Electronic Supplementary Information

Reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster size and charge state

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Figure S1 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 4. The relative energies (eV) take WO_3^+ + CO as the reference.

Figure S2 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 5. The relative energies (eV) take $W_2O_6^+$ + CO as the reference.

Figure S3 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 6. The relative energies (eV) take $W_3O_9^+$ + CO as the reference.

Figure S4 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 7. The relative energies (eV) take $W_4O_{12}^+$ + CO as the reference.

Figure S5 B3LYP optimized structures for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 8. The relative energies (eV) take WO_3 + CO as the reference.

Figure S6 B3LYP optimized structures for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 9. The relative energies (eV) take WO_3^- + CO as the reference.

Figure S7 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 4.

Figure S8 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 5.

Figure S9 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 6.

Figure S10 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 7.

TABLE S1 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 4 at B3LYP level.

TABLE S2 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 5 at B3LYP level.

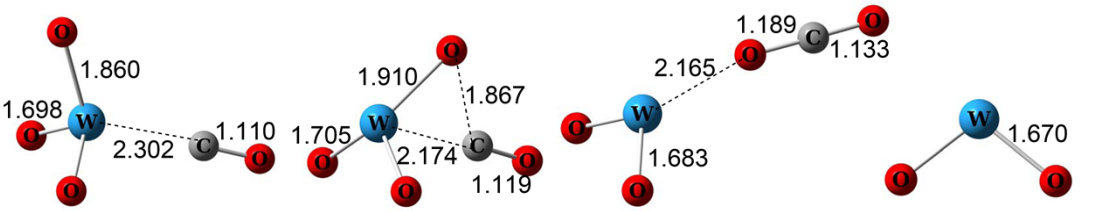
TABLE S3 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 6 at B3LYP level.

TABLE S4 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 7 at B3LYP level.

TABLE S5 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 8 at B3LYP level.

TABLE S6 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 9 at B3LYP level.

Figure S1 B3LYP optimized structures intermediates, transition states and the product shown in the energy profile of Figure 4. The relative energies (eV) take WO_3^+ + CO as the reference.



(a) $[WO_3–CO]^+$ IM1 (C_s ^{2}A") -1.84 eV (b) $[WO_3–CO]^+$ TS (C_s ^{2}A') -0.47 eV (c) $[WO_2^+–CO_2]$ IM2 (C_s ^{2}A') -3.32 eV (d) WO_2^+ (C_{2v} $^2A_1$)

Figure S2 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 5. The relative energies (eV) take $W_2O_6^+$ + CO as the reference.

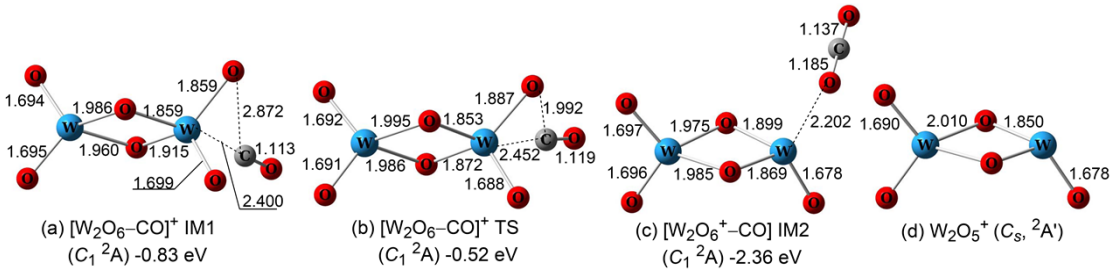


Figure S3 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 6. The relative energies (eV) take $W_3O_9^+$ + CO as the reference.

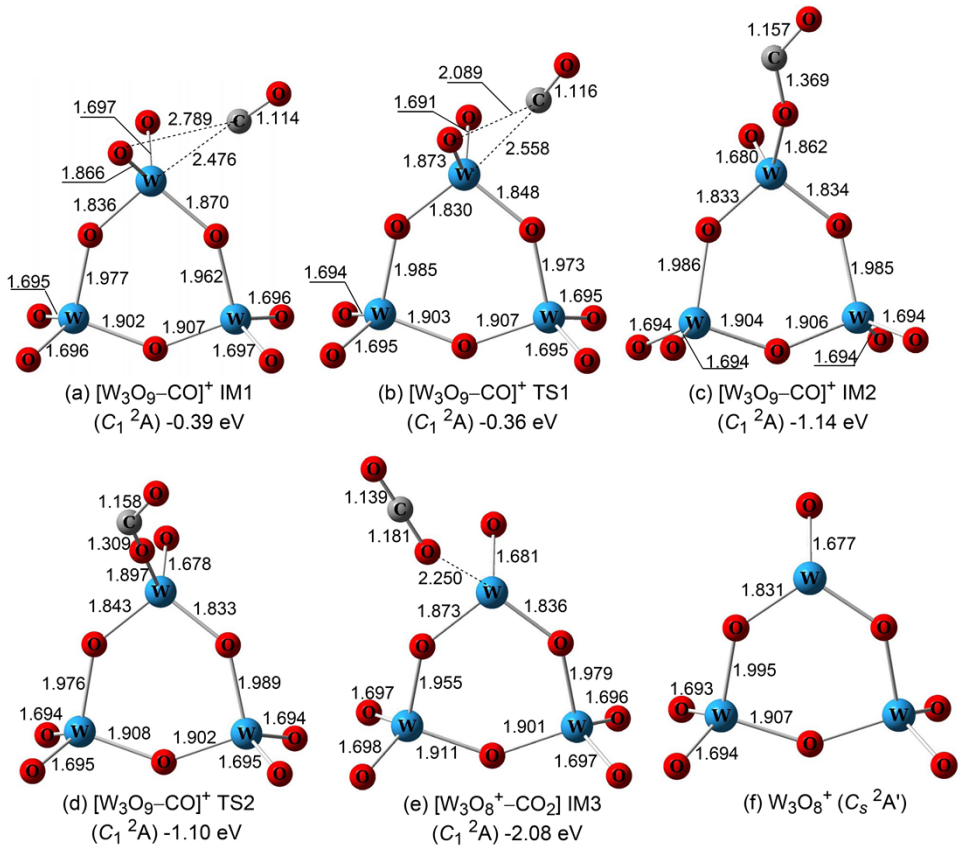
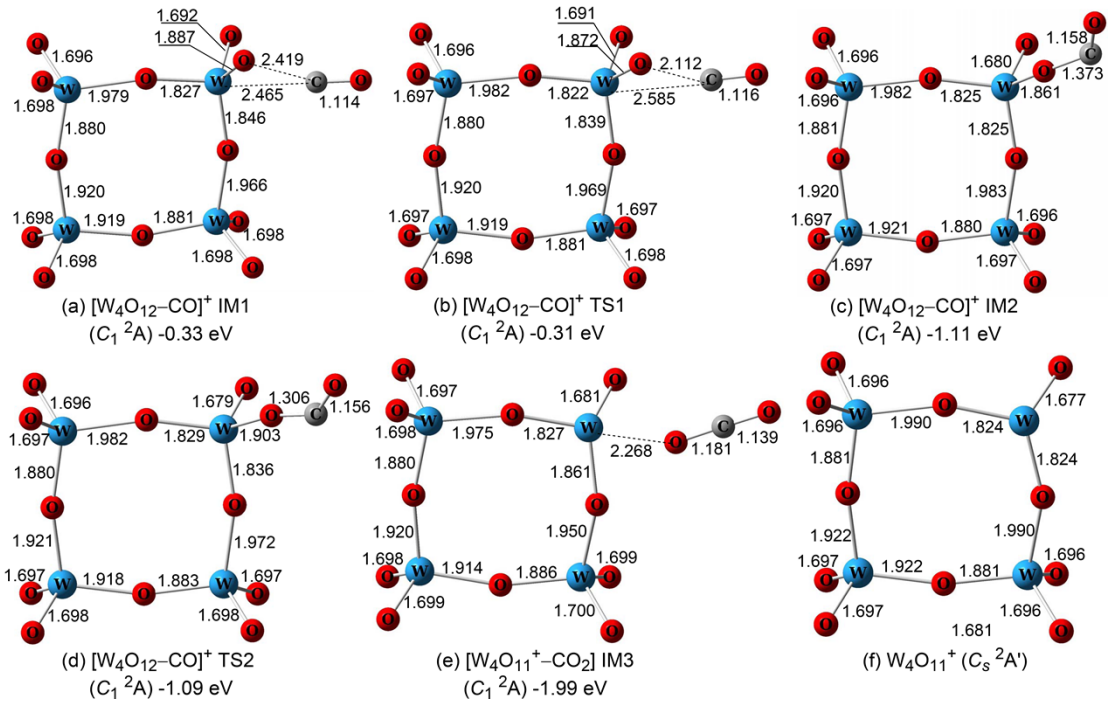


Figure S4 B3LYP optimized structures for the intermediates, transition states and the product shown in the energy profile of Figure 7. The relative energies (eV) take $W_4O_{12}^+ + CO$ as the reference.



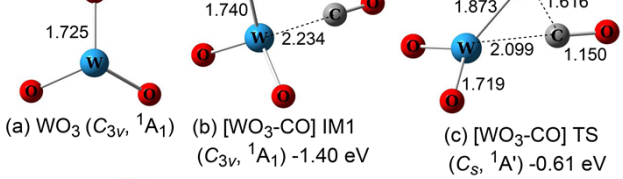


Figure S5 B3LY[illegible] iediates, transition states and the proc[illegible] e relative energies (eV) take WO_3 + C[illegible]

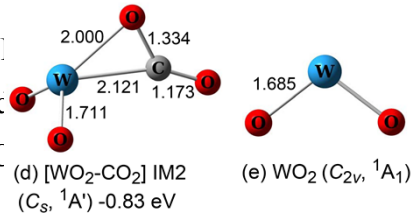
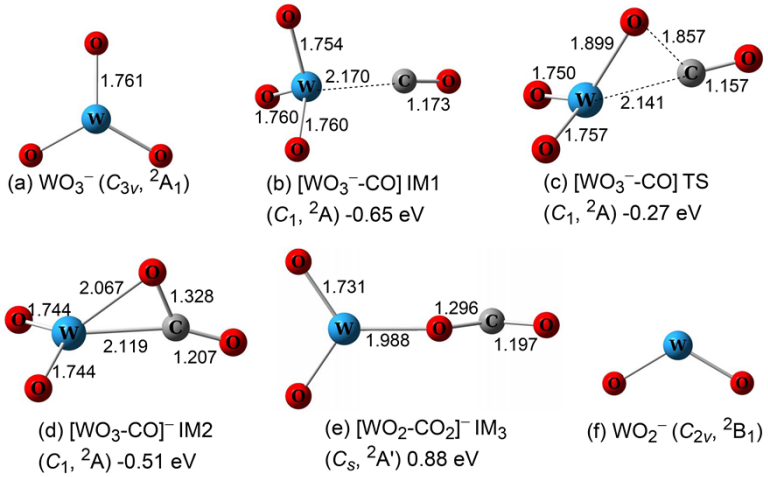
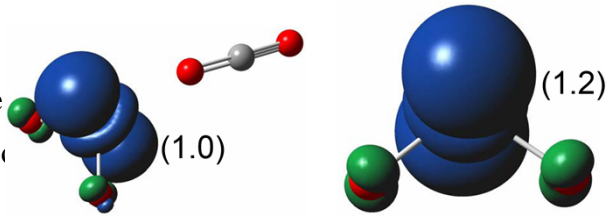


Figure S6 B3LYP optimized structures for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 9. The relative energies (eV) take WO_3^- + CO as the reference.



(a) WO_3^+ (C_s, $^2A''$) (b) IM1 (c) TS



(d) IM2 (e) WO_2^+ (C_{2v}, $^2A_1$)

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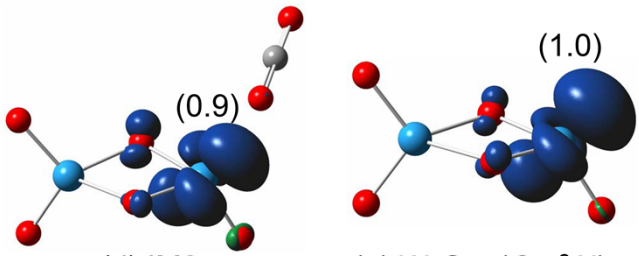
(a) $W_2O_6^+$ (C_s, $^2A'$) (b) IM1 (c) TS



(d) IM2 (e) $W_2O_5^+$ (C_s, $^2A'$)

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Figure S9 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 6.

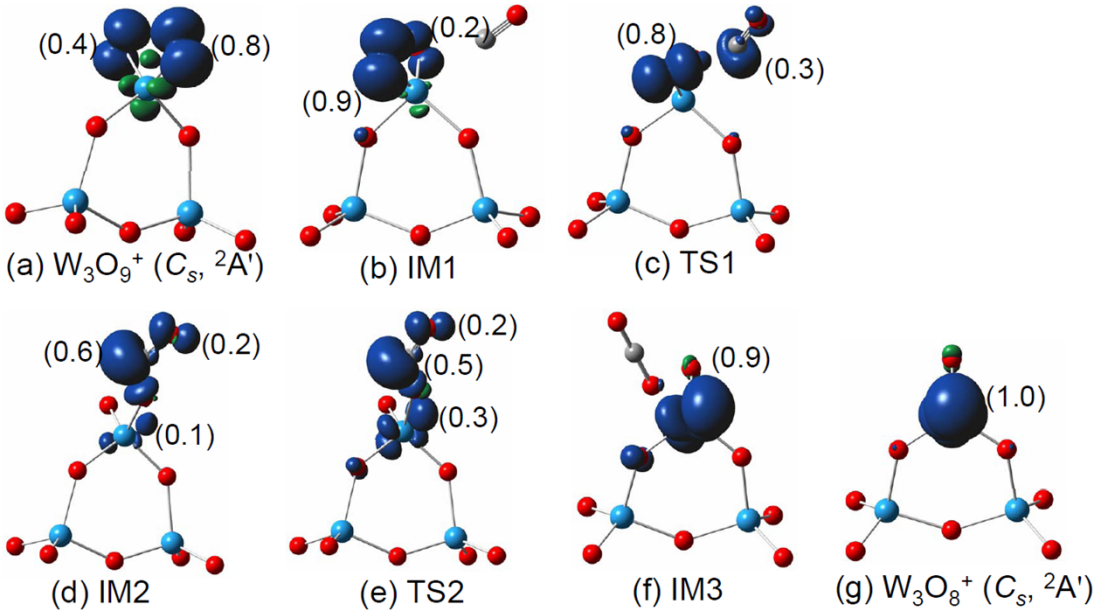

Figure S10 Numerical electron spin density (in |e|) for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 7.

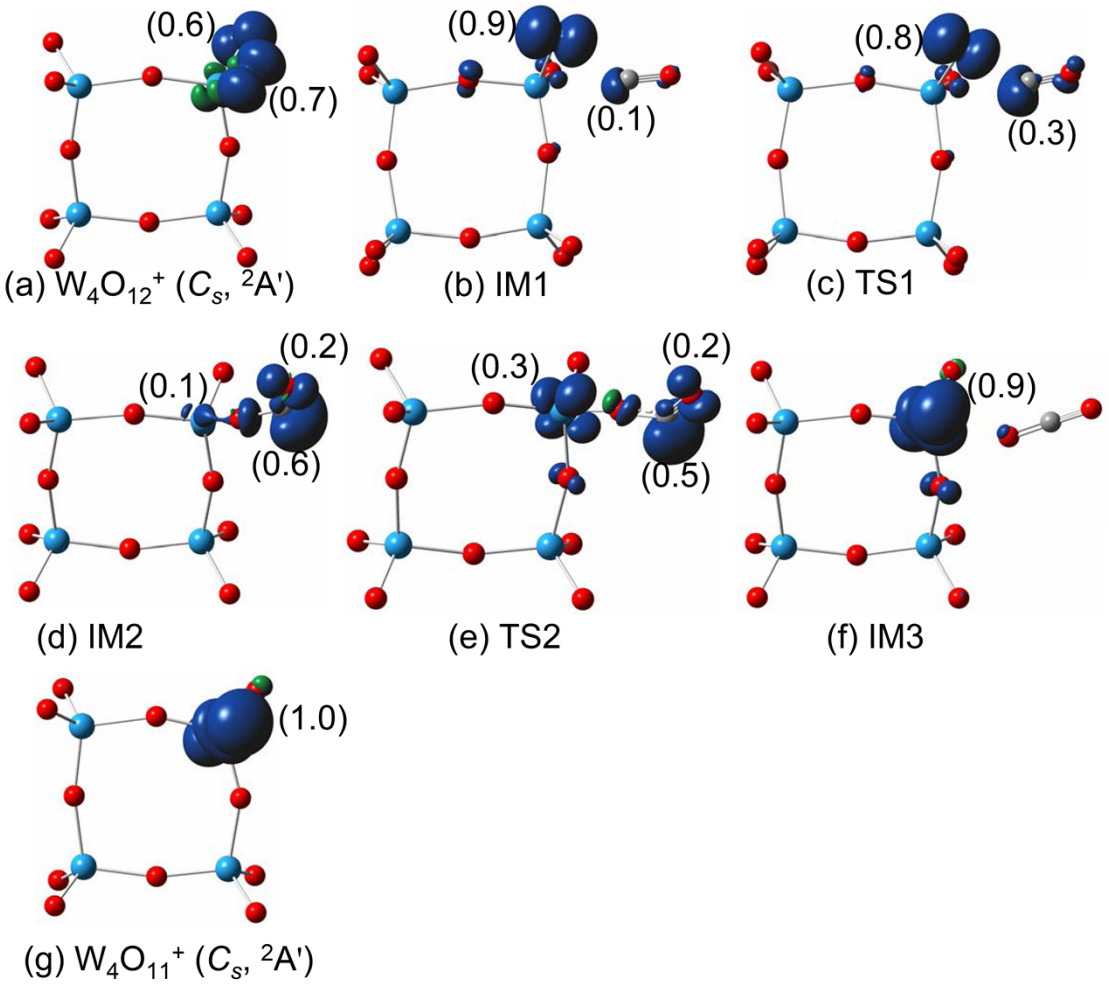

TABLE S1 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 4 at B3LYP level.

	x	y	z
[a] WO_3^+ (C_s ^{2}A")			
74	-0.1808770	0.0215270	0.0000000
8	0.5577040	0.7261190	1.3503030
8	0.5577040	0.7261190	-1.3503030
8	0.5577040	-1.6513590	0.0000000
[b] IM1			
74	-0.2282650	0.0712200	0.0000000
8	-0.8290060	-0.7125120	1.3808230
8	-0.8290060	-0.7125120	-1.3808230
8	-0.8290060	1.8319360	0.0000000
6	2.0133880	-0.4507200	0.0000000
8	3.0884310	-0.7276560	0.0000000
[c] TS			
74	-0.4308960	0.0321800	0.0000000
8	-0.4308960	-0.9552040	1.3894510
8	-0.4308960	-0.9552040	-1.3894510
8	0.6804950	1.5857670	0.0000000
6	1.7426520	0.0503480	0.0000000
8	2.8601010	-0.0107840	0.0000000
[d] IM2			
74	-0.1149330	0.5234010	0.0000000
8	0.3799240	1.3971420	1.3501820
8	0.3799240	1.3971420	-1.3501820
8	-0.1667380	-1.6410510	0.0000000
6	0.1201240	-2.7953340	0.0000000
8	0.3799240	-3.8981920	0.0000000
[e] WO_2^+ (C_{2v} $^2A_1$)			
74	0.0000000	0.0000000	0.1844200
8	0.0000000	1.3089790	-0.8529450
8	0.0000000	-1.3089790	-0.8529450

TABLE S2 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 5 at B3LYP level.

	x	y	z
[a] $W_2O_6^+$ (C_s $^2A'$)			
74	0.0030000	1.4430910	0.0000000
8	0.0030000	0.0882020	1.2606910
8	0.0030000	0.0882020	-1.2606910
74	-0.0039030	-1.4736430	0.0000000
8	-1.4095670	2.3936120	0.0000000
8	1.4182240	2.6125980	0.0000000
8	1.3750660	-2.4495210	0.0000000
8	-1.3813620	-2.4504900	0.0000000
[b] IM1			
74	-1.2299770	-0.3631620	0.0115070
8	-0.0144400	1.1147660	0.0791410
8	0.3468480	-1.3409590	-0.0984150
74	1.6778120	0.1308480	-0.0104000
8	-2.0075890	-0.8304330	1.4478440
8	-2.2836960	-0.9664180	-1.3963530
8	2.6103550	0.4217230	-1.3955830
8	2.6559300	0.2216410	1.3698660
6	-2.7274440	1.5116000	-0.0135190
8	-3.4043000	2.3948830	-0.0066040
[c] TS			
74	1.1736280	-0.3608760	0.1224440
8	0.0144730	0.7172110	-0.8762570
8	-0.3695330	-0.9418150	0.9669890
74	-1.6966050	0.1565400	-0.0385950
8	1.8200750	-1.5955960	-0.8295480
8	2.4703690	0.4305850	1.2421380
8	-2.5120420	1.3582480	0.8303500
8	-2.7920210	-0.6640940	-1.0319770
6	3.0552840	1.0979080	-0.4627490
8	3.9147630	1.7621370	-0.7302360
[d] IM2			
74	1.6509470	0.2967520	0.0307640
8	0.5902600	-1.0781850	-0.9299730
8	-0.1611140	0.7983230	0.6337280
74	-1.0618930	-0.6758410	-0.1554620

8	2.7118140	-0.2630130	1.2292340
8	2.4158390	1.4868850	-0.9068610
8	-2.7998670	0.6688200	-0.2915060
8	-1.5752130	-1.8051450	0.9745740
6	-3.4290270	1.6045610	0.0712970
8	-4.0586960	2.4954680	0.3907860

[e] $W_2O_5^+$ (C_s ^{1}A')

74	0.1507240	-1.5324040	0.0000000
8	0.1507240	-0.1947310	1.2772960
8	0.1507240	-0.1947310	-1.2772960
74	-0.0255900	1.3467610	0.0000000
8	-1.1982670	-2.5296500	0.0000000
8	-1.5012040	2.1695690	0.0000000
8	1.2405380	2.4667430	0.0000000

TABLE S3 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 6 at B3LYP level.

	x	y	z
[a] $W_3O_9^+$ (C_s $^2A'$)			
74	-0.0023370	1.0388190	1.7972640
8	-0.0206470	-0.9231350	1.4525680
74	0.0031060	-2.0404300	0.0000000
8	-0.0206470	-0.9231350	-1.4525680
74	-0.0023370	1.0388190	-1.7972640
8	-0.0039010	1.6720560	0.0000000
8	-1.3659130	1.5454740	2.6642560
8	1.3744630	1.5275390	2.6530510
8	-1.3385540	-3.2423110	0.0000000
8	1.3811430	-3.0736800	0.0000000
8	-1.3659130	1.5454740	-2.6642560
8	1.3744630	1.5275390	-2.6530510
[b] IM1			
74	-1.9695240	-1.0718800	-0.0188650
8	-0.0669460	-1.6087670	-0.0259670
74	1.6590100	-0.9870510	0.0438370
8	1.2163860	0.8289710	-0.0192030
74	-0.3106340	2.0615820	-0.0029400
8	-1.7569250	0.8181270	-0.0141370
8	-2.7872300	-1.6341630	-1.3945720
8	-2.7903400	-1.6364620	1.3522820
8	2.4353270	-1.9850720	-1.3288650
8	2.2921830	-1.5314370	1.5208960
8	-0.3002550	3.0672910	-1.3695420
8	-0.3042150	3.0451340	1.3791850
6	3.8873110	0.0767790	-0.1378860
8	4.8921490	0.5542690	-0.2004530
[c] TS1			
74	-1.8840650	-1.2234060	-0.0722370
8	0.0520500	-1.6561570	-0.0065740
74	1.6715800	-0.8164750	0.1393600
8	1.1826520	0.9615460	0.0237690
74	-0.4620790	2.0512830	0.0004770
8	-1.7805560	0.6766450	-0.0916450
8	-2.6278130	-1.8498920	-1.4602510
8	-2.7211330	-1.8087720	1.2791270

8	2.7791960	-1.4761850	-1.2186850
8	2.2985690	-1.1387730	1.6758670
8	-0.5055020	3.0860370	-1.3415450
8	-0.6182690	2.9985360	1.3974920
6	4.0650860	-0.0684270	-0.3650900
8	5.1317040	0.1528700	-0.6090340

[d] IM2

74	-1.2542980	1.7934860	0.1080340
8	0.6798080	1.4302760	-0.1630290
74	1.7883370	-0.0090620	-0.4085000
8	0.6670140	-1.4393080	-0.1646400
74	-1.2679510	-1.7886380	0.1082740
8	-1.9028220	0.0056000	0.2079030
8	-1.5362810	2.6664610	1.5325680
8	-1.9370220	2.6578390	-1.1785620
8	3.2410020	0.0148940	0.7568470
8	2.3463120	-0.0165220	-1.9931060
8	-1.5577470	-2.6579010	1.5332920
8	-1.9587120	-2.6474980	-1.1776720
6	4.5027150	0.3798750	1.1440020
8	5.3701040	-0.2597720	1.5661750

[e] TS2

74	-1.2325090	1.7955390	0.1241280
8	0.6859780	1.4245600	-0.1695970
74	1.7859980	-0.0218050	-0.4780600
8	0.6715620	-1.4486370	-0.1909980
74	-1.2644560	-1.7839360	0.1206800
8	-1.8923590	0.0085060	0.2267410
8	-1.4837270	2.6639170	1.5584150
8	-1.9261380	2.6721550	-1.1491990
8	3.2941400	0.1761240	0.6554920
8	2.2774190	0.0099540	-2.0825410
8	-1.5236790	-2.6497930	1.5542760
8	-1.9803350	-2.6467490	-1.1491640
6	4.3350750	0.3127700	1.4381230
8	5.2022710	-0.3502490	1.8255700

[f] IM3

74	0.3779160	2.0419430	0.0381240
8	-1.1958270	0.8845940	-0.0334650
74	-1.5316910	-0.9450950	0.1841730
8	0.1184980	-1.7149640	-0.0490760

74	2.0057530	-1.1279540	-0.1428160
8	1.7873900	0.7601800	-0.1105210
8	0.3627930	3.1568250	-1.2421660
8	0.4509270	2.9084510	1.4958360
8	-3.5087440	-0.3849470	-0.7320250
8	-2.2127450	-1.4075270	1.6493200
8	2.7488940	-1.6685320	-1.5688980
8	2.9113110	-1.6973800	1.1726890
6	-4.6890970	-0.3412720	-0.7360070
8	-5.8264780	-0.2930140	-0.7648840

[g] $W_3O_8^+$ (C_s ^{2}A')

74	-0.9280550	-0.0165910	1.8064430
8	-1.5378550	-0.0153440	0.0000000
74	-0.9280550	-0.0165910	-1.8064430
8	1.0306270	0.2092640	-1.5054390
74	2.0713090	0.1518650	0.0000000
8	1.0306270	0.2092640	1.5054390
8	-1.5723880	1.2572810	2.7177310
8	-1.2876110	-1.4663390	2.6037700
8	-1.5723880	1.2572810	-2.7177310
8	-1.2876110	-1.4663390	-2.6037700
8	3.2060120	-1.0828860	0.0000000

TABLE S4 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 7 at B3LYP level.

	x	y	z
[a] $W_4O_{12}^+$ (C_s ^{2}A')			
8	0.0045730	-1.4945640	1.5171880
8	0.0364560	1.5855160	-1.4833020
8	0.0364560	1.5855160	1.4833020
8	0.0045730	-1.4945640	-1.5171880
74	0.0095850	-2.6741340	0.0000000
74	0.0083850	2.6477580	0.0000000
74	-0.0068940	-0.0086860	2.6690070
74	-0.0068940	-0.0086860	-2.6690070
8	-1.3548670	-3.6829390	0.0000000
8	-1.3620890	3.7055600	0.0000000
8	-1.4003800	0.0152590	3.6350330
8	-1.4003800	0.0152590	-3.6350330
8	1.3389700	-0.0083800	-3.7008030
8	1.3389700	-0.0083800	3.7008030
8	1.3326350	3.8525870	0.0000000
8	1.3863980	-3.6661980	0.0000000
[b] IM1			
8	2.1079720	0.9561450	-0.0437870
8	-1.7723210	-0.8730100	-0.0380220
8	-0.8391070	1.8501590	-0.0702560
8	1.1349340	-1.9139220	-0.0239790
74	2.7367030	-0.8577020	-0.0578690
74	-2.3745210	0.8692910	0.0591570
74	1.0299220	2.4953700	0.0092020
74	-0.6554580	-2.4885210	0.0419300
8	3.7180330	-1.1801360	1.2892430
8	-3.0443730	1.1887270	1.5799560
8	1.2858260	3.3779640	1.4347490
8	-0.9787800	-3.3430970	1.4729750
8	-1.0380760	-3.5050110	-1.2633770
8	1.3399570	3.5287520	-1.3013870
8	-3.3509030	1.6440720	-1.3577990
8	3.6504560	-1.1755730	-1.4530150
6	-4.5773420	-0.1676430	-0.3265360
8	-5.5945830	-0.5998850	-0.4652830

	x	y	z
[c] TS1			
8	2.0914790	0.9833850	-0.0519200
8	-1.7599110	-0.9072300	-0.0499270
8	-0.8643020	1.8574160	-0.1023250
8	1.1624630	-1.9020120	-0.0268840
74	2.7476180	-0.8210650	-0.0666660
74	-2.3566200	0.8274140	0.0754970
74	1.0025080	2.5148880	0.0010180
74	-0.6172490	-2.5079020	0.0472020
8	3.7385930	-1.1275800	1.2770170
8	-2.9885190	1.0952320	1.6207060
8	1.2397630	3.3880080	1.4356520
8	-0.9222780	-3.3521120	1.4879340
8	-0.9830890	-3.5454020	-1.2456710
8	1.3196590	3.5597890	-1.2975940
8	-3.5339260	1.3973980	-1.2636800
8	3.6611260	-1.1258550	-1.4648360
6	-4.7323340	-0.0916750	-0.3660490
8	-5.7921800	-0.3756300	-0.5716570
[d] IM2			
8	-1.6957220	1.5236180	0.0795580
8	1.3809820	-1.4709620	-0.0645830
8	1.3805720	1.4559910	-0.0758950
8	-1.6991690	-1.5101540	0.0868510
74	-2.8711820	0.0091600	0.1855730
74	2.4494600	-0.0086810	-0.2862670
74	-0.1980930	2.6538940	-0.0532130
74	-0.2121880	-2.6522910	-0.0488670
8	-3.9930520	0.0074080	-1.0878580
8	3.0497820	-0.0068670	-1.8556350
8	-0.2533020	3.5864940	-1.4687650
8	-0.2736840	-3.5778840	-1.4687440
8	-0.1213430	-3.7247140	1.2625510
8	-0.0983190	3.7193050	1.2630340
8	3.8845530	-0.0250000	0.8984890
8	-3.7419490	0.0133920	1.6426460
6	5.1638640	-0.3746400	1.2554410
8	6.0037760	0.2711010	1.7224290

	x	y	z
[e] TS2			
8	-1.8415970	1.3315630	0.1451250
8	1.5204240	-1.2657180	-0.1404480
8	1.2191130	1.6535050	-0.0875330
8	-1.5244550	-1.6836180	0.0113190
74	-2.8483220	-0.3043730	0.1713070
74	2.4307740	0.3122010	-0.3672790
74	-0.4972450	2.6392030	0.0076000
74	0.1007450	-2.6315450	-0.0607110
8	-3.9565630	-0.3655970	-1.1130180
8	3.0267810	0.3801890	-1.9357620
8	-0.7035500	3.5927260	-1.3801000
8	0.1715520	-3.6490410	-1.4166640
8	0.3202400	-3.5938400	1.3211310
8	-0.4916440	3.6764160	1.3506140
8	3.8993040	0.2101820	0.8381920
8	-3.7231640	-0.4590500	1.6180850
6	4.9452160	-0.2240850	1.4885890
8	5.9045950	0.1970940	1.9766410
[f] IM3			
8	-1.7688570	-0.8128850	-0.1065460
8	2.1707420	0.8789280	-0.0796570
8	1.0917190	-1.9559850	-0.0090410
8	-0.7209680	1.9728230	-0.0818390
74	-2.2343410	0.9726690	0.1359160
74	2.7240080	-0.9593910	-0.0811150
74	-0.7266310	-2.4514140	0.0742170
74	1.1872060	2.4813290	-0.0459970
8	-2.9929630	1.3668160	1.5837720
8	3.7176400	-1.3033280	1.2526400
8	-1.0930540	-3.2070500	1.5514900
8	1.5227980	3.3811400	1.3532400
8	1.5334330	3.4610080	-1.3889600
8	-1.1474780	-3.5211800	-1.1781930
8	3.5992400	-1.3267960	-1.4899730
8	-4.1803920	0.2576430	-0.7836380
6	-5.3616560	0.2461520	-0.7822160
8	-6.5003560	0.2247290	-0.8045670

	x	y	z
[g] $W_4O_{11}^+$ (C_s ^{2}A')			
8	-1.6914640	-0.2433630	1.5513940
8	1.3818870	-0.0146710	-1.5193080
8	1.3818870	-0.0146710	1.5193080
8	-1.6914640	-0.2433630	-1.5513940
74	-2.6440910	-0.1374800	0.0000000
74	2.5585210	0.0141650	0.0000000
74	-0.0841400	0.0029960	2.6978640
74	-0.0841400	0.0029960	-2.6978640
8	-3.8028540	1.0753550	0.0000000
8	3.5348210	1.4019620	0.0000000
8	-0.1798270	1.4748290	3.5345810
8	-0.1798270	1.4748290	-3.5345810
8	0.0058730	-1.2434630	-3.8447210
8	0.0058730	-1.2434630	3.8447210
8	3.5831940	-1.3387460	0.0000000

TABLE S5 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 8 at B3LYP level.

	x	y	z
[a] WO_3 (C_{3v} $^1A_1$)			
74	0.0000000	0.0000000	0.1529910
8	0.0000000	1.6078470	-0.4717210
8	-1.3924360	-0.8039230	-0.4717210
8	1.3924360	-0.8039230	-0.4717210
[b] IM1			
74	0.0000000	0.0000000	0.2629610
8	0.0000000	1.6813410	0.7110110
8	1.4560840	-0.8406700	0.7110110
8	-1.4560840	-0.8406700	0.7110110
6	0.0000000	0.0000000	-1.9710750
8	0.0000000	0.0000000	-3.0871190
[c] TS			
74	0.0151920	0.3235060	0.0000000
8	-0.4121300	1.1537060	1.4435580
8	-0.4121300	1.1537060	-1.4435580
8	1.2540950	-1.0815580	0.0000000
6	-0.2109800	-1.7634740	0.0000000
8	-0.4121300	-2.8956840	0.0000000
[d] IM2			
74	-0.1024460	0.3768560	0.0000000
8	0.6747230	0.9482640	1.4136510
8	0.6747230	0.9482640	-1.4136510
8	-1.1589040	-1.3210250	0.0000000
6	0.1098080	-1.7336960	0.0000000
8	0.6747230	-2.7611510	0.0000000
[e] WO_2 (C_{2v} $^1A_1$)			
74	0.0000000	0.0000000	0.1834410
8	0.0000000	1.3319750	-0.8484150
8	0.0000000	-1.3319750	-0.8484150

TABLE S6 Cartesian coordinates for the reactant, intermediates, transition states and the product shown in the energy profile of Figure 9 at B3LYP level.

	x	y	z
[a] WO_3^- (C_{3v} $^2A_1$)			
74	0.0000000	0.0000000	0.0895520
8	0.0000000	1.7222690	-0.2761180
8	-1.4915280	-0.8611340	-0.2761180
8	1.4915280	-0.8611340	-0.2761180
[b] IM1			
74	0.2398420	0.0000000	0.0007710
8	0.6993350	-1.4822580	-0.8291190
8	0.8133390	-0.0001650	1.6586610
8	0.6994360	1.4823720	-0.8288610
6	-1.9139990	0.0000640	-0.2646660
8	-2.9951500	0.0000010	0.1906830
[b] TS			
74	-0.3101060	0.0095330	-0.0203770
8	0.9839780	-0.7860110	1.1192380
8	-1.5556080	-1.1339280	-0.4982110
8	-0.8774140	1.6451220	0.2374480
6	1.8117840	0.0836380	-0.2974120
8	2.9586830	0.1239130	-0.4469230
[c] IM2			
74	-0.0004780	0.3505370	0.0000000
8	-0.4092150	1.1474980	1.4969030
8	-0.4092150	1.1474980	-1.4969030
8	1.2373200	-1.3043990	0.0000000
6	-0.0070040	-1.7685470	0.0000000
8	-0.4092150	-2.9066550	0.0000000
[d] IM3			
74	0.0329260	0.4758300	0.0000000
8	-0.0292300	1.4301590	1.4423980
8	-0.0292300	1.4301590	-1.4423980
8	0.1374270	-1.5090040	0.0000000
6	-0.4724020	-2.6519980	0.0000000
8	-0.0292300	-3.7637400	0.0000000

	x	y	z
[e] WO_2^- (C_{2v} $^2B_1$)			
74	0.0000000	0.0000000	0.1625690
8	0.0000000	1.4736540	-0.7518790
8	0.0000000	-1.4736540	-0.7518790