.151344	W	-0.968307	-1.632917	4.917029
O	1.742181	2.756380	-1.480401	W	0.001102	0.000814	0.002807
O	1.517827	-2.888451	-1.479290	H	0.001332	-0.005542	-2.745669
O	-3.255841	0.129733	-1.478663	O	0.000746	-0.001272	-3.744219
O	-0.215924	3.808218	0.016108	O	-0.003024	0.001017	3.754347
O	-3.192152	-2.088282	0.015457	H	-0.007955	0.004773	2.756497
O	3.530413	1.452010	-0.017456	O	-0.705324	1.350761	-1.253947
O	-3.021856	2.329774	-0.016554	O	1.526725	-0.064196	-1.260736
O	-0.509036	-3.778360	-0.015186	O	-0.811349	-1.290198	-1.258440
O	3.406537	-1.719733	0.016212	O	-0.815490	-1.282941	1.240460
O	-3.237572	0.130440	1.529572	O	1.519574	-0.056401	1.236597
O	1.505897	-2.866872	1.523063	O	-0.710465	1.350828	1.244707
O	1.732181	2.739871	1.523030				

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**Coordinates of  $\gamma$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2$ ]<sup>8-</sup>**

W	1.003361	-1.612559	-4.923717	O	3.246761	0.007717	1.557960
W	-1.896405	-0.062440	-4.921983	O	2.024195	3.515225	2.045001
W	0.895394	1.674639	-4.922199	O	-4.056059	-0.003876	2.044452
W	-3.084302	-1.624683	-1.815590	O	2.031361	-3.509430	2.045616
W	2.933823	1.822586	-1.895037	O	4.540341	2.364364	2.279333
W	2.947883	-1.860067	-1.816550	O	-0.253903	5.092547	2.323504
W	0.110110	-3.450699	-1.894899	O	-4.315096	2.754055	2.278853
W	0.133773	3.481098	-1.814980	O	-4.282739	-2.765725	2.325781
W	-3.045679	1.627930	-1.894233	O	-0.227739	-5.112071	2.277380
O	-3.218980	-0.053670	-6.048205	O	4.537118	-2.329834	2.324599
O	1.655198	-2.761869	-6.051757	O	0.088517	-2.785092	3.642601
O	1.562103	2.814763	-6.050830	O	2.342783	-1.465870	3.670940
O	1.549871	0.022725	-5.755963	O	2.369791	1.471722	3.645160
O	-0.755692	-1.356283	-5.754544	O	-2.455164	1.317409	3.641866
O	-0.795265	1.329702	-5.754998	O	-2.437661	-1.294188	3.667782
O	2.371112	-1.470363	-3.645355	O	0.098138	2.760249	3.668362
O	-2.455197	-1.318823	-3.641731	O	-0.756856	1.356246	5.754328
O	0.086806	2.787123	-3.643816	O	-0.794722	-1.330233	5.754795
O	0.100309	-2.759418	-3.668356	O	1.549444	-0.021217	5.755957
O	2.340442	1.467180	-3.670552	O	1.652778	2.763499	6.051962
O	-2.437753	1.292324	-3.666995	O	1.564231	-2.812175	6.051131
O	-4.284469	2.763080	-2.325383	O	-3.219861	0.052719	6.048035
O	-0.229252	5.113566	-2.276531	W	2.946022	1.860407	1.816068
O	4.535636	2.330251	-2.325098	W	-3.044790	-1.629435	1.895128
O	4.542640	-2.363062	-2.278299	W	0.135909	-3.479892	1.814426
O	-0.251034	-5.092199	-2.324169	W	2.935096	-1.822431	1.894541
O	-4.316471	-2.754347	-2.279352	W	-3.083175	1.623075	1.816286
O	2.029462	3.510018	-2.045461	W	0.109710	3.451549	1.894687
O	2.025894	-3.514228	-2.044922	W	0.897101	-1.673555	4.921564
O	-4.057195	0.001994	-2.045053	W	1.002495	1.613587	4.924005
O	-1.630145	-2.810381	-1.549971	W	-1.896007	0.060794	4.923177
O	-1.617446	2.812738	-1.549644	W	-0.000889	-0.000238	-0.000179
O	3.246143	-0.006841	-1.557374	H	0.003028	-0.002132	-2.760221
O	3.141447	2.180522	-0.020811	O	0.001746	-0.000479	-3.758471
O	-3.461761	1.626870	-0.020298	O	0.001782	0.000817	3.758469
O	3.142436	-2.178554	0.020525	H	0.002679	0.003213	2.760251
O	0.323226	3.809493	0.020492	O	0.764063	1.319540	-1.246357
O	0.324895	-3.809901	-0.020946	O	0.760499	-1.323322	-1.247476
O	-3.461882	-1.629450	0.020391	O	-1.527420	0.000591	-1.246404
O	-1.629147	2.807291	1.548533	O	0.761623	1.322427	1.247401
O	-1.615528	-2.812001	1.547846	O	-1.526767	-0.001223	1.246597
				O	0.765363	-1.320080	1.246158

**Coordinates of  $\alpha^*-\text{[WO}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$**

W	-1.604275	0.995095	-4.876966	O	-0.030556	-3.987166	1.925256
W	1.677815	0.888671	-4.905219	O	3.486986	1.959810	1.927585
W	-0.055727	-1.902737	-4.877967	O	-3.548099	2.062412	2.031960
W	1.722513	3.133105	-1.937457	O	-5.126231	-0.063255	2.349020
W	-1.867622	-2.980327	-1.807903	O	-2.746293	-4.410355	2.400661
W	-3.470711	-0.094526	-1.885021	O	2.670757	-4.441436	2.331541
W	-1.605517	3.047785	-1.785433	O	5.188383	-0.177112	2.370194
W	1.819181	-3.014347	-1.893659	O	2.481040	4.466096	2.299850
W	3.544216	-0.075313	-1.847660	O	-2.454977	4.500950	2.393103
O	2.841266	1.544663	-6.013627	O	1.356546	2.390834	3.603704
O	-2.750651	1.659080	-6.002303	O	-1.293084	2.417956	3.655097
O	-0.052707	-3.248712	-5.974941	O	-2.758569	-0.061442	3.638075
O	-1.326007	-0.758853	-5.732927	O	1.416860	-2.380128	3.606131
O	0.045125	1.526925	-5.740594	O	2.756713	-0.094333	3.620914
O	1.340172	-0.810722	-5.726268	O	-1.444653	-2.361918	3.651424
O	1.472973	2.335845	-3.649467	O	-0.002282	-1.558788	5.729224
O	1.313373	-2.421999	-3.625089	O	1.371792	0.733859	5.725010
O	-2.735176	0.070631	-3.645134	O	-1.290876	0.779101	5.748034
O	-1.402274	2.358716	-3.624031	O	-2.801961	-1.570777	6.023866
O	-1.338036	-2.408596	-3.600767	O	0.095821	3.222122	5.991693
O	2.783703	0.035673	-3.620386	O	2.789705	-1.682643	5.981495
O	5.193706	0.112192	-2.330186	W	-3.481982	0.139047	1.807444
O	2.439867	-4.557472	-2.365906	W	3.543724	0.063972	1.899267
O	-2.473396	-4.519762	-2.324434	W	1.816751	2.945312	1.780524
O	-5.124379	0.117169	-2.379245	W	-1.855987	2.944138	1.894125
O	-2.555312	4.407505	-2.332377	W	1.678243	-3.111608	1.846469
O	2.771658	4.416478	-2.430125	W	-1.729333	-3.094125	1.924721
O	0.069355	4.046978	-1.986132	W	0.071335	1.894000	4.871732
O	3.435971	-1.997189	-1.923570	W	-1.665693	-0.896014	4.895649
O	-3.515076	-2.021849	-1.971292	W	1.621907	-0.997194	4.895982
O	2.958177	1.694073	-1.690610	W	-0.010202	-0.001331	-0.007407
O	-0.019002	-3.344305	-1.650133	H	0.037316	0.006255	-2.727885
O	-2.921679	1.705376	-1.687750	O	0.018382	-0.001675	-3.719561
O	1.968745	3.364310	-0.062197	O	0.003535	-0.014426	3.719527
O	-1.980577	-3.348524	0.033648	H	-0.011853	-0.035848	2.727539
O	-1.953182	3.391767	0.033972	O	1.288919	-0.727365	-1.147029
O	1.909381	-3.346004	-0.011932	O	-1.465077	-0.758595	-1.134081
O	3.854412	-0.024654	0.014187	O	-0.116473	1.639713	-1.144964
O	-3.911260	0.031492	-0.015058	O	-0.043532	-1.500152	1.140129
O	2.925012	-1.713415	1.669564	O	1.293076	0.873909	1.116654
O	0.000517	3.340586	1.659256	O	-1.499566	0.857198	1.189966
O	-2.942890	-1.678258	1.690498				

**Coordinates of  $\beta^*-\text{[WO}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{]}^{8-}$**

W	0.994586	-1.592495	-4.921507	O	3.322063	0.054919	1.808743
W	0.855050	1.702039	-4.883601	O	-1.647842	-2.975762	1.837439
W	-1.915533	-0.068161	-4.906556	O	-1.707303	2.874857	1.840524
W	-2.953623	1.848316	-1.904205	O	-0.174953	5.129998	2.397646
W	3.002141	1.674598	-1.897342	O	4.614081	-2.393620	2.307342
W	-0.050094	-3.496779	-1.920052	O	-4.421980	-2.839331	2.357640
W	-0.174929	3.484267	-1.776694	O	4.495196	2.541830	2.321206
W	3.141246	-1.653096	-1.877000	O	-0.024018	-5.236045	2.253817
W	-3.013953	-1.839467	-1.835978	O	-4.435197	2.544214	2.328600
O	1.518586	2.834589	-6.023340	O	2.373290	1.574440	3.663453
O	1.668841	-2.748599	-6.025955	O	0.225568	-2.888833	3.627243
O	-3.244694	-0.087690	-6.023258	O	-2.528716	1.186968	3.641644
O	-0.824628	1.309642	-5.748011	O	0.143102	2.796458	3.707103
O	1.519636	0.036810	-5.744174	O	2.398400	-1.584606	3.651005
O	-0.760797	-1.364794	-5.741356	O	-2.521140	-1.351584	3.660340
O	-2.458367	1.276572	-3.656618	O	-0.760531	1.284718	5.728173
O	0.027139	2.792231	-3.637812	O	1.587450	-0.060145	5.717017
O	2.377071	-1.414135	-3.635021	O	-0.761649	-1.420782	5.689858
O	-2.447290	-1.354431	-3.628123	O	1.615972	2.699657	6.126782
O	2.309311	1.469065	-3.659693	O	1.616776	-2.823988	6.079864
O	0.106927	-2.746332	-3.651892	O	-3.171760	-0.052588	6.087989
O	0.023941	5.135432	-2.311965	W	2.949295	1.932755	1.805883
O	-4.538208	2.408752	-2.351861	W	0.143885	-3.570315	1.829787
O	4.331513	2.703506	-2.351213	W	-3.081313	1.591089	1.791591
O	0.201517	-5.150888	-2.354740	W	3.054869	-1.786150	1.869359
O	4.437815	-2.692439	-2.351462	W	-3.121321	-1.792960	1.918755
O	-4.563410	-2.460022	-2.290836	W	0.965339	-1.711301	4.918893
O	4.018107	0.027526	-2.017483	W	-1.896515	-0.018760	4.910822
O	-1.959088	-3.443370	-1.994826	W	1.003128	1.606994	4.923506
O	-2.102487	3.542109	-2.056407	W	0.083583	3.476603	1.915753
O	1.712009	-2.874044	-1.652629	W	0.013380	0.016832	0.007543
O	1.633069	2.949575	-1.655718	H	-0.043089	-0.018019	-2.740157
O	-3.327244	-0.020668	-1.619021	O	-0.020945	0.001328	-3.732830
O	-0.119880	3.902364	0.044569	O	0.027015	-0.042866	3.729430
O	-3.337033	1.974268	-0.023262	H	0.055795	-0.030250	2.738218
O	3.388998	-1.795910	-0.017242	O	-0.843945	1.520035	-1.204376
O	-3.235510	-2.046777	0.030400	O	1.584518	0.170114	-1.147169
O	3.355523	1.942207	-0.011959	O	-0.734867	-1.256263	-1.156872
O	-0.045736	-3.783063	-0.029446	O	0.816693	1.516529	1.180380
O	-4.011142	-0.115901	1.814348	O	0.791043	-1.249725	1.135691
O	2.050824	-3.432839	1.758244	O	-1.549824	0.146425	1.107174
O	2.019692	3.603254	1.905890				

**Coordinates of  $\gamma^*-\text{[}(W\text{O}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{]}^{8-}$**

W	0.906367	1.686207	4.937996	O	-2.059644	-3.575324	-1.946658
W	1.045166	-1.627087	4.924153	O	1.647017	-2.864440	-1.797599
W	-1.894455	-0.101748	4.930098	O	1.661758	2.901331	-1.771387
W	-3.095114	1.612021	1.941791	O	-3.325983	-0.004412	-1.761202
W	0.110691	-3.454679	1.881633	O	-4.503768	-2.438906	-2.363818
W	3.000902	1.841335	1.911063	O	4.392856	-2.737997	-2.362601
W	-3.093193	-1.630482	1.779121	O	0.163489	5.207776	-2.343303
W	3.045619	-1.873756	1.826277	O	0.136729	-5.147105	-2.335393
W	0.071846	3.548815	1.843949	O	4.420607	2.734760	-2.280742
O	1.705400	-2.732137	6.088402	O	-4.506199	2.462001	-2.288197
O	1.563986	2.796457	6.098241	O	-0.141894	-2.826318	-3.682240
O	-3.158208	-0.092235	6.123223	O	2.536582	1.310690	-3.646503
O	-0.708438	-1.376129	5.743176	O	-2.361307	1.545600	-3.628578
O	1.600774	0.031219	5.714509	O	-2.346946	-1.534883	-3.711983
O	-0.776183	1.326178	5.739103	O	2.542113	-1.240268	-3.691604
O	-2.516972	-1.299674	3.671120	O	-0.155425	2.833925	-3.657423
O	0.206350	-2.806083	3.677418	O	-1.539668	-0.001921	-5.738374
O	2.356636	1.556070	3.666563	O	0.826414	-1.310563	-5.750271
O	-2.498076	1.256335	3.708930	O	0.768300	1.397499	-5.712349
O	2.420519	-1.546114	3.635861	O	-1.522229	-2.770452	-6.133385
O	0.155174	2.847871	3.659245	O	3.207152	0.102509	-6.105517
O	-4.391461	-2.662960	2.321645	O	-1.653174	2.760819	-6.065811
O	-4.382468	2.686827	2.396045	W	-0.155124	-3.509355	-1.827561
O	-0.111682	-5.121780	2.326519	W	3.110067	1.697125	-1.840236
O	4.556585	2.463961	2.335607	W	-2.965177	1.843725	-1.765016
O	4.607511	-2.461615	2.276105	W	3.086358	-1.691507	-1.927015
O	-0.183803	5.195305	2.308473	W	-0.105149	3.557287	-1.907993
O	2.056669	-3.493187	1.856644	W	1.917852	0.084530	-4.944411
O	1.990455	3.474921	1.854007	W	-1.015824	1.637551	-4.905502
O	-4.126130	-0.000469	1.934111	W	-0.884746	-1.676235	-4.944533
O	3.341516	-0.001878	1.775888	W	-2.927751	-1.838853	-1.923537
O	-1.668970	-2.887310	1.796520	W	-0.008533	-0.000893	0.001336
O	-1.665497	2.863804	1.784825	H	0.000655	-0.007838	2.753233
O	-3.342322	-1.966472	-0.027006	O	0.016888	-0.005312	3.745823
O	-3.361558	1.920378	0.054981	O	0.015511	0.002968	-3.746186
O	3.308425	-1.897151	-0.029175	H	0.022001	-0.035915	-2.754148
O	-0.009673	3.825414	-0.013669	O	-1.705405	-0.046151	1.195110
O	-0.005576	-3.853522	-0.003058	O	0.679943	-1.430208	1.134579
O	3.271302	1.902364	0.018176	O	0.719821	1.294127	1.147606
O	-2.010720	3.524866	-1.858570	O	-0.881897	-1.453940	-1.204576
O	4.001525	0.006225	-1.855242	O	1.476658	-0.015849	-1.149433
				O	-0.905836	1.310309	-1.117301

**Coordinates of  $\alpha$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{6-}$**

W	0.094121	-3.680678	1.690856	O	-4.335997	2.720295	-2.455610
W	-3.145195	1.626713	-1.867184	O	-1.794337	-1.381640	-5.201549
W	-1.581857	-0.935695	-3.553619	O	0.357578	-5.005448	-2.748456
W	0.025234	-3.700982	-1.671713	O	5.671621	1.670888	-0.001862
W	-3.135909	1.618393	1.842177	O	4.259170	-0.103183	-1.489696
W	-1.539152	-0.914183	3.560465	O	0.791499	2.841500	3.461017
W	-3.686958	-3.344058	-1.667429	O	3.791224	-2.214640	-0.000989
W	-3.621459	-3.337199	1.673597	O	4.499116	3.697842	1.363777
W	-5.148109	-0.908877	-0.005186	O	3.139437	1.802664	-2.816648
W	0.033871	3.593123	-1.832031	O	0.763561	2.828568	-3.452220
W	3.216397	-1.618104	1.721905	O	4.459073	3.651223	-1.348745
W	3.160559	-1.661999	-1.725220	O	2.159939	-0.590091	2.908671
W	1.549744	1.099552	-3.591974	O	2.137814	-0.605202	-2.916757
W	1.593062	1.118349	3.587217	O	-1.626667	2.701297	-2.182240
W	0.042423	3.595281	1.848955	O	1.798127	4.077160	-1.286381
W	4.644546	1.745082	-1.642327	O	3.193662	1.819952	2.836880
W	3.208333	4.224244	0.003314	O	-0.111536	0.303615	3.824006
W	4.698627	1.802863	1.649691	O	4.298880	-0.075009	1.507498
O	-5.271854	-2.296882	-1.351951	O	1.808611	4.094475	1.294383
O	-3.004815	-2.013381	-2.832437	O	-0.152961	0.286199	-3.810013
O	-2.747269	0.584383	3.397782	O	-0.450263	3.705597	0.004132
O	-2.784697	0.570743	-3.413140	O	-0.446586	5.133409	-2.438812
O	-5.202500	-2.283403	1.337771	O	3.532540	5.924195	-0.011269
O	-1.849041	-3.936818	-1.534458	O	5.948788	1.755962	-2.771129
O	0.329488	-4.589188	0.007317	O	6.019623	1.811031	2.765773
O	-3.998025	-4.240127	0.008654	O	-0.434189	5.137820	2.452641
O	-2.985076	2.063540	-0.008587	O	2.093385	1.090761	5.232213
O	-0.400966	-2.244768	-2.885799	O	4.256738	-2.504442	2.763647
O	1.816059	-2.941384	1.636914	O	4.212460	-2.534812	-2.767964
O	-1.809478	-3.910679	1.522104	O	2.051682	1.078283	-5.236022
O	-4.345542	0.251895	1.282597	I	0.026767	0.189269	0.004833
O	-1.591530	2.688748	2.166802	H	2.265486	1.646830	0.288115
O	-4.360095	0.250306	-1.290270	H	-2.516816	-1.081553	-0.443943
O	-2.956977	-1.970327	2.794157	H	-1.371407	-2.138909	0.093819
O	1.773096	-2.949315	-1.621548	O	3.169204	2.014188	0.052541
O	-0.368227	-2.242739	2.911983	O	0.819716	1.474296	1.273455
O	0.387537	-4.997663	2.765545	O	1.762624	-0.639724	-0.006327
O	-4.254620	-4.471987	2.800606	O	0.673951	1.444029	-1.325214
O	-4.335980	-4.508779	-2.767854	O	-3.074454	-1.863922	-0.094929
O	-6.793651	-0.387003	0.011371	O	-1.380988	-0.008540	1.317184
O	-1.779261	-1.361150	5.203721	O	-1.489115	-0.090599	-1.270685
O	-4.303992	2.729270	2.441072	O	-0.370606	-2.149658	0.028833

### Coordinates of $\beta$ 1-[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$

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W	-3.093569	-1.729452	-1.858491	O	4.609475	2.389405	-2.280150
W	3.057208	1.807223	-1.821809	O	4.612287	-2.476225	-2.333187
W	3.042060	-1.929793	-1.874267	O	-0.184758	-5.235773	-2.317795
W	0.139621	-3.599912	-1.884083	O	0.771075	-1.330450	5.711622
W	0.098546	3.560921	-1.794609	O	2.456483	-1.255924	3.614310
W	-3.135940	1.688356	-1.832734	O	-3.985614	0.019305	2.122579
W	0.941806	-1.677865	-4.914924	O	1.942066	-3.360232	2.055311
W	-1.919109	0.003840	-4.900223	O	-1.555397	0.004056	5.728945
W	0.920926	1.657232	-4.823151	O	2.507624	1.321087	3.660256
W	0.079637	3.569426	1.951309	O	1.997123	3.473471	2.131346
W	0.045011	-3.526917	1.858562	O	0.787616	1.370230	5.768490
W	3.027351	-1.794432	1.877544	O	-1.703212	-2.886291	1.545089
W	3.048068	1.895855	1.926747	O	3.348676	0.037202	1.546785
W	-3.165663	-1.686732	1.893442	O	3.181127	2.142455	0.045113
W	-3.106719	1.728379	1.918445	O	-0.132316	2.856593	3.703316
W	1.894246	0.022100	4.930992	O	-2.379350	-1.496032	3.627542
W	-0.954441	1.664160	4.961779	O	-3.439221	1.696440	0.037322
W	-0.953926	-1.632401	4.883403	O	-0.116641	-2.756671	3.600574
O	1.511299	-0.004149	-5.636853	O	-2.370947	1.554509	3.678101
O	2.368770	-1.539207	-3.635754	O	3.168438	-2.141112	-0.005553
O	-1.657784	2.864954	-1.554747	O	-1.691659	2.959967	1.595205
O	3.351498	-0.041410	-1.607796	O	-0.162095	5.227375	2.352893
O	-0.791659	1.341586	-5.686333	O	-1.603867	2.770417	6.123202
O	0.117552	-2.853378	-3.651973	O	3.207175	-0.006454	6.056604
O	-1.633573	-2.901495	-1.612844	O	-1.593508	-2.778815	6.002350
O	-0.790574	-1.350430	-5.689786	O	-4.421033	2.763807	2.332343
O	1.992514	3.425158	-1.934046	O	-4.456758	-2.737900	2.323080
O	2.058787	-3.582434	-2.003005	O	-0.197820	-5.170062	2.300653
O	-3.429498	-1.671764	0.021484	O	4.573388	-2.406081	2.312676
O	-2.490877	-1.312030	-3.619278	O	4.609890	2.479647	2.348788
O	0.077074	2.788193	-3.567622	I	-0.069066	0.129054	0.134957
O	0.265945	3.815432	0.066340	H	0.126922	0.329639	2.797259
O	2.354502	1.476539	-3.576165	H	-0.493839	0.213428	-2.721069
O	-2.473798	1.292997	-3.597815	H	0.611704	-0.898480	-2.246569
O	0.272994	-3.808216	-0.012172	O	0.011996	0.076571	3.760185
O	-3.984353	-0.015098	-1.940956	O	-1.585632	0.097521	1.343373
O	-4.368766	-2.801591	-2.287501	O	0.730063	-1.277705	1.183005
O	-3.230896	0.005064	-6.024638	O	0.691976	1.358593	1.472523
O	1.595196	-2.776669	-6.065865	O	-0.057383	0.008475	-3.614208
O	1.582129	2.781503	-5.954777	O	0.780544	1.278487	-1.172841
O	-4.402161	2.756008	-2.297803	O	0.838372	-1.407645	-1.417052
O	-0.183727	5.193703	-2.255423	O	-1.440650	-0.019443	-1.300555

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### Coordinates of $\beta$ 2-[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$

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W	-3.167685	-1.686321	-1.958674	O	4.606979	2.456298	-2.370680
W	3.041659	1.901068	-1.926821	O	4.567705	-2.398699	-2.308351
W	3.019278	-1.815520	-1.842393	O	-0.223949	-5.170785	-2.323523
W	0.050067	-3.539622	-1.857356	O	0.755025	-1.308145	5.631431
W	0.082579	3.569354	-1.887747	O	2.517822	-1.304237	3.631066
W	-3.125776	1.693116	-1.926468	O	-3.902728	-0.019906	2.023526
W	0.921580	-1.627812	-4.875752	O	2.038844	-3.540194	2.104016
W	-1.919447	0.013496	-4.991323	O	-1.544924	0.014062	5.645767
W	0.913497	1.666947	-4.926149	O	2.516266	1.300489	3.602102
W	0.104267	3.564266	1.852691	O	1.990391	3.396001	2.044840
W	0.127409	-3.611475	1.883176	O	0.775131	1.374687	5.695423
W	3.039180	-1.906015	1.908031	O	-1.659731	-2.958787	1.529246
W	3.066638	1.804002	1.819870	O	3.364122	-0.033409	1.531835
W	-3.091828	-1.758495	1.788909	O	3.170677	2.145724	-0.036536
W	-3.098207	1.697088	1.829494	O	-0.111648	2.812535	3.597190
W	1.909580	0.041284	4.880001	O	-2.343683	-1.499275	3.558103
W	-0.950993	1.668237	4.874801	O	-3.408023	1.674957	-0.048632
W	-0.976584	-1.646356	4.843917	O	-0.107125	-2.822400	3.610341
O	1.520719	0.006124	-5.705162	O	-2.342584	1.515043	3.576860
O	2.321433	-1.445881	-3.589314	O	3.156272	-2.140831	0.025363
O	-1.687359	2.922084	-1.670521	O	-1.648338	2.894320	1.495212
O	3.323726	0.034828	-1.602949	O	-0.148223	5.207973	2.293040
O	-0.802483	1.364595	-5.784196	O	-1.617724	2.798141	5.996699
O	0.058772	-2.754707	-3.601202	O	3.194147	0.032170	6.037508
O	-1.695262	-2.865084	-1.608945	O	-1.633343	-2.761344	5.976872
O	-0.793111	-1.347514	-5.750227	O	-4.403162	2.733279	2.255171
O	2.009983	3.504509	-2.025330	O	-4.393850	-2.783799	2.249462
O	1.954614	-3.409421	-1.962319	O	-0.149962	-5.252604	2.332853
O	-3.444957	-1.691739	-0.059491	O	4.607490	-2.489315	2.321715
O	-2.505533	-1.305203	-3.693803	O	4.621294	2.403899	2.249340
O	0.099049	2.834612	-3.672312	I	-0.075498	0.121760	-0.114168
O	0.268407	3.838162	-0.020757	H	0.182917	0.568029	2.714905
O	2.355403	1.500862	-3.655279	H	-0.339786	0.077944	-2.798276
O	-2.530263	1.305907	-3.708588	H	0.478669	-1.002218	2.293233
O	0.267882	-3.840209	0.016255	O	0.071838	0.068862	3.599556
O	-4.051911	-0.000621	-2.027777	O	-1.500443	-0.040036	1.186426
O	-4.428952	-2.772359	-2.390127	O	0.794780	-1.433009	1.444646
O	-3.220693	-0.008319	-6.131481	O	0.751877	1.247103	1.320025
O	1.593307	-2.778318	-5.974705	O	-0.075929	0.037461	-3.764950
O	1.586312	2.776955	-6.065875	O	0.707270	1.421394	-1.318197
O	-4.409108	2.764509	-2.347335	O	0.735750	-1.276569	-1.152990
O	-0.198423	5.211814	-2.328538	O	-1.513250	0.083109	-1.459686

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**Coordinates of  $\gamma$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$**

W	-0.132223	-3.610419	-1.898141	O	0.163884	5.200010	-2.335634
W	-0.102686	3.564445	-1.874818	O	4.422169	2.744156	-2.249954
W	3.133402	1.702389	-1.790479	O	4.395957	-2.776490	-2.260883
W	3.101267	-1.742549	-1.798173	O	0.788445	-1.351066	5.766147
W	-3.041401	1.809638	-1.861596	O	2.516907	-1.284075	3.710510
W	-3.044574	-1.931673	-1.883906	O	-3.342806	0.034706	1.638781
W	1.901430	0.020080	-4.811196	O	1.691488	-2.868311	1.667214
W	-0.984583	-1.663719	-4.927164	O	-1.530397	0.008388	5.698102
W	-0.958876	1.653495	-4.921218	O	2.541415	1.312579	3.736921
W	-0.081413	3.583569	1.881286	O	1.699963	2.944403	1.726853
W	-0.059860	-3.542916	1.856730	O	0.789342	1.368490	5.784514
W	3.158864	-1.677067	1.965441	O	-1.963246	-3.404666	1.941311
W	3.129090	1.711621	1.969822	O	4.043664	0.012321	2.009671
W	-3.029723	-1.808427	1.870384	O	-0.186844	3.840699	0.013392
W	-3.044950	1.908356	1.902157	O	-0.117685	2.848306	3.670607
W	1.910546	0.014818	5.014770	O	-2.337803	-1.457448	3.609515
W	-0.928555	1.671676	4.912971	O	-3.190635	-2.095974	-0.012770
W	-0.923366	-1.632846	4.890645	O	-0.086982	-2.764243	3.613478
O	0.769253	1.344714	-5.685253	O	-2.364912	1.519107	3.643236
O	2.469539	1.321249	-3.566688	O	3.389608	1.744059	0.075752
O	-3.330255	-0.043237	-1.663396	O	-2.009959	3.511213	1.982687
O	1.658723	2.890541	-1.606451	O	0.175114	5.227691	2.330421
O	-1.568818	-0.001714	-5.701632	O	-1.599863	2.773301	6.061902
O	2.468935	-1.296044	-3.562992	O	3.201934	-0.002191	6.165940
O	1.652763	-2.943134	-1.646165	O	-1.597143	-2.771695	6.000118
O	0.754930	-1.320254	-5.630555	O	-4.603427	2.485220	2.343480
O	-2.000254	3.441760	-1.924954	O	-4.574970	-2.407331	2.326995
O	3.962227	-0.009189	-1.892009	O	0.196538	-5.175961	2.326729
O	-0.207398	-3.830951	-0.016183	O	4.432290	-2.748216	2.399960
O	-0.151828	-2.842477	-3.651178	O	4.427351	2.764604	2.387626
O	-2.372368	1.517962	-3.632246	I	0.073655	0.124982	0.127072
O	-3.191569	2.080702	0.014466	H	0.355840	0.062748	2.807773
O	-0.120348	2.799554	-3.625556	H	-0.088754	0.536773	-2.725960
O	-2.406964	-1.557905	-3.661034	H	-0.461643	-0.984464	-2.256123
O	3.403350	-1.737105	0.065399	O	0.073923	0.033805	3.771009
O	-2.059142	-3.579189	-1.975766	O	-0.747339	-1.270121	1.167850
O	0.159485	-5.248420	-2.351025	O	1.510392	0.085599	1.475970
O	-1.601535	-2.775561	-6.085466	O	-0.710380	1.433177	1.318877
O	3.199046	0.007403	-5.950661	O	-0.025543	0.048817	-3.616094
O	-1.606755	2.782070	-6.057261	O	-0.787031	-1.434714	-1.424399
O	-4.615188	-2.485475	-2.325931	O	-0.735915	1.239347	-1.318243
O	-4.599781	2.390584	-2.302954	O	1.507395	-0.033219	-1.167119

**Coordinates of  $\alpha^*-\text{[IO}_6\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$**

W	3.574205	-0.042311	1.914715	O	-5.199185	0.119953	2.393155
W	-3.559786	-0.031290	1.895686	O	-2.509821	-4.533487	2.358590
W	-1.822148	-3.037560	1.861106	O	2.529493	-4.551124	2.396078
W	1.850710	-3.050497	1.900541	O	1.323208	0.764641	-5.631302
W	-1.732925	3.166694	1.919872	O	2.750717	-0.069949	-3.541535
W	1.742816	3.162628	1.899491	O	-3.401585	1.955071	-1.901529
W	-0.003787	-1.879790	4.891106	O	3.417212	1.961026	-1.884947
W	1.638105	0.970407	4.906434	O	-1.343397	0.783963	-5.683483
W	-1.646354	0.964813	4.911159	O	1.444352	-2.367806	-3.553302
W	-1.736190	-3.183513	-1.890337	O	0.008610	-3.996820	-1.929054
W	1.849242	3.063768	-1.844020	O	0.004291	-1.516670	-5.616966
W	3.583580	0.036735	-1.807393	O	0.001844	3.462632	-1.641580
W	1.762137	-3.194891	-1.847572	O	3.012248	-1.763281	-1.647357
W	-1.845131	3.068826	-1.829228	O	1.951251	3.419879	0.036886
W	-3.576788	0.035670	-1.838109	O	-1.469759	-2.380965	-3.592844
W	1.660742	-0.944763	-4.809723	O	-1.321533	2.456084	-3.579898
W	-1.662099	-0.927692	-4.853984	O	-1.947908	3.382912	0.039378
W	-0.009925	1.910381	-4.847262	O	1.313149	2.440196	-3.569408
O	-1.343262	-0.766178	5.723612	O	-2.799462	-0.082851	-3.593244
O	-1.304177	-2.406522	3.590914	O	-1.907422	-3.378633	-0.016191
O	0.003681	3.982722	1.981207	O	-2.988003	-1.751064	-1.660074
O	-3.390954	-1.942951	1.912334	O	-2.716760	-4.509273	-2.375399
O	-0.006021	1.557103	5.743261	O	-2.787733	-1.599725	-5.980486
O	1.326569	-2.421416	3.616078	O	2.808041	-1.605574	-5.906657
O	3.421629	-1.959431	1.936616	O	0.005834	3.230259	-5.958948
O	1.330285	-0.763370	5.724968	O	-5.216595	-0.131091	-2.329486
O	-3.001439	1.765713	1.714186	O	-2.525224	4.567689	-2.332923
O	0.015893	-3.456174	1.680880	O	2.530136	4.561161	-2.350270
O	3.947832	-0.002302	0.043798	O	5.210181	-0.122274	-2.345665
O	2.754853	0.081223	3.631532	O	2.734074	-4.510738	-2.378358
O	-1.470244	2.393125	3.649988	I	0.035111	0.098909	0.071176
O	-3.887004	0.028651	0.022493	H	-0.479175	0.435828	-2.697576
O	-2.751489	0.086490	3.620640	H	0.010249	0.060817	2.751712
O	1.465997	2.380269	3.637949	H	0.105306	-1.060042	-2.171790
O	1.945035	-3.409859	0.007874	O	-0.097608	0.016207	-3.542699
O	2.995246	1.746294	1.699607	O	-1.280153	0.784301	-1.236610
O	5.205199	0.128834	2.434797	O	1.408267	0.811089	-1.082222
O	2.792060	1.617268	6.019360	O	0.050666	-1.562674	-1.292807
O	-0.010556	-3.220584	5.980643	O	-0.000800	0.028851	3.737595
O	-2.806029	1.609248	6.018164	O	-0.004336	1.610179	1.242136
O	2.716047	4.485186	2.413048	O	-1.350113	-0.776322	1.097199
O	-2.699983	4.504687	2.402719	O	1.364001	-0.788959	1.161867

**Coordinates of  $\beta$ 1\*- $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$**

W	-1.906860	0.012880	4.883334	O	-1.708913	2.970256	-1.783997
W	0.952044	1.648906	4.938836	O	-1.689987	-2.980132	-1.813638
W	0.947464	-1.629963	4.921167	O	3.457318	-0.028868	-1.800782
W	3.116200	-1.707824	1.902553	O	-4.476420	2.699430	-2.333040
W	-0.083322	3.608771	1.951364	O	-0.099807	-5.292788	-2.326335
W	-3.063139	-1.807255	1.869079	O	4.577169	2.505952	-2.308598
W	3.104437	1.750845	1.912651	O	4.615314	-2.573634	-2.337005
W	-3.096356	1.884355	1.902189	O	-0.083341	5.242031	-2.292246
W	-0.066866	-3.539766	1.898776	O	-4.454840	-2.723543	-2.334403
O	-3.226435	-0.011981	5.996605	O	0.149276	2.850873	-3.576907
O	1.600715	-2.790246	6.023115	O	-2.555371	-1.275195	-3.630467
O	1.615365	2.785133	6.060571	O	-2.549226	1.269622	-3.621217
O	1.556620	0.002516	5.756647	O	0.175666	-2.880833	-3.610880
O	-0.776720	1.341141	5.732448	O	2.358497	1.549417	-3.574131
O	-0.775214	-1.329328	5.718771	O	2.364630	-1.588252	-3.591284
O	0.093536	2.809034	3.668370	O	-0.791397	1.344539	-5.661658
O	-2.429343	-1.292350	3.603766	O	-0.785699	-1.364961	-5.649279
O	-2.479999	1.334907	3.636885	O	1.519383	-0.013418	-5.579473
O	0.088040	-2.751952	3.620818	O	1.580321	2.749255	-5.996637
O	2.349849	1.479884	3.650551	O	-3.200626	-0.006381	-6.077986
O	2.358867	-1.461468	3.635534	O	1.597407	-2.772042	-6.048686
O	0.118885	5.249146	2.427995	W	3.073805	1.823854	-1.823632
O	-4.572723	-2.472344	2.357416	W	0.082570	3.604576	-1.788795
O	4.448551	-2.690954	2.368255	W	-3.119909	-1.743511	-1.870819
O	4.426322	2.740466	2.397141	W	3.106830	-1.902656	-1.854852
O	-4.615772	2.534301	2.380734	W	-3.138724	1.729683	-1.850594
O	0.112125	-5.183872	2.370307	W	0.093478	-3.652375	-1.851992
O	-1.997534	3.459192	2.032079	W	-1.930273	0.001121	-4.907900
O	3.932727	0.018089	1.998344	W	0.946152	-1.692171	-4.879880
O	-1.969322	-3.384202	1.964760	W	0.925539	1.672789	-4.816329
O	1.700761	3.002034	1.677524	I	-0.038087	0.110396	0.086962
O	1.721972	-2.968710	1.654467	H	0.174632	0.022716	2.765181
O	-3.466172	0.032662	1.664586	O	0.024861	0.020239	3.743268
O	3.400632	1.871647	0.042799	O	1.526161	0.006479	1.234705
O	3.374578	-1.876367	0.011584	O	-0.064608	0.019739	-3.560271
O	-3.331622	2.023211	0.026814	O	0.811473	1.402368	-1.074447
O	-0.051171	-3.867260	0.005426	O	-0.822195	1.410385	1.236484
O	-0.093534	3.921813	0.063319	O	-0.791002	-1.349441	1.101790
O	-3.314805	-1.977436	0.002965	O	-1.498309	0.051125	-1.234149
O	1.988349	3.434029	-1.758524	O	0.820915	-1.321033	-1.278790
O	2.009210	-3.491426	-1.779749	H	-0.553962	0.236495	-2.701817
O	-3.954409	-0.004459	-1.772491	H	0.603625	-0.840705	-2.140728

### Coordinates of $\beta$ 2\*- $[(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$

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W	3.069935	1.828549	-1.924036	O	-0.795571	1.376590	-5.719830
W	0.084943	3.566322	-1.905897	O	-0.784997	-1.329632	-5.688720
W	-3.113349	-1.747909	-1.887288	O	-2.528746	1.274765	-3.612118
W	-0.075489	3.631579	1.852360	O	0.167963	-2.859460	-3.666838
W	-3.059553	-1.825210	1.847671	O	-3.940906	-0.010927	-1.771511
W	0.951330	1.660927	-4.960612	O	-3.202081	0.017746	-6.053269
W	3.118499	1.749490	1.806103	O	-4.476071	2.675251	-2.300527
W	0.975980	1.643843	4.820498	O	-0.091081	-5.274215	-2.386446
W	3.087788	-1.894278	-1.893628	O	-1.991208	3.466174	1.996897
W	0.960924	-1.652065	-4.916454	O	-1.966091	-3.409266	1.964095
W	3.129048	-1.730023	1.849174	O	-0.742660	1.307941	5.628499
W	0.954105	-1.669635	4.860232	O	-0.762099	-1.363521	5.694263
W	-3.122914	1.717927	-1.842452	O	-3.424130	0.018817	1.632680
W	0.084633	-3.628714	-1.917138	O	-2.469173	1.313757	3.615787
W	-1.913591	0.022049	-4.903248	O	0.106400	-2.806618	3.590652
W	-3.078326	1.882412	1.909705	O	-3.260865	2.026726	0.030626
W	-0.064875	-3.587835	1.837319	O	-0.078469	-3.889347	-0.035799
W	-1.895756	-0.035950	4.872640	O	-3.196658	-0.019084	6.010639
O	3.426828	-0.023577	-1.846484	O	-4.610108	2.513354	2.369209
O	1.559284	0.009788	-5.731387	O	0.125463	-5.229392	2.319127
O	2.362691	1.562398	-3.672886	O	0.171679	2.842796	-3.662065
O	1.990240	3.422349	-1.813135	O	-2.524481	-1.266558	-3.631510
O	1.591594	2.772911	-6.119416	O	-0.077835	5.220204	-2.347875
O	4.580945	2.492943	-2.409168	O	-4.467325	-2.700589	-2.353915
O	3.938215	0.003784	1.918697	O	0.089524	2.779141	3.568333
O	1.541374	-0.009562	5.634190	O	-2.471930	-1.326130	3.610740
O	1.720038	3.014436	1.620366	O	-0.100381	3.852079	-0.007583
O	2.354309	1.442113	3.546590	O	-3.279235	-2.026687	-0.012369
O	3.409193	1.895062	-0.049814	O	0.132154	5.267572	2.342191
O	1.641000	2.781369	5.924560	O	-4.582062	-2.474249	2.317500
O	4.445212	2.719217	2.316009	I	0.071623	-0.088624	-0.075384
O	2.375774	-1.570994	-3.658072	H	0.092550	0.165536	-2.762679
O	2.004883	-3.487612	-1.857270	H	-0.194526	-0.621740	2.708294
O	1.585257	-2.742182	-6.101162	H	-0.425284	0.957939	2.175911
O	4.596871	-2.548543	-2.398300	O	0.016215	0.029739	-3.740019
O	1.723234	-2.988555	1.605766	O	0.762758	1.322018	-1.219588
O	2.360829	-1.476380	3.574547	O	-0.070925	-0.072306	3.556753
O	3.417932	-1.921096	-0.037761	O	1.611891	0.000050	1.084096
O	1.630681	-2.799160	5.975405	O	0.804504	-1.429788	-1.211709
O	4.459682	-2.706757	2.335538	O	-1.572605	-0.013976	-1.081310
O	-1.709816	2.976649	-1.835744	O	-0.720168	-1.323659	1.257482
O	-1.709486	-3.012419	-1.858752	O	-0.736191	1.372873	1.305871

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### Coordinates of $\gamma^*-[({\rm IO}_6){\rm W}_{18}{\rm O}_{54}({\rm OH})_2{\rm H}]^{6-}$

W	-1.846785	-3.039889	-1.868478	O	2.767155	4.415365	-2.326880
W	1.770961	3.100854	-1.835546	O	5.277524	0.068205	-2.356068
W	3.639112	-0.128308	-1.870091	O	2.499536	-4.655749	-2.326045
W	1.888098	-3.118124	-1.860068	O	-1.372379	-0.768849	5.731138
W	-1.701246	3.175313	-1.809410	O	-1.305585	-2.493880	3.640191
W	-3.579202	-0.045845	-1.843660	O	0.003094	3.426061	1.796223
W	1.648821	-1.006202	-4.889768	O	-3.000898	-1.659562	1.816297
W	-1.684146	-0.943291	-4.906290	O	0.006202	1.560694	5.733060
W	-0.015390	1.908354	-4.831907	O	1.251788	-2.509739	3.641626
W	3.570778	0.061224	1.890154	O	2.952803	-1.726827	1.792846
W	-3.615355	0.130909	1.917016	O	1.332958	-0.793085	5.720570
W	-1.763435	-3.091955	1.876392	O	-3.470190	2.052997	1.899326
W	1.687518	-3.126669	1.895182	O	-0.041360	-3.946685	1.836646
W	-1.864325	3.107918	1.936144	O	3.865602	-0.060109	0.001244
W	1.855006	3.055713	1.901748	O	2.814445	0.127947	3.645696
W	-0.034704	-1.904664	4.925779	O	-1.542185	2.404845	3.681545
W	1.652935	0.937998	4.928894	O	-1.947876	3.393187	0.052190
W	-1.660242	0.976161	4.949694	O	-2.858703	0.201420	3.677899
O	1.326077	0.734549	-5.602081	O	1.542726	2.350037	3.650947
O	2.826521	-0.202503	-3.602679	O	1.927923	-3.331025	0.003338
O	-2.943027	1.741046	-1.751856	O	3.449112	1.969611	1.858885
O	3.003720	1.665087	-1.756757	O	5.214522	-0.137967	2.356042
O	-1.350877	0.780712	-5.676146	O	2.774721	1.572212	6.079622
O	1.546143	-2.417136	-3.615381	O	-0.040094	-3.200143	6.068604
O	0.004176	-3.406102	-1.760483	O	-2.754255	1.623760	6.119251
O	-0.017663	-1.570934	-5.660024	O	2.511444	4.568949	2.392036
O	0.038964	3.973143	-1.809055	O	-2.482812	4.640683	2.413001
O	3.488004	-2.054203	-1.844293	O	-5.263257	-0.059896	2.372661
O	-3.859323	0.050878	0.033943	O	-2.758102	-4.415894	2.342690
O	-1.570588	-2.362011	-3.627838	O	2.656065	-4.471327	2.354845
O	-1.281159	2.540899	-3.590746	I	-0.075609	0.080231	0.084812
O	1.978601	3.349550	0.031332	H	-0.037480	0.034648	2.769901
O	1.296648	2.490378	-3.584203	H	-0.590485	-0.046200	-2.710948
O	-2.835562	-0.133221	-3.620258	H	0.941241	-0.447191	-2.150566
O	-1.967152	-3.284224	0.009083	O	-0.022248	0.011135	3.756575
O	-3.444133	-1.953498	-1.818767	O	-1.388049	0.819408	1.258181
O	-2.501781	-4.564730	-2.321003	O	-0.016196	-1.550773	1.121494
O	-2.794655	-1.583914	-6.063834	O	1.361461	0.772408	1.177282
O	2.752016	-1.635080	-6.048597	O	-0.066624	-0.009153	-3.574008
O	0.022308	3.177740	-6.001527	O	-1.320479	-0.696871	-1.233295
O	-5.221736	0.161242	-2.314634	O	0.010704	1.612961	-1.092052
O	-2.671195	4.508153	-2.304398	O	1.370908	-0.757550	-1.291884

**Coordinates of  $\alpha$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{7-}$**

W	0.099527	-3.687631	1.655108	O	-4.330338	2.718921	-2.443572
W	-3.133566	1.617612	-1.864586	O	-1.782816	-1.374541	-5.194031
W	-1.582765	-0.929919	-3.538673	O	0.353882	-5.002888	-2.763090
W	0.019414	-3.704648	-1.669764	O	5.680782	1.676621	0.013122
W	-3.136365	1.604517	1.849833	O	4.272946	-0.098568	-1.486532
W	-1.525195	-0.888990	3.459035	O	0.805360	2.868328	3.485066
W	-3.694016	-3.350451	-1.677740	O	3.820090	-2.218693	0.007700
W	-3.617486	-3.345595	1.656400	O	4.508825	3.706889	1.381806
W	-5.146036	-0.913873	-0.014285	O	3.145505	1.826152	-2.789351
W	0.056149	3.563325	-1.832232	O	0.773414	2.886053	-3.490794
W	3.206484	-1.604182	1.720770	O	4.470991	3.657649	-1.329751
W	3.150352	-1.659933	-1.701918	O	2.156588	-0.579035	2.908235
W	1.516478	1.127417	-3.497019	O	2.113002	-0.592148	-2.858839
W	1.588196	1.139391	3.585778	O	-1.626436	2.692997	-2.193864
W	0.050102	3.563397	1.838385	O	1.810535	4.095515	-1.279820
W	4.646122	1.746628	-1.626982	O	3.210737	1.827736	2.855984
W	3.212221	4.230860	0.016779	O	-0.107014	0.332430	3.807320
W	4.705794	1.810243	1.663371	O	4.316474	-0.071075	1.526994
O	-5.280198	-2.308508	-1.366033	O	1.815795	4.121944	1.301752
O	-3.011393	-2.030440	-2.846741	O	-0.178885	0.305076	-3.785445
O	-2.788243	0.589194	3.414614	O	-0.445527	3.681939	0.002262
O	-2.810896	0.562638	-3.422233	O	-0.451924	5.111186	-2.421536
O	-5.207046	-2.301122	1.321830	O	3.556999	5.931263	-0.000138
O	-1.854739	-3.953205	-1.547904	O	5.954078	1.766744	-2.757769
O	0.338140	-4.632614	-0.010403	O	6.034976	1.825678	2.776004
O	-4.001390	-4.257684	-0.007319	O	-0.443120	5.113250	2.436899
O	-2.980659	2.046860	-0.006599	O	2.088132	1.095990	5.235802
O	-0.399772	-2.242812	-2.880698	O	4.233014	-2.498368	2.777722
O	1.825088	-2.959409	1.622154	O	4.195286	-2.519681	-2.771272
O	-1.811662	-3.929227	1.505879	O	2.022714	1.070815	-5.149642
O	-4.362867	0.244801	1.281006	Te	0.033602	0.191457	0.005363
O	-1.596024	2.678110	2.177791	H	2.260153	1.666707	0.333394
O	-4.382030	0.249687	-1.296407	H	-2.496747	-1.087980	-0.461436
O	-2.965629	-1.978983	2.766601	H	-1.361473	-2.164831	0.076531
O	1.777602	-2.967021	-1.613934	O	3.171091	2.024510	0.075280
O	-0.357976	-2.241043	2.860652	O	0.815029	1.530434	1.267728
O	0.379901	-5.003491	2.745189	O	1.773458	-0.640644	0.014991
O	-4.254804	-4.481950	2.787033	O	0.681991	1.467104	-1.398509
O	-4.347390	-4.518681	-2.778500	O	-3.084667	-1.867317	-0.112524
O	-6.802213	-0.409580	0.005166	O	-1.369475	-0.042253	1.374088
O	-1.749314	-1.337996	5.115075	O	-1.508956	-0.096164	-1.252460
O	-4.307918	2.730255	2.427755	O	-0.365554	-2.191706	0.009055

**Coordinates of  $\beta$ 1-[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>7-</sup>**

W	-3.072282	-1.707140	-1.857674	O	4.541011	2.352713	-2.247574
W	2.969571	1.780981	-1.797426	O	4.610942	-2.469045	-2.340624
W	3.030749	-1.937920	-1.876690	O	-0.190892	-5.227847	-2.310239
W	0.151990	-3.589920	-1.877199	O	0.772830	-1.348476	5.735666
W	0.119137	3.575434	-1.794359	O	2.474824	-1.267129	3.634040
W	-3.114709	1.690614	-1.841890	O	-4.025927	0.033566	2.151690
W	0.935209	-1.671554	-4.915992	O	1.963199	-3.376509	2.085030
W	-1.923113	0.004866	-4.913661	O	-1.560754	-0.006158	5.753656
W	0.910324	1.661605	-4.823563	O	2.486867	1.312740	3.678032
W	0.095361	3.532894	1.951782	O	2.010152	3.525864	2.178742
W	0.063917	-3.503053	1.865852	O	0.777543	1.350027	5.770346
W	3.021614	-1.788897	1.869436	O	-1.664356	-2.843244	1.527437
W	2.975153	1.899122	1.922736	O	3.310317	0.038084	1.535426
W	-3.102704	-1.614768	1.882405	O	3.148404	2.173249	0.056707
W	-3.082232	1.696451	1.903928	O	-0.139531	2.855900	3.722981
W	1.895948	0.006592	4.934812	O	-2.367700	-1.489880	3.648971
W	-0.963758	1.656220	4.964128	O	-3.435525	1.684384	0.024378
W	-0.955816	-1.643943	4.913188	O	-0.123299	-2.776834	3.629431
O	1.506585	-0.007172	-5.646595	O	-2.375276	1.550314	3.691953
O	2.368860	-1.536864	-3.640511	O	3.166810	-2.171019	-0.007355
O	-1.640193	2.864719	-1.564410	O	-1.669002	2.926983	1.579904
O	3.327378	-0.059492	-1.583693	O	-0.176415	5.198731	2.343445
O	-0.794922	1.336195	-5.709862	O	-1.610369	2.755564	6.137915
O	0.117348	-2.851804	-3.653002	O	3.203328	-0.011199	6.072168
O	-1.620822	-2.889183	-1.607481	O	-1.605765	-2.788084	6.038271
O	-0.795066	-1.358815	-5.702812	O	-4.387100	2.762223	2.307497
O	2.001621	3.470726	-1.973756	O	-4.389197	-2.695765	2.284839
O	2.070675	-3.604674	-2.022418	O	-0.207093	-5.154130	2.282283
O	-3.402780	-1.620409	0.011479	O	4.587155	-2.374125	2.293813
O	-2.495809	-1.313425	-3.638666	O	4.553409	2.461279	2.348422
O	0.074609	2.806873	-3.590451	Te	-0.041790	0.140616	0.128220
O	0.282622	3.838807	0.057444	H	0.029252	0.131729	2.795636
O	2.339199	1.463755	-3.590281	H	-0.512666	0.179724	-2.713312
O	-2.486652	1.302140	-3.631138	H	0.621598	-0.907140	-2.230667
O	0.301745	-3.799769	-0.010726	O	-0.004931	0.036612	3.784760
O	-3.987124	-0.002728	-1.966843	O	-1.610714	0.094961	1.371701
O	-4.349886	-2.792026	-2.268225	O	0.742125	-1.254770	1.224126
O	-3.230866	-0.004304	-6.050292	O	0.731773	1.443732	1.451243
O	1.590607	-2.775766	-6.067429	O	-0.074235	0.007807	-3.628184
O	1.579665	2.774462	-5.968967	O	0.857569	1.291219	-1.206265
O	-4.376696	2.775286	-2.299541	O	0.850246	-1.424659	-1.411047
O	-0.193338	5.205837	-2.264009	O	-1.417580	0.007840	-1.324726

### Coordinates of $\beta$ 2-[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>7-</sup>

W	-3.130777	-1.631799	-1.958161	O	4.533199	2.408823	-2.333206
W	2.941796	1.886042	-1.908330	O	4.569011	-2.370181	-2.297969
W	3.002480	-1.818888	-1.833454	O	-0.252074	-5.164631	-2.311619
W	0.050514	-3.530837	-1.852333	O	0.766301	-1.314621	5.642831
W	0.095635	3.532670	-1.881963	O	2.527024	-1.307665	3.645455
W	-3.107372	1.664879	-1.927793	O	-3.935333	-0.005559	2.059976
W	0.919437	-1.627228	-4.879977	O	2.066393	-3.569016	2.126844
W	-1.924165	0.019526	-5.007913	O	-1.534125	0.009810	5.657470
W	0.906094	1.671659	-4.938399	O	2.530354	1.296681	3.620117
W	0.106074	3.547355	1.852522	O	1.992201	3.405165	2.078495
W	0.154935	-3.602498	1.884310	O	0.780959	1.374671	5.708114
W	3.030496	-1.910402	1.915229	O	-1.622477	-2.938422	1.513959
W	3.045804	1.798773	1.821198	O	3.351956	-0.037467	1.530213
W	-3.022574	-1.699105	1.762080	O	3.122492	2.162125	-0.021470
W	-3.104120	1.683682	1.829193	O	-0.117041	2.826315	3.618154
W	1.911628	0.043091	4.889960	O	-2.324381	-1.491206	3.568485
W	-0.949727	1.666631	4.874105	O	-3.421483	1.657855	-0.045630
W	-0.965972	-1.647076	4.845577	O	-0.095754	-2.831305	3.622128
O	1.515264	0.007378	-5.717107	O	-2.349148	1.521312	3.592403
O	2.324166	-1.452987	-3.602496	O	3.156426	-2.164765	0.033748
O	-1.671662	2.886921	-1.652452	O	-1.644649	2.877912	1.496073
O	3.267281	0.024689	-1.572454	O	-0.160762	5.196600	2.285548
O	-0.805437	1.369023	-5.807290	O	-1.613627	2.786418	6.014996
O	0.059925	-2.766142	-3.615930	O	3.194542	0.031516	6.055821
O	-1.677927	-2.841247	-1.595829	O	-1.628758	-2.761635	5.982619
O	-0.794852	-1.344562	-5.765571	O	-4.396062	2.745748	2.250563
O	2.017198	3.550248	-2.058241	O	-4.329057	-2.740908	2.212604
O	1.963094	-3.430888	-1.981211	O	-0.141345	-5.245811	2.338065
O	-3.440530	-1.646566	-0.073553	O	4.610007	-2.481252	2.328409
O	-2.501756	-1.297039	-3.720218	O	4.612082	2.394761	2.235088
O	0.090609	2.842587	-3.695923	Te	-0.081916	0.112185	-0.119110
O	0.288182	3.831128	-0.014474	H	0.202432	0.562381	2.700122
O	2.335704	1.491910	-3.670887	H	-0.346882	0.069520	-2.809404
O	-2.540221	1.315541	-3.737720	H	0.499104	-1.018464	2.297709
O	0.295524	-3.854640	0.019113	O	0.079861	0.078844	3.608925
O	-4.093619	0.010208	-2.064041	O	-1.534230	-0.090605	1.197549
O	-4.377500	-2.748272	-2.384804	O	0.821493	-1.459111	1.461437
O	-3.223460	-0.008244	-6.156982	O	0.730179	1.240872	1.338868
O	1.589729	-2.771465	-5.992314	O	-0.084782	0.039296	-3.779733
O	1.590512	2.778043	-6.081251	O	0.741845	1.458136	-1.343078
O	-4.377180	2.768837	-2.340851	O	0.725788	-1.289236	-1.162679
O	-0.223828	5.180541	-2.310346	O	-1.567306	0.084413	-1.482484

### Coordinates of $\gamma$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{7-}$

W	-0.159774	-3.601112	-1.905984	O	0.187100	5.183867	-2.338001
W	-0.103541	3.544939	-1.882931	O	4.409393	2.754494	-2.239671
W	3.136391	1.685881	-1.778617	O	4.322822	-2.743199	-2.220085
W	3.028730	-1.687875	-1.765849	O	0.794164	-1.354235	5.783208
W	-3.023564	1.799987	-1.866723	O	2.529228	-1.284027	3.738973
W	-3.034534	-1.942057	-1.888021	O	-3.283160	0.023538	1.603052
W	1.895790	0.027306	-4.805242	O	1.691953	-2.848592	1.669189
W	-0.988242	-1.657425	-4.936985	O	-1.519079	0.008309	5.705995
W	-0.960273	1.656063	-4.933803	O	2.554133	1.319075	3.770947
W	-0.108077	3.557885	1.868088	O	1.681714	2.928906	1.714170
W	-0.055353	-3.524997	1.844119	O	0.798436	1.369645	5.805935
W	3.164763	-1.654561	1.980818	O	-1.967882	-3.426063	1.961465
W	3.093420	1.692800	1.979204	O	4.071205	0.016782	2.043033
W	-3.007938	-1.811844	1.864221	O	-0.209325	3.842136	0.003645
W	-2.950119	1.894979	1.880694	O	-0.108688	2.856075	3.686848
W	1.916300	0.012691	5.037617	O	-2.341007	-1.461810	3.621964
W	-0.915919	1.674636	4.915583	O	-3.189268	-2.125960	-0.022537
W	-0.918029	-1.632436	4.891124	O	-0.085799	-2.771416	3.625677
O	0.765185	1.344681	-5.703156	O	-2.345337	1.507528	3.655604
O	2.470655	1.328947	-3.576665	O	3.399089	1.723457	0.078651
O	-3.316098	-0.049404	-1.664158	O	-2.030657	3.566508	2.018594
O	1.651233	2.869778	-1.600072	O	0.177278	5.207120	2.313477
O	-1.577142	-0.000052	-5.719806	O	-1.594802	2.770265	6.072489
O	2.443999	-1.293063	-3.568713	O	3.205494	-0.007354	6.197656
O	1.613151	-2.927171	-1.624189	O	-1.590072	-2.766235	6.012833
O	0.749275	-1.318055	-5.640007	O	-4.536246	2.432830	2.312164
O	-2.002193	3.451371	-1.956338	O	-4.571899	-2.381260	2.315402
O	3.991583	-0.000443	-1.919525	O	0.225482	-5.160753	2.310697
O	-0.235755	-3.842847	-0.021716	O	4.429648	-2.745004	2.411590
O	-0.158731	-2.848640	-3.667626	O	4.389049	2.770024	2.380415
O	-2.379024	1.522115	-3.655939	Te	0.073795	0.125093	0.137085
O	-3.159646	2.098961	-0.004451	H	0.401317	0.064495	2.817418
O	-0.119034	2.809947	-3.653243	H	-0.126023	0.530030	-2.716197
O	-2.416172	-1.563385	-3.678569	H	-0.488233	-1.001676	-2.256824
O	3.406378	-1.705968	0.091231	O	0.092331	0.034324	3.781472
O	-2.088316	-3.613813	-2.003261	O	-0.733025	-1.288180	1.175150
O	0.154836	-5.240811	-2.362122	O	1.527832	0.138894	1.508714
O	-1.603522	-2.768808	-6.103105	O	-0.772885	1.484049	1.332457
O	3.192658	0.004405	-5.952658	O	-0.040483	0.059486	-3.629032
O	-1.608628	2.781118	-6.080426	O	-0.822833	-1.466879	-1.442548
O	-4.617016	-2.474730	-2.338351	O	-0.716291	1.235560	-1.340208
O	-4.593695	2.370748	-2.301043	O	1.538652	-0.093523	-1.169086

**Coordinates of  $\alpha^*-\text{[}(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}\text{]}^{7-}$**

W	3.495687	-0.057434	1.859899	O	-2.481356	-4.529055	2.328863
W	-3.527102	-0.038427	1.903211	O	2.511826	-4.556374	2.411290
W	-1.806677	-3.009340	1.869166	O	1.309447	0.749234	-5.641502
W	1.865494	-3.031298	1.932772	O	2.757057	-0.068654	-3.563743
W	-1.676126	3.140284	1.919490	O	-3.418681	1.976749	-1.919307
W	1.677766	3.155362	1.858490	O	3.496077	1.976032	-1.938255
W	-0.025478	-1.879269	4.926285	O	-1.355484	0.774695	-5.704703
W	1.628806	0.963878	4.857466	O	1.432428	-2.358357	-3.545697
W	-1.654686	0.955319	4.929852	O	0.025349	-3.990881	-1.912675
W	-1.701961	-3.162638	-1.884735	O	-0.005387	-1.526767	-5.628315
W	1.845791	2.981027	-1.843983	O	0.005281	3.421129	-1.646603
W	3.613638	0.063137	-1.839792	O	3.017296	-1.741112	-1.655613
W	1.774600	-3.163324	-1.817044	O	1.954535	3.453281	0.025468
W	-1.843555	3.062326	-1.819426	O	-1.457580	-2.379104	-3.598204
W	-3.536340	0.050375	-1.832730	O	-1.327199	2.470631	-3.600237
W	1.648945	-0.954883	-4.808602	O	-1.953941	3.390356	0.035783
W	-1.665698	-0.929086	-4.862001	O	1.314893	2.426333	-3.595642
W	-0.023904	1.902939	-4.850076	O	-2.808650	-0.080781	-3.613209
O	-1.370577	-0.780600	5.765185	O	-1.891492	-3.315657	-0.011044
O	-1.315950	-2.437233	3.629497	O	-2.963653	-1.738698	-1.674011
O	-0.002337	4.079390	2.024658	O	-2.685233	-4.499614	-2.347260
O	-3.400857	-1.952005	1.933183	O	-2.794557	-1.613541	-5.984355
O	-0.012023	1.535516	5.735567	O	2.791652	-1.625880	-5.910228
O	1.318434	-2.431940	3.643007	O	0.000996	3.213536	-5.981750
O	3.460958	-1.997148	1.953764	O	-5.190312	-0.121362	-2.295419
O	1.311776	-0.765101	5.720806	O	-2.502306	4.574478	-2.331864
O	-2.946230	1.739346	1.708960	O	2.533473	4.488599	-2.349339
O	0.025622	-3.410814	1.677386	O	5.235295	-0.138327	-2.393600
O	3.980059	0.006449	0.001648	O	2.745541	-4.480678	-2.362304
O	2.734124	0.058403	3.620007	Te	0.065795	0.149529	0.089087
O	-1.471673	2.384488	3.668178	H	-0.504015	0.417475	-2.686047
O	-3.827688	0.015573	0.027067	H	-0.297919	-0.162000	2.757815
O	-2.787142	0.087124	3.661715	H	0.135950	-1.040609	-2.134551
O	1.438272	2.370065	3.625205	O	-0.114000	0.034202	-3.557673
O	1.960482	-3.402841	0.026964	O	-1.288430	0.777473	-1.253501
O	2.916652	1.717286	1.663672	O	1.440871	0.901320	-1.110937
O	5.134040	0.134232	2.389558	O	0.085814	-1.536422	-1.260815
O	2.783998	1.609059	5.972645	O	-0.066032	-0.016418	3.723768
O	-0.019695	-3.218326	6.027192	O	0.007287	1.756707	1.220369
O	-2.802034	1.611112	6.051874	O	-1.263496	-0.712289	1.267627
O	2.689210	4.449187	2.407048	O	1.469007	-0.748795	1.147678
O	-2.679333	4.466996	2.389591				
O	-5.181510	0.137191	2.362747				

**Coordinates of  $\beta$ 1<sup>\*</sup>-[TeO<sub>6</sub>]W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H]<sup>7-</sup>**

W	-1.915763	-0.015373	4.848293	O	-1.670191	-2.950876	-1.838006
W	0.935385	1.619944	4.965917	O	3.451903	-0.013793	-1.792530
W	0.940025	-1.647454	4.943935	O	-4.473290	2.719982	-2.364453
W	3.092800	-1.691639	1.918055	O	-0.093132	-5.260644	-2.332995
W	-0.140698	3.545368	1.970229	O	4.565570	2.521819	-2.259427
W	-2.976229	-1.815491	1.807440	O	4.616699	-2.549621	-2.305507
W	3.069750	1.737146	1.937861	O	-0.097991	5.244579	-2.264520
W	-3.021470	1.865444	1.859060	O	-4.423105	-2.707487	-2.390038
W	-0.074832	-3.553787	1.910486	O	0.163127	2.880732	-3.583320
O	-3.244529	-0.046979	5.955765	O	-2.542449	-1.258789	-3.679176
O	1.586357	-2.806309	6.059142	O	-2.569737	1.288116	-3.671900
O	1.575116	2.758017	6.106938	O	0.196751	-2.856641	-3.616784
O	1.551266	-0.021783	5.794883	O	2.367365	1.570559	-3.566710
O	-0.793229	1.301674	5.739356	O	2.377701	-1.563476	-3.584295
O	-0.784844	-1.354886	5.715905	O	-0.769919	1.372887	-5.687393
O	0.067278	2.779915	3.697699	O	-0.761031	-1.343282	-5.673957
O	-2.416029	-1.323154	3.589591	O	1.543044	0.014416	-5.573812
O	-2.467642	1.316168	3.628627	O	1.601607	2.774784	-5.992515
O	0.091498	-2.791543	3.640669	O	-3.165585	0.010340	-6.136374
O	2.351231	1.485569	3.700904	O	1.622568	-2.739596	-6.045723
O	2.366188	-1.490534	3.674471	W	3.051415	1.833943	-1.797775
O	0.100452	5.191358	2.438826	W	0.080867	3.602939	-1.758159
O	-4.505039	-2.469796	2.294781	W	-3.099440	-1.709172	-1.907816
O	4.431305	-2.687529	2.357617	W	3.094039	-1.885776	-1.841258
O	4.380746	2.756810	2.410871	W	-3.145194	1.728815	-1.878187
O	-4.569035	2.478316	2.339137	W	0.106965	-3.619657	-1.844738
O	0.147102	-5.205773	2.350766	W	-1.913943	0.029609	-4.938667
O	-2.053135	3.521326	2.074392	W	0.958075	-1.660726	-4.876773
O	3.935032	0.020696	2.038043	W	0.934814	1.702666	-4.808453
O	-1.974222	-3.464259	1.967157	Te	-0.081407	0.114703	0.106308
O	1.650941	2.948597	1.686703	H	0.378929	-0.012435	2.776478
O	1.705481	-2.951227	1.657459	O	0.062286	-0.005990	3.736153
O	-3.382289	0.018177	1.618738	O	1.451764	0.006469	1.355668
O	3.377881	1.850003	0.070223	O	-0.077655	0.046496	-3.586133
O	3.349949	-1.841130	0.026230	O	0.798884	1.410846	-1.066870
O	-3.342356	2.025135	-0.010949	O	-0.909387	1.492602	1.244507
O	-0.044890	-3.860866	0.004255	O	-0.874965	-1.372435	1.131397
O	-0.121391	3.922699	0.078089	O	-1.526927	0.039277	-1.278519
O	-3.319320	-1.987083	-0.048152	O	0.817664	-1.329839	-1.253182
O	1.992403	3.467839	-1.747415	H	-0.556483	0.222216	-2.702096
O	2.028708	-3.493077	-1.781824	H	0.605539	-0.836355	-2.098310
O	-3.993505	0.006279	-1.829578				
O	-1.709264	2.963191	-1.811515				

**Coordinates of  $\beta$ 2<sup>\*</sup>-[TeO<sub>6</sub>]W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H]<sup>7-</sup>**

W	3.060625	1.822406	-1.935344	O	-0.789046	-1.322719	-5.691083
W	0.099502	3.546696	-1.911949	O	-2.545710	1.279759	-3.629825
W	-3.100913	-1.736830	-1.889168	O	0.169083	-2.850074	-3.672608
W	-0.076419	3.618637	1.843827	O	-3.975596	-0.013000	-1.787114
W	-3.036164	-1.822798	1.847631	O	-3.197856	0.029736	-6.077457
W	0.951221	1.667746	-4.979259	O	-4.456953	2.679006	-2.280733
W	3.084462	1.686704	1.784227	O	-0.084114	-5.219748	-2.354138
W	0.967828	1.639572	4.817486	O	-1.994793	3.479775	1.998037
W	3.038550	-1.899230	-1.874008	O	-1.977666	-3.434257	1.991650
W	0.960243	-1.644858	-4.912458	O	-0.750854	1.311586	5.640794
W	3.092092	-1.676718	1.845798	O	-0.771846	-1.364735	5.720666
W	0.947870	-1.669195	4.870572	O	-3.410960	0.018801	1.640322
W	-3.110844	1.696950	-1.833617	O	-2.460521	1.314831	3.624994
W	0.123936	-3.566598	-1.891395	O	0.107466	-2.830901	3.627895
W	-1.917301	0.031222	-4.912441	O	-3.252366	2.018530	0.036100
W	-3.056256	1.877573	1.915049	O	-0.082890	-3.881042	-0.017539
W	-0.073649	-3.582074	1.851003	O	-3.201790	-0.012223	6.022599
W	-1.894465	-0.040522	4.885215	O	-4.594559	2.507079	2.371063
O	3.390322	-0.024172	-1.858177	O	0.140399	-5.229683	2.324075
O	1.555496	0.015484	-5.745625	O	0.177553	2.858256	-3.686601
O	2.374354	1.585786	-3.707965	O	-2.547304	-1.263681	-3.654493
O	2.009300	3.445658	-1.833305	O	-0.084692	5.206196	-2.345299
O	1.578889	2.775697	-6.155176	O	-4.444326	-2.722364	-2.341862
O	4.589011	2.468368	-2.414211	O	0.079343	2.776732	3.572981
O	4.006404	0.000737	1.957475	O	-2.480921	-1.326703	3.629887
O	1.528271	-0.005462	5.653989	O	-0.099577	3.854496	-0.013498
O	1.693255	2.968251	1.605902	O	-3.272565	-2.023458	-0.006752
O	2.338550	1.423288	3.550933	O	0.155911	5.255397	2.338098
O	3.410348	1.884985	-0.063032	O	-4.566882	-2.468204	2.316361
O	1.639462	2.782684	5.918826	Te	0.081241	-0.098614	-0.081299
O	4.399129	2.685525	2.298254	H	0.082330	0.230744	-2.768479
O	2.374788	-1.570815	-3.672371	H	-0.225971	-0.623205	2.699996
O	2.049297	-3.550694	-1.887948	H	-0.419500	0.958756	2.163476
O	1.576315	-2.734733	-6.107666	O	0.013792	0.050693	-3.746437
O	4.565641	-2.529001	-2.385752	O	0.785079	1.314185	-1.259152
O	1.696676	-2.953383	1.616058	O	-0.075987	-0.097918	3.578697
O	2.353398	-1.466136	3.597872	O	1.677042	-0.009646	1.112601
O	3.413820	-1.916148	-0.034676	O	0.854320	-1.507264	-1.215428
O	1.630738	-2.784883	6.004409	O	-1.566760	-0.026577	-1.128422
O	4.415316	-2.683684	2.322044	O	-0.719755	-1.318463	1.304855
O	-1.691341	2.948421	-1.838143	O	-0.730828	1.368857	1.300412
O	-1.682520	-2.966243	-1.848758				
O	-0.800861	1.386160	-5.735412				

**Coordinates of  $\gamma^*-[({\rm TeO}_6){\rm W}_{18}{\rm O}_{54}({\rm OH})_2{\rm H}]^{7-}$**

W	-1.820562	-3.007811	-1.844474	O	2.750354	4.448672	-2.372193
W	1.741666	3.145942	-1.857222	O	5.264936	0.137268	-2.365868
W	3.625059	-0.075436	-1.874637	O	2.539599	-4.606417	-2.276532
W	1.909342	-3.062431	-1.841358	O	-1.366971	-0.809303	5.761487
W	-1.667813	3.136710	-1.781422	O	-1.278468	-2.547221	3.699231
W	-3.569874	-0.062829	-1.873727	O	-0.032196	3.348489	1.748160
W	1.652652	-0.994553	-4.891723	O	-2.947305	-1.643841	1.823745
W	-1.675792	-0.972636	-4.922076	O	-0.003761	1.517745	5.706330
W	-0.041390	1.899522	-4.833249	O	1.279341	-2.536550	3.692702
W	3.584037	0.105796	1.879734	O	2.936561	-1.672523	1.796206
W	-3.583355	0.148828	1.872723	O	1.358395	-0.807355	5.750133
W	-1.722505	-3.066480	1.908312	O	-3.569334	2.071640	1.946200
W	1.687196	-3.081443	1.917516	O	-0.011147	-3.953028	1.853127
W	-1.895370	3.024616	1.930263	O	3.881371	-0.012761	-0.000695
W	1.809195	2.986365	1.864377	O	2.837379	0.138786	3.653123
W	-0.006818	-1.924917	4.984753	O	-1.548028	2.370014	3.688813
W	1.650614	0.924960	4.911144	O	-2.006808	3.389375	0.050089
W	-1.673453	0.921108	4.929283	O	-2.868193	0.170305	3.680603
O	1.318873	0.736050	-5.610899	O	1.520044	2.335665	3.648604
O	2.824727	-0.173980	-3.610332	O	1.905591	-3.252834	0.015672
O	-2.931981	1.708073	-1.767506	O	3.489962	2.006072	1.878893
O	2.983848	1.702395	-1.770340	O	5.227474	-0.123558	2.348788
O	-1.357147	0.754270	-5.694962	O	2.755232	1.578664	6.072988
O	1.578654	-2.403029	-3.619397	O	0.001164	-3.215643	6.142794
O	0.030842	-3.375077	-1.783117	O	-2.757040	1.569097	6.112909
O	-0.001103	-1.589674	-5.670914	O	2.432823	4.525408	2.359956
O	0.028623	4.042399	-1.851580	O	-2.476249	4.581123	2.415826
O	3.510308	-2.006684	-1.836244	O	-5.230701	-0.094431	2.338658
O	-3.871234	0.027456	0.012480	O	-2.743086	-4.394553	2.327297
O	-1.575669	-2.379677	-3.641457	O	2.699119	-4.417205	2.326105
O	-1.296347	2.526301	-3.606500	Te	-0.101405	0.132907	0.101370
O	1.972569	3.384566	-0.003902	H	-0.003362	-0.314937	2.777952
O	1.281447	2.497571	-3.603988	H	-0.585285	-0.101277	-2.705429
O	-2.858864	-0.164296	-3.660166	H	0.944343	-0.406193	-2.117575
O	-1.891647	-3.240247	0.027866	O	-0.013321	-0.069905	3.751150
O	-3.456593	-1.974152	-1.825853	O	-1.511374	0.890920	1.244336
O	-2.466994	-4.552333	-2.264502	O	-0.013602	-1.441973	1.291317
O	-2.767460	-1.624248	-6.098260	O	1.376408	0.889107	1.166405
O	2.766161	-1.614003	-6.052324	O	-0.084752	-0.026183	-3.592161
O	-0.011802	3.160207	-6.019513	O	-1.313677	-0.707445	-1.255982
O	-5.219097	0.158544	-2.335358	O	-0.058333	1.683208	-1.119462
O	-2.657487	4.458041	-2.305425	O	1.377030	-0.707222	-1.265571

**Coordinates of  $\alpha$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{7-}$**

O	0.178755	3.736111	0.050413	O	1.597664	-1.545006	2.866090
O	-0.780995	1.428669	1.266177	O	4.267084	-2.517347	2.774117
O	1.495554	1.016837	0.021521	O	1.247189	-6.026651	2.808415
O	-0.833319	1.245701	-1.280914	O	1.218737	-6.150247	-2.758263
O	-0.260679	-3.582804	-0.128917	O	-3.560421	-5.812781	0.040436
O	-0.830456	-1.100255	1.354256	O	0.083621	-2.194915	5.115358
O	-0.825099	-1.312682	-1.281208	O	-4.653645	-1.938771	2.380424
O	1.431429	-1.461837	0.064786	O	-4.672462	-1.977654	-2.393389
W	3.027312	-2.001151	1.684973	O	0.089880	-2.217998	-5.127777
W	-3.059553	-1.653894	-1.850077	O	4.277363	-2.560486	-2.784751
W	-0.195173	-1.823857	-3.467656	O	1.895752	5.612714	-0.010183
W	3.029355	-2.098440	-1.686696	O	2.532214	3.433533	-1.473287
W	-3.041168	-1.629001	1.833753	O	-1.860014	2.329348	3.485618
W	-0.195708	-1.756826	3.465616	O	4.047878	1.865026	-0.000437
W	0.620414	-4.945959	-1.662928	O	-0.434198	5.815681	1.344012
W	0.666100	-4.876801	1.662873	O	0.323734	3.604202	-2.795399
W	-2.196358	-4.744041	0.000477	O	-1.875242	2.271578	-3.468878
W	-2.877930	2.048542	-1.829581	O	-0.415071	5.752308	-1.352380
W	3.172298	1.720934	1.694810	O	1.712534	1.439080	2.870100
W	3.171396	1.634439	-1.686792	O	1.692592	1.384700	-2.844985
W	-0.017083	1.886346	-3.550399	O	-3.115008	0.205508	-2.219862
W	0.000720	1.953130	3.572096	O	-2.270970	3.798499	-1.292081
W	-2.860011	2.078333	1.846005	O	0.356222	3.681595	2.833838
W	1.243988	4.810111	-1.645199	O	-0.353761	0.109995	3.797715
W	-1.618014	5.034824	-0.010365	O	2.538072	3.496229	1.489360
W	1.221635	4.894680	1.645357	O	-2.294036	3.843141	1.291681
O	-1.133043	-5.667722	-1.347226	O	-0.376697	0.043445	-3.756389
O	-0.072733	-3.646504	-2.840401	O	-3.262113	1.748966	0.006511
O	-2.105808	-1.956134	3.466730	O	-4.426963	2.555620	-2.411678
O	-2.109880	-2.013840	-3.466791	O	-2.827167	6.278845	-0.038418
O	-1.092546	-5.587661	1.340588	O	1.991500	5.870398	-2.787110
O	2.160511	-3.771127	-1.530728	O	1.982676	5.984640	2.756477
O	3.905579	-2.344381	-0.001023	O	-4.408273	2.589669	2.432543
O	1.197794	-5.715131	0.010320	O	0.352827	2.333611	5.216714
O	-3.335179	-1.245626	-0.007599	O	4.472314	2.058917	2.773085
O	1.583407	-1.594932	-2.840253	O	4.455945	1.987808	-2.777917
O	3.463147	-0.176202	1.607339	O	0.340725	2.261644	-5.193326
O	2.153695	-3.705619	1.498991	W	-0.109705	0.122050	0.028152
O	-2.672742	-3.430460	1.286439	H	-0.016100	2.775298	0.255134
O	-3.094657	0.244639	2.211427	H	-0.565676	-2.660873	-0.544715
O	-2.725814	-3.473218	-1.293050	H	0.887112	-2.297435	0.129500
O	-0.091932	-3.546808	2.759712				
O	3.436470	-0.233939	-1.591716				

**Coordinates of  $\beta$ 1-[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{7-}$**

W	-3.041203	-1.638509	-1.855334	O	4.586556	-2.448429	-2.325435
W	2.933078	1.794255	-1.787485	O	-0.233483	-5.240044	-2.311432
W	3.014656	-1.904203	-1.851949	O	0.776941	-1.350210	5.717360
W	0.115511	-3.606891	-1.877121	O	2.451981	-1.276052	3.625495
W	0.113490	3.575368	-1.783099	O	-3.996716	0.003118	2.153314
W	-3.066782	1.641837	-1.842700	O	1.977172	-3.412691	2.082088
W	0.921105	-1.660521	-4.895541	O	-1.543389	-0.019219	5.741372
W	-1.931882	0.003521	-4.932259	O	2.517223	1.303747	3.681266
W	0.889538	1.664921	-4.813312	O	2.033741	3.479428	2.183314
W	0.113780	3.500558	1.947560	O	0.786154	1.344060	5.778415
W	0.080996	-3.510352	1.859950	O	-1.648324	-2.829987	1.520108
W	3.009142	-1.810235	1.885375	O	3.309524	0.025685	1.541722
W	3.041862	1.885165	1.933198	O	3.142742	2.179082	0.071978
W	-3.128268	-1.663977	1.877015	O	-0.117336	2.836965	3.724213
W	-3.067983	1.677782	1.876710	O	-2.351773	-1.489994	3.625665
W	1.897670	0.013444	4.940040	O	-3.448024	1.655717	0.023832
W	-0.961015	1.646876	4.951104	O	-0.090881	-2.757181	3.604378
W	-0.947079	-1.646304	4.887713	O	-2.347955	1.519352	3.671847
O	1.494091	0.000617	-5.632336	O	3.154714	-2.174097	0.008953
O	2.338354	-1.504839	-3.610069	O	-1.667841	2.932517	1.590818
O	-1.616978	2.839827	-1.533321	O	-0.144787	5.165947	2.349834
O	3.327419	-0.045421	-1.559458	O	-1.618071	2.748560	6.119261
O	-0.801856	1.343297	-5.716694	O	3.212541	-0.029335	6.068057
O	0.094263	-2.844022	-3.640627	O	-1.593974	-2.807774	5.992356
O	-1.608248	-2.861277	-1.581820	O	-4.371618	2.733717	2.309041
O	-0.797987	-1.355505	-5.713261	O	-4.388795	-2.764259	2.290746
O	1.997646	3.490440	-1.975211	O	-0.220359	-5.149160	2.295308
O	2.027342	-3.558566	-2.008349	O	4.577216	-2.382789	2.310326
O	-3.410270	-1.600797	0.023712	O	4.626584	2.425884	2.347913
O	-2.500295	-1.310885	-3.659018	W	-0.024424	0.107014	0.127635
O	0.062260	2.815144	-3.580524	H	0.112041	0.286894	2.775975
O	0.309440	3.829939	0.066158	H	-0.599354	0.136617	-2.700577
O	2.309976	1.447960	-3.568846	H	0.623523	-0.825181	-2.197033
O	-2.496460	1.302499	-3.655749	O	0.020106	0.062669	3.748114
O	0.301140	-3.818333	-0.008510	O	-1.561628	0.153049	1.217238
O	-4.035419	0.001042	-1.989084	O	0.736675	-1.239625	1.125675
O	-4.303326	-2.755566	-2.243975	O	0.662575	1.391266	1.397268
O	-3.240399	-0.005872	-6.069951	O	-0.107542	0.012532	-3.612730
O	1.595435	-2.768459	-6.032895	O	0.840647	1.276324	-1.114023
O	1.575453	2.781558	-5.944448	O	0.817964	-1.305823	-1.347724
O	-4.307525	2.765867	-2.283261	O	-1.465264	0.017012	-1.335360
O	-0.226862	5.205130	-2.237591				
O	4.506803	2.356808	-2.240060				

### Coordinates of $\beta$ 2-[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>7-</sup>

W	-3.150832	-1.690550	-1.968451	O	4.598594	2.381877	-2.345200
W	3.008289	1.876371	-1.915154	O	4.563049	-2.365172	-2.297721
W	2.990509	-1.836594	-1.834374	O	-0.240952	-5.169622	-2.316562
W	0.072493	-3.537393	-1.864776	O	0.759574	-1.313431	5.639338
W	0.104137	3.512685	-1.857311	O	2.516367	-1.294927	3.634924
W	-3.083037	1.635213	-1.910121	O	-3.964627	0.014526	2.055979
W	0.930572	-1.637819	-4.886670	O	2.036200	-3.502752	2.105392
W	-1.916989	0.000969	-4.993834	O	-1.542269	0.008519	5.653489
W	0.911540	1.655379	-4.918508	O	2.525571	1.309061	3.632107
W	0.122529	3.499679	1.852167	O	2.010408	3.460770	2.102510
W	0.122496	-3.571822	1.862150	O	0.771564	1.374912	5.722517
W	3.052418	-1.885004	1.913750	O	-1.638364	-2.925332	1.498608
W	2.964338	1.810451	1.811884	O	3.321180	-0.030736	1.515572
W	-3.025706	-1.653172	1.757211	O	3.103534	2.165984	-0.040540
W	-3.103689	1.693168	1.828774	O	-0.121481	2.835427	3.636350
W	1.901060	0.054135	4.887998	O	-2.313883	-1.460722	3.548367
W	-0.954170	1.668211	4.874227	O	-3.438137	1.644307	-0.044636
W	-0.963273	-1.636923	4.837848	O	-0.094646	-2.797452	3.597719
O	1.529961	-0.006672	-5.707825	O	-2.354423	1.523130	3.590007
O	2.318427	-1.452366	-3.589898	O	3.145497	-2.165837	0.027395
O	-1.672371	2.889272	-1.650349	O	-1.635617	2.852727	1.480062
O	3.254272	0.017187	-1.565723	O	-0.180294	5.152101	2.269100
O	-0.787859	1.340871	-5.799471	O	-1.628076	2.780125	6.019248
O	0.069739	-2.773696	-3.616942	O	3.184654	0.029550	6.054522
O	-1.666036	-2.845678	-1.606272	O	-1.634594	-2.767374	5.953256
O	-0.777681	-1.361778	-5.759297	O	-4.376720	2.782010	2.242422
O	2.026914	3.502885	-2.063108	O	-4.323834	-2.704096	2.211285
O	1.981286	-3.458995	-1.993079	O	-0.164745	-5.215036	2.316097
O	-3.441591	-1.647957	-0.086314	O	4.634113	-2.445127	2.317455
O	-2.498352	-1.330100	-3.719396	O	4.545958	2.391206	2.208872
O	0.090769	2.795458	-3.668396	W	-0.071427	0.074997	-0.113525
O	0.315807	3.833029	-0.012667	H	0.268268	0.627188	2.685549
O	2.345669	1.461425	-3.650547	H	-0.335668	0.063071	-2.782039
O	-2.513583	1.289796	-3.730097	H	0.422430	-0.956735	2.243185
O	0.304013	-3.837774	0.001634	O	0.084544	0.116665	3.594227
O	-4.066431	-0.025717	-2.075072	O	-1.515345	-0.078311	1.122519
O	-4.390937	-2.813325	-2.387073	O	0.727671	-1.361251	1.382918
O	-3.213631	-0.025090	-6.145379	O	0.745016	1.282815	1.359116
O	1.614782	-2.789751	-5.981279	O	-0.077870	0.017981	-3.752185
O	1.596422	2.773863	-6.048408	O	0.653336	1.433573	-1.189991
O	-4.356063	2.728311	-2.346221	O	0.703310	-1.266904	-1.095986
O	-0.203334	5.154927	-2.314650	O	-1.520008	0.119610	-1.394231

### Coordinates of $\gamma$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{7-}$

W	-0.139173	-3.579626	-1.905410	O	0.211578	5.131649	-2.322057
W	-0.117671	3.490832	-1.885643	O	4.392203	2.776421	-2.226017
W	3.137430	1.685484	-1.764305	O	4.324646	-2.718121	-2.224964
W	3.032673	-1.665024	-1.764398	O	0.783842	-1.363115	5.777011
W	-2.941968	1.789710	-1.845398	O	2.516021	-1.295642	3.739565
W	-3.081638	-1.954247	-1.901422	O	-3.262790	0.025706	1.606500
W	1.881765	0.046110	-4.793581	O	1.660070	-2.817244	1.648719
W	-0.995728	-1.655890	-4.936049	O	-1.522358	0.002557	5.696271
W	-0.974361	1.656719	-4.945103	O	2.551292	1.309353	3.779792
W	-0.095449	3.560023	1.853319	O	1.699262	2.936330	1.732258
W	-0.078826	-3.522339	1.838901	O	0.792317	1.355310	5.808908
W	3.150614	-1.658723	1.979823	O	-1.986503	-3.440050	1.965132
W	3.101964	1.681271	1.986504	O	4.072236	0.003528	2.065327
W	-3.003342	-1.819471	1.859165	O	-0.224793	3.846323	0.011193
W	-3.001423	1.901185	1.901952	O	-0.104300	2.835775	3.676980
W	1.916781	0.004035	5.036987	O	-2.330366	-1.452709	3.604164
W	-0.910362	1.673805	4.907910	O	-3.193268	-2.129366	-0.023367
W	-0.923815	-1.634718	4.888173	O	-0.090762	-2.762596	3.611113
O	0.761470	1.353420	-5.704011	O	-2.343576	1.489744	3.645754
O	2.463648	1.339149	-3.562134	O	3.423752	1.713321	0.093164
O	-3.287089	-0.067205	-1.663749	O	-2.022858	3.529945	2.028093
O	1.640926	2.836168	-1.566217	O	0.180357	5.204128	2.322586
O	-1.583036	0.001653	-5.727983	O	-1.595498	2.772549	6.057218
O	2.414815	-1.278020	-3.546973	O	3.205239	-0.024966	6.196985
O	1.633245	-2.936464	-1.617004	O	-1.606351	-2.779612	5.990869
O	0.744022	-1.304668	-5.628136	O	-4.585679	2.425019	2.332377
O	-2.017108	3.486647	-1.961666	O	-4.570004	-2.363574	2.321415
O	4.008027	0.010098	-1.925210	O	0.227039	-5.151209	2.307507
O	-0.255396	-3.830677	-0.020338	O	4.395333	-2.774784	2.402648
O	-0.157037	-2.850289	-3.678007	O	4.397677	2.752736	2.399397
O	-2.383601	1.533478	-3.668904	W	0.087728	0.112264	0.161988
O	-3.120111	2.093847	0.027499	H	0.405987	0.076818	2.808857
O	-0.122996	2.813526	-3.669075	H	-0.202393	0.561833	-2.700204
O	-2.440640	-1.582333	-3.691706	H	-0.420713	-1.006329	-2.273535
O	3.410354	-1.682141	0.091964	O	0.095191	0.032051	3.766533
O	-2.087822	-3.591338	-2.004629	O	-0.714771	-1.249385	1.080320
O	0.160486	-5.227061	-2.355989	O	1.524291	0.148111	1.449919
O	-1.596015	-2.764409	-6.112361	O	-0.641101	1.469387	1.224490
O	3.189598	0.012041	-5.927651	O	-0.062136	0.080485	-3.614375
O	-1.617915	2.786104	-6.092079	O	-0.740122	-1.466445	-1.452327
O	-4.670283	-2.476166	-2.331379	O	-0.739892	1.260269	-1.330804
O	-4.532020	2.345132	-2.243484	O	1.515200	-0.076132	-1.078985

**Coordinates of  $\alpha^*-\text{[WO}_6\text{W}_{18}\text{O}_{54}\text{(OH)}_2\text{H}]^{7-}$**

W	3.582905	-0.060682	1.914220	O	-5.190089	0.213027	2.389639
W	-3.548494	-0.017944	1.917309	O	-2.509272	-4.438538	2.312303
W	-1.831099	-2.926416	1.810308	O	2.493289	-4.462293	2.364405
W	1.830776	-2.935038	1.886331	O	1.317957	0.764318	-5.649301
W	-1.697454	3.188498	1.924899	O	2.713091	-0.061130	-3.563681
W	1.746634	3.161688	1.926178	O	-3.410488	1.973570	-1.882721
W	-0.038367	-1.869022	4.892833	O	3.463378	1.991175	-1.887755
W	1.652187	0.953899	4.914871	O	-1.344466	0.808970	-5.702423
W	-1.637969	0.994394	4.924715	O	1.455613	-2.403930	-3.610284
W	-1.677057	-3.174638	-1.923028	O	-0.006107	-4.133938	-2.002267
W	1.874949	3.023005	-1.828397	O	-0.014097	-1.503832	-5.654173
W	3.467533	0.040897	-1.795365	O	0.019594	3.377102	-1.620054
W	1.689263	-3.205172	-1.842893	O	2.927017	-1.755422	-1.654782
W	-1.822863	3.023928	-1.828700	O	1.947410	3.380350	0.053619
W	-3.513979	0.040274	-1.820122	O	-1.494934	-2.388061	-3.650911
W	1.643070	-0.969824	-4.824476	O	-1.318578	2.448809	-3.585484
W	-1.677581	-0.903230	-4.876757	O	-1.903958	3.368266	0.055133
W	0.009812	1.904908	-4.847450	O	1.328659	2.419425	-3.562151
O	-1.347904	-0.734860	5.752457	O	-2.803173	-0.059939	-3.616037
O	-1.324355	-2.369231	3.605176	O	-1.898972	-3.349378	-0.046297
O	0.027982	4.028417	2.000275	O	-2.935471	-1.731223	-1.678334
O	-3.471782	-1.925673	1.952459	O	-2.706127	-4.486022	-2.387735
O	0.007237	1.568611	5.747800	O	-2.810541	-1.549082	-6.018280
O	1.317990	-2.379538	3.635320	O	2.799770	-1.599162	-5.938504
O	3.497430	-1.969634	1.977032	O	0.032464	3.244316	-5.943158
O	1.318967	-0.754768	5.742915	O	-5.168383	-0.138497	-2.281717
O	-2.931918	1.761041	1.727552	O	-2.468509	4.553038	-2.301462
O	0.000760	-3.360765	1.686853	O	2.502821	4.552482	-2.319013
O	3.908913	-0.025604	0.060548	O	5.112834	-0.134875	-2.308356
O	2.759023	0.073672	3.646610	O	2.704120	-4.504539	-2.376057
O	-1.441928	2.417241	3.663900	W	0.041548	0.145727	0.139709
O	-3.829978	0.031108	0.044361	H	-0.452927	0.373610	-2.682417
O	-2.752961	0.106127	3.652247	H	-0.032717	-0.046022	2.759984
O	1.463300	2.387878	3.656265	H	0.086032	-1.177486	-2.215307
O	1.899313	-3.411416	-0.004942	O	-0.103895	0.019033	-3.574166
O	2.956634	1.719899	1.713770	O	-1.248522	0.713152	-1.197670
O	5.212494	0.176658	2.427429	O	1.438997	0.704231	-1.046487
O	2.807398	1.609355	6.024632	O	0.030389	-1.717208	-1.380218
O	-0.041931	-3.213900	5.986493	O	-0.008559	0.032095	3.743372
O	-2.793132	1.656631	6.030337	O	0.012909	1.610068	1.203668
O	2.761642	4.466350	2.413525	O	-1.301109	-0.825753	1.111787
O	-2.693607	4.512684	2.397815	O	1.344492	-0.863287	1.138258

**Coordinates of  $\beta$ 1<sup>\*</sup>-[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>7-</sup>**

W	-1.907242	0.008291	4.894412	O	-1.665875	-2.953468	-1.824907
W	0.949457	1.647527	4.931174	O	3.437403	-0.025134	-1.807451
W	0.944161	-1.631976	4.938795	O	-4.448304	2.713125	-2.303063
W	3.104085	-1.682324	1.908561	O	-0.090014	-5.258589	-2.309300
W	-0.122404	3.570366	1.943902	O	4.567046	2.492699	-2.309441
W	-3.038651	-1.813104	1.869687	O	4.618367	-2.547400	-2.332744
W	3.088121	1.729955	1.898332	O	-0.100151	5.229233	-2.268779
W	-3.028897	1.885522	1.895864	O	-4.417594	-2.709819	-2.304372
W	-0.091905	-3.518508	1.909502	O	0.166252	2.880885	-3.610062
O	-3.231887	0.005198	6.009381	O	-2.572783	-1.270976	-3.658766
O	1.603811	-2.785990	6.049739	O	-2.590417	1.273279	-3.659720
O	1.610101	2.795200	6.046164	O	0.186290	-2.880323	-3.624936
O	1.548315	0.006387	5.766565	O	2.354123	1.563098	-3.597667
O	-0.772787	1.336146	5.742279	O	2.374496	-1.587892	-3.604631
O	-0.777519	-1.328504	5.748112	O	-0.799949	1.361812	-5.689134
O	0.066183	2.793422	3.671904	O	-0.782813	-1.356056	-5.660769
O	-2.436888	-1.299731	3.633012	O	1.520082	-0.000680	-5.592338
O	-2.445540	1.341405	3.646608	O	1.575746	2.754447	-6.030640
O	0.081642	-2.760424	3.653338	O	-3.192095	-0.009580	-6.115885
O	2.344514	1.469820	3.656096	O	1.599540	-2.755771	-6.057914
O	2.355767	-1.453495	3.658438	W	3.045751	1.824990	-1.837924
O	0.138178	5.214349	2.400740	W	0.106264	3.582120	-1.792556
O	-4.579857	-2.431322	2.343027	W	-3.080036	-1.707096	-1.868503
O	4.422411	-2.692385	2.378917	W	3.093039	-1.899395	-1.844679
O	4.385719	2.762506	2.379165	W	-3.119092	1.706110	-1.852913
O	-4.577345	2.494041	2.360138	W	0.123019	-3.611191	-1.835075
O	0.124518	-5.168451	2.367172	W	-1.935345	0.009327	-4.922275
O	-2.034136	3.528534	2.060499	W	0.948596	-1.681232	-4.876686
O	3.975243	0.022269	2.023712	W	0.913859	1.683393	-4.843268
O	-2.002331	-3.434318	2.011549	W	-0.067105	0.158344	0.137496
O	1.655687	2.939027	1.671967	H	0.096656	-0.075188	2.760266
O	1.695733	-2.927347	1.670856	O	0.012546	0.000540	3.745577
O	-3.388193	0.032272	1.665831	O	1.522736	0.000441	1.169804
O	3.386011	1.864066	0.034510	O	-0.096486	0.042097	-3.596109
O	3.387132	-1.879850	0.019588	O	0.800454	1.363462	-1.062440
O	-3.283285	2.020338	0.024667	O	-0.853421	1.453421	1.205919
O	-0.056799	-3.851958	0.018214	O	-0.764369	-1.315476	1.126301
O	-0.111353	3.882095	0.057088	O	-1.490898	0.013602	-1.207903
O	-3.274685	-1.979138	0.011734	O	0.822027	-1.369933	-1.255596
O	2.012975	3.480211	-1.775516	H	-0.523981	0.211089	-2.689523
O	2.048938	-3.530789	-1.796201	H	0.609963	-0.894866	-2.098988
O	-3.991670	0.001339	-1.778751				
O	-1.678511	2.927826	-1.817390				

### Coordinates of $\beta$ 2\*- $[(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{7-}$

W	3.038591	1.825288	-1.914550	O	-0.793863	1.365266	-5.736652
W	0.100614	3.550630	-1.899312	O	-0.789303	-1.346555	-5.705624
W	-3.091376	-1.726714	-1.890689	O	-2.543352	1.268469	-3.642484
W	-0.073720	3.631442	1.851982	O	0.182363	-2.887136	-3.683087
W	-3.023595	-1.809833	1.847011	O	-4.003744	-0.019093	-1.810572
W	0.946885	1.656756	-4.956922	O	-3.199970	0.014162	-6.094661
W	3.115539	1.730706	1.818814	O	-4.439745	2.682891	-2.300129
W	0.966560	1.644007	4.829404	O	-0.108328	-5.283450	-2.369998
W	3.075133	-1.909992	-1.899741	O	-2.001286	3.520155	2.011931
W	0.951329	-1.667330	-4.925985	O	-1.981508	-3.438997	1.979327
W	3.120779	-1.692995	1.853686	O	-0.742266	1.308626	5.652005
W	0.948261	-1.665161	4.869890	O	-0.761442	-1.364812	5.725122
W	-3.114208	1.677274	-1.839295	O	-3.407747	0.026740	1.656050
W	0.108420	-3.635066	-1.912832	O	-2.459077	1.317585	3.634636
W	-1.922522	0.016787	-4.924951	O	0.109178	-2.829213	3.624547
W	-3.035567	1.893746	1.909612	O	-3.270487	2.007207	0.029601
W	-0.076293	-3.550471	1.844886	O	-0.069473	-3.864109	-0.041228
W	-1.891559	-0.038758	4.883435	O	-3.189934	-0.014999	6.031590
O	3.370386	-0.032275	-1.845764	O	-4.574266	2.528454	2.371446
O	1.553072	-0.003112	-5.722828	O	0.137006	-5.205085	2.293831
O	2.361989	1.560263	-3.683622	O	0.174036	2.845910	-3.679076
O	2.016982	3.467749	-1.847637	O	-2.548448	-1.271859	-3.667513
O	1.591943	2.757342	-6.128044	O	-0.114599	5.200213	-2.359087
O	4.574534	2.449969	-2.393996	O	-4.426198	-2.726961	-2.335116
O	3.999363	0.007806	1.940242	O	0.091495	2.786897	3.587598
O	1.542219	-0.007273	5.648535	O	-2.485419	-1.333794	3.642906
O	1.720167	3.008536	1.640000	O	-0.077013	3.890667	-0.005849
O	2.361433	1.439616	3.566049	O	-3.246593	-1.997757	-0.018612
O	3.390148	1.891422	-0.043747	O	0.148203	5.268019	2.358821
O	1.636917	2.778180	5.940227	O	-4.561772	-2.461655	2.290325
O	4.442787	2.719140	2.311530	W	0.106355	-0.118991	-0.126719
O	2.375277	-1.589751	-3.669599	H	-0.045134	0.112805	-2.755813
O	2.034579	-3.537584	-1.877679	H	-0.220424	-0.590604	2.683749
O	1.582940	-2.749469	-6.117958	H	-0.449631	1.000146	2.136748
O	4.610537	-2.523771	-2.390513	O	-0.010480	0.015250	-3.741826
O	1.705384	-2.947040	1.615958	O	0.763760	1.337359	-1.160613
O	2.369957	-1.473874	3.592045	O	-0.065743	-0.106798	3.585180
O	3.389844	-1.914302	-0.042505	O	1.587979	0.015577	1.060929
O	1.633816	-2.786462	5.997790	O	0.809269	-1.438955	-1.178407
O	4.444491	-2.702025	2.311840	O	-1.531347	-0.013010	-1.116930
O	-1.672475	2.912462	-1.821318	O	-0.729184	-1.284327	1.252493
O	-1.670976	-2.974406	-1.875842	O	-0.763850	1.403275	1.285118

**Coordinates of  $\gamma^*-[W_6O_{18}O_{54}(OH)_2H]^{7-}$**

W	-1.814157	-3.009185	-1.858089	O	2.723458	4.429647	-2.321171
W	1.722947	3.105651	-1.843224	O	5.272147	0.125701	-2.355538
W	3.628969	-0.099166	-1.871600	O	2.534546	-4.605780	-2.304509
W	1.915394	-3.059795	-1.845210	O	-1.366565	-0.784231	5.744425
W	-1.696504	3.162077	-1.811638	O	-1.281025	-2.536778	3.688216
W	-3.547709	-0.078416	-1.868336	O	-0.029713	3.352416	1.784327
W	1.655702	-0.988347	-4.892017	O	-2.921730	-1.635274	1.820244
W	-1.678819	-0.967516	-4.927217	O	-0.010284	1.550880	5.720809
W	-0.048120	1.903926	-4.849711	O	1.276692	-2.523282	3.685116
W	3.553352	0.107906	1.882389	O	2.909607	-1.668381	1.796685
W	-3.584566	0.145860	1.887068	O	1.345811	-0.786072	5.750935
W	-1.719372	-3.082757	1.891106	O	-3.554165	2.069955	1.931482
W	1.675481	-3.101229	1.904332	O	-0.014397	-3.999350	1.881641
W	-1.899398	3.048394	1.930457	O	3.875444	-0.007549	0.002355
W	1.827986	3.043073	1.900005	O	2.823404	0.157356	3.666130
W	-0.010630	-1.916952	4.958776	O	-1.563325	2.386140	3.686312
W	1.649507	0.942055	4.936182	O	-1.977472	3.343722	0.046538
W	-1.674075	0.947243	4.942313	O	-2.862901	0.185380	3.680429
O	1.315179	0.751612	-5.610343	O	1.530558	2.361306	3.665996
O	2.842169	-0.176992	-3.622922	O	1.927103	-3.302231	0.013116
O	-2.913167	1.700031	-1.783756	O	3.473146	2.023691	1.887666
O	2.981511	1.689826	-1.777384	O	5.196615	-0.123391	2.356774
O	-1.370007	0.771055	-5.699041	O	2.755692	1.593785	6.097949
O	1.587061	-2.403727	-3.635383	O	-0.007672	-3.199533	6.123710
O	0.035718	-3.377178	-1.793013	O	-2.768523	1.593726	6.115224
O	-0.003127	-1.571642	-5.678686	O	2.426071	4.591289	2.375540
O	0.004160	4.030368	-1.824477	O	-2.479103	4.608256	2.389184
O	3.548410	-2.034438	-1.853377	O	-5.230972	-0.112782	2.339483
O	-3.832360	0.038066	0.022780	O	-2.760772	-4.388416	2.331439
O	-1.583555	-2.386191	-3.659789	O	2.702817	-4.416064	2.345725
O	-1.305124	2.559795	-3.617867	W	-0.128590	0.118404	0.140253
O	1.945186	3.339333	0.027290	H	0.053562	-0.129681	2.769786
O	1.261169	2.507929	-3.599943	H	-0.558433	-0.094821	-2.695929
O	-2.873034	-0.173497	-3.668528	H	0.971946	-0.467794	-2.102231
O	-1.897325	-3.274455	0.020870	O	-0.006201	-0.026758	3.754823
O	-3.463676	-1.990477	-1.823116	O	-1.459109	0.844984	1.205214
O	-2.453867	-4.557149	-2.282604	O	-0.009266	-1.501288	1.160893
O	-2.767688	-1.611820	-6.111773	O	1.337377	0.770999	1.145959
O	2.761233	-1.599579	-6.065425	O	-0.103393	-0.020385	-3.604579
O	-0.010738	3.169052	-6.029506	O	-1.288259	-0.724232	-1.213551
O	-5.204168	0.150950	-2.301067	O	0.007461	1.589665	-1.063992
O	-2.715942	4.472944	-2.285780	O	1.399476	-0.771661	-1.261809

**Coordinates of  $\alpha$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H]<sup>8-</sup>**

W	0.098012	-3.693058	1.639720	O	-1.786003	-1.357569	-5.197090
W	-3.133793	1.632055	-1.858574	O	0.343919	-5.001011	-2.770595
W	-1.585104	-0.914304	-3.535732	O	5.689614	1.675362	0.029064
W	0.011343	-3.702060	-1.670040	O	4.306599	-0.102970	-1.500199
W	-3.161731	1.611005	1.872537	O	0.816578	2.879680	3.515290
W	-1.533984	-0.875356	3.385395	O	3.841936	-2.229301	0.014416
W	-3.700678	-3.343824	-1.689105	O	4.520632	3.707985	1.394388
W	-3.624159	-3.353756	1.640111	O	3.170638	1.835433	-2.787787
W	-5.143709	-0.910124	-0.026097	O	0.793426	2.922554	-3.535537
W	0.088497	3.534110	-1.839359	O	4.483291	3.656406	-1.316274
W	3.212385	-1.600860	1.732807	O	2.173340	-0.575228	2.921200
W	3.154009	-1.663220	-1.696115	O	2.124019	-0.583164	-2.842063
W	1.514409	1.151540	-3.457595	O	-1.632662	2.698611	-2.193328
W	1.579294	1.150641	3.607393	O	1.828168	4.108764	-1.279119
W	0.059707	3.516342	1.818723	O	3.226268	1.826988	2.874556
W	4.662347	1.743808	-1.615793	O	-0.093448	0.332143	3.818816
W	3.220344	4.230504	0.030098	O	4.352348	-0.081658	1.557385
W	4.710464	1.809675	1.683197	O	1.828474	4.134318	1.304875
O	-5.291136	-2.313772	-1.380475	O	-0.177039	0.306427	-3.779134
O	-3.020658	-2.038864	-2.868341	O	-0.434312	3.678832	-0.005977
O	-2.837987	0.606927	3.437859	O	-0.439163	5.083457	-2.438656
O	-2.825065	0.571867	-3.429012	O	3.581249	5.932036	0.010841
O	-5.212500	-2.310005	1.306576	O	5.981898	1.782433	-2.738373
O	-1.861351	-3.957453	-1.555297	O	6.050083	1.840858	2.788774
O	0.339000	-4.650918	-0.021836	O	-0.426200	5.073166	2.440187
O	-4.007188	-4.266419	-0.023968	O	2.096828	1.104814	5.257528
O	-3.003845	2.046584	-0.000075	O	4.224254	-2.520203	2.792273
O	-0.407506	-2.240002	-2.880339	O	4.195535	-2.530240	-2.772992
O	1.822609	-2.971831	1.630209	O	2.013899	1.074387	-5.122217
O	-1.821628	-3.939573	1.496605	Sb	0.032504	0.170404	0.009123
O	-4.390620	0.250198	1.282667	H	2.271149	1.650065	0.344565
O	-1.618568	2.680820	2.180123	H	-2.478642	-1.070344	-0.514642
O	-4.411297	0.259703	-1.307028	H	-1.364283	-2.169023	0.071098
O	-2.988758	-1.996708	2.766077	O	3.179595	2.020887	0.088866
O	1.777274	-2.972795	-1.621567	O	0.796402	1.574358	1.290665
O	-0.369569	-2.259701	2.855430	O	1.820120	-0.630119	0.025788
O	0.362965	-5.024058	2.723842	O	0.686014	1.506420	-1.460270
O	-4.270967	-4.500000	2.762199	O	-3.091118	-1.856083	-0.134602
O	-4.355161	-4.521155	-2.786990	O	-1.385133	-0.062874	1.447690
O	-6.812729	-0.432588	-0.004014	O	-1.553380	-0.106738	-1.243565
O	-1.761133	-1.291213	5.066266	O	-0.368756	-2.215438	0.009393
O	-4.340765	2.745912	2.431360				
O	-4.339066	2.731779	-2.440873				

**Coordinates of  $\beta$ 1-[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>8-</sup>**

W	-3.075916	-1.680753	-1.849277	O	4.607707	-2.471162	-2.318236
W	2.912667	1.773884	-1.777932	O	-0.196666	-5.217203	-2.283585
W	3.021458	-1.932144	-1.867831	O	0.783237	-1.384524	5.774264
W	0.149594	-3.572528	-1.864840	O	2.516488	-1.293660	3.673376
W	0.136100	3.619711	-1.805351	O	-4.070931	0.033896	2.165556
W	-3.104916	1.720067	-1.874916	O	1.975292	-3.390734	2.110503
W	0.927907	-1.656992	-4.905525	O	-1.557479	-0.025883	5.743490
W	-1.927855	-0.002047	-4.925239	O	2.482482	1.295291	3.695681
W	0.898653	1.668136	-4.818103	O	2.037696	3.575603	2.210417
W	0.116101	3.496199	1.939381	O	0.759779	1.317826	5.752407
W	0.071736	-3.499400	1.882886	O	-1.646623	-2.828837	1.531938
W	3.023874	-1.785182	1.882348	O	3.294846	0.037311	1.549701
W	2.937228	1.914123	1.926557	O	3.173067	2.190522	0.070159
W	-3.073517	-1.576182	1.896184	O	-0.133990	2.843788	3.723323
W	-3.068651	1.662422	1.863866	O	-2.358688	-1.509913	3.667778
W	1.896367	-0.012671	4.942540	O	-3.448269	1.708688	-0.009250
W	-0.973558	1.634380	4.924435	O	-0.134210	-2.833213	3.670186
W	-0.938476	-1.666322	4.944989	O	-2.379943	1.531650	3.678737
O	1.508384	-0.007972	-5.644798	O	3.138079	-2.169660	0.004816
O	2.365497	-1.524063	-3.626075	O	-1.649906	2.896858	1.568144
O	-1.637335	2.892511	-1.599818	O	-0.161107	5.172175	2.341812
O	3.331378	-0.059220	-1.578325	O	-1.621988	2.727919	6.102595
O	-0.796364	1.327241	-5.725963	O	3.188322	-0.016453	6.107073
O	0.116934	-2.843543	-3.642374	O	-1.605367	-2.796263	6.085173
O	-1.621787	-2.874321	-1.613725	O	-4.372580	2.741101	2.286114
O	-0.794179	-1.371402	-5.712464	O	-4.369160	-2.671456	2.267335
O	2.008290	3.525790	-1.996567	O	-0.207545	-5.165228	2.257056
O	2.069617	-3.603272	-2.022465	O	4.604404	-2.367627	2.278483
O	-3.394736	-1.614334	0.006986	O	4.524735	2.460715	2.377224
O	-2.511171	-1.307348	-3.657036	Sb	-0.033718	0.144497	0.123732
O	0.073302	2.835777	-3.611716	H	0.170178	-0.296069	2.784611
O	0.270556	3.891045	0.037534	H	-0.572741	0.140978	-2.688558
O	2.332239	1.473420	-3.603938	H	0.622205	-0.885472	-2.188256
O	-2.515209	1.317905	-3.677278	O	0.025999	-0.056804	3.761313
O	0.317735	-3.763560	-0.000843	O	-1.693214	0.096789	1.360105
O	-3.994334	0.020172	-1.984176	O	0.718734	-1.206254	1.374580
O	-4.354577	-2.770409	-2.269415	O	0.789330	1.549246	1.421986
O	-3.221296	-0.023104	-6.085648	O	-0.096080	0.010326	-3.627664
O	1.594067	-2.770162	-6.048929	O	0.920832	1.336334	-1.217748
O	1.566675	2.764593	-5.986964	O	0.857473	-1.414875	-1.378387
O	-4.369652	2.809866	-2.334626	O	-1.411847	0.036831	-1.383554
O	-0.193158	5.245707	-2.296998				
O	4.490831	2.362413	-2.240304				

**Coordinates of  $\beta$ 2-[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{8-}$**

W	-3.153600	-1.588607	-1.893944	O	4.564164	-2.364866	-2.291322
W	2.909981	1.896896	-1.885767	O	-0.290406	-5.158483	-2.320725
W	2.976258	-1.817267	-1.876850	O	0.796931	-1.335376	5.646496
W	0.030376	-3.507115	-1.916774	O	2.517369	-1.300505	3.620937
W	0.103821	3.474251	-1.888786	O	-4.003046	0.033465	2.117138
W	-3.100021	1.631769	-1.882876	O	2.051278	-3.548197	2.107707
W	0.944229	-1.637324	-4.971912	O	-1.502783	-0.005859	5.670128
W	-1.916724	-0.003467	-4.931264	O	2.555979	1.306592	3.641128
W	0.943400	1.645521	-4.941276	O	1.982116	3.429152	2.102298
W	0.081967	3.559672	1.846614	O	0.805138	1.363010	5.720313
W	0.141382	-3.585038	1.838140	O	-1.644266	-2.925858	1.520829
W	3.012687	-1.890599	1.882453	O	3.338084	-0.016228	1.522194
W	3.025613	1.820855	1.839620	O	3.104125	2.172969	-0.008589
W	-2.997040	-1.635122	1.798743	O	-0.124531	2.848909	3.643905
W	-3.156181	1.703900	1.866308	O	-2.333516	-1.489453	3.614771
W	1.918679	0.038879	4.889636	O	-3.494715	1.696145	-0.000302
W	-0.936751	1.661018	4.869116	O	-0.094468	-2.817905	3.597462
W	-0.935965	-1.655635	4.849393	O	-2.366827	1.533668	3.629228
O	1.564925	-0.007141	-5.777317	O	3.099905	-2.138829	0.006405
O	2.351373	-1.497431	-3.671261	O	-1.671947	2.887573	1.527047
O	-1.662092	2.846931	-1.610429	O	-0.187234	5.211244	2.293956
O	3.243390	0.024079	-1.598615	O	-1.582726	2.756136	6.052108
O	-0.769976	1.329043	-5.759416	O	3.214028	0.003556	6.048090
O	0.084472	-2.807939	-3.689165	O	-1.580779	-2.782640	5.991432
O	-1.685982	-2.821265	-1.608911	O	-4.423021	2.791031	2.319958
O	-0.776189	-1.355249	-5.778454	O	-4.333412	-2.663439	2.252511
O	2.033755	3.580549	-2.075282	O	-0.148485	-5.233872	2.291360
O	1.959968	-3.448899	-2.002044	O	4.599535	-2.464372	2.273946
O	-3.498598	-1.658159	-0.046468	O	4.600848	2.420327	2.236012
O	-2.493121	-1.307691	-3.698074	Sb	-0.106658	0.096530	-0.099818
O	0.099892	2.822922	-3.708299	H	0.253052	0.604906	2.670173
O	0.288308	3.836678	-0.001079	H	0.122747	-0.230216	-2.792336
O	2.359452	1.491812	-3.684086	H	0.465221	-0.995255	2.244306
O	-2.518634	1.319734	-3.715138	O	0.092426	0.099932	3.605957
O	0.284381	-3.809336	-0.013630	O	-1.619615	-0.122732	1.245603
O	-4.164713	0.019094	-2.086820	O	0.790288	-1.441269	1.410134
O	-4.385228	-2.716503	-2.375122	O	0.700687	1.253283	1.395088
O	-3.198524	-0.017654	-6.102676	O	0.007154	-0.028386	-3.775409
O	1.606298	-2.783754	-6.097825	O	0.762123	1.508133	-1.346319
O	1.609060	2.760756	-6.092198	O	0.675200	-1.229588	-1.344168
O	-4.360966	2.753816	-2.330177	O	-1.736998	0.078619	-1.393218
O	-0.237029	5.133574	-2.304086				
O	4.517351	2.407357	-2.298613				

### Coordinates of $\gamma$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H]<sup>8-</sup>

W	-0.179074	-3.604730	-1.904552	O	0.217868	5.184157	-2.352690
W	-0.079953	3.539854	-1.900125	O	4.436170	2.766697	-2.245574
W	3.176527	1.677314	-1.776570	O	4.293866	-2.702444	-2.190049
W	2.969160	-1.647527	-1.766314	O	0.785239	-1.355627	5.801749
W	-3.010501	1.808370	-1.868232	O	2.547665	-1.284741	3.760815
W	-3.029789	-1.940336	-1.887556	O	-3.271660	0.018363	1.618356
W	1.894637	0.044689	-4.811104	O	1.701644	-2.847969	1.711868
W	-0.982258	-1.655580	-4.937291	O	-1.524604	0.014791	5.714646
W	-0.969655	1.655994	-4.944522	O	2.558864	1.324140	3.798031
W	-0.146920	3.535858	1.851798	O	1.661833	2.931823	1.711684
W	-0.040505	-3.521683	1.854277	O	0.799394	1.366137	5.809322
W	3.200171	-1.640947	1.976447	O	-1.973005	-3.443229	1.971230
W	3.038833	1.673370	1.984520	O	4.102032	0.017193	2.064962
W	-3.004472	-1.817416	1.873359	O	-0.209567	3.845995	-0.014896
W	-2.912653	1.894492	1.883925	O	-0.115077	2.863750	3.695613
W	1.921166	-0.006106	5.040756	O	-2.363845	-1.480899	3.651762
W	-0.906891	1.680929	4.924650	O	-3.195901	-2.120057	-0.026169
W	-0.929822	-1.635716	4.911270	O	-0.108675	-2.800068	3.664064
O	0.759857	1.345379	-5.720812	O	-2.350447	1.519954	3.675503
O	2.494413	1.334171	-3.594872	O	3.407712	1.726342	0.069986
O	-3.311706	-0.047012	-1.687086	O	-2.068273	3.612621	2.032665
O	1.665668	2.863327	-1.626292	O	0.142676	5.194713	2.300852
O	-1.581630	-0.007558	-5.731979	O	-1.582535	2.776085	6.089654
O	2.453310	-1.291838	-3.595553	O	3.195411	-0.017012	6.223569
O	1.601603	-2.937461	-1.636972	O	-1.601146	-2.751641	6.056956
O	0.751129	-1.319158	-5.642184	O	-4.518566	2.423459	2.293533
O	-1.993730	3.461286	-1.974167	O	-4.580963	-2.385317	2.306075
O	4.038819	0.010378	-1.941801	O	0.240580	-5.165943	2.313295
O	-0.223969	-3.850913	-0.017142	O	4.455470	-2.742082	2.429208
O	-0.161084	-2.859578	-3.671860	O	4.352110	2.756806	2.365749
O	-2.390503	1.534749	-3.682144	Sb	0.070485	0.113013	0.128153
O	-3.151568	2.089988	-0.012842	H	0.377455	0.036396	2.820829
O	-0.125789	2.833429	-3.690946	H	-0.173105	0.550223	-2.699777
O	-2.417863	-1.576228	-3.687997	H	-0.490403	-1.010358	-2.253079
O	3.411024	-1.714509	0.109310	O	0.090545	0.022994	3.791206
O	-2.105153	-3.632439	-2.001239	O	-0.730435	-1.303705	1.222120
O	0.132855	-5.249203	-2.366963	O	1.574489	0.179118	1.516203
O	-1.595018	-2.768824	-6.109597	O	-0.814054	1.543707	1.348722
O	3.180552	0.015970	-5.976914	O	-0.048563	0.073052	-3.632654
O	-1.617099	2.763922	-6.115556	O	-0.835764	-1.493127	-1.454450
O	-4.616232	-2.470964	-2.346481	O	-0.698489	1.237920	-1.389834
O	-4.585186	2.381082	-2.305633	O	1.597444	-0.147143	-1.190802

**Coordinates of  $\alpha^*-\text{[}(SbO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}\text{]}^{8-}$**

W	3.422304	-0.068493	1.825548	O	-2.477027	-4.531254	2.309031
W	-3.523704	-0.035755	1.912105	O	2.500109	-4.591303	2.423998
W	-1.798436	-2.999834	1.872995	O	1.303984	0.740340	-5.644826
W	1.888214	-3.044167	1.955606	O	2.767111	-0.080453	-3.576514
W	-1.631579	3.119763	1.929673	O	-3.437537	1.996617	-1.946226
W	1.645950	3.168248	1.847934	O	3.560904	1.977294	-1.992219
W	-0.034492	-1.881300	4.936335	O	-1.364533	0.774358	-5.722522
W	1.624001	0.960576	4.843043	O	1.427378	-2.364221	-3.550538
W	-1.658118	0.948505	4.947387	O	0.037041	-3.998189	-1.910424
W	-1.674636	-3.145899	-1.886163	O	-0.012230	-1.532068	-5.637432
W	1.830390	2.917141	-1.836519	O	0.005996	3.426993	-1.666740
W	3.649910	0.086541	-1.862289	O	3.008688	-1.724535	-1.652578
W	1.788069	-3.144958	-1.801501	O	1.940828	3.474255	0.034235
W	-1.851355	3.075072	-1.818393	O	-1.455777	-2.375611	-3.607768
W	-3.529346	0.058644	-1.839880	O	-1.331076	2.505285	-3.627536
W	1.640193	-0.961355	-4.806814	O	-1.954238	3.381951	0.026227
W	-1.669047	-0.922545	-4.872626	O	1.317928	2.433581	-3.618346
W	-0.030905	1.902924	-4.851593	O	-2.837874	-0.084803	-3.640900
O	-1.386414	-0.787259	5.783801	O	-1.886327	-3.279960	-0.011242
O	-1.328834	-2.464727	3.657819	O	-2.956713	-1.727832	-1.688834
O	0.001249	4.145352	2.073892	O	-2.659541	-4.491716	-2.336393
O	-3.414841	-1.953959	1.953684	O	-2.790253	-1.619854	-6.001714
O	-0.017862	1.528106	5.743361	O	2.776449	-1.638880	-5.917583
O	1.316707	-2.454984	3.664558	O	0.005967	3.196223	-6.011296
O	3.484223	-2.045357	1.984179	O	-5.195234	-0.113266	-2.279390
O	1.298416	-0.768378	5.726513	O	-2.505582	4.595090	-2.333222
O	-2.927324	1.736017	1.716523	O	2.578167	4.420342	-2.319004
O	0.029005	-3.389978	1.684205	O	5.266889	-0.169212	-2.422070
O	3.995753	0.019694	-0.025416	O	2.764643	-4.460740	-2.357036
O	2.726174	0.048926	3.628355	Sb	0.059122	0.162147	0.093375
O	-1.480900	2.392588	3.692175	H	-0.549555	0.414677	-2.665702
O	-3.795195	0.021313	0.026664	H	-0.399868	-0.212655	2.755709
O	-2.824489	0.103953	3.691567	H	0.137978	-1.039364	-2.133943
O	1.433996	2.369957	3.635095	O	-0.134629	0.051350	-3.566248
O	1.964849	-3.413829	0.041122	O	-1.286110	0.782636	-1.322705
O	2.885386	1.711625	1.660930	O	1.479209	0.976242	-1.126425
O	5.080204	0.080051	2.359033	O	0.090876	-1.541488	-1.268403
O	2.775580	1.597691	5.973023	O	-0.097194	-0.032905	3.720676
O	-0.030331	-3.211898	6.054525	O	-0.001370	1.837306	1.249719
O	-2.794814	1.608876	6.084784	O	-1.244796	-0.696588	1.366663
O	2.680866	4.444669	2.422437	O	1.543872	-0.743937	1.153644
O	-2.644793	4.464107	2.362349				
O	-5.190655	0.149090	2.342665				

**Coordinates of  $\beta$ 1\*- $[(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{8-}$**

W	-1.912334	-0.019832	4.845230	O	-1.711574	2.965771	-1.832749
W	0.940235	1.607762	4.980693	O	-1.670680	-2.946152	-1.848172
W	0.945128	-1.652055	4.953587	O	3.459756	-0.006818	-1.806550
W	3.084889	-1.691218	1.922112	O	-4.478437	2.735325	-2.373562
W	-0.179378	3.512335	1.990183	O	-0.086263	-5.243577	-2.332268
W	-2.902254	-1.801398	1.784882	O	4.573086	2.539686	-2.250876
W	3.057609	1.737797	1.941357	O	4.622125	-2.551117	-2.300002
W	-2.989279	1.867007	1.850376	O	-0.100525	5.260495	-2.262696
W	-0.081445	-3.583165	1.931838	O	-4.427685	-2.715723	-2.412899
O	-3.232925	-0.055086	5.968424	O	0.163712	2.904157	-3.600217
O	1.582583	-2.803347	6.088475	O	-2.560406	-1.262822	-3.713718
O	1.566505	2.744084	6.138744	O	-2.601322	1.298433	-3.711815
O	1.560833	-0.029503	5.816668	O	0.204832	-2.851366	-3.619238
O	-0.790160	1.291873	5.751631	O	2.375910	1.589575	-3.581062
O	-0.779768	-1.362201	5.722066	O	2.386329	-1.563309	-3.590166
O	0.061888	2.782138	3.725059	O	-0.771298	1.375948	-5.708332
O	-2.416921	-1.332724	3.606626	O	-0.761452	-1.344743	-5.691453
O	-2.476430	1.314100	3.644608	O	1.547343	0.021678	-5.572386
O	0.103140	-2.824830	3.662762	O	1.588476	2.775228	-6.008695
O	2.362616	1.508396	3.730777	O	-3.154777	0.010939	-6.176284
O	2.385620	-1.518464	3.703520	O	1.619968	-2.725483	-6.051348
O	0.081463	5.170193	2.438290	W	3.053978	1.838722	-1.803964
O	-4.425724	-2.516343	2.260355	W	0.084836	3.617958	-1.739154
O	4.434082	-2.689997	2.345259	W	-3.107618	-1.704696	-1.923829
O	4.363219	2.774590	2.414531	W	3.090814	-1.887607	-1.847176
O	-4.545478	2.493121	2.324463	W	-3.149229	1.733389	-1.891801
O	0.179666	-5.239496	2.349847	W	0.112995	-3.599826	-1.833794
O	-2.089906	3.569651	2.121157	W	-1.921318	0.035884	-4.952444
O	3.941058	0.023681	2.062903	W	0.949121	-1.646611	-4.879229
O	-1.966099	-3.527194	1.992013	W	0.920913	1.715686	-4.807513
O	1.622508	2.921687	1.689058	Sb	-0.086626	0.118280	0.104088
O	1.699405	-2.945633	1.665873	H	0.472460	-0.014302	2.772777
O	-3.370613	0.018381	1.630718	O	0.088367	-0.013812	3.737136
O	3.379429	1.845398	0.074747	O	1.429374	0.001070	1.443940
O	3.341611	-1.820726	0.025635	O	-0.101497	0.052471	-3.603578
O	-3.346500	2.013616	-0.023060	O	0.813001	1.437499	-1.087598
O	-0.038877	-3.862120	0.011879	O	-0.952896	1.557554	1.277896
O	-0.139016	3.937205	0.082436	O	-0.939640	-1.403484	1.163522
O	-3.326255	-1.965729	-0.072227	O	-1.533054	0.038177	-1.345994
O	2.004243	3.505074	-1.765248	O	0.819217	-1.360678	-1.261958
O	2.046733	-3.508399	-1.785912	H	-0.589848	0.187446	-2.693479
O	-4.021673	0.011838	-1.866638	H	0.597265	-0.850744	-2.089355

**Coordinates of  $\beta$ 2<sup>\*</sup>-[ $(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>8-</sup>**

W	3.067574	1.812088	-1.951368	O	-0.781003	-1.314257	-5.677663
W	0.105264	3.536262	-1.929728	O	-2.569900	1.285865	-3.651485
W	-3.102107	-1.753331	-1.905098	O	0.173742	-2.847581	-3.675265
W	-0.074504	3.620025	1.838165	O	-4.010648	-0.018158	-1.815375
W	-3.036439	-1.823136	1.847313	O	-3.177043	0.037752	-6.100417
W	0.960225	1.675347	-5.002773	O	-4.468461	2.682351	-2.275912
W	3.060006	1.637621	1.770150	O	-0.041492	-5.196271	-2.323548
W	0.956443	1.638098	4.816652	O	-2.000471	3.499878	2.002462
W	3.014973	-1.919166	-1.851218	O	-1.990704	-3.449982	2.019701
W	0.971847	-1.630825	-4.903531	O	-0.761471	1.318103	5.649218
W	3.074331	-1.639518	1.856428	O	-0.786439	-1.366774	5.743029
W	0.934680	-1.667498	4.877919	O	-3.411323	0.022403	1.646182
W	-3.123946	1.688887	-1.824831	O	-2.466852	1.322606	3.638080
W	0.160619	-3.526360	-1.879909	O	0.112742	-2.860555	3.662815
W	-1.912866	0.046889	-4.912507	O	-3.260262	2.026890	0.038120
W	-3.042551	1.879100	1.924402	O	-0.099552	-3.872036	-0.002706
W	-0.077813	-3.585860	1.861112	O	-3.201764	0.000003	6.042843
W	-1.897504	-0.044677	4.894096	O	-4.585520	2.513395	2.377090
O	3.371855	-0.028685	-1.867464	O	0.148300	-5.239226	2.332221
O	1.565493	0.020744	-5.763097	O	0.189550	2.885846	-3.723911
O	2.397995	1.612455	-3.747322	O	-2.569028	-1.270180	-3.676138
O	2.021449	3.459188	-1.857045	O	-0.090435	5.205592	-2.342713
O	1.576532	2.773249	-6.201354	O	-4.448609	-2.754007	-2.340551
O	4.610917	2.447754	-2.420470	O	0.074820	2.792772	3.583692
O	4.063676	-0.006008	2.000771	O	-2.515283	-1.321197	3.652596
O	1.514508	-0.001278	5.666946	O	-0.100244	3.842879	-0.021498
O	1.680776	2.947533	1.607007	O	-3.281670	-2.030653	-0.002376
O	2.329617	1.419990	3.560524	O	0.170526	5.262809	2.324764
O	3.397905	1.885668	-0.074978	O	-4.572261	-2.466516	2.323596
O	1.631644	2.777698	5.926959	Sb	0.070711	-0.099828	-0.085880
O	4.385417	2.640629	2.283219	H	0.150845	0.338497	-2.770711
O	2.384927	-1.571894	-3.678912	H	-0.278023	-0.647744	2.672213
O	2.094160	-3.609132	-1.918655	H	-0.435133	0.955707	2.172885
O	1.578783	-2.722507	-6.107871	O	0.030276	0.082497	-3.743760
O	4.555650	-2.529560	-2.375778	O	0.787001	1.298670	-1.344940
O	1.679061	-2.931550	1.626939	O	-0.091865	-0.121292	3.590504
O	2.353288	-1.468864	3.622598	O	1.748544	-0.010767	1.141736
O	3.420910	-1.919593	-0.027685	O	0.898224	-1.586533	-1.226036
O	1.620648	-2.765272	6.035814	O	-1.602251	-0.040415	-1.155736
O	4.397389	-2.669380	2.317818	O	-0.720388	-1.311410	1.385753
O	-1.687416	2.930722	-1.858459	O	-0.745685	1.377339	1.319859
O	-1.676590	-2.960912	-1.852685				
O	-0.795543	1.392636	-5.754463				

**Coordinates of  $\gamma^*-[{\rm (SbO}_6){\rm W}_{18}{\rm O}_{54}{\rm (OH)}_2{\rm H}]^{8-}$**

W	-1.811377	-2.998111	-1.852463	O	5.265802	0.183394	-2.363371
W	1.734165	3.203132	-1.862343	O	2.563701	-4.572956	-2.250896
W	3.619891	-0.035858	-1.877939	O	-1.379381	-0.838952	5.778835
W	1.926037	-3.021794	-1.832723	O	-1.286311	-2.596617	3.731467
W	-1.627659	3.099892	-1.740224	O	-0.054106	3.323199	1.739849
W	-3.574241	-0.062406	-1.909859	O	-2.934030	-1.638395	1.840032
W	1.654378	-0.988056	-4.895469	O	-0.012271	1.486662	5.707609
W	-1.668366	-0.976999	-4.944158	O	1.280873	-2.576786	3.727300
W	-0.042064	1.899477	-4.816123	O	2.929392	-1.653090	1.813498
W	3.611779	0.132846	1.883314	O	1.355467	-0.832956	5.764078
W	-3.558453	0.167692	1.842601	O	-3.632518	2.097277	1.987265
W	-1.716027	-3.064582	1.917125	O	-0.006822	-3.962429	1.857729
W	1.689785	-3.059122	1.931770	O	3.894354	-0.006871	0.007797
W	-1.925689	2.988508	1.948950	O	2.851539	0.131840	3.664928
W	1.769301	2.923487	1.850448	O	-1.550506	2.359839	3.710159
W	-0.012536	-1.948552	5.007839	O	-2.041290	3.388603	0.066794
W	1.641114	0.899508	4.905495	O	-2.886455	0.163361	3.690809
W	-1.683599	0.887591	4.927426	O	1.506657	2.319933	3.662146
O	1.326535	0.737218	-5.613251	O	1.880194	-3.213712	0.018859
O	2.841127	-0.166893	-3.620622	O	3.534896	2.016333	1.911287
O	-2.944609	1.710928	-1.791712	O	5.253642	-0.127803	2.357701
O	2.975858	1.720791	-1.767620	O	2.735290	1.554051	6.082840
O	-1.346848	0.751507	-5.708403	O	-0.001861	-3.229616	6.183330
O	1.600235	-2.399202	-3.628968	O	-2.758431	1.534940	6.125589
O	0.037335	-3.355985	-1.814451	O	2.422760	4.468631	2.340883
O	0.009014	-1.599126	-5.687598	O	-2.487780	4.561738	2.436381
O	0.049628	4.106711	-1.886353	O	-5.216008	-0.082444	2.305748
O	3.531959	-1.985775	-1.832523	O	-2.748774	-4.401712	2.298518
O	-3.859857	0.017963	-0.009223	O	2.715956	-4.401780	2.304499
O	-1.602619	-2.394191	-3.675558	Sb	-0.113619	0.138172	0.103807
O	-1.295198	2.525838	-3.612918	H	-0.017421	-0.432871	2.774484
O	1.979759	3.407956	-0.022026	H	-0.596478	-0.175289	-2.690037
O	1.294189	2.496548	-3.604944	H	0.948740	-0.393455	-2.119353
O	-2.887199	-0.169668	-3.704084	O	-0.022150	-0.113531	3.751259
O	-1.867289	-3.202493	0.023318	O	-1.585305	0.922662	1.275451
O	-3.472860	-1.979950	-1.849393	O	-0.013158	-1.412360	1.393437
O	-2.457869	-4.554632	-2.250619	O	1.403970	0.962819	1.173367
O	-2.743429	-1.620342	-6.146589	O	-0.095839	-0.046106	-3.601601
O	2.770251	-1.604490	-6.062295	O	-1.306783	-0.696866	-1.338087
O	-0.008174	3.154624	-6.015445	O	-0.110374	1.760741	-1.128780
O	-5.234150	0.161305	-2.351152	O	1.392022	-0.694590	-1.276853
O	-2.583648	4.455798	-2.287707				
O	2.775079	4.478623	-2.398055				

**Coordinates of  $\alpha$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$**

W	3.153825	-1.747208	-1.861648	O	0.156711	5.242499	-2.244300
W	-3.052627	1.821399	-1.831926	O	4.417239	2.800451	-2.259159
W	-0.132339	3.586160	-1.903056	O	1.606433	0.070444	5.723421
W	3.130940	1.718840	-1.908318	O	2.412836	1.587400	3.638059
W	-3.002892	-1.913395	-1.788334	O	-1.994202	-3.504042	2.252847
W	-0.128094	-3.558799	-1.794700	O	4.061469	0.031295	2.123837
W	0.926830	1.649476	-4.904358	O	-0.718847	-1.289539	5.766463
W	0.941206	-1.781467	-4.881967	O	0.160720	2.884199	3.646303
W	-2.036798	-0.083204	-4.881124	O	-2.026223	3.511974	2.148723
W	-2.982468	1.852673	1.925813	O	-0.731691	1.404961	5.728847
W	3.118972	-1.633885	1.907087	O	1.631285	-2.774956	1.551002
W	3.100100	1.679736	1.859556	O	1.603108	2.802389	1.479594
W	-0.121236	3.522538	1.869172	O	-3.030037	2.149990	0.021334
W	-0.087848	-3.506060	1.966103	O	-2.512102	1.323871	3.697768
W	-2.966459	-1.863716	1.970774	O	0.195138	-2.814538	3.726719
W	0.990465	1.713342	4.912003	O	-0.359364	-3.699095	0.076987
W	-1.871753	0.039728	4.964519	O	2.431973	-1.497698	3.681336
W	1.009107	-1.600977	4.957996	O	-2.508018	-1.272805	3.733748
O	-0.828598	1.236076	-5.593519	O	-0.386853	3.666554	-0.037074
O	0.120814	2.871923	-3.681426	O	-3.207348	-0.008089	1.562845
O	-2.033634	-3.554951	-2.085119	O	-4.585149	2.383329	2.263838
O	-2.031986	3.440058	-2.161418	O	-3.138086	0.053759	6.139717
O	-0.807302	-1.385432	-5.576765	O	1.640333	2.841789	6.047381
O	2.396061	1.582023	-3.692821	O	1.671057	-2.689137	6.125600
O	3.960885	-0.012435	-2.169048	O	-4.563853	-2.399686	2.326108
O	1.464827	-0.070633	-5.594822	O	0.260703	-5.155835	2.315040
O	-3.283369	-0.039832	-1.466808	O	4.390923	-2.743458	2.245808
O	1.622581	2.858896	-1.575635	O	4.364361	2.808187	2.163201
O	3.403270	-1.545207	-0.006521	O	0.210284	5.185517	2.165596
O	2.364237	-1.611797	-3.634179	Na	-0.067119	-0.050582	0.072138
O	-2.573217	-1.359560	-3.597455	H	0.021459	0.016687	2.775651
O	-3.000746	-2.194700	0.084538	H	-0.535366	0.593125	-2.700268
O	-2.583773	1.223317	-3.623038	H	0.792228	-0.093562	-2.651314
O	0.120669	-2.900089	-3.603290	O	0.030223	0.034340	3.762281
O	3.358692	1.541026	-0.045181	O	0.067794	0.112522	-3.389742
O	1.645195	-2.859526	-1.491878	F	-0.815841	-1.436805	1.581370
O	4.428486	-2.836220	-2.233763	F	1.665062	0.007334	1.496308
O	1.557168	-2.877465	-6.049613	F	-0.829413	1.438056	1.517062
O	1.517714	2.696303	-6.139674	F	-0.854780	-1.495479	-1.429882
O	-3.303254	-0.100751	-6.038996	F	-0.903592	1.312263	-1.497150
O	0.191427	-5.215478	-2.134269	F	1.531822	-0.022272	-1.489065
O	-4.596873	-2.472112	-2.121314				
O	-4.643425	2.367028	-2.196882				

**Coordinates of  $\beta$ 1-[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>6-</sup>**

W	-3.195410	-1.689907	-1.867608	O	4.608849	2.442847	-2.211738
W	3.014420	1.921763	-1.825637	O	4.657238	-2.410261	-2.278096
W	3.076748	-1.867861	-1.881127	O	-0.229407	-5.229222	-2.230896
W	0.091028	-3.581570	-1.870882	O	0.768647	-1.354984	5.747200
W	0.151746	3.571588	-1.824823	O	2.518724	-1.299661	3.682306
W	-3.124127	1.693263	-1.867655	O	-4.049672	0.013793	2.140382
W	0.974554	-1.751557	-4.955766	O	2.024829	-3.490942	2.126647
W	-2.000071	-0.038881	-4.948527	O	-1.560469	-0.009327	5.746429
W	0.973620	1.688408	-4.849110	O	2.530279	1.311173	3.710592
W	0.119350	3.538111	1.948691	O	2.034179	3.531192	2.177781
W	0.111479	-3.503640	1.911517	O	0.766296	1.332540	5.750017
W	2.990901	-1.837401	1.907117	O	-1.627015	-2.798574	1.569668
W	2.998540	1.877662	1.951056	O	3.241603	0.022026	1.573577
W	-3.104625	-1.649948	1.920757	O	3.080106	2.138414	0.044192
W	-3.099712	1.675621	1.906842	O	-0.134914	2.848715	3.709314
W	1.905216	-0.007993	4.951512	O	-2.403726	-1.535540	3.690941
W	-0.967597	1.650236	4.948294	O	-3.363000	1.607941	0.009796
W	-0.962203	-1.661278	4.946872	O	-0.134735	-2.836120	3.682961
O	1.491341	-0.028010	-5.589737	O	-2.393059	1.539579	3.685991
O	2.393721	-1.581616	-3.683321	O	3.086105	-2.087830	-0.003219
O	-1.613051	2.829084	-1.642322	O	-1.606361	2.813550	1.568744
O	3.265643	0.011627	-1.667095	O	-0.209637	5.190079	2.307499
O	-0.774041	1.278757	-5.588808	O	-1.613303	2.755515	6.109005
O	0.145880	-2.902536	-3.693825	O	3.188045	-0.017496	6.108972
O	-1.648504	-2.815896	-1.688406	O	-1.605374	-2.782446	6.093334
O	-0.780057	-1.352983	-5.642504	O	-4.366715	2.784877	2.265740
O	2.074155	3.594753	-2.004262	O	-4.386931	-2.750165	2.249956
O	2.016542	-3.489984	-1.981814	O	-0.197705	-5.163186	2.247882
O	-3.338085	-1.580643	0.004278	O	4.581390	-2.390213	2.265505
O	-2.603404	-1.321782	-3.684580	O	4.592017	2.424067	2.309191
O	0.145982	2.888020	-3.646792	Na	0.002557	0.088644	0.076339
O	0.315679	3.741795	0.046317	H	-0.002947	-0.014978	2.778917
O	2.426520	1.581259	-3.651313	H	-0.706736	0.323638	-2.693103
O	-2.557281	1.280781	-3.679101	H	0.517137	-0.515635	-2.643687
O	0.274890	-3.672831	0.001666	O	-0.004915	-0.003174	3.765762
O	-4.079533	0.002077	-1.993296	F	-1.662350	0.009265	1.520064
O	-4.454945	-2.799585	-2.221483	F	0.832095	-1.419810	1.505153
O	-3.238204	-0.016525	-6.137326	F	0.845175	1.467815	1.550597
O	1.606447	-2.816723	-6.142690	O	0.012280	0.049247	-3.370196
O	1.577923	2.743070	-6.067187	F	0.878834	1.524240	-1.386768
O	-4.376425	2.805900	-2.265613	F	0.779184	-1.302545	-1.491446
O	-0.198708	5.212662	-2.210880	F	-1.602191	0.128821	-1.481475

**Coordinates of  $\beta$ 2-[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ] $^{6-}$**

W	-3.129085	-1.646929	-1.922058	O	4.581447	-2.373576	-2.263314
W	2.973220	1.879086	-1.907084	O	-0.250903	-5.164311	-2.287807
W	2.973972	-1.870939	-1.907148	O	0.754252	-1.318110	5.596396
W	0.118404	-3.523350	-1.921518	O	2.612801	-1.309846	3.662255
W	0.117332	3.532290	-1.915929	O	-4.060980	0.001707	2.131600
W	-3.129023	1.652961	-1.922179	O	1.993453	-3.458426	2.118503
W	0.955460	-1.652378	-4.961016	O	-1.507852	-0.000022	5.613164
W	-1.921095	0.002859	-4.963070	O	2.611952	1.317631	3.662822
W	0.952115	1.664263	-4.958229	O	1.991453	3.465983	2.120041
W	0.076997	3.620864	1.867247	O	0.753399	1.323589	5.597346
W	0.078427	-3.615111	1.861929	O	-1.645763	-2.861717	1.547121
W	3.081748	-1.873508	1.874167	O	3.358146	0.004228	1.569995
W	3.081554	1.880664	1.874116	O	3.044691	2.116324	0.003600
W	-3.121586	-1.658414	1.851250	O	-0.159827	2.862097	3.645308
W	-3.121664	1.662664	1.850634	O	-2.394672	-1.536859	3.646693
W	1.968009	0.003389	4.887087	O	-3.369849	1.581231	-0.021301
W	-1.001627	1.712535	4.905221	O	-0.156979	-2.858586	3.643704
W	-0.999122	-1.713423	4.904255	O	-2.395588	1.538795	3.646044
O	1.555632	0.005694	-5.746208	O	3.044637	-2.106567	0.003032
O	2.398319	-1.544774	-3.704019	O	-1.646154	2.864900	1.547154
O	-1.608774	2.774963	-1.645747	O	-0.219998	5.267324	2.255761
O	3.185235	0.004457	-1.644208	O	-1.635966	2.795014	6.075963
O	-0.778684	1.350225	-5.752018	O	3.191058	0.003518	6.102182
O	0.130552	-2.855047	-3.711141	O	-1.630341	-2.797246	6.075156
O	-1.606997	-2.767574	-1.646184	O	-4.402561	2.749573	2.225136
O	-0.777345	-1.342293	-5.752987	O	-4.402402	-2.745372	2.226118
O	2.040705	3.562183	-2.029615	O	-0.217235	-5.262323	2.247982
O	2.042633	-3.553905	-2.031200	O	4.652618	-2.477626	2.212111
O	-3.369737	-1.578616	-0.020950	O	4.651955	2.485330	2.213108
O	-2.549815	-1.310992	-3.719703	Na	-0.068555	0.002997	-0.070828
O	0.128751	2.863535	-3.708328	H	0.343013	0.748488	2.672454
O	0.295595	3.744387	0.000272	H	-0.010925	0.002538	-2.782379
O	2.397385	1.553593	-3.703414	H	0.340772	-0.740929	2.673647
O	-2.551456	1.316990	-3.719986	O	0.188508	0.004539	3.395640
O	0.299115	-3.734206	-0.002735	F	-1.702025	0.001533	1.451416
O	-4.117994	0.002359	-2.053107	F	0.773384	-1.358622	1.488437
O	-4.364595	-2.789978	-2.284951	F	0.773529	1.366149	1.487753
O	-3.192148	0.001857	-6.132670	O	-0.006017	0.003878	-3.768680
O	1.596610	-2.758180	-6.122565	F	0.822092	1.461078	-1.491612
O	1.592998	2.770447	-6.119586	F	0.822905	-1.452392	-1.493875
O	-4.366030	2.794928	-2.283377	F	-1.687415	0.003103	-1.529747
O	-0.252187	5.172581	-2.284971				
O	4.580269	2.382989	-2.263403				

### Coordinates of $\gamma$ -[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}]^{6-}$

W	-0.110614	-3.562698	-1.866486	O	0.229280	5.248777	-2.300123
W	-0.074481	3.605261	-1.904762	O	4.437023	2.764306	-2.214902
W	3.173093	1.659736	-1.834501	O	4.402185	-2.778199	-2.209527
W	3.155810	-1.653802	-1.826110	O	0.763951	-1.337019	5.764600
W	-3.054109	1.876253	-1.884070	O	2.565601	-1.296364	3.751913
W	-3.019847	-1.907321	-1.874633	O	-3.218757	-0.002838	1.698771
W	1.962356	0.002620	-4.862104	O	1.612269	-2.773273	1.713642
W	-1.023144	-1.721139	-4.959822	O	-1.567970	0.016139	5.736735
W	-1.030606	1.718656	-4.973530	O	2.567623	1.312119	3.748663
W	-0.125555	3.533254	1.895028	O	1.615649	2.785877	1.708807
W	-0.123041	-3.525618	1.926343	O	0.767217	1.365150	5.757734
W	3.130268	-1.648840	1.958386	O	-2.049177	-3.557226	2.008989
W	3.129014	1.661897	1.954491	O	4.115183	0.006792	2.037668
W	-2.988830	-1.877561	1.918001	O	-0.201749	3.718510	-0.018396
W	-2.987957	1.873627	1.908371	O	-0.160633	2.879976	3.703062
W	1.909568	0.008802	4.993380	O	-2.421492	-1.568308	3.718781
W	-0.961511	1.679054	4.954813	O	-3.049819	-2.041286	0.002947
W	-0.970291	-1.650944	4.967262	O	-0.159110	-2.865711	3.727069
O	0.727674	1.307946	-5.593196	O	-2.414848	1.578052	3.705460
O	2.605556	1.310592	-3.664972	O	3.341716	1.658954	0.039727
O	-3.247528	-0.008957	-1.732251	O	-2.048994	3.557141	1.973984
O	1.651332	2.840934	-1.723661	O	0.215408	5.179063	2.266434
O	-1.553094	-0.004430	-5.649741	O	-1.602191	2.776279	6.124797
O	2.594364	-1.304814	-3.658007	O	3.165851	0.009277	6.178642
O	1.617499	-2.785810	-1.680392	O	-1.607672	-2.740176	6.146100
O	0.732047	-1.311369	-5.589365	O	-4.587954	2.406037	2.255245
O	-2.011139	3.496786	-1.966452	O	-4.591572	-2.407062	2.256507
O	4.143452	0.000617	-1.970661	O	0.229097	-5.170698	2.291888
O	-0.235236	-3.700693	0.013898	O	4.376364	-2.777385	2.330841
O	-0.179896	-2.864974	-3.682538	O	4.377928	2.789093	2.320901
O	-2.437359	1.595483	-3.711158	Na	0.055456	-0.048478	0.067419
O	-3.081055	2.026289	-0.008898	H	0.025889	0.010073	2.791656
O	-0.184254	2.878904	-3.704952	H	-0.184931	0.704495	-2.645401
O	-2.438877	-1.607225	-3.703731	H	-0.064109	-0.777602	-2.721337
O	3.348378	-1.646033	0.048907	O	0.002155	0.009163	3.778144
O	-2.042118	-3.556040	-1.976321	F	-0.831727	-1.450459	1.516383
O	0.235812	-5.200867	-2.260746	F	1.686599	0.004950	1.545588
O	-1.619144	-2.800904	-6.153816	F	-0.830363	1.452017	1.485591
O	3.169947	-0.000171	-6.087593	O	0.053976	-0.010677	-3.377217
O	-1.632842	2.786412	-6.173350	F	-0.780216	-1.450086	-1.493601
O	-4.611909	-2.447238	-2.226916	F	-0.734263	1.340087	-1.506533
O	-4.637502	2.427995	-2.253686	F	1.748435	0.007055	-1.392019

**Coordinates of  $\alpha^*-\text{[}(SbO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}\text{]}^{8-}$**

W	3.516004	-0.075341	1.889688	O	-2.501982	-4.593075	2.316285
W	-3.564238	-0.047924	1.920979	O	2.531705	-4.624588	2.386397
W	-1.820508	-3.062518	1.935965	O	1.308161	0.739586	-5.613739
W	1.898503	-3.083261	1.974146	O	2.837565	-0.097223	-3.642373
W	-1.676960	3.145545	1.942230	O	-3.445610	2.001473	-1.969642
W	1.679005	3.151617	1.902962	O	3.526297	2.005705	-1.977509
W	-0.012467	-1.892209	4.952775	O	-1.296431	0.748611	-5.607821
W	1.642188	0.961798	4.888499	O	1.493253	-2.377112	-3.622627
W	-1.656452	0.953215	4.942165	O	0.008014	-3.997996	-1.948546
W	-1.717909	-3.158175	-1.865421	O	0.013635	-1.517314	-5.608819
W	1.853284	3.025072	-1.867144	O	0.002705	3.452890	-1.722436
W	3.633935	0.098413	-1.890016	O	2.951792	-1.683362	-1.685098
W	1.740195	-3.124362	-1.826538	O	1.886842	3.310876	0.014151
W	-1.862464	3.114590	-1.861630	O	-1.522818	-2.442636	-3.649427
W	-3.596926	0.073113	-1.879954	O	-1.305554	2.494201	-3.637222
W	1.720162	-0.993380	-4.892888	O	-1.890823	3.292244	0.004164
W	-1.689950	-0.989558	-4.875843	O	1.341260	2.490811	-3.658186
W	0.011931	1.969864	-4.897943	O	-2.880138	-0.118786	-3.665323
O	-1.362272	-0.770991	5.766388	O	-1.832374	-3.216836	0.019573
O	-1.334285	-2.512135	3.702833	O	-2.943655	-1.703123	-1.707009
O	0.000364	4.102627	2.001380	O	-2.726416	-4.493325	-2.244751
O	-3.423005	-1.971332	1.968323	O	-2.769783	-1.623162	-6.059001
O	-0.008930	1.543097	5.729485	O	2.823050	-1.643545	-6.034271
O	1.336634	-2.494382	3.694402	O	0.011481	3.236810	-6.054809
O	3.495136	-2.037276	2.002176	O	-5.257717	-0.125076	-2.266289
O	1.319970	-0.756671	5.736875	O	-2.515444	4.632634	-2.326160
O	-2.927761	1.722879	1.720326	O	2.546993	4.537895	-2.316938
O	0.024513	-3.431017	1.755922	O	5.273575	-0.148976	-2.333992
O	3.813858	0.011199	-0.009358	O	2.738510	-4.444147	-2.291339
O	2.801159	0.086830	3.667900	Na	0.064730	0.065290	0.048136
O	-1.483801	2.416688	3.683488	H	-0.659909	0.475769	-2.641558
O	-3.722029	0.018764	0.007400	H	-0.243932	-0.144911	2.760202
O	-2.846871	0.121755	3.689413	H	0.125463	-0.808092	-2.670575
O	1.458599	2.402913	3.657119	O	-0.153738	-0.091282	-3.357318
O	1.894791	-3.284816	0.047919	F	-1.364729	0.815906	-1.454220
O	2.903356	1.699133	1.705701	F	1.416209	0.970034	-1.382687
O	5.171291	0.119302	2.335602	F	0.096141	-1.612439	-1.435161
O	2.768473	1.619030	6.019232	O	-0.047192	-0.020565	3.732308
O	-0.003035	-3.187623	6.096639	F	-0.015852	1.762218	1.422099
O	-2.777237	1.618918	6.077259	F	-1.300488	-0.758233	1.522949
O	2.711182	4.454507	2.350133	F	1.522177	-0.750178	1.413568
O	-2.696703	4.473634	2.338740				
O	-5.226423	0.149809	2.308787				

**Coordinates of  $\beta$ 1<sup>\*</sup>-[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>6-</sup>**

W	-1.947626	-0.020820	4.927472	O	-1.644484	-2.871467	-2.000870
W	0.914526	1.635134	4.975657	O	3.361027	0.030510	-1.922280
W	0.927500	-1.669179	4.943511	O	-4.510323	2.754165	-2.269244
W	3.106870	-1.663154	1.932995	O	-0.096252	-5.260159	-2.202844
W	-0.131745	3.532722	1.966371	O	4.668738	2.555636	-2.172022
W	-3.006291	-1.858907	1.892182	O	4.625440	-2.495794	-2.237266
W	3.084564	1.682958	1.970984	O	-0.061755	5.245372	-2.179856
W	-3.019360	1.847335	1.904102	O	-4.477802	-2.750025	-2.244271
W	-0.105087	-3.515349	1.910381	O	0.264391	2.984115	-3.656282
O	-3.246754	-0.030366	6.066001	O	-2.723862	-1.263955	-3.751132
O	1.566510	-2.793603	6.088628	O	-2.688179	1.266505	-3.719634
O	1.550783	2.749588	6.131624	O	0.274747	-2.985854	-3.709713
O	1.506125	-0.020896	5.771012	O	2.485878	1.731866	-3.653200
O	-0.819548	1.314065	5.758482	O	2.437533	-1.681593	-3.682865
O	-0.811657	-1.363292	5.733232	O	-0.750545	1.307235	-5.515707
O	0.077316	2.823500	3.726406	O	-0.768477	-1.327838	-5.582791
O	-2.543134	-1.342884	3.672193	O	1.540020	0.002517	-5.527434
O	-2.541499	1.305777	3.681205	O	1.589299	2.747090	-6.124790
O	0.090462	-2.857373	3.687929	O	-3.184418	0.024334	-6.246893
O	2.370336	1.506589	3.731510	O	1.604364	-2.734703	-6.192576
O	2.374444	-1.516959	3.703164	W	3.110849	1.926930	-1.818484
O	0.144447	5.189340	2.345587	W	0.114306	3.572217	-1.804485
O	-4.585266	-2.465803	2.210237	W	-3.144093	-1.724999	-1.900902
O	4.406319	-2.727121	2.311701	W	3.079913	-1.841536	-1.857915
O	4.377830	2.755882	2.343749	W	-3.163585	1.755407	-1.899035
O	-4.596558	2.440892	2.254871	W	0.124276	-3.590667	-1.875616
O	0.168324	-5.186130	2.220635	W	-2.030233	-0.006670	-4.978540
O	-2.051634	3.509005	2.086592	W	0.998026	-1.735012	-4.935145
O	4.040782	0.012337	2.107165	W	1.019165	1.742486	-4.851057
O	-2.028292	-3.511512	2.035552	Na	0.007701	0.023204	0.072713
O	1.628434	2.864359	1.689108	H	-0.018491	-0.005002	2.775036
O	1.654165	-2.856067	1.656053	O	-0.026230	-0.010972	3.762133
O	-3.325190	-0.004818	1.634146	F	1.663392	0.005725	1.518515
O	3.273364	1.738952	0.047372	O	0.099970	0.017942	-3.344435
O	3.285422	-1.715186	0.023728	F	0.754828	1.547141	-1.337366
O	-3.126695	1.965675	-0.015321	F	-0.855114	1.446701	1.515022
O	-0.143267	-3.607520	-0.015930	F	-0.834154	-1.425577	1.512337
O	-0.165601	3.717002	0.054385	F	-1.548551	0.032360	-1.530797
O	-3.072362	-1.946853	-0.029740	F	0.935471	-1.319780	-1.450451
O	2.069480	3.541733	-1.733350	H	-0.669304	0.170897	-2.659393
O	2.034636	-3.484101	-1.749767	H	0.687100	-0.415602	-2.628703
O	-3.999712	0.005283	-1.775212				
O	-1.687974	2.937652	-1.952784				

**Coordinates of  $\beta$ 2<sup>\*</sup>-[ $(\text{NaF}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}$ ]<sup>6-</sup>**

W	3.083308	1.873489	-1.947747	O	-0.798885	-1.360869	-5.695554
W	0.101718	3.530309	-1.923994	O	-2.656841	1.273573	-3.709911
W	-3.120315	-1.673171	-1.904502	O	0.215400	-2.939743	-3.724758
W	-0.063709	3.610026	1.871500	O	-4.085426	-0.001940	-1.802000
W	-3.080623	-1.870867	1.892874	O	-3.162860	0.002999	-6.166796
W	0.962934	1.673008	-4.969562	O	-4.469589	2.709239	-2.246963
W	3.127028	1.672054	1.846518	O	-0.145923	-5.223522	-2.288229
W	1.017230	1.703305	4.903297	O	-1.985969	3.455220	2.032719
W	3.023650	-1.886197	-1.923229	O	-1.986377	-3.461939	2.031563
W	0.961200	-1.675480	-4.962338	O	-0.729978	1.313785	5.614993
W	3.126984	-1.681398	1.860857	O	-0.734946	-1.314838	5.617923
W	1.008428	-1.714751	4.909511	O	-3.431017	0.001058	1.702464
W	-3.137531	1.676629	-1.901273	O	-2.573490	1.337630	3.684025
W	0.117966	-3.561948	-1.926072	O	0.135222	-2.843964	3.656391
W	-1.937176	0.007196	-4.951405	O	-3.122200	1.921820	0.005514
W	-3.083014	1.863405	1.893624	O	-0.089334	-3.734067	-0.001077
W	-0.061725	-3.623603	1.874371	O	-3.179998	0.002158	6.104702
W	-1.949646	0.002354	4.897951	O	-4.629400	2.521721	2.242176
O	3.311988	-0.006928	-1.940602	O	0.172667	-5.274484	2.286316
O	1.561716	-0.006854	-5.718969	O	0.222206	2.934405	-3.740501
O	2.432910	1.661512	-3.739855	O	-2.653205	-1.269250	-3.709887
O	2.047461	3.488146	-1.824606	O	-0.095532	5.204234	-2.283140
O	1.568604	2.719575	-6.202237	O	-4.433602	-2.731394	-2.248330
O	4.646037	2.481037	-2.320068	O	0.142323	2.836134	3.650314
O	4.067177	-0.005607	2.018880	O	-2.572211	-1.332606	3.681814
O	1.521879	-0.004432	5.624125	O	-0.105484	3.714183	-0.004772
O	1.691096	2.918472	1.651349	O	-3.128230	-1.914411	0.013184
O	2.412070	1.497705	3.642470	O	0.180531	5.261610	2.275731
O	3.270769	1.756955	-0.043802	O	-4.626294	-2.527978	2.248029
O	1.662488	2.796303	6.057306	Na	0.033631	-0.021780	-0.063939
O	4.442293	2.709531	2.238482	H	0.014094	0.079017	-2.766500
O	2.420521	-1.675727	-3.734340	H	-0.325611	-0.748774	2.681192
O	2.045242	-3.554194	-1.830470	H	-0.335369	0.745044	2.673875
O	1.555281	-2.734535	-6.188306	O	0.001558	0.011402	-3.752587
O	4.584601	-2.507936	-2.295340	F	0.711872	1.458312	-1.508525
O	1.694197	-2.938721	1.670368	O	-0.176408	0.001008	3.393034
O	2.407214	-1.505485	3.650893	F	1.712681	-0.004252	1.410167
O	3.252490	-1.772988	-0.027681	F	0.850059	-1.471104	-1.490557
O	1.651446	-2.807023	6.065370	F	-1.677754	0.003893	-1.481863
O	4.445173	-2.715943	2.250451	F	-0.770926	-1.378919	1.488745
O	-1.677436	2.897388	-1.921884	F	-0.773978	1.366329	1.484957
O	-1.635469	-2.848906	-1.885546				
O	-0.795061	1.361218	-5.714956				

**Coordinates of  $\gamma^*-\text{[}( \text{NaF}_6 )\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}\text{]}^{6-}$**

W	-1.884016	-3.060096	-1.877078	O	5.293960	0.156111	-2.258014
W	1.741034	3.209946	-1.847783	O	2.519358	-4.623817	-2.175433
W	3.630893	-0.065632	-1.889774	O	-1.375390	-0.805826	5.740452
W	1.883334	-3.060600	-1.861570	O	-1.304401	-2.636539	3.738582
W	-1.665859	3.146574	-1.825751	O	0.003095	3.261878	1.831371
W	-3.627268	-0.058030	-1.905003	O	-2.847886	-1.614324	1.838856
W	1.735485	-1.046423	-4.947945	O	-0.008630	1.534446	5.732401
W	-1.731400	-1.034936	-4.962402	O	1.271741	-2.643706	3.744542
W	0.022006	1.984701	-4.869098	O	2.829595	-1.635097	1.847641
W	3.548834	0.119778	1.918387	O	1.344114	-0.812610	5.741801
W	-3.556368	0.145514	1.905902	O	-3.557178	2.073551	1.921287
W	-1.681752	-3.104235	1.923589	O	-0.018741	-4.079016	1.891615
W	1.650640	-3.115179	1.934561	O	3.696907	0.041710	0.005755
W	-1.874432	3.021012	1.956131	O	2.904910	0.186485	3.732522
W	1.876966	3.000688	1.950918	O	-1.618283	2.417289	3.747239
W	-0.018795	-1.948544	4.985595	O	-1.902672	3.186678	0.039539
W	1.664069	0.933091	4.973449	O	-2.927511	0.204979	3.726124
W	-1.684421	0.941697	4.971612	O	1.614432	2.407550	3.743537
O	1.335059	0.725754	-5.543543	O	1.746140	-3.140348	0.008770
O	2.951503	-0.254591	-3.696277	O	3.556091	2.047855	1.926740
O	-2.922378	1.700655	-1.914030	O	5.204744	-0.174476	2.285305
O	2.922106	1.685577	-1.897012	O	2.729144	1.549550	6.184121
O	-1.294628	0.732968	-5.546976	O	-0.023309	-3.187601	6.188007
O	1.696129	-2.473867	-3.706602	O	-2.748174	1.562436	6.181207
O	-0.005596	-3.335825	-1.932398	O	2.448606	4.584614	2.307838
O	0.003643	-1.569091	-5.602351	O	-2.430681	4.608167	2.324939
O	0.042628	4.101200	-1.815409	O	-5.217427	-0.140930	2.255492
O	3.495437	-2.007595	-1.804017	O	-2.771279	-4.400809	2.229822
O	-3.684518	0.065590	-0.011025	O	2.729654	-4.420247	2.241383
O	-1.704556	-2.465959	-3.725161	Na	-0.018598	0.035906	0.087808
O	-1.256878	2.678734	-3.677958	H	-0.011908	-0.077242	2.789269
O	1.905955	3.165166	0.022687	H	-0.715733	-0.161419	-2.655552
O	1.312331	2.685587	-3.670877	H	0.753433	-0.149452	-2.636955
O	-2.939244	-0.232986	-3.712741	O	-0.011001	-0.029568	3.775320
O	-1.774761	-3.132642	-0.001695	F	-1.472225	0.850257	1.517266
O	-3.497481	-1.993095	-1.823874	F	-0.011336	-1.640472	1.545695
O	-2.525303	-4.620476	-2.195529	F	1.465415	0.839450	1.508977
O	-2.763317	-1.597411	-6.212325	O	0.027345	0.023286	-3.357855
O	2.769290	-1.625459	-6.189542	F	-1.377636	-0.741359	-1.503456
O	0.028982	3.144153	-6.138801	F	-0.112431	1.711435	-1.359056
O	-5.289839	0.164520	-2.273865	F	1.387480	-0.735040	-1.474262
O	-2.665492	4.497997	-2.211031				
O	2.794199	4.517237	-2.206225				

**Coordinates of  $\alpha$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ]<sup>5-</sup>**

O	3.020367	1.934084	-0.096508	O	-1.268261	-0.836789	3.389279
O	0.531004	1.917331	0.794079	O	-0.685443	-3.364438	4.653542
O	1.633686	-0.512626	0.783165	O	-5.111063	-3.128054	3.221366
O	1.113177	0.743272	-1.487543	O	-3.716926	-5.536605	-1.607780
O	-3.020360	-1.934267	-0.096578	O	-6.570807	-0.765807	-1.599648
O	-1.633767	0.512955	0.782703	O	-3.203319	0.843726	4.610682
O	-1.113284	-0.743040	-1.487564	O	-4.633340	3.209828	-0.188355
O	-0.530941	-1.917359	0.793978	O	-3.383467	1.124891	-4.440744
W	-0.609200	-2.638327	3.100783	O	-0.445097	-3.589235	-4.422962
W	-2.472703	0.451142	-3.152796	O	0.789619	-5.707769	-0.166199
W	-0.659351	-2.488813	-3.124205	O	5.503487	1.830567	0.769869
W	0.267476	-4.094849	0.100099	O	4.483354	-0.475509	-0.132709
W	-3.406440	2.038038	0.063666	O	-0.026388	4.086496	2.015707
W	-2.497572	0.564279	3.073697	O	3.481069	-1.778039	1.956763
W	-3.301991	-3.981917	-0.987532	O	4.101337	4.084191	0.766493
W	-4.149095	-2.553715	1.923632	O	3.851222	0.612342	-2.370918
W	-5.021490	-1.159458	-0.962011	O	1.763062	1.129532	-3.943615
W	0.659316	2.488928	-3.124293	O	4.850368	2.984116	-1.564666
W	2.497826	-0.564141	3.074427	O	1.268925	0.836788	3.391069
W	3.405922	-2.037746	0.063865	O	2.762067	-1.655173	-1.683733
W	2.472803	-0.451062	-3.152909	O	-0.845932	1.382397	-3.444373
W	0.609472	2.638351	3.100843	O	2.273628	3.237549	-2.400378
W	-0.267844	4.094669	0.100317	O	2.384368	3.010995	2.509634
W	5.021407	1.159560	-0.962161	O	-1.110652	1.872114	3.193344
W	3.301745	3.981837	-0.987382	O	3.700239	0.795545	2.467011
W	4.149350	2.553548	1.923861	O	1.601791	4.342171	-0.146888
O	-4.850167	-2.984156	-1.565025	O	0.845500	-1.382067	-3.444203
O	-2.273251	-3.237998	-2.400034	O	-0.233050	3.323058	-1.675365
O	-3.480924	1.778464	1.956670	O	0.445452	3.588961	-4.423343
O	-1.763666	-1.129941	-3.943339	O	3.716852	5.536341	-1.608041
O	-5.503458	-1.831543	0.769383	O	6.571601	0.765327	-1.597043
O	-1.601986	-4.342710	-0.146462	O	5.112148	3.128134	3.220846
O	0.026795	-4.086401	2.015619	O	-0.789383	5.707966	-0.164920
O	-4.101112	-4.084827	0.766699	O	0.686021	3.365018	4.653420
O	-2.762881	1.655502	-1.684091	O	3.205148	-0.843466	4.610772
O	0.233094	-3.322330	-1.674901	O	4.632467	-3.209750	-0.189232
O	1.111068	-1.871880	3.194057	O	3.382521	-1.127969	-4.439762
O	-2.383958	-3.011513	2.509383	I	-0.000013	0.000020	-0.058102
O	-4.484168	0.475800	-0.132522	H	2.401269	1.349741	-0.651301
O	-1.949112	3.254812	0.300242	H	-2.401306	-1.349950	-0.651465
O	-3.850659	-0.612297	-2.370006	H	-1.528477	-1.976247	0.586491
O	-3.699102	-0.795887	2.466082	H	1.528520	1.976267	0.586458
O	1.948854	-3.254670	0.300925				

**Coordinates of  $\beta$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ]<sup>5-</sup>**

O	0.004916	3.610432	-0.045660	O	2.926291	-1.588431	1.657033
O	0.030406	1.448995	1.548957	O	5.223474	-2.460851	0.149255
O	1.345129	1.077612	-0.747471	O	2.643877	-6.020958	1.657871
O	-1.272898	1.355960	-0.722158	O	-0.148697	-6.089121	-3.175985
O	-0.136218	-3.589763	-0.093508	O	-2.922424	-5.934487	1.635026
O	0.000602	-1.120251	1.509592	O	2.730020	-2.314958	4.391834
O	-1.299869	-1.321419	-0.791240	O	-2.789095	-2.210893	4.397940
O	1.328574	-1.494949	-0.785448	O	-5.265328	-2.178367	0.133672
W	3.600967	-1.970363	-0.117441	O	-2.480857	-2.250839	-4.646046
W	-3.614109	-1.786626	-0.116320	O	2.451666	-2.433822	-4.646998
W	-1.859605	-1.843513	-3.099416	O	0.083925	5.685546	-1.583971
W	1.854986	-2.003251	-3.096884	O	1.514828	3.521107	-2.382163
W	-1.755872	-1.807038	3.090264	O	0.031680	2.025561	4.065539
W	1.723464	-1.832587	3.090348	O	3.440926	1.847034	-1.970592
W	-0.138780	-4.917679	-1.910351	O	1.397110	5.618731	0.728849
W	1.548748	-4.885662	0.985068	O	-1.434512	3.644539	-2.375442
W	-1.771446	-4.851013	0.955347	O	-3.439670	2.032349	-1.995351
W	-3.543109	1.967743	-0.062849	O	-1.263376	5.746085	0.746667
W	3.583690	1.778303	-0.050267	O	2.916616	1.577656	1.707737
W	1.872981	1.750429	-3.056338	O	0.005625	1.563119	-3.326322
W	-1.859937	1.908605	-3.048162	O	-3.787948	0.091117	-0.265755
W	1.744827	1.914156	3.199203	O	-2.774187	3.713811	-0.144727
W	-1.685211	1.951594	3.196248	O	1.347873	3.636905	2.483556
W	-1.587948	4.968811	-0.982846	O	1.714018	0.034352	3.452195
W	0.049518	4.948472	1.903736	O	2.817662	3.519271	-0.110858
W	1.702337	4.796885	-0.998284	O	-1.256807	3.704777	2.520376
O	-1.487625	-5.680533	-0.760685	O	-2.125582	0.024761	-3.171294
O	-1.376534	-3.621879	-2.535989	O	-2.865590	1.739459	1.692147
O	-0.025891	-1.984450	3.877135	O	-5.175670	2.415608	0.214914
O	-3.440945	-2.009792	-2.000158	O	0.097868	6.099507	3.174310
O	-0.128148	-5.638706	1.552908	O	-2.685114	6.111844	-1.657731
O	1.230625	-3.699082	-2.533589	O	2.866868	5.886200	-1.648749
O	3.443805	-2.183204	-2.018851	O	-2.745881	2.413855	4.463528
O	1.196012	-5.667561	-0.739132	O	2.820013	2.367033	4.457480
O	-2.933650	-1.449868	1.647029	O	5.221183	2.219451	0.202278
O	-0.005140	-1.597365	-3.408247	O	2.464469	2.197240	-4.602781
O	3.850435	-0.108730	-0.255269	O	-2.417470	2.357472	-4.606904
O	2.738786	-3.659863	0.118203	I	-0.055530	-0.009361	-0.041403
O	-1.568447	-3.541329	2.341045	H	-0.341938	2.768254	-0.484100
O	-1.699591	0.089041	3.413959	H	-0.685472	-2.745440	-0.225935
O	-2.880732	-3.540301	0.120391	H	0.896546	-2.365317	-0.474172
O	1.407095	-3.573460	2.338644	H	0.102361	2.312175	1.019979
O	2.122544	-0.123220	-3.189993				

**Coordinates of  $\gamma$ -[ $(\text{IO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ]<sup>5-</sup>**

O	-0.068110	0.012049	3.610027	O	3.849318	0.078686	0.067443
O	-1.249543	0.796938	1.337859	O	-0.109564	-4.065419	-2.007402
O	-0.025996	-1.526138	1.103436	O	2.648909	-4.549234	-2.403376
O	1.370276	0.733931	1.467561	O	-0.043001	-3.165768	-6.129798
O	-0.028346	0.048912	-3.610408	O	2.841034	1.570287	-5.939237
O	-1.270732	0.752634	-1.344289	O	-2.703733	1.730315	-6.079330
O	1.352659	0.706820	-1.100159	O	-2.888372	-4.401874	-2.422807
O	-0.033090	-1.558011	-1.465177	O	-5.212934	-0.048831	-2.348175
W	1.630068	-3.250997	-1.933238	O	-2.340019	4.665843	-2.304020
W	-1.793665	3.098375	-1.871468	O	2.592402	4.537911	-2.232881
W	1.941050	3.014890	-1.789560	O	5.193145	-0.331247	-2.279838
W	3.565948	-0.051976	-1.816286	O	1.257490	-0.821605	5.648155
W	-3.566414	0.158439	-1.912436	O	2.805937	0.057846	3.674015
W	-1.804571	-3.151496	-1.969778	O	-2.950311	-1.584199	1.599166
W	1.681199	0.957103	-4.823588	O	2.885162	-1.737726	1.674968
W	-0.046431	-1.905919	-4.966133	O	-1.407142	-0.758159	5.674346
W	-1.619611	1.027790	-4.940050	O	1.606671	2.355814	3.717600
W	-1.755534	3.115687	1.899360	O	0.119895	3.365208	1.748253
W	1.647815	-3.155701	1.828683	O	0.006721	1.532565	5.722442
W	3.629486	0.015127	1.945422	O	-0.114922	-3.939509	1.864544
W	1.992508	3.035449	1.970799	O	3.572856	1.935644	2.015701
W	-1.820766	-3.087663	1.790438	O	-1.954335	3.239717	0.019867
W	-3.580475	0.207876	1.858519	O	-1.493223	2.417738	3.664005
W	1.663683	0.911482	4.970236	O	-1.409350	-2.447688	3.553482
W	-1.664352	0.993095	4.931903	O	-1.848059	-3.356378	-0.092808
W	-0.111183	-1.920955	4.828000	O	1.196398	-2.507859	3.567363
O	0.062313	1.586390	-5.677779	O	-2.813995	0.189830	3.609441
O	1.562401	2.355685	-3.553323	O	2.161599	3.162182	0.093666
O	-2.943810	-1.627783	-1.755084	O	-3.402519	2.101164	1.927161
O	0.089123	3.344421	-1.606570	O	-2.315370	4.679737	2.329010
O	-1.345679	-0.708895	-5.725189	O	-2.782401	1.648130	6.066468
O	2.791199	0.056005	-3.558264	O	2.784815	1.479923	6.137005
O	2.858437	-1.795175	-1.661596	O	-0.141523	-3.231065	5.945335
O	1.319824	-0.763224	-5.640592	O	-5.226998	-0.011833	2.286651
O	-3.403310	2.085875	-1.943445	O	-2.889375	-4.353369	2.233554
O	3.468584	1.874372	-1.856061	O	2.631956	-4.478405	2.299879
O	1.666577	-3.471086	-0.054153	O	5.246519	-0.307165	2.421378
O	1.227310	-2.537650	-3.664146	O	2.617122	4.569197	2.419322
O	-2.818554	0.235789	-3.674758	I	-0.053951	0.031306	-0.000604
O	-3.773067	0.283600	-0.033835	H	-0.610635	0.095042	2.761867
O	-1.425757	2.419083	-3.619485	H	-0.349484	0.497627	-2.764099
O	-1.364556	-2.502631	-3.716205	H	0.046693	-1.026467	-2.327638
				H	0.929381	0.424680	2.329235

**Coordinates of  $\alpha^*-\text{[IO}_6\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]^{5-}}$**

O	0.969288	-1.626037	0.062799	O	-3.865554	-2.069918	-1.271197
O	-1.237672	-0.825066	1.396845	O	-0.000034	0.000150	3.970106
O	-1.238533	-0.796489	-1.324316	O	-3.851784	0.103325	0.065193
O	-0.969353	1.625970	0.062669	O	-5.219573	-0.014702	2.585414
O	1.238536	0.796263	-1.324414	O	-5.615946	-3.856900	0.048794
O	1.237764	0.825118	1.397001	O	-1.266839	-6.005914	2.852458
W	-3.659097	-0.271730	1.925130	O	-1.293269	-6.058067	-2.730084
W	1.904283	-3.087728	-1.688674	O	-5.186870	0.014649	-2.454928
W	1.926328	-3.045202	1.827631	O	-1.014618	-2.149663	-5.200586
W	-0.934023	-1.633812	3.710681	O	2.865554	-4.158304	-2.622324
W	-0.931736	-1.632726	-3.566357	O	2.875347	-4.125873	2.760815
W	-3.624126	-0.233742	-1.794419	O	-1.024764	-2.160139	5.339197
W	-1.365448	-4.734370	1.707050	O	-1.712861	-3.098229	0.001838
W	-3.940104	-3.450024	0.029013	O	3.301889	4.705073	-1.291157
W	-1.404524	-4.762584	-1.603809	O	3.864863	2.069495	-1.271013
W	0.934183	1.633983	3.711003	O	-2.592863	3.437552	0.068610
W	0.931941	1.632724	-3.566356	O	2.656196	0.818358	-3.359405
W	3.623792	0.233253	-1.794115	O	1.235262	5.709569	0.059983
W	3.658929	0.272154	1.925713	O	3.859259	2.076913	1.383913
W	-1.904530	3.087548	-1.688407	O	2.649627	0.801892	3.484463
W	-1.925821	3.045363	1.827425	O	3.255132	4.651237	1.370531
W	3.939966	3.449730	0.028875	O	-0.756979	2.277140	-2.963305
W	1.366038	4.734634	1.707508	O	3.850416	-0.102874	0.065716
W	1.404052	4.762644	-1.603576	O	1.587496	3.197324	2.835149
O	1.712715	3.098172	0.002030	O	-0.427310	4.242025	-1.377913
O	3.004669	-1.504494	2.053589	O	1.585355	3.242196	-2.745237
O	-2.995198	1.533036	-1.930961	O	-0.439964	4.208876	1.490376
O	2.995267	-1.533579	-1.930830	O	-0.759152	2.271330	3.107028
O	-1.234861	-5.709869	0.059675	O	1.023851	2.161229	5.339291
O	0.440214	-4.208394	1.490120	O	1.268274	6.006439	2.852611
O	-2.655873	-0.818110	-3.359586	O	5.615446	3.856977	0.047623
O	2.592342	-3.438132	0.068534	O	1.293043	6.058595	-2.729210
O	-3.302173	-4.705824	-1.290221	O	-2.874486	4.125536	2.761413
O	-1.587351	-3.197088	2.834851	O	-2.866490	4.157746	-2.621719
O	-2.649439	-0.801431	3.483718	O	1.014506	2.149099	-5.200706
O	-3.254850	-4.651084	1.370983	O	5.186875	-0.014553	-2.454021
O	0.757095	-2.277383	-2.963732	O	5.219288	0.013310	2.585527
O	0.759705	-2.271714	3.108008	I	0.000051	-0.000035	-0.091787
O	-3.004772	1.504599	2.053254	H	-1.463806	-2.332250	-0.606372
O	-3.858699	-2.076655	1.383279	H	-1.381728	-1.760646	1.003144
O	-1.585527	-3.241935	-2.744936	H	1.463779	2.332210	-0.606221
O	0.000181	-0.000108	-3.854221	H	1.381718	1.760713	1.003222
O	0.426652	-4.241742	-1.378229				

**Coordinates of  $\beta^*-\text{[}(IO_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{5-}$**

O	0.805227	-1.248121	-1.104364	O	-2.560237	1.234498	-3.627093
O	-1.508208	0.040852	-1.291817	O	-0.079395	-3.777737	0.031136
O	0.854867	1.456396	-1.154322	O	-3.980542	-0.014606	-1.789797
O	-0.816772	1.413105	1.071848	O	-4.542665	-2.731883	-2.323742
O	1.570492	0.085277	1.304086	O	-3.209103	-0.032581	-6.083398
O	-0.765073	-1.265829	1.293388	O	1.622709	-2.771770	-6.046591
W	-3.203809	-1.757901	-1.884785	O	1.561217	2.746196	-6.053981
W	3.112332	1.935487	-1.864569	O	-4.511122	2.726435	-2.404886
W	3.106765	-1.800826	-1.853039	O	-0.142065	5.258609	-2.373492
W	0.062628	-3.571291	-1.852432	O	4.611621	2.614250	-2.349389
W	0.059414	3.630100	-1.872074	O	4.600033	-2.498712	-2.327161
W	-3.186145	1.759746	-1.903713	O	-0.066318	-5.225495	-2.280373
W	0.975451	-1.666224	-4.895810	O	0.055739	-0.016654	-3.550224
W	-1.951851	-0.040032	-4.919196	O	-0.766771	1.343589	5.648252
W	0.967699	1.657924	-4.858738	O	0.086800	2.772713	3.580150
W	-0.011230	-3.590779	1.910399	O	-3.458451	-0.031593	1.632552
W	-0.070132	3.593500	1.869808	O	1.729541	3.013702	1.632373
W	3.174231	1.800740	1.890497	O	-0.741378	-1.294995	5.638652
W	3.185506	-1.697980	1.893205	O	2.386845	1.530557	3.618865
W	-3.084601	1.818870	1.838186	O	1.763555	-2.941850	1.652820
W	-3.082916	-1.888245	1.879103	O	1.565324	0.044159	5.703881
W	0.965300	1.681230	4.886165	O	-1.978171	3.389380	1.922113
W	1.003130	-1.614356	4.890636	O	3.971744	0.057806	2.000740
W	-1.900347	0.018295	4.846925	O	2.425301	-1.453846	3.634386
O	0.108464	-0.030594	3.557052	O	-2.421445	-1.314542	3.575628
O	3.429074	1.925992	0.008346	O	-2.421434	1.305709	3.557112
O	-3.371769	1.971498	-0.033832	O	0.146568	-2.786504	3.624883
O	3.421482	-1.781651	0.020813	O	-1.931683	-3.416699	1.988436
O	1.553240	-0.007058	-5.659384	O	0.207647	-5.233705	2.348112
O	2.372523	-1.531096	-3.599443	O	1.644803	-2.738229	6.029945
O	-1.732775	2.967006	-1.819034	O	1.584317	2.842550	5.993964
O	3.455925	0.062186	-1.824699	O	-3.223226	0.013170	5.937256
O	-0.784780	1.297001	-5.607261	O	-4.588195	-2.552756	2.359778
O	0.193618	-2.841371	-3.605644	O	-4.587185	2.472645	2.344142
O	-1.731351	-2.968708	-1.837419	O	0.090341	5.227054	2.370678
O	-0.777290	-1.369511	-5.640725	O	4.479683	2.804358	2.374320
O	1.992796	3.497914	-1.825566	O	4.514865	-2.680813	2.349306
O	1.972741	-3.345868	-1.732308	I	0.144367	0.155031	0.016991
O	-3.265978	-2.007223	-0.000600	H	0.585888	-0.229469	-2.736024
O	-2.579916	-1.302546	-3.631175	H	-0.998374	0.040875	-2.177027
O	0.159262	2.844601	-3.614548	H	0.695346	0.161528	2.757967
O	-0.065373	3.928791	-0.011026	H	-0.584866	-0.806001	2.190450
O	2.399988	1.600326	-3.622937				

**Coordinates of  $\gamma^*-\text{[IO}_6\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{5-}$**

O	0.801527	-1.252151	-1.122247	O	-2.541517	1.251033	-3.623634
O	-1.511595	0.035836	-1.301740	O	0.007560	-3.791943	0.013928
O	0.843877	1.450586	-1.177245	O	-3.995001	-0.011470	-1.836107
O	-0.808710	1.408425	1.066090	O	-4.520984	-2.742119	-2.317924
O	1.564868	0.086178	1.293116	O	-3.215057	-0.028874	-6.064047
O	-0.762647	-1.270181	1.279303	O	1.625057	-2.774885	-6.049800
W	-3.198446	-1.746851	-1.875567	O	1.572680	2.749581	-6.059893
W	3.103965	1.939151	-1.861646	O	-4.498590	2.741117	-2.380847
W	3.089889	-1.802762	-1.851863	O	-0.168997	5.255951	-2.397535
W	0.063681	-3.572125	-1.880339	O	4.613623	2.593124	-2.349725
W	0.056891	3.627784	-1.906107	O	4.597217	-2.469738	-2.327589
W	-3.183435	1.752628	-1.895820	O	-0.098222	-5.222914	-2.310297
W	0.975511	-1.661370	-4.908065	O	0.058224	-0.012106	-3.568032
W	-1.945216	-0.034215	-4.913249	O	0.802851	1.357751	5.679908
W	0.974526	1.651799	-4.875384	O	2.553701	1.312349	3.646988
W	-0.018394	-3.623508	1.882291	O	-3.429721	-0.041391	1.785888
W	-0.078062	3.619505	1.834558	O	1.715044	2.986317	1.760422
W	3.180240	1.784370	1.902152	O	-1.491214	-0.013141	5.611983
W	3.192873	-1.692274	1.903838	O	2.589131	-1.246300	3.655863
W	-3.076264	1.818895	1.858303	O	1.742820	-2.924032	1.797288
W	-3.072083	-1.911676	1.896829	O	0.821089	-1.342915	5.680947
W	1.957961	0.023336	4.941458	O	-1.983123	3.413407	1.807220
W	-0.904550	-1.687722	4.909464	O	4.010944	0.051294	1.854455
W	-0.918059	1.666927	4.846015	O	-0.113731	-2.858138	3.637396
O	0.074360	0.022436	3.572736	O	-2.346166	1.524690	3.590594
O	3.381549	1.983373	0.008450	O	-0.129741	2.833682	3.589552
O	-3.371054	1.889373	-0.023768	O	-2.322636	-1.564739	3.613333
O	3.358004	-1.855932	0.021696	O	-1.941617	-3.460960	1.844033
O	1.556089	-0.006397	-5.682606	O	0.208666	-5.263511	2.325754
O	2.362152	-1.514705	-3.606128	O	-1.554745	-2.777518	6.063150
O	-1.726505	2.962327	-1.781362	O	3.230562	0.033642	6.100623
O	3.430657	0.061581	-1.782934	O	-1.580619	2.756518	6.002796
O	-0.780662	1.298629	-5.620915	O	-4.576299	-2.587622	2.364219
O	0.167375	-2.831617	-3.623561	O	-4.584538	2.479747	2.337205
O	-1.721059	-2.955190	-1.787903	O	0.088580	5.252340	2.335145
O	-0.775398	-1.360884	-5.653823	O	4.484883	2.793108	2.377468
O	1.989508	3.504417	-1.873487	O	4.517876	-2.685511	2.349172
O	1.972850	-3.363722	-1.794340	I	0.147542	0.152084	0.004573
O	-3.290774	-1.929487	0.008046	H	0.589283	-0.211348	-2.751607
O	-2.549819	-1.304378	-3.621657	H	-1.003228	0.033959	-2.186000
O	0.141077	2.839484	-3.634496	H	0.610790	0.255418	2.755566
O	0.005040	3.927037	-0.029377	H	-0.580554	-0.796496	2.163406
O	2.392580	1.585647	-3.626818				

**Coordinates of  $\alpha$ -[(TeO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H<sub>2</sub>]<sup>6-</sup>**

O	3.009358	2.008969	-0.015897	O	0.259158	-3.313333	1.657617
O	1.245322	0.756608	1.587761	O	0.773631	-5.730073	0.171555
O	1.675366	-0.518095	-0.734450	O	-3.649013	-5.508647	1.632370
O	0.464451	1.873214	-0.676043	O	-5.181780	-3.182739	-3.183631
O	-3.111695	-1.825567	-0.095051	O	-6.577900	-0.798237	1.623216
O	-0.962704	-0.619271	1.518421	O	-0.473866	-3.551672	4.376806
O	-1.831022	0.356116	-0.823233	O	-3.349261	1.170234	4.367134
O	-0.508891	-1.932241	-0.777328	O	-4.668337	3.247077	0.149872
W	0.296316	-4.101486	-0.113513	O	-3.162624	0.877234	-4.609320
W	-3.465323	2.049570	-0.133092	O	-0.675857	-3.348804	-4.641055
W	-2.523931	0.564180	-3.039307	O	5.513901	1.842245	-0.767660
W	-0.634838	-2.631388	-3.076756	O	3.715545	0.811283	-2.470979
W	-2.442892	0.489361	3.072472	O	1.825869	1.123620	4.056660
W	-0.636213	-2.436574	3.077837	O	3.521404	-1.801041	-1.932599
W	-4.187631	-2.545456	-1.919705	O	4.809709	2.970992	1.533510
W	-3.275761	-3.968905	0.966630	O	2.398351	3.024325	-2.510295
W	-5.028182	-1.150018	0.948303	O	-0.005627	4.064209	-1.958341
W	-0.279279	3.988533	-0.037522	O	4.152631	4.161076	-0.788720
W	3.412305	-2.041503	-0.025741	O	2.829933	-1.670729	1.738069
W	2.506823	-0.575799	-3.001708	O	1.247601	0.814341	-3.302942
W	0.599359	2.604861	-3.013065	O	-1.979934	3.209228	-0.339446
W	2.530014	-0.458159	3.221456	O	1.604921	4.360911	0.155905
W	0.741740	2.475743	3.195305	O	3.883287	0.613177	2.396389
W	4.153025	2.583136	-1.907811	O	0.920842	-1.399098	3.494622
W	3.291141	4.013701	0.936477	O	4.501230	-0.470868	0.137271
W	5.024290	1.153600	0.957787	O	2.296240	3.245970	2.401875
O	-5.576507	-1.839971	-0.773810	O	-1.141783	1.860519	-3.086904
O	-3.788862	-0.809886	-2.553509	O	-0.209005	3.298198	1.725585
O	-1.729070	-1.083679	3.902657	O	-0.828506	5.600995	0.226139
O	-3.608560	1.803569	-2.010923	O	3.724721	5.557070	1.585683
O	-4.809337	-2.966563	1.543854	O	5.131838	3.153130	-3.210791
O	-2.423186	-3.023636	-2.539855	O	6.578984	0.779478	1.587999
O	0.028450	-4.108940	-2.017297	O	0.535517	3.593693	4.488007
O	-4.106302	-4.092958	-0.758516	O	3.472867	-1.128458	4.495607
O	-2.776115	1.675191	1.626130	O	4.658049	-3.201342	0.221365
O	-1.298661	-0.840747	-3.379727	O	3.171812	-0.862135	-4.563060
O	1.994967	-3.304290	-0.289072	O	0.629489	3.304755	-4.584743
O	-1.590146	-4.308784	0.125421	Te	-0.024250	0.047271	-0.026052
O	-3.840034	-0.593514	2.336013	H	2.056800	1.891122	-0.391216
O	-0.808827	1.429251	3.451400	H	-2.645928	-0.920218	-0.254424
O	-4.571222	0.508549	0.125105	H	-1.460500	-2.041161	-0.463927
O	-2.252873	-3.153110	2.335337	H	2.018387	1.154433	1.078434
O	1.092210	-1.870466	-3.140957				

**Coordinates of  $\beta$ -[ $(\text{TeO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ] $^{6-}$**

O	-0.021693	3.634600	-0.057340	O	2.128500	-0.137932	-3.197070
O	0.028810	1.443725	1.574547	O	2.929454	-1.596392	1.653557
O	1.360426	1.097406	-0.749072	O	5.224195	-2.473218	0.149453
O	-1.273775	1.394423	-0.717550	O	2.636312	-6.029084	1.648297
O	-0.167716	-3.613088	-0.097073	O	-0.150576	-6.109455	-3.171086
O	0.004151	-1.144707	1.526563	O	-2.915211	-5.956312	1.629647
O	-1.299724	-1.357226	-0.792315	O	2.727693	-2.309719	4.379451
O	1.343551	-1.495098	-0.796785	O	-2.778307	-2.195428	4.382810
W	3.601091	-1.971828	-0.125403	O	-5.254244	-2.157871	0.125059
W	-3.593004	-1.785994	-0.130480	O	-2.478702	-2.237077	-4.644562
W	-1.853253	-1.840543	-3.090489	O	2.458489	-2.453399	-4.644312
W	1.860764	-2.019676	-3.089865	O	0.078565	5.704475	-1.588825
W	-1.730962	-1.808602	3.073257	O	1.524322	3.534113	-2.392673
W	1.710838	-1.825306	3.078961	O	0.033581	2.040154	4.092747
W	-0.150220	-4.927255	-1.908895	O	3.465225	1.858572	-1.979951
W	1.541598	-4.885289	0.977583	O	1.394612	5.625114	0.725835
W	-1.775573	-4.853253	0.947825	O	-1.457919	3.677366	-2.396566
W	-3.532472	1.971547	-0.058970	O	-3.457625	2.044211	-2.001547
W	3.567988	1.779868	-0.049457	O	-1.271819	5.762756	0.746993
W	1.873974	1.734483	-3.033496	O	2.922902	1.588365	1.719966
W	-1.858302	1.914984	-3.026745	O	0.006002	1.573235	-3.320397
W	1.740651	1.923107	3.207530	O	-3.775565	0.094869	-0.267561
W	-1.678210	1.952877	3.204356	O	-2.797584	3.739530	-0.154489
W	-1.593763	4.980148	-0.986609	O	1.348817	3.648184	2.489996
W	0.043501	4.950881	1.893086	O	1.722970	0.041576	3.467891
W	1.690022	4.797285	-1.006551	O	2.819102	3.531577	-0.113546
O	-1.499495	-5.702107	-0.768133	O	-1.258057	3.716838	2.529739
O	-1.381134	-3.642805	-2.556531	O	-2.121081	0.023916	-3.161237
O	-0.022496	-2.002875	3.910316	O	-2.874098	1.761468	1.704979
O	-3.458204	-2.029559	-2.016388	O	-5.174459	2.405252	0.221763
O	-0.131119	-5.649120	1.546445	O	0.096471	6.110981	3.161999
O	1.231605	-3.715826	-2.534255	O	-2.682995	6.144222	-1.651828
O	3.467246	-2.199859	-2.031186	O	2.853100	5.899532	-1.649066
O	1.192977	-5.680015	-0.744722	O	-2.741302	2.423967	4.473365
O	-2.924311	-1.456834	1.640830	O	2.820282	2.382502	4.466149
O	0.000952	-1.614026	-3.418688	O	5.211707	2.216368	0.208961
O	3.867093	-0.113599	-0.255395	O	2.458259	2.177787	-4.590109
O	2.739368	-3.668520	0.112728	O	-2.411221	2.342196	-4.599485
O	-1.577526	-3.560061	2.348104	Te	-0.048840	-0.009097	-0.034891
O	-1.703417	0.097206	3.422073	H	-0.386448	2.750191	-0.437790
O	-2.910072	-3.564849	0.126019	H	-0.673926	-2.724285	-0.256630
O	1.409731	-3.585458	2.340183	H	0.919779	-2.351647	-0.477196
				H	0.110263	2.293358	1.046432

**Coordinates of  $\gamma$ -[(TeO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H<sub>2</sub>]<sup>6-</sup>**

O	-0.087004	0.026039	3.637929	O	3.853147	0.092133	0.070938
O	-1.245690	0.843381	1.374539	O	-0.108052	-4.091290	-2.028248
O	-0.039357	-1.526535	1.136695	O	2.658730	-4.547699	-2.405345
O	1.387804	0.744332	1.457108	O	-0.039092	-3.156228	-6.139006
O	-0.048626	0.059228	-3.638549	O	2.831569	1.574573	-5.953981
O	-1.309314	0.728999	-1.380831	O	-2.706906	1.717887	-6.106774
O	1.348329	0.720382	-1.133642	O	-2.893266	-4.399289	-2.432639
O	-0.033738	-1.577880	-1.454644	O	-5.170615	-0.050829	-2.319202
W	1.623605	-3.255893	-1.934087	O	-2.323176	4.668000	-2.292787
W	-1.798478	3.080784	-1.884126	O	2.569612	4.527237	-2.217232
W	1.934881	2.988855	-1.780202	O	5.168211	-0.337576	-2.273782
W	3.536068	-0.043718	-1.815870	O	1.255063	-0.824381	5.658220
W	-3.513663	0.169099	-1.896331	O	2.809368	0.056641	3.682455
W	-1.797046	-3.154113	-1.975066	O	-2.934202	-1.571095	1.600566
W	1.670226	0.967539	-4.830165	O	2.882867	-1.729590	1.674548
W	-0.044236	-1.896561	-4.968350	O	-1.414075	-0.756658	5.695342
W	-1.625034	1.026834	-4.950237	O	1.609667	2.359035	3.729653
W	-1.741525	3.064172	1.883828	O	0.131062	3.358980	1.749273
W	1.626945	-3.133238	1.828042	O	0.006822	1.536371	5.740699
W	3.630973	0.022646	1.946306	O	-0.117634	-3.966286	1.884663
W	1.998459	3.030417	1.975786	O	3.595408	1.945615	2.036628
W	-1.801434	-3.071266	1.781131	O	-1.961963	3.210100	0.009852
W	-3.566772	0.220067	1.871431	O	-1.500561	2.419958	3.683482
W	1.655793	0.906319	4.971948	O	-1.417610	-2.458255	3.571470
W	-1.666402	0.998006	4.942868	O	-1.841399	-3.373129	-0.101369
W	-0.125566	-1.915782	4.833977	O	1.191069	-2.504992	3.580825
O	0.057616	1.591270	-5.698864	O	-2.840724	0.195385	3.642810
O	1.567739	2.367847	-3.571323	O	2.179786	3.164086	0.102317
O	-2.933182	-1.635323	-1.756043	O	-3.433546	2.113228	1.952305
O	0.084456	3.323552	-1.607002	O	-2.293298	4.643385	2.301346
O	-1.347925	-0.710869	-5.744023	O	-2.774072	1.655829	6.094212
O	2.786084	0.059866	-3.572024	O	2.777999	1.472886	6.145348
O	2.848918	-1.796272	-1.661021	O	-0.147961	-3.223958	5.960173
O	1.321568	-0.759399	-5.651399	O	-5.221721	-0.025458	2.274337
O	-3.427630	2.107858	-1.969342	O	-2.890217	-4.329983	2.217182
O	3.492537	1.889095	-1.876755	O	2.624611	-4.455813	2.291223
O	1.655849	-3.479843	-0.057967	O	5.249702	-0.315017	2.424394
O	1.230452	-2.541151	-3.673226	O	2.614080	4.571807	2.430157
O	-2.823528	0.239807	-3.694044	Te	-0.056371	0.034010	-0.000175
O	-3.748557	0.303255	-0.023712	H	-0.585736	0.151262	2.753795
O	-1.442845	2.439719	-3.652694	H	-0.387780	0.449884	-2.756153
O	-1.365351	-2.507180	-3.728357	H	0.059437	-1.051743	-2.304935
				H	0.957698	0.424924	2.306529

**Coordinates of  $\alpha^*-\text{[TeO}_6\text{)W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]^{6-}}$**

O	0.953012	-1.677894	0.088838	O	-3.881658	-2.087506	-1.271065
O	-1.254161	-0.816495	1.430397	O	0.000459	-0.000540	3.993507
O	-1.278147	-0.828211	-1.300738	O	-3.837900	0.082743	0.076750
O	-0.953209	1.677667	0.088614	O	-5.215007	-0.035451	2.583392
O	1.278067	0.828181	-1.300703	O	-5.625478	-3.871826	0.053183
O	1.254241	0.816486	1.430272	O	-1.267038	-5.998998	2.848769
W	-3.644053	-0.297018	1.936224	O	-1.315506	-6.079561	-2.726269
W	1.888125	-3.087301	-1.662906	O	-5.155917	0.019957	-2.433381
W	1.901214	-3.001218	1.775471	O	-1.001240	-2.134109	-5.188415
W	-0.944480	-1.625404	3.699386	O	2.853726	-4.131611	-2.631905
W	-0.944065	-1.627383	-3.543717	O	2.848780	-4.077950	2.729186
W	-3.586744	-0.242391	-1.776028	O	-1.011309	-2.176535	5.326381
W	-1.371014	-4.727948	1.695893	O	-1.727251	-3.136657	-0.027038
W	-3.944974	-3.465543	0.021588	O	3.323283	4.730456	-1.296501
W	-1.416956	-4.767896	-1.608949	O	3.881132	2.087347	-1.271059
W	0.943917	1.625017	3.699169	O	-2.625625	3.488065	0.056836
W	0.944720	1.627966	-3.543682	O	2.677302	0.830454	-3.381127
W	3.586775	0.242286	-1.775953	O	1.248271	5.722600	0.057609
W	3.644094	0.297523	1.936356	O	3.854308	2.098382	1.389055
W	-1.888332	3.087241	-1.663065	O	2.673917	0.808801	3.526583
W	-1.901215	3.001386	1.775327	O	3.267831	4.665956	1.371274
W	3.944897	3.465451	0.020656	O	-0.733381	2.275714	-2.931721
W	1.371631	4.727502	1.696233	O	3.838288	-0.081917	0.076841
W	1.416342	4.767912	-1.608661	O	1.600828	3.194039	2.827552
O	1.727406	3.136659	-0.027232	O	-0.421934	4.272893	-1.389922
O	3.005589	-1.483304	2.050373	O	1.600731	3.269431	-2.767346
O	-2.970983	1.524756	-1.917437	O	-0.428390	4.207168	1.476706
O	2.971254	-1.525168	-1.916314	O	-0.739494	2.245297	3.070639
O	-1.248245	-5.722606	0.057248	O	1.010790	2.176396	5.326111
O	0.429180	-4.208357	1.477580	O	1.267216	5.998565	2.849051
O	-2.677471	-0.831138	-3.380969	O	5.625597	3.871154	0.051685
O	2.625304	-3.489101	0.057036	O	1.314430	6.079706	-2.725974
O	-3.323542	-4.730105	-1.295682	O	-2.847672	4.079011	2.728808
O	-1.600335	-3.194150	2.827308	O	-2.854230	4.131046	-2.632274
O	-2.674007	-0.808467	3.526439	O	1.002600	2.134381	-5.188429
O	-3.267656	-4.665506	1.372268	O	5.155744	-0.021295	-2.432991
O	0.733773	-2.274871	-2.931775	O	5.214359	0.035181	2.584542
O	0.739564	-2.245443	3.070809	Te	-0.000024	-0.000063	-0.071486
O	-3.005525	1.483620	2.051258	H	-1.472823	-2.312073	-0.576118
O	-3.853509	-2.097726	1.388796	H	-1.380494	-1.741451	1.043347
O	-1.600631	-3.269264	-2.767539	H	1.473060	2.311887	-0.576184
O	-0.000332	0.000413	-3.825875	H	1.380345	1.741468	1.043264
O	0.421381	-4.272365	-1.390251				

**Coordinates of  $\beta^*-\text{[TeO}_6\text{)W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2]^{\text{6}-}$**

O	0.784841	-1.255286	-1.200816	O	-2.558134	1.227601	-3.637720
O	-1.549659	0.038530	-1.294898	O	-0.079270	-3.749386	0.041937
O	0.841530	1.466238	-1.171596	O	-4.025308	-0.015611	-1.805945
O	-0.853641	1.405400	1.112455	O	-4.525711	-2.739493	-2.322155
O	1.554634	0.059516	1.352726	O	-3.194225	-0.042487	-6.093075
O	-0.778750	-1.298410	1.294824	O	1.615077	-2.778356	-6.081369
W	-3.202043	-1.737658	-1.880174	O	1.551491	2.736006	-6.070201
W	3.089463	1.939729	-1.855265	O	-4.514831	2.714878	-2.418861
W	3.065743	-1.794746	-1.857819	O	-0.153872	5.248610	-2.370824
W	0.080175	-3.514777	-1.840973	O	4.603453	2.609780	-2.327930
W	0.049823	3.615115	-1.865673	O	4.587461	-2.470220	-2.294590
W	-3.189410	1.740962	-1.915060	O	-0.083627	-5.176772	-2.253607
W	0.983254	-1.670178	-4.916368	O	0.063046	-0.043032	-3.588658
W	-1.934610	-0.054089	-4.924034	O	-0.761577	1.338989	5.666560
W	0.973491	1.652517	-4.857082	O	0.096197	2.787559	3.606939
W	-0.030247	-3.572138	1.918092	O	-3.412574	-0.037695	1.624117
W	-0.079337	3.581510	1.879388	O	1.714811	2.983950	1.635056
W	3.160647	1.778774	1.897312	O	-0.737532	-1.299150	5.657143
W	3.154976	-1.676841	1.887531	O	2.406293	1.544421	3.650631
W	-3.009414	1.807681	1.813060	O	1.750655	-2.937305	1.669308
W	-3.063783	-1.892698	1.877857	O	1.574850	0.039732	5.732375
W	0.971384	1.675725	4.897497	O	-1.985267	3.439150	1.954117
W	1.008341	-1.609995	4.903561	O	3.994562	0.058017	2.024437
W	-1.886713	0.015176	4.845456	O	2.433391	-1.464054	3.658551
O	0.134564	-0.011555	3.594792	O	-2.407663	-1.323980	3.581569
O	3.421456	1.905856	0.012601	O	-2.402240	1.301858	3.565089
O	-3.366536	1.968965	-0.051429	O	0.135720	-2.777043	3.637688
O	3.375289	-1.751265	0.018601	O	-1.956341	-3.450837	2.001878
O	1.557976	-0.013442	-5.681088	O	0.197805	-5.221128	2.347727
O	2.394588	-1.563171	-3.638874	O	1.642188	-2.742570	6.045697
O	-1.741930	2.965305	-1.833309	O	1.584030	2.830405	6.025136
O	3.424449	0.066892	-1.846385	O	-3.217460	0.008268	5.933898
O	-0.782383	1.288500	-5.617471	O	-4.584584	-2.529742	2.365413
O	0.202657	-2.841968	-3.622850	O	-4.526105	2.454204	2.316362
O	-1.718589	-2.926252	-1.831439	O	0.117705	5.220933	2.365152
O	-0.778307	-1.388531	-5.663703	O	4.465467	2.802307	2.361047
O	1.997753	3.521783	-1.843199	O	4.493058	-2.670014	2.318854
O	2.000470	-3.386323	-1.747503	Te	0.127064	0.143229	0.011820
O	-3.277699	-2.013656	0.000346	H	0.496939	-0.317432	-2.720515
O	-2.587950	-1.304886	-3.639687	H	-1.041426	0.052052	-2.165271
O	0.157524	2.842399	-3.627884	H	0.684444	0.132144	2.741182
O	-0.073481	3.929064	-0.007279	H	-0.606029	-0.826498	2.171505
O	2.414782	1.616936	-3.647520				

**Coordinates of  $\gamma^*-[({\rm TeO}_6){\rm W}_{18}{\rm O}_{54}({\rm OH})_2{\rm H}_2]^{6-}$**

O	0.774186	-1.255273	-1.220839	O	2.406087	1.603772	-3.649001
O	-1.555764	0.039256	-1.297352	O	-2.535942	1.242746	-3.627976
O	0.830295	1.463315	-1.188513	O	0.014012	-3.760287	0.021864
O	-0.843553	1.399526	1.117870	O	-4.038330	-0.012106	-1.848308
O	1.550776	0.056404	1.345041	O	-4.505563	-2.747368	-2.321304
O	-0.779588	-1.306246	1.278956	O	-3.198478	-0.035248	-6.067933
W	-3.198596	-1.726902	-1.870313	O	1.616536	-2.782187	-6.089037
W	3.080425	1.943776	-1.844545	O	1.571948	2.736238	-6.078210
W	3.051754	-1.797056	-1.858838	O	-4.502838	2.728709	-2.395608
W	0.077559	-3.515868	-1.876024	O	-0.181027	5.249902	-2.396219
W	0.046341	3.613436	-1.912310	O	4.602732	2.590323	-2.324683
W	-3.187493	1.735820	-1.901063	O	4.586490	-2.445701	-2.292333
W	0.983476	-1.666304	-4.932271	O	-0.118393	-5.175340	-2.284560
W	-1.924662	-0.044641	-4.913480	O	0.068863	-0.038357	-3.608122
W	0.987858	1.642911	-4.876966	O	0.812896	1.355762	5.706816
W	-0.035889	-3.612576	1.883582	O	2.582765	1.316309	3.687032
W	-0.093100	3.607736	1.828779	O	-3.386510	-0.049502	1.766364
W	3.161860	1.765023	1.917721	O	1.696394	2.955300	1.765653
W	3.159770	-1.669755	1.899526	O	-1.486314	-0.011926	5.625489
W	-3.004807	1.803028	1.841327	O	2.612917	-1.247194	3.685066
W	-3.052311	-1.918404	1.896012	O	1.729585	-2.920235	1.824784
W	1.965581	0.018165	4.960105	O	0.828265	-1.354463	5.701719
W	-0.896173	-1.678386	4.915869	O	-1.997098	3.463669	1.841070
W	-0.899357	1.669184	4.851271	O	4.031637	0.053537	1.869995
O	0.111456	0.016099	3.613419	O	-0.123696	-2.868297	3.651182
O	3.370698	1.965373	0.016490	O	-2.324124	1.513414	3.600824
O	-3.364299	1.897371	-0.038134	O	-0.124486	2.850003	3.612178
O	3.300067	-1.829452	0.018279	O	-2.316673	-1.562580	3.617854
O	1.564148	-0.013418	-5.708000	O	-1.964898	-3.497684	1.858347
O	2.385006	-1.549643	-3.649406	O	0.203278	-5.259621	2.313646
O	-1.736966	2.965145	-1.799483	O	-1.555071	-2.766526	6.073358
O	3.401372	0.065668	-1.808345	O	3.227941	0.022712	6.138800
O	-0.774679	1.292668	-5.629183	O	-1.571764	2.751709	6.015631
O	0.173115	-2.833210	-3.646320	O	-4.573005	-2.563294	2.373864
O	-1.711156	-2.916841	-1.781888	O	-4.531928	2.445049	2.317584
O	-0.775141	-1.376842	-5.678768	O	0.116433	5.242447	2.326732
O	1.992216	3.528591	-1.889120	O	4.461588	2.800002	2.369570
O	1.995695	-3.399846	-1.816812	O	4.493387	-2.677243	2.310654
O	-3.305135	-1.941482	0.008569	Te	0.129594	0.141812	0.003953
O	-2.552705	-1.306505	-3.626372	H	0.494656	-0.310016	-2.734799
O	0.140986	2.840606	-3.652653	H	-1.049212	0.051197	-2.166516
O	-0.006788	3.926855	-0.030339	H	0.617237	0.186761	2.745285
				H	-0.603405	-0.821513	2.143915

**Coordinates of  $\alpha$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ] $^{6-}$**

O	3.038344	1.928346	-0.131296	O	-1.266394	-0.828859	3.362145
O	0.508493	1.884061	0.773566	O	-0.694230	-3.331872	4.647503
O	1.556093	-0.518965	0.769204	O	-5.110273	-3.122620	3.220548
O	1.043942	0.783230	-1.483386	O	-3.727276	-5.539958	-1.611444
O	-3.038521	-1.928267	-0.131239	O	-6.580888	-0.766190	-1.588982
O	-1.556112	0.518853	0.769038	O	-3.191051	0.828546	4.584958
O	-1.044036	-0.783155	-1.483420	O	-4.605654	3.185278	-0.221642
O	-0.508563	-1.884109	0.773626	O	-3.368482	1.151010	-4.404522
W	-0.609788	-2.623069	3.081453	O	-0.432277	-3.532385	-4.376156
W	-2.458103	0.424001	-3.138333	O	0.784438	-5.697887	-0.166278
W	-0.672032	-2.428341	-3.073134	O	5.510201	1.838542	0.767897
W	0.261542	-4.080480	0.108171	O	4.481575	-0.461103	-0.121523
W	-3.385866	2.012082	0.081425	O	-0.014491	4.101315	2.025344
W	-2.501667	0.572479	3.031682	O	3.526002	-1.806848	1.977386
W	-3.305451	-3.980445	-0.994682	O	4.110143	4.090986	0.764943
W	-4.149124	-2.558025	1.913183	O	3.879334	0.615588	-2.384840
W	-5.019903	-1.165141	-0.967590	O	1.803918	1.142590	-3.981864
W	0.671774	2.428332	-3.073091	O	4.871381	2.996630	-1.566473
W	2.501802	-0.572445	3.031869	O	1.266470	0.828863	3.362477
W	3.386083	-2.012066	0.081718	O	2.725904	-1.612842	-1.654235
W	2.458016	-0.424010	-3.138065	O	-0.826503	1.330883	-3.441670
W	0.609895	2.623090	3.081418	O	2.289477	3.245021	-2.402762
W	-0.261640	4.080600	0.108472	O	2.390144	3.010898	2.500744
W	5.019793	1.165190	-0.967463	O	-1.122370	1.886395	3.175280
W	3.305548	3.980475	-0.994584	O	3.700848	0.792849	2.435629
W	4.149136	2.557986	1.913006	O	1.611886	4.343427	-0.147081
O	-4.871543	-2.996524	-1.566575	O	0.826476	-1.330900	-3.441196
O	-2.289622	-3.244952	-2.402732	O	-0.232303	3.316663	-1.661251
O	-3.526022	1.806909	1.977262	O	0.432168	3.532434	-4.376157
O	-1.804090	-1.142570	-3.981874	O	3.727044	5.540090	-1.611646
O	-5.510446	-1.838441	0.767946	O	6.581030	0.766997	-1.588357
O	-1.611911	-4.343262	-0.147077	O	5.111128	3.121207	3.220578
O	0.014454	-4.101073	2.025111	O	-0.784998	5.697477	-0.167202
O	-4.110334	-4.090915	0.764846	O	0.694444	3.332252	4.647290
O	-2.725985	1.612706	-1.654501	O	3.191803	-0.828966	4.584612
O	0.231932	-3.316341	-1.661060	O	4.606011	-3.185140	-0.221522
O	1.122385	-1.886382	3.175433	O	3.368195	-1.151821	-4.403973
O	-2.390088	-3.011400	2.500883	W	0.000021	-0.000108	-0.058656
O	-4.481802	0.461189	-0.121487	H	2.357976	1.379448	-0.666093
O	-1.946473	3.252883	0.324908	H	-2.358141	-1.379353	-0.666005
O	-3.879561	-0.615523	-2.384829	H	-1.490178	-1.976427	0.592173
O	-3.700404	-0.793011	2.435704	H	1.490100	1.976408	0.592076
O	1.946650	-3.253076	0.325259				

**Coordinates of  $\beta$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ] $^{6-}$**

O	3.044083	1.960245	0.075579	O	1.759199	-2.955784	-1.646822
O	0.733928	1.414438	1.224961	O	-0.417766	-2.328283	2.951931
O	1.654838	-0.720265	0.012271	O	0.331703	-5.088128	2.797284
O	0.736869	1.374792	-1.325269	O	-4.307085	-4.492903	2.809344
O	-3.089070	-1.863607	-0.082664	O	-4.323303	-4.499321	-2.786677
O	-1.324772	-0.091945	1.428527	O	-6.817338	-0.387752	0.005311
O	-1.367962	-0.012611	-1.228924	O	-1.813730	-1.364767	5.178245
O	-0.407715	-2.076192	0.065847	O	-4.318209	2.678697	2.450281
W	0.037923	-3.754030	1.750065	O	-4.330481	2.708562	-2.378113
W	-3.148760	1.590570	-1.819737	O	-1.808673	-1.372178	-5.157210
W	-1.588822	-0.914914	-3.514474	O	0.331591	-5.013893	-2.754172
W	0.020044	-3.708663	-1.676621	O	5.185445	2.325025	-1.309276
W	-3.150249	1.548943	1.888063	O	3.016778	2.018339	-2.789969
W	-1.557769	-0.918148	3.531627	O	0.656184	2.773610	3.495868
W	-3.689443	-3.349484	-1.663192	O	3.739876	-2.359688	0.011903
W	-3.665333	-3.357262	1.689757	O	5.260705	2.355347	1.349699
W	-5.180536	-0.934844	-0.006026	O	1.846583	3.986677	-1.530680
W	-0.006986	3.620352	-1.918589	O	0.646503	2.805225	-3.535572
W	3.166364	-1.700156	1.704379	O	4.056495	4.356678	0.000979
W	3.155218	-1.664317	-1.690643	O	2.186933	-0.556891	2.850121
W	1.551745	1.105435	-3.605223	O	2.197293	-0.552434	-2.893884
W	1.573459	1.117436	3.557278	O	-1.630796	2.704347	-2.152408
W	0.028772	3.522225	1.813978	O	1.880554	3.979497	1.534326
W	3.663120	3.430584	-1.641338	O	4.313497	-0.197303	1.334840
W	3.703416	3.444186	1.661605	O	-0.108179	0.242418	3.831820
W	5.087875	0.941686	0.043202	O	4.279075	-0.180038	-1.277459
O	-5.291512	-2.315270	-1.348602	O	3.069406	2.032741	2.810777
O	-3.014153	-1.988366	-2.793049	O	-0.132858	0.268636	-3.810295
O	-2.801734	0.568876	3.469458	O	-0.345446	3.720489	-0.042113
O	-2.778955	0.590407	-3.401576	O	-0.466050	5.184007	-2.472435
O	-5.243747	-2.309854	1.333799	O	4.346259	4.583593	2.790624
O	-1.858508	-3.935221	-1.515342	O	4.312305	4.544315	-2.780904
O	0.304854	-4.568332	0.020557	O	6.724201	0.395022	0.013896
O	-4.019246	-4.243431	0.007211	O	-0.463871	5.075642	2.383111
O	-2.984866	1.984947	0.019767	O	2.123383	1.060245	5.186884
O	-0.422871	-2.248234	-2.860547	O	4.221933	-2.516132	2.788228
O	1.773507	-3.003441	1.702208	O	4.215046	-2.497458	-2.757000
O	-1.850543	-3.959349	1.529764	O	2.107206	1.066016	-5.233474
O	-4.360360	0.202616	1.293018	W	-0.024867	0.014353	0.097663
O	-1.613566	2.633234	2.129777	H	2.204600	1.636052	0.583254
O	-4.368193	0.211475	-1.291882	H	-2.552218	-1.079278	-0.421237
O	-2.996468	-1.999370	2.792410	H	-1.404484	-2.142768	0.130495
				H	1.635907	1.583774	-0.941846

**Coordinates of  $\gamma$ -[ $(\text{WO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2$ ] $^{6-}$**

O	-0.096604	0.026330	3.622906	O	3.843238	0.118414	0.064296
O	-1.210202	0.861447	1.293256	O	-0.107799	-4.077675	-2.036550
O	-0.023964	-1.486701	1.042370	O	2.662245	-4.515338	-2.391998
O	1.347033	0.739629	1.427208	O	-0.035986	-3.162156	-6.125886
O	-0.053373	0.067771	-3.623716	O	2.835652	1.580487	-5.941864
O	-1.309770	0.689332	-1.298316	O	-2.714380	1.724271	-6.095745
O	1.319564	0.688886	-1.039434	O	-2.893965	-4.390794	-2.421813
O	-0.048051	-1.538756	-1.424033	O	-5.151472	-0.051311	-2.311453
W	1.615890	-3.231218	-1.924109	O	-2.282712	4.658141	-2.291768
W	-1.787022	3.063149	-1.878271	O	2.545787	4.525532	-2.216107
W	1.944987	2.975525	-1.777939	O	5.155825	-0.346078	-2.275643
W	3.529989	-0.028719	-1.815650	O	1.250470	-0.824014	5.650673
W	-3.495086	0.176022	-1.887569	O	2.793288	0.049959	3.674957
W	-1.794786	-3.146014	-1.968772	O	-2.886991	-1.554262	1.576737
W	1.664915	0.969593	-4.830812	O	2.857178	-1.722563	1.650727
W	-0.046859	-1.897366	-4.961491	O	-1.414423	-0.757521	5.694621
W	-1.628419	1.026634	-4.946618	O	1.601099	2.359917	3.727425
W	-1.739423	3.044429	1.875210	O	0.132289	3.356879	1.735890
W	1.611036	-3.134366	1.827882	O	0.006586	1.529978	5.739444
W	3.605887	0.018321	1.936203	O	-0.119359	-3.986867	1.899901
W	1.992098	3.024622	1.969362	O	3.583984	1.939484	2.044096
W	-1.784570	-3.073924	1.778342	O	-1.979108	3.206488	0.007544
W	-3.545950	0.217580	1.865647	O	-1.489502	2.416277	3.682407
W	1.655168	0.908968	4.965164	O	-1.414984	-2.446661	3.561701
W	-1.667701	1.001223	4.939073	O	-1.818217	-3.381097	-0.096743
W	-0.130364	-1.912192	4.834450	O	1.184904	-2.487748	3.569301
O	0.057875	1.592312	-5.697939	O	-2.825818	0.189309	3.639057
O	1.558869	2.359714	-3.561797	O	2.196682	3.146857	0.097478
O	-2.930322	-1.635300	-1.741995	O	-3.433881	2.108988	1.963306
O	0.090723	3.274095	-1.584269	O	-2.284137	4.626733	2.293358
O	-1.342701	-0.708047	-5.742737	O	-2.784018	1.657564	6.083465
O	2.767897	0.057322	-3.560682	O	2.784333	1.471958	6.132998
O	2.830736	-1.776336	-1.637148	O	-0.152061	-3.230850	5.947438
O	1.318945	-0.755613	-5.644674	O	-5.194351	-0.058277	2.275142
O	-3.424302	2.110020	-1.979548	O	-2.899673	-4.306890	2.216548
O	3.510776	1.900186	-1.891809	O	2.625261	-4.441577	2.294766
O	1.627805	-3.483186	-0.051333	O	5.222716	-0.334059	2.410691
O	1.228701	-2.522915	-3.665491	O	2.607412	4.568174	2.418614
O	-2.814617	0.231392	-3.692174	W	-0.053749	0.033110	0.000278
O	-3.754409	0.320840	-0.020988	H	-0.588678	0.155917	2.743218
O	-1.431842	2.429795	-3.649245	H	-0.393244	0.450245	-2.745637
O	-1.370262	-2.499400	-3.726031	H	0.031496	-1.054370	-2.294226
				H	0.947857	0.451221	2.296590

**Coordinates of  $\alpha^*-\text{[}(W\text{O}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{6-}$**

O	0.890903	-1.571313	0.291425	O	-3.866631	-2.086509	-1.283882
O	-1.351564	-0.844388	1.491381	O	0.000000	0.000000	3.991535
O	-1.200337	-0.766256	-1.276026	O	-3.830735	0.071147	0.081788
O	-0.890903	1.571313	0.291425	O	-5.216185	-0.047075	2.593889
O	1.200337	0.766256	-1.276026	O	-5.629384	-3.885274	0.012056
O	1.351564	0.844388	1.491381	O	-1.258647	-6.027773	2.828030
W	-3.634787	-0.311391	1.961166	O	-1.308463	-6.071765	-2.747958
W	1.913242	-3.129140	-1.710700	O	-5.164814	0.054626	-2.416647
W	1.874226	-2.972990	1.762297	O	-1.006168	-2.119837	-5.186465
W	-0.959950	-1.625341	3.716780	O	2.878780	-4.158449	-2.687612
W	-0.947862	-1.633247	-3.538898	O	2.845170	-4.066183	2.680069
W	-3.601995	-0.237771	-1.766508	O	-1.013052	-2.164525	5.351012
W	-1.373502	-4.733397	1.701786	O	-1.729084	-3.169401	-0.020249
W	-3.952273	-3.469422	0.013230	O	3.319092	4.733132	-1.313049
W	-1.417652	-4.780500	-1.609338	O	3.866631	2.086509	-1.283882
W	0.959950	1.625341	3.716780	O	-2.605962	3.452437	0.025615
W	0.947862	1.633247	-3.538898	O	2.666212	0.812009	-3.361738
W	3.601995	0.237771	-1.766508	O	1.245691	5.729990	0.044626
W	3.634787	0.311391	1.961166	O	3.892215	2.112769	1.377938
W	-1.913242	3.129140	-1.710700	O	2.725029	0.845760	3.592774
W	-1.874226	2.972990	1.762297	O	3.269946	4.677288	1.354113
W	3.952273	3.469422	0.013230	O	-0.738982	2.292952	-2.947772
W	1.373502	4.733397	1.701786	O	3.830735	-0.071147	0.081788
W	1.417652	4.780500	-1.609338	O	1.600324	3.236898	2.871493
O	1.729084	3.169401	-0.020249	O	-0.431022	4.273109	-1.398854
O	3.006118	-1.467659	2.071609	O	1.602114	3.253243	-2.748813
O	-2.932830	1.521947	-1.892656	O	-0.417440	4.202105	1.459523
O	2.932830	-1.521947	-1.892656	O	-0.729423	2.272020	3.099673
O	-1.245691	-5.729990	0.044626	O	1.013052	2.164525	5.351012
O	0.417440	-4.202105	1.459523	O	1.258647	6.027773	2.828030
O	-2.666212	-0.812009	-3.361738	O	5.629384	3.885274	0.012056
O	2.605962	-3.452437	0.025615	O	1.308463	6.071765	-2.747958
O	-3.319092	-4.733132	-1.313049	O	-2.845170	4.066183	2.680069
O	-1.600324	-3.236898	2.871493	O	-2.878780	4.158449	-2.687612
O	-2.725029	-0.845760	3.592774	O	1.006168	2.119837	-5.186465
O	-3.269946	-4.677288	1.354113	O	5.164814	-0.054626	-2.416647
O	0.738982	-2.292952	-2.947772	O	5.216185	0.047075	2.593889
O	0.729423	-2.272020	3.099673	W	0.000000	0.000000	-0.118767
O	-3.006118	1.467659	2.071609	H	-1.426287	-2.351680	-0.514237
O	-3.892215	-2.112769	1.377938	H	-1.460732	-1.770741	1.142042
O	-1.602114	-3.253243	-2.748813	H	1.426287	2.351680	-0.514237
O	0.000000	0.000000	-3.786552	H	1.460732	1.770741	1.142042
O	0.431022	-4.273109	-1.398854				

**Coordinates of  $\beta^*-\text{[}(W\text{O}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{6-}$**

O	0.654913	-1.263589	-1.132233	O	-2.596616	1.238461	-3.684083
O	-1.626829	0.027215	-1.353251	O	-0.083833	-3.775313	0.054734
O	0.823101	1.433983	-1.117029	O	-4.091606	-0.001894	-1.847743
O	-0.936943	1.246160	1.015948	O	-4.524757	-2.721386	-2.316511
O	1.532922	0.071555	1.250511	O	-3.184530	-0.056401	-6.130011
O	-0.790046	-1.387673	1.355167	O	1.629512	-2.772726	-6.079175
W	-3.211879	-1.699753	-1.871446	O	1.555864	2.747893	-6.064023
W	3.087100	1.945998	-1.866303	O	-4.501343	2.749892	-2.427358
W	3.085583	-1.804071	-1.868883	O	-0.153172	5.249849	-2.338934
W	0.067371	-3.487640	-1.828920	O	4.612961	2.593209	-2.320721
W	0.065201	3.611228	-1.868696	O	4.616778	-2.457830	-2.292966
W	-3.190954	1.744194	-1.933750	O	-0.091979	-5.147288	-2.259607
W	0.987730	-1.668180	-4.916050	O	0.063332	-0.042287	-3.604297
W	-1.948511	-0.059289	-4.935260	O	-0.753373	1.351903	5.672144
W	0.970638	1.650944	-4.868475	O	0.087805	2.779300	3.597436
W	-0.038823	-3.581538	1.928124	O	-3.438813	-0.056652	1.657527
W	-0.080973	3.602239	1.896516	O	1.704278	2.978519	1.641001
W	3.155413	1.778126	1.901281	O	-0.725071	-1.282444	5.667508
W	3.162232	-1.682558	1.891574	O	2.395263	1.528520	3.636515
W	-3.005332	1.777432	1.796785	O	1.749168	-2.933247	1.687179
W	-3.061926	-1.925316	1.889919	O	1.586268	0.055113	5.734650
W	0.971628	1.677837	4.911185	O	-1.966885	3.417601	1.928784
W	1.014375	-1.610742	4.909312	O	3.990222	0.059102	2.004403
W	-1.892628	0.018684	4.847443	O	2.431991	-1.437309	3.651926
O	0.122170	-0.006289	3.619985	O	-2.446552	-1.332425	3.618603
O	3.377071	1.899899	0.007535	O	-2.376465	1.301103	3.557864
O	-3.375853	1.953279	-0.064741	O	0.155529	-2.798303	3.670817
O	3.357093	-1.752296	0.018180	O	-1.982776	-3.510846	2.048871
O	1.577462	-0.003165	-5.675664	O	0.201093	-5.231301	2.366803
O	2.406794	-1.557328	-3.636289	O	1.671537	-2.719421	6.060131
O	-1.725756	2.946615	-1.848828	O	1.598680	2.851448	6.009227
O	3.391105	0.066388	-1.834435	O	-3.213813	0.043590	5.947831
O	-0.774967	1.293656	-5.617677	O	-4.587333	-2.566327	2.368259
O	0.213249	-2.829087	-3.624151	O	-4.508621	2.450662	2.311722
O	-1.723846	-2.906905	-1.838232	O	0.124133	5.242995	2.359110
O	-0.762239	-1.378006	-5.674340	O	4.458800	2.806795	2.346783
O	2.005248	3.527663	-1.826819	O	4.496921	-2.676380	2.320017
O	2.002847	-3.368410	-1.738962	W	0.185213	0.169592	0.003408
O	-3.287596	-2.007704	0.008632	H	0.445546	-0.317511	-2.721451
O	-2.607732	-1.305777	-3.665607	H	-1.138065	-0.007578	-2.219507
O	0.172026	2.843747	-3.617368	H	0.607197	0.152334	2.756656
O	-0.075732	3.860923	-0.002115	H	-0.649550	-0.927449	2.226816
O	2.410050	1.621082	-3.637772				

**Coordinates of  $\gamma^*-\text{[WO}_6\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]^{6-}}$**

O	0.676842	-1.264100	-1.154881	O	2.402163	1.604740	-3.642124
O	-1.613087	0.023497	-1.349815	O	-2.572397	1.254462	-3.674855
O	0.818971	1.439362	-1.130047	O	0.007460	-3.774263	0.033645
O	-0.918337	1.232606	1.028940	O	-4.089635	0.002440	-1.884340
O	1.548121	0.073983	1.223290	O	-4.512156	-2.726998	-2.311380
O	-0.779850	-1.403789	1.345031	O	-3.193189	-0.047273	-6.108564
W	-3.209352	-1.694140	-1.861558	O	1.630446	-2.775415	-6.088355
W	3.080503	1.946273	-1.865683	O	1.569349	2.748632	-6.071579
W	3.055412	-1.808115	-1.867738	O	-4.482866	2.767140	-2.399540
W	0.066245	-3.494779	-1.863272	O	-0.169063	5.252806	-2.361185
W	0.071858	3.613562	-1.904692	O	4.618282	2.562897	-2.324423
W	-3.181555	1.742429	-1.920637	O	4.600485	-2.433543	-2.287480
W	0.984878	-1.665083	-4.932873	O	-0.126846	-5.154019	-2.280455
W	-1.943968	-0.052539	-4.927085	O	0.066342	-0.040478	-3.620550
W	0.977979	1.643440	-4.886675	O	0.814551	1.377587	5.700770
W	-0.034723	-3.609348	1.896977	O	2.574830	1.319989	3.667663
W	-0.090254	3.635511	1.859097	O	-3.390924	-0.073485	1.800893
W	3.166693	1.770269	1.910176	O	1.690010	2.953907	1.778649
W	3.177321	-1.669220	1.900266	O	-1.488713	-0.002293	5.637747
W	-2.992587	1.769481	1.822351	O	2.613584	-1.232862	3.673214
W	-3.044942	-1.957396	1.905860	O	1.730301	-2.906103	1.846443
W	1.956172	0.026515	4.951352	O	0.819062	-1.335425	5.692997
W	-0.922747	-1.695437	4.937395	O	-1.971729	3.439150	1.811540
W	-0.912022	1.671707	4.866885	O	4.033547	0.059794	1.857466
O	0.100961	0.037365	3.632383	O	-0.140920	-2.892380	3.694660
O	3.331378	1.966338	0.007549	O	-2.307511	1.523179	3.594102
O	-3.368063	1.878296	-0.052130	O	-0.125259	2.860664	3.613554
O	3.284193	-1.828407	0.020637	O	-2.353475	-1.601330	3.666046
O	1.579769	-0.003579	-5.700549	O	-1.990196	-3.561155	1.896972
O	2.392213	-1.541856	-3.645579	O	0.227921	-5.256820	2.332093
O	-1.712574	2.946578	-1.809078	O	-1.558441	-2.762039	6.125843
O	3.359641	0.064519	-1.792961	O	3.223454	0.035348	6.124434
O	-0.770317	1.296334	-5.629479	O	-1.584024	2.764741	6.021672
O	0.188158	-2.829236	-3.649360	O	-4.577596	-2.597155	2.363131
O	-1.717095	-2.900890	-1.800711	O	-4.511605	2.433394	2.301354
O	-0.762224	-1.367966	-5.689836	O	0.117046	5.276669	2.319649
O	2.009479	3.537453	-1.879741	O	4.465482	2.808735	2.346421
O	1.999451	-3.395393	-1.808846	O	4.507975	-2.677048	2.308346
O	-3.304732	-1.939350	0.014020	W	0.195076	0.167768	-0.010229
O	-2.580479	-1.307172	-3.657511	H	0.452032	-0.312006	-2.737723
O	0.157677	2.842031	-3.638131	H	-1.133748	-0.015111	-2.220519
O	0.007139	3.863244	-0.019369	H	0.505357	0.265511	2.750947
				H	-0.624877	-0.920329	2.199053

**Coordinates of  $\alpha$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H<sub>2</sub>]<sup>7-</sup>**

O	3.014378	2.030659	-0.036569	O	0.248381	-3.336141	1.665162
O	1.257697	0.759410	1.615452	O	0.766585	-5.749587	0.166351
O	1.718344	-0.507192	-0.751359	O	-3.671291	-5.513327	1.622259
O	0.485942	1.935496	-0.665513	O	-5.197122	-3.193317	-3.176053
O	-3.139082	-1.811529	-0.098147	O	-6.601199	-0.827083	1.611105
O	-1.003564	-0.633985	1.538698	O	-0.476525	-3.544414	4.389977
O	-1.880854	0.338356	-0.865537	O	-3.351119	1.177688	4.383246
O	-0.505945	-1.960322	-0.787749	O	-4.676265	3.271909	0.149413
W	0.295159	-4.113703	-0.117711	O	-3.153403	0.898126	-4.565132
W	-3.485624	2.057133	-0.142890	O	-0.688598	-3.370996	-4.644829
W	-2.511823	0.557118	-2.990818	O	5.518468	1.848015	-0.767469
W	-0.634864	-2.640996	-3.080971	O	3.740252	0.823548	-2.502754
W	-2.456085	0.491226	3.075033	O	1.835195	1.126266	4.082821
W	-0.643125	-2.435481	3.077822	O	3.545482	-1.807992	-1.948871
W	-4.193208	-2.543931	-1.919395	O	4.817762	2.978414	1.536642
W	-3.283184	-3.970664	0.961702	O	2.417045	3.048609	-2.545915
W	-5.036620	-1.148186	0.942582	O	0.001436	4.095671	-1.989039
W	-0.259036	3.942600	-0.051172	O	4.164603	4.175651	-0.789719
W	3.416247	-2.036971	-0.028985	O	2.856751	-1.671597	1.747113
W	2.513953	-0.568677	-3.009643	O	1.267546	0.830203	-3.323011
W	0.601678	2.626164	-3.023841	O	-1.980622	3.187231	-0.341313
W	2.538154	-0.454978	3.232214	O	1.616413	4.384797	0.156658
W	0.745615	2.477131	3.205057	O	3.902603	0.615675	2.408083
W	4.153960	2.593386	-1.909918	O	0.936825	-1.412544	3.502595
W	3.293417	4.017039	0.933247	O	4.531177	-0.476223	0.145733
W	5.028574	1.161709	0.957844	O	2.303910	3.256656	2.406429
O	-5.594432	-1.845739	-0.778650	O	-1.128469	1.861395	-3.072755
O	-3.811637	-0.816148	-2.567174	O	-0.196361	3.307592	1.734174
O	-1.745776	-1.088053	3.927193	O	-0.828997	5.561804	0.193591
O	-3.647790	1.824286	-2.015809	O	3.744156	5.561564	1.581653
O	-4.815900	-2.969438	1.541045	O	5.158332	3.176058	-3.194163
O	-2.433062	-3.030916	-2.546241	O	6.591285	0.803456	1.587244
O	0.033224	-4.133822	-2.028194	O	0.554193	3.603742	4.499504
O	-4.114578	-4.099903	-0.762019	O	3.487709	-1.119888	4.510952
O	-2.807225	1.677467	1.634015	O	4.660419	-3.209899	0.206985
O	-1.309331	-0.854411	-3.387231	O	3.175740	-0.871795	-4.576247
O	1.998442	-3.321697	-0.277110	O	0.618552	3.313933	-4.606800
O	-1.597307	-4.329487	0.126525	Sb	-0.021960	0.043328	-0.023274
O	-3.877547	-0.585268	2.354852	H	2.029457	1.913330	-0.379856
O	-0.817407	1.453033	3.467689	H	-2.639746	-0.908156	-0.289526
O	-4.614361	0.524067	0.134230	H	-1.447358	-2.053904	-0.462969
O	-2.262805	-3.179193	2.348066	H	2.019441	1.143624	1.093476
O	1.087639	-1.873619	-3.169503				

**Coordinates of  $\beta$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H<sub>2</sub>]<sup>7-</sup>**

O	-0.039965	3.651720	-0.063031	O	2.889961	-1.580661	1.626220
O	0.043916	1.428550	1.578153	O	5.233517	-2.469405	0.194142
O	1.431836	1.153363	-0.792606	O	2.630080	-6.043252	1.647393
O	-1.314327	1.443281	-0.675447	O	-0.155735	-6.120599	-3.172312
O	-0.185901	-3.623066	-0.105975	O	-2.905068	-5.976800	1.632960
O	-0.000881	-1.197364	1.616090	O	2.679637	-2.286988	4.324749
O	-1.289266	-1.401436	-0.840837	O	-2.752701	-2.159010	4.322988
O	1.351054	-1.486532	-0.778782	O	-5.268338	-2.140616	0.169324
W	3.608958	-1.971976	-0.114659	O	-2.464526	-2.202350	-4.574753
W	-3.603722	-1.794453	-0.133489	O	2.460351	-2.451840	-4.641102
W	-1.830162	-1.814454	-3.011397	O	0.070702	5.726112	-1.595871
W	1.868318	-2.027771	-3.076879	O	1.519243	3.552574	-2.395112
W	-1.663324	-1.803794	3.024586	O	0.043108	2.069236	4.100755
W	1.631717	-1.810366	3.031611	O	3.520697	1.906884	-2.018932
W	-0.155665	-4.931442	-1.909347	O	1.386821	5.638487	0.720627
W	1.541392	-4.890602	0.970769	O	-1.473931	3.712533	-2.422221
W	-1.777084	-4.859740	0.941468	O	-3.469177	2.072307	-2.033437
W	-3.445131	1.949930	-0.081093	O	-1.277717	5.780718	0.746217
W	3.476918	1.768174	-0.093267	O	2.878729	1.567239	1.703040
W	1.865519	1.713075	-2.951999	O	-0.005350	1.553581	-3.253079
W	-1.862113	1.937108	-3.033470	O	-3.749311	0.080928	-0.306230
W	1.751683	1.924539	3.209446	O	-2.789178	3.756418	-0.158950
W	-1.668776	1.947491	3.208419	O	1.355004	3.658775	2.488323
W	-1.599566	4.997543	-0.987129	O	1.696549	0.053778	3.482333
W	0.040068	4.947226	1.885299	O	2.800334	3.551562	-0.112020
W	1.678171	4.807108	-1.014593	O	-1.260775	3.721104	2.522093
O	-1.507297	-5.716759	-0.775731	O	-2.132608	0.041423	-3.116965
O	-1.378161	-3.653224	-2.556809	O	-2.847807	1.744747	1.707501
O	-0.027564	-2.051811	3.982886	O	-5.099172	2.371473	0.208848
O	-3.491444	-2.060572	-2.009458	O	0.091971	6.112405	3.156324
O	-0.132167	-5.664250	1.533632	O	-2.693017	6.171396	-1.640897
O	1.231278	-3.727488	-2.538751	O	2.844935	5.914620	-1.653837
O	3.477866	-2.235980	-2.023283	O	-2.743328	2.426982	4.471668
O	1.193946	-5.690044	-0.752680	O	2.856900	2.387837	4.452238
O	-2.867719	-1.439487	1.599284	O	5.131902	2.181310	0.201248
O	0.016499	-1.602462	-3.395321	O	2.405764	2.135896	-4.541464
O	3.857810	-0.128068	-0.296053	O	-2.375079	2.333517	-4.633233
O	2.750358	-3.684434	0.119808	Sb	-0.034499	-0.010118	-0.024596
O	-1.569238	-3.579858	2.344288	H	-0.448733	2.751020	-0.403376
O	-1.669781	0.106377	3.436741	H	-0.683683	-2.716840	-0.310410
O	-2.940048	-3.588430	0.139878	H	0.922932	-2.336075	-0.457828
O	1.392964	-3.601526	2.330278	H	0.125741	2.272608	1.049021
O	2.156510	-0.154762	-3.158121				

**Coordinates of  $\gamma$ -[(SbO<sub>6</sub>)W<sub>18</sub>O<sub>54</sub>(OH)<sub>2</sub>H<sub>2</sub>]<sup>7-</sup>**

O	-0.126889	-0.011529	3.656226	O	-0.106660	-4.117759	-2.049841
O	-1.293543	0.792546	1.407018	O	2.610750	-4.417401	-2.309034
O	-0.198518	-1.661792	1.317989	O	-0.039510	-3.133590	-6.093514
O	1.350704	0.618969	1.313671	O	2.843607	1.582484	-6.013628
O	-0.079312	0.037035	-3.654039	O	-2.699247	1.724727	-6.134653
O	-1.356420	0.670808	-1.439135	O	-2.839972	-4.327211	-2.393566
O	1.324779	0.680973	-1.301969	O	-5.155846	-0.056893	-2.330088
O	-0.054224	-1.710777	-1.351028	O	-2.291324	4.662789	-2.276653
W	1.542364	-3.124629	-1.862309	O	2.582466	4.553057	-2.240504
W	-1.776309	3.059696	-1.902241	O	5.209709	-0.346000	-2.325900
W	1.964256	2.995337	-1.840449	O	1.252043	-0.826811	5.672164
W	3.583954	-0.004185	-1.864267	O	2.763241	0.020990	3.639630
W	-3.498915	0.187070	-1.882331	O	-2.980423	-1.613046	1.658765
W	-1.722065	-3.092350	-1.905925	O	2.840344	-1.790304	1.679266
W	1.675048	0.969291	-4.904530	O	-1.423041	-0.762329	5.738741
W	-0.050890	-1.875945	-4.903092	O	1.546502	2.308797	3.660376
W	-1.637824	1.018061	-4.961224	O	0.111874	3.282214	1.679373
W	-1.757460	2.962843	1.859743	O	-0.005772	1.534014	5.728801
W	1.590993	-3.239950	1.895173	O	-0.120091	-4.102735	1.991306
W	3.582747	-0.059040	1.904506	O	3.547920	1.875283	2.000868
W	1.965616	2.950345	1.914879	O	-1.967887	3.131700	-0.017832
W	-1.757929	-3.071237	1.816046	O	-1.507704	2.381952	3.679249
W	-3.621486	0.168460	1.893576	O	-1.438698	-2.522460	3.666545
W	1.619228	0.881644	4.931868	O	-1.852552	-3.423821	-0.046106
W	-1.690017	0.971706	4.950365	O	1.190592	-2.566108	3.652733
W	-0.141547	-1.943022	4.877428	O	-2.909107	0.182494	3.688114
O	0.067835	1.613481	-5.708236	O	2.171121	3.063542	0.035647
O	1.598945	2.369713	-3.609531	O	-3.484396	2.071698	1.965194
O	-2.905239	-1.604060	-1.705629	O	-2.296643	4.560161	2.257246
O	0.106838	3.309209	-1.646967	O	-2.772319	1.659589	6.115810
O	-1.335528	-0.689122	-5.773060	O	2.765311	1.485423	6.070101
O	2.794588	0.075850	-3.599226	O	-0.145764	-3.213257	6.053180
O	2.822730	-1.718075	-1.621238	O	-5.283588	-0.078491	2.289284
O	1.336170	-0.741949	-5.665811	O	-2.857014	-4.342643	2.264426
O	-3.440782	2.117398	-1.991598	O	2.633135	-4.535718	2.356149
O	3.558019	1.921811	-1.921497	O	5.205652	-0.390819	2.384895
O	1.618303	-3.492281	0.019554	O	2.584174	4.499779	2.345326
O	1.241528	-2.505546	-3.665310	Sb	-0.183954	-0.165505	-0.008875
O	-2.837281	0.237987	-3.722382	H	-0.610697	0.140294	2.752678
O	-3.787077	0.286364	-0.005729	H	-0.605918	0.133662	-2.764829
O	-1.455032	2.451983	-3.683150	H	0.925383	0.391252	-2.174220
O	-1.377951	-2.470532	-3.719044	H	0.931684	0.309980	2.166467
O	3.839437	0.094861	0.029865				

**Coordinates of  $\alpha^*-\text{[}( \text{SbO}_6 )\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{7-}$**

O	0.979605	-1.740164	0.145931	O	-3.913899	-2.096668	-1.271063
O	-1.289286	-0.831168	1.469524	O	0.000578	-0.000220	4.007910
O	-1.304495	-0.883422	-1.271645	O	-3.835804	0.068819	0.091521
O	-0.980220	1.739862	0.145497	O	-5.201261	-0.058095	2.602331
O	1.303989	0.883512	-1.271603	O	-5.628733	-3.893150	0.057598
O	1.289531	0.831552	1.469586	O	-1.276888	-6.015544	2.842002
W	-3.621877	-0.317766	1.959147	O	-1.339014	-6.102103	-2.714612
W	1.899220	-3.117172	-1.671755	O	-5.149979	0.032008	-2.415771
W	1.856774	-2.949842	1.697653	O	-1.003698	-2.117674	-5.182217
W	-0.943083	-1.632618	3.710488	O	2.860084	-4.131615	-2.684327
W	-0.949363	-1.628600	-3.526016	O	2.852413	-4.026927	2.628032
W	-3.577410	-0.237774	-1.754195	O	-0.984546	-2.190642	5.341359
W	-1.381281	-4.731465	1.696372	O	-1.736094	-3.153206	-0.046479
W	-3.946789	-3.471466	0.015920	O	3.334265	4.745838	-1.298508
W	-1.421993	-4.773517	-1.608069	O	3.911459	2.095991	-1.269849
W	0.943274	1.632752	3.710636	O	-2.658258	3.549457	0.013926
W	0.949927	1.629398	-3.526158	O	2.690172	0.835657	-3.380016
W	3.577096	0.237651	-1.754628	O	1.252650	5.732386	0.057722
W	3.621923	0.317795	1.959083	O	3.855513	2.116562	1.394241
W	-1.899526	3.117343	-1.671911	O	2.690275	0.837043	3.576574
W	-1.856708	2.949366	1.697050	O	3.276055	4.679640	1.373170
W	3.946747	3.470823	0.015747	O	-0.723372	2.281668	-2.917761
W	1.381264	4.731332	1.696751	O	3.835396	-0.068150	0.091856
W	1.422057	4.773536	-1.607814	O	1.604727	3.216295	2.853576
O	1.736192	3.153272	-0.045956	O	-0.428885	4.306404	-1.414805
O	2.992241	-1.451059	2.064923	O	1.606951	3.296210	-2.788000
O	-2.959938	1.528682	-1.909626	O	-0.416408	4.219525	1.476444
O	2.960340	-1.529028	-1.908186	O	-0.726580	2.241949	3.054898
O	-1.252928	-5.731735	0.058073	O	0.983201	2.190826	5.341546
O	0.417239	-4.220544	1.477320	O	1.275546	6.016352	2.841178
O	-2.690845	-0.836771	-3.379792	O	5.628864	3.892096	0.056425
O	2.657997	-3.549157	0.014230	O	1.338325	6.101477	-2.715264
O	-3.334238	-4.745973	-1.297398	O	-2.851341	4.027080	2.628025
O	-1.604157	-3.215135	2.852261	O	-2.860231	4.132216	-2.684073
O	-2.689677	-0.835488	3.576498	O	1.004793	2.118204	-5.182481
O	-3.276320	-4.678109	1.374846	O	5.149975	-0.032122	-2.414924
O	0.723090	-2.280874	-2.916692	O	5.201332	0.057504	2.601980
O	0.727214	-2.243028	3.056485	Sb	0.000004	-0.000015	-0.033484
O	-2.993036	1.451620	2.064211	H	-1.490324	-2.279864	-0.572533
O	-3.854388	-2.115587	1.393205	H	-1.404936	-1.743526	1.065964
O	-1.606837	-3.296833	-2.788649	H	1.490163	2.280169	-0.572274
O	-0.000911	0.000626	-3.799344	H	1.405092	1.743855	1.065896
O	0.429308	-4.307522	-1.415440				

**Coordinates of  $\beta^*-\text{[}(\text{SbO}_6)\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{7-}$**

O	0.770135	-1.259796	-1.298595	O	-2.560919	1.221458	-3.652168
O	-1.605907	0.023039	-1.318649	O	-0.081820	-3.730868	0.042360
O	0.830664	1.491066	-1.184224	O	-4.076491	-0.021487	-1.834406
O	-0.928266	1.430511	1.148786	O	-4.515492	-2.743338	-2.315902
O	1.527467	0.056921	1.438081	O	-3.180978	-0.054997	-6.104965
O	-0.790537	-1.327527	1.326902	O	1.605608	-2.777169	-6.124056
W	-3.195931	-1.723414	-1.880308	O	1.546091	2.719059	-6.084002
W	3.076311	1.949168	-1.847083	O	-4.530897	2.703037	-2.440063
W	3.057556	-1.793006	-1.872699	O	-0.172766	5.253415	-2.373696
W	0.085606	-3.504467	-1.850875	O	4.598421	2.622513	-2.310927
W	0.024666	3.615556	-1.858821	O	4.597000	-2.467533	-2.270251
W	-3.208924	1.719874	-1.924517	O	-0.086393	-5.178458	-2.239145
W	0.989636	-1.677153	-4.935429	O	0.072127	-0.074100	-3.613025
W	-1.921336	-0.064853	-4.928404	O	-0.761522	1.337423	5.681805
W	0.976447	1.645947	-4.851911	O	0.111743	2.813260	3.631408
W	-0.047699	-3.556751	1.917031	O	-3.401619	-0.036992	1.633038
W	-0.084658	3.610774	1.899071	O	1.708014	2.972484	1.642793
W	3.151437	1.775918	1.909404	O	-0.742850	-1.305961	5.671455
W	3.144780	-1.674082	1.888750	O	2.428707	1.564764	3.684990
W	-2.914611	1.792109	1.792518	O	1.745321	-2.943179	1.685113
W	-3.065792	-1.895137	1.884848	O	1.577035	0.032564	5.751813
W	0.972832	1.670782	4.903589	O	-1.973345	3.510829	1.998132
W	1.006691	-1.608081	4.908990	O	4.004712	0.056116	2.047628
W	-1.881898	0.012896	4.855032	O	2.448376	-1.493759	3.685094
O	0.154883	-0.002275	3.613378	O	-2.428143	-1.329569	3.599900
O	3.419635	1.883187	0.017897	O	-2.401915	1.301436	3.586394
O	-3.367155	1.954949	-0.075236	O	0.124278	-2.776389	3.647624
O	3.337038	-1.728327	0.017235	O	-1.984189	-3.472596	2.014350
O	1.562104	-0.022366	-5.697026	O	0.176060	-5.212117	2.345790
O	2.422653	-1.605231	-3.678059	O	1.621653	-2.745695	6.064303
O	-1.757399	2.970485	-1.849569	O	1.576476	2.810888	6.058650
O	3.418352	0.066788	-1.874984	O	-3.210460	0.009571	5.953670
O	-0.780277	1.279479	-5.629215	O	-4.600140	-2.523571	2.358738
O	0.212936	-2.871158	-3.650948	O	-4.428829	2.501244	2.273316
O	-1.716131	-2.921404	-1.841389	O	0.163388	5.250282	2.376905
O	-0.780247	-1.407491	-5.681293	O	4.463613	2.806846	2.357462
O	2.001999	3.543897	-1.862937	O	4.495628	-2.669745	2.296142
O	2.017641	-3.413389	-1.761510	Sb	0.106861	0.126654	0.011413
O	-3.273993	-2.003843	0.001660	H	0.445908	-0.393881	-2.706625
O	-2.597053	-1.313400	-3.652058	H	-1.074116	0.054043	-2.165624
O	0.156718	2.847535	-3.642777	H	0.713359	0.104441	2.714165
O	-0.079782	3.951384	0.002069	H	-0.601715	-0.846033	2.188416
O	2.428170	1.625839	-3.666276				

**Coordinates of  $\gamma^*-\text{[}( \text{SbO}_6 )\text{W}_{18}\text{O}_{54}(\text{OH})_2\text{H}_2\text{]}^{7-}$**

O	0.757494	-1.225608	-1.340710	O	2.397186	1.594384	-3.652079
O	-1.584566	0.035129	-1.325489	O	-2.539855	1.236604	-3.648473
O	0.864062	1.565653	-1.213870	O	0.018029	-3.711746	0.013013
O	-0.908662	1.435092	1.129084	O	-4.069908	-0.013943	-1.875533
O	1.529756	0.067771	1.403808	O	-4.501244	-2.749238	-2.315239
O	-0.784679	-1.332577	1.297739	O	-3.185406	-0.051728	-6.085592
W	-3.196809	-1.714393	-1.870554	O	1.609728	-2.784238	-6.138179
W	2.983476	1.950242	-1.809512	O	1.571982	2.724704	-6.073398
W	3.047377	-1.788804	-1.878998	O	-4.485743	2.754059	-2.422741
W	0.083637	-3.495632	-1.892787	O	-0.181871	5.176680	-2.359666
W	0.080792	3.529775	-1.888294	O	4.530602	2.573204	-2.281036
W	-3.192618	1.729172	-1.911667	O	4.607340	-2.413005	-2.282182
W	0.988812	-1.677545	-4.959168	O	-0.121259	-5.168390	-2.264737
W	-1.914648	-0.059995	-4.919569	O	0.068270	-0.078352	-3.628749
W	0.987667	1.625373	-4.870908	O	0.822485	1.346661	5.726805
W	-0.050726	-3.585316	1.872405	O	2.620212	1.316464	3.733281
W	-0.105455	3.647960	1.844068	O	-3.367835	-0.048687	1.766568
W	3.145831	1.777601	1.944071	O	1.695491	2.971311	1.818403
W	3.151076	-1.654468	1.892838	O	-1.484694	-0.013973	5.631987
W	-2.924376	1.794152	1.817467	O	2.636526	-1.255153	3.708435
W	-3.047569	-1.916334	1.901246	O	1.722683	-2.911723	1.849805
W	1.973381	0.002775	4.972962	O	0.827960	-1.371649	5.716638
W	-0.894713	-1.675505	4.922813	O	-1.997256	3.532578	1.873733
W	-0.880209	1.670519	4.852946	O	4.037075	0.061367	1.879453
O	0.140679	0.013498	3.632092	O	-0.141473	-2.878128	3.660676
O	3.328857	1.958382	0.040810	O	-2.302687	1.511359	3.608392
O	-3.387558	1.887227	-0.056651	O	-0.120352	2.878677	3.640482
O	3.263296	-1.825837	0.013882	O	-2.330628	-1.569151	3.631209
O	1.570495	-0.023637	-5.726134	O	-1.988408	-3.515747	1.860308
O	2.412199	-1.589105	-3.694627	O	0.188557	-5.243731	2.280998
O	-1.715669	2.908528	-1.773384	O	-1.557505	-2.761332	6.086753
O	3.344101	0.063552	-1.805144	O	3.217056	-0.005842	6.178841
O	-0.772084	1.280081	-5.642706	O	-1.558792	2.736854	6.035707
O	0.184344	-2.865813	-3.684825	O	-4.583796	-2.548748	2.364964
O	-1.708357	-2.907892	-1.802636	O	-4.454743	2.465439	2.289737
O	-0.774301	-1.395606	-5.704769	O	0.131430	5.282807	2.346805
O	2.023704	3.604364	-1.931593	O	4.459880	2.814869	2.372045
O	2.008176	-3.414168	-1.832745	O	4.494006	-2.665756	2.287828
O	-3.298676	-1.935163	0.004409	Sb	0.112826	0.146204	-0.009809
O	-2.564967	-1.318046	-3.644371	H	0.437181	-0.425089	-2.721921
O	0.129038	2.815944	-3.659787	H	-1.073802	0.046630	-2.186082
O	0.019074	3.930120	-0.002211	H	0.647186	0.147178	2.729561
				H	-0.592576	-0.837457	2.146092

