Supporting information for the paper:

Closed-Cage Tungsten Oxide Clusters in the Gas Phase

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Table S1. The Cartesian coordinates of the atoms of $W_6O_{19}^{2-}$ cluster at B3LYP/LANL2DZ level of theory.

Atomic Number	B3LYP/LANL2DZ		
	X	Y	Z
74	-0.018158	-0.032988	-0.045521
74	-0.026654	-0.027128	3.318159
74	2.892322	-0.034025	1.643048
8	0.95025	1.342556	1.635937
8	-0.583065	-0.821666	1.636491
8	1.716357	-0.826068	0.317841
8	1.709467	-0.820463	2.967323
8	0.957566	1.337002	-1.014355
8	-0.724988	-1.034951	-1.272225
8	-1.341162	1.34293	0.3051
8	-1.34852	1.348093	2.954911
8	-0.738255	-1.025836	4.54489
8	4.307041	-1.037654	1.649845
74	1.918656	2.718096	3.317392
74	1.927156	2.712237	-0.046287
74	-0.991823	2.719133	1.628822
8	2.483568	3.506776	1.63538
8	0.184145	3.511176	2.954031
8	0.191033	3.505569	0.30455
8	0.942935	1.348105	4.28623
8	2.625488	3.720059	4.544096
8	3.241659	1.342178	2.966771
8	3.249022	1.337016	0.31696
8	2.638732	3.71093	-1.273043
8	-2.406533	3.722775	1.62204

Table S2. The Cartesian coordinates of the atoms of $W_{13}O_{29}^-$ cluster at B3LYP/LANL2DZ level of theory.

Atomic Number	B3LYP/LANL2DZ		
	X	Y	Z
74	0	0	4.102475
74	0	-1.64556	-3.22108
74	0	1.64556	-3.22108
74	-1.37128	-3.66529	-0.8573
74	-1.37128	3.66529	-0.8573
74	1.37128	-3.66529	-0.8573
74	1.37128	3.66529	-0.8573
74	-2.11314	0	-1.25053
74	2.11314	0	-1.25053
74	-2.08058	0	2.177555
74	2.08058	0	2.177555
74	0	-2.9941	2.037585
74	0	2.9941	2.037585
8	1.74787	1.15999	-2.81753
8	-1.74787	1.15999	-2.81753
8	1.74787	-1.15999	-2.81753
8	-1.74787	-1.15999	-2.81753
8	1.27233	-3.53764	-2.63313
8	-1.27233	3.53764	-2.63313
8	-1.27233	-3.53764	-2.63313
8	1.27233	3.53764	-2.63313
8	1.8937	-1.93168	-0.5997
8	-1.8937	-1.93168	-0.5997
8	1.8937	1.93168	-0.5997
8	-1.8937	1.93168	-0.5997
8	0	5.00742	-0.78632
8	0	-5.00742	-0.78632
8	-3.07278	0	0.331475
8	3.07278	0	0.331475
8	1.32272	3.99369	1.252455
8	-1.32272	3.99369	1.252455
8	-1.32272	-3.99369	1.252455
8	1.32272	-3.99369	1.252455
8	0	1.87202	3.781475
8	0	-1.87202	3.781475
8	2.03465	0	4.011095
8	-2.03465	0	4.011095
8	1.45364	-1.64133	1.805325
8	-1.45364	-1.64133	1.805325
8	-1.45364	1.64133	1.805325

8	1.45364	1.64133	1.805325
8	0	0	-4.1887

Table. S3. The Cartesian coordinates of the atoms of $W_{14}O_{32}^{-}$ cluster at B3LYP/LANL2DZ level of theory.

Atomic Number	B3LYP/LANL2DZ		
	X	Y	Z
74	4.133302	0	0
74	-0.05901	-3.01179	-1.62102
74	-0.05901	3.01179	-1.62102
74	-0.05901	-3.01179	1.621028
74	-0.05901	3.01179	1.621028
74	-1.25973	0	-1.91511
74	-1.25973	0	1.915117
74	1.833303	0	-2.15
74	1.833301	0	2.149998
74	2.020681	-2.14182	0
74	2.020683	2.141819	0
74	-2.11425	-2.06732	0
74	-2.11425	2.067321	0
74	-4.3667	0.000001	0
8	-3.79183	-1.60207	0
8	-3.79183	1.602071	0
8	-3.30669	0.000001	-1.64207
8	-3.30669	0.000001	1.642076
8	-2.52175	1.510061	-1.79961
8	-2.52175	1.510061	1.799617
8	-2.52175	-1.51006	1.799617
8	-2.52175	-1.51006	-1.79961
8	-0.8667	1.69574	-2.71375
8	-0.8667	1.69574	2.713757
8	-0.8667	-1.69574	-2.71375
8	-0.8667	-1.69574	2.713757
8	-0.15474	-4.03771	0
8	-0.15474	4.03771	0
8	0.433301	0	3.099998
8	0.433303	0	-3.1
8	1.767183	3.443789	1.253438
8	1.76718	-3.44378	1.253438
8	1.767181	-3.44378	-1.25343

8	1.767184	3.443789	-1.25343
8	2.267421	-1.74091	1.740918
8	2.267422	-1.74091	-1.74091
8	2.267423	1.740909	-1.74091
8	2.267422	1.740909	1.740918
8	3.601073	1.767769	0
8	3.601071	-1.76777	0
8	3.601071	0	1.767769
8	3.601073	0	-1.76776
8	-1.97174	-3.27641	1.192517
8	-1.97174	-3.27641	-1.19251
8	-1.97174	3.276411	1.192517
8	-1.97174	3.276411	-1.19251