Supporting Information for

Hydration Enthalpies of $Ba^{2+}(H_2O)_x$, $x = 1 – 8$: A Threshold Collision-Induced Dissociation and Theoretical Investigation

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Table S1. Theoretical 0 K Bond Enthalpies (kJ/mol) for H_2O Loss from Ground Structure $Ba^{2+}(H_2O)_x$ (x = 1 – 8)[a]

geometry[b]	single point[c]	x = 1	2	3	4	5	6	7	8[d]	MAD[e]
B3LYP/SDD/ 6-311+G(d,p)	B3LYP/SDD/ 6-311+G(2d,2p)	160 (160)	140 (141)	125 (126)	111 (112)	91 (93)	83 (85)	66 (69)	67 (69)	*3 ± 2 (5 ± 2)* **7 ± 5 (8 ±6)**
	B3P86/SDD/ 6-311+G(2d,2p)	163 (164)	142 (144)	127 (128)	112 (113)	91 (93)	82 (85)	69 (72)	69 (72)	*2 ± 1 (4 ± 1)* **7 ± 6 (8 ± 8)**
	M06/SDD/ 6-311+G(2d,2p)	164 (166)	144 (145)	129 (130)	115 (116)	98 (99)	84 (86)	84 (86)	75 (77)	*4 ± 4 (4 ± 4)* **10 ± 10 (11 ± 11)**
	MP2(full)/SDD/ 6-311+G(2d,2p)	152 (158)	136 (141)	123 (129)	111 (117)	95 (102)	88 (97)	70 (80)	66 (77)	*5 ± 4 (6 ± 4)* **10 ± 6 (14 ± 9)**
B3LYP/HW*/ 6-311+G(d,p)	B3LYP/HW*/ 6-311+G(2d,2p)	158 (159)	139 (140)	124 (125)	110 (112)	90 (91)	82 (83)	67 (69)	67 (70)	*4 ± 2 (6 ± 2)* **8 ± 5 (8 ± 6)**
	B3P86/HW*/ 6-311+G(2d,2p)	161 (163)	141 (143)	126 (127)	112 (113)	90 (91)	81 (83)	69 (72)	69 (72)	*2 ± 2 (4 ± 2)* **8 ± 6 (8 ± 8)**
	M06/HW*/ 6-311+G(2d,2p)	162 (165)	142 (143)	128 (130)	115 (116)	96 (97)	83 (85)	83 (86)	73 (75)	*4 ± 4 (4 ± 4)* **10 ± 10 (11 ± 11)**
	MP2(full)/HW*/ 6-311+G(2d,2p)	149 (155)	133 (138)	121 (127)	109 (116)	92 (100)	84 (95)	68 (77)	68 (77)	*6 ± 6 (6 ± 4)* **10 ± 7 (14 ± 8)**
B3LYP/SDD/ def2-TZVP	B3LYP/SDD/ def2-TZVPP	162 (166)	142 (146)	126 (130)	113 (117)	91 (96)	82 (87)	69 (73)	69 (73)	*1 ± 2 (1 ± 2)* **8 ± 6 (9 ± 8)**
	B3P86/SDD/ def2-TZVPP	164 (167)	144 (147)	127 (130)	113 (116)	91 (95)	82 (86)	72 (75)	72 (75)	*1 ± 1 (2 ± 1)* **8 ± 8 (9 ± 9)**
	M06/SDD/ def2-TZVPP	165 (168)	143 (146)	127 (131)	114 (118)	96 (99)	84 (88)	82 (86)	71 (76)	*3 ± 4 (3 ± 3)* **10 ± 9 (11 ± 11)**
	MP2(full)/SDD/ def2-TZVPP	154 (161)	137 (144)	125 (131)	112 (119)	95(102)	86 (93)	72 (80)	69 (76)	*4 ± 4 (5 ± 3)* **10 ± 6 (13± 9)**

geometry[b]	single point[c]	x = 1	2	3	4	5	6	7	8[d]	MAD[e]
B3LYP/SDD/ def2-TZVPP	B3LYP/SDD/ def2-TZVPP	162 (166)	142 (146)	126 (130)	113 (117)	92 (96)	83 (87)	70 (74)	70 (74)	*1 ± 1 (1 ± 1)* **8 ± 7 (9± 8)**
	GD3BJ[f]	172 (176)	144 (148)[g]	132 (137)	121 (125)	101 (106)	92 (97)	78 (82)	77 (81)	*7 ± 4 (7 ± 4)* **13 ± 10 (17 ± 10)**
	B3P86/SDD/ def2-TZVPP	165 (168)	144 (147)	127 (130)	113 (117)	91 (95)	82 (86)	72 (75)	72 (75)	*1 ± 1 (2 ± 0)* **8 ± 8 (9± 9)**
	M06/SDD/ def2-TZVPP	164 (168)	143 (146)	127 (131)	115 (118)	96 (99)	84 (88)	82 (86)	72 (75)	*4 ± 4 (3 ± 4)* **11 ± 9 (11 ± 11)**
	GD3[f]	164 (168)	143 (146)	128 (132)	115 (118)	99 (102)	86 (90)	85 (89)	71 (76)	*4 ± 5 (4 ± 5)* **10 ± 10 (12 ± 11)**
	MP2(full)/SDD/ def2-TZVPP	155 (161)	137 (144)	125 (131)	113 (120)	95(102)	86 (94)	72 (80)	69 (76)	*3 ± 3 (4 ± 3)* **10 ± 7 (13 ± 9)**
B3LYP/DHF/ def2-TZVPP	B3LYP/DHF/ def2-TZVPP	167 (170)	145 (149)	128 (132)	114 (118)	92 (96)	83 (87)	70 (74)	70 (74)	*(4 ± 0)*[h] **7 ± 7 (10 ± 8)**
	GD3BJ[f]	172 (176)	144 (148)[g]	132 (137)	119 (124)	100 (104)	91 (95)			*5 ± 2 (5 ± 2)* **7 ± 5 (11 ± 5)**
	B3P86/DHF/ def2-TZVPP	169 (172)	147 (150)	129 (132)	114 (118)	92 (96)	82 (86)	72 (75)	72 (75)	*1 ± 1 (1 ± 1)* **7 ± 8 (10 ± 8)**
	M06/DHF/ def2-TZVPP	168 (173)	146 (149)	130 (133)	115 (119)	97 (100)	84 (88)	81 (85)	72 (75)	*3 ± 3 (3 ± 3)* **9 ± 10 (13 ± 10)**
	GD3[f]	164 (168)	143 (146)	128 (132)	115 (119)	98 (102)	86 (90)			*3 ± 2 (2 ± 2)* **5 ± 3 (7 ± 5)**
	MP2(full)/DHF/ def2-TZVPP	162 (168)	143 (149)	128 (135)	115 (122)	97 (106)	87 (95)	74 (85)	69 (76)	*3 ± 2 (5 ± 4)* **9 ± 7 (15 ± 10)**
GF[i]		(166)	(148)	(134)	(121)	(102)	(93)			*6 ± 4 (4 ± 2)* **(9 ± 5)**

geometry[b]	single point[c]	x = 1	2	3	4	5	6	7	8[d]	MAD[e]
KS[j]	HF	(167)	(152)							*4 ± 3 (3 ± 0)* **(5 ± 4)**
	MP2	(177)	(159)							*12 ± 2 (8 ± 2)* **(11 ± 4)**
	MP4	(175)								
MX[k]	MP2/ADZ	(165)	(141)	(135)	(119)	(98)	(91)			*5 ± 2 (4 ± 2)* **(8 ± 4)**
	MP2/ATZ	(163)	(141)	(137)	(122)	(106)	(96)			*9 ± 4 (7 ± 2)* **(11 ± 5)**
Experimental[l]		169	145	129	107	92	77	55	48	*7 ± 7 (10 ± 8)*

[a] Values in parenthesis do not include counterpoise corrections. [b] Level of theory and basis set for geometry optimization. [c] Level of theory and basis set for single point energy calculations. [d] (8,0) structures are converged using analytic gradients for the SDD/6-311+G(d,p), SDD/def2-TZVPP, and DHF/def2-TZVPP basis sets but not using explicit force constant calculations. [e] Mean absolute deviations from B3LYP/DHF/def2-TZVPP with (and without) counterpoise corrections in *italics* and from current experimental results in **bold**. Uncertainties are one standard deviation. [f] Empirical dispersion corrections to geometry optimizations and single point energy calculations for the level of theory in the preceding row. B3LYP uses GD3BJ and M06 uses GD3 terms found in the Gaussian09 package. [g] $Ba^{2+}(H_2O)_2$ structure changed from C_2 symmetry to a nonsymmetric structure when dispersion corrections were used. See Table S3. [h] MAD from B3LYP/DHF/def2-TZVPP with counterpoise corrections. [i] From ref. 1. [j] From refs. 2 and 3. [k] From ref.4 . [l] Current experimental results taken from Table 6.

References

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Table S2. Relative Free Energies (kJ/mol) at 0 (298) K for $Ba^{2+}(H_2O)_x$ (x = 7 and 8) Isomers Including Values Having Empirical Dispersion Corrections[a]

x	complex name	B3LYP/SDD/ def2-TZVPP	B3LYP-GD3BJ/ SDD /def2-TZVPP	M06/SDD/ def2-TZVPP	M06-GD3/ SDD/ def2-TZVPP	MP2(full)/SDD/ def2-TZVPP
7[b]	(7,0)	6.6 (4.9)		2.1 (0.2)		1.9 **(0.0)**
	(7,0)_C_2	4.6 (4.8)	1.5 (2.5)	**0.0 (0.0)**	**0.0 (0.0)**	**0.0 (0.0)**
	(6,1)_2D_AA	**0.0** (0.6)	**0.0 (0.0)**	8.2 (8.6)	9.2 (8.1)	3.1 (3.5)
	(6,1)_D_A	6.9 **(0.0)**		19.8 (12.7)		12.7 (5.6)
8	(8,0)[c]	20.8 (23.4)	9.0 (4.0)	5.3 (12.7)	**0.0 (0.0)**	6.4 (13.7)
	(7,1)	7.2 (2.4)	4.4 (1.6)	**0.0 (0.0)**	2.3 (4.5)	0.1 **(0.0)**
	(6,2)adj	**0.0 (0.0)**	**0.0 (0.0)**	4.4 (9.2)	7.6 (12.5)	**0.0** (4.7)

[a] Relative ΔG_{298} are in parentheses. Bold values represent the predicted ground structures. Single-point energies are calculated at the level shown using B3LYP/SDD/def2-TZVPP or B3LYP-GD3BJ/SDD/def2-TZVPP geometries and ZPE corrections. [b] Dispersion corrected single-point energies for x = 7 were only performed for (7,0)_C_2 and (6,1)_2D_AA structures. [c] (8,0) structures converged using analytic gradients but not using explicit force constant calculations.

Table S3. Ba-O bond Lengths for Ground Structures Calculated at the B3LYP/SDD/def2-TZVP, B3LYP/SDD/def2-TZVPP, B3LYP-GD3BJ/SDD/def2-TZVPP, and B3LYP/DHF/def2-TZVPP Levels of Theory

	Ba-O bond lengths (Å)[a]										
level of theory	(1,0)	(2,0)	(3,0)	(4,0)	(5,0)	(6,0)	(6,1) _2D_AA	(7,0)_C2	(6,2)adj	(7,1)	(8,0)
B3LYP/SDD/	2.602	2.647 (2)	2.680 (3)	2.712 (2)	2.737	2.784 (6)	2.738	2.796 (2)	2.748 (2)	2.770	2.839 (3)
def2-TZVP				2.713 (2)	2.743 (2)		2.744	2.810 (2)	2.752 (2)	2.776	2.840 (5)
					2.765 (2)		2.782	2.813	2.802 (2)	2.802	
							2.792 (2)	2.827 (2)	4.561 (2)	2.808	
							2.813			2.812	
							4.530			2.822	
										2.847	
										4.591	
B3LYP/SDD/	2.602	2.647 (2)	2.678(2)	2.711	2.737	2.784 (4)	2.737	2.797 (2)	2.747 (2)	2.769	2.839 (3)
def2-TZVPP			2.679	2.712	2.744 (2)	2.785 (2)	2.743	2.810 (2)	2.752 (2)	2.776	2.840 (5)
				2.713 (2)	2.765 (2)		2.784	2.814	2.803 (2)	2.804	
							2.793 (2)	2.828 (2)	4.559 (2)	2.809	
							2.814			2.815	
							4.527			2.822	
										2.848	
										4.589	

level of theory	(1,0)	(2,0)	(3,0)	(4,0)	(5,0)	(6,0)	(6,1) _2D_AA	(7,0)_C2	(6,2)adj	(7,1)	(8,0)
B3LYP-GD3BJ/	2.602	2.634	2.671 (2)	2.705(4)	2.730 (3)	2.771 (4)	2.724	2.792 (2)	2.735 (2)	2.754	2.824 (2)
SDD/		2.642	2.672		2.754 (2)	2.772 (2)	2.729	2.795	2.738 (2)	2.760	2.825 (5)
def2-TZVPP							2.765	2.780 (2)	2.787 (2)	2.787	2.826
							2.768	2.810 (2)	4.526 (2)	2.789	
							2.791			2.797	
							2.798			2.808	
							4.492			2.823	
										4.544	
B3LYP/	2.587	2.634 (2)	2.668	2.702	2.728	2.776 (6)	2.729	2.789 (2)	2.740 (2)	2.762	2.835 (3)
DHF/def2-			2.667 (2)	2.703 (2)	2.735 (2)		2.735	2.806 (2)	2.744 (2)	2.769	2.836 (5)
TZVPP				2.704	2.757 (2)		2.776	2.809	2.796 (2)	2.798	
							2.785 (2)	2.821 (2)	4.550 (2)	2.803	
							2.806			2.809	
							4.521			2.817	
										2.842	
										4.583	

[a] Degeneracies are in parentheses.

Table S4. Conversion from 0 K Primary and Secondary Binding Energies (kJ/mol) for H_2O Loss from $Ba^{2+}(H_2O)_x$ (x = 1 – 8) to Enthalpies and Free Energies at 298 K[a]

complex	ΔH_0[b]	$\Delta H_{298} - \Delta H_0$[c]	ΔH_{298}	$T\Delta S_{298}$[c]	ΔG_{298}
$Ba^{2+}(H_2O)$	168.6 (4.8)	4.0 (0.2)	172.6 (4.8)	27.7 (0.4)	144.9 (4.8)
	189.3 (35.6)		193.3 (35.6)		165.6 (35.6)
$Ba^{2+}(H_2O)_2$	144.9 (6.5)	0.7 (0.4)	145.6 (6.5)	26.3 (2.6)	119.3 (7.0)
	144.0 (7.7)		144.7 (7.7)		118.4 (8.1)
$Ba^{2+}(H_2O)_3$	127.4 (3.9)	0.7 (0.4)	129.2 (3.9)	32.0 (2.6)	97.2 (3.9)
	152.1 (6.6)		152.8 (6.6)		120.8 (7.1)
$Ba^{2+}(H_2O)_4$	107.2 (4.0)	0.3 (0.6)	107.5 (4.0)	26.3 (2.7)	81.2 (4.8)
	130.8 (3.8)		131.1 (3.8)		104.8 (4.7)
$Ba^{2+}(H_2O)_5$	91.6 (6.3)	1.1 (0.5)	92.7 (6.3)	38.1 (1.3)	54.6 (6.4)
	104.5 (5.5)		105.6 (5.5)		67.5 (5.7)
$Ba^{2+}(H_2O)_6$	76.7 (5.4)	0.7 (0.4)	77.4 (5.4)	35.0 (2.2)	42.4 (5.8)
	81.0 (4.0)		81.7 (4.0)		46.7 (4.6)
$Ba^{2+}(H_2O)_6(H_2O)$	55.6 (5.7)	4.4 (0.4)	60.0 (5.7)	41.5 (0.8)	18.5 (5.8)
	66.3 (6.7)		70.7 (6.7)		29.2 (6.7)
$Ba^{2+}(H_2O)_7$	55.0 (5.8)	0.7 (0.4)	55.7 (5.8)	33.5 (2.3)	22.2 (6.2)
$Ba^{2+}(H_2O)_6(H_2O)_2$	51.9 (4.8)	4.9 (0.5)	56.8 (4.8)	50.7 (1.0)	6.1 (4.9)
$Ba^{2+}(H_2O)_7(H_2O)$	47.5 (4.7)	4.6 (0.4)	52.1 (4.7)	47.5 (1.6)	4.6 (5.0)
$Ba^{2+}(H_2O)_8$	46.3 (3.2)	1.7 (0.4)	48.0 (3.2)	42.6 (2.2)	5.4 (3.9)

[a] Uncertainties (in parentheses) are reported to two standard deviations. [b] 0 K primary (top) and secondary (bottom) binding energies taken from Tables 1 and 2. [c] Values calculated from standard formulae and molecular constants determined at the B3LYP/def2-TZVP level of theory. Uncertainties are evaluated by scaling the frequencies up and down by 10%

Table S5. Parameters of Eq 1 Used to Model Cross Sections for Collision-Induced Dissociation of $Ba^{2+}(H_2O)_3$

reactant	product	σ_0	n	E_0 (eV)
$Ba^{2+}(H_2O)_3$[a]	$Ba^{2+}(H_2O)_2$[b]	39 (4)	0.8 (0.1)	1.33 (0.04)
$Ba^{2+}(H_2O)_3$[b]	$Ba^{2+}(H_2O)_2$[c]	36	0.9	1.16
	$BaOH^+$[c]			1.05
	$Ba^{2+}(H_2O)_2$[d]	0.3	0.9	0.43
	$BaOH^+$[d]			0.42

[a] Reactant beam produced under thermalized conditions. Fitting parameters are taken from Table 1 and represent a modeled zero pressure extrapolated thermalized cross section. [b] Reactant beam produced under conditions to optimize intensity with P(Xe) = 0.19 mTorr. [c] Values are from simultaneously modeling cross sections of the primary water loss channel (no tail) and the $BaOH^+$ product. [d] Values are from simultaneously modeling the tail and $BaOH^+$ channel (unable to accurately produce the threshold of the latter).

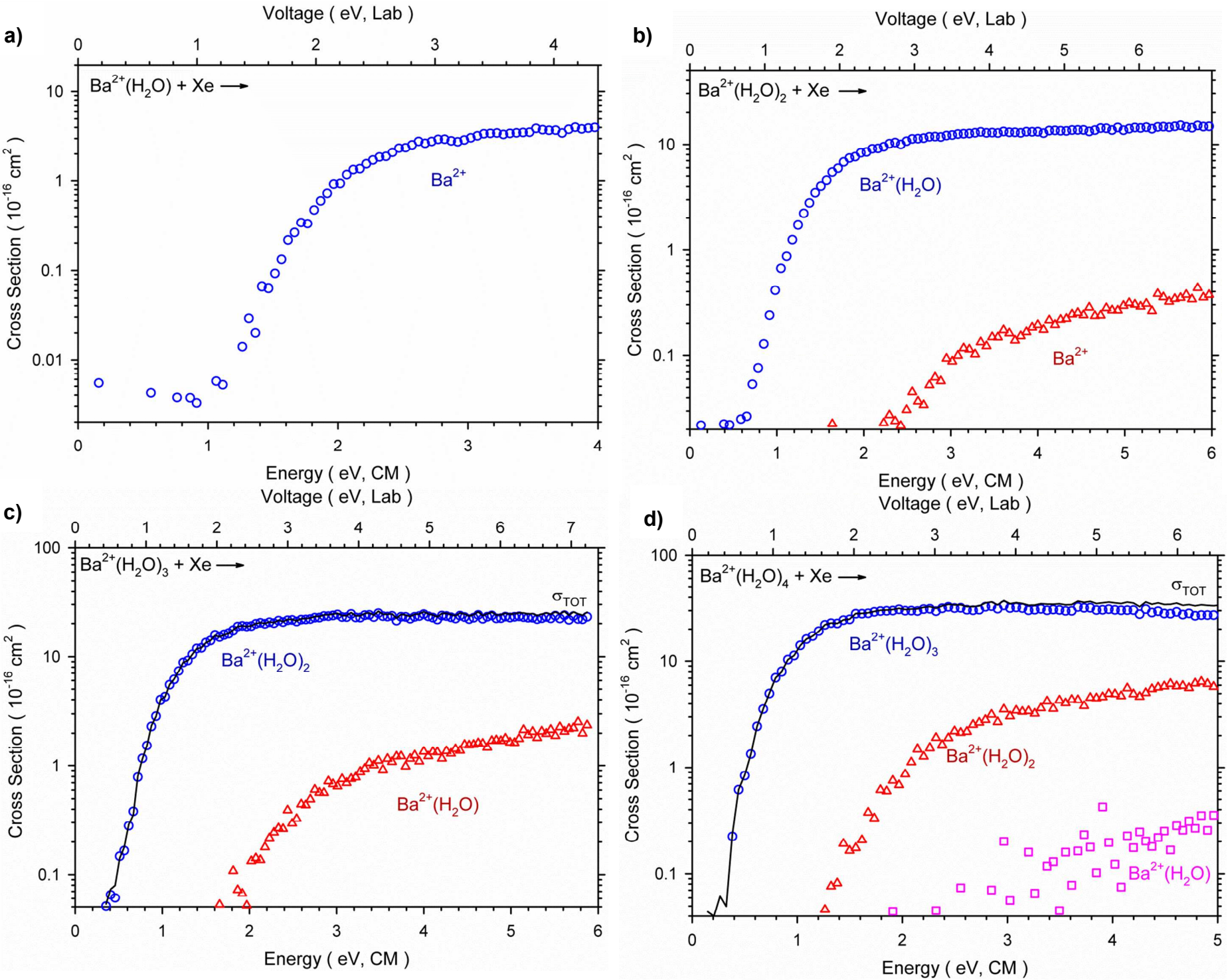
Figure Captions

Figure S1. Cross sections for collision-induced dissociation of $Ba^{2+}(H_2O)_x$ where $x = 1 – 8$ (parts a – h, respectively) with xenon at ≈ 0.2 mTorr as a function of kinetic energy in the CM frame (lower x-axis) and the laboratory frame voltage (upper x-axis).

Figure S2. Zero pressure extrapolated total cross sections for CID of $Ba^{2+}(H_2O)_x$ where $x = 1 – 8$ with xenon (parts a – h, respectively) as a function of kinetic energy in the CM frame (lower x-axis) and the laboratory frame voltage (upper x-axis). Solid lines represent the best fits to the experimental data using eq 1 convoluted over the neutral and ion kinetic and internal energy distributions. Dashed lines show the models in the absence of experimental kinetic energy broadening for reactants having an internal energy of 0 K.

Figure S3. Zero pressure extrapolated total cross sections for sequential water loss from $Ba^{2+}(H_2O)_x$, $x = 2 – 8$ with xenon (parts a – g, respectively) as a function of kinetic energy in the CM frame (lower x-axis) and the laboratory frame (upper x-axis). Solid lines represents the best fit to the experimental data using the modified version of eq 1 for sequential channels convoluted over the neutral and ion kinetic and internal energy distributions. Dashed lines show the models in the absence of experimental kinetic energy broadening for reactants having an internal energy of 0 K.

Figure S4. Reaction coordinates for water loss and charge separation pathways of $Ba^{2+}(H_2O)_2$. Energies (kJ/mol) are calculated at the B3LYP/def2-TZVPP level of theory and include zero-point energies.


a)
Voltage (eV, Lab)
Ba2+(H2O) + Xe
Ba2+
Cross Section (10-16 cm2)
Energy (eV, CM)
b)
Voltage (eV, Lab)
Ba2+(H2O)2 + Xe
Ba2+(H2O)
Ba2+
Cross Section (10-16 cm2)
Energy (eV, CM)
c)
Voltage (eV, Lab)
Ba2+(H2O)3 + Xe
σTOT
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)
d)
Voltage (eV, Lab)
Ba2+(H2O)4 + Xe
σTOT
Ba2+(H2O)3
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)

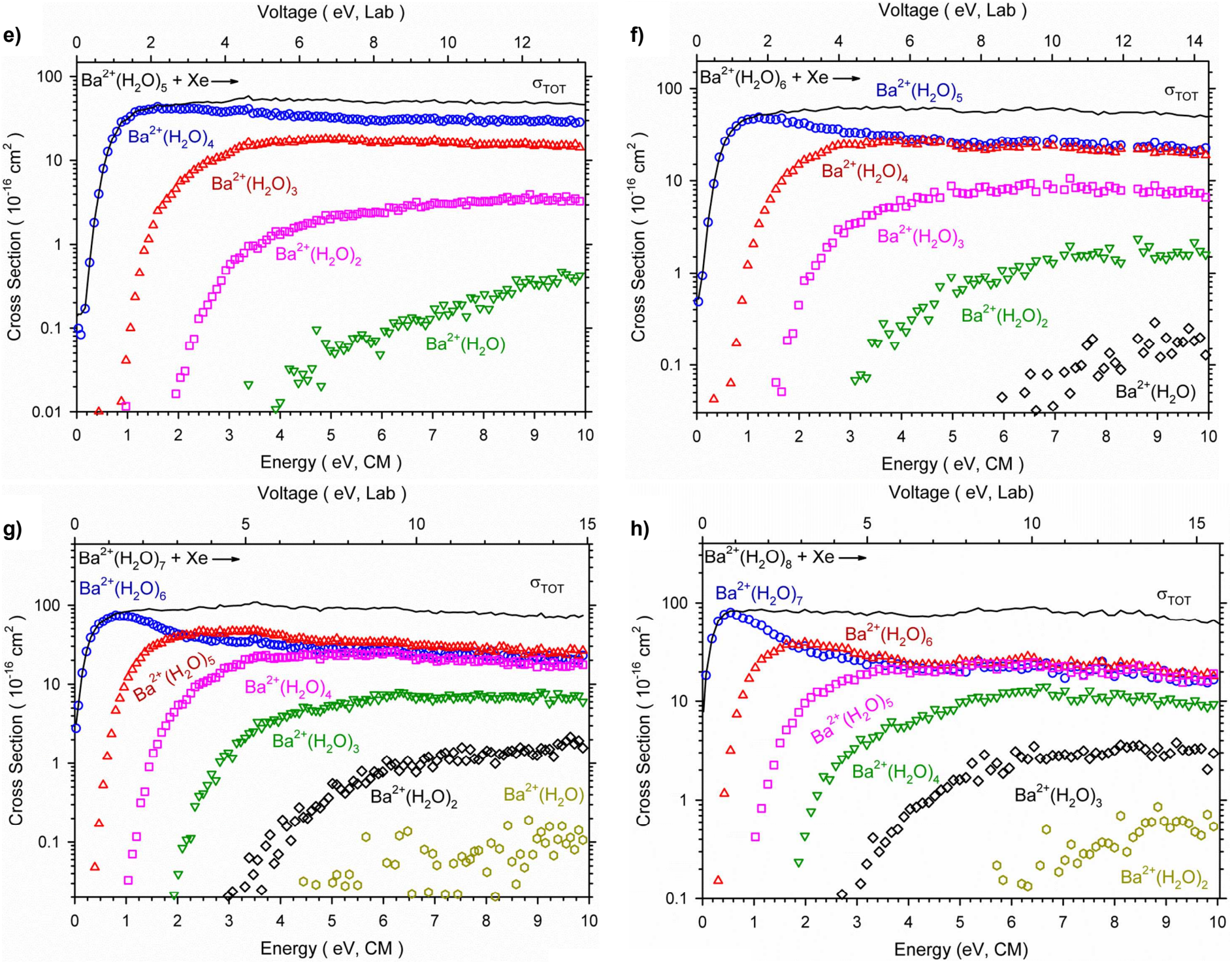
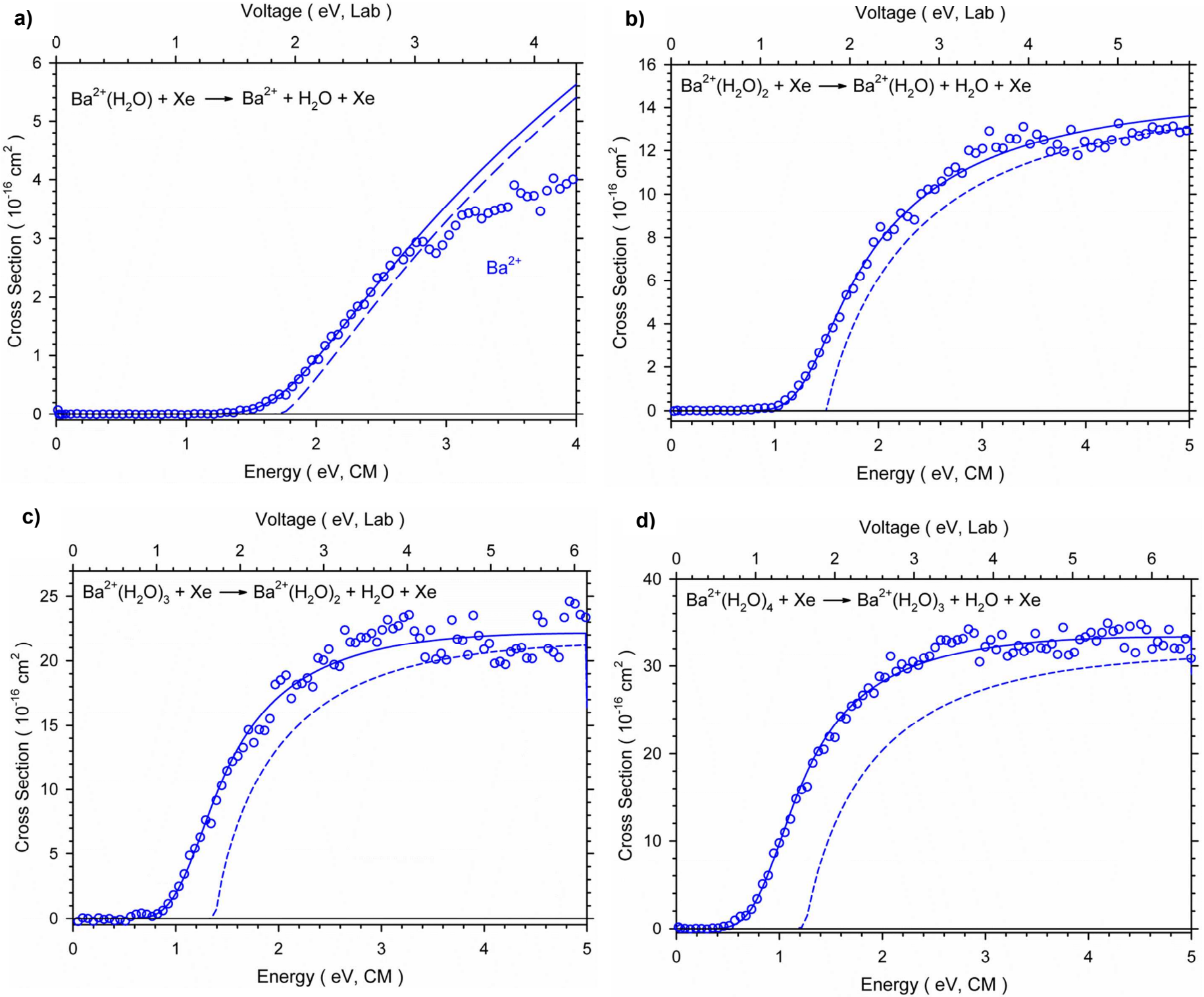

e)
Voltage (eV, Lab)
Ba2+(H2O)5 + Xe
σTOT
Ba2+(H2O)4
Ba2+(H2O)3
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)
f)
Voltage (eV, Lab)
Ba2+(H2O)6 + Xe
σTOT
Ba2+(H2O)5
Ba2+(H2O)4
Ba2+(H2O)3
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)
g)
Voltage (eV, Lab)
Ba2+(H2O)7 + Xe
σTOT
Ba2+(H2O)6
Ba2+(H2O)5
Ba2+(H2O)4
Ba2+(H2O)3
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)
h)
Voltage (eV, Lab)
Ba2+(H2O)8 + Xe
σTOT
Ba2+(H2O)7
Ba2+(H2O)6
Ba2+(H2O)5
Ba2+(H2O)4
Ba2+(H2O)3
Ba2+(H2O)2
Cross Section (10-16 cm2)
Energy (eV, CM)

Figure S1


a)
Voltage (eV, Lab)
Ba2+(H2O) + Xe ⟶ Ba2+ + H2O + Xe
Ba2+
Cross Section (10-16 cm2)
Energy (eV, CM)
b)
Voltage (eV, Lab)
Ba2+(H2O)2 + Xe ⟶ Ba2+(H2O) + H2O + Xe
Cross Section (10-16 cm2)
Energy (eV, CM)
c)
Voltage (eV, Lab)
Ba2+(H2O)3 + Xe ⟶ Ba2+(H2O)2 + H2O + Xe
Cross Section (10-16 cm2)
Energy (eV, CM)
d)
Voltage (eV, Lab)
Ba2+(H2O)4 + Xe ⟶ Ba2+(H2O)3 + H2O + Xe
Cross Section (10-16 cm2)
Energy (eV, CM)

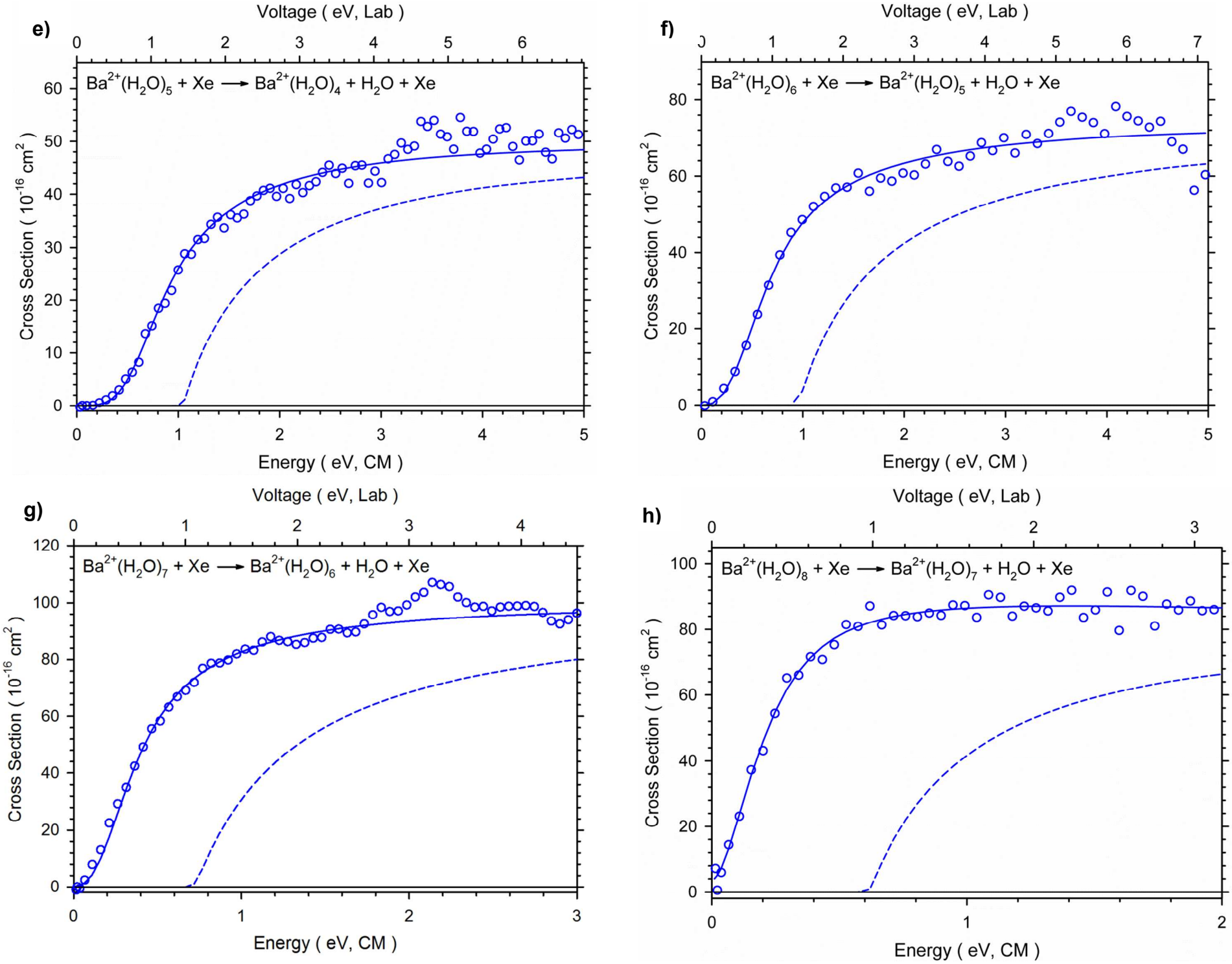
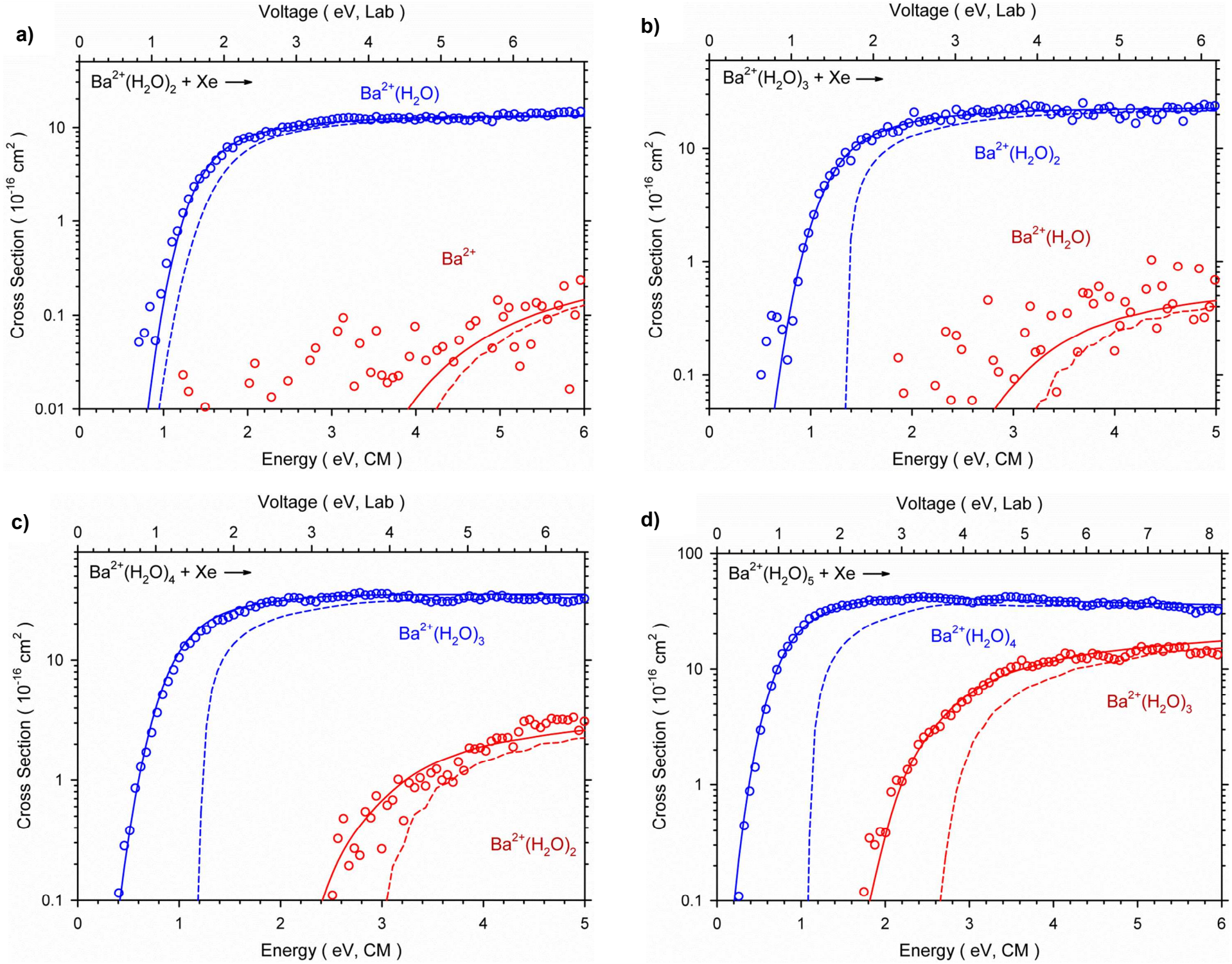
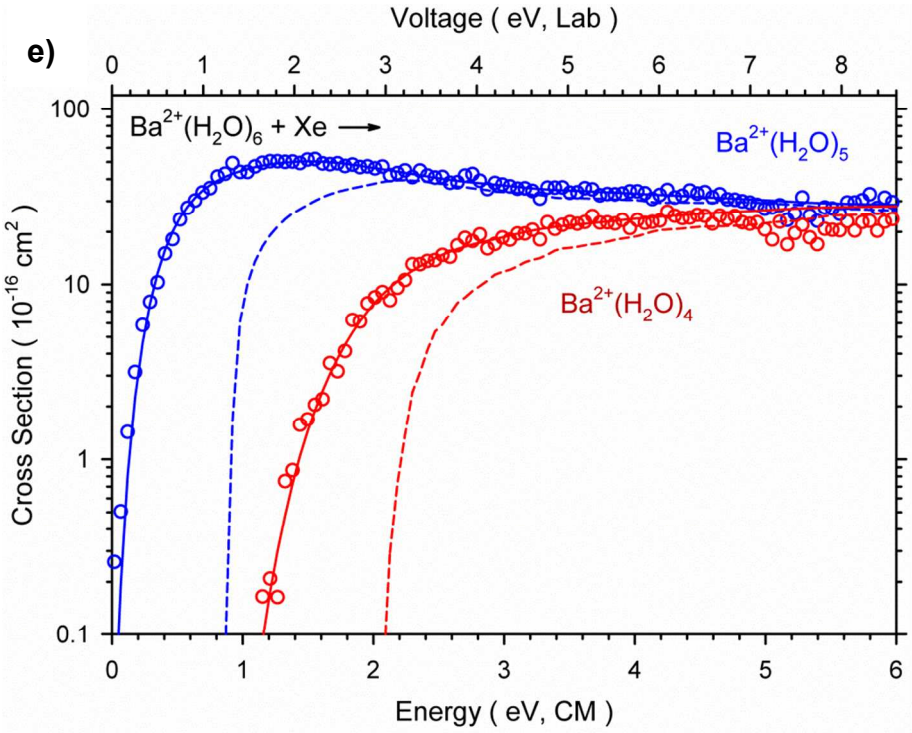
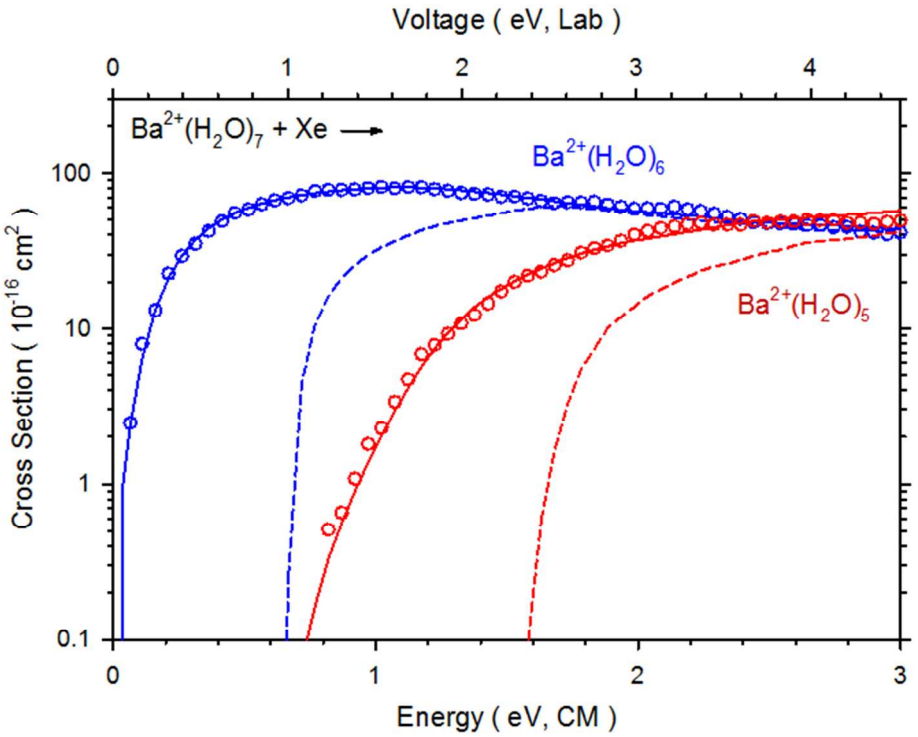

e)
Voltage (eV, Lab)
$Ba^{2+}(H_2O)_5 + Xe \longrightarrow Ba^{2+}(H_2O)_4 + H_2O + Xe$
Cross Section (10^{-16} cm^2)
Energy (eV, CM)
f)
Voltage (eV, Lab)
$Ba^{2+}(H_2O)_6 + Xe \longrightarrow Ba^{2+}(H_2O)_5 + H_2O + Xe$
Cross Section (10^{-16} cm^2)
Energy (eV, CM)
g)
Voltage (eV, Lab)
$Ba^{2+}(H_2O)_7 + Xe \longrightarrow Ba^{2+}(H_2O)_6 + H_2O + Xe$
Cross Section (10^{-16} cm^2)
Energy (eV, CM)
h)
Voltage (eV, Lab)
$Ba^{2+}(H_2O)_8 + Xe \longrightarrow Ba^{2+}(H_2O)_7 + H_2O + Xe$
Cross Section (10^{-16} cm^2)
Energy (eV, CM)

Figure S2


a)
Voltage (eV, Lab)
Ba2+(H2O)2 + Xe
Ba2+(H2O)
Ba2+
Cross Section (10-16 cm2)
Energy (eV, CM)
b)
Voltage (eV, Lab)
Ba2+(H2O)3 + Xe
Ba2+(H2O)2
Ba2+(H2O)
Cross Section (10-16 cm2)
Energy (eV, CM)
c)
Voltage (eV, Lab)
Ba2+(H2O)4 + Xe
Ba2+(H2O)3
Ba2+(H2O)2
Cross Section (10-16 cm2)
Energy (eV, CM)
d)
Voltage (eV, Lab)
Ba2+(H2O)5 + Xe
Ba2+(H2O)4
Ba2+(H2O)3
Cross Section (10-16 cm2)
Energy (eV, CM)


e)
Voltage (eV, Lab)
0 1 2 3 4 5 6 7 8
Ba2+(H2O)6 + Xe ⟶
Ba2+(H2O)5
Ba2+(H2O)4
Cross Section (10-16 cm2)
100
10
1
0.1
0 1 2 3 4 5 6
Energy (eV, CM)


f)
Voltage (eV, Lab)
0 1 2 3 4
Ba2+(H2O)7 + Xe ⟶
Ba2+(H2O)6
Ba2+(H2O)5
Cross Section (10-16 cm2)
100
10
1
0.1
0 1 2 3
Energy (eV, CM)

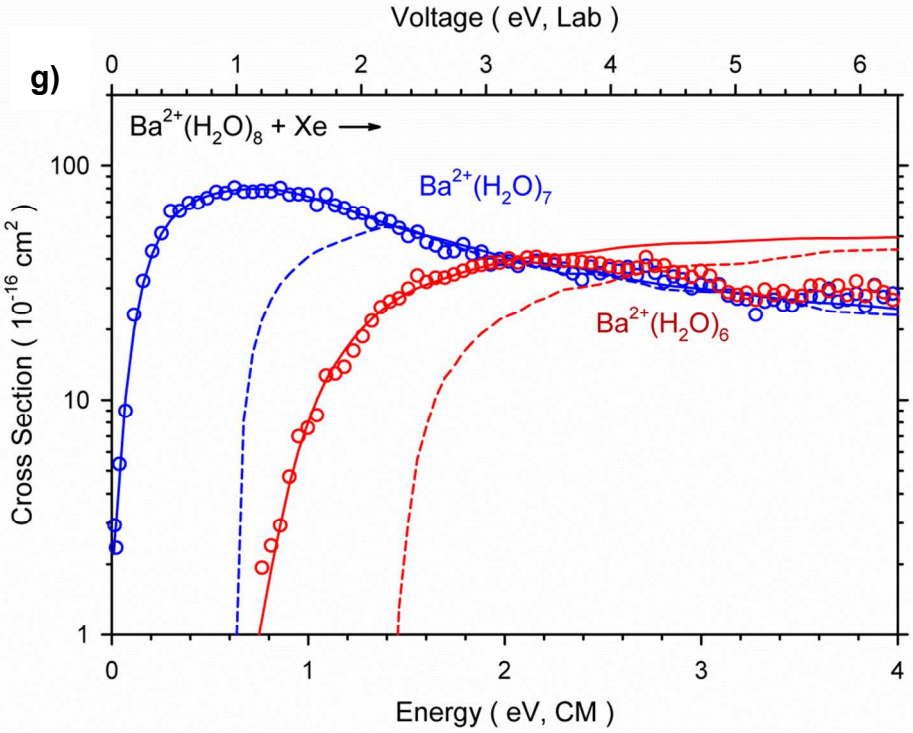

g)
Voltage (eV, Lab)
0 1 2 3 4 5 6
Ba2+(H2O)8 + Xe ⟶
Ba2+(H2O)7
Ba2+(H2O)6
Cross Section (10-16 cm2)
100
10
1
0 1 2 3 4
Energy (eV, CM)

Figure S3

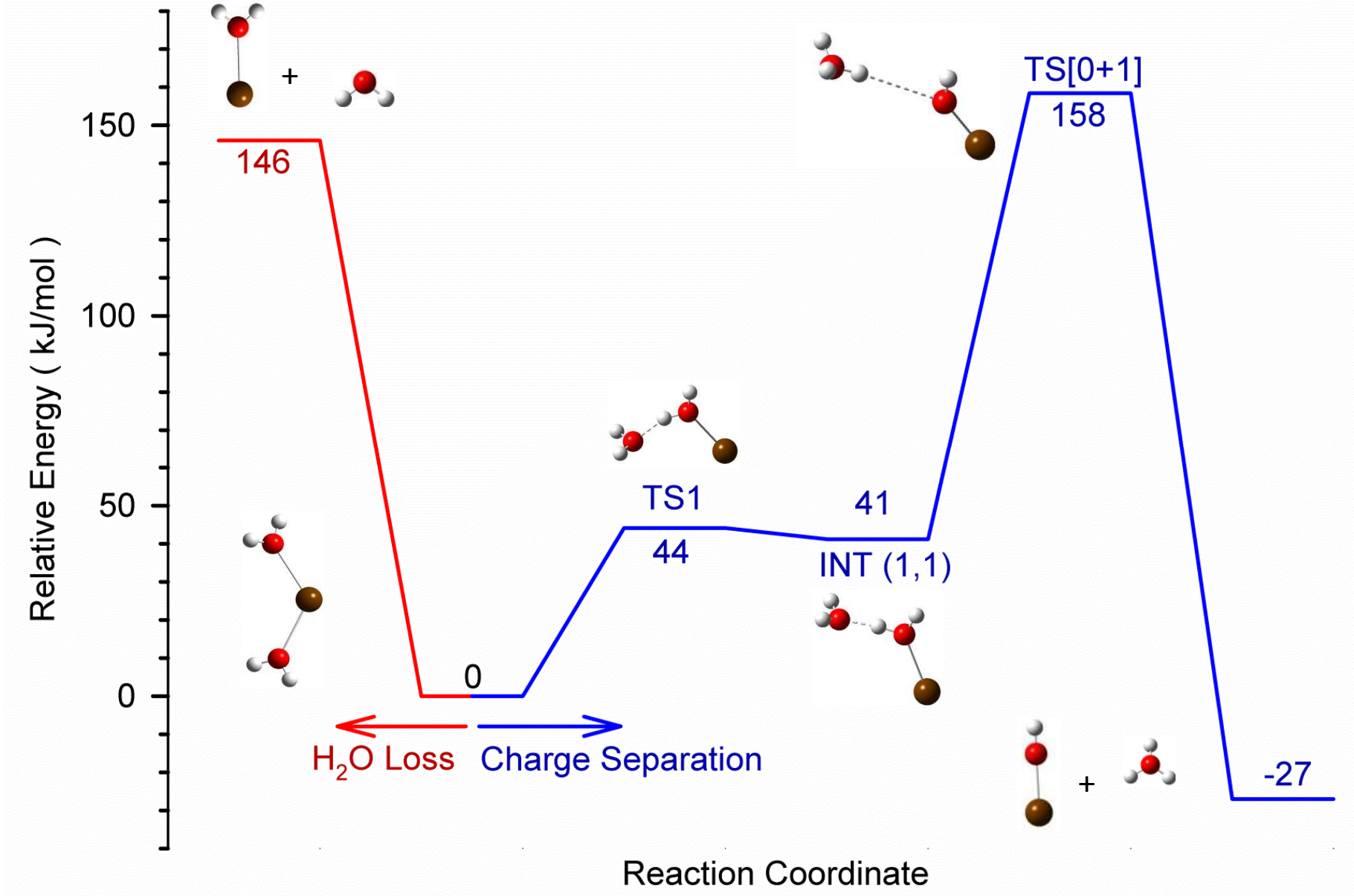

Relative Energy (kJ/mol)
150
100
50
0
146
0
TS1
44
41
INT (1,1)
TS[0+1]
158
-27
+
+
H2O Loss
Charge Separation
Reaction Coordinate

Figure S4