

Available Supporting Materials

The Mechanisms of the Reactions of W and W⁺ with H₂O: Computational Studies

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Complete Ref. 8:

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Table S1. The B3LYP calculated relative energies (in kcal/mol, relative to the ground-state reactants) of the intermediates, transition states and products of the reactions $W + H_2O$ and $W^+ + H_2O$ for several low-lying electronic states.^{a)}

Structure	M = W					M = W ⁺				
	State	ΔE	+ZPC	ΔH	ΔG	State	ΔE	+ ZPC	ΔH	ΔG
M + H₂O	⁷ S	0.0	0.0	0.0	0.0	⁶ D	0.0	0.0	0.0	0.0
	⁵ D	5.2	---	---	---	⁴ D	36.5	---	---	---
	³ D	37.6	---	---	---	² D	49.1	---	---	---
	¹ S	68.3	---	---	---					
M(H₂O)	⁷ A \square	(5.1)	(4.1)	(4.4)	(3.3)	⁶ A \square	-70.6(0.0)	-69.1(0.0)	-68.4(0.0)	-75.7(0.0)
	⁵ A \square	-27.7(0.0)	-26.4(0.0)	-25.9(0.0)	-32.9(0.0)	⁴ A \square	(29.4)	(29.4)	(29.2)	(30.0)
	³ A''	(35.0)	(34.7)	(34.8)	(35.1)	² A \square	(52.2)	(52.7)	(52.4)	(53.7)
	¹ A \square	(48.3)	(48.1)	(48.2)	(49.2)					
TS1	⁷ A	---	---	---	---	⁶ A	(24.3)	(23.3)	(23.8)	(22.5)
	⁵ A	-11.7(0.0)	-14.6(0.0)	-14.3(0.0)	-20.8(0.0)	⁴ A	-27.0(0.0)	-24.3(0.0)	-24.2(0.0)	-30.4(0.0)
	³ A	(23.6)	(23.7)	(23.8)	(24.0)	² A	(23.9)	(22.7)	(23.4)	(20.7)
	¹ A	((44.6)	(44.7)	(44.7)	(45.6)					
HM(OH)	⁷ A	(79.4)	(77.8)	(78.0)	(78.0)	⁶ A	(61.1)	(58.1)	(58.1)	(58.2)
	⁵ A	-68.1(0.0)	-70.2(0.0)	-69.6(0.0)	-76.5(0.0)	⁴ A	-75.3(0.0)	-74.6(0.0)	-76.6(0.0)	-83.3(0.0)
	³ A	(12.7)	(15.2)	(15.0)	(15.7)	² A	(30.6)	(20.7)	(20.7)	(21.2)
	¹ A	(32.4)	(33.4)	(32.4)	(33.4)					
TS2	⁵ A	(30.8)	(30.7)	(30.7)	(30.2)	⁶ A	(22.3)	(24.4)	(24.5)	(24.1)
	³ A	-38.1(0.0)	-43.6(0.0)	-43.2(0.0)	(-49.6)(0.0)	⁴ A	-19.1(0.0)	-25.8(0.0)	-25.4(0.0)	-32.0(0.0)
	¹ A	(71.1)	(73.7)	(73.6)	(74.4)	² A	(21.3)	(24.6)	(24.4)	(25.1)

(H)₂MO	⁵ A _g	(44.8)	(45.4)	(45.6)	(45.2)	⁶ A _g	(140.0)	(136.2)	(136.5)	(135.1)
	³ A _g	-95.3(0.0)	-99.6(0.0)	-99.1(0.0)	-105.7(0.0)	⁴ A _g	(54.4)	(51.7)	(51.8)	(51.1)
	¹ A _g	(10.6)	(11.5)	(11.3)	(12.3)	² A _g	-87.3(0.0)	-90.3(0.0)	-90.1(0.0)	-96.1(0.0)
WO + H₂	⁵ □ ⁺	(17.9)	(17.7)	(17.7)	(17.4)	⁶ □ ⁺	(93.0)	(92.5)	(92.5)	(92.1)
	³ □ ⁺	-60.7(0.0)	-66.2(0.0)	-64.4(0.0)	-77.6(0.0)	⁴ □ ⁺	-62.2(0.0)	-67.6(0.0)	-65.8(0.0)	-79.2(0.0)
	¹ □ ⁺	(19.3)	(19.3)	(19.3)	(20.0)	² □ ⁺	(35.5)	(35.6)	(35.6)	(36.0)

a) Important geometry parameters of these structures are given in Figure 1. Total energies and full cartesian coordinates of all these structures are given in Tables S2 and S4 in the Supporting Material, respectively.

Table S2. The B3LYP calculated total energies (in a.u.) of the reactants, intermediates, transition states and products of the reactions $W + H_2O$ and $W^+ + H_2O$ for several low-lying electronic states.

Structures	M = W					M = W ⁺				
	State	-E _{tot}	+ZPC	-H	-G	State	-E _{tot}	+ ZPC	-H	-G
M(H ₂ O)	¹ A□	143.332677	143.309376	143.304764	143.335724	² A□	143.100770	143.076248	143.071922	143.102876
	³ A''	143.353777	143.330836	143.326116	143.358216	⁴ A□	143.137234	143.113341	143.108869	143.140720
	⁵ A□	143.409485	143.386096	143.381507	143.413997	⁶ A□	143.184034	143.160219	143.155432	143.188452
	⁷ A□	143.401456	143.379519	143.374541	143.408798					
TS1	¹ A	143.312802	143.296045	143.291791	143.322148	² A	143.067967	143.050786	143.046418	143.077570
	³ A	143.346324	143.329390	143.325167	143.356536	⁴ A	143.106030	143.089022	143.084933	143.116262
	⁵ A	143.383944	143.367207	143.363024	143.394816	⁶ A	143.067273	143.051815	143.047077	143.080404
HM(OH)	¹ A	143.422128	143.404220	143.399653	143.430447	² A	143.158692	143.140066	143.135586	143.166859
	³ A	143.453605	143.431542	143.427351	143.458622	⁴ A	143.191561	143.173051	143.168578	143.200537
	⁵ A	143.473817	143.455865	143.451268	143.483697	⁶ A	143.094131	143.080538	143.075937	143.107838
	⁷ A	143.347248	143.331823	143.326928	143.359355					
TS2	¹ A	143.312802	143.296045	143.291791	143.322148	² A	143.068069	143.052117	143.048035	143.078824
	³ A	143.426037	143.413442	143.409049	143.440649	⁴ A	143.102019	143.091300	143.086880	143.118874
	⁵ A	143.376992	143.364533	143.360150	143.392520	⁶ A	143.066482	143.052346	143.047887	143.080546
(H) ₂ MO	¹ A□	143.500289	143.484349	143.480121	143.510492	² A□	143.210619	143.194112	143.189886	143.220885
	³ A''	143.517235	143.502735	143.498178	143.530152	⁴ A□	143.123885	143.111785	143.107321	143.139413
	⁵ A□	143.445909	143.430326	143.425559	143.458165	⁶ A□	142.987557	142.977119	142.972311	143.005556
MO	¹ □ ⁺	142.252842	142.250341	142.247011	142.273710	² □ ₊	141.935474	141.932906	141.929579	141.956913
	³ □ ⁺	142.283595	142.281126	142.277795	142.305538	⁴ □ ⁺	141.992095	141.989586	141.986257	142.014251

Table S3. The calculated CCSD(T) energetics (in a.u., at their B3LYP optimized geometries) and $\langle S^2 \rangle$ (at the B3LYP level) values of the intermediates, transition states and products of the reactions of W and W⁺ with the water molecule.

Structures	State	M = W		State	M = W ⁺	
		E _{tot}	$\langle S^2 \rangle$		E _{tot}	$\langle S^2 \rangle$
M	⁷ S	-66.4622	12.00/12.00	⁶ D	-66.18821	8.75/8.75
	⁵ D	-66.4548	6.19/6.00	⁴ D	-66.14421	3.82/3.75
	³ D	-66.3903	2.16/2.00	² D	-66.11331	0.89/0.76
	¹ S	-66.3483				
M(H ₂ O)	⁷ A□	---	12.00/12.00	⁶ A□	-142.5539	8.75/8.75
	⁵ A□	-142.7657	6.06/6.00	⁴ A□	-142.5052	3.84/3.75
	³ A''	-142.7006	2.05/2.00	² A□	-142.4669	0.75/0.75
	¹ A□	-142.6753				
TS1	⁵ A	-142.7273	6.03/6.00	⁶ A	-142.4321	8.76/8.75
	³ A	-142.6859	2.02/2.00	⁴ A	-142.4624	3.82/3.75
	¹ A	-142.6453		² A	-142.4553	1.65/0.82
t-HMOH	⁵ A	-142.8222	6.01/6.00	⁶ A	-142.4592	8.76/8.75
	³ A	-142.7981	2.15/2.00	⁴ A	-142.5574	3.77/3.75
	¹ A	-142.7634		² A	-142.5118	0.76/0.75
c-HMOH	⁵ A	---		⁶ A	----	
	³ A	-142.8049	2.13/2.00	⁴ A	-142.5494	3.78/3.75
	¹ A	-142.7733		² A	-142.5022	0.75/0.75
TS2	⁵ A	---	6.01/6.00	⁶ A	-142.3239	8.75/8.75
	³ A	-142.7707	2.02/2.00	⁴ A	-142.4585	3.77/3.75
	¹ A	-142.7456		² A	-142.4489	0.81/0.75
(H) ₂ MO	⁵ A□	-142.7169	6.01/6.00	⁶ A□	-142.3416	8.76/8.75
	³ A''	-142.8671	2.01/2.00	⁴ A□	-142.4811	3.76/3.75
	¹ A□	-142.8467		² A□	-142.5713	0.76/0.75
TS3	⁵ A	-142.7948	6.02/6.00	⁶ A	---	
	³ A	-142.7795	2.02/2.00	⁴ A	-142.5486	
	¹ A	-142.7718		² A	-142.5013	
TS4	⁵ A	---	6.01/6.00	⁶ A	---	
	³ A	-142.7925	2.03/2.00	⁴ A	---	
	¹ A	-142.7612		² A	---	
M(OH)	⁶ A	-142.2058	8.75/8.75	⁷ A	-141.8375	12.00/12.00

	⁴ A	-142.2043	3.78/3.75	⁵ A	-141.9508	6.01/6.00
	² A	-142.1299	0.87/0.75	³ A	-141.9208	2.03/2.00
MO	⁵ □ ⁺	-141.6122	6.20/6.00	⁶ □ ⁺	-141.2153	8.75/8.75
	³ □ ⁺	-141.648	2.32/2.06	⁴ □ ⁺	-141.3666	4.25/3.84
	¹ □ ⁺	-141.6111		² □ ⁺	-141.3245	1.23/0.91
HMO	⁶ A	-142.1174	8.76/8.75	⁷ A	-141.7434	12.00/12.00
	⁴ A	-142.2431	3.76/3.75	⁵ A	-141.8696	6.01/6.00
	² A	-142.2172	0.79/0.75	³ A	-141.9656	2.02/2.00
TS5	⁶ A	-142.0983	8.76/8.75	⁷ A	-141.7476	12.00/12.00
	⁴ A	-142.1475	3.76/3.75	⁵ A	-141.8253	6.01/6.00
	² A	-142.1412	0.78/0.75	³ A	-141.8853	2.03/2.00
MH	⁶ □ ⁺	-67.06193	8.76/8.75	⁷ □ ⁺	-66.69764	12.00/12.00
	⁴ □ ⁺	-67.03651	3.76/3.75	⁵ □ ⁺	-66.77588	6.01/6.00
	² □ ⁺	-66.97888	1.61/0.76	³ □ ⁺	-66.73865	2.00/2.00
H ₂ O	¹ A ₁	-76.28634				
H ₂	¹ □ _g	-1.16834				
OH		-75.59623				
H		-0.49981				

Table S4. Cartesian coordinates (in Å) of all reported structures in this paper.

(a) For the reaction $W^+ + H_2O$

$W(H_2O)^+$, 6A_1

W	-0.00188	-0.26693	0.00000
O	-0.00188	1.86436	0.00000
H	0.07722	2.41880	0.79520
H	0.07722	2.41880	-0.79520

$W(H_2O)^+$, 4A_1

W	0.00002	-0.25377	0.00000
O	0.00002	1.76727	0.00000
H	-0.00088	2.32023	0.80844
H	-0.00088	2.32023	-0.80844

$W(H_2O)^+$, 2A_1

W	-0.00005	-0.25416	0.00000
O	-0.00005	1.76862	0.00000
H	0.00195	2.32937	0.80074
H	0.00195	2.32937	-0.80074

TS1, 2A_1

W	0.23405	-0.00533	0.00223
O	-1.71490	-0.05318	-0.10441
H	-1.20918	1.11930	0.11073
H	-2.39116	-0.29948	0.55925

TS1, 4A_1

W	0.23166	-0.00476	0.00192
O	-1.69730	-0.04515	-0.11525
H	-1.29095	1.10986	0.17799
H	-2.27389	-0.39639	0.60164

TS1, 6A_1

W	0.24304	-0.02139	0.00242
O	-1.97999	-0.09757	-0.03797
H	0.35370	1.66380	-0.11714
H	-2.49898	0.69998	0.24156

cis-HWOH $^+$, 2A_1

W	-0.19361	-0.02398	0.00001
O	1.57944	-0.04434	-0.00011
H	-0.67232	1.58603	-0.00021
H	2.36372	0.54283	0.00057

cis-HWOH $^+$, 4A_1

W	0.02585	-0.19178	0.00000
O	0.02585	1.61770	0.00000
H	-1.44147	-1.04824	0.00000
H	-0.67833	2.29847	0.00000

trans-HWOH $^+$, 2A_1

W	-0.19361	-0.02398	0.00001
O	1.57944	-0.04434	-0.00011
H	-0.67232	1.58603	-0.00021
H	2.36372	0.54283	0.00057

trans-HWOH $^+$, 4A_1

W	0.19350	-0.03092	-0.00000
O	-1.61089	0.16119	-0.00006
H	0.90454	1.49746	0.00019
H	-2.33638	-0.49886	0.00042

trans-HWOH $^+$, 6A_1

W	0.17601	0.00628	-0.00341
O	-1.65737	-0.11894	0.01170
H	2.56045	-0.10758	0.11653
H	-2.32620	0.59465	0.04247

TS(cis-trans), 2A_1

W	-0.01781	-0.06249	-0.00670
O	0.00943	-0.00729	1.74483
H	1.60902	0.04629	-0.39497
H	0.02458	0.02345	2.71932

TS(cis-trans), 4A_1

W	-0.19255	-0.02795	0.00002
O	1.59524	0.06580	-0.00048
H	-1.07833	1.42551	0.00000
H	2.56507	0.11664	0.00251

TS2, 2A_1

W	0.00106	-0.16647	0.00000
O	0.00106	1.52881	0.00000
H	1.46976	-1.02632	0.00000
H	-1.55664	1.11445	0.00000

TS2, 4A_1

W	-0.00087	-0.16968	0.00000
O	-0.00087	1.51308	0.00000
H	-1.61930	-0.72883	0.00000
H	1.69048	1.18039	0.00000

(H) $_2$ WO $^+$, 2A_1

W	0.02455	-0.15358	0.00000
O	0.02455	1.50006	0.00000
H	-1.00665	-0.31779	1.31752
H	-1.00665	-0.31779	-1.31752

(H) $_2$ WO $^+$, 4A_1

W	-0.00000	-0.14961	0.00000
O	-0.00000	1.50620	0.00000
H	0.00006	-0.48925	1.79624
H	0.00006	-0.48925	-1.79624

(H)₂WO⁺, ⁶A□

W	0.17003	0.00000	-0.00000
O	-1.73604	0.00000	0.00001
H	0.65304	1.75123	0.00015
H	0.65304	-1.75123	0.00015

WO⁺, ²□_g

W	.000000	.000000	.161256
O	.000000	.000000	-1.491622

WO⁺, ⁴□_g

W	.000000	.000000	.161498
O	.000000	.000000	-1.493861

WO⁺, ⁶□_g

W	.000000	.000000	.186511
O	.000000	.000000	-1.725224

WH⁺, ¹□_g

W	.000000	.000000	.022468
H	.000000	.000000	-1.662634

WH⁺, ³□_g

W	.000000	.000000	.022044
H	.000000	.000000	-1.631253

WH⁺, ⁵□_g

W	.000000	.000000	.022361
H	.000000	.000000	-1.654735

WH⁺, ⁷□_g

W	.000000	.000000	.028614
H	.000000	.000000	-2.117426

W(OH)⁺, ¹A

W	.000020	-1.99959	.000000
O	.000020	1.535546	.000000
H	-.001615	2.512633	.000000

W(OH)⁺, ³A

W	-.000006	-.200185	.000000
O	-.000006	1.537377	.000000
H	.000505	2.514657	.000000

W(OH)⁺, ⁵A

W	.009451	-.205414	.000000
O	.009451	1.623652	.000000
H	-.774960	2.211409	.000000

W(OH)⁺, ⁷A

W	.010148	-.249740	.000000
O	.010148	1.995600	.000000
H	-.832142	2.515987	.000000

TS5, ³A

W	0.01443	-0.18274	0.00000
O	0.01443	1.53483	0.00000
H	-1.18302	1.24417	0.00000

TS5, ⁵A

W	0.02027	-0.18278	0.00000
O	0.02027	1.71174	0.00000
H	-1.66206	-0.16826	0.00000

TS5, ⁷A

W	0.02011	-0.22520	0.00000
O	0.02011	2.14304	0.00000
H	-1.64903	-0.47984	0.00000

(a) For the reaction W + H₂O

W(H₂O), ³A

W	0.00001	-0.26404	0.00000
O	0.00001	1.84348	0.00000
H	-0.00031	2.39546	0.80447
H	-0.00031	2.39546	-0.80447

W(H₂O), ⁵A□

W	-0.01081	-0.26991	0.00000
O	-0.01081	1.92639	0.00000
H	0.44325	2.28098	0.78890
H	0.44325	2.28098	-0.78890

TS1, ¹A

W	-0.24665	-0.00501	0.00041
O	1.84201	-0.00890	-0.11812
H	1.26334	0.96562	0.31625
H	2.25272	-0.52390	0.59865

TS1, ³A

W	-0.24858	-0.00488	0.00046
O	1.85733	-0.01249	-0.12055
H	1.27358	0.95735	0.30969
H	2.26264	-0.49651	0.62106

TS1, ⁵A

W	-0.24370	-0.00501	0.00120
O	1.81455	-0.03877	-0.12178
H	1.25988	1.06830	0.20981
H	2.25723	-0.38698	0.67566

trans-HWOH, ¹A

W	-0.18899	-0.02946	-0.00184
O	1.64709	0.19680	-0.01942

H	-1.31726	1.24669	0.11300
H	2.12604	-0.64107	0.17830

trans-HWOH, ³A

W	0.00668	-0.19334	0.00000
O	0.00668	1.66403	0.00000
H	-1.44359	-1.08676	0.00000
H	0.89548	2.08189	0.00000

trans-HWOH, ⁵A

W	-0.19951	-0.02719	0.00508
O	1.71314	0.03479	-0.10898
H	-1.20547	1.38435	-0.12829
H	2.26379	0.34926	0.62458

cis-HWOH, ¹A

W	0.19057	-0.02392	0.00000
O	-1.64697	-0.01967	-0.00004
H	1.36845	1.22909	-0.00010
H	-2.29514	0.69876	0.00018

cis-HWOH, ³A

W	-0.19142	-0.02398	0.00000
O	1.65564	-0.02165	-0.00001
H	-1.36442	1.23412	-0.00004
H	2.28430	0.71394	0.00006

TS2, ¹A

W	-0.17261	-0.02648	-0.01097
O	1.56014	0.17403	-0.05406
H	1.38304	-0.76462	0.76482
H	-1.09096	1.33164	0.47954

TS2, ³A

W	-0.17286	-0.02733	-0.00929
O	1.59599	0.13138	-0.08537
H	1.29087	-0.31112	1.05860
H	-1.26706	1.28283	0.31203

TS2, ⁵A

W	0.17940	0.00245	-0.02838
O	-1.78533	-0.09265	0.04991
H	-0.15898	1.51581	0.67474
H	1.16642	-0.95565	1.02616

(H)₂WO, ¹A□

W	0.01897	-0.15052	0.00000
O	0.01897	1.52469	0.00000
H	-0.77763	-0.52959	1.46689
H	-0.77763	-0.52959	-1.46689

(H)₂WO, ³A"

W	-0.00001	-0.14297	0.00000
O	-0.00001	1.55209	0.00000
H	0.00034	-0.91837	1.57097
H	0.00034	-0.91837	-1.57097

(H)₂WO, ⁵A□

W	0.02283	-0.12105	0.00000
O	0.02283	1.60429	0.00000
H	-0.93601	-1.93839	0.40383
H	-0.93601	-1.93839	-0.40383

WO, ¹□_g

W	.000000	.000000	.162620
O	.000000	.000000	-1.504231

WO, ³□_g

W	.000000	.000000	.162981
O	.000000	.000000	-1.507571

WO, ⁵□_g

W	.000000	.000000	.168300
O	.000000	.000000	-1.556771

WH, ²□_g

W	.000000	.000000	.022443
H	.000000	.000000	-1.660777

WH, ⁴□_g

W	.000000	.000000	.022348
H	.000000	.000000	-1.653762

WO, ⁶□_g

W	.000000	.000000	.022908
H	.000000	.000000	-1.695190

WHO, ²A

W	.010404	-.205594	.000000
O	.010404	1.639347	.000000
H	-.853105	2.099155	.000000

WHO, ⁴A

W	.010515	-.206714	.000000
O	.010515	1.651069	.000000
H	-.862204	2.088254	.000000

WHO, ⁶A

W	.010246	-.216007	.000000
O	.010246	1.724465	.000000
H	-.840163	2.188787	.000000

TS5, ²A

W	0.01394	-0.18576	0.00000
O	0.01394	1.55804	0.00000
H	-1.14283	1.28171	0.00000

TS5, ⁴A

W	0.01562	-0.18629	0.00000
O	0.01562	1.58717	0.00000
H	-1.28041	1.08837	0.00000

TS5, 6A

W	0.01960	-0.19666	0.00000
O	0.01960	1.78061	0.00000
H	-1.60723	0.30827	0.00000