TABLE I. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_2H clusters.

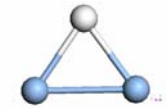
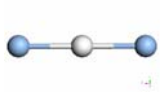
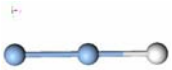
Ag_2H	Charge (au)	Ee(Hartree)	ZPE (Hartree)	$<S^2>$
 2-N-a	-0.48317	-292.173939	0. 004954	0.7526
 2-N-b 2nd order TS	-0.48317	-292.173688	0.003838	0.7526
2-N-c	-0.24141	-292.169071	0.004400	0.7542:
 2-N-d 2nd order TS	-0.21349	-292.167212	0.003871	0.7549

TABLE II. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_3H clusters.

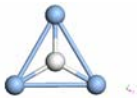
Ag_2H	Charge (au)	Ee(Hartree)	ZPE (Hartree)	$<S^2>$
3-N-a	-0.36334	-438.022143	0.005398	0.0000
3-N-b	-0.38695	-438.016514	0.006112	0.0000
3-N-c	-0.61257	-438.011491	0.004723	0.0000
3-N-d many order TS	-0.24386	-437.997703	0.004314	0.7773
 3-N-e 2nd order TS	-0.54425	-437.970646	0.004523	0.9998

TABLE III. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_4H clusters.

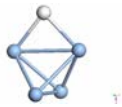
Ag_4H	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
4-N-a	-0.47832	-583.858862	0.006634	0.7525
4-N-b TS	-0.31804	-583.834732	0.005281	0.7543
 4-N-c TS	-0.48693	-583.833193	0.006074	0.7524
4-N-d TS	-0.56181	-583.820062	0.004253	0.7541
4-N-e many order TS	-0.23156	-583.811124	0.004516	0.7568

TABLE IV. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_5H clusters.

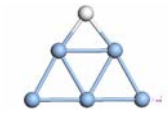
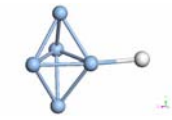
Ag_5H	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 5-N-a	-0.48799	-729.725599	0.007587	0.000
5-N-b TS	-0.33154	-729.701234	0.006578	0.000
5-N-c	-0.45922	-729.69381	0.006727	0.000
5-N-d TS	-0.45932	-729.691239	0.006983	0.000
 5-N-e TS	-0.32190	-729.687125	0.006394	0.000
5-N-f TS	-0.55213	-729.683583	0.006300	0.000

TABLE V. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_6H clusters.

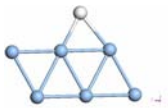
Ag_6H	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
6-N-a	-0.46442	-875.548949	0.008010	0.7525
 6-N-b	-0.48373	-875.547454	0.008188	0.7529
6-N-c	-0.48346	-875.542895	0.007866	0.7534
6-N-d	-0.31798	-875.533759	0.007248	0.7525
6-N-e TS	-0.48270	-875.529869	0.007413	0.7545

TABLE V. Continued.

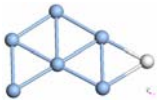
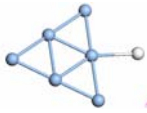
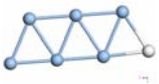
Ag_6H	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
6-N-f	-0.43251	-875.527105	0.007323	0.7544
 6-N-g	-0.47797	-875.525587	0.007205	0.7534
6-N-h	-0.45694	-875.525453	0.006601	0.7545
 6-N-i	-0.27601	-875.52474	0.006525	0.7548
 6-N-j TS	-0.48614	-875.51939	0.007325	0.7539
6-N-k TS	-0.29013	-875.51917	0.006927	0.7531

TABLE VI. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the optimized neutral Ag_7H clusters.

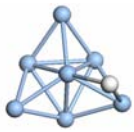
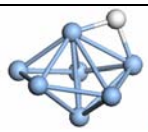
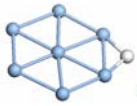
Ag_7H	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
7-N-a	-0.52428	-1021.404769	0.007928	0.0000
 7-N-b	-0.44046	-1021.402683	0.008432	0.0000
 7-N-c	-0.44582	-1021.402296	0.008294	0.0000
7-N-d	-0.46373	-1021.401451	0.008640	0.0000
7-N-e	-0.48663	-1021.400502	0.007698	0.0000
 7-N-f	-0.54855	-1021.394521	0.008284	0.0000

TABLE VII. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_2H^- clusters.

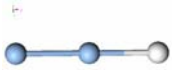
Ag_2H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 2-A-a	-0.51510	-292.257465	0. 004989	0.0000
2-A-b	-0.42387	-292.228584	0.004695	0.0000

TABLE VIII. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_3H^-

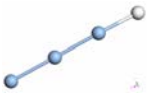
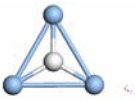
Ag_2H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
3-A-a	-0.47530	-438.085845	0.005455	0.7548
 3-A-b	-0.46101	-438.080559	0.004873	0.7560
3-A-c	-0.51304	-438.076864	0.005874	0.7517
3-A-d	-0.56635	-438.069819	0.004935	0.7551
 3-A-e 2nd order TS	-0.49416	-438.034282	0.004814	0.9028

TABLE IX NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_4H^- clusters.

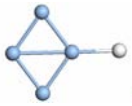
Ag_4H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 4-A-a	-0.44087	-583.937595	0.006051	0.0000
4-A-b	-0.46276	-583.93613	0.006013	0.0000
4-A-c 2nd order TS	-0.43139	-583.924538	0.005467	0.0000
4-A-d	-0.44426	-583.908089	0.005708	0.0000
4-A-e	-0.51638	-583.895068	0.005662	0.9664
4-A-f Many order TS	-0.59567	-583.882799	0.003069	1.0036

TABLE X NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_5H^- clusters.

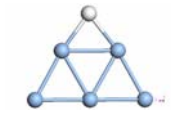
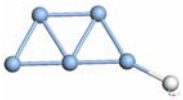
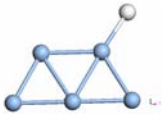
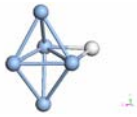
Ag_5H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 5-A-a	-0.51286	-729.770364	0.007146	0.7536
 5-A-b	-0.46211	-729.768879	0.006385	0.7533
5-A-c	-0.42009	-729.768227	0.006605	0.7536
 5-A-d	-0.44259	-729.766119	0.006415	0.7534
5-A-e	-0.40648	-729.762935	0.006109	0.7556
5-A-f	-0.48127	-729.762129	0.006790	0.7540
 5-A-g	-0.50887	-729.756376	0.006273	0.7532

TABLE XI. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_6H^- clusters.

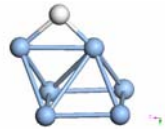
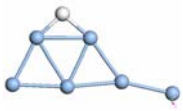
Ag_6H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
6-A-a	-0.50473	-875.63064	0.008080	0.0000
6-A-b	-0.49551	-875.627144	0.007042	0.0000
6-A-c	-0.39904	-875.624198	0.007257	0.0000
 6-A-d	-0.50270	-875.623215	0.007373	0.0000
6-A-e TS	-0.41616	-875.621912	0.007085	0.0000
 6-A-f	-0.50887	-875.621337	0.007501	0.0000
6-A-g 2nd order TS	-0.43325	-875.621145	0.006863	0.0000

TABLE XI. Continued.

Ag_6H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
6-A-h	-0.47484	-875.620251	0.007010	0.0000
6-A-i	-0.55463	-875.619979	0.007178	0.0000
6-A-j	-0.48117	-875.619493	0.006950	0.0000
6-A-k TS	-0.40481	-875.613772	0.006974	0.0000
6-A-l TS	-0.50797	-875.61333	0.006625	0.0000

TABLE XII. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the optimized anionic Ag_7H^- clusters.

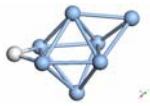
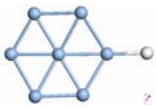
Ag_7H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
7-A-a	-0.54305	-1021.464916	0.008002	0.7541
7-A-b	-0.45341	-1021.461795	0.007808	0.7528
7-A-c	-0.50756	-1021.461601	0.007375	0.7526
 7-A-d	-0.50453	-1021.460769	0.007766	0.7536
7-A-e	-0.49015	-1021.460064	0.008399	0.7531
7-A-f	-0.50942	-1021.458694	0.007633	0.7533
7-A-g	-0.40209	-1021.457609	0.007418	0.7544
7-A-h	-0.51703	-1021.457521	0.007620	0.7547
 7-A-i	-0.43584	-1021.455642	0.007225	0.7536

TABLE XII. Continued.

Ag_7H^-	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
7-A-j	-0.50844	-1021.45551	0.007610	0.7539
7-A-k	-0.38973	-1021.454074	0.007423	0.7549
7-A-l TS	-0.63844	-1021.45302	0.006728	0.7533
7-A-m	-0.46666	-1021.452798	0.008000	0.7543
7-A-n 2nd order TS	-0.55662	-1021.452126	0.007516	0.7527
7-A-o	-0.55147	-1021.449903	0.006453	0.7533

TABLE XIII. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_2H^+ clusters.

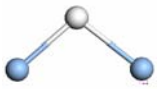
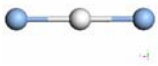
Ag_2H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 2-C-a	-0.49003	-291.943167	0.005694	0.000
 2-C-b 2nd order TS	-0.68411	-291.937929	0.004453	0.0000
2-C-c 2nd order TS	0.07202	-291.863796	0.003325	0.4466

TABLE XIV NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the neutral Ag_3H^+ clusters.

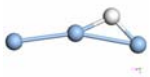
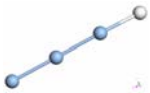
Ag_3H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 3-C-a	-0.45548	-437.76232	0.006117	0.7517
3-C-b	-0.41048	-437.759699	0.005664	0.7528
3-C-c 2nd order TS	-0.65670	-437.739679	0.005626	0.7515
3-C-d 2nd order TS	-0.47804	-437.728728	0.002444	0.7550
 3-C-e 2nd order TS	-0.02914	-437.706494	0.003872	0.7773

TABLE XV. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the anionic Ag_4H^+.

Ag_4H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
4-C-a	-0.44864	-583.637419	0.006965	0.0000
4-C-b TS	-0.45154	-583.636912	0.006847	0.0000
4-C-c TS	-0.62500	-583.620195	0.005895	0.0000
4-C-d TS,	-0.52116	-583.6168	0.006130	0.0000
4-C-e 2nd order TS	-0.44611	-583.601819	0.006406	0.0000
4-C-f 2nd order TS	-0.07504	-583.597566	0.005277	0.0000
4-C-g 2nd order TS	-0.67012	-583.590386	0.003767	0.0000

TABLE XVI. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the cationic Ag_5H^+.

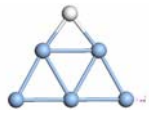
Ag_5H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
5-C-a	-0.40897	-729.462827	0.007422	0.7517
5-C-b	-0.54036	-729.459304	0.006894	0.7518
5-C-c TS	-0.43022	-729.458457	0.007139	0.7517
 5-C-d TS	-0.48991	-729.457022	0.007387	0.7521
5-C-e TS	-0.45320	-729.455669	0.007171	0.7523
5-C-f	-0.47166	-729.451417	0.006280	0.7524
5-C-g TS	-0.53670	-729.447117	0.005720	0.7518

TABLE XVI. Continued.

Ag_5H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 5-C-h Many order TS	-0.51992	-729.439567	0.005755	0.7518
 5-C-i 2nd order TS	-0.22489	-729.434457	0.005919	0.7519

TABLE XVII. NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the cationic Ag_6H^+.

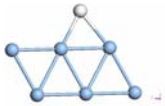
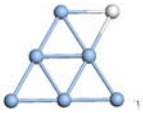
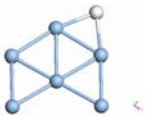
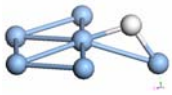
Ag_6H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
6-C-a	-0.44616	-875.331698	0.008164	0.0000
6-C-b	-0.45600	-875.328103	0.008092	0.0000
6-C-c	-0.47795	-875.327896	0.007197	0.0000
 6-C-d TS	-0.46425	-875.321299	0.008091	0.0000
 6-C-e TS	-0.36287	-875.316523	0.007983	0.0000
 6-C-f TS	-0.39097	-875.315781	0.007799	0.0000
 6-C-g TS	-0.41072	-875.311016	0.007621	0.0000
6-C-h	-0.44087	-875.312723	0.007840	0.0000

TABLE XVIII NBO net atomic charges of the adsorbates, zero-point vibrational energies (ZPE), electronic energies (E_e), and $<S^2>$ for the cationic Ag_7H^+.

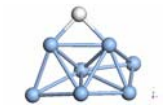
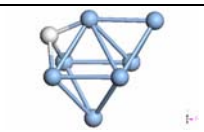
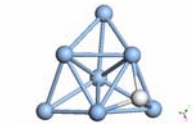
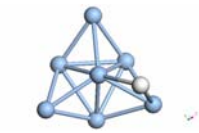
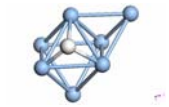
Ag_7H^+	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 7-C-a	-0.44906	-1021.1718	0.008732	0.7521
7-C-b	-0.47891	-1021.164563	0.007983	0.7520
 7-C-c	-0.50603	-1021.163713	0.007804	0.7519
7-C-d	-0.40405	-1021.163337	0.008248	0.7524
 7-C-e	-0.45703	-1021.162147	0.008067	0.7518
 7-C-f	-0.40771	-1021.161693	0.008434	0.7520
 7-C-g	-0.49248	-1021.161632	0.007677	0.7520

TABLE XVIII Continued.

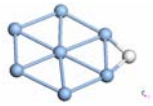
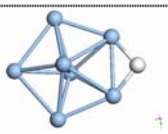
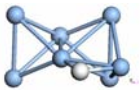
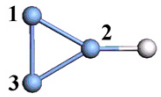
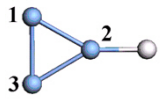
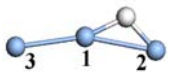
Ag_7Br	Charge (au)	E_e (Hartree)	ZPE (Hartree)	$<S^2>$
 7-C-h	-0.41820	-1021.160948	0.008438	0.7536
 7-C-i 2nd order TS	-0.44453	-1021.151998	0.007559	0.7526
 7-C-j TS	-0.41977	-1021.151783	0.008179	0.7518
7-C-k 2nd order TS	-0.47142	-1021.139668	0.006346	0.7520
7-C-l 2nd order TS	-0.14667	-1021.137316	0.006672	0.7557

TABLE XIX. NBO population analysis for Ag_3, Ag_3^-, Ag_3^+, Ag_3H, Ag_3H, and Ag_3H.

H					H
	charges				0
	s				100
	p				
	d				
Species		Ag_1	Ag_2	Ag_3	H
Ag_3	charges	-0.065	0.130	-0.065	
	s	3.07	2.86	3.07	
	p	6.02	6.03	6.02	
	D	9.97	9.98	9.97	
Ag_3H	charges	+0.121	+0.122	+0.121	-0.363
	s	2.88	2.97	2.88	1.36
	p	6.02	6.01	6.02	
	d	9.97	9.90	9.97	
Ag_3^-	charges	-0.319	-0.362	-0.319	
	s	3.32	3.36	3.32	
	p	6.03	6.03	6.03	
	d	9.97	9.97	9.97	
Ag_3H^-	charges	-0.350	+0.176	-0.350	-0.475
	s	3.36	2.89	3.36	1.47
	p	6.03	6.02	6.03	
	d	9.97	9.91	9.97	
Ag_3^+	charges	-0.302	+0.651	+0.651	
	s	3.31	2.36	2.36	
	p	6.01	6.01	6.01	
	d	9.98	9.99	9.99	
Ag_3H^+	charges	+0.345	+0.693	+0.417	-0.455
	s	2.68	2.37	2.61	1.45
	p	6.04	6.00	6.01	
	d	9.94	9.94	9.97	

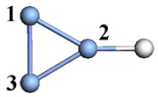
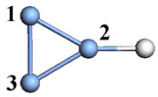
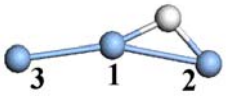
 **neutral**	 **anionic**	 **cationic**

TABLE XX. NBO population analysis for Ag_4, Ag_4^-, Ag_4^+, Ag_4H, Ag_4H^-, and Ag_4H^+.

H						H
	charges					0
	s					1.00
	p					
	d					

Species		Ag_1	Ag_2	Ag_3	Ag_4	H
Ag_4	charges	0.268	-0.268	-0.268	-0.101	
	s	2.71	3.30	3.30	3.13	
	p	6.05	6.01	6.01	6.08	
	d	9.97	9.96	9.96	9.89	
Ag_4H	charges	+0.308	+0.283	-0.029	-0.084	-0.478
	s	2.74	2.75	3.03	3.11	1.48
	p	6.04	6.03	6.03	6.01	
	d	9.92	9.94	9.97	9.96	
Ag_4^-	charges	-0.138	-0.362	-0.138	-0.362	
	s	3.14	3.37	3.14	3.37	
	p	6.04	6.02	6.04	6.02	
	d	9.96	9.97	9.96	9.97	
Ag_4H^-	charges	+0.201	-0.347	-0.067	-0.347	-0.441
	s	2.87	3.36	3.07	3.36	1.44
	p	6.03	6.02	6.04	6.02	
	d	9.90	9.97	9.96	9.97	
Ag_4^+	charges	-0.041	+0.318	+0.318	+0.406	
	s	3.03	2.69	2.69	2.61	
	p	6.05	6.02	6.02	6.01	
	d	9.96	9.97	9.97	9.98	
Ag_4H^+	charges	+0.248	+0.272	+0.272	+0.657	-0.449
	s	2.80	2.74	2.74	2.40	1.45
	p	6.04	6.02	6.02	6.00	
	d	9.92	9.97	9.97	9.94	

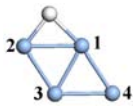
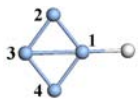
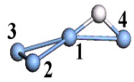
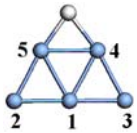
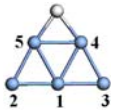
 **neutral**	 **anionic**	 **cationic**

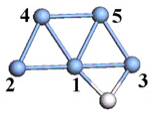
TABLE XXI NBO population analysis for Ag_5, Ag_5^-, Ag_5^+, Ag_5H, Ag_5H^-, and Ag_5H^+.

Species							H
H	charges						0
	s						1.00
	p						
	d						

Species		Ag_1	Ag_2	Ag_3	Ag_4	Ag_5	H
Ag_5	charges	0.085	-0.053	-0.053	0.010	0.010	
	s	2.91	3.07	3.07	2.99	2.99	
	p	6.06	6.01	6.01	6.03	6.03	
	d	9.95	9.97	9.97	9.96	9.96	
Ag_5H	charges	+0.070	-0.103	-0.103	+0.312	+0.312	-0.488
	s	2.93	3.13	3.13	2.72	2.72	1.49
	p	6.04	6.01	6.01	6.03	6.03	
	d	9.96	9.96	9.96	9.93	9.93	
Ag_5^-	charges	0.037	-0.309	-0.309	-0.206	-0.206	
	s	2.96	3.32	3.32	3.22	3.22	
	p	6.04	6.02	6.02	6.03	6.03	
	d	9.96	9.97	9.97	9.96	9.96	
Ag_5H^-	charges	-0.320	-0.332	-0.332	+0.249	+0.249	-0.513
	s	3.32	3.34	3.34	2.78	2.78	1.51
	p	6.04	6.03	6.03	6.04	6.04	
	d	9.96	9.96	9.96	9.93	9.93	
Ag_5^+	charges	+0.184	+0.189	+0.204	+0.197	+0.225	
	s	2.79	2.83	2.81	2.81	2.78	
	p	6.09	6.01	6.01	6.03	6.03	
	d	9.94	9.96	9.97	9.96	9.97	
Ag_5H^+	charges	+0.257	+0.305	+0.543	+0.135	+0.170	-0.409
	s	2.78	2.71	2.51	2.88	2.84	1.41
	p	6.07	6.01	6.02	6.03	6.02	
	d	9.90	9.97	9.93	9.96	9.97	







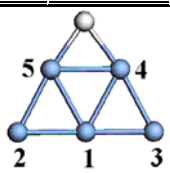
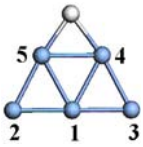
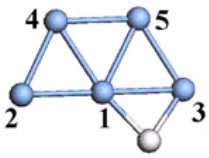
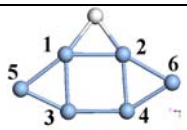
 **neutral**	 **anionic**	 **cationic**

TABLE XXII. NBO population analysis for Ag_6, Ag_6^-, Ag_6^+, Ag_6H, Ag_6H^-, and Ag_6H^+.

Species								H
H	charges							0
	s							1.00
	p							
	d							

Species		Ag_1	Ag_2	Ag_3	Ag_4	Ag_5	Ag_6	H
Ag_6	charges	-0.146	-0.168	-0.168	-0.146	0.314	0.314	
	s	3.17	3.18	3.18	3.17	2.64	2.64	
	p	6.02	6.04	6.04	6.02	6.09	6.09	
	d	9.96	9.95	9.95	9.96	9.96	9.96	
Ag_6H	charges	-0.051	+0.314	+0.314	-0.051	-0.031	-0.031	-0.464
	s	3.07	2.71	2.71	3.07	3.02	3.02	1.46
	p	6.02	6.05	6.05	6.02	6.05	6.05	
	d	9.96	9.93	9.93	9.96	9.96	9.96	
Ag_6^-	charges	-0.036	-0.090	-0.160	-0.187	-0.284	-0.242	
	s	3.03	3.09	3.18	3.21	3.30	3.25	
	p	6.04	6.04	6.03	6.03	6.02	6.02	
	d	9.96	9.96	9.96	9.95	9.97	9.97	
Ag_6H^-	charges	+0.295	+0.280	-0.165	-0.115	-0.410	-0.382	-0.505
	s	2.74	2.75	3.18	3.13	3.44	3.41	1.50
	p	6.04	6.04	6.03	6.03	6.01	6.01	
	d	9.93	9.93	9.96	9.96	9.96	9.96	
Ag_6^+	charges	0.054	0.079	0.079	0.054	0.368	0.368	
	s	2.97	2.93	2.93	2.97	2.58	2.58	
	p	6.02	6.05	6.05	6.02	6.09	6.09	
	d	9.95	9.95	9.95	9.95	9.96	9.96	
Ag_6H^+	charges	+0.348	+0.352	+0.352	+0.348	+0.030	+0.030	-0.446
	s	2.61	2.69	2.69	2.61	3.00	3.00	1.44
	p	6.08	6.04	6.04	6.08	6.02	6.02	
	d	9.96	9.92	9.92	9.96	9.95	9.95	

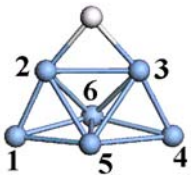
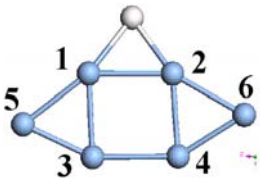
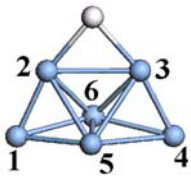
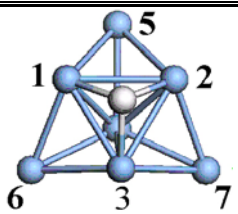
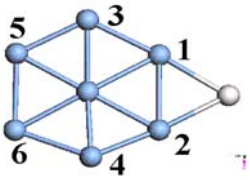
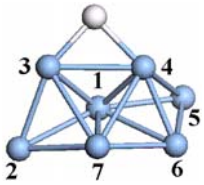
		
neutral	**Anionic**	**cationic**

TABLE XXIII NBO population analysis for Ag_7, Ag_7^-, Ag_7^+, Ag_7H, Ag_7H^-, and Ag_7H^+.

Species									H
H	charges								0
	s								1.00
	p								
	d								

Species		Ag_1	Ag_2	Ag_3	Ag_4	Ag_5	Ag_6	Ag_7	H
Ag_7	charges	+0.032	+0.032	+0.032	+0.028	-0.041	-0.041	-0.041	
	s	2.95	2.95	2.95	2.94	3.06	3.06	3.06	
	p	6.06	6.06	6.06	6.08	6.02	6.02	6.02	
	d	9.95	9.95	9.95	9.95	9.96	9.96	9.96	
Ag_7H	charges	+0.240	+0.241	+0.240	+0.031	-0.075	-0.075	-0.076	-0.524
	s	2.76	2.76	2.76	2.94	3.10	3.10	3.10	1.52
	p	6.06	6.06	6.06	6.08	6.02	6.02	6.02	
	d	9.94	9.94	9.94	9.95	9.96	9.96	9.96	
Ag_7^-	charges	-0.186	-0.186	-0.175	-0.175	-0.186	-0.186	+0.096	
	s	3.20	3.20	3.18	3.18	3.20	3.20	2.87	
	p	6.03	6.03	6.03	6.03	6.03	6.03	6.09	
	d	9.96	9.96	9.96	9.96	9.96	9.96	9.94	
Ag_7H^-	charges	+0.131	+0.132	-0.141	-0.141	-0.252	-0.252	+0.066	-0.543
	s	2.91	2.91	3.15	3.15	3.27	3.27	2.91	1.54
	p	6.03	6.03	6.03	6.03	6.02	6.02	6.08	
	d	9.93	9.93	9.96	9.96	9.96	9.96	9.95	
Ag_7^+	charges	+0.087	-0.046	-0.007	-0.220	+0.379	+0.295	+0.513	
	s	2.86	3.06	3.00	3.21	2.64	2.73	2.48	
	p	6.11	6.02	6.05	6.06	6.03	6.02	6.06	
	d	9.94	9.96	9.96	9.95	9.95	9.96	9.95	
Ag_7H^+	charges	+0.136	+0.120	+0.404	+0.347	+0.167	+0.146	+0.130	-0.449
	s	2.83	2.91	2.63	2.67	2.86	2.86	2.86	1.45
	p	6.09	6.02	6.04	6.06	6.02	6.04	6.05	
	d	9.94	9.95	9.93	9.92	9.96	9.95	9.96	

 **neutral**	 **anionic**	 **cationic**