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

Electronic properties and collision cross sections the $AgO_kH_m^{\pm}$ (k, m = 1 – 4) aerosol ionic clusters (Electronic Supplementary Information)

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Table S1
The cartesian coordinates (in Å) of the $AgO_kH_m^{\pm}$ clusters, where k, m = 1 - 4, obtained from the geometry optimization calculations at the CCSD level.

$AgOH^+$			
Ag	0.01333000	-0.38559000	0.00000000
H	-0.73288000	2.57842000	0.00000000
O	0.01333000	1.94305000	0.00000000
$AgOH_2^+$			
Ag	0.00000000	0.41741000	0.00000000
H	0.77397000	-2.42234000	0.00000000
H	-0.77397000	-2.42234000	0.00000000
O	0.00000000	-1.84669000	0.00000000
$AgOH_3^+$			
Ag	-0.37413000	-0.00004000	0.00003000
H	2.41821000	-0.77598000	0.00249000
H	2.41794000	0.77629000	0.00249000
H	-2.00672000	0.00102000	-0.00007000
O	1.84435000	0.00006000	-0.00079000
$AgOH_4^+$			
Ag	0.32770000	0.00021000	0.00005000
H	2.32823000	-0.00176000	0.38010000
H	-2.46399000	-0.77663000	0.00071000
H	-2.46441000	0.77541000	-0.00022000
H	2.32804000	-0.00365000	-0.38118000
O	-1.89124000	-0.00044000	-0.00019000
AgO_2H^+			
Ag	0.72043000	-0.02834000	-0.00001000
H	-3.21988000	-0.09012000	0.00005000
O	-2.30764000	-0.45131000	0.00003000
O	-1.52242000	0.62910000	0.00002000
$AgO_2H_2^+$			
Ag	-0.67570000	-0.00002000	0.00000000
H	2.29433000	-1.03173000	-0.60076000
H	2.29336000	1.03237000	0.60106000
O	1.69828000	-0.72878000	0.10635000
O	1.69797000	0.72883000	-0.10638000
$AgO_2H_3^+$			
Ag	-0.03777000	0.00675000	0.00005000
H	2.75221000	-0.78820000	-0.00524000
H	2.76980000	0.76368000	0.00579000
H	-2.91355000	0.64673000	-0.01126000
O	2.18895000	-0.00568000	-0.00043000
O	-2.29312000	-0.11174000	0.00146000
$AgO_2H_4^+$			
Ag	0.00001000	0.00004000	0.00002000
H	2.80149000	-0.55364000	0.54368000
H	2.80085000	0.55024000	-0.54756000

H	-2.80202000	0.54878000	0.54786000
H	-2.80045000	-0.55035000	-0.54809000
O	-2.22977000	0.00002000	-0.00011000
O	2.22974000	0.00038000	0.00049000

AgO_3H^+

Ag	0.87471000	-0.00270000	0.00001000
H	-1.99991000	1.79812000	0.00134000
O	-2.17855000	-0.15463000	0.00004000
O	-1.33139000	1.08570000	-0.00028000
O	-1.37901000	-1.13997000	0.00000000

$AgO_3H_2^+$

Ag	0.30313000	0.03598000	-0.00007000
H	3.11529000	-0.16969000	0.77527000
H	3.11564000	-0.16551000	-0.77495000
O	-2.11502000	0.41551000	0.00064000
O	-2.98698000	-0.43993000	-0.00039000
O	2.54223000	-0.14506000	0.00009000

$AgO_3H_3^+$

Ag	-0.29959000	-0.07671000	0.00001000
H	-3.07740000	0.28467000	0.77577000
H	-3.07740000	0.28419000	-0.77583000
H	3.58016000	0.31765000	-0.00001000
O	-2.50592000	0.25758000	-0.00002000
O	1.94373000	-0.52770000	0.00003000
O	2.64410000	0.60998000	-0.00004000

$AgO_3H_4^+$

Ag	0.29839000	-0.10409000	0.00559000
H	3.14618000	-0.10093000	-0.61082000
H	-3.01258000	0.88375000	-0.67781000
H	-2.43888000	-1.01035000	0.65002000
H	2.97399000	0.91567000	0.54817000
O	-2.38478000	0.81623000	0.06190000
O	-1.95269000	-0.57934000	-0.07315000
O	2.50083000	0.28863000	-0.01027000

AgO_4H^+

Ag	0.00182000	-0.03478000	-0.00015000
H	-3.90983000	0.19772000	0.00068000
O	2.38906000	0.52095000	-0.00044000
O	3.31622000	-0.27455000	0.00053000
O	-2.24321000	-0.58909000	0.00002000
O	-2.98404000	0.52231000	0.00065000

$AgO_4H_2^+$

Ag	-0.46825000	-0.07555000	0.00006000
H	-3.16802000	1.04094000	0.00103000
H	-3.35287000	-0.49851000	-0.00070000
O	-2.69148000	0.20292000	0.00017000
O	2.53287000	0.02616000	-0.00022000
O	1.76842000	-0.99996000	-0.00006000
O	1.95627000	1.14693000	-0.00026000

$AgO_4H_3^+$

Ag	-0.55648000	0.08167000	0.00595000
H	-1.61113000	-2.63456000	0.56793000
H	-0.29248000	2.88510000	-0.74702000
H	-0.03133000	2.84777000	0.78000000
O	-0.15771000	2.29285000	0.00182000
O	2.03680000	-0.81115000	0.31819000
O	2.98611000	-0.30262000	-0.25818000
O	-1.35399000	-2.04616000	-0.17189000

$AgO_4H_4^+$

Ag	0.57312000	0.12638000	0.00174000
H	0.10124000	2.88701000	-0.79235000
H	2.12052000	-2.35772000	0.02328000
H	0.62979000	-2.78649000	0.02992000
H	0.16240000	2.90869000	0.75555000
O	-2.04457000	-0.89965000	-0.14610000
O	0.11191000	2.32448000	-0.00958000
O	-3.02833000	-0.22631000	0.11586000
O	1.21717000	-2.02246000	0.02756000

$AgOH^-$

Ag	0.01678700	-0.35331400	0.00000000
H	-0.92328200	2.03586900	0.00000000
O	0.01678700	1.82123900	0.00000000

$AgOH_2^-$

Ag	-0.31053000	0.00163000	-0.00001000
H	-1.96540000	0.03558000	0.00020000
H	2.17800000	0.77602000	0.00001000
O	1.79778000	-0.11101000	0.00002000

$AgOH_3^-$

Ag	0.65673000	0.00000000	-0.00003000
H	2.38351000	0.00006000	0.00100000
H	-2.82914000	0.74367000	-0.00009000
H	-2.82898000	-0.74357000	-0.00009000
O	-3.44898000	-0.00001000	0.00007000

$AgOH_4^-$

Ag	0.61897000	-0.01508000	0.00000000
H	-2.81824000	0.94130000	-0.00008000
H	-0.67402000	-1.15159000	-0.00006000
H	1.89599000	1.11200000	-0.00001000
H	-2.31611000	-0.48064000	-0.00003000
O	-3.14739000	0.03599000	0.00001000

AgO_2H^-

Ag	-0.04075000	-0.00217000	-0.00001000
H	2.40389000	0.79390000	0.00002000
O	2.04379000	-0.10151000	0.00002000
O	-2.10489000	0.01502000	0.00003000

$AgO_2H_2^-$

Ag	0.00000000	-0.00256000	-0.00004000
H	2.43803000	0.59949000	-0.52556000
H	-2.43788000	0.60006000	0.52521000
O	-2.08601000	-0.06749000	-0.07662000

O	2.08599000	-0.06741000	0.07689000

$AgO_2H_3^-$

Ag	0.89002000	-0.10398000	0.00002000
H	-3.06423000	-1.19826000	0.38958000
H	-2.52569000	0.15792000	-0.08224000
H	-1.02122000	1.69028000	0.51113000
O	-3.36225000	-0.38814000	-0.03524000
O	-1.04022000	0.91777000	-0.06721000

$AgO_2H_4^-$

Ag	0.84376000	-0.07803000	-0.00103000
H	2.29495000	-0.86243000	0.02800000
H	-3.07866000	-1.21729000	0.38963000
H	-2.52829000	0.13402000	-0.08299000
H	-1.04659000	1.68487000	0.49212000
O	-1.04366000	0.89581000	-0.06137000
O	-3.36861000	-0.40476000	-0.03595000

AgO_3H^-

Ag	0.26938000	-0.07448000	-0.00062000
H	2.59936000	0.81564000	-0.61453000
O	2.33346000	0.20982000	0.08823000
O	-1.81967000	-0.55199000	-0.03995000
O	-2.42132000	0.67781000	0.03219000

$AgO_3H_2^-$

Ag	-0.32077000	0.08877000	-0.00338000
H	-2.68455000	-0.48690000	0.80677000
H	2.95130000	-0.63646000	0.74529000
O	-2.35752000	-0.34434000	-0.09013000
O	1.71980000	0.62607000	0.01818000
O	2.48891000	-0.66286000	-0.10219000

$AgO_3H_3^-$

Ag	0.00756000	-0.20026000	-0.00049000
H	2.43550000	0.35224000	0.05260000
H	-2.45262000	0.01369000	-0.59513000
H	-0.79924000	2.14009000	0.38098000
O	0.04779000	1.92564000	-0.03700000
O	2.03340000	-0.52309000	-0.00913000
O	-2.02355000	-0.53929000	0.06921000

$AgO_3H_4^-$

Ag	-0.52388000	-0.11374000	-0.00289000
H	-2.54141000	1.35219000	0.58852000
H	1.49280000	-1.62577000	0.59291000
H	2.77433000	0.08715000	-0.05847000
H	3.06594000	1.56835000	0.21536000
O	3.51510000	0.75340000	-0.02836000
O	1.41777000	-0.91162000	-0.05020000
O	-2.45406000	0.65370000	-0.07173000

AgO_4H^-

Ag	0.51164000	-0.12119000	-0.00003000
H	2.66070000	1.28925000	0.00161000
O	-1.48211000	-1.00753000	0.00015000

O	2.55359000	0.32987000	-0.00011000
O	-1.95051000	1.22068000	-0.00008000
O	-2.45946000	0.00780000	0.00003000

$AgO_4H_2^-$

Ag	0.72468000	0.16657000	-0.00172000
H	2.50037000	-1.50860000	0.78432000
H	-0.55129000	2.39285000	0.05291000
O	-2.96684000	-0.66112000	-0.61096000
O	-2.92925000	-0.70648000	0.60787000
O	2.28762000	-1.21221000	-0.10936000
O	-0.89263000	1.49067000	0.01793000

$AgO_4H_3^-$

Ag	-0.81295000	-0.04430000	-0.00295000
H	3.05312000	-0.75972000	-0.01681000
H	-3.19484000	-0.80576000	0.54663000
H	4.19981000	0.18835000	0.01620000
O	4.02939000	-0.75993000	-0.00723000
O	1.78837000	1.29745000	0.02977000
O	1.33366000	0.02285000	-0.00800000
O	-2.88261000	-0.12799000	-0.06546000

$AgO_4H_4^-$

Ag	-0.00003400	0.00030300	0.00021500
H	-0.37399900	-2.34978900	-0.00113900
H	2.35052000	-0.37488500	-0.00111300
H	0.37338400	2.35095800	0.00075200
H	-2.35121600	0.37211800	-0.00096000
O	-0.50188300	1.94226600	-0.00028500
O	-1.94205200	-0.50281700	-0.00028100
O	0.50187200	-1.94184000	-0.00001800
O	1.94242900	0.50080800	-0.00037300

Table S2
Zero-point vibrational energy corrected stabilization energy ΔE (in eV) of the $AgO_kH_m^{\pm}$ clusters (where k, m = 1 - 4) with respect to specific dissociation channels (DCs).

a. **$AgOH_m^+$:**

Species	DC	ΔE (eV)
$AgOH^+$	$Ag^+ + OH$	0.86
	$AgO^+ + H$	5.12
	$Ag + OH^+$	6.43
$AgOH_2^+$	$Ag^+ + H_2O$	1.20
	$AgOH^+ + H$	5.35
	$Ag + H_2O^+$	6.41
	$AgO^+ + 2H$	10.48
$AgOH_3^+$	$AgOH_2^+ + H$	0.57
	$AgH^+ + H_2O$	1.34
	$Ag^+ + H_2O + H$	1.77
	$AgH + H_2O^+$	4.67
	$Ag + H_2O^+ + H$	6.98
$AgOH_4^+$	$AgOH_2^+ + H_2$	0.41
	$AgH_2+ + H_2O$	1.25
	$Ag^+ + H_2O + H_2$	1.61
	$AgOH_3^+ + H$	4.28
	$AgH_2 + H_2O^+$	6.81
	$Ag + H_2O^+ + H_2$	6.82
	$AgOH_2 + H_2^+$	9.66
	$Ag + H_2O + H_2^+$	9.72

b. **$AgO_2H_m^+$:**

Species	DC	ΔE (eV)
AgO_2H^+	$Ag^+ + HO_2$	1.02
	$AgO_2+ H$	2.80
	$AgO^+ + OH$	3.61
	$Ag + HO_2^+$	5.01
$AgO_2H_2^+$	$Ag^+ + H_2O_2$	1.18
	$AgOH^+ + OH$	2.28
	$AgO_2H^+ + H$	3.79
	$Ag + H_2O_2^+$	4.76
	$AgOH + OH^+$	6.32
$AgO_2H_3^+$	$AgOH_2^+ + OH$	0.84
	$AgOH^+ + H_2O$	1.18
	$Ag^+ + H_2O + OH$	2.04
	$AgOH + H_2O^+$	4.86
	$AgO^+ + H_2O + H$	6.91
	$Ag + H_2O^+ + OH$	7.24
	$Ag + H_2O + OH^+$	7.61
	$AgO + H_2O^+ + H$	10.68
$AgO_2H_4^+$	$AgOH_2^+ + H_2O$	1.14
	$Ag^+ + 2H_2O$	2.34
	$AgO_2H_3^+ + H$	5.31
	$AgOH^+ + H_2O + H$	6.49
	$AgOH_2 + H_2O^+$	7.48
	$Ag + H_2O + H_2O^+$	7.54

	$AgOH + H_2O^+ + H$	10.16
	$AgO^+ + H_2O + 2H$	11.62
	$AgO_2^+ + 4H$	15.81
	$AgO + H_2O^+ + 2H$	16.00

c. **$AgO_3H_m^+$:**

Species	DC	ΔE (eV)
AgO_3H^+	$AgO_2^+ + OH$	0.77
	$Ag^+ + O_2 + OH$	1.04
	$AgO_3^+ + H$	3.78
	$Ag^+ + O_3 + H$	4.56
	$AgO^+ + O_2 + H$	5.31
	$Ag + O_2^+ + OH$	5.67
	$AgO_2 + OH^+$	6.61
	$AgO + O_2^+ + H$	9.12
	$Ag + O_3^+ + H$	9.83
$AgO_3H_2^+$	$AgOH_2^+ + O_2$	0.26
	$AgO_2^+ + H_2O$	1.19
	$Ag^+ + H_2O + O_2$	1.47
	$AgOH_2 + O_2^+$	6.03
	$Ag + H_2O + O_2^+$	6.10
	$Ag + H_2O^+ + O_2$	6.67
	$AgO_2 + H_2O^+$	6.67
$AgO_3H_3^+$	$AgOH_2^+ + HO_2$	0.97
	$Ag^+ + H_2O + HO_2$	2.17
	$AgO_3H_2^+ + H$	2.75
	$AgO^+ + OH + H_2O$	4.76
	$AgOH_2 + HO_2^+$	6.09
	$Ag + H_2O + HO_2^+$	6.16
	$AgOH^+ + H + HO_2$	6.32
	$Ag + H_2O^+ + HO_2$	7.38
	$AgOH + H + HO_2^+$	8.78
	$AgO + H_2O^+ + OH$	9.14
	$AgO + H_2O + OH^+$	9.51
	$AgO^+ + HO_2 + 2H$	11.45
	$AgO + HO_2^+ + 2H$	14.61
$AgO_3H_4^+$	$AgOH_2^+ + H_2O_2$	1.08
	$AgO_2H_2^+ + H_2O$	1.11
	$Ag^+ + H_2O_2 + H_2O$	2.28
	$AgOH^+ + H_2O + OH$	3.39
	$AgO_2H^+ + H_2O + H$	4.90
	$AgO_3H_3^+ + H$	3.75
	$AgOH_2^+ + H_2O_2$	5.80
	$Ag + H_2O_2^+ + H_2O$	5.87
	$AgOH^+ + H_2O_2 + H$	6.44
	$AgO_3H_2^+ + 2H$	6.51
	$AgOH + H_2O^+ + OH$	7.06
	$AgOH + H_2O + OH^+$	7.43
	$Ag + H_2O_2 + H_2O^+$	7.49
	$AgO_2^+ + H_2O + 2H$	7.70
	$AgOH + H_2O_2^+ + H$	8.48
	$AgO^+ + H_2O + OH + H$	8.51
	$AgO_2H + H_2O^+ + H$	9.86
	$AgO^+ + H_2O_2 + 2H$	11.56
	$AgO + H_2O^+ + OH + H$	12.89

	$AgO_2 + H_2O + 2H$	13.18
	$AgO + H_2O + OH^+ + H$	13.27
	$AgO + H_2O_2^+ + 2H$	14.32

d. **$AgO_4H_m^+$:**

Species	DC	ΔE (eV)
AgO_4H^+	$AgO_2H^+ + O_2$	-1.13
	$AgO_2^+ + HO_2$	-0.38
	$Ag^+ + O_2 + HO_2$	-0.10
	$AgO_4^+ + H$	1.85
	$AgO_2H + O_2^+$	3.26
	$AgO_2 + HO_2^+$	3.87
	$Ag + O_2 + HO_2^+$	3.88
	$Ag + O_2^+ + HO_2$	4.52
$AgO_4H_2^+$	$AgOH_2^+ + O_3$	0.76
	$AgO_3^+ + H_2O$	1.18
	$Ag^+ + O_3 + H_2O$	1.97
	$AgO_2^+ + H_2O + O$	2.48
	$AgO^+ + H_2O + O_2$	2.72
	$AgO + H_2O + O_2^+$	6.53
	$AgO + H_2O^+ + O_2$	7.10
	$AgOH_2 + O_3^+$	7.16
	$Ag + H_2O^+ + O_3$	7.17
	$Ag + H_2O + O_3^+$	7.23
	$AgO_2 + H_2O^+ + O$	7.95
	$AgO_2 + H_2O + O^+$	8.88
$AgO_4H_3^+$	$AgO_2H_3^+ + O_2$	-0.34
	$AgO_3H_2^+ + OH$	0.23
	$AgOH_2^+ + OH + O_2$	0.50
	$AgOH^+ + H_2O + O_2$	0.85
	$AgO_2^+ + OH + H_2O$	1.42
	$Ag^+ + OH + O_2 + H_2O$	1.70
	$AgO_2H_3 + O_2^+$	3.26
	$AgOH + O_2^+ + H_2O$	3.95
	$AgOH + O_2 + H2O^+$	4.52
	$AgOH_2 + OH + O_2^+$	6.26
	$Ag + OH + O_2^+ + H_2O$	6.33
	$AgO_3H_2 + OH^+$	6.87
	$AgO_2 + OH + H_2O$	6.90
	$Ag + OH + O_2 + H_2O^+$	6.91
	$AgOH_2 + OH^+ + O_2$	7.21
	$AgO_2 + OH^+ + H_2O$	7.27
	$Ag + OH^+ + O_2 + H_2O$	7.28
$AgO_4H_4^+$	$AgO_2H_4^+ + O2$	0.08
	$AgO_3H_2^+ + H_2O$	0.95
	$AgOH_2^+ + O_2 + H_2O$	1.22
	$AgO_2^+ + 2H_2O$	2.14
	$Ag^+ + O_2 + 2H_2O$	2.42
	$AgO_2H_3^+ + H + O_2$	5.39
	$AgO_4H_3^+ + H$	5.73
	$AgOH^+ + O_2 + H_2O + H$	6.57
	$AgO_2H_4 + O_2^+$	6.67
	$AgOH_2 + O_2^+ + H_2O$	6.99
	$Ag + O_2^+ + 2H_2O$	7.06
	$AgO_3H_2 + H_2O^+$	7.22

	$AgOH_2 + O_2 + H_2O^+$	7.56
	$AgO_2 + H_2O + H_2O^+$	7.62
	$Ag + O_2 + H_2O + H_2O^+$	7.63
	$AgO_2H_3 + H + O_2^+$	8.99
	$AgOH + H + O_2^+ + H_2O$	9.67
	$AgOH + H + O_2 + H_2O^+$	10.24
	$AgO^+ + O_2 + H_2O + 2H$	11.70
	$AgO + 2H + O_2^+ + H_2O$	15.50
	$AgO + 2H + O_2 + H_2O^+$	16.08

e. **$AgOH_m^-$:**

Species	DC	ΔE (eV)
$AgOH^-$	$Ag + OH^-$	1.68
	$Ag^- + OH$	2.43
	$AgO^- + H$	4.39
	$AgO + H^-$	6.13
$AgOH_2^-$	$AgH + OH^-$	2.70
	$AgOH^- + H$	3.32
	$AgOH + H^-$	3.62
	$AgH^- + OH$	4.01
	$Ag + H + OH^-$	5.01
	$Ag^- + H + OH$	5.75
	$Ag + H^- + OH$	5.75
$AgOH_3^-$	$AgH^- + H_2O$	0.40
	$AgH + H_2O^-$	1.41
	$Ag^- + H + H_2O$	2.15
	$AgOH_2 + H^-$	2.33
	$Ag + H^- + H_2O$	2.40
	$Ag + H + H_2O^-$	3.71
$AgOH_4^-$	$AgH_2^- + H_2O$	0.47
	$AgH_2 + H_2O^-$	2.55
	$AgOH_3 + H^-$	2.83
	$AgOH_3^- + H$	3.28
	$Ag^- + 2H + H_2O$	5.42
	$Ag + H + H^- + H_2O$	5.68
	$Ag + 2H + H_2O^-$	6.99

f. **$AgO_2H_m^-$:**

Species	DC	ΔE (eV)
AgO_2H^-	$AgOH + O^-$	2.58
	$AgOH^- + O$	2.88
	$AgO^- + OH$	2.97
	$AgO + OH^-$	3.70
	$AgO_2^- + H$	3.73
	$Ag + O + OH^-$	4.56
	$Ag + O^- + OH$	4.96
	$AgO_2 + H^-$	4.99
	$Ag^- + O + OH$	5.31
$AgO_2H_2^-$	$AgOH + OH^-$	3.12
	$AgOH^- + OH$	3.82
	$AgO_2H^- + H$	5.25
	$Ag + OH^- + OH$	5.51
	$Ag^- + 2OH$	6.26
	$AgO_2^- + 2H$	8.99

	$AgO_2 + H + H^-$	10.25
$AgO_2H_3^-$	$AgOH^- + H_2O$	0.73
	$AgOH + H_2O^-$	2.34
	$Ag + OH^- + H_2O$	2.41
	$Ag^- + OH + H_2O$	3.16
	$Ag + OH + H_2O^-$	4.73
	$AgO^- + H + H_2O$	5.12
	$AgO + H^- + H_2O$	6.86
	$AgO + H + H_2O^-$	8.17
$AgO_2H_4^-$	$AgOH_2^- + H_2O$	0.70
	$AgOH_3 + OH^-$	2.85
	$AgO_2H_3^- + H$	3.29
	$AgO_2H_3 + H^-$	3.63
	$AgOH^- + H + H_2O$	4.01
	$AgOH_3^- + OH$	4.30
	$AgOH + H^- + H_2O$	4.32
	$AgOH + H + H_2O^-$	5.62
	$Ag + H + OH^- + H_2O$	5.70
	$Ag^- + H + OH + H_2O$	6.45
	$Ag + H^- + OH + H_2O$	6.70
	$Ag + H + OH + H_2O^-$	8.01

g. **$AgO_3H_m^-$:**

Species	DC	ΔE (eV)
AgO_3H^-	$AgOH^- + O_2$	1.55
	$AgOH + O_2^-$	2.19
	$AgO_2 + OH^-$	3.23
	$Ag + OH^- + O_2$	3.23
	$AgO_2H^- + O$	3.55
	$Ag^- + OH + O_2$	3.98
	$Ag + OH + O_2^-$	4.58
	$AgO_2H + O^-$	4.62
	$AgO_3^- + H$	4.63
	$AgO^- + H + O_2$	5.94
	$AgO_3 + H^-$	6.47
	$AgO_2^- + H + O$	7.28
	$AgO + H^- + O_2$	7.68
	$AgO_2 + H + O^-$	7.93
	$AgO + H + O_2^-$	8.02
	$AgO_2 + H^- + O$	8.54
$AgO_3H_2^-$	$AgO_2H^- + OH$	2.58
	$AgOH + HO_2^-$	2.82
	$AgOH^- + HO_2$	2.83
	$AgO_2H + OH^-$	3.25
	$AgO_3H^- + H$	3.33
	$Ag + OH^- + HO_2$	4.51
	$AgO_3H + H^-$	5.01
	$Ag + OH + HO_2^-$	5.21
	$Ag^- + OH + HO_2$	5.26
	$AgO^- + 2OH$	5.54
	$AgO + OH + OH^-$	6.28
	$AgO_2^- + H + OH$	6.31
	$AgO_2 + H + OH^-$	6.56
	$AgO^- + H + HO_2$	7.22
	$AgO_2 + H^- + OH$	7.57

	$AgO_3^- + 2H$	7.97
	$AgO + H + HO_2^-$	8.65
	$AgO + H^- + HO_2$	8.96
	$AgO_3 + H + H^-$	9.81
$AgO_3H_3^-$	$AgO_2H_2^- + OH$	0.92
	$AgO_2H_2 + OH^-$	3.03
	$AgOH + OH + OH^-$	4.04
	$AgOH^- + 2OH$	4.74
	$AgO_2H^- + H + OH$	6.17
	$Ag + 2OH + OH^-$	6.42
	$AgO_2H + H + OH^-$	6.84
	$Ag^- + 3OH$	7.18
	$AgO_2H + H^- + OH$	7.85
	$AgO_3H + H + H^-$	8.61
	$AgO^- + H + 2OH$	9.14
	$AgO + H + OH + OH^-$	9.87
	$AgO_2^- + 2H + OH$	9.90
	$AgO_2 + 2H + OH^-$	10.16
	$AgO + H^- + 2OH$	10.88
	$AgO_2 + H + H^- + OH$	11.16
	$AgO_3^- + 3H$	11.56
	$AgO_3 + 2H + H^-$	13.41
$AgO_3H_4^-$	$AgO_2H_2^- + H_2O$	0.66
	$AgO_2H_3 + OH^-$	3.10
	$AgO_2H_3^- + OH$	3.76
	$AgOH + OH^- + H_2O$	3.79
	$AgOH^- + OH + H_2O$	4.49
	$AgO_2H_2 + H_2O^-$	5.10
	$AgO_2H^- + H + H_2O$	5.92
	$AgOH + OH + H_2O^-$	6.10
	$Ag + OH + OH^- + H_2O$	6.18
	$AgO + H + OH^- + H_2O$	6.62
	$Ag^- + 2OH + H_2O$	6.93
	$AgO_2H + H^- + H_2O$	7.60
	$Ag + 2OH + H_2O^-$	8.49
	$AgO^- + H + OH + H_2O$	8.89
	$AgO + H^- + OH + H_2O$	10.63
	$AgO + H + OH + H_2O^-$	11.93

h. **$AgO_4H_m^-$:**

Species	DC	ΔE (eV)
AgO_4H^-	$AgO_2H^- + O_2$	1.35
	$AgOH + O_3^-$	2.32
	$AgO_3H^- + O$	2.68
	$AgO_2H + O_2^-$	3.36
	$AgOH^- + O_3$	3.44
	$AgO_3H + O^-$	3.75
	$Ag + OH + O_3^-$	4.70
	$Ag + OH^- + O_3$	5.12
	$Ag^- + OH + O_3$	5.87
	$AgO^- + H + O_3$	7.83
	$AgO + H + O_3^-$	8.15
	$AgO + H^- + O_3$	9.57
$AgO_4H_2^-$	$AgO_2H_2^- + O_2$	0.04

	$AgO_3H^- + OH$	2.32
	$AgO_3H + OH^-$	2.99
	$AgOH + OH^- + O_2$	3.16
	$AgO_2H_2 + O_2^-$	3.50
	$AgOH^- + OH + O_2$	3.86
	$AgOH + OH + O_2^-$	4.51
	$Ag + OH + OH^- + O_2$	5.55
	$Ag^- + 2OH + O_2$	6.30
	$Ag + 2OH + O_2^-$	6.89
	$AgO^- + H + OH + O_2$	8.26
	$AgO + H + OH^- + O_2$	8.99
	$AgO + H^- + OH + O_2$	10.00
	$AgO + H + OH + O_2^-$	10.34
$AgO_4H_3^-$	$AgO_3H- + H_2O$	0.40
	$AgOH^- + O_2 + H_2O$	1.95
	$AgOH + O_2^- + H_2O$	2.59
	$AgO_3H + H_2O^-$	3.39
	$AgOH + O_2 + H_2O$	3.56
	$Ag + OH^- + O_2 + H_2O$	3.64
	$AgO_2H^- + O + H_2O$	3.95
	$Ag^- + OH + O_2 + H_2O$	4.39
	$Ag + OH + O_2^- + H_2O$	4.98
	$AgO_2H + O^- + H_2O$	5.02
	$Ag + OH + O_2 + H_2O-$	5.95
	$AgO^- + H + O_2 + H_2O$	6.35
	$AgO^- + O + OH + H_2O$	6.91
	$AgO_2H + O + H_2O^-$	6.93
	$AgO + O + OH^- + H_2O$	7.65
	$AgO + O^- + OH + H_2O$	8.05
	$AgO + H^- + O_2 + H_2O$	8.08
	$AgO + H + O_2^- + H_2O$	8.42
	$AgO + H + O_2 + H_2O-$	9.39
	$AgO + O + OH + H_2O$	9.96
$AgO_4H_4^-$	$AgO_3H_3^- + OH$	2.45
	$AgO_2H_2^- + 2OH$	3.37
	$AgO_3H_3 + OH^-$	3.70
	$AgO_2H_2 + OH + OH^-$	5.49
	$AgOH + 2OH + OH^-$	6.49
	$AgOH^- + 3OH$	7.20
	$Ag + 3OH + OH^-$	8.88
	$Ag^- + 4OH$	9.63
	$AgO^- + H + 3OH$	11.59
	$AgO + H + 2OH + OH^-$	12.32
	$AgO_2^- + 2H + 2OH$	12.35
	$AgO_2 + 2H + OH + OH^-$	12.61
	$AgO + H^- + 3OH$	13.33
	$AgO_2 + H^- + H + 2OH$	13.61
	$AgO_3^- + 3H + OH$	14.01
	$AgO_4^- + 4H$	14.92

Table S3
The values of electronic energy (EE; Hartree); energy of HOMO ($\varepsilon_{HOMO;}$ eV); energy of LUMO (ε_{LUMO}; eV); the HOMO-LUMO energy gap (HLG; eV); chemical hardness (η; eV); chemical potential (μ; eV); electrophilicity index (ω; eV) of the $AgO_kH_m^{\pm}$ clusters, where k, m = 1 – 4, obtained at the ωB97XD calculations. Note that only EE values are reported for the open-shell systems.

Systems	EE	ε_{HOMO}	ε_{LUMO}	HLG	η	μ	ω
$AgOH^+$	-222.454675						
$AgOH_2^+$	-223.167256	-17.057191	-6.515769	10.541422	5.270711	-11.786480	13.178593
$AgOH_3^+$	-223.699083						
$AgOH_4^+$	-224.364072	-16.569563	-5.279827	11.289736	5.644868	-10.924695	10.571457
AgO_2H^+	-297.640595						
$AgO_2H_2^+$	-298.286436	-16.238400	-6.523660	9.714740	4.857370	-11.381030	13.333125
$AgO_2H_3^+$	-298.944186						
$AgO_2H_4^+$	-299.653947	-15.506414	-4.709476	10.796938	5.398469	-10.107945	9.462919
AgO_3H^+	-372.796833						
$AgO_3H_2^+$	-373.512219						
$AgO_3H_3^+$	-374.127709						
$AgO_3H_4^+$	-374.773231	-15.229402	-4.775056	10.454346	5.227173	-10.002229	9.569665
AgO_4H^+	-447.985657						
$AgO_4H_2^+$	-448.621258	-16.014723	-8.467370	7.547353	3.773676	-12.241046	19.853745
$AgO_4H_3^+$	-449.192647						
$AgO_4H_4^+$	-449.990535						
$AgOH^-$	-222.822651						
$AgOH_2^-$	-223.457333	-3.291490	4.089329	7.380819	3.690410	0.398920	0.021561
$AgOH_3^-$	-224.018024						
$AgOH_4^-$	-224.654394	-3.556802	3.852317	7.409119	3.704560	0.147758	0.002947
AgO_2H^-	-298.029123						
$AgO_2H_2^-$	-298.709174	-3.569047	3.895583	7.464630	3.732315	0.163268	0.003571
$AgO_2H_3^-$	-299.292106						
$AgO_2H_4^-$	-299.926084	-3.745649	3.795990	7.541639	3.770819	0.025171	0.000084
AgO_3H^-	-373.220980						
$AgO_3H_2^-$	-373.843461	-3.350811	3.756805	7.107616	3.553808	0.202997	0.005798
$AgO_3H_3^-$	-374.492472						
$AgO_3H_4^-$	-375.176759	-4.116268	3.600340	7.716608	3.858304	-0.257964	0.008624
AgO_4H^-	-448.386446						
$AgO_4H_2^-$	-449.044976						
$AgO_4H_3^-$	-449.684175						
$AgO_4H_4^-$	-450.324761	-4.887983	3.193529	8.081512	4.040756	-0.847227	0.088819

Table S4
Natural electronic configuration and natural charges of the $AgO_kH_m^{\pm}$ clusters, where k, m = 1 – 4, obtained from NBO calculations at the ωB97XD level of theory.

Systems	atom	Natural Charge	Electron Configuration
$AgOH^+$	Ag	0.97585	[core]5s(0.04)4d(9.97)5p(0.01)
	H	0.46571	1s(0.53)
	O	-0.44156	[core]2s(1.88)2p(4.55)3d(0.01)
$AgOH_2^+$	Ag	0.97511	[core]5s(0.04)4d(9.98)5p(0.01)
	H	0.52045	1s(0.48)
	H	0.52045	1s(0.48)
	O	-1.01602	[core]2s(1.74)2p(5.27)
$AgOH_3^+$	Ag	0.91632	[core]5s(0.29)4d(9.75)5p(0.05)
	H	0.52694	1s(0.47)
	H	0.52693	1s(0.47)
	H	0.02939	1s(0.97)
	O	-0.99958	[core]2s(1.73)2p(5.26)3p(0.01)
$AgOH_4^+$	Ag	0.90012	[core]5s(0.15)4d(9.93)5p(0.02)
	H	0.02102	1s(0.97)2p(0.01)
	H	0.52309	1s(0.47)
	H	0.52308	1s(0.47)
	H	0.02106	1s(0.97)2p(0.01)
	O	-0.98837	[core]2s(1.73)2p(5.25)
AgO_2H^+	Ag	0.95057	[core]5s(0.06)4d(9.98)5p(0.01)
	H	0.49785	1s(0.50)
	O	-0.22909	[core]2s(1.75)2p(4.46)3p(0.01)3d(0.01)
	O	-0.21933	[core]2s(1.86)2p(4.33)3s(0.01)3p(0.01)3d(0.01)
$AgO_2H_2^+$	Ag	0.96289	[core]5s(0.03)4d(9.99)5p(0.01)
	H	0.49907	1s(0.50)
	H	0.49907	1s(0.50)
	O	-0.48047	[core]2s(1.79)2p(4.68)3p(0.01)4d(0.01)
	O	-0.48057	[core]2s(1.78)2p(4.68)3p(0.01)4d(0.01)
$AgO_2H_3^+$	Ag	0.90584	[core]5s(0.17)4d(9.90)5p(0.02)
	H	0.52043	1s(0.48)
	H	0.52015	1s(0.48)
	H	0.46245	1s(0.53)
	O	-0.98835	[core]2s(1.73)2p(5.25)3p(0.01)
	O	-0.42052	[core]2s(1.87)2p(4.54)3d(0.01)
$AgO_2H_4^+$	Ag	0.896	[core]5s(0.16)4d(9.92)5p(0.02)
	H	0.51809	1s(0.48)
	H	0.51806	1s(0.48)
	H	0.5181	1s(0.48)
	H	0.51804	1s(0.48)
	O	-0.98414	[core]2s(1.73)2p(5.25)3p(0.01)

	O	-0.98415	[core]2s(1.73)2p(5.25)3p(0.01)
AgO_3H^+	Ag	0.94152	[core]5s(0.06)4d(9.98)5p(0.02)
	H	0.51625	1s(0.48)
	O	0.18701	[core]2s(1.75)2p(4.03)3s(0.01)3p(0.01)3d(0.01)
	O	-0.51411	[core]2s(1.80)2p(4.69)3p(0.01)3d(0.01)
	O	-0.13066	[core]2s(1.83)2p(4.27)3s(0.01)3p(0.01)3d(0.01)
$AgO_3H_2^+$	Ag	0.92367	[core]5s(0.10)4d(9.95)5p(0.02)
	H	0.52007	1s(0.48)
	H	0.52007	1s(0.48)
	O	-0.10427	[core]2s(1.80)2p(4.27)3s(0.02)3p(0.01)3d(0.01)
	O	0.14068	[core]2s(1.81)2p(4.02)3s(0.01)3p(0.01)3d(0.01)
	O	-1.00022	[core]2s(1.73)2p(5.26)3p(0.01)
$AgO_3H_3^+$	Ag	0.87774	[core]5s(0.17)4d(9.92)5p(0.02)
	H	0.51849	1s(0.48)
	H	0.51849	1s(0.48)
	H	0.49447	1s(0.50)
	O	-0.98723	[core]2s(1.73)2p(5.25)3p(0.01)
	O	-0.19018	[core]2s(1.85)2p(4.31)3s(0.01)3p(0.01)3d(0.01)
	O	-0.23178	[core]2s(1.75)2p(4.46)3p(0.01)3d(0.01)
$AgO_3H_4^+$	Ag	0.88631	[core]5s(0.15)4d(9.93)5p(0.03)
	H	0.51756	1s(0.48)
	H	0.48262	1s(0.51)
	H	0.50465	1s(0.49)
	H	0.51759	1s(0.48)
	O	-0.41605	[core]2s(1.79)2p(4.61)3p(0.01)4d(0.01)
	O	-0.50609	[core]2s(1.77)2p(4.72)3p(0.01)4d(0.01)
	O	-0.98659	[core]2s(1.73)2p(5.25)3p(0.01)
AgO_4H^+	Ag	0.89931	[core]5s(0.12)4d(9.95)5p(0.03)
	H	0.49744	1s(0.50)
	O	-0.10606	[core]2s(1.80)2p(4.27)3s(0.01)3p(0.01)3d(0.01)
	O	0.14224	[core]2s(1.81)2p(4.02)3s(0.01)3p(0.01)3d(0.01)
	O	-0.20361	[core]2s(1.85)2p(4.32)3s(0.01)3p(0.01)3d(0.01)
	O	-0.22933	[core]2s(1.75)2p(4.46)3p(0.01)3d(0.01)
$AgO_4H_2^+$	Ag	0.84868	[core]5s(0.17)4d(9.94)5p(0.05)
	H	0.51875	1s(0.48)
	H	0.51883	1s(0.48)
	O	-0.98804	[core]2s(1.73)2p(5.25)3p(0.01)
	O	0.35444	[core]2s(1.66)2p(3.94)3p(0.01)4s(0.01)3d(0.02)
	O	-0.16853	[core]2s(1.84)2p(4.30)3s(0.01)3p(0.01)
	O	-0.08412	[core]2s(1.84)2p(4.23)3s(0.01)3p(0.01)
$AgO_4H_3^+$	Ag	0.94676	[core]5s(0.22)4d(9.78)5p(0.05)
	H	0.46656	1s(0.53)
	H	0.52022	1s(0.48)
	H	0.51946	1s(0.48)

	O	-0.97704	[core]2s(1.72)2p(5.24)3p(0.01)
	O	0.093	[core]2s(1.81)2p(4.06)3s(0.01)3p(0.01)3d(0.01)
	O	0.16018	[core]2s(1.82)2p(3.99)3s(0.01)3p(0.01)3d(0.01)
	O	-0.72914	[core]2s(1.86)2p(4.86)3d(0.01)
$AgO_4H_4^+$	Ag	0.87306	[core]5s(0.16)4d(9.93)5p(0.04)
	H	0.51564	1s(0.48)
	H	0.51605	1s(0.48)
	H	0.51613	1s(0.48)
	H	0.51563	1s(0.48)
	O	-0.05878	[core]2s(1.80)2p(4.22)3s(0.02)3p(0.01)3d(0.01)
	O	-0.97712	[core]2s(1.73)2p(5.24)3p(0.01)
	O	0.07874	[core]2s(1.81)2p(4.08)3s(0.01)3p(0.01)3d(0.01)
	O	-0.97935	[core]2s(1.72)2p(5.24)3p(0.01)
$AgOH^-$	Ag	-0.15658	[core]5s(1.05)4d(9.93)5p(0.16)6s(0.01)
	H	0.40732	1s(0.58)2p(0.01)
	O	-1.25074	[core]2s(1.85)2p(5.39)3p(0.01)3d(0.01)
$AgOH_2^-$	Ag	0.34306	[core]5s(0.71)4d(9.84)5p(0.11)
	H	-0.52319	1s(1.51)2s(0.01)
	H	0.41388	1s(0.58)
	O	-1.23375	[core]2s(1.82)2p(5.40)3p(0.01)3d(0.01)
$AgOH_3^-$	Ag	-0.37102	[core]5s(1.13)4d(9.94)5p(0.28)6s(0.02)
	H	-0.558	1s(1.55)
	H	0.44815	1s(0.53)2s(0.02)
	H	0.44815	1s(0.53)2s(0.02)
	O	-0.9673	[core]2s(1.76)2p(5.20)3p(0.01)3d(0.01)
$AgOH_4^-$	Ag	0.13164	[core]5s(0.83)4d(9.89)5p(0.15)
	H	0.45138	1s(0.54)
	H	-0.56779	1s(1.56)
	H	-0.53377	1s(1.53)
	H	0.50514	1s(0.49)
	O	-0.98659	[core]2s(1.75)2p(5.22)3p(0.01)3d(0.01)
AgO_2H^-	Ag	0.59406	[core]5s(0.57)4d(9.75)5p(0.08)
	H	0.41553	1s(0.58)2p(0.01)
	O	-1.21411	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
	O	-0.79548	[core]2s(1.96)2p(4.83)3d(0.01)
$AgO_2H_2^-$	Ag	0.60099	[core]5s(0.54)4d(9.78)5p(0.07)
	H	0.41441	2s(0.58)
	H	0.4144	2s(0.58)
	O	-1.2149	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
	O	-1.2149	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
$AgO_2H_3^-$	Ag	-0.11783	[core]5s(1.03)4d(9.94)5p(0.14)6s(0.01)
	H	0.43826	1s(0.56)
	H	0.51298	1s(0.48)
	H	0.42724	1s(0.57)

	O	-1.00693	[core]2s(1.75)2p(5.24)3p(0.01)3d(0.01)
	O	-1.25371	[core]2s(1.83)2p(5.40)3p(0.01)
$AgO_2H_4^-$	Ag	0.3538	[core]5s(0.71)4d(9.84)5p(0.09)
	H	-0.50802	1s(1.50)2s(0.01)
	H	0.43885	1s(0.55)
	H	0.51247	1s(0.48)
	H	0.43189	1s(0.56)
	O	-1.2237	[core]2s(1.81)2p(5.39)3p(0.01)
	O	-1.00528	[core]2s(1.75)2p(5.24)3p(0.01)3d(0.01)
AgO_3H^-	Ag	0.6194	[core]5s(0.50)4d(9.80)5p(0.07)
	H	0.41727	1s(0.57)
	O	-1.21579	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
	O	-0.4646	[core]2s(1.83)2p(4.60)3s(0.01)3p(0.01)3d(0.01)
	O	-0.35628	[core]2s(1.86)2p(4.47)3s(0.01)3p(0.01)
$AgO_3H_2^-$	Ag	0.60541	[core]5s(0.53)4d(9.78)5p(0.07)
	H	0.41542	1s(0.58)
	H	0.4225	1s(0.57)
	O	-1.21494	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
	O	-0.67707	[core]2s(1.88)2p(4.77)3s(0.01)3p(0.01)
	O	-0.55132	[core]2s(1.77)2p(4.76)3p(0.01)4d(0.01)
$AgO_3H_3^-$	Ag	1.00091	[core]5s(0.34)4d(9.48)5p(0.17)
	H	0.43357	1s(0.56)
	H	0.4251	1s(0.57)
	H	0.42091	1s(0.57)
	O	-1.00939	[core]2s(1.84)2p(5.16)3p(0.01)3d(0.01)
	O	-1.13127	[core]2s(1.82)2p(5.29)3p(0.01)3d(0.01)
	O	-1.13983	[core]2s(1.82)2p(5.30)3p(0.01)3d(0.01)
$AgO_3H_4^-$	Ag	0.6224	[core]5s(0.52)4d(9.78)5p(0.07)
	H	0.41706	1s(0.57)
	H	0.43298	1s(0.56)
	H	0.5115	1s(0.48)
	H	0.44001	1s(0.55)
	O	-1.00224	[core]2s(1.75)2p(5.24)3p(0.01)3d(0.01)
	O	-1.21248	[core]2s(1.82)2p(5.38)3p(0.01)3d(0.01)
	O	-1.20922	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
AgO_4H^-	Ag	0.63203	[core]5s(0.46)4d(9.82)5p(0.08)
	H	0.41793	1s(0.57)2p(0.01)
	O	-0.55785	[core]2s(1.86)2p(4.67)3s(0.01)3p(0.01)
	O	-1.22153	[core]2s(1.83)2p(5.38)3d(0.01)
	O	-0.35447	[core]2s(1.85)2p(4.48)3p(0.01)3d(0.01)
	O	0.08389	[core]2s(1.71)2p(4.16)3s(0.02)3p(0.01)3d(0.01)
$AgO_4H_2^-$	Ag	0.60302	[core]5s(0.54)4d(9.78)5p(0.07)
	H	0.41488	1s(0.58)2p(0.01)
	H	0.4161	1s(0.58)2p(0.01)

	O	-0.00081	[core]2s(1.81)2p(4.16)3s(0.02)3p(0.01)3d(0.01)
	O	-0.00156	[core]2s(1.81)2p(4.16)3s(0.02)3p(0.01)3d(0.01)
	O	-1.21419	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
	O	-1.21745	[core]2s(1.83)2p(5.37)3p(0.01)3d(0.01)
$AgO_4H_3^-$	Ag	0.63983	[core]5s(0.49)4d(9.80)5p(0.06)
	H	0.4939	1s(0.50)
	H	0.41968	1s(0.57)
	H	0.45844	1s(0.53)
	O	-0.97854	[core]2s(1.75)2p(5.21)3p(0.01)3d(0.01)
	O	-0.33363	[core]2s(1.85)2p(4.46)3s(0.01)3p(0.01)
	O	-0.48865	[core]2s(1.82)2p(4.63)3s(0.01)3p(0.02)3d(0.01)
	O	-1.21102	[core]2s(1.83)2p(5.37)3d(0.01)
$AgO_4H_4^-$	Ag	1.19441	[core]5s(0.34)4d(9.15)5p(0.30)
	H	0.44713	2s(0.55)
	H	0.4471	2s(0.55)
	H	0.44702	2s(0.55)
	H	0.44702	2s(0.55)
	O	-0.99575	[core]2s(1.81)2p(5.17)3d(0.01)
	O	-0.99579	[core]2s(1.81)2p(5.17)3d(0.01)
	O	-0.99554	[core]2s(1.81)2p(5.17)3d(0.01)
	O	-0.9956	[core]2s(1.81)2p(5.17)3d(0.01)

Table S5
The values of second order perturbation energies ($E^{(2)}$) corresponding to the most dominant donor (D)-acceptor (A) interactions of the $AgO_kH_m^{\pm}$ clusters, where k, m = 1 – 4, obtained at the ωB97XD level of theory. For open-shell systems, the most dominant D-A interactions for both α and β spin orbitals are provided.

Systems	Donor NBO (i)	Acceptor NBO (j)	$E^{(2)}$ (eV)
$AgOH^+$	LP (2) O 3	LV (1) Ag 1	0.35346
	LP (3) O 3	LV (1) Ag 1	0.23048
$AgOH_2^+$	LP (2) O 4	LV (1) Ag 1	0.49192
$AgOH_3^+$	LP (2) O 5	BD*(1) Ag 1 - H 4	0.49063
	LP (2) O 5	LV (1) Ag 1	0.35518
$AgOH_4^+$	BD (1) H 2 - H 5	LV (1) Ag 1	1.22808
AgO_2H^+	LP (2) O 4	LV (1) Ag 1	0.42570
	LP (3) O 4	LV (1) Ag 1	0.31304
$AgO_2H_2^+$	LP (2) O 5	LV (1) Ag 1	0.2365
$AgO_2H_3^+$	LP (2) O 6	LV (1) Ag 1	0.66521
	LP (3) O 6	LV (1) Ag 1	0.47902
$AgO_2H_4^+$	LP (2) O 7	LV (1) Ag 1	0.90687
AgO_3H^+	LP (2) O 5	BD*(1) O 3 - O 4	1.02985
	LP (3) O 5	BD*(1) O 3 - O 4	0.84624
$AgO_3H_2^+$	LP (2) O 6	LV (1) Ag 1	0.31390
	LP (2) O 6	LV (1) Ag 1	0.31605
$AgO_3H_3^+$	LP (2) O 6	LV (1) Ag 1	0.63812
	LP (3) O 6	LV (1) Ag 1	0.50396
AgO_3H4^+	LP (2) O 7	LV (1) Ag 1	0.85570
AgO_4H^+	LP (2) O 5	LV (1) Ag 1	0.51127
	LP (3) O 5	LV (1) Ag 1	0.38528
$AgO_4H_2^+$	LP (3) O 6	BD*(1) O 5 - O 7	10.50748
$AgO_4H_3^+$	LP (2) O 8	LV (1) Ag 1	0.59856
	LP (3) O 8	LV (1) Ag 1	0.43731
$AgO_4H_4^+$	LP (2) O 7	LV (1) Ag 1	0.43774
	LP (2) O 7	LV (1) Ag 1	0.43215

$AgOH^-$	LP (6) Ag 1	RY (1) O 3	0.58265
	LP (3) O 3	RY (1) Ag 1	0.49278
$AgOH_2^-$	LP (3) O 4	BD*(1) Ag 1 - H 2	3.09041
$AgOH_3^-$	LP (1) H 2	RY (1) Ag 1	2.79543
	LP (1) H 2	RY (10) H 2	1.85760
$AgOH_4^-$	LP (1) H 3	BD*(1) Ag 1 - H 4	11.41134
AgO_2H^-	LP (3) O 3	BD*(1) Ag 1 - O 4	1.71871
	LP (3) O 3	BD*(1) Ag 1 - O 4	1.63529
$AgO_2H_2^-$	LP (3) O 4	BD*(1) Ag 1- O 5	3.41291
$AgO_2H_3^-$	LP (6) Ag 1	RY (1) O 6	0.74648
	LP (2) O 6	BD*(1) H 3 - O 5	0.53062
$AgO_2H_4^-$	LP (3) O 6	BD*(1) Ag 1 - H 2	2.70556
AgO_3H^-	LP (2) O 4	BD*(1) Ag 1 - O 3	1.46587
	LP (3) O 4	BD*(1) Ag 1- O 3	1.20744
$AgO_3H_2^-$	LP (3) O 5	BD*(1) Ag 1- O 4	3.25983
$AgO_3H_3^-$	LP (3) O 7	BD*(1) Ag 1 - O 6	2.53528
	LP (3) O 6	LV (1) Ag 1	1.69033
$AgO_3H_4^-$	LP (3) O 7	BD*(1) Ag 1- O 8	2.99882
AgO_4H^-	LP (3) O 3	BD*(1) O 5 - O 6	1.94876
	LP (3) O 3	BD*(1) Ag 1 - O 4	1.04275
$AgO_4H_2^-$	LP (3) O 7	BD*(1) Ag 1 - O 6	1.68947
	LP (3) O 7	BD*(1) Ag 1- O 6	1.6856
$AgO_4H_3^-$	LP (2) O 7	BD*(1) Ag 1 - O 8	1.22593
	LP (3) O 7	BD*(1) Ag 1- O 8	1.07672
$AgO_4H_4^-$	LP (3) O 8	BD*(1) Ag 1- O 6	6.56825
	LP (3) O 7	BD*(1) Ag 1- O 9	6.56438

Table S6
QTAIM topology parameters including electron density ρ(**BCP**), Laplacian of electron density $\nabla^2\rho$(**BCP**), kinetic electron density *G*(**BCP**), potential of electron density *V*(**BCP**), and *G*(**BCP**)/|*V*(**BCP**)| ratio of the $AgO_kH_m^{\pm}$ clusters, where *k*, *m* = 1 – 4, calculated at the ωB97XD level of theory.

Systems	BCP(3,-1)	ρ(**BCP**)	$\nabla^2\rho$(**BCP**)	*G*(**BCP**)	*V*(**BCP**)	*G*(**BCP**)/|*V*(**BCP**)|
$AgOH^+$	4	0.0493	0.2346	0.0618	-0.0651	0.949308756
	5	0.3521	-2.6673	0.0591	-0.7850	0.075286624
$AgOH_2^+$	5	0.3625	-2.7555	0.0653	-0.8195	0.079682733
	6	0.0561	0.2747	0.0739	-0.0791	0.93426043
	7	0.3625	-2.7555	0.0653	-0.8195	0.079682733
$AgOH_3^+$	6	0.3613	-2.7573	0.0642	-0.8177	0.078512902
	7	0.1259	-0.0444	0.0694	-0.1498	0.463284379
	8	0.0604	0.3090	0.0836	-0.0900	0.928888889
	9	0.3613	-2.7574	0.0642	-0.8177	0.078512902
$AgOH_4^+$	7	0.3622	-2.7599	0.0648	-0.8195	0.079072605
	8	0.0623	0.3039	0.0836	-0.0913	0.915662651
	9	0.0554	0.1924	0.0546	-0.0611	0.893617021
	10	0.2536	-1.0906	0.0027	-0.2781	0.009708738
	11	0.3622	-2.7596	0.0648	-0.8195	0.079072605
AgO_2H^+	5	0.3573	-2.7494	0.0548	-0.7970	0.068757842
	6	0.3767	-0.0033	0.2940	-0.5888	0.499320652
	7	0.0509	0.2282	0.0615	-0.0660	0.931818182
$AgO_2H_2^+$	6	0.3630	-2.7567	0.0620	-0.8132	0.076242007
	7	0.0329	0.1610	0.0397	-0.0392	1.012755102
	8	0.2654	0.1239	0.1817	-0.3325	0.546466165
	9	0.0329	0.1611	0.0398	-0.0392	1.015306122
	10	0.3629	-2.7565	0.0620	-0.8132	0.076242007
$AgO_2H_3^+$	7	0.3629	-2.7621	0.0652	-0.8210	0.079415347
	8	0.0610	0.2981	0.0818	-0.0890	0.919101124
	9	0.0581	0.2793	0.0763	-0.0828	0.921497585
	10	0.3631	-2.7633	0.0653	-0.8214	0.079498417
	11	0.3531	-2.6642	0.0599	-0.7859	0.07621835
$AgO_2H_4^+$	8	0.3636	-2.7630	0.0657	-0.8222	0.079907565
	9	0.3636	-2.7631	0.0657	-0.8222	0.079907565
	10	0.0602	0.2967	0.0812	-0.0881	0.921679909
	11	0.3636	-2.7631	0.0657	-0.8222	0.079907565
	12	0.0602	0.2967	0.0812	-0.0881	0.921679909
	13	0.3636	-2.7631	0.0657	-0.8222	0.079907565

AgO_3H^+	6	0.4513	-0.1872	0.3904	-0.8275	0.471782477
	7	0.0331	0.1376	0.0346	-0.0349	0.991404011
	8	0.0200	0.1015	0.0221	-0.0189	1.169312169
	9	0.2500	0.2178	0.1876	-0.3207	0.584970377
	10	0.0344	0.1643	0.0408	-0.0405	1.007407407
	11	0.3534	-2.6974	0.0590	-0.7924	0.074457345
$AgO_3H_2^+$	7	0.3628	-2.7588	0.0654	-0.8204	0.079717211
	8	0.0584	0.2855	0.0775	-0.0837	0.925925926
	9	0.0348	0.1611	0.0406	-0.0409	0.992665037
	10	0.3628	-2.7588	0.0654	-0.8204	0.079717211
	11	0.5146	-0.4960	0.4577	-1.0394	0.440350202
$AgO_3H_3^+$	8	0.0562	0.2572	0.0708	-0.0774	0.914728682
	9	0.3764	-0.0034	0.2935	-0.5878	0.499319496
	10	0.3584	-2.7497	0.0556	-0.7986	0.069621838
	11	0.0602	0.2953	0.0807	-0.0877	0.92018244
	12	0.3634	-2.7618	0.0656	-0.8217	0.079834489
	13	0.3634	-2.7618	0.0656	-0.8217	0.079834489
$AgO_3H_4^+$	9	0.3637	-2.7620	0.0658	-0.8222	0.08002919
	10	0.3637	-2.7703	0.0621	-0.8167	0.076037713
	11	0.0524	0.2497	0.0672	-0.0721	0.932038835
	12	0.0593	0.2917	0.0795	-0.0861	0.923344948
	13	0.2688	0.1224	0.1848	-0.3389	0.545293597
	14	0.3637	-2.7620	0.0658	-0.8222	0.08002919
	15	0.3655	-2.7549	0.0638	-0.8163	0.07815754
AgO_4H^+	7	0.0537	0.2419	0.0660	-0.0715	0.923076923
	8	0.3767	-0.0037	0.2939	-0.5886	0.499320421
	9	0.3575	-2.7494	0.0550	-0.7974	0.068974166
	10	0.0346	0.1600	0.0402	-0.0404	0.995049505
	11	0.5144	-0.4948	0.4575	-1.0387	0.44045441
$AgO_4H_2^+$	8	0.3633	-2.7606	0.0656	-0.8213	0.079873371
	9	0.0418	0.1840	0.0482	-0.0503	0.958250497
	10	0.4386	-0.0600	0.3979	-0.8108	0.490749877
	11	0.0590	0.2902	0.0789	-0.0853	0.924970692
	12	0.0200	0.0841	0.0190	-0.0170	1.117647059
	13	0.3633	-2.7611	0.0656	-0.8215	0.079853926
	14	0.0223	0.0867	0.0208	-0.0199	1.045226131
	15	0.4620	-0.1514	0.4264	-0.8907	0.478724599
$AgO_4H_3^+$	9	0.3526	-2.5693	0.0674	-0.7771	0.086732724
	10	0.0586	0.2136	0.0609	-0.0683	0.891654466
	11	0.0203	0.0608	0.0140	-0.0128	1.09375

	12	0.5172	-0.4545	0.4711	-1.0558	0.446201932
	13	0.0576	0.2829	0.0767	-0.0826	0.928571429
	14	0.3632	-2.7611	0.0655	-0.8212	0.079761325
	15	0.3630	-2.7610	0.0653	-0.8209	0.079546839
$AgO_4H_4^+$	10	0.3640	-2.7608	0.0661	-0.8225	0.080364742
	11	0.3641	-2.7637	0.0661	-0.8232	0.080296404
	12	0.0584	0.2871	0.0781	-0.0844	0.92535545
	13	0.0160	0.0646	0.0146	-0.0130	1.123076923
	14	0.5161	-0.5047	0.4595	-1.0452	0.439628779
	15	0.0582	0.2851	0.0776	-0.0839	0.924910608
	16	0.3639	-2.7579	0.0662	-0.8218	0.08055488
	17	0.3639	-2.7578	0.0662	-0.8218	0.08055488
$AgOH^-$	4	0.0750	0.3137	0.0928	-0.1071	0.866479925
	5	0.3683	-2.4219	0.0946	-0.7946	0.119053612
$AgOH_2^-$	5	0.1172	0.0837	0.0845	-0.1481	0.570560432
	6	0.0851	0.3702	0.1119	-0.1312	0.852896341
	7	0.3672	-2.4120	0.0938	-0.7906	0.118644068
$AgOH_3^-$	6	0.3631	-2.6342	0.0759	-0.8104	0.093657453
	7	0.0054	0.0056	0.0015	-0.0017	0.882352941
	8	0.0985	0.1010	0.0708	-0.1164	0.608247423
	9	0.3631	-2.6343	0.0759	-0.8104	0.093657453
$AgOH_4^-$	6	0.0998	0.1245	0.0766	-0.1222	0.626841244
	7	0.0216	0.0339	0.0101	-0.0117	0.863247863
	8	0.1050	0.1072	0.0775	-0.1282	0.604524181
	9	0.3483	-2.5853	0.0711	-0.7884	0.09018265
	10	0.3706	-2.6298	0.0803	-0.8181	0.09815426
AgO_2H^-	5	0.0981	0.4039	0.1283	-0.1556	0.824550129
	6	0.0916	0.3777	0.1178	-0.1412	0.83427762
	7	0.3679	-2.4374	0.0924	-0.7941	0.116358141
$AgO_2H_2^-$	6	0.3678	-2.4303	0.0928	-0.7931	0.117009204
	7	0.3678	-2.4303	0.0928	-0.7931	0.117009204
	8	0.0911	0.3762	0.1171	-0.1402	0.835235378
	9	0.0911	0.3762	0.1171	-0.1402	0.835235378
$AgO_2H_3^-$	7	0.3722	-2.5978	0.0838	-0.8171	0.102557826
	8	0.3229	-2.3871	0.0697	-0.7363	0.094662502
	9	0.0511	0.0980	0.0378	-0.0510	0.741176471
	10	0.0722	0.3139	0.0913	-0.1041	0.877041306
	11	0.3669	-2.4497	0.0913	-0.7950	0.114842767
$AgO_2H_4^-$	8	0.3723	-2.6003	0.0837	-0.8175	0.102385321

	9	0.1189	0.0803	0.0853	-0.1506	0.566401062
	10	0.3239	-2.3968	0.0697	-0.7387	0.094354948
	11	0.0510	0.0990	0.0379	-0.0510	0.743137255
	12	0.0815	0.3648	0.1085	-0.1259	0.861795075
	13	0.3683	-2.4755	0.0910	-0.8009	0.113622175
AgO_3H^-	6	0.0808	0.3523	0.1057	-0.1234	0.856564019
	7	0.0923	0.3751	0.1176	-0.1414	0.831683168
	8	0.3676	-2.4426	0.0920	-0.7946	0.115781525
	9	0.3408	0.1004	0.2647	-0.5042	0.524990083
$AgO_3H_2^-$	7	0.0871	0.3727	0.1140	-0.1348	0.845697329
	8	0.2404	0.1698	0.1693	-0.2961	0.571766295
	9	0.3760	-2.6595	0.0792	-0.8233	0.096198227
	10	0.0923	0.3784	0.1184	-0.1423	0.832044975
	11	0.3677	-2.4352	0.0924	-0.7936	0.116431452
$AgO_3H_3^-$	8	0.1016	0.3916	0.1278	-0.1576	0.810913706
	9	0.0985	0.3937	0.1261	-0.1538	0.819895969
	10	0.3680	-2.5049	0.0881	-0.8023	0.109809298
	11	0.3683	-2.4761	0.0901	-0.7992	0.112737738
	12	0.0855	0.3092	0.0976	-0.1179	0.82782019
	13	0.3665	-2.4725	0.0873	-0.7928	0.110116044
$AgO_3H_4^-$	9	0.3688	-2.4914	0.0900	-0.8029	0.11209366
	10	0.0877	0.3745	0.1147	-0.1358	0.844624448
	11	0.0490	0.0980	0.0365	-0.0486	0.751028807
	12	0.0936	0.3830	0.1203	-0.1449	0.830227743
	13	0.3268	-2.4238	0.0696	-0.7451	0.09341028
	14	0.3678	-2.4425	0.0921	-0.7948	0.115878208
	15	0.3723	-2.6057	0.0834	-0.8182	0.101931068
AgO_4H^-	7	0.3100	0.1965	0.2490	-0.4488	0.554812834
	8	0.0720	0.3242	0.0940	-0.1069	0.879326473
	9	0.0190	0.0790	0.0178	-0.0159	1.119496855
	10	0.0912	0.3728	0.1163	-0.1395	0.833691756
	11	0.3960	0.0104	0.3334	-0.6643	0.50188168
	12	0.0194	0.0728	0.0170	-0.0158	1.075949367
	13	0.3674	-2.4403	0.0919	-0.7939	0.115757652
$AgO_4H_2^-$	8	0.3677	-2.4308	0.0927	-0.7930	0.116897856
	9	0.5165	-0.5096	0.4591	-1.0457	0.439036052
	10	0.0914	0.3773	0.1176	-0.1409	0.834634493
	11	0.0058	0.0262	0.0051	-0.0037	1.378378378
	12	0.0906	0.3754	0.1167	-0.1396	0.835959885
	13	0.3678	-2.4369	0.0923	-0.7938	0.11627614

$AgO_4H_3^-$	9	0.3676	-2.4535	0.0913	-0.7959	0.114712904
	10	0.3523	-2.6166	0.0709	-0.7959	0.089081543
	11	0.0956	0.3849	0.1220	-0.1478	0.825439783
	12	0.0299	0.0877	0.0237	-0.0255	0.929411765
	13	0.0788	0.3517	0.1046	-0.1213	0.862324815
	14	0.3698	-2.6495	0.0787	-0.8198	0.095999024
	15	0.3561	0.0675	0.2794	-0.5419	0.515593283
$AgO_4H_4^-$	11	0.3683	-2.5699	0.0836	-0.8098	0.103235367
	12	0.3684	-2.5712	0.0837	-0.8101	0.103320578
	13	0.1153	0.3781	0.1342	-0.1738	0.772151899
	14	0.1152	0.3781	0.1341	-0.1737	0.772020725
	15	0.3686	-2.5738	0.0837	-0.8109	0.103218646
	16	0.1153	0.3784	0.1343	-0.1740	0.77183908
	17	0.3685	-2.5725	0.0837	-0.8106	0.103256847

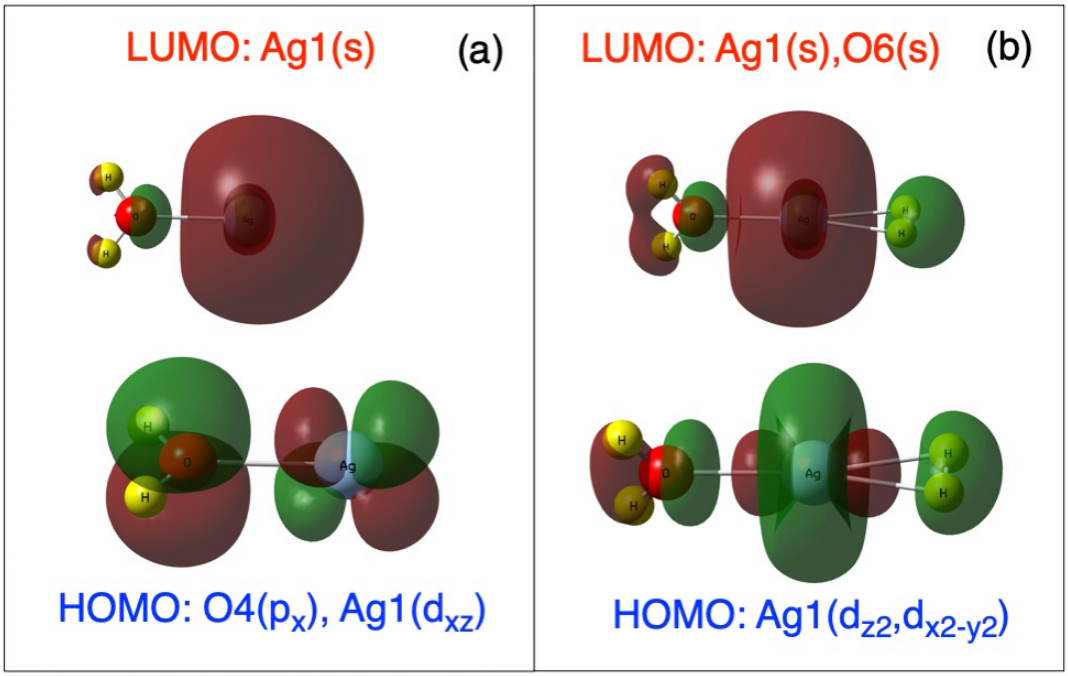

Figure S1. Schematic representation of HOMO (bottom) and LUMO (top) for (a) $AgOH_2^+$ and (b) $AgOH_4^+$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

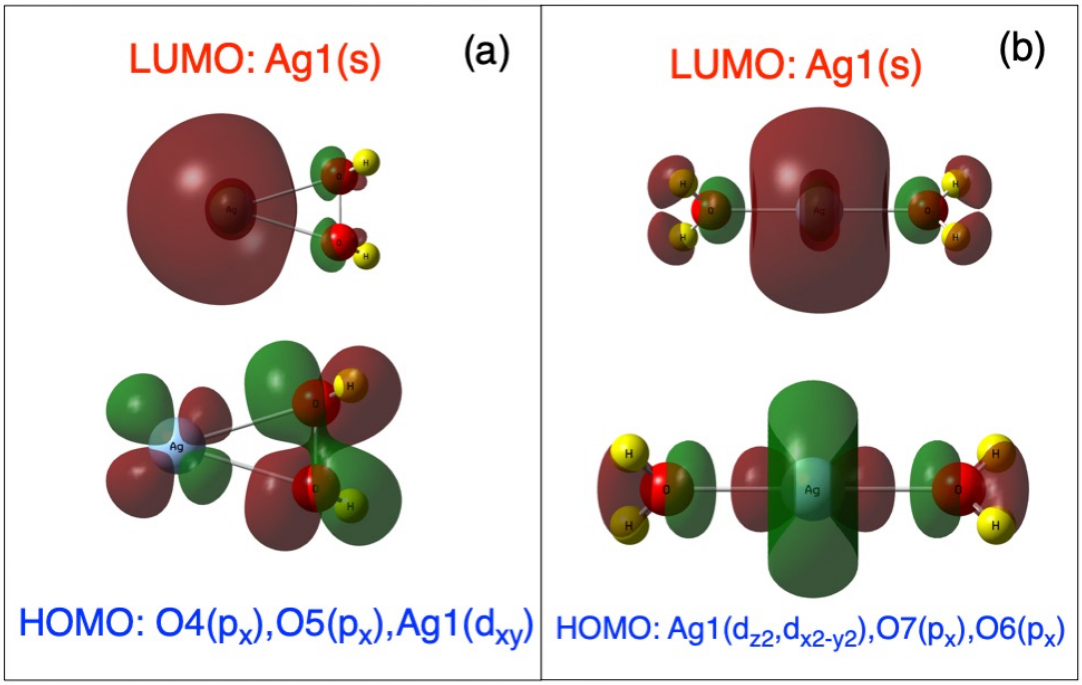

Figure S2. Schematic representation of HOMO (bottom) and LUMO (top) for (a) $AgO_2H_2^+$ and (b) $AgO_2H_4^+$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

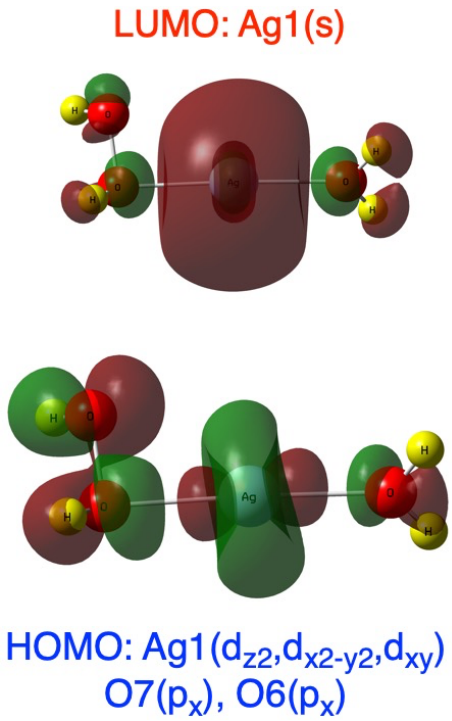

Figure S3. Schematic representation of HOMO (bottom) and LUMO (top) for $AgO_3H_4^+$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

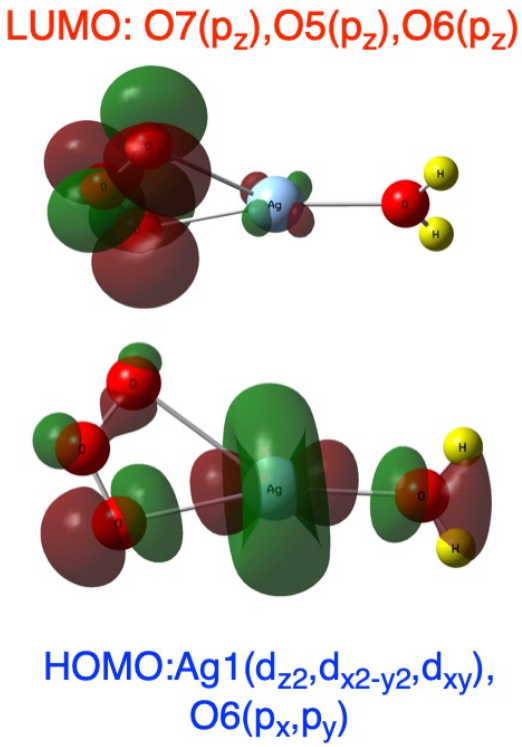

Figure S4. Schematic representation of HOMO (bottom) and LUMO (top) for $AgO_4H_2^+$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

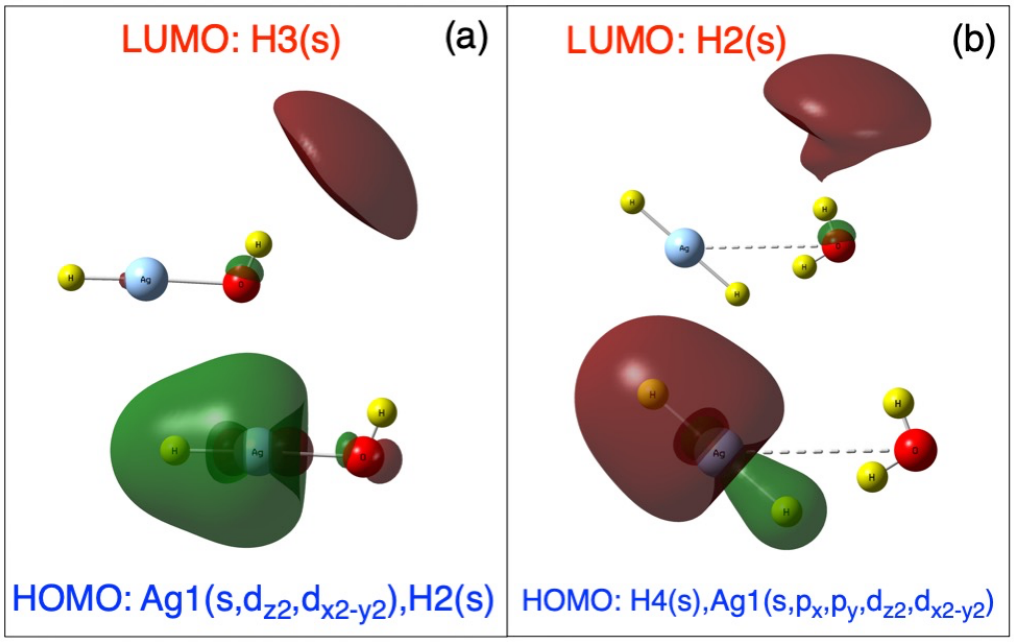

Figure S5. Schematic representation of HOMO (bottom) and LUMO (top) for (a) $AgOH_2^-$ and (b) $AgOH_4^-$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

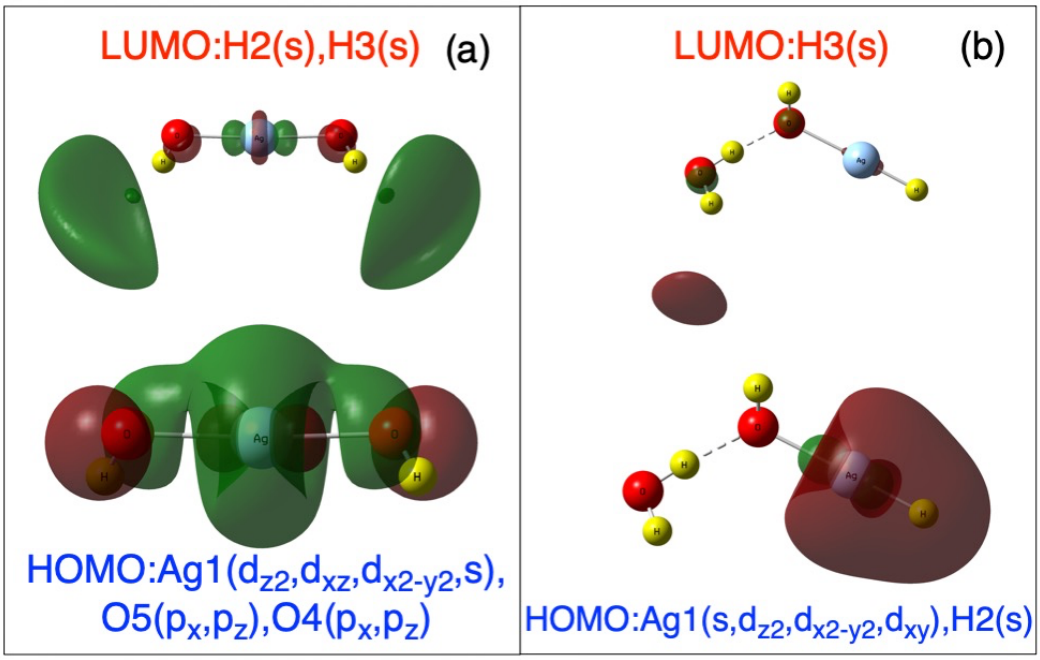

Figure S6. Schematic representation of HOMO (bottom) and LUMO (top) for (a) $AgO_2H_2^-$ and (b) $AgO_2H_4^-$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

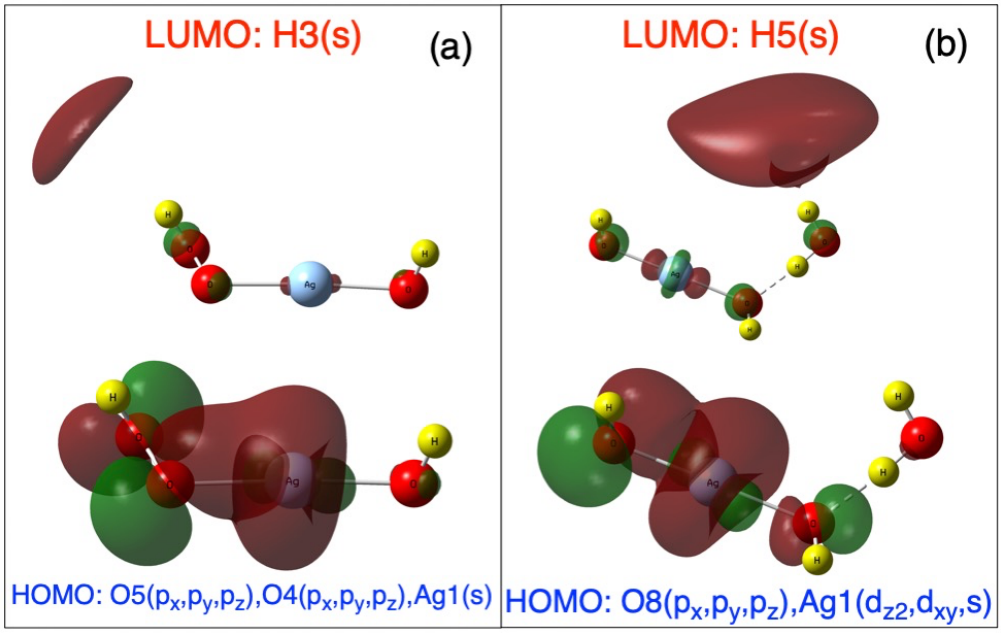

Figure S7. Schematic representation of HOMO (bottom) and LUMO (top) orbitals for (a) $AgO_3H_2^-$ and (b) $AgO_3H_4^-$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

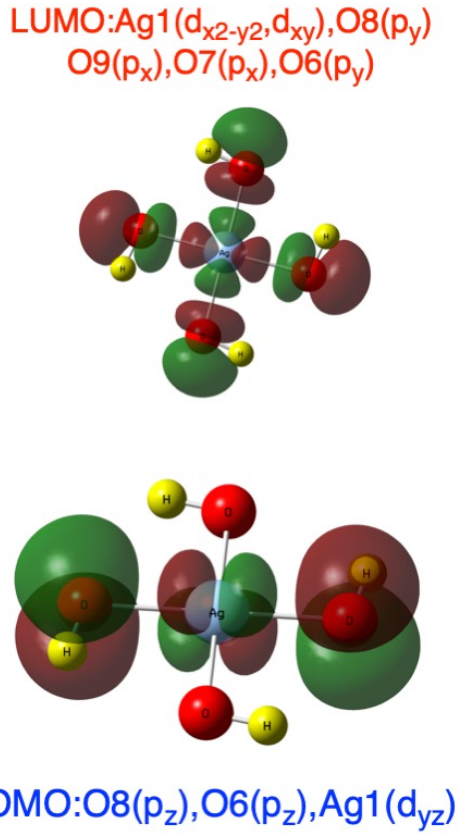

Figure S8. Schematic representation of HOMO (bottom) and LUMO (top) orbitals for $AgO_4H_4^-$ using isovalues of 0.03 obtained at ωB97XD level of theory. The dominant atomic orbital contributions to HOMO and LUMO are reported. The atom numbers correspond to the same as in Table S1.

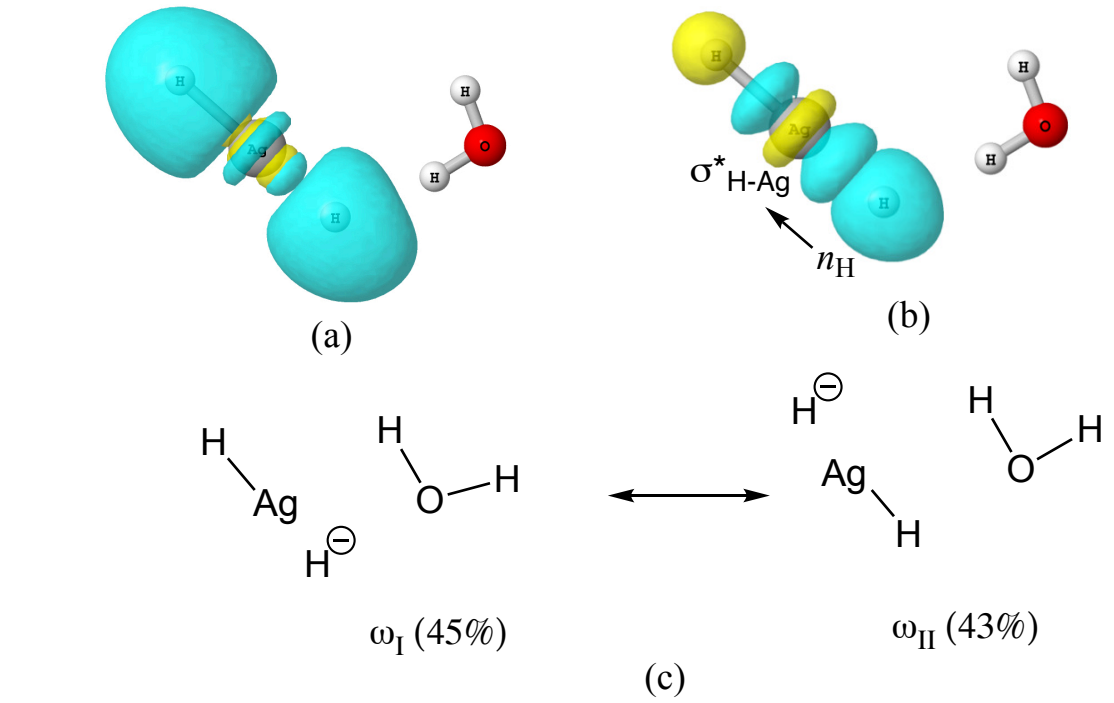

Figure S9. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of H (n_H) and empty σ* NBO of H-Ag bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgOH_4^-$ cluster.

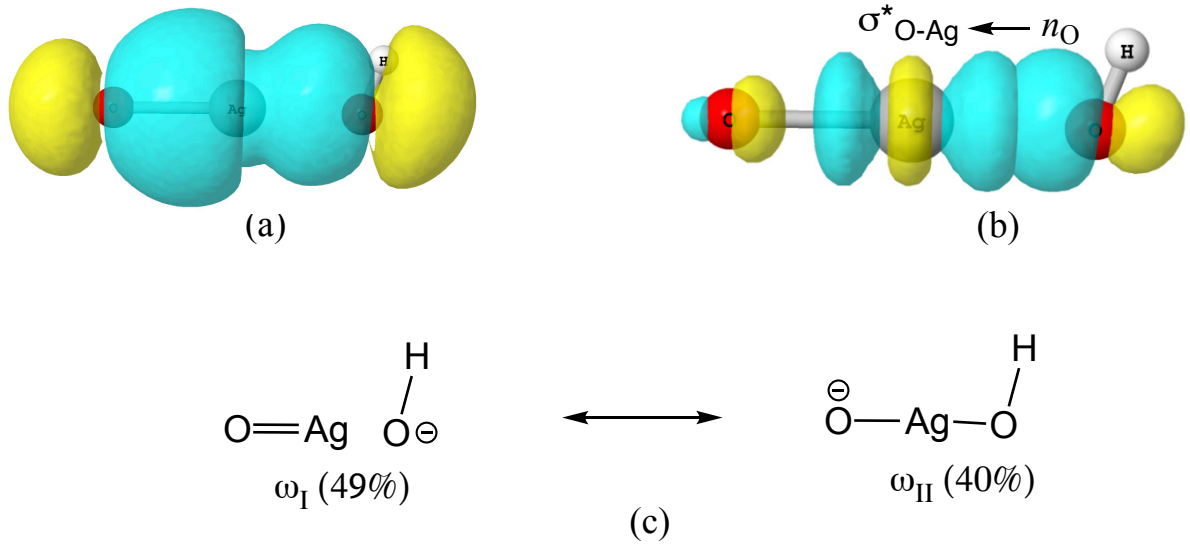

Figure S10. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for AgO_2H^- cluster.

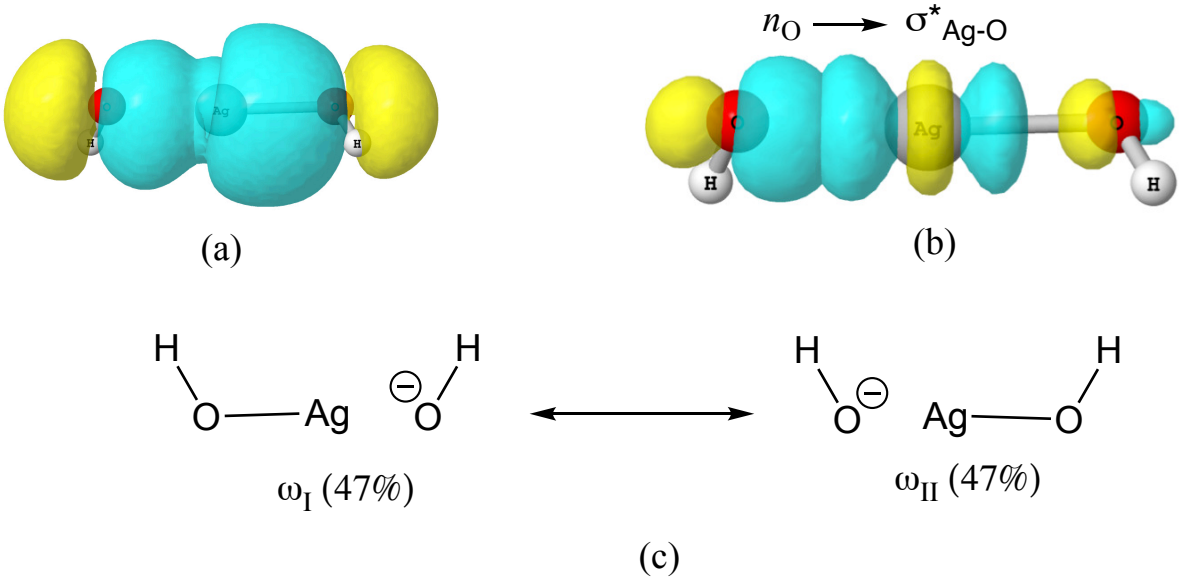

Figure S11. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_2H_2^-$ cluster.

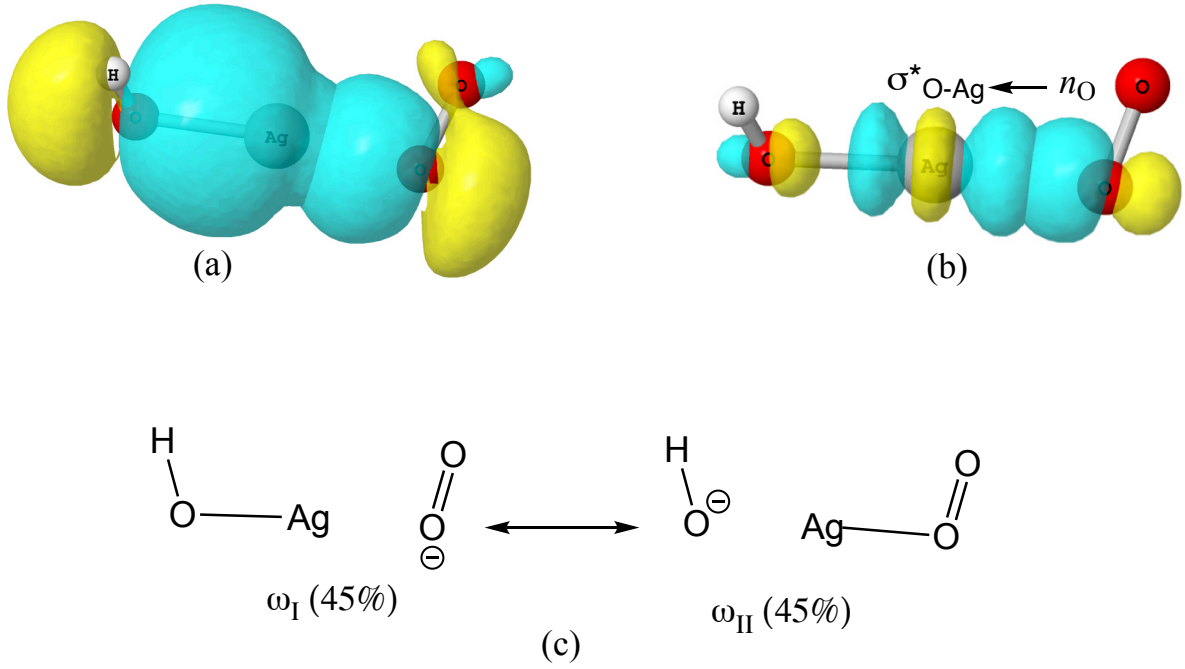

Figure S12. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for AgO_3H^- cluster.

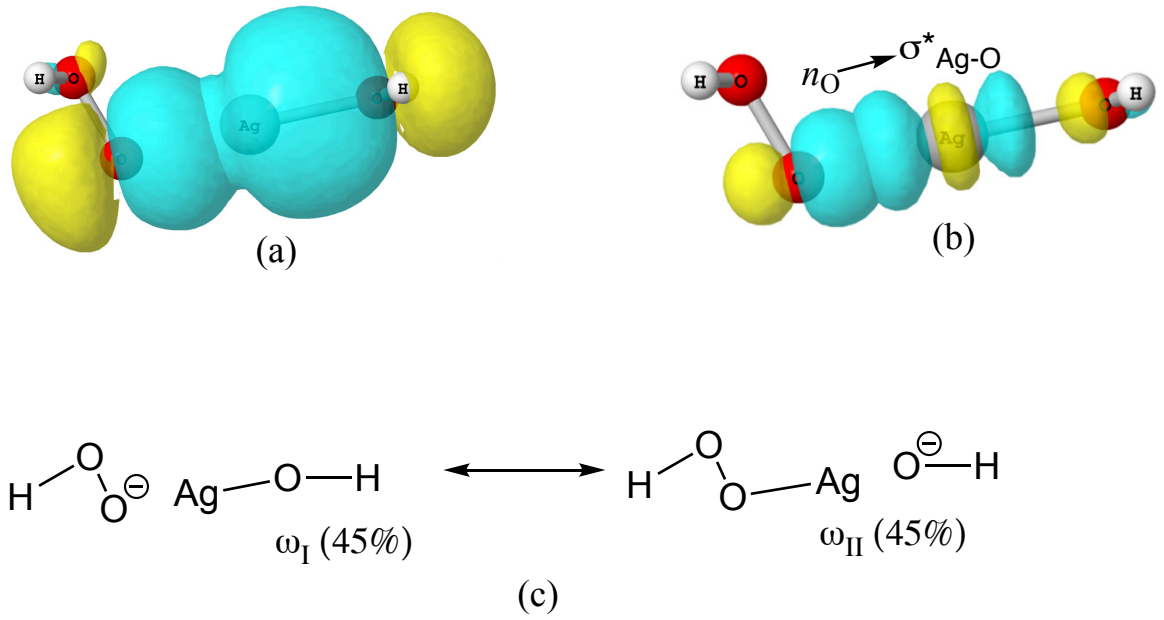

Figure S13. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_3H_2^-$ cluster.

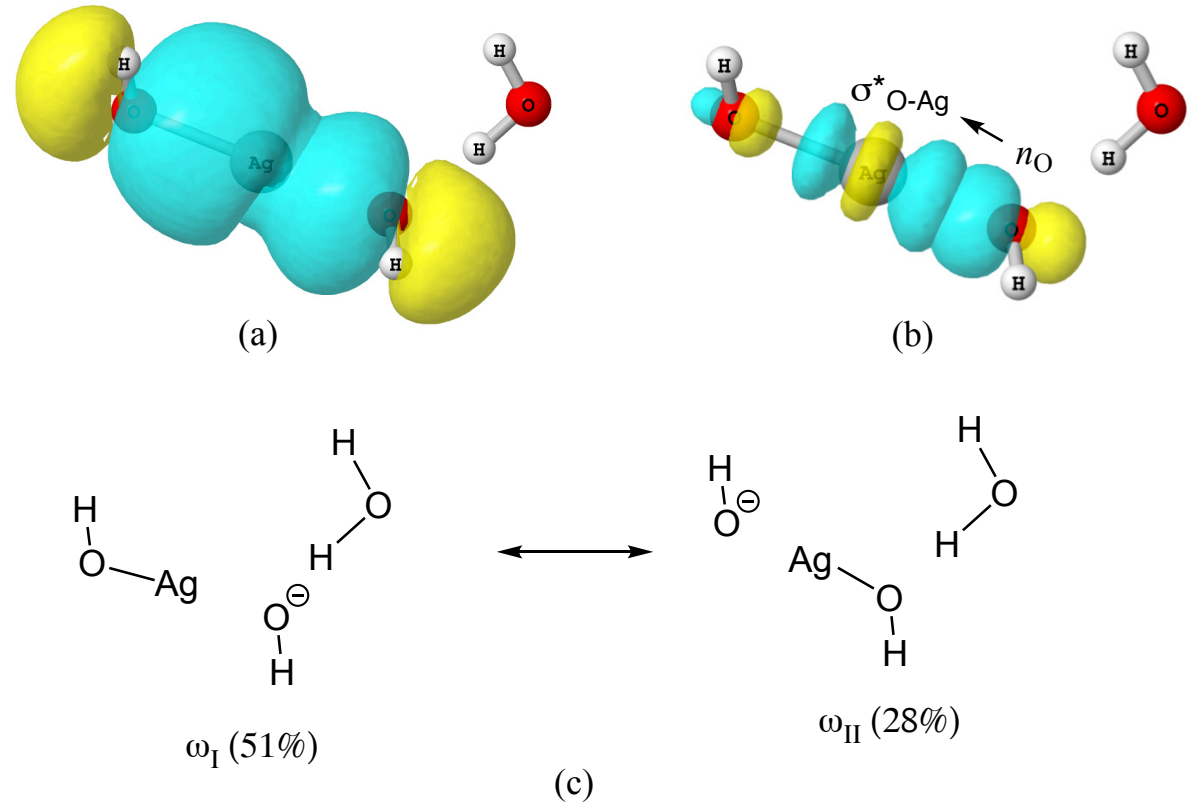

Figure S14. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_3H_4^-$ cluster.

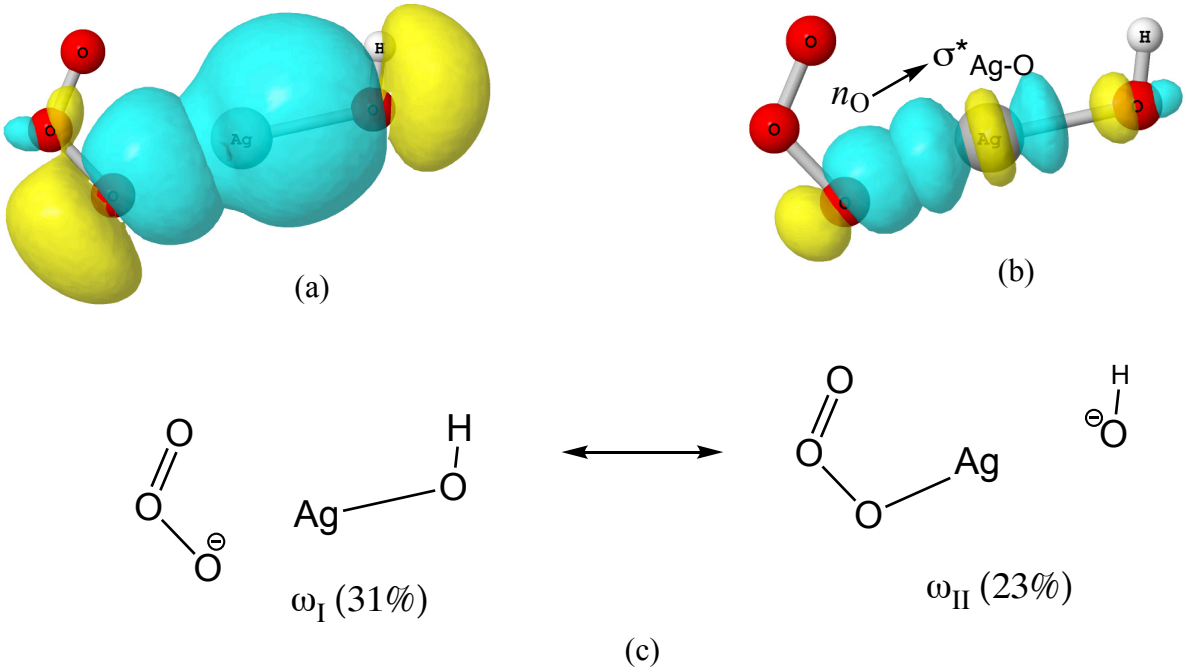

Figure S15. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for AgO_4H^- cluster.

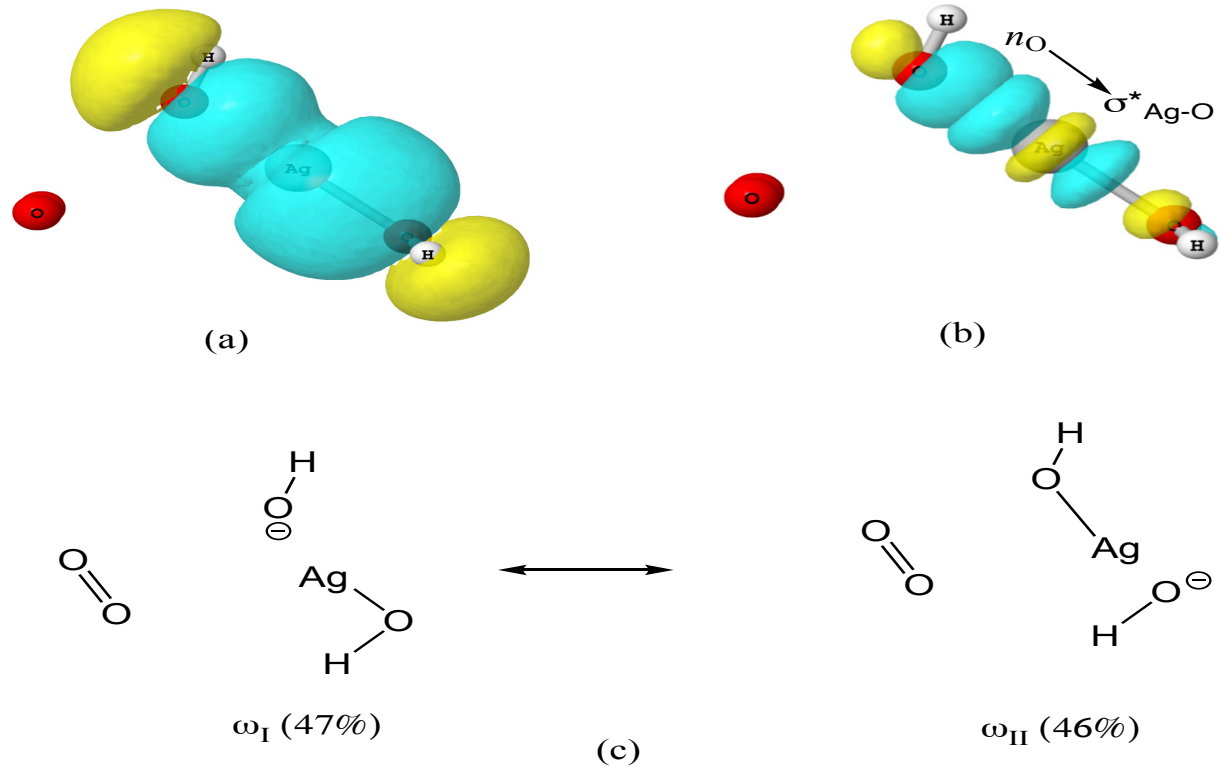

Figure S16. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_4H_2^-$ cluster.

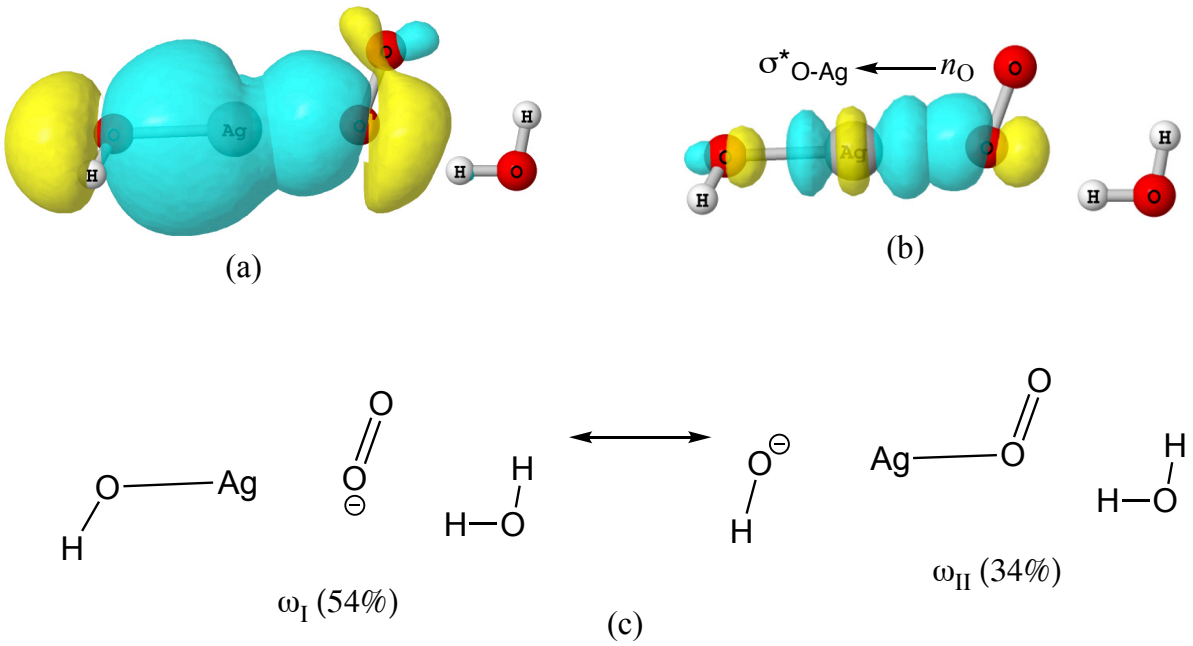

Figure S17. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_4H_3^-$ cluster.

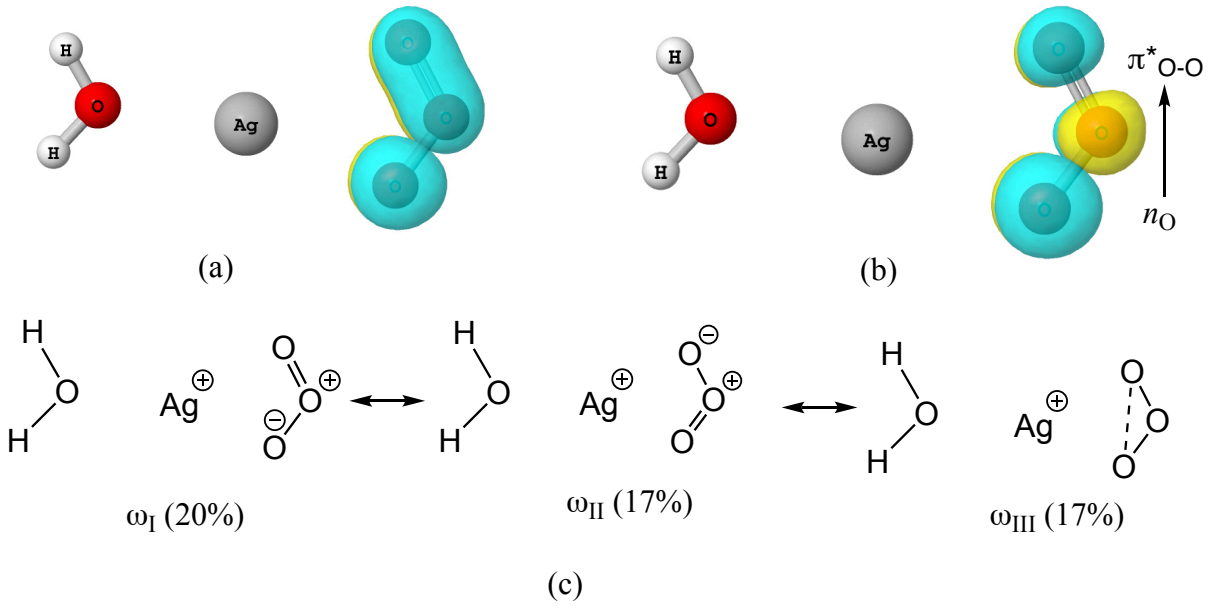

Figure S18. (a) 3-d surface views of leading 3c/4e Lewis-type NBOs (b) lone-pair NBO of O (n_O) and empty **π*** NBO of O-O bond donor-acceptor pair (c) resonance structures with weights (***ω***) for $AgO_4H_2^+$ cluster.

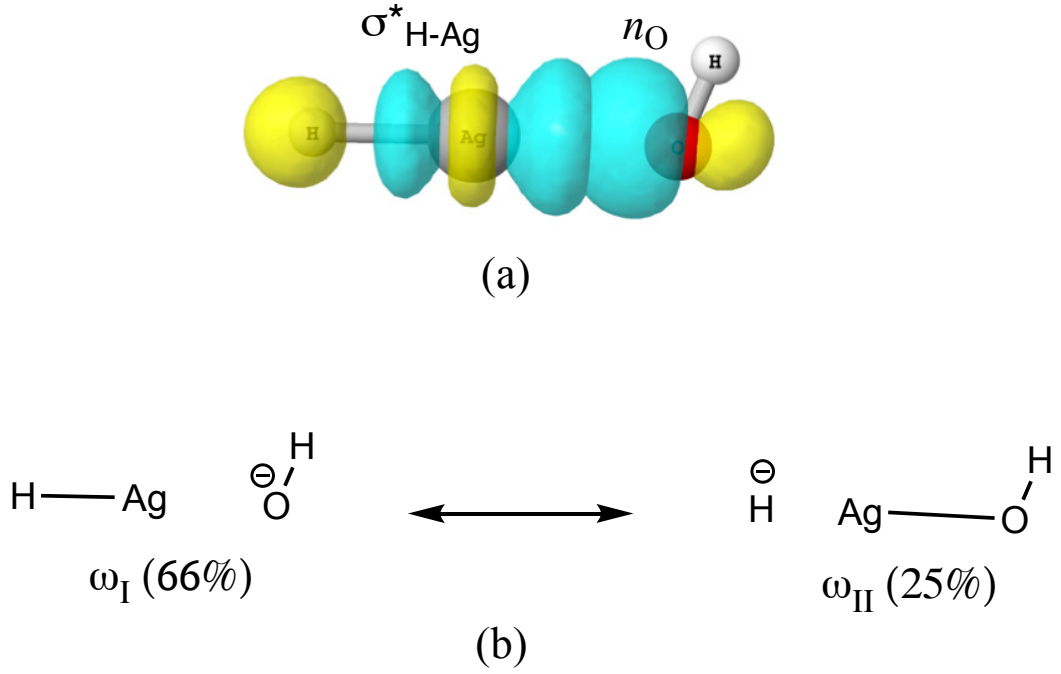

Figure S19. (a) Lone-pair NBO of O (n_O) and empty σ* NBO of Ag-H bond donor-acceptor pair (b) resonance structures with weights (***ω***) for $AgOH_2^-$ cluster.

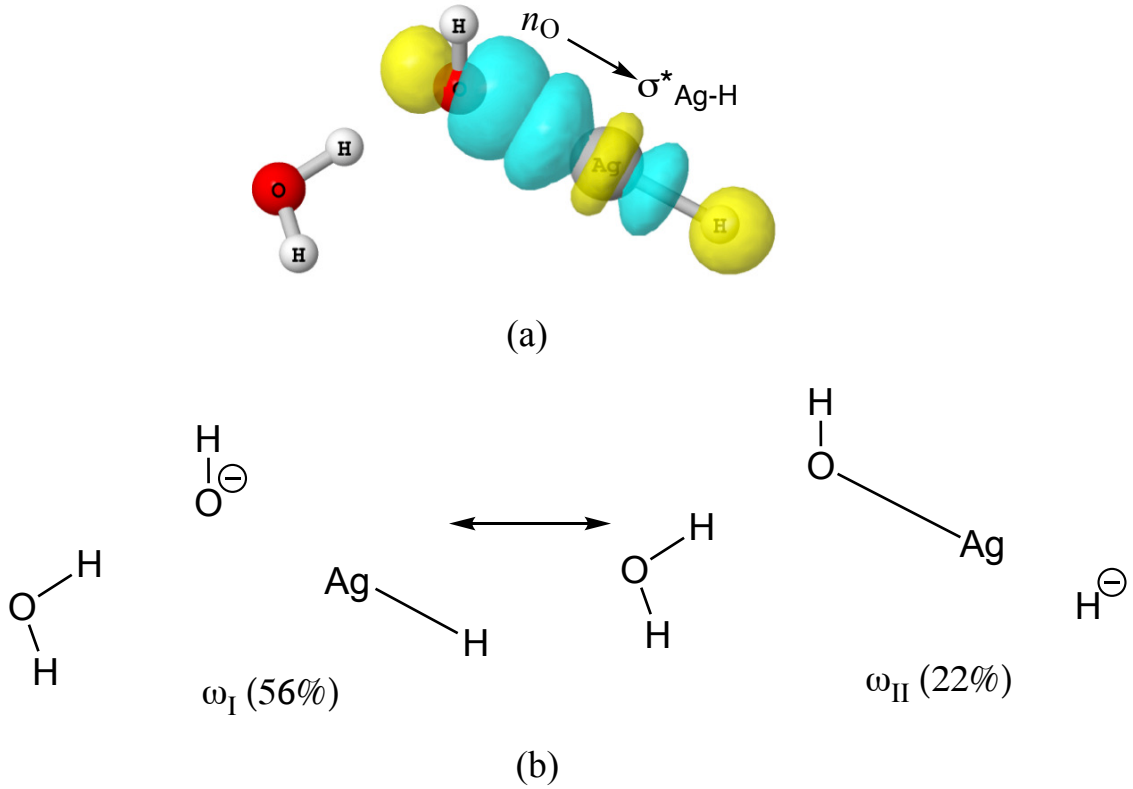

Figure S20. (a) Lone-pair NBO of O (n_O) and empty σ* NBO of Ag-H bond donor-acceptor pair (b) resonance structures with weights (***ω***) for $AgO_2H_4^-$ cluster.

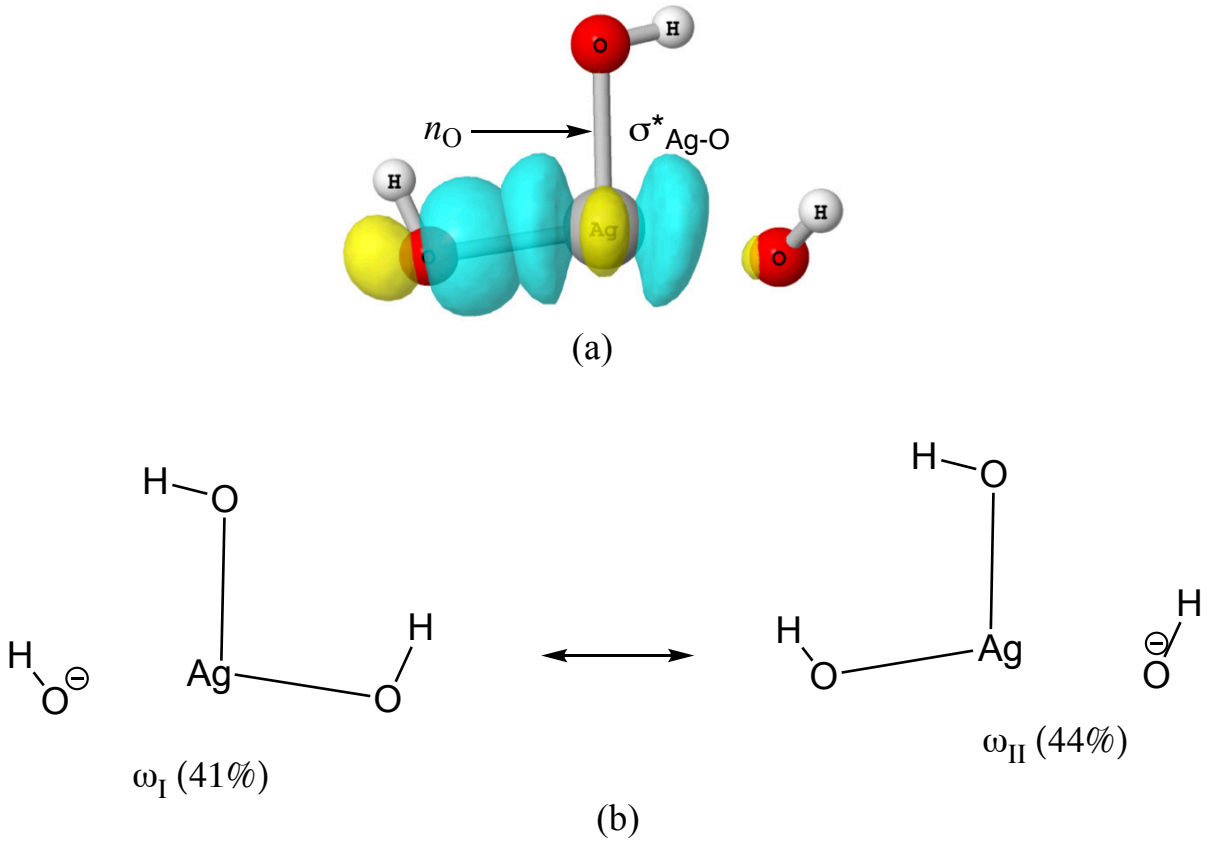

Figure S21. (a) Lone-pair NBO of O (n_O) and empty σ* NBO of Ag-O bond donor-acceptor pair (b) resonance structures with weights (***ω***) for $AgO_3H_3^-$ cluster.

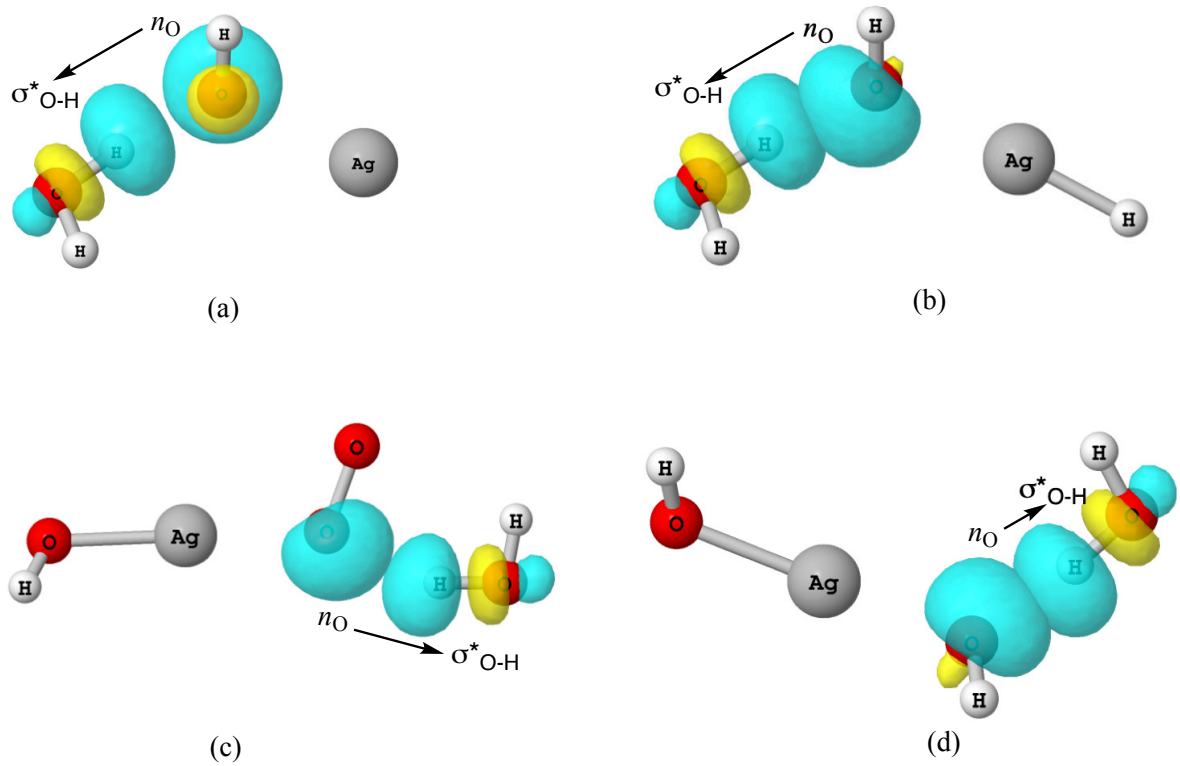

Figure S22. Lone-pair NBO of O (n_O) and empty σ* NBO of O-H bond donor-acceptor pair interactions leading to hydrogen bonding in (a) $AgO_2H_3^-$ (b) $AgO_2H_4^-$ (c) $AgO_4H_3^-$ and (d) $AgO_3H_4^-$ clusters.

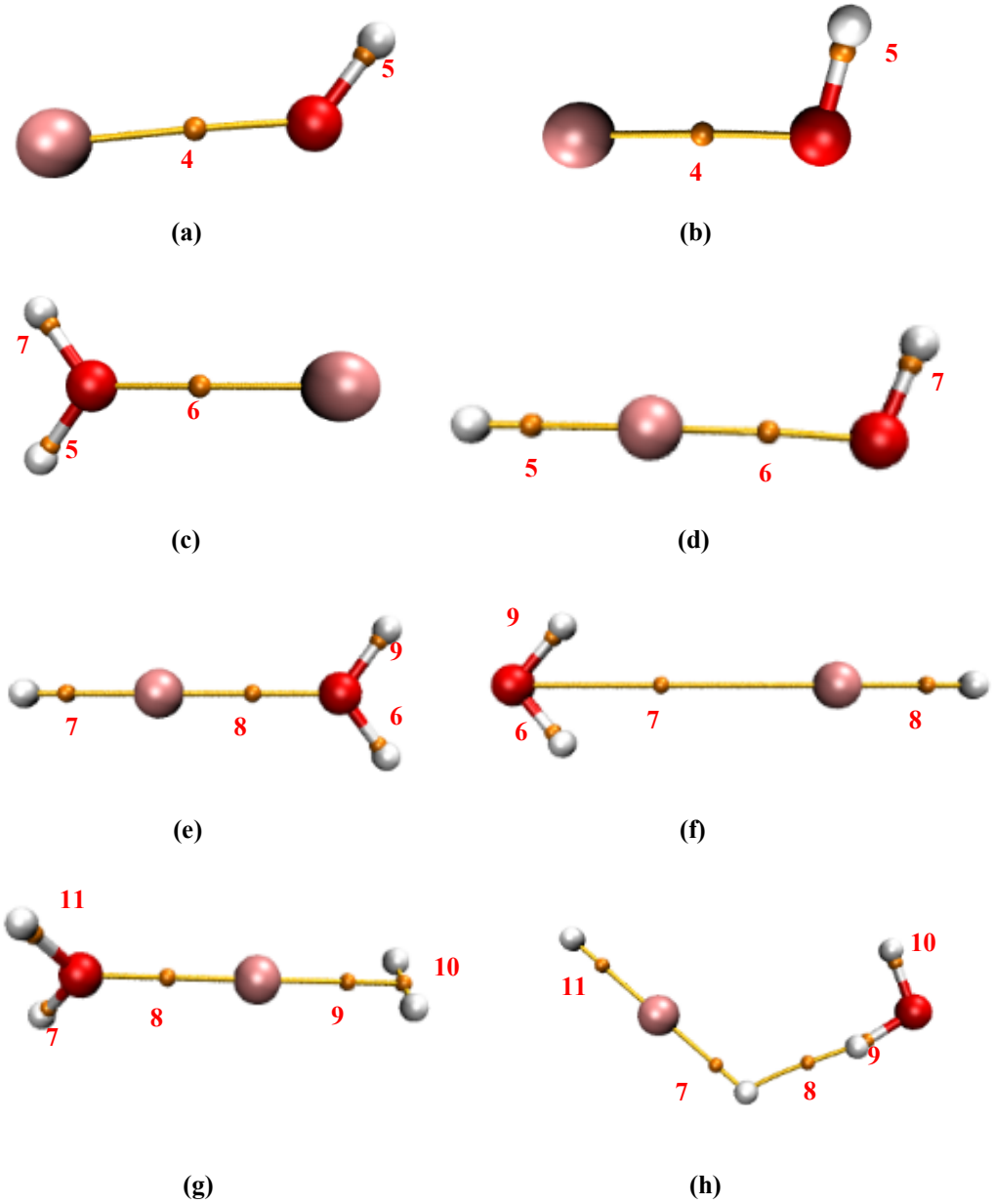

Figure S23. AIM trajectories for (a) $AgOH^{+}$; (b) $AgOH^{-}$; (c) $AgOH_2^{+}$; (d) $AgOH_2^{-}$; (e) $AgOH_3^{+}$; (f) $AgOH_3^{-}$; (g) $AgOH_4^{+}$; and (h) $AgOH_4^{-}$ calculated at the ωB97XD level. Numbers are located at bond critical point (3,-1).

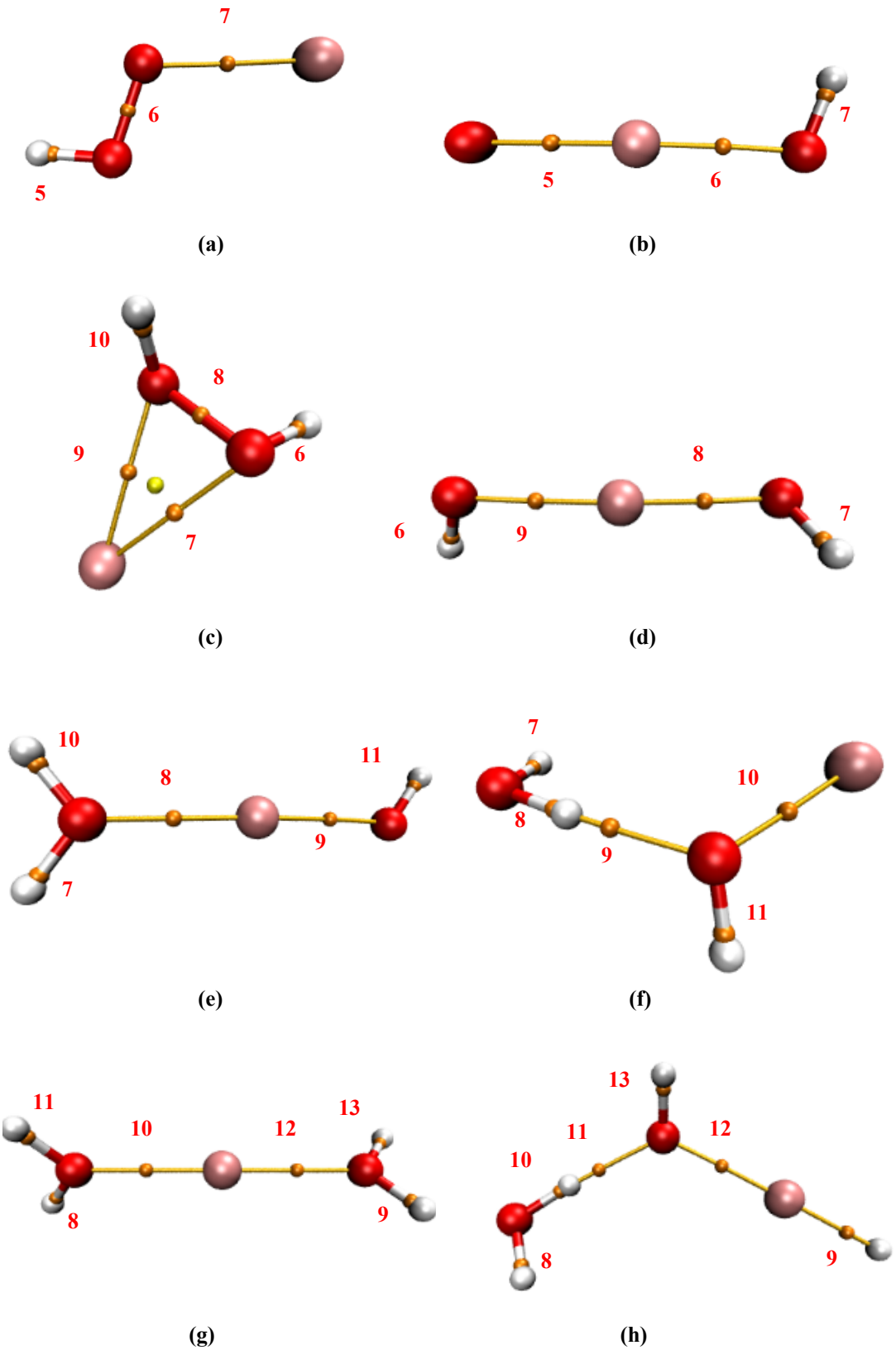

Figure S24. AIM trajectories for (a) AgO_2H^+; (b) AgO_2H^-; (c) $AgO_2H_2^+$; (d) $AgO_2H_2^-$; (e) $AgO_2H_3^+$; (f) $AgO_2H_3^-$; (g) $AgO_2H_4^+$; and (h) $AgO_2H_4^-$ calculated at the ωB97XD level. Numbers are located at bond critical point (3,-1).

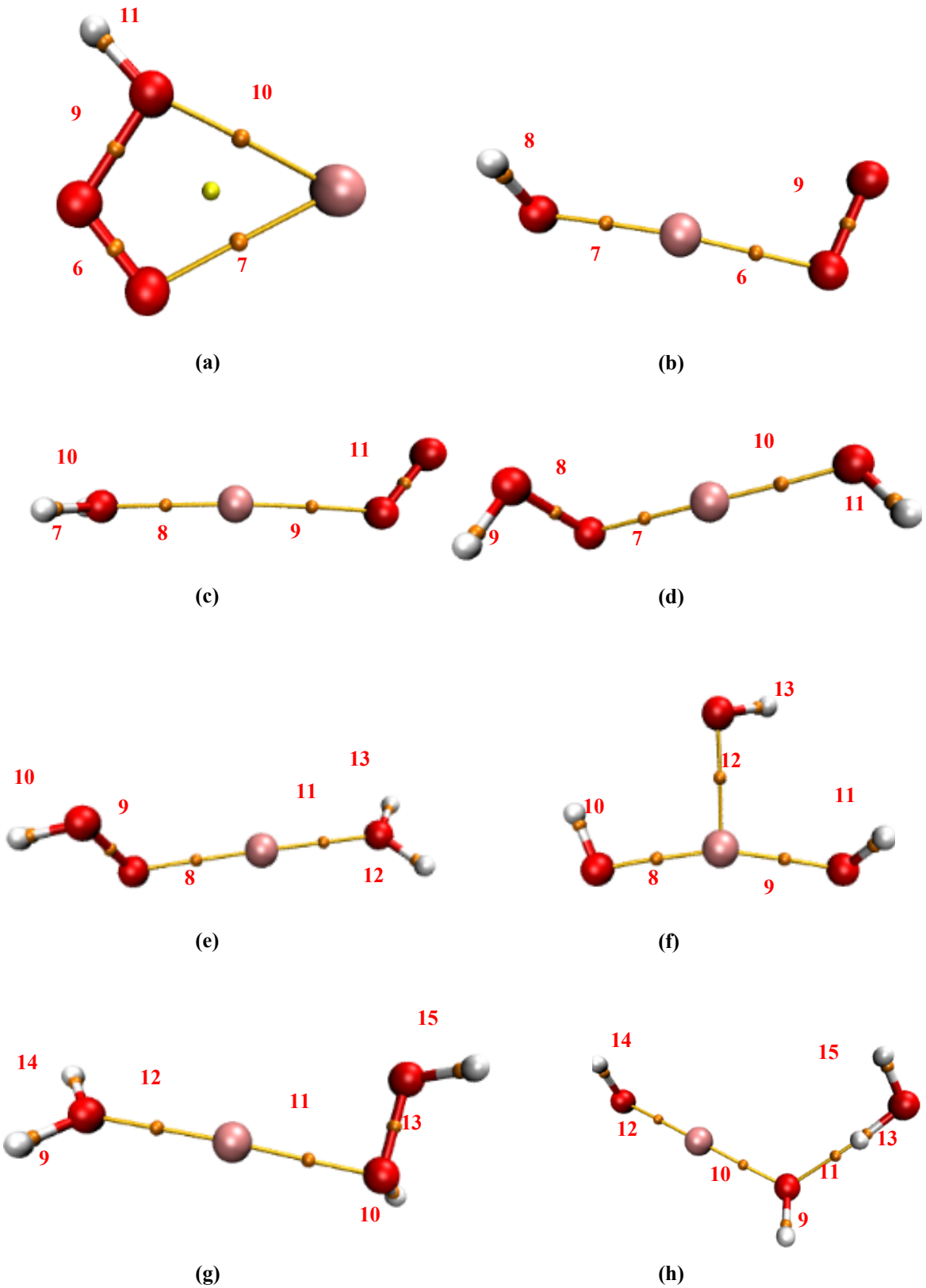

Figure S25. AIM trajectories for (a) AgO_3H^+; (b) AgO_3H^-; (c) $AgO_3H_2^+$; (d) $AgO_3H_2^-$; (e) $AgO_3H_3^+$; (f) $AgO_3H_3^-$; (g) $AgO_3H_4^+$; and (h) $AgO_3H_4^-$ calculated at the ωB97XD level. Numbers are located at bond critical point (3,-1).

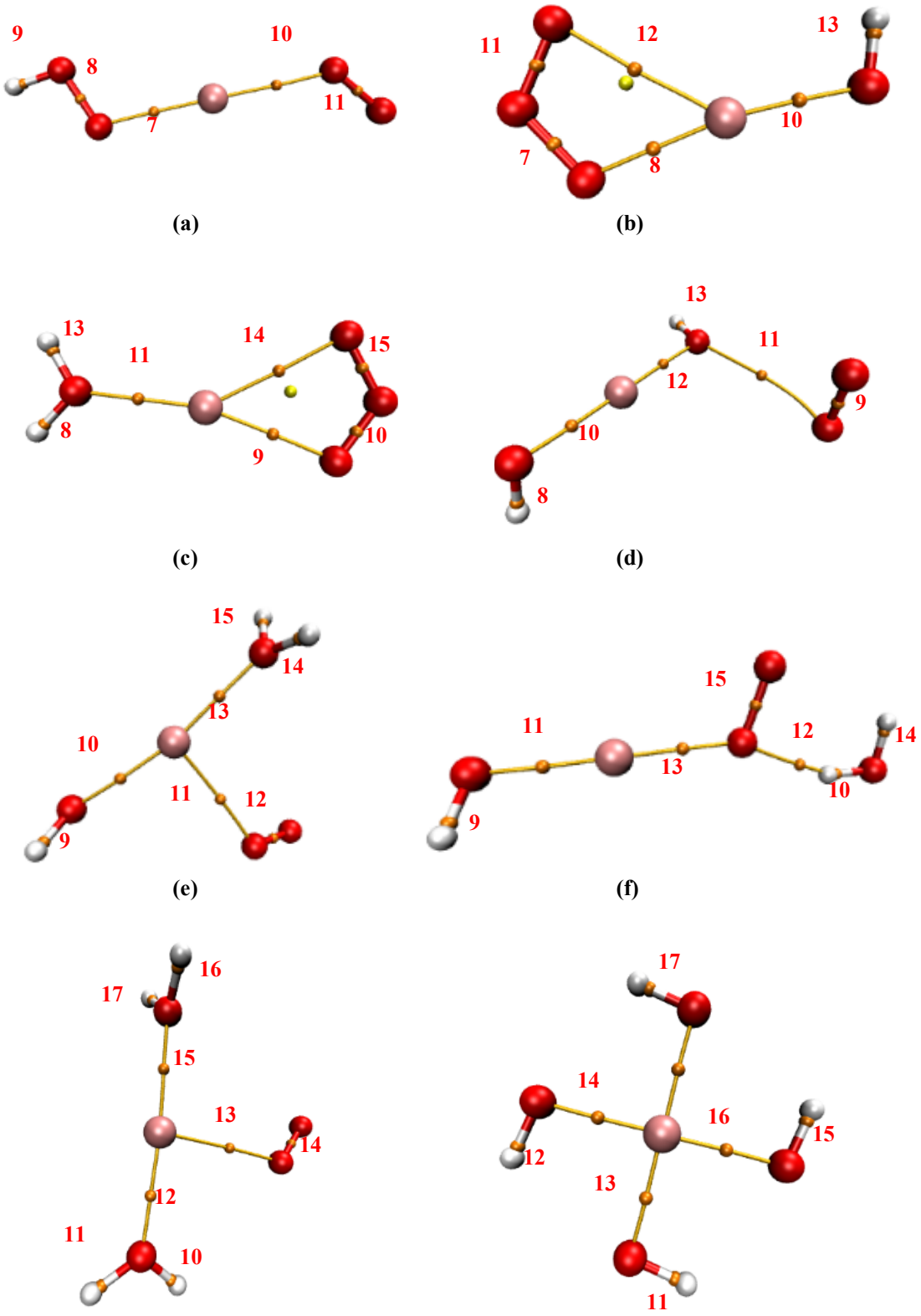

Figure S26. AIM trajectories for (a) AgO_4H^+; (b) AgO_4H^-; (c) $AgO_4H_2^+$; (d) $AgO_4H_2^-$; (e) $AgO_4H_3^+$; (f) $AgO_4H_3^-$; (g) $AgO_4H_4^+$; and (h) $AgO_4H_4^-$ calculated at the ωB97XD level. Numbers are located at bond critical point (3,-1).