Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for:

"Binding Energies of Hydrated Cobalt(II) By Collision-Induced Dissociation and Theoretical Studies: Evidence for a New Critical Size"

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Table S1 is an extension of Table 1 in the manuscript and includes calculated values for all isomers explored. Table S1 provides the relative single point energies for low energy conformers of $Co^{2+}(H_2O)_x$ (x = 4 – 11). Tables S2 and S3 provide the electronic energies of all complexes listed in Table S1 including zero point corrections from the geometry optimization and single point energy calculations, where Table S2 refers to calculations performed from the B3LYP/6-311+G(d,p) geometry optimizations and Table S3 refers to calculations performed from the B3LYP-GD3BJ/6-311+G(d,p) geometry optimizations . Figures S1 – S3 show the reaction coordinates comparing the loss of water versus charge separation pathways from $Co^{2+}(H_2O)_x$ for x = 7, 6, and 4, respectively.

Table S1. Theoretical Relative Enthalpy (ΔH_0) and Free Energies (ΔG_{298})[a] (kJ/mol) for Hydrated Cobalt Complexes [a]

	complex (*x*,*y*,*z*)[b]	B3LYP	B3LYP-GD3BJ[c]	B3P86	MP2(full)
$Co^{2+}(H_2O)_4$	(4,0)	**0.0 (0.0)**	**0.0 (0.0)**	**0.0 (0.0)**	**0.0 (0.0)**
	(3,1)_A	52.8 (52.7)	56.6 (56.5)	50.8 (50.6)	80.5 (80.4)
$Co^{2+}(H_2O)_5$	(4,1)_AA	**0.0 (0.0)**	**0.0 (0.0)**	**0.0 (0.0)**	**0.0 (0.0)**
	(4,1)_A	2.0 (6.2)	5.1 (9.3)	1.8 (6.1)	6.4 (10.7)
	(5,0)	17.0 (26.4)	13.5 (22.8)	16.4 (25.8)	7.8 (17.1)
$Co^{2+}(H_2O)_6$	(4,2)_4D_2AA	**0.0 (0.0)**	3.0 **(0.0)**	**0.0 (0.0)**	19.5 (12.7)
	(4,2)_3D_AA_A	5.3 (8.8)	11.2 (11.6)	5.1 (8.6)	29.6 (26.2)
	(4,2)_2D,DD_2AA	11.1 (10.0)	13.7 (9.6)	11.6 (10.6)	31.8 (24.0)
	(5,1)_A_aA_b	7.1 (10.1)	6.9 (6.8)	7.5 (10.5)	39.2 (35.4)
	(5,1)_A_bA_b	16.5 (17.9)	16.2 (14.5)	15.6 (16.9)	27.3 (21.9)
	(6,0) T_h	6.3 (10.5)	16.6 (17.8)	7.2 (11.4)	17.5 (14.9)
	(6,0) D_{2h}	4.9 (11.7)	**0.0** (3.7)	5.8 (12.5)	**0.0 (0.0)**
$Co^{2+}(H_2O)_7$	(4,3)_3D,DD_2AA,A	**0.0 (0.0)**	4.5 **(0.0)**	**0.0 (0.0)**	20.3 (17.4)
	(4,3)_2D,2DD_3AA	8.3 (5.2)	9.0 (4.1)	9.1 (6.0)	20.3 (20.7.)
	(4,3)_4D_AA_2A	1.0 (2.0)	8.0 (7.4)	0.5 (1.6)	26.7 (20.7)
	(5,2)_2D,DD_2AA	9.2 (8.4)	7.2 (4.6)	8.0 (7.2)	11.6 (9.0)
	(5,2)_4D_2AA	5.2 (3.7)	3.3 (2.7)	3.6 (2.0)	9.3 (4.9)
	(6,1)_AA	6.8 (9.7)	**0.0** (1.1)	7.0 (9.9)	**0.0 (0.0)**
$Co^{2+}(H_2O)_8$	(4,4)_2D,2DD_2A,2AA	5.7 (8.6)	15.0 (18.0)	6.6 (9.6)	20.8 (20.6)
	(4,4)_2D,2DD_2AA,AD_2,AA_2	19.0 (18.2)	23.5 (22.8)	20.4 (19.6)	32.1 (28.2)
	(4,4)_3D,DD_A,AA,AD_2,AA_2	12.9 (14.9)	21.2 (23.2)	13.9 (15.9)	28.9 (27.6)
	(4,4)_4DD_4AA	10.0 (7.2)	12.6 (9.8)	12.2 (9.4)	20.3 (14.4)
	(5,3)_2D,2DD_3A_bA_b	**0.0 (0.0)**	4.3 **(0.0)**	**0.0 (0.0)**	16.1 (12.9)
	(5,3)_2D,2DD_2A_bA_b,A_aA_b	6.8 (5.6)	6.7 (5.5)	5.4 (4.2)	8.4 (4.0)
	(5,3)_4D,DD_3AA	9.3 (8.6)	9.2 (8.4)	8.2 (7.5)	10.2 (6.2)
	(6,2)_2D,DD_2AA	21.7 (24.9)	16.7 (19.9)	21.4 (24.7)	7.6 (7.7)

	complex (*x*,*y*,*z*)[b]	B3LYP	B3LYP-GD3BJ[c]	B3P86	MP2(full)
	(6,2)_4D_2AA$_g$	9.9 (13.1)	4.9 (8.1)	10.4 (13.6)	15.9 (15.9)
	(6,2)_4D_2AA$_t$	13.8 (17.0)	**0.0** (2.0)	13.9 (17.0)	**0.0 (0.0)**
$Co^{2+}(H_2O)_9$	(4,4,1)_2D,2DD_2AA,2AD_AA	16.1 (18.4)	28.1 (27.1)	18.2 (20.5)	45.7 (44.8)
	(4,4,1)_2D,2DD_A,2AD_2AA	14.2 (18.1)	28.6 (29.3)	15.8 (19.7)	47.5 (48.1)
	(4,5)_2D,2DD_AA,2A,AD$_2$,AA$_2$	8.9 (14.4)	24.1 (26.3)	11.1 (16.6)	41.1 (43.3)
	(4,5)_D,3DD_2AA,3A	2.4 (8.9)	18.7 (21.9)	4.5 (10.9)	34.0 (37.2)
	(4,5)_D,3DD_2AA,A,AD$_2$,AA$_2$	11.7 (15.1)	23.4 (23.5)	14.2 (17.6)	45.4 (45.4)
	(5,4)_2D,3DD_4AA	**0.0 (0.0)**	4.5 (1.3)	**0.0 (0.0)**	16.7 (13.4)
	(5,4)_3D,2DD_A,3AA	6.4 (9.2)	12.9 (12.5)	6.3 (9.1)	24.5 (24.1)
	(5,4)_4D,DD_2AA,AD$_2$,AA$_2$	14.1 (15.9)	20.0 (18.5)	13.9 (15.7)	33.6 (32.1)
	(5,4)_4DD_4AA	1.2 (1.7)	4.9 (2.1)	0.7 (1.2)	16.1 (13.4)
	(6,3)_2D,2DD_3AA	6.5 (11.1)	5.3 (6.6)	7.7 (12.2)	6.3 (7.6)
	(6,3)_4D,DD_3AA	2.6 (6.6)	1.8 (2.6)	3.9 (7.9)	1.9 (2.7)
	(6,3)_6D_3AA	0.6 (3.9)	**0.0 (0.0)**	1.7 (5.0)	**0.0 (0.0)**
$Co^{2+}(H_2O)_{10}$	(4,4,2)_4D,4AD_2AA	20.7 (22.5)	36.8 (37.2)	22.1 (23.9)	55.9 (56.3)
	(4,4,2)_4DD,2AA_2AAD,2A	17.2 (16.2)	29.1 (26.6)	18.4 (17.4)	48.1 (45.6)
	(4,5,1)_2D,2DD_2AA,A,2AD_AA	11.5 (13.1)	25.7 (25.9)	14.1 (15.8)	41.3 (41.5)
	(4,5,1)_D,3DD_2A,AA,AAD,AD_AA	19.9 (22.0)	34.0 (34.6)	21.6 (23.7)	50.6 (51.2)
	(4,6)_4DD,2AA_4A	0.2 (6.7)	18.8 (23.8)	3.1 (9.6)	31.3 (36.4)
	(5,4,1)_4DD,4AA_A	7.3 (6.4)	13.2 (10.8)	6.0 (5.1)	24.0 (21.6)
	(5,5)_D,4DD_3AA,AAD_AA	9.5 (6.7)	10.3 (6.1)	9.3 (6.5)	20.4 (16.2)
	(5,5)_D,4DD_4AA,A	**0.0 (0.0)**	5.9 (4.5)	**0.0 (0.0)**	15.8 (14.4)
	(6,4)_4D,2DD_4AA S_4	3.2 (4.6)	**0.0 (0.0)**	4.6 (6.0)	**0.0 (0.0)**
	(6,4)_4D,2DD_4AA C_1	13.7 (14.8)	11.8 (11.4)	13.7 (14.8)	12.4 (12.0)
	(6,4)_4DD,4AA	17.4 (19.8)	14.8 (15.7)	18.7 (21.0)	14.1 (15.0)
	(6,4)_5D,DD_2AA,AAD$_2$,AA$_2$	5.7 (6.3)	2.3 (1.4)	30.1 (30.7)	1.2 (0.3)
$Co^{2+}(H_2O)_{11}$	(4,4,3)_4DD,AA_3AAD,3A	19.6 (16.6)	35.3 (35.2)	17.3 (16.8)	55.4 (55.4)
	(4,6,1)_4DD,4A_AA,AAD_A	6.1 (9.8)	28.4 (34.9)	5.4 (11.5)	42.6 (49.1)

complex $(x,y,z)^{b}$	B3LYP	B3LYP-GD3BJ^{c}	B3P86	MP2(full)
(5,4,2)_4DD,2AA_2AAD,2A	10.5 (7.0)	20.0 (19.4)	5.4 (4.4)	32.4 (31.8)
(5,5,1)_D,4DD_A,3AA,AAD_A	3.8 (1.3)	13.4 (13.8)	**0.0 (0.0)**	24.6 (25.0)
(5,6)_5DD_4AA,2A	**0.0 (0.0)**	9.3 (12.2)	0.6 (3.1)	34.4 (37.3)
(6,5)_4D,2DD_AA,2AAD$_2$,2AA$_2$	8.5 (3.1)	3.6 (1.1)	6.1 (3.1)	23.7 (21.2)
(6,5)_D,4DD_4AA,A	22.2 (21.7)	22.4 (24.9)	20.5 (22.6)	22.6 (25.1)
(6,5)_3D,3DD_3AA,AAD$_2$_AA$_2$	6.2 (1.9)	3.4 (2.0)	3.9 (2.1)	30.6 (29.3)
(6,5)_2D,4DD_5AA	3.5 (0.5)	**0.0 (0.0)**	1.3 (0.9)	**0.0 (0.0)**
(6,4,1)_4D,2DD_3AA,AAD_A	17.6 (15.9)	19.1 (20.3)	13.7 (14.5)	21.1 (22.3)

$^{a}\Delta G_{298}$ values are given in parentheses. Values are single-point energies calculated at the level shown using a 6-311+G(2d,2p) basis set from geometries optimized at the B3LYP/6-311+G(d,p) level except as noted. Zero point energy corrections are included. ^{b}To differentiate otherwise similar structures, several additions to the nomenclature were made: 1) the point group symmetry may be added; 2) subscripts "a" and "b" refer to apex and base sites in an inner shell of five waters; 3) O – M^{2+} – O angles denoted as subscript "g" (gauche) for angles between 45° and 135°, and "t" (trans) for angles >135°; 4) waters that can be assigned to two shells and always indicate a cyclic structure are denoted with a subscript "2". ^{c}Geometries optimized at B3LYP-GD3BJ/6-311+G(d,p) level.

Table S2. Electronic Energies and Electronic (Hartrees) for $Co^{2+}(H_2O)_n$ Complexes[a]

n	Complex (*x*,*y*,*z*)	B3LYP/6-311+G(d,p)	B3LYP[b]	B3P86[b]	MP2(full)[b]
4	(4,0)	-1688.0685 (-1687.9697)	-1688.0807 (-1687.9819)	-1689.3160 (-1689.2172)	-1686.8288 (-1686.7300)
	(3,1)_A	-1688.0475 (-1687.9496)	-1688.0583 (-1687.9604)	-1689.2958 (-1689.1979)	-1686.7973 (-1686.6994)
5	(4,1)_AA	-1764.5753 (-1764.4504)	-1764.5912 (-1764.4662)	-1766.0003 (-1765.8753)	-1763.1922 (-1763.0672)
	(4,1)_A	-1764.5724 (-1764.4496)	-1764.5871 (-1764.4643)	-1765.9974 (-1765.8746)	-1763.1876 (-1763.0648)
	(5,0)	-1764.5680 (-1764.4439)	-1764.5852 (-1764.4610)	-1765.9932 (-1765.8690)	-1763.1884 (-1763.0643)
6	(4,2)_4D_2AA	-1841.0798 (-1840.9293)	-1841.0991 (-1840.9485)	-1842.6819 (-1842.5314)	-1839.5537 (-1839.4031)
	(4,2)_3D_AA_A	-1841.0764 (-1840.9272)	-1841.0946 (-1840.9454)	-1842.6786 (-1842.5294)	-1839.5484 (-1839.3992)
	(4,2)_2D,DD_2AA	-1841.0760 (-1840.9250)	-1841.0955 (-1840.9445)	-1842.6779 (-1842.5269)	-1839.5494 (-1839.3992)
	(5,1)_A_aA_b	-1841.0760 (-1840.9265)	-1841.0965 (-1840.9471)	-1842.6779 (-1842.5285)	-1839.5450 (-1839.3956)
	(5,1)_A_bA_b	-1841.0730 (-1840.9230)	-1841.0936 (-1840.9435)	-1842.6755 (-1842.5254)	-1839.5502 (-1839.4001)
	(6,0) T_h	-1841.0748 (-1840.9268)	-1841.0913 (-1840.9434)	-1842.6765 (-1842.5286)	-1839.5584 (-1839.4105)
	(6,0) D_{2h}	-1841.0753 (-1840.9274)	-1841.0967 (-1840.9497)	-1842.6771 (-1842.5292)	-1839.5518 (-1839.4038)
7	(4,3)_3D,DD_2AA,A	-1917.5761 (-1917.4014)	-1917.5977 (-1917.4230)	-1919.3552 (-1919.1805)	-1915.9057 (-1915.7310)
	(4,3)_2D,2DD_3AA	-1917.5754 (-1917.3983)	-1917.5984 (-1917.4212)	-1919.3541 (-1919.1770)	-1915.9056 (-1915.7285)
	(4,3)_4D_AA_2A	-1917.5746 (-1917.4011)	-1917.5951 (-1917.4216)	-1919.3537 (-1919.1803)	-1915.9022 (-1915.7287)
	(5,2)_2D,DD_2AA	-1917.5740 (-1917.3979)	-1917.5979 (-1917.4219)	-1919.3535 (-1919.1774)	-1915.9080 (-1915.7320)
	(5,2)_4D_2AA	-1917.5758 (-1917.3994)	-1917.5997 (-1917.4234)	-1919.3554 (-1919.1791)	-1915.9077 (-1915.7313)
	(6,1)_AA	-1917.5723 (-1917.3988)	-1917.5981 (-1917.4247)	-1919.3513 (-1919.1778)	-1915.9122 (-1915.7387)
8	(4,4)_2D,2DD_2A,2AA	-1994.0702 (-1993.8716)	-1994.0939 (-1993.8953)	-1996.0259 (-1995.8274)	-1992.2557 (-1992.0572)
	(4,4)_2D,2DD_2AA,AD_2,AA_2	-1994.0673 (-1993.8665)	-1994.0929 (-1993.8921)	-1996.0229 (-1995.8221)	-1992.2536 (-1992.0529)
	(4,4)_3D,DD_A,AA,AD_2,AA_2	-1994.0676 (-1993.8689)	-1994.0918 (-1993.8930)	-1996.0234 (-1995.8246)	-1992.2529 (-1992.0541)
	(4,4)_4DD_4AA	-1994.0730 (-1993.8700)	-1994.0994 (-1993.8963)	-1996.0283 (-1995.8252)	-1992.2604 (-1992.0573)
	(5,3)_2D,2DD_3A_bA_b	-1994.0750 (-1993.8738)	-1994.1023 (-1993.9011)	-1996.0311 (-1995.8299)	-1992.2602 (-1992.0590)
	(5,3)_2D,2DD_2A_bA_b,A_aA_b	-1994.0732 (-1993.8712)	-1994.1005 (-1993.8985)	-1996.0298 (-1995.8278)	-1992.2639 (-1992.0619)
	(5,3)_4D,DD_3AA	-1994.0720 (-1993.8702)	-1994.0994 (-1993.8976)	-1996.0286 (-1995.8268)	-1992.2630 (-1992.0612)
	(6,2)_2D,DD_2AA	-1994.0648 (-1993.8655)	-1994.0940 (-1993.8947)	-1996.0210 (-1995.8218)	-1992.2615 (-1992.0622)

n	Complex (x,y,z)	B3LYP/6-311+G(d,p)	B3LYP[b]	B3P86[b]	MP2(full)[b]
	(6,2)_4D_2AA$_g$	-1994.0693 (-1993.8700)	-1994.0985 (-1993.8992)	-1996.0252 (-1995.8260)	-1992.2583 (-1992.0590)
	(6,2)_4D_2AA$_t$	-1994.0678 (-1993.8685)	-1994.0970 (-1993.8977)	-1996.0239 (-1995.8246)	-1992.2644 (-1992.0651)
9	(4,4,1)_2D,2DD_2AA,2AD_AA	-2070.5585 (-2070.3337)	-2070.5861 (-2070.3613)	-2072.6909 (-2072.4660)	-2068.6012 (-2068.3763)
	(4,4,1)_2D,2DD_A,2AD_2AA	-2070.5579 (-2070.3345)	-2070.5845 (-2070.3610)	-2072.6904 (-2072.4670)	-2068.5991 (-2068.3757)
	(4,5)_2D,2DD_AA,2A,AD$_2$,AA$_2$	-2070.5595 (-2070.3364)	-2070.5858 (-2070.3628)	-2072.6918 (-2072.4687)	-2068.6011 (-2068.3781)
	(4,5)_D,3DD_2AA,3A	-2070.5618 (-2070.3389)	-2070.5877 (-2070.3648)	-2072.6941 (-2072.4713)	-2068.6037 (-2068.3808)
	(4,5)_D,3DD_2AA,A,AD$_2$,AA$_2$	-2070.5600 (-2070.3354)	-2070.5877 (-2070.3630)	-2072.6922 (-2072.4675)	-2068.6011 (-2068.3765)
	(5,4)_2D,3DD_4AA	-2070.5676 (-2070.3398)	-2070.5980 (-2070.3702)	-2072.7008 (-2072.4730)	-2068.6152 (-2068.3874)
	(5,4)_3D,2DD_A,3AA	-2070.5631 (-2070.3374)	-2070.5927 (-2070.3670)	-2072.6963 (-2072.4706)	-2068.6101 (-2068.3844)
	(5,4)_4D,DD_2AA,AD$_2$,AA$_2$	-2070.5605 (-2070.3345)	-2070.5903 (-2070.3643)	-2072.6937 (-2072.4677)	-2068.6070 (-2068.3810)
	(5,4)_4DD_4AA	-2070.5669 (-2070.3394)	-2070.5976 (-2070.3701)	-2072.7002 (-2072.4727)	-2068.6151 (-2068.3876)
	(6,3)_2D,2DD_3AA	-2070.5620 (-2070.3374)	-2070.5946 (-2070.3699)	-2072.6947 (-2072.4700)	-2068.6161 (-2068.3914)
	(6,3)_4D,DD_3AA	-2070.5638 (-2070.3389)	-2070.5962 (-2070.3713)	-2072.6964 (-2072.4715)	-2068.6179 (-2068.3930)
	(6,3)_6D_3AA	-2070.5650 (-2070.3396)	-2070.5973 (-2070.3719)	-2072.6977 (-2072.4723)	-2068.6191 (-2068.3938)
10	(4,4,2)_4D,4AD_2AA	-2147.0446 (-2146.7970)	-2147.0736 (-2146.8261)	-2149.3539 (-2149.1064)	-2144.9415 (-2144.6940)
	(4,4,2)_4DD,2AA_2AAD,2A	-2147.0497 (-2146.7984)	-2147.0803 (-2146.8290)	-2149.3590 (-2149.1078)	-2144.9482 (-2144.6970)
	(4,5,1)_2D,2DD_2AA,A,2AD_AA	-2147.0497 (-2146.8006)	-2147.0794 (-2146.8303)	-2149.3585 (-2149.1094)	-2144.9487 (-2144.6996)
	(4,5,1)_D,3DD_2A,AA,AAD,AD_AA	-2147.0465 (-2146.7974)	-2147.0762 (-2146.8271)	-2149.3557 (-2149.1065)	-2144.9451 (-2144.6960)
	(4,6)_4DD,2AA_4A	-2147.0513 (-2146.8048)	-2147.0794 (-2146.8329)	-2149.3601 (-2149.1136)	-2144.9499 (-2144.7034)
	(5,4,1)_4DD,4AA_A	-2147.0540 (-2146.8021)	-2147.0869 (-2146.8350)	-2149.3644 (-2149.1125)	-2144.9580 (-2144.7062)
	(5,5)_D,4DD_3AA,AAD_AA	-2147.0544 (-2146.8013)	-2147.0892 (-2146.8361)	-2149.3643 (-2149.1112)	-2144.9606 (-2144.7075)
	(5,5)_D,4DD_4AA,A	-2147.0564 (-2146.8049)	-2147.0893 (-2146.8378)	-2149.3662 (-2149.1148)	-2144.9607 (-2144.7093)
	(6,4)_4D,2DD_4AA S_4	-2147.0540 (-2146.8037)	-2147.0898 (-2146.8395)	-2149.3633 (-2149.1130)	-2144.9656 (-2144.7153)
	(6,4)_4D,2DD_4AA C_1	-2147.0503 (-2146.7997)	-2147.0861 (-2146.8356)	-2149.3601 (-2149.1095)	-2144.9611 (-2144.7106)
	(6,4)_4DD,4AA	-2147.0481 (-2146.7983)	-2147.0843 (-2146.8344)	-2149.3575 (-2149.1077)	-2144.9597 (-2144.7099)
	(6,4)_5D,DD_2AA,AAD$_2$,AA$_2$	-2147.0534 (-2146.8028)	-2147.0898 (-2146.8392)	-2149.3539 (-2149.1033)	-2144.9654 (-2144.7148)
11	(4,4,3)_4DD,AA_3AAD,3A	-2223.5361 (-2223.2609)	-2223.5688 (-2223.2937)	-2226.0224 (-2225.7472)	-2221.2907 (-2221.0155)
	(4,6,1)_4DD,4A_AA,AAD_A	-2223.5373 (-2223.2661)	-2223.5676 (-2223.2963)	-2226.0230 (-2225.7517)	-2221.2916 (-2221.0204)

n	Complex (x,y,z)	B3LYP/6-311+G(d,p)	B3LYP[b]	B3P86[b]	MP2(full)[b]
	(5,4,2)_4DD,2AA_2AAD,2A	-2223.5405 (-2223.2644)	-2223.5755 (-2223.2995)	-2226.0277 (-2225.7517)	-2221.3003 (-2221.0243)
	(5,5,1)_D,4DD_A,3AA,AAD_A	-2223.5426 (-2223.2670)	-2223.5776 (-2223.3020)	-2226.0294 (-2225.7537)	-2221.3028 (-2221.0272)
	(5,6)_5DD_4AA,2A	-2223.5427 (-2223.2684)	-2223.5778 (-2223.3035)	-2226.0278 (-2225.7535)	-2221.2978 (-2221.0235)
	(6,5)_4D,2DD_AA,2AAD$_2$,2AA$_2$	-2223.5424 (-2223.2652)	-2223.5830 (-2223.3057)	-2226.0287 (-2225.7514)	-2221.3048 (-2221.0276)
	(6,5)_D,4DD_4AA,A	-2223.5344 (-2223.2600)	-2223.5730 (-2223.2986)	-2226.0204 (-2225.7459)	-2221.3024 (-2221.0280)
	(6,5)_3D,3DD_3AA,AAD$_2$_AA$_2$	-2223.5428 (-2223.2660)	-2223.5826 (-2223.3058)	-2226.0291 (-2225.7523)	-2221.3017 (-2221.0249)
	(6,5)_2D,4DD_5AA	-2223.5431 (-2223.2671)	-2223.5831 (-2223.3071)	-2226.0293 (-2225.7532)	-2221.3126 (-2221.0366)
	(6,4,1)_4D,2DD_3AA,AAD_A	-2223.5366 (-2223.2617)	-2223.5747 (-2223.2998)	-2226.0234 (-2225.7485)	-2221.3034 (-2221.0286)

[a]Zero-(scaled by 0.989) corrected electronic energy values are given in the parentheses. [b]Values from single-point energies calculated at the level shown using a 6-311+G(2d,2p) basis set from geometries optimized at the B3LYP/6-311+G(d,p) level.

Table S3. Electronic Energies and Electronic (Hartrees) for $Co^{2+}(H_2O)_n$ Complexes[a]

n	Complex (*x*,*y*,*z*)	B3LYP-GD3BJ/6-311+G(d,p)	B3LYP-GD3BJ[b]
4	(4,0)	-1688.0741 (-1687.9753)	-1688.0807 (-1687.9819)
	(3,1)_A	-1688.0509 (-1687.9530)	-1688.0583 (-1687.9604)
5	(4,1)_AA	-1764.5828 (-1764.4579)	-1764.5912 (-1764.4662)
	(4,1)_A	-1764.5788 (-1764.4560)	-1764.5871 (-1764.4643)
	(5,0)	-1764.5771 (-1764.4529)	-1764.5852 (-1764.4610)
6	(4,2)_4D_2AA	-1841.0899 (-1840.9384)	-1841.0991 (-1840.9485)
	(4,2)_3D_AA_A	-1841.0848 (-1840.9393)	-1841.0946 (-1840.9454)
	(4,2)_2D,DD_2AA	-1841.0858 (-1840.9356)	-1841.0955 (-1840.9445)
	(5,1)_A_aA_b	-1841.0875 (-1840.9381)	-1841.0965 (-1840.9471)
	(5,1)_A_bA_b	-1841.0842 (-1840.9342)	-1841.0936 (-1840.9435)
	(6,0) T_h	-1841.0764 (-1840.9285)	-1841.0913 (-1840.9434)
	(6,0) D_{2h}	-1841.0886 (-1840.9407)	-1841.0967 (-1840.9497)
7	(4,3)_3D,DD_2AA,A	-1917.5857 (-1917.4110)	-1917.5977 (-1917.4230)
	(4,3)_2D,2DD_3AA	-1917.5877 (-1917.4105)	-1917.5984 (-1917.4212)
	(4,3)_4D_AA_2A	-1917.5838 (-1917.4103)	-1917.5951 (-1917.4216)
	(5,2)_2D,DD_2AA	-1917.5872 (-1917.4111)	-1917.5979 (-1917.4219)
	(5,2)_4D_2AA	-1917.5890 (-1917.4126)	-1917.5997 (-1917.4234)
	(6,1)_AA	-1917.5876 (-1917.4142)	-1917.5981 (-1917.4247)
8	(4,4)_2D,2DD_2A,2AA	-1994.0812 (-1993.8827)	-1994.0939 (-1993.8953)
	(4,4)_2D,2DD_2AA,AD_2,AA_2	-1994.0800 (-1993.8792)	-1994.0929 (-1993.8921)
	(4,4)_3D,DD_A,AA,AD_2,AA_2	-1994.0788 (-1993.8801)	-1994.0918 (-1993.8930)
	(4,4)_4DD_4AA	-1994.0879 (-1993.8848)	-1994.0994 (-1993.8963)
	(5,3)_2D,2DD_3A_bA_b	-1994.0906 (-1993.8893)	-1994.1023 (-1993.9011)
	(5,3)_2D,2DD_2A_bA_b,A_aA_b	-1994.0881 (-1993.8861)	-1994.1005 (-1993.8985)
	(5,3)_4D,DD_3AA	-1994.0869 (-1993.8851)	-1994.0994 (-1993.8976)
	(6,2)_2D,DD_2AA	-1994.0817 (-1993.8824)	-1994.0940 (-1993.8947)

n	Complex (*x*,*y*,*z*)	B3LYP-GD3BJ/6-311+G(d,p)	B3LYP-GD3BJ[b]
	(6,2)_4D_2AA$_g$	-1994.0571 (-1993.8870)	-1994.0985 (-1993.8992)
	(6,2)_4D_2AA$_t$	-1994.0863 (-1993.8857)	-1994.0970 (-1993.8977)
9	(4,4,1)_2D,2DD_2AA,2AD_AA	-2070.0850 (-2070.3468	-2070.5861 (-2070.3613)
	(4,4,1)_2D,2DD_A,2AD_2AA	-2070.5716 (-2070.3465)	-2070.5845 (-2070.3610)
	(4,5)_2D,2DD_AA,2A,AD$_2$,AA$_2$	-2070.5699 (-2070.3477)	-2070.5858 (-2070.3628)
	(4,5)_D,3DD_2AA,3A	-2070.5708 (-2070.3505)	-2070.5877 (-2070.3648)
	(4,5)_D,3DD_2AA,A,AD$_2$,AA$_2$	-2070.5733 (-2070.3485)	-2070.5877 (-2070.3630)
	(5,4)_2D,3DD_4AA	-2070.5731 (-2070.3556)	-2070.5980 (-2070.3702)
	(5,4)_3D,2DD_A,3AA	-2070.5834 (-2070.3529)	-2070.5927 (-2070.3670)
	(5,4)_4D,DD_2AA,AD$_2$,AA$_2$	-2070.5786 (-2070.3497)	-2070.5903 (-2070.3643)
	(5,4)_4DD_4AA	-2070.5757 (-2070.3554)	-2070.5976 (-2070.3701)
	(6,3)_2D,2DD_3AA	-2070.5829 (-2070.3563)	-2070.5946 (-2070.3699)
	(6,3)_4D,DD_3AA	-2070.5810 (-2070.3577)	-2070.5962 (-2070.3713)
	(6,3)_6D_3AA	-2070.5826 (-2070.3586)	-2070.5973 (-2070.3719)
10	(4,4,2)_4D,4AD_2AA	-2147.5840 (-2146.8100)	-2147.0736 (-2146.8261)
	(4,4,2)_4DD,2AA_2AAD,2A	-2147.0576 (-2146.8140)	-2147.0803 (-2146.8290)
	(4,5,1)_2D,2DD_2AA,A,2AD_AA	-2147.0653 (-2146.8143)	-2147.0794 (-2146.8303)
	(4,5,1)_D,3DD_2A,AA,AAD,AD_AA	-2147.0595 (-2146.8104)	-2147.0762 (-2146.8271)
	(4,6)_4DD,2AA_4A	-2147.0634 (-2146.8169)	-2147.0794 (-2146.8329)
	(5,4,1)_4DD,4AA_A	-2147.0710 (-2146.8191)	-2147.0869 (-2146.8350)
	(5,5)_D,4DD_3AA,AAD_AA	-2147.0699 (-2146.8199)	-2147.0892 (-2146.8361)
	(5,5)_D,4DD_4AA,A	-2147.0735 (-2146.8220)	-2147.0893 (-2146.8378)
	(6,4)_4D,2DD_4AA S_4	-2147.0707 (-2146.8243)	-2147.0898 (-2146.8395)
	(6,4)_4D,2DD_4AA C_1	-2147.0687 (-2146.8202)	-2147.0861 (-2146.8356)
	(6,4)_4DD,4AA	-2147.0745 (-2146.8188)	-2147.0843 (-2146.8344)
	(6,4)_5D,DD_2AA,AAD$_2$,AA$_2$	-2147.0710 (-2146.8238)	-2147.0898 (-2146.8392)
11	(4,4,3)_4DD,AA_3AAD,3A	-2223.5523 (-2223.2771)	-2223.5688 (-2223.2937)
	(4,6,1)_4DD,4A_AA,AAD_A	-2223.5499 (-2223.2786)	-2223.5676 (-2223.2963)

n	Complex (x,y,z)	B3LYP-GD3BJ/6-311+G(d,p)	B3LYP-GD3BJ[b]
	(5,4,2)_4DD,2AA_2AAD,2A	-2223.5579 (-2223.2818)	-2223.5755 (-2223.2995)
	(5,5,1)_D,4DD_A,3AA,AAD_A	-2223.5599 (-2223.2843)	-2223.5776 (-2223.3020)
	(5,6)_5DD_4AA,2A	-2223.5607 (-2223.2865)	-2223.5778 (-2223.3035)
	(6,5)_4D,2DD_AA,2AAD$_2$,2AA$_2$	-2223.5623 (-2223.2881)	-2223.5830 (-2223.3057)
	(6,5)_D,4DD_4AA,A	-2223.5553 (-2223.2809)	-2223.5730 (-2223.2986)
	(6,5)_3D,3DD_3AA,AAD$_2$_AA$_2$	-2223.5653 (-2223.2885)	-2223.5826 (-2223.3058)
	(6,5)_2D,4DD_5AA	-2223.5651 (-2223.2891)	-2223.5831 (-2223.3071)
	(6,4,1)_4D,2DD_3AA,AAD_A	-2223.5574 (-2223.2825)	-2223.5747 (-2223.2998)

[a]Zero-(scaled by 0.989) corrected electronic energy values are given in the parentheses. [b]Values from single-point energies calculated at the level shown using a 6-311+G(2d,2p) basis set from geometries optimized at the B3LYP-GD3BJ/6-311+G(d,p) level.

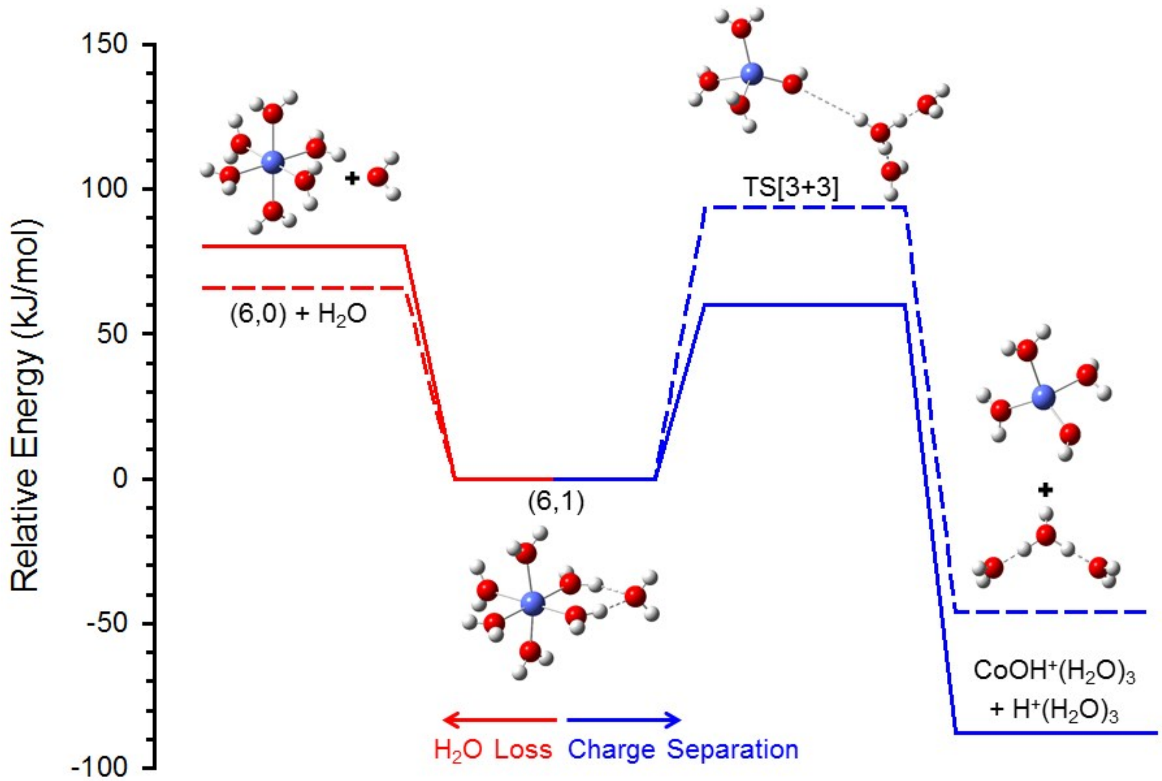

Figure S1. Simplified reaction coordinates for water loss and charge separation pathways of $Co^{2+}(H_2O)_7$ from the (6,1) GS. Single point energies are calculated at the B3LYP (solid line) and MP2 (dashed line) levels of theory with the 6-311+G(d,p) basis set and include zero point energies.

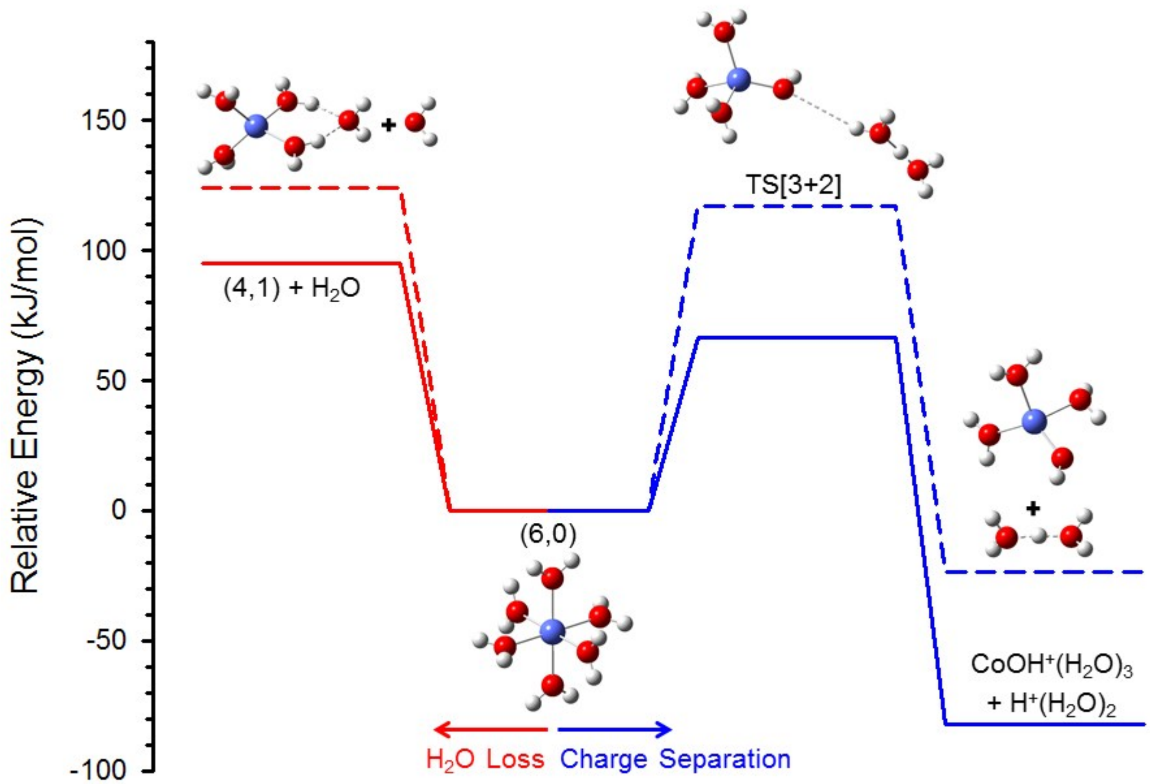

Figure S2. Simplified reaction coordinates for water loss and charge separation pathways of $Co^{2+}(H_2O)_6$ from the (6,0) GS. Single point energies are calculated at the B3LYP (solid line) and MP2 (dashed line) levels of theory with the 6-311+G(d,p) basis set and include zero point energies.

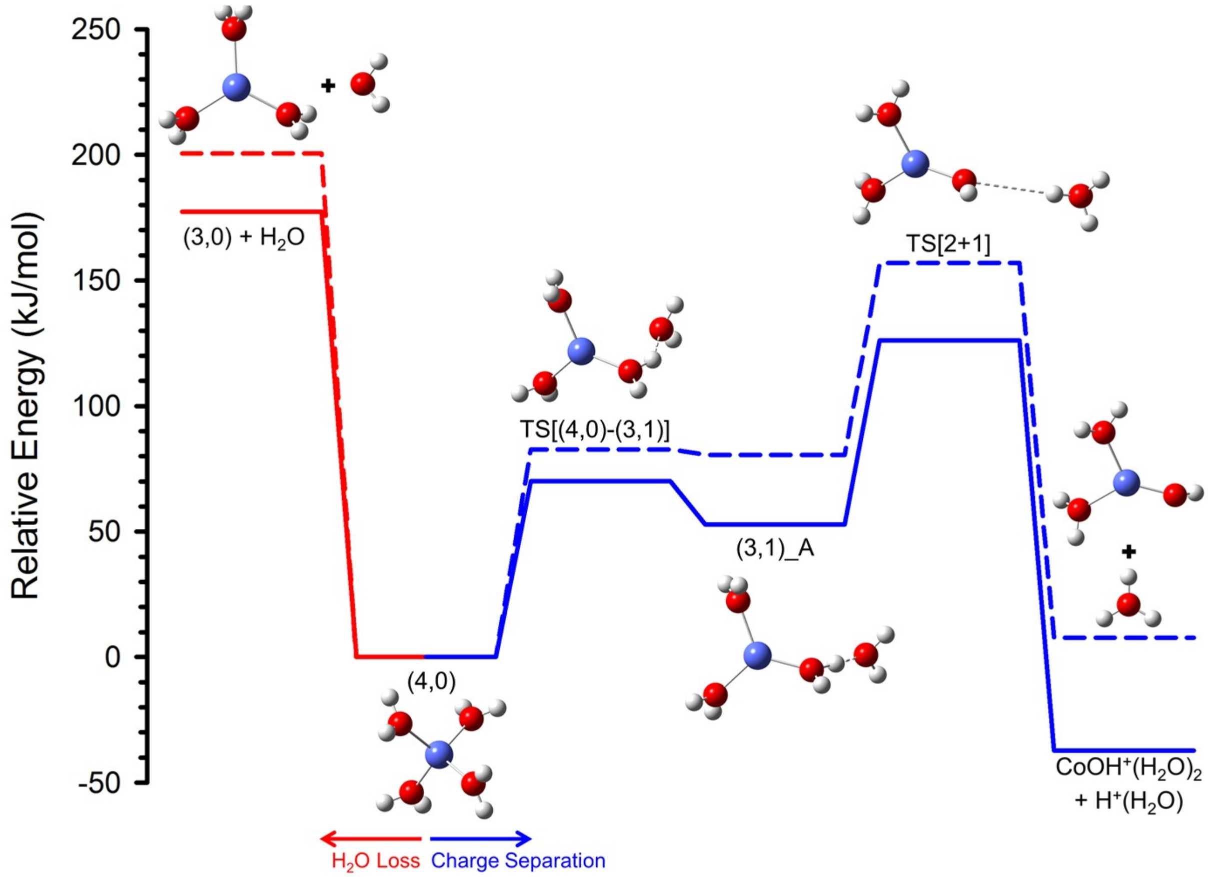

Figure S3. Reaction coordinates for water loss and charge separation pathways of $Co^{2+}(H_2O)_4$ from the (4,0) GS. Single point energies are calculated at the B3LYP (solid line) and MP2 (dashed line) levels of theory with the 6-311+G(d,p) basis set and include zero point energies.