Supporting Information for:

Shape Modulation of Octanuclear Cu(I) or Ag(I) Dichalcogeno Template Clusters with Respect to the Nature of their Encapsulated Anions: A Combined Theoretical and Experimental Investigation

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1 Reagents and general procedures. All chemicals were purchased from commercial sources and used as received. Solvents were purified following standard protocols. All reactions were carried out under N_2 atmosphere by using standard Schlenk techniques. The preparations of $[Cu_8\{S_2P(OR)_2\}_6](PF_6)_2$ (R = Et, ^{i}Pr) had been reported previously.[7b,SI1] $[NH_4][S_2P(OR)_2]$ ligands (R = ^{i}Pr, **i** and ^{n}Pr, **iii**) were prepared by following the method reported by Wystrach,[SI2] whereas $[NH_4][S_2P(OEt)_2]$ (**ii**) was obtained from Aldrich. Melting points were measured by using a Fargo MP-2D melting point apparatus. The elemental analyses were done using an Elementar vario EL III-CHNS elemental analyzer. Ambient temperature NMR spectra were recorded on a Bruker Advance DPX300 FT-NMR spectrometer that operates at 300 MHz while recording ^{1}H, 121.5 MHz for $^{31}P\{^1H\}$, and 376.5 MHz for ^{19}F. The $^{31}P\{^1H\}$ NMR are referenced externally against 85% H_3PO_4 (δ = 0 ppm). The chemical shift (δ) and coupling constant (J) are reported in ppm and Hz, respectively. MALDI-TOF mass spectra were recorded on an Autoflex time-of-flight mass spectrometer (Bruker Daltonic, Bremen, Germany) equipped with 337-nm nitrogen laser (10 Hz, 3-ns pulse width).

2 Synthesis of $[Cu_8(F)\{S_2P(O^iPr)_2\}_6](PF_6)$, 1.

Method (a). $[Cu(MeCN)_4](PF_6)$ (0.430 g, 1.153 mmol) and $[NH_4][S_2P(O^iPr)_2]$ (0.200 g, 0.865 mmol) were charged in a 100 mL Schlenk flask first, then 30 mL of acetone was added to it. $[^nBu_4N]F{\cdot}xH_2O$ (0.038 g, 0.144 mmol) was dissolved in de-ionized water (5mL) and transferred to the solution. The solution was stirred at room temperature for 1h. The reaction mixture was filtered and the filtrate was evaporated to dryness under vacuum to obtain light blue solid.[SI3] The solid was washed with de-ionized water and dried under vacuum to get $[Cu_8(F)\{S_2P(O^iPr)_2\}_6](PF_6)$ as a pale blue powder. Yield: (0.225 g) 80%.

Method (b). To a solution of $[Cu_8\{S_2P(O^iPr)_2\}_6](PF_6)_2$ (0.281 g, 0.144 mmol) in 30 mL of acetone was added $[^nBu_4N]F{\cdot}xH_2O$ (0.038 g, 0.144 mmol). The mixture was stirred at room temperature for 1h. The reaction mixture was filtered and the filtrate was evaporated to dryness under vacuum to obtain light blue solid. The solid was washed with de-ionized water and dried under vacuum to get $[Cu_8(F)\{S_2P(O^iPr)_2\}_6](PF_6)$. Yield: (0.203 g) 72%. Mp: 162 ^oC (decomposed) Anal. calcd for $Cu_8H_{84}C_{36}O_{12}P_7F_7S_{12}{\cdot}(CH_3)_2CO$: C 23.30; H 4.51. Found: C 23.21; H 4.76%. ^1H NMR (300 MHz, acetone-d_6, δ, ppm): 1.43 (d, $^3J_{HH}$ = 6Hz, 72H, OCH(CH_3)$_2$), 4.90 (m, 12H, OC*H*(CH_3)$_2$); $^{31}P\{^1H\}$ NMR (121.5 MHz, acetone-d_6, δ, ppm): 94.8 (s, 6P) -143.0 (septet, $^1J_{PF}$ = 708.0 Hz, PF_6); ^{19}F NMR (376.5 MHz, acetone-d_6, δ, ppm) : -72.9 (d, $^1J_{FP}$ = 708.4 Hz, PF_6), -177.7 (s). Positive ion MALDI-TOF-MS (*m/z*)(Cal.): 1804.7(1807.0) (M^+).

3 Synthesis of $[Cu_8(F)\{S_2P(OEt)_2\}_6](PF_6)$, 2. The synthetic method is similar to $[Cu_8(F)\{S_2P(O^iPr)_2\}_6](PF_6)$ by using $NH_4[S_2P(OEt)_2]$ instead of $NH_4[S_2P(O^iPr)_2]$. Yield: (0.251 g) 86%. Anal. calcd for $Cu_8H_{84}C_{36}O_{12}P_7F_7S_{12}{\cdot}0.5[(CH_3)_2CO]$: C 16.9; H 3.50. Found: C 16.9; H 3.81%. ^1H NMR (300 MHz, acetone-d_6, δ, ppm): 1.40(t, $^3J_{HH}$ = 7 Hz, 36H, C*H*$_3$), 4.28 (m, 24H, OC*H*$_2$); $^{31}P\{^1H\}$ NMR (121.5 MHz, acetone-d_6, δ, ppm): 99.7 (s, 6P), -143.0 (septet, $^1J_{PF}$ = 708.0 Hz, PF_6); ^{19}F NMR (376.5 MHz, acetone-d_6, δ, ppm) : -72.9 (d, $^1J_{FP}$ = 708.4 Hz, PF_6), -178.5 (s). Positive ion MALDI-TOF-MS (*m/z*)(Cal.): 1637.3(1638.7) (M^+).

4 Synthesis of $[Ag_8(F)\{S_2P(O^nPr)_2\}_6](PF_6)$, 3. $[Ag(CH_3CN)_4](PF_6)$ (0.534 g, 1.28 mmol) and $NH_4[S_2P(O^nPr)_2]$ (0.223 g, 0.96 mmol) were charged in a 100 mL flask and 20 mL of THF was added to it. The solution was stirred at –20 °C for 1 h, then tetrabutylammonium fluoride $[^nBu_4N]F{\cdot}xH_2O$ (0.04, 0.16 mmol) was added to the flask and stirring was continued for 12h. It was then filtered to get rid of any solid, and the filtrate was evaporated to dryness under a vacuum. The solid was washed with deionized water to remove any NH_4PF_6 formed during the reaction and dried under a vacuum to obtain $[Ag_8(F)\{S_2P(O^nPr)_2\}_6](PF_6)$ as a white

powder. ESI-MS (*m/z*)(Cal.): 2162.2(2161.6) (M^+). ^{1}H NMR (300 MHz, acetone-d_6, δ, ppm): 0.92 (t, $^3J_{HH}$ = 7.0Hz, 24H, $OCH_2CH_2CH_3$), 1.85 (m, 24H, $OCH_2CH_2CH_3$), 4.30 (m, 36H, $OCH_2CH_2CH_3$); $^{31}P\{^1H\}$ NMR (121.5 MHz, acetone-d_6, δ, ppm): 104.3 (s, 6P), -143.0 (septet, $^1J_{PF}$ = 708.0 Hz, PF_6). ^{19}F NMR (376.5 MHz, acetone-d_6, δ, ppm) : -72.9 (d, $^1J_{FP}$ = 708.4 Hz, PF_6), -150.8 (s).

5 Synthesis of $Cu_4Ag_4(O)[S_2P(OEt)_2]_6$, 4. A solution of $[Ag_7(H)\{S_2P(OEt)_2\}_6]$ (0.12g, 0.0643mmol) and $[Cu(CH_3CN)_4]PF_6$ (0.024g, 0.0643 mmol) in 30 mL of chloroform was stirred at room temperature for 24 h under nitrogen. It was then filtered to get rid of any solid, and the filtrate was evaporated to dryness to get a white solid. It was washed with deionized water then dried under vacuum. Crystallizations in chloroform obtain $Ag_4Cu_4(O)[S_2P(OEt)_2]_6$ as a colorless crystal. ^{1}H NMR (300MHz, acetone-d6): 1.32 (t, 36H, CH_3), 4.15 (m, 24H, CH_2), ^{31}P NMR (acetone-d6): 110.3 ppm. EDX analysis: Cu K (48.58%), Ag L (51.42%).

1. Wu, C.-C.; Lee, B.-H.; Liao, P.-K.; Fang, C.-S.; Liu, C. W. *J. Chin. Chem. Soc*. **2012**, *59*, 480–484
2. Wystrach, V. P.; Hook, E. O.; Christopher G. L. M. *J. Org. Chem.*, **1956**, *21*, 705.
3. The blue color is due to the presence of minute amount of Cu(II), a water oxidized product. Similarly, the original syntheses of an encapsulated S^{2-} gave a red material, presumably due to Mo(III) impurities (Wu, D. M.; Huang, J. Q.; Lin, H. Y.;Huang, J. L. *Scientia Sinica B.* **1988**, *31*, 121). Simple HOMO-LUMO gap considerations suggest that there is no reason for the encapsulated species not to be as colorless as their empty relatives.

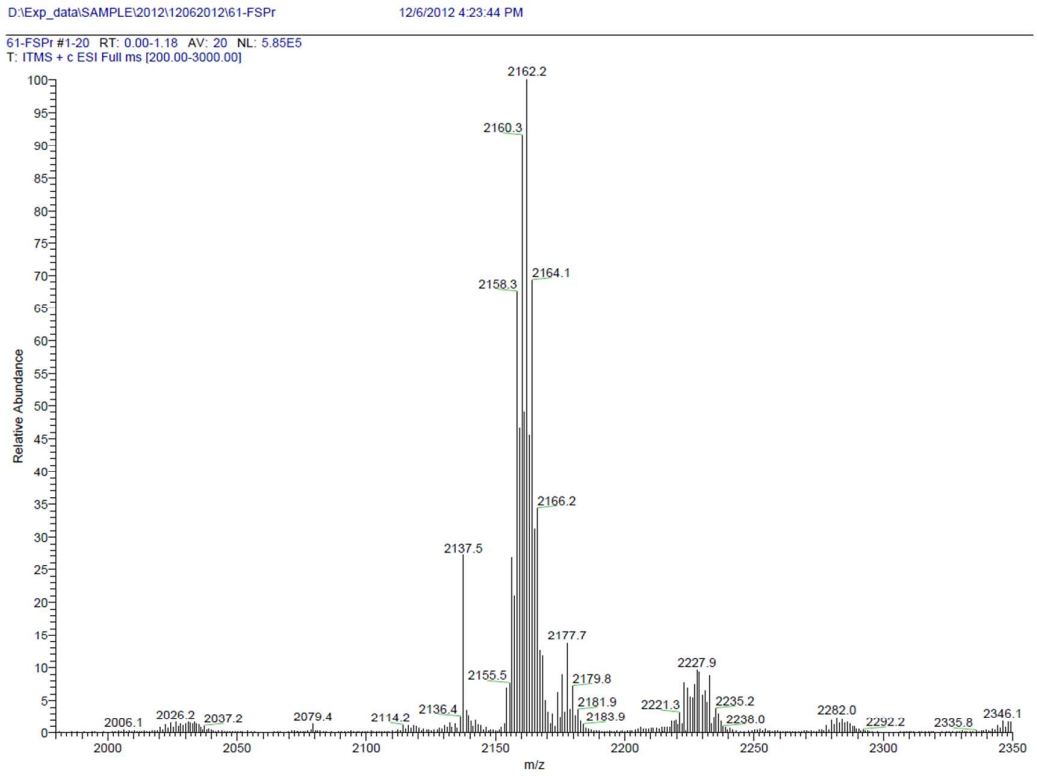

Figure S1. The MS spectrum of compound **3**.

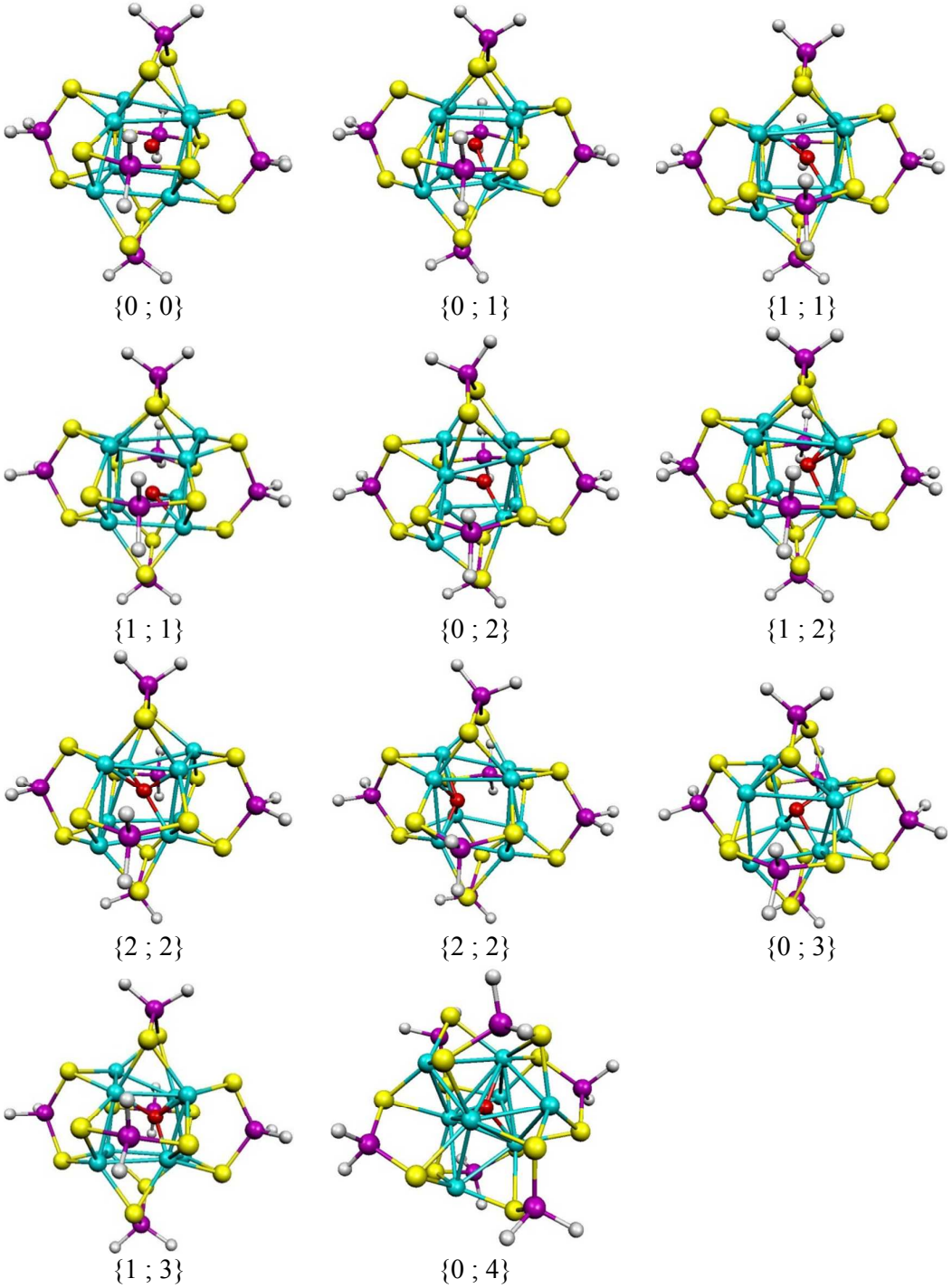

Figure S2: Various structures of the $[Cu_8(H)(Se_2PH_2)_6]^+$ cluster that were visited during a MetaD simulation at 300 K using CV_1 and CV_2 as CVs. For each structure, the corresponding values of CV_1 and CV_2 are indicated in curly brackets $\{CV_1 ; CV_2\}$.

Table S1. Relevant computed data corresponding to the optimized geometries of $[Cu_8(X)(Se_2PH_2)_6]^q$ (X = □ (vacancy), H, F, Cl, Br, O, S, Se, N, P, C). The metal atom numbering corresponds to that of Scheme 1 (left side) and refers to the values of the T_h and T structures only.

q	$[Cu_8(X)(Se_2PH_2)_6]^q$	Symm.	Imag.Freq. (cm^{-1})	ΔE (eV) [a]	Cu_1-Cu_2(Å) Cu_1-Cu_3(Å)	Cu_1-X (Å) Cu_2-X (Å)	DI (%) [b]
+2	X= □	T_h	-	-	3.38 4.78	2.93	0
+1	X=H	T	-	0.00	2.71 2.87	1.76 2.73	86
		T_h	407.i (t_u), 67.i (a_u), 41.i (t_g)	0.54	2.60 3.68	2.25	0
	X= F	T	-	0.00	3.03 3.87	2.37 2.84	33
		T_h	79.i (t_u), 41.i (a_u), 21.i(t_g)	0.04	3.00 4.24	2.60	0
	X=Cl	T_h	-	0.00	3.22 4.55	2.79	0
	X=Br	T_h	-	0.00	3.28 4.64	2.84	0
0	X=O	T	-	0.00	2.82 3.30	2.02 2.75	59
		T_h	75.i (a_u), 38.i (t_g)	0.33	2.69 3.81	2.33	0
	X=S	T_h	-	0.00	2.84 4.02	2.46	0
	X=Se	T_h	-	0.00	2.96 4.19	2.56	0
-1	X=N	S_6	-	0.00	6*2.62, 6*2.75, 6*2.81	6*1.97, 2*3.24	-
		C_3	-	0.01	3*2.58, 3*2.59, 3*2.62, 3*2.65, 3*2.69	3*2.17, 3*2.01, 1*2.13, 1*3.39	-
		T_h	72.i (a_u), 30.i (t_g)	0.45	2.55 3.60	2.21	0
	X=P	T_h	-	0.00	2.72 3.86	2.36	0
-2	X=C	S_6	-	0.00	6*2.65, 6*2.7, 6*2.78	6*1.92, 2*3.31	-
		T_h	32.i (t_u), 24.i (t_g)	1.83	2.49 3.53	2.16	0

[a] Relative energies between different geometries of the same compound.

[b] Distortion index measuring the degree of tetrahedral distortion away from the ideal T_h cubic structure, as defined in the text.

Table S2. Relevant computed data corresponding to the optimized geometries of $[Ag_8(X)(S_2PH_2)_6]^q$ (X = □ (vacancy), H, F, Cl, Br, O, S, Se, N, P, C). The metal atom numbering corresponds to that of Scheme 2 (left side) and refers to the values of the T_h and T structures only.

q	$[Ag_8(X)(S_2PH_2)_6]^q$	Symm.	Imag.Freq. (cm^{-1})	ΔE (eV) [a]	Ag_1-Ag_2(Å) Ag_1-Ag_3(Å)	Ag_1-X (Å) Ag_2-X (Å)	DI (%) [b]
+2	X= □	T_h	-	-	3.53 4.99	3.06	0
+1	X=H	T	-	0.00	3.11 3.26	2.00 3.15	88
		T_h	208.i (t_u), 45.i (a_u), 28.i (t_g)	0.59	2.98 4.22	2.58	0
	X= F	T	-	0.00	3.23 4.17	2.55 3.01	30
		T_h	25.i (a_u)	0.03	3.18 4.51	2.76	0
	X=Cl	T_h	-	0.00	3.42 4.83	2.96	0
	X=Br	T_h	-	0.00	3.45 4.87	2.98	0
0	X=O	T	-	0.00	3.04 3.84	2.36 2.86	36
		T_h	28.i (a_u)	0.04	2.98 4.21	2.58	0
	X=S	T_h	-	0.00	3.16 4.47	2.74	0
	X=Se	T_h	-	0.00	3.25 4.58	2.81	0
-1	X=N	S_6	-	0.00	6*3.06, 6*3.16, 6*3.13	6*2.20, 2*3.78	-
		C_3	-	0.98	3*2.97, 3*2.91, 3*3.04, 3* 2.96, 3*3.12	3* 2.30, 3* 2.44, 2.47, 3.80	-
		T_h	30.i (a_u)	1.48	2.90 4.09	2.51	0
	X=P	T_h	-	0.00	3.05 4.32	2.64	0
-2	X=C	S_6	-	0.00	6*3.02, 6*3.15, 6*3.07	6*2.18, 2*3.68	-
		T_h	29.i (e_u)	3.21	2.84 4.02	2.46	0

[a] Relative energies between different geometries of the same compound.

[b] Distortion index measuring the degree of tetrahedral distortion away from the ideal T_h cubic structure, as defined in the text.

Table S3. Relevant computed data corresponding to the optimized geometries of $[Ag_8(X)(Se_2PH_2)_6]^q$ (X = □ (vacancy), H, F, Cl, Br, O, S, Se, N, P, C). The metal atom numbering corresponds to that of Scheme 1 (left side) and refers to the values of the T_h and T structures only.

q	$[Ag_8(X)(Se_2PH_2)_6]^q$	Symm.	Imag.Freq. (cm^{-1})	ΔE (eV) [a]	Ag_1-Ag_2(Å) Ag_1-Ag_3(Å)	Ag_1-X (Å) Ag_2-X (Å)	DI (%) [b]
+2	X= □	T_h	-	-	3.62 5.12	3.14	0
+1	X=H	T	-	0.00	3.14 3.24	1.98 3.18	92
		T_h	244.i (t_u), 45.i (a_u), 30.i (t_g)	0.66	2.99 4.23	2.59	0
	X= F	T	-	0.00	3.26 4.13	2.53 3.07	36
		T_h	23.i (a_u)	0.04	3.20 4.53	2.77	0
	X=Cl	T_h	-	0.00	3.45 4.87	2.98	0
	X=Br	T_h	-	0.00	3.49 4.93	3.02	0
0	X=O	T	-	0.00	3.08 3.80	2.33 2.93	44
		T_h	35.i (a_u)	0.09	2.99 4.23	2.59	0
	X=S	T_h	-	0.00	3.18 4.50	2.76	0
	X=Se	T_h	-	0.00	3.27 4.62	2.83	0
-1	X=N	S_6	-	0.00	6*3.06, 6*3.12, 6*3.18	6*2.21, 2*3.74	-
		C_3	-	0.39	3*2.94, 3*2.96, 3*2.98, 3*3.07, 3*3.15	3*2.49, 3*2.31, 2.41, 3.78	-
		T_h	34.i (a_u)	0.95	2.91 4.11	2.52	0
	X=P	T_h	-	0.00	3.06 4.33	2.65	0
-2	X=C	S_6	-	0.00	6*3.02 6*3.16 6*3.08	6*2.19 2*3.69	-
		T_h	12.i (a_u), 7.i (e_u)	2.70	2.85 4.04	2.48	0

[a] Relative energies between different geometries of the same compound.

[b] Distortion index measuring the degree of tetrahedral distortion away from the ideal T_h cubic structure, as defined in the text.

Table S4. Relevant bonding parameters computed for $[Cu_8(X)(Se_2PH_2)_6]^q$ (X = H, F, Cl, Br, q = +1; X = O, S, Se, q = 0; X = N, P, q = -1; X = C, q = -2). BE: bonding energy, DE: dissociation energy, ΔE_{Dist}: cage distortion energy (see text for definitions)

q	$[Cu_8(X)(Se_2PH_2)_6]^q$	Symm.	BE (eV)	DE (eV)	ΔE_{Dist} (eV)	Cu-X Wiberg indices [a]	NAO charge and population analysis of X
+1	X=H	T	11.73	10.78	0.95	4*0.104 4*0.006	-0.64 ($1s^{1.63}$)
		T_h	11.23	10.24	0.99	8*0.047	-0.65 ($1s^{1.64}$)
	X= F	T	9.37	8.90	0.47	4*0.041 4*0.011	-0.86 ($2s^{1.97}$ $2p^{5.88}$)
		T_h	9.14	8.86	0.28	8*0.026	-0.85 ($2s^{1.98}$ $2p^{5.87}$)
	X=Cl	T_h	7.77	7.62	0.15	8*0.036	-0.82 ($3s^{1.95}$ $3p^{5.85}$)
	X=Br	T_h	7.30	7.14	0.16	8*0.040	-0.81 ($4s^{1.95}$ $4p^{5.83}$)
0	X=O	T	26.80	25.89	0.91	4*0.084 4*0.020	-1.70 ($2s^{1.91}$ $2p^{5.77}$)
		T_h	26.49	25.66	0.83	8*0.054	-1.67 ($2s^{1.93}$ $2p^{5.72}$)
	X=S	T_h	22.01	21.17	0.84	8*0.081	-1.58 ($3s^{1.86}$ $3p^{5.67}$)
	X=Se	T_h	20.33	19.54	0.79	8*0.083	-1.56 ($4s^{1.87}$ $4p^{5.63}$)
-1	X=N	S_6	b	46.40	b	6*0.140 2*0.027	-2.34 ($2s^{1.79}$ $2p^{5.53}$)
		C_3	b	46.39	b	3*0.159 3*0.091 1*0.034 1*0.067	-2.31 ($2s^{1.83}$ $2p^{5.46}$)
		T_h	47.63	45.95	1.68	8*0.091	-2.38 ($2s^{1.85}$ $2p^{5.51}$)
	X=P	T_h	38.55	36.90	1.65	8*0.133	-2.17 ($3s^{1.74}$ $3p^{5.35}$)
-2	X=C	S_6	b	64.53	b	6*0.267 2*0.074	-2.76 ($2s^{1.60}$ $2p^{5.12}$)
		T_h	66.04	62.70	3.34	8*0.140	-2.90 ($2s^{1.71}$ $2p^{5.16}$)

[a] Expressed in the NAO basis.

[b] Could not be calculated due to convergence problems.

Table S5. Relevant bonding parameters computed for $[Ag_8(X)(S_2PH_2)_6]^q$ (X = H, F, Cl, Br, q = +1; X = O, S, Se, q = 0; X = N, P, q = -1; X = C, q = -2).BE: bonding energy, DE: dissociation energy, ΔE_{Dist}: cage distortion energy (see text for definitions).

q	$[Ag_8(X)(S_2PH_2)_6]^q$	Symm.	BE (eV)	DE (eV)	ΔE_{Dist} (eV)	Ag-X Wiberg indices [a]	NAO charge and population analysis of X
+1	X=H	*T*	11.42	10.55	0.86	4*0.105 4*0.006	-0.66 ($1s^{1.65}$)
		T_h	10.65	9.96	0.69	8*0.048	-0.67 ($1s^{1.67}$)
	X= F	*T*	9.78	9.48	0.30	4*0.035 4*0.016	-0.86 ($2s^{1.97}$ $2p^{5.89}$)
		T_h	9.71	9.45	0.26	8*0.027	-0.86 ($2s^{1.97}$ $2p^{5.88}$)
	X=Cl	T_h	8.24	8.13	0.11	8*0.038	-0.82 ($3s^{1.94}$ $3p^{5.86}$)
	X=Br	T_h	7.78	7.65	0.13	8*0.041	-0.81 ($4s^{1.94}$ $4p^{5.86}$)
0	X=O	*T*	26.66	25.85	0.81	4*0.076 4*0.046	-1.65 ($2s^{1.94}$ $2p^{5.72}$)
		T_h	26.69	25.81	0.88	8*0.066	-1.62 ($2s^{1.94}$ $2p^{5.68}$)
	X=S	T_h	22.02	21.31	0.71	8*0.075	-1.62 ($3s^{1.88}$ $3p^{5.71}$)
	X=Se	T_h	20.62	19.90	0.72	8*0.079	-1.62 ($4s^{1.88}$ $4p^{5.71}$)
-1	X=N	S_6	b	46.83	b	6*0.210 2*0.046	-2.10 ($2s^{1.81}2p^{5.27}$)
		C_3	b	45.85	b	3* 0.190 3*0.098 1*0.069 1*0.050	-2.27 ($2s^{1.88}2p^{5.37}$)
		T_h	47.13	45.35	1.78	8*0.113	-2.32 ($2s^{1.89}2p^{5.42}$)
	X=P	T_h	38.32	36.55	1.77	8*0.133	-2.30 ($3s^{1.79}$ $3p^{5.47}$)
-2	X=C	S_6	b	64.60	b	6*0.305 2*0.084	-2.55 ($2s^{1.52}$ $2p^{4.97}$)
		T_h	64.91	61.39	3.52	8*0.172	-2.98 ($2s^{1.77}$ $2p^{5.18}$)

[a] Expressed in the NAO basis.

[b] Could not be calculated due to convergence problems.

Table S6. Relevant bonding parameters computed for $[Ag_8(X)(Se_2PH_2)_6]^q$ (X = H, F, Cl, Br, q = +1; X = O, S, Se, q = 0; X = N, P, q = -1; X = C, q = -2).BE: bonding energy, DE: dissociation energy, ΔE_{Dist}: cage distortion energy (see text for definitions).

q	$[Ag_8(X)(Se_2PH_2)_6]^q$	Symm.	BE (eV)	DE (eV)	ΔE_{Dist} (eV)	Ag-X Wiberg indices [a]	NAO charge and population analysis of X
+1	X=H	*T*	11.32	10.49	0.83	4*0.107 4*0.005	-0.63 ($1s^{1.63}$)
		T_h	10.51	9.83	0.68	8*0.047	-0.65 ($1s^{1.65}$)
	X= F	*T*	9.60	9.27	0.33	4*0.039 4*0.015	-0.85 ($2s^{1.97}$ $2p^{5.88}$)
		T_h	9.49	9.23	0.26	8*0.027	-0.85 ($2s^{1.97}$ $2p^{5.87}$)
	X=Cl	T_h	8.14	8.02	0.12	8*0.039	-0.80 ($3s^{1.94}$ $3p^{5.85}$)
	X=Br	T_h	7.71	7.59	0.12	8*0.041	-0.78 ($4s^{1.94}$ $4p^{5.84}$)
0	X=O	*T*	26.36	25.63	0.73	4*0.080 4*0.042	-1.63 ($2s^{1.93}$ $2p^{5.69}$)
		T_h	26.36	25.54	0.82	8*0.064	-1.61 ($2s^{1.94}$ $2p^{5.66}$)
	X=S	T_h	21.79	21.19	0.60	8*0.075	-1.59 ($3s^{1.88}$ $3p^{5.69}$)
	X=Se	T_h	20.42	19.83	0.59	8*0.078	-1.60 ($4s^{1.88}$ $4p^{5.68}$)
-1	X=N	S_6	b	46.19	b	6*0.202 2*0.045	-2.12 ($2s^{1.82}$ $2p^{5.28}$)
		C_3	b	45.80	b	3*0.183 3*0.096 1*0.070 1*0.043	-2.24 ($2s^{1.88}$ $2p^{5.33}$)
		T_h	46.80	45.24	1.56	8*0.110	-2.27 ($2s^{1.89}$ $2p^{5.37}$)
	X=P	T_h	38.01	36.59	1.43	8*0.121	-2.27 ($3s^{1.78}$ $3p^{5.44}$)
-2	X=C	S_6	b	64.30	b	6*0.286 2*0.098	-2.65 ($2s^{1.67}$ $2p^{4.94}$)
		T_h	64.30	61.60	2.70	8*0.160	-2.85 ($2s^{1.77}$ $2p^{5.05}$)

[a] Expressed in the NAO basis.

[b] Could not be calculated due to convergence problems.

Computed optimized structure of $[Cu_8(\square)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -19961.3695196 a. u.

	X	Y	Z
Cu	1.604154	1.604154	1.604154
Cu	-1.604154	1.604154	1.604154
Cu	-1.604154	1.604154	-1.604154
Cu	1.604154	1.604154	-1.604154
Cu	1.604154	-1.604154	1.604154
Cu	-1.604154	-1.604154	1.604154
Cu	-1.604154	-1.604154	-1.604154
Cu	1.604154	-1.604154	-1.604154
S	1.798268	3.192630	0.000000
S	0.000000	1.798268	3.192630
S	-1.798268	3.192630	0.000000
S	0.000000	1.798268	-3.192630
S	1.798268	-3.192630	0.000000
S	0.000000	-1.798268	3.192630
S	-1.798268	-3.192630	0.000000
S	0.000000	-1.798268	-3.192630
S	3.192630	0.000000	1.798268
S	-3.192630	0.000000	1.798268
S	-3.192630	0.000000	-1.798268
S	3.192630	0.000000	-1.798268
P	4.207559	0.000000	0.000000
P	0.000000	0.000000	4.207559
P	-4.207559	0.000000	0.000000
P	0.000000	0.000000	-4.207559
P	0.000000	4.207559	0.000000
P	0.000000	-4.207559	0.000000
H	5.083190	-1.113293	0.000000
H	5.083190	1.113293	0.000000
H	-1.113293	0.000000	5.083190
H	1.113293	0.000000	5.083190
H	-5.083190	-1.113293	0.000000
H	-5.083190	1.113293	0.000000
H	1.113293	0.000000	-5.083190
H	-1.113293	0.000000	-5.083190
H	0.000000	5.083190	1.113293
H	0.000000	5.083190	-1.113293
H	0.000000	-5.083190	-1.113293
H	0.000000	-5.083190	1.113293

Computed optimized structure of $[Cu_8(H)(S_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E= -19962.2712308 a. u.

X	Y	Z
Cu	1.025185	1.025185	1.025185
Cu	-1.555796	1.555796	1.555796
Cu	-1.025185	1.025185	-1.025185
Cu	1.555796	1.555796	-1.555796
Cu	1.555796	-1.555796	1.555796
Cu	-1.025185	-1.025185	1.025185
Cu	-1.555796	-1.555796	-1.555796
Cu	1.025185	-1.025185	-1.025185
S	1.769492	3.150131	0.074731
S	0.074731	1.769492	3.150131
S	-1.769492	3.150131	-0.074731
S	-0.074731	1.769492	-3.150131
S	1.769492	-3.150131	-0.074731
S	-0.074731	-1.769492	3.150131
S	-1.769492	-3.150131	0.074731
S	0.074731	-1.769492	-3.150131
S	3.150131	0.074731	1.769492
S	-3.150131	-0.074731	1.769492
S	-3.150131	0.074731	-1.769492
S	3.150131	-0.074731	-1.769492
P	4.176194	0.000000	0.000000
P	0.000000	0.000000	4.176194
P	-4.176194	0.000000	0.000000
P	0.000000	0.000000	-4.176194
P	0.000000	4.176194	0.000000
P	0.000000	-4.176194	0.000000
H	5.065045	-1.104099	0.015370
H	5.065045	1.104099	-0.015370
H	-1.104099	0.015370	5.065045
H	1.104099	-0.015370	5.065045
H	-5.065045	-1.104099	-0.015370
H	-5.065045	1.104099	0.015370
H	1.104099	0.015370	-5.065045
H	-1.104099	-0.015370	-5.065045
H	-0.015370	5.065045	1.104099
H	0.015370	5.065045	-1.104099
H	-0.015370	-5.065045	-1.104099
H	0.015370	-5.065045	1.104099
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(F)(S_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E= -20061.5803034 a. u.

Cu	1.408695	1.408695	1.408695
Cu	-1.567805	1.567805	1.567805
Cu	-1.408695	1.408695	-1.408695
Cu	1.567805	1.567805	-1.567805
Cu	1.567805	-1.567805	1.567805
Cu	-1.408695	-1.408695	1.408695
Cu	-1.567805	-1.567805	-1.567805
Cu	1.408695	-1.408695	-1.408695
S	1.790834	3.195224	0.009229
S	0.009229	1.790834	3.195224
S	-1.790834	3.195224	-0.009229
S	-0.009229	1.790834	-3.195224
S	1.790834	-3.195224	-0.009229
S	-0.009229	-1.790834	3.195224
S	-1.790834	-3.195224	0.009229
S	0.009229	-1.790834	-3.195224
S	3.195224	0.009229	1.790834
S	-3.195224	-0.009229	1.790834
S	-3.195224	0.009229	-1.790834
S	3.195224	-0.009229	-1.790834
P	4.199118	0.000000	0.000000
P	0.000000	0.000000	4.199118
P	-4.199118	0.000000	0.000000
P	0.000000	0.000000	-4.199118
P	0.000000	4.199118	0.000000
P	0.000000	-4.199118	0.000000
H	5.087868	-1.105277	-0.004354
H	5.087868	1.105277	0.004354
H	-1.105277	-0.004354	5.087868
H	1.105277	0.004354	5.087868
H	-5.087868	-1.105277	0.004354
H	-5.087868	1.105277	-0.004354
H	1.105277	-0.004354	-5.087868
H	-1.105277	0.004354	-5.087868
H	0.004354	5.087868	1.105277
H	-0.004354	5.087868	-1.105277
H	0.004354	-5.087868	-1.105277
H	-0.004354	-5.087868	1.105277
F	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Cl)(S_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E= -20421.9675313 a. u.

Cu	1.581888	1.581888	1.581888
Cu	1.581888	1.581888	-1.581888
Cu	1.581888	-1.581888	-1.581888
Cu	1.581888	-1.581888	1.581888
Cu	-1.581888	1.581888	1.581888
Cu	-1.581888	1.581888	-1.581888
Cu	-1.581888	-1.581888	-1.581888
Cu	-1.581888	-1.581888	1.581888
S	3.232658	0.000000	1.814290
S	1.814290	3.232658	0.000000
S	3.232658	0.000000	-1.814290
S	1.814290	-3.232658	0.000000
S	-3.232658	0.000000	1.814290
S	-1.814290	3.232658	0.000000
S	-3.232658	0.000000	-1.814290
S	-1.814290	-3.232658	0.000000
S	0.000000	1.814290	3.232658
S	0.000000	1.814290	-3.232658
S	0.000000	-1.814290	-3.232658
S	0.000000	-1.814290	3.232658
P	0.000000	0.000000	4.202178
P	0.000000	4.202178	0.000000
P	0.000000	0.000000	-4.202178
P	0.000000	-4.202178	0.000000
P	4.202178	0.000000	0.000000
P	-4.202178	0.000000	0.000000
H	-1.107555	0.000000	5.087166
H	1.107555	0.000000	5.087166
H	0.000000	5.087166	-1.107555
H	0.000000	5.087166	1.107555
H	-1.107555	0.000000	-5.087166
H	1.107555	0.000000	-5.087166
H	0.000000	-5.087166	1.107555
H	0.000000	-5.087166	-1.107555
H	5.087166	1.107555	0.000000
H	5.087166	-1.107555	0.000000
H	-5.087166	-1.107555	0.000000
H	-5.087166	1.107555	0.000000
Cl	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Br)(S_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E= -22536.1359960 a. u.

Cu	1.609606	1.609606	1.609606
Cu	-1.609606	1.609606	1.609606
Cu	-1.609606	1.609606	-1.609606
Cu	1.609606	1.609606	-1.609606
Cu	1.609606	-1.609606	1.609606
Cu	-1.609606	-1.609606	1.609606
Cu	-1.609606	-1.609606	-1.609606
Cu	1.609606	-1.609606	-1.609606
S	1.822808	3.249213	0.000000
S	0.000000	1.822808	3.249213
S	-1.822808	3.249213	0.000000
S	0.000000	1.822808	-3.249213
S	1.822808	-3.249213	0.000000
S	0.000000	-1.822808	3.249213
S	-1.822808	-3.249213	0.000000
S	0.000000	-1.822808	-3.249213
S	3.249213	0.000000	1.822808
S	-3.249213	0.000000	1.822808
S	-3.249213	0.000000	-1.822808
S	3.249213	0.000000	-1.822808
P	4.205740	0.000000	0.000000
P	0.000000	0.000000	4.205740
P	-4.205740	0.000000	0.000000
P	0.000000	0.000000	-4.205740
P	0.000000	4.205740	0.000000
P	0.000000	-4.205740	0.000000
H	5.089032	-1.108541	0.000000
H	5.089032	1.108541	0.000000
H	-1.108541	0.000000	5.089032
H	1.108541	0.000000	5.089032
H	-5.089032	-1.108541	0.000000
H	-5.089032	1.108541	0.000000
H	1.108541	0.000000	-5.089032
H	-1.108541	0.000000	-5.089032
H	0.000000	5.089032	1.108541
H	0.000000	5.089032	-1.108541
H	0.000000	-5.089032	-1.108541
H	0.000000	-5.089032	1.108541
Br	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(O)(S_2PH_2)_6]$ (*T*)
BP86/Def2TZVP
E= -20037.1055692 a. u.

Cu	1.187206	1.187206	1.187206
Cu	1.545927	-1.545927	1.545927
Cu	-1.187206	-1.187206	1.187206
Cu	-1.545927	1.545927	1.545927
Cu	1.545927	1.545927	-1.545927
Cu	1.187206	-1.187206	-1.187206
Cu	-1.545927	-1.545927	-1.545927
Cu	-1.187206	1.187206	-1.187206
S	0.038284	1.786807	3.201793
S	3.201793	0.038284	1.786807
S	-0.038284	-1.786807	3.201793
S	-3.201793	-0.038284	1.786807
S	-0.038284	1.786807	-3.201793
S	3.201793	-0.038284	-1.786807
S	0.038284	-1.786807	-3.201793
S	-3.201793	0.038284	-1.786807
S	1.786807	3.201793	0.038284
S	1.786807	-3.201793	-0.038284
S	-1.786807	-3.201793	0.038284
S	-1.786807	3.201793	-0.038284
P	0.000000	4.188512	0.000000
P	4.188512	0.000000	0.000000
P	0.000000	-4.188512	0.000000
P	-4.188512	0.000000	0.000000
P	0.000000	0.000000	4.188512
P	0.000000	0.000000	-4.188512
H	-0.003502	5.089300	-1.098717
H	0.003502	5.089300	1.098717
H	5.089300	-1.098717	-0.003502
H	5.089300	1.098717	0.003502
H	0.003502	-5.089300	-1.098717
H	-0.003502	-5.089300	1.098717
H	-5.089300	1.098717	-0.003502
H	-5.089300	-1.098717	0.003502
H	1.098717	0.003502	5.089300
H	-1.098717	-0.003502	5.089300
H	-1.098717	0.003502	-5.089300
H	1.098717	-0.003502	-5.089300
O	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(S)(S_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E= -20360.1557617 a. u.

Cu	1.422259	1.422259	1.422259
Cu	-1.422259	1.422259	1.422259
Cu	-1.422259	1.422259	-1.422259
Cu	1.422259	1.422259	-1.422259
Cu	1.422259	-1.422259	1.422259
Cu	-1.422259	-1.422259	1.422259
Cu	-1.422259	-1.422259	-1.422259
Cu	1.422259	-1.422259	-1.422259
S	1.810227	3.265875	0.000000
S	0.000000	1.810227	3.265875
S	-1.810227	3.265875	0.000000
S	0.000000	1.810227	-3.265875
S	1.810227	-3.265875	0.000000
S	0.000000	-1.810227	3.265875
S	-1.810227	-3.265875	0.000000
S	0.000000	-1.810227	-3.265875
S	3.265875	0.000000	1.810227
S	-3.265875	0.000000	1.810227
S	-3.265875	0.000000	-1.810227
S	3.265875	0.000000	-1.810227
P	4.215618	0.000000	0.000000
P	0.000000	0.000000	4.215618
P	-4.215618	0.000000	0.000000
P	0.000000	0.000000	-4.215618
P	0.000000	4.215618	0.000000
P	0.000000	-4.215618	0.000000
H	5.112801	-1.100695	0.000000
H	5.112801	1.100695	0.000000
H	-1.100695	0.000000	5.112801
H	1.100695	0.000000	5.112801
H	-5.112801	-1.100695	0.000000
H	-5.112801	1.100695	0.000000
H	1.100695	0.000000	-5.112801
H	-1.100695	0.000000	-5.112801
H	0.000000	5.112801	1.100695
H	0.000000	5.112801	-1.100695
H	0.000000	-5.112801	-1.100695
H	0.000000	-5.112801	1.100695
S	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Se)(S_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E= -22363.7359330 a. u.

Cu	1.475276	1.475276	1.475276
Cu	-1.475276	1.475276	1.475276
Cu	-1.475276	1.475276	-1.475276
Cu	1.475276	1.475276	-1.475276
Cu	1.475276	-1.475276	1.475276
Cu	-1.475276	-1.475276	1.475276
Cu	-1.475276	-1.475276	-1.475276
Cu	1.475276	-1.475276	-1.475276
S	1.821488	3.284077	0.000000
S	0.000000	1.821488	3.284077
S	-1.821488	3.284077	0.000000
S	0.000000	1.821488	-3.284077
S	1.821488	-3.284077	0.000000
S	0.000000	-1.821488	3.284077
S	-1.821488	-3.284077	0.000000
S	0.000000	-1.821488	-3.284077
S	3.284077	0.000000	1.821488
S	-3.284077	0.000000	1.821488
S	-3.284077	0.000000	-1.821488
S	3.284077	0.000000	-1.821488
P	4.219613	0.000000	0.000000
P	0.000000	0.000000	4.219613
P	-4.219613	0.000000	0.000000
P	0.000000	0.000000	-4.219613
P	0.000000	4.219613	0.000000
P	0.000000	-4.219613	0.000000
H	5.114133	-1.102313	0.000000
H	5.114133	1.102313	0.000000
H	-1.102313	0.000000	5.114133
H	1.102313	0.000000	5.114133
H	-5.114133	-1.102313	0.000000
H	-5.114133	1.102313	0.000000
H	1.102313	0.000000	-5.114133
H	-1.102313	0.000000	-5.114133
H	0.000000	5.114133	1.102313
H	0.000000	5.114133	-1.102313
H	0.000000	-5.114133	-1.102313
H	0.000000	-5.114133	1.102313
Se	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(N)(S_2PH_2)_6]^-$ (S_6)
BP86/Def2TZVP
E= -20016.6945370 a. u.

Cu	0.000000	0.000000	3.361311
Cu	1.283916	0.949023	1.064062
Cu	1.463836	-0.637392	-1.064062
Cu	0.179920	-1.586416	1.064062
Cu	-1.463836	0.637392	1.064062
Cu	-0.179920	1.586416	-1.064062
Cu	0.000000	0.000000	-3.361311
Cu	-1.283916	-0.949023	-1.064062
S	2.190280	-0.264990	4.294664
S	-0.865652	2.029333	4.294664
S	3.033714	2.116939	1.870214
S	3.350180	-1.568803	-1.870214
S	-3.033714	-2.116939	-1.870214
S	-3.350180	1.568803	1.870214
S	-2.190280	0.264990	-4.294664
S	0.865652	-2.029333	-4.294664
S	-1.324628	-1.764343	4.294664
S	-0.316466	3.685743	-1.870214
S	1.324628	1.764343	-4.294664
S	0.316466	-3.685743	1.870214
P	0.000000	-3.186739	3.801494
P	-2.759797	1.593369	3.801494
P	0.000000	3.186739	-3.801494
P	2.759797	-1.593369	-3.801494
P	2.759797	1.593369	3.801494
P	-2.759797	-1.593369	-3.801494
H	-0.332715	-4.389521	4.501679
H	1.249752	-2.893300	4.419652
H	-3.635080	2.482900	4.501679
H	-3.130547	0.364333	4.419652
H	-1.249752	2.893300	-4.419652
H	0.332715	4.389521	-4.501679
H	3.635080	-2.482900	-4.501679
H	3.130547	-0.364333	-4.419652
H	1.880796	2.528967	4.419652
H	3.967794	1.906621	4.501679
H	-1.880796	-2.528967	-4.419652
H	-3.967794	-1.906621	-4.501679
N	0.000000	0.000000	0.000000
XX	0.566505	0.170103	-0.806311

Computed optimized structure of $[Cu_8(N)(S_2PH_2)_6]^-$ (C_3)
BP86/Def2TZVP
E= -20016.6508321 a. u.

Cu	0.000000	0.000000	2.994569
Cu	0.748515	1.341498	0.931940
Cu	2.139966	0.000000	-0.825582
Cu	0.787514	-1.318982	0.931940
Cu	-1.536029	-0.022516	0.931940
Cu	-1.069983	1.853265	-0.825582
Cu	0.000000	0.000000	-2.494021
Cu	-1.069983	-1.853265	-0.825582
S	1.920106	-1.330077	2.981627
S	0.191827	2.327899	2.981627
S	3.318093	1.266271	0.905932
S	2.929764	-2.214674	-1.046867
S	-3.382846	-1.429913	-1.046867
S	-2.755669	2.240417	0.905932
S	-1.976658	1.256290	-2.965672
S	-0.099650	-2.339981	-2.965672
S	-2.111933	-0.997822	2.981627
S	0.453082	3.644587	-1.046867
S	2.076308	1.083691	-2.965672
S	-0.562424	-3.506688	0.905932
P	-1.781667	-2.969761	2.413128
P	-1.681055	3.027849	2.413128
P	1.416743	3.000423	-2.689682
P	1.890071	-2.727147	-2.689682
P	3.462722	-0.058088	2.413128
P	-3.306814	-0.273276	-2.689682
H	-3.086053	-3.492802	2.198376
H	-1.404502	-3.682630	3.586301
H	-1.481829	4.419001	2.198376
H	-2.487000	3.057649	3.586301
H	0.649202	3.313193	-3.847304
H	2.541033	3.851796	-2.891819
H	2.065237	-4.126497	-2.891819
H	2.544708	-2.218822	-3.847304
H	3.891502	0.624981	3.586301
H	4.567882	-0.926199	2.198376
H	-3.193910	-1.094371	-3.847304
H	-4.606270	0.274701	-2.891819
N	0.000000	0.000000	-0.351684

Computed optimized structure of $[Cu_8(P)(S_2PH_2)_6]^-$ (T_h)
BP86/Def2TZVP
E= -20303.3512097 a. u.

Cu	1.362851	1.362851	1.362851
Cu	-1.362851	1.362851	1.362851
Cu	-1.362851	1.362851	-1.362851
Cu	1.362851	1.362851	-1.362851
Cu	1.362851	-1.362851	1.362851
Cu	-1.362851	-1.362851	1.362851
Cu	-1.362851	-1.362851	-1.362851
Cu	1.362851	-1.362851	-1.362851
S	1.826620	3.319148	0.000000
S	0.000000	1.826620	3.319148
S	-1.826620	3.319148	0.000000
S	0.000000	1.826620	-3.319148
S	1.826620	-3.319148	0.000000
S	0.000000	-1.826620	3.319148
S	-1.826620	-3.319148	0.000000
S	0.000000	-1.826620	-3.319148
S	3.319148	0.000000	1.826620
S	-3.319148	0.000000	1.826620
S	-3.319148	0.000000	-1.826620
S	3.319148	0.000000	-1.826620
P	4.232731	0.000000	0.000000
P	0.000000	0.000000	4.232731
P	-4.232731	0.000000	0.000000
P	0.000000	0.000000	-4.232731
P	0.000000	4.232731	0.000000
P	0.000000	-4.232731	0.000000
H	5.138491	-1.096226	0.000000
H	5.138491	1.096226	0.000000
H	-1.096226	0.000000	5.138491
H	1.096226	0.000000	5.138491
H	-5.138491	-1.096226	0.000000
H	-5.138491	1.096226	0.000000
H	1.096226	0.000000	-5.138491
H	-1.096226	0.000000	-5.138491
H	0.000000	5.138491	1.096226
H	0.000000	5.138491	-1.096226
H	0.000000	-5.138491	-1.096226
H	0.000000	-5.138491	1.096226
P	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(C)(S_2PH_2)_6]^{2-}$ (*S6*)
BP86/Def2TZVP
E= -20000.0065514 a. u.

Cu	0.286612	0.757769	3.262216
Cu	1.082061	-0.995593	1.232580
Cu	-0.672498	-1.676064	-0.647973
Cu	-1.482368	0.039170	1.217524
Cu	0.672498	1.676064	0.647973
Cu	1.482368	-0.039170	-1.217524
Cu	-0.286612	-0.757769	-3.262216
Cu	-1.082061	0.995593	-1.232580
S	0.181476	-1.169675	4.680878
S	2.355535	1.843986	3.789836
S	2.376914	-2.499644	2.298828
S	-1.600495	-3.710277	-0.924561
S	-2.376914	2.499644	-2.298828
S	1.600495	3.710277	0.924561
S	-0.181476	1.169675	-4.680878
S	-2.355535	-1.843986	-3.789836
S	-1.438422	2.230238	4.033444
S	3.499002	-0.054223	-2.221845
S	1.438422	-2.230238	-4.033444
S	-3.499002	0.054223	2.221845
P	-2.848900	0.805890	3.980072
P	1.810961	3.570949	2.928379
P	2.848900	-0.805890	-3.980072
P	-1.810961	-3.570949	-2.928379
P	2.010374	-1.805828	4.159813
P	-2.010374	1.805828	-4.159813
H	-3.998831	1.268552	4.695086
H	-2.458862	-0.267462	4.832064
H	2.724750	4.595700	3.331514
H	0.626521	4.051749	3.557694
H	2.458862	0.267462	-4.832064
H	3.998831	-1.268552	-4.695086
H	-2.724750	-4.595700	-3.331514
H	-0.626521	-4.051749	-3.557694
H	2.962903	-0.795207	4.478307
H	2.425625	-2.819695	5.080292
H	-2.962903	0.795207	-4.478307
H	-2.425625	2.819695	-5.080292
C	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(\square)(Se_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -44004.3871729 a. u.

Cu	1.691707	1.691707	1.691707
Cu	-1.691707	1.691707	1.691707
Cu	-1.691707	1.691707	-1.691707
Cu	1.691707	1.691707	-1.691707
Cu	1.691707	-1.691707	1.691707
Cu	-1.691707	-1.691707	1.691707
Cu	-1.691707	-1.691707	-1.691707
Cu	1.691707	-1.691707	-1.691707
Se	1.961213	3.348710	0.000000
Se	0.000000	1.961213	3.348710
Se	-1.961213	3.348710	0.000000
Se	0.000000	1.961213	-3.348710
Se	1.961213	-3.348710	0.000000
Se	0.000000	-1.961213	3.348710
Se	-1.961213	-3.348710	0.000000
Se	0.000000	-1.961213	-3.348710
Se	3.348710	0.000000	1.961213
Se	-3.348710	0.000000	1.961213
Se	-3.348710	0.000000	-1.961213
Se	3.348710	0.000000	-1.961213
P	4.423857	0.000000	0.000000
P	0.000000	0.000000	4.423857
P	-4.423857	0.000000	0.000000
P	0.000000	0.000000	-4.423857
P	0.000000	4.423857	0.000000
P	0.000000	-4.423857	0.000000
H	5.311899	-1.104895	0.000000
H	5.311899	1.104895	0.000000
H	-1.104895	0.000000	5.311899
H	1.104895	0.000000	5.311899
H	-5.311899	-1.104895	0.000000
H	-5.311899	1.104895	0.000000
H	1.104895	0.000000	-5.311899
H	-1.104895	0.000000	-5.311899
H	0.000000	5.311899	1.104895
H	0.000000	5.311899	-1.104895
H	0.000000	-5.311899	-1.104895
H	0.000000	-5.311899	1.104895

Computed optimized structure of $[Cu_8(H)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E= -44005.2935027 a. u.

Cu	1.014283	1.014283	1.014283
Cu	-1.576045	1.576045	1.576045
Cu	-1.014283	1.014283	-1.014283
Cu	1.576045	1.576045	-1.576045
Cu	1.576045	-1.576045	1.576045
Cu	-1.014283	-1.014283	1.014283
Cu	-1.576045	-1.576045	-1.576045
Cu	1.014283	-1.014283	-1.014283
Se	1.904711	3.257816	0.118961
Se	0.118961	1.904711	3.257816
Se	-1.904711	3.257816	-0.118961
Se	-0.118961	1.904711	-3.257816
Se	1.904711	-3.257816	-0.118961
Se	-0.118961	-1.904711	3.257816
Se	-1.904711	-3.257816	0.118961
Se	0.118961	-1.904711	-3.257816
Se	3.257816	0.118961	1.904711
Se	-3.257816	-0.118961	1.904711
Se	-3.257816	0.118961	-1.904711
Se	3.257816	-0.118961	-1.904711
P	4.374875	0.000000	0.000000
P	0.000000	0.000000	4.374875
P	-4.374875	0.000000	0.000000
P	0.000000	0.000000	-4.374875
P	0.000000	4.374875	0.000000
P	0.000000	-4.374875	0.000000
H	5.273812	-1.096715	0.029957
H	5.273812	1.096715	-0.029957
H	-1.096715	0.029957	5.273812
H	1.096715	-0.029957	5.273812
H	-5.273812	-1.096715	-0.029957
H	-5.273812	1.096715	0.029957
H	1.096715	0.029957	-5.273812
H	-1.096715	-0.029957	-5.273812
H	-0.029957	5.273812	1.096715
H	0.029957	5.273812	-1.096715
H	-0.029957	-5.273812	-1.096715
H	0.029957	-5.273812	1.096715
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(F)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E= -44104.5886101 a. u.

Cu	1.370121	1.370121	1.370121
Cu	-1.638053	1.638053	1.638053
Cu	-1.370121	1.370121	-1.370121
Cu	1.638053	1.638053	-1.638053
Cu	1.638053	-1.638053	1.638053
Cu	-1.370121	-1.370121	1.370121
Cu	-1.638053	-1.638053	-1.638053
Cu	1.370121	-1.370121	-1.370121
Se	1.935087	3.327661	0.030918
Se	0.030918	1.935087	3.327661
Se	-1.935087	3.327661	-0.030918
Se	-0.030918	1.935087	-3.327661
Se	1.935087	-3.327661	-0.030918
Se	-0.030918	-1.935087	3.327661
Se	-1.935087	-3.327661	0.030918
Se	0.030918	-1.935087	-3.327661
Se	3.327661	0.030918	1.935087
Se	-3.327661	-0.030918	1.935087
Se	-3.327661	0.030918	-1.935087
Se	3.327661	-0.030918	-1.935087
P	4.415705	0.000000	0.000000
P	0.000000	0.000000	4.415705
P	-4.415705	0.000000	0.000000
P	0.000000	0.000000	-4.415705
P	0.000000	4.415705	0.000000
P	0.000000	-4.415705	0.000000
H	5.315960	-1.097092	-0.001888
H	5.315960	1.097092	0.001888
H	-1.097092	-0.001888	5.315960
H	1.097092	0.001888	5.315960
H	-5.315960	-1.097092	0.001888
H	-5.315960	1.097092	-0.001888
H	1.097092	-0.001888	-5.315960
H	-1.097092	0.001888	-5.315960
H	0.001888	5.315960	1.097092
H	-0.001888	5.315960	-1.097092
H	0.001888	-5.315960	-1.097092
H	-0.001888	-5.315960	1.097092
F	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Cl)(Se_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E= -44464.9844334 a. u.

Cu	1.608701	1.608701	1.608701
Cu	-1.608701	1.608701	1.608701
Cu	-1.608701	1.608701	-1.608701
Cu	1.608701	1.608701	-1.608701
Cu	1.608701	-1.608701	1.608701
Cu	-1.608701	-1.608701	1.608701
Cu	-1.608701	-1.608701	-1.608701
Cu	1.608701	-1.608701	-1.608701
Se	1.964176	3.373765	0.000000
Se	0.000000	1.964176	3.373765
Se	-1.964176	3.373765	0.000000
Se	0.000000	1.964176	-3.373765
Se	1.964176	-3.373765	0.000000
Se	0.000000	-1.964176	3.373765
Se	-1.964176	-3.373765	0.000000
Se	0.000000	-1.964176	-3.373765
Se	3.373765	0.000000	1.964176
Se	-3.373765	0.000000	1.964176
Se	-3.373765	0.000000	-1.964176
Se	3.373765	0.000000	-1.964176
P	4.421152	0.000000	0.000000
P	0.000000	0.000000	4.421152
P	-4.421152	0.000000	0.000000
P	0.000000	0.000000	-4.421152
P	0.000000	4.421152	0.000000
P	0.000000	-4.421152	0.000000
H	5.319009	-1.098584	0.000000
H	5.319009	1.098584	0.000000
H	-1.098584	0.000000	5.319009
H	1.098584	0.000000	5.319009
H	-5.319009	-1.098584	0.000000
H	-5.319009	1.098584	0.000000
H	1.098584	0.000000	-5.319009
H	-1.098584	0.000000	-5.319009
H	0.000000	5.319009	1.098584
H	0.000000	5.319009	-1.098584
H	0.000000	-5.319009	-1.098584
H	0.000000	-5.319009	1.098584
Cl	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Br)(Se_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E= -46579.1583471 a. u.

Cu	1.640066	1.640066	1.640066
Cu	-1.640066	1.640066	1.640066
Cu	-1.640066	1.640066	-1.640066
Cu	1.640066	1.640066	-1.640066
Cu	1.640066	-1.640066	1.640066
Cu	-1.640066	-1.640066	1.640066
Cu	-1.640066	-1.640066	-1.640066
Cu	1.640066	-1.640066	-1.640066
Se	1.975293	3.389143	0.000000
Se	0.000000	1.975293	3.389143
Se	-1.975293	3.389143	0.000000
Se	0.000000	1.975293	-3.389143
Se	1.975293	-3.389143	0.000000
Se	0.000000	-1.975293	3.389143
Se	-1.975293	-3.389143	0.000000
Se	0.000000	-1.975293	-3.389143
Se	3.389143	0.000000	1.975293
Se	-3.389143	0.000000	1.975293
Se	-3.389143	0.000000	-1.975293
Se	3.389143	0.000000	-1.975293
P	4.418909	0.000000	0.000000
P	0.000000	0.000000	4.418909
P	-4.418909	0.000000	0.000000
P	0.000000	0.000000	-4.418909
P	0.000000	4.418909	0.000000
P	0.000000	-4.418909	0.000000
H	5.315441	-1.099296	0.000000
H	5.315441	1.099296	0.000000
H	-1.099296	0.000000	5.315441
H	1.099296	0.000000	5.315441
H	-5.315441	-1.099296	0.000000
H	-5.315441	1.099296	0.000000
H	1.099296	0.000000	-5.315441
H	-1.099296	0.000000	-5.315441
H	0.000000	5.315441	1.099296
H	0.000000	5.315441	-1.099296
H	0.000000	-5.315441	-1.099296
H	0.000000	-5.315441	1.099296
Br	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(O)(Se_2PH_2)_6]$ (*T*)
BP86/Def2TZVP
E= -44080.1217198 a. u.

Cu	1.165380	1.165380	1.165380
Cu	-1.590244	1.590244	1.590244
Cu	-1.165380	1.165380	-1.165380
Cu	1.590244	1.590244	-1.590244
Cu	1.590244	-1.590244	1.590244
Cu	-1.165380	-1.165380	1.165380
Cu	-1.590244	-1.590244	-1.590244
Cu	1.165380	-1.165380	-1.165380
Se	1.929043	3.324395	0.068778
Se	0.068778	1.929043	3.324395
Se	-1.929043	3.324395	-0.068778
Se	-0.068778	1.929043	-3.324395
Se	1.929043	-3.324395	-0.068778
Se	-0.068778	-1.929043	3.324395
Se	-1.929043	-3.324395	0.068778
Se	0.068778	-1.929043	-3.324395
Se	3.324395	0.068778	1.929043
Se	-3.324395	-0.068778	1.929043
Se	-3.324395	0.068778	-1.929043
Se	3.324395	-0.068778	-1.929043
P	4.395951	0.000000	0.000000
P	0.000000	0.000000	4.395951
P	-4.395951	0.000000	0.000000
P	0.000000	0.000000	-4.395951
P	0.000000	4.395951	0.000000
P	0.000000	-4.395951	0.000000
H	5.306039	-1.091218	0.003645
H	5.306039	1.091218	-0.003645
H	-1.091218	0.003645	5.306039
H	1.091218	-0.003645	5.306039
H	-5.306039	-1.091218	-0.003645
H	-5.306039	1.091218	0.003645
H	1.091218	0.003645	-5.306039
H	-1.091218	-0.003645	-5.306039
H	-0.003645	5.306039	1.091218
H	0.003645	5.306039	-1.091218
H	-0.003645	-5.306039	-1.091218
H	0.003645	-5.306039	1.091218
O	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(S)(Se_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E= -44403.1774496 a. u.

Cu	1.421279	1.421279	1.421279
Cu	-1.421279	1.421279	1.421279
Cu	-1.421279	1.421279	-1.421279
Cu	1.421279	1.421279	-1.421279
Cu	1.421279	-1.421279	1.421279
Cu	-1.421279	-1.421279	1.421279
Cu	-1.421279	-1.421279	-1.421279
Cu	1.421279	-1.421279	-1.421279
Se	1.954855	3.388963	0.000000
Se	0.000000	1.954855	3.388963
Se	-1.954855	3.388963	0.000000
Se	0.000000	1.954855	-3.388963
Se	1.954855	-3.388963	0.000000
Se	0.000000	-1.954855	3.388963
Se	-1.954855	-3.388963	0.000000
Se	0.000000	-1.954855	-3.388963
Se	3.388963	0.000000	1.954855
Se	-3.388963	0.000000	1.954855
Se	-3.388963	0.000000	-1.954855
Se	3.388963	0.000000	-1.954855
P	4.417934	0.000000	0.000000
P	0.000000	0.000000	4.417934
P	-4.417934	0.000000	0.000000
P	0.000000	0.000000	-4.417934
P	0.000000	4.417934	0.000000
P	0.000000	-4.417934	0.000000
H	5.326511	-1.091728	0.000000
H	5.326511	1.091728	0.000000
H	-1.091728	0.000000	5.326511
H	1.091728	0.000000	5.326511
H	-5.326511	-1.091728	0.000000
H	-5.326511	1.091728	0.000000
H	1.091728	0.000000	-5.326511
H	-1.091728	0.000000	-5.326511
H	0.000000	5.326511	1.091728
H	0.000000	5.326511	-1.091728
H	0.000000	-5.326511	-1.091728
H	0.000000	-5.326511	1.091728
S	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(Se)(Se_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E= -46406.7619882 a. u.

Cu	1.481394	1.481394	1.481394
Cu	1.481394	1.481394	-1.481394
Cu	1.481394	-1.481394	-1.481394
Cu	1.481394	-1.481394	1.481394
Cu	-1.481394	1.481394	1.481394
Cu	-1.481394	1.481394	-1.481394
Cu	-1.481394	-1.481394	-1.481394
Cu	-1.481394	-1.481394	1.481394
Se	3.409233	0.000000	1.970153
Se	1.970153	3.409233	0.000000
Se	3.409233	0.000000	-1.970153
Se	1.970153	-3.409233	0.000000
Se	-3.409233	0.000000	1.970153
Se	-1.970153	3.409233	0.000000
Se	-3.409233	0.000000	-1.970153
Se	-1.970153	-3.409233	0.000000
Se	0.000000	1.970153	3.409233
Se	0.000000	1.970153	-3.409233
Se	0.000000	-1.970153	-3.409233
Se	0.000000	-1.970153	3.409233
P	0.000000	0.000000	4.418972
P	0.000000	4.418972	0.000000
P	0.000000	0.000000	-4.418972
P	0.000000	-4.418972	0.000000
P	4.418972	0.000000	0.000000
P	-4.418972	0.000000	0.000000
H	-1.093064	0.000000	5.325208
H	1.093064	0.000000	5.325208
H	0.000000	5.325208	-1.093064
H	0.000000	5.325208	1.093064
H	-1.093064	0.000000	-5.325208
H	1.093064	0.000000	-5.325208
H	0.000000	-5.325208	1.093064
H	0.000000	-5.325208	-1.093064
H	5.325208	1.093064	0.000000
H	5.325208	-1.093064	0.000000
H	-5.325208	-1.093064	0.000000
H	-5.325208	1.093064	0.000000
Se	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(N)(Se_2PH_2)_6]^-$ (S_6)
BP86/Def2TZVP
E= -44059.6833988 a. u.

Cu	0.000000	0.000000	3.245047
Cu	0.752070	1.396264	1.166055
Cu	1.585235	0.046821	-1.166055
Cu	0.833165	-1.349444	1.166055
Cu	-1.585235	-0.046821	1.166055
Cu	-0.833165	1.349444	-1.166055
Cu	0.000000	0.000000	-3.245047
Cu	-0.752070	-1.396264	-1.166055
Se	2.142192	-1.201766	3.284537
Se	-0.030336	2.456076	3.284537
Se	3.247331	1.874847	1.246306
Se	3.247331	-1.874848	-1.246306
Se	-3.247331	-1.874847	-1.246306
Se	-3.247331	1.874848	1.246306
Se	-2.142192	1.201766	-3.284537
Se	0.030336	-2.456076	-3.284537
Se	-2.111856	-1.254310	3.284537
Se	0.000000	3.749695	-1.246306
Se	2.111856	1.254310	-3.284537
Se	0.000000	-3.749695	1.246306
P	-1.205061	-3.287758	2.973622
P	-2.244751	2.687492	2.973622
P	1.205061	3.287758	-2.973622
P	2.244751	-2.687492	-2.973622
P	3.449812	0.600265	2.973622
P	-3.449812	-0.600265	-2.973622
H	-2.288536	-4.204803	3.076464
H	-0.517157	-3.595633	4.181411
H	-2.497199	4.084332	3.076464
H	-2.855331	2.245688	4.181411
H	0.517157	3.595633	-4.181411
H	2.288536	4.204803	-3.076464
H	2.497199	-4.084332	-3.076464
H	2.855331	-2.245688	-4.181411
H	3.372488	1.349946	4.181411
H	4.785734	0.120472	3.076464
H	-3.372488	-1.349946	-4.181411
H	-4.785734	-0.120472	-3.076464
N	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(N)(Se_2PH_2)_6]^-$ (C_3)
BP86/Def2TZVP
E= -44059.6830092 a. u.

Cu	0.000000	0.000000	3.057880
Cu	-1.341406	0.741125	0.963576
Cu	0.000000	2.122860	-0.810930
Cu	1.312537	0.791129	0.963576
Cu	0.028870	-1.532255	0.963576
Cu	-1.838450	-1.061430	-0.810930
Cu	0.000000	0.000000	-2.463248
Cu	1.838450	-1.061430	-0.810930
Se	1.395384	2.010272	3.112809
Se	-2.438639	0.203302	3.112809
Se	-1.467980	3.405621	0.865798
Se	2.300702	3.066410	-0.989912
Se	1.505238	-3.525671	-0.989912
Se	-2.215365	-2.974118	0.865798
Se	-1.374571	-2.033985	-3.102073
Se	2.448768	-0.173421	-3.102073
Se	1.043255	-2.213574	3.112809
Se	-3.805940	0.459261	-0.989912
Se	-1.074197	2.207406	-3.102073
Se	3.683344	-0.431503	0.865798
P	3.169827	-1.731557	2.533928
P	-3.084486	-1.879372	2.533928
P	-3.100502	1.363138	-2.834387
P	2.730764	2.003544	-2.834387
P	-0.085341	3.610930	2.533928
P	0.369738	-3.366683	-2.834387
H	3.791291	-3.001243	2.382418
H	3.838315	-1.276993	3.704925
H	-4.494798	-1.782733	2.382418
H	-3.025066	-2.685582	3.704925
H	-3.292657	0.454165	-3.911752
H	-4.018680	2.385019	-3.206940
H	4.074827	2.287770	-3.206940
H	2.039647	2.624442	-3.911752
H	-0.813249	3.962575	3.704925
H	0.703507	4.783976	2.382418
H	1.253010	-3.078607	-3.911752
H	-0.056147	-4.672789	-3.206940
N	0.000000	0.000000	-0.335041

Computed optimized structure of $[Cu_8(P)(Se_2PH_2)_6]^-$ (T_h)
BP86/Def2TZVP
E= -44346.3897331 a. u.

Cu	1.363130	1.363130	1.363130
Cu	1.363130	1.363130	-1.363130
Cu	1.363130	-1.363130	-1.363130
Cu	1.363130	-1.363130	1.363130
Cu	-1.363130	1.363130	1.363130
Cu	-1.363130	1.363130	-1.363130
Cu	-1.363130	-1.363130	-1.363130
Cu	-1.363130	-1.363130	1.363130
Se	3.428563	0.000000	1.980824
Se	1.980824	3.428563	0.000000
Se	3.428563	0.000000	-1.980824
Se	1.980824	-3.428563	0.000000
Se	-3.428563	0.000000	1.980824
Se	-1.980824	3.428563	0.000000
Se	-3.428563	0.000000	-1.980824
Se	-1.980824	-3.428563	0.000000
Se	0.000000	1.980824	3.428563
Se	0.000000	1.980824	-3.428563
Se	0.000000	-1.980824	-3.428563
Se	0.000000	-1.980824	3.428563
P	0.000000	0.000000	4.412545
P	0.000000	4.412545	0.000000
P	0.000000	0.000000	-4.412545
P	0.000000	-4.412545	0.000000
P	4.412545	0.000000	0.000000
P	-4.412545	0.000000	0.000000
H	-1.087582	0.000000	5.327421
H	1.087582	0.000000	5.327421
H	0.000000	5.327421	-1.087582
H	0.000000	5.327421	1.087582
H	-1.087582	0.000000	-5.327421
H	1.087582	0.000000	-5.327421
H	0.000000	-5.327421	1.087582
H	0.000000	-5.327421	-1.087582
H	5.327421	1.087582	0.000000
H	5.327421	-1.087582	0.000000
H	-5.327421	-1.087582	0.000000
H	-5.327421	1.087582	0.000000
P	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_8(C)(Se_2PH_2)_6]^{2-}$ (S_6)
BP86/Def2TZVP
E=-44043.0139878 a. u.

Cu	0.000000	0.000000	-3.308876
Cu	1.390765	0.801728	-1.054907
Cu	0.001066	1.605302	1.054907
Cu	-1.389700	0.803574	-1.054907
Cu	-0.001066	-1.605302	-1.054907
Cu	1.389700	-0.803574	1.054907
Cu	0.000000	0.000000	3.308876
Cu	-1.390765	-0.801728	1.054907
Se	0.411357	2.297107	-4.287575
Se	1.783675	-1.504799	-4.287575
Se	3.273878	2.035497	-1.835099
Se	-0.125853	3.853010	1.835099
Se	-3.273878	-2.035497	1.835099
Se	0.125853	-3.853010	-1.835099
Se	-0.411357	-2.297107	4.287575
Se	-1.783675	1.504799	4.287575
Se	-2.195032	-0.792308	-4.287575
Se	3.399731	-1.817513	1.835099
Se	2.195032	0.792308	4.287575
Se	-3.399731	1.817513	-1.835099
P	-3.096291	1.134687	-3.884869
P	0.565478	-3.248810	-3.884869
P	3.096291	-1.134687	3.884869
P	-0.565478	3.248810	3.884869
P	2.530813	2.114123	-3.884869
P	-2.530813	-2.114123	3.884869
H	-4.346380	1.222988	-4.571709
H	-2.374569	2.131348	-4.603753
H	1.114051	-4.375570	-4.571709
H	-0.658517	-3.122111	-4.603753
H	2.374569	-2.131348	4.603753
H	4.346380	-1.222988	4.571709
H	-1.114051	4.375570	4.571709
H	0.658517	3.122111	4.603753
H	3.033086	0.990763	-4.603753
H	3.232329	3.152581	-4.571709
H	-3.033086	-0.990763	4.603753
H	-3.232329	-3.152581	4.571709
C	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(\square)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -48438.8527471 a. u.

Ag	1.764391	1.764391	1.764391
Ag	1.764391	1.764391	-1.764391
Ag	1.764391	-1.764391	-1.764391
Ag	1.764391	-1.764391	1.764391
Ag	-1.764391	1.764391	1.764391
Ag	-1.764391	1.764391	-1.764391
Ag	-1.764391	-1.764391	-1.764391
Ag	-1.764391	-1.764391	1.764391
S	3.618444	0.000000	1.806981
S	1.806981	3.618444	0.000000
S	3.618444	0.000000	-1.806981
S	1.806981	-3.618444	0.000000
S	-3.618444	0.000000	1.806981
S	-1.806981	3.618444	0.000000
S	-3.618444	0.000000	-1.806981
S	-1.806981	-3.618444	0.000000
S	0.000000	1.806981	3.618444
S	0.000000	1.806981	-3.618444
S	0.000000	-1.806981	-3.618444
S	0.000000	-1.806981	3.618444
P	0.000000	0.000000	4.574952
P	0.000000	4.574952	0.000000
P	0.000000	0.000000	-4.574952
P	0.000000	-4.574952	0.000000
P	4.574952	0.000000	0.000000
P	-4.574952	0.000000	0.000000
H	-1.109382	0.000000	5.454212
H	1.109382	0.000000	5.454212
H	0.000000	5.454212	-1.109382
H	0.000000	5.454212	1.109382
H	-1.109382	0.000000	-5.454212
H	1.109382	0.000000	-5.454212
H	0.000000	-5.454212	1.109382
H	0.000000	-5.454212	-1.109382
H	5.454212	1.109382	0.000000
H	5.454212	-1.109382	0.000000
H	-5.454212	-1.109382	0.000000
H	-5.454212	1.109382	0.000000

Computed optimized structure of $[Ag_8(H)(S_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E= -48439.7510450 a. u.

Ag	1.154711	1.154711	1.154711
Ag	1.817732	-1.817732	1.817732
Ag	-1.154711	-1.154711	1.154711
Ag	-1.817732	1.817732	1.817732
Ag	1.817732	1.817732	-1.817732
Ag	1.154711	-1.154711	-1.154711
Ag	-1.817732	-1.817732	-1.817732
Ag	-1.154711	1.154711	-1.154711
S	0.103204	1.790238	3.559612
S	3.559612	0.103204	1.790238
S	-0.103204	-1.790238	3.559612
S	-3.559612	-0.103204	1.790238
S	-0.103204	1.790238	-3.559612
S	3.559612	-0.103204	-1.790238
S	0.103204	-1.790238	-3.559612
S	-3.559612	0.103204	-1.790238
S	1.790238	3.559612	0.103204
S	1.790238	-3.559612	-0.103204
S	-1.790238	-3.559612	0.103204
S	-1.790238	3.559612	-0.103204
P	0.000000	4.523898	0.000000
P	4.523898	0.000000	0.000000
P	0.000000	-4.523898	0.000000
P	-4.523898	0.000000	0.000000
P	0.000000	0.000000	4.523898
P	0.000000	0.000000	-4.523898
H	0.034527	5.415631	-1.100784
H	-0.034527	5.415631	1.100784
H	5.415631	-1.100784	0.034527
H	5.415631	1.100784	-0.034527
H	-0.034527	-5.415631	-1.100784
H	0.034527	-5.415631	1.100784
H	-5.415631	1.100784	0.034527
H	-5.415631	-1.100784	-0.034527
H	1.100784	-0.034527	5.415631
H	-1.100784	0.034527	5.415631
H	-1.100784	-0.034527	-5.415631
H	1.100784	0.034527	-5.415631
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(F)(S_2PH_2)_6]^{2+}$ (*T*)
BP86/Def2TZVP
E= -48539.0752369 a. u.

Ag	1.475957	1.475957	1.475957
Ag	1.737284	-1.737284	1.737284
Ag	-1.475957	-1.475957	1.475957
Ag	-1.737284	1.737284	1.737284
Ag	1.737284	1.737284	-1.737284
Ag	1.475957	-1.475957	-1.475957
Ag	-1.737284	-1.737284	-1.737284
Ag	-1.475957	1.475957	-1.475957
S	0.021124	1.800185	3.623397
S	3.623397	0.021124	1.800185
S	-0.021124	-1.800185	3.623397
S	-3.623397	-0.021124	1.800185
S	-0.021124	1.800185	-3.623397
S	3.623397	-0.021124	-1.800185
S	0.021124	-1.800185	-3.623397
S	-3.623397	0.021124	-1.800185
S	1.800185	3.623397	0.021124
S	1.800185	-3.623397	-0.021124
S	-1.800185	-3.623397	0.021124
S	-1.800185	3.623397	-0.021124
P	0.000000	4.573396	0.000000
P	4.573396	0.000000	0.000000
P	0.000000	-4.573396	0.000000
P	-4.573396	0.000000	0.000000
P	0.000000	0.000000	4.573396
P	0.000000	0.000000	-4.573396
H	-0.000433	5.464263	-1.102078
H	0.000433	5.464263	1.102078
H	5.464263	-1.102078	-0.000433
H	5.464263	1.102078	0.000433
H	0.000433	-5.464263	-1.102078
H	-0.000433	-5.464263	1.102078
H	-5.464263	1.102078	-0.000433
H	-5.464263	-1.102078	0.000433
H	1.102078	0.000433	5.464263
H	-1.102078	-0.000433	5.464263
H	-1.102078	0.000433	-5.464263
H	1.102078	-0.000433	-5.464263
F	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Cl)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -48899.4684809 a. u.

Ag	1.710789	1.710789	1.710789
Ag	-1.710789	1.710789	1.710789
Ag	-1.710789	1.710789	-1.710789
Ag	1.710789	1.710789	-1.710789
Ag	1.710789	-1.710789	1.710789
Ag	-1.710789	-1.710789	1.710789
Ag	-1.710789	-1.710789	-1.710789
Ag	1.710789	-1.710789	-1.710789
S	1.812366	3.664389	0.000000
S	0.000000	1.812366	3.664389
S	-1.812366	3.664389	0.000000
S	0.000000	1.812366	-3.664389
S	1.812366	-3.664389	0.000000
S	0.000000	-1.812366	3.664389
S	-1.812366	-3.664389	0.000000
S	0.000000	-1.812366	-3.664389
S	3.664389	0.000000	1.812366
S	-3.664389	0.000000	1.812366
S	-3.664389	0.000000	-1.812366
S	3.664389	0.000000	-1.812366
P	4.595675	0.000000	0.000000
P	0.000000	0.000000	4.595675
P	-4.595675	0.000000	0.000000
P	0.000000	0.000000	-4.595675
P	0.000000	4.595675	0.000000
P	0.000000	-4.595675	0.000000
H	5.484556	-1.103338	0.000000
H	5.484556	1.103338	0.000000
H	-1.103338	0.000000	5.484556
H	1.103338	0.000000	5.484556
H	-5.484556	-1.103338	0.000000
H	-5.484556	1.103338	0.000000
H	1.103338	0.000000	-5.484556
H	-1.103338	0.000000	-5.484556
H	0.000000	5.484556	1.103338
H	0.000000	5.484556	-1.103338
H	0.000000	-5.484556	-1.103338
H	0.000000	-5.484556	1.103338
Cl	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Br)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -51013.6424889 a. u.

Ag	1.744921	1.744921	1.744921
Ag	1.744921	1.744921	-1.744921
Ag	1.744921	-1.744921	-1.744921
Ag	1.744921	-1.744921	1.744921
Ag	-1.744921	1.744921	1.744921
Ag	-1.744921	1.744921	-1.744921
Ag	-1.744921	-1.744921	-1.744921
Ag	-1.744921	-1.744921	1.744921
S	3.679301	0.000000	1.817096
S	1.817096	3.679301	0.000000
S	3.679301	0.000000	-1.817096
S	1.817096	-3.679301	0.000000
S	-3.679301	0.000000	1.817096
S	-1.817096	3.679301	0.000000
S	-3.679301	0.000000	-1.817096
S	-1.817096	-3.679301	0.000000
S	0.000000	1.817096	3.679301
S	0.000000	1.817096	-3.679301
S	0.000000	-1.817096	-3.679301
S	0.000000	-1.817096	3.679301
P	0.000000	0.000000	4.603252
P	0.000000	4.603252	0.000000
P	0.000000	0.000000	-4.603252
P	0.000000	-4.603252	0.000000
P	4.603252	0.000000	0.000000
P	-4.603252	0.000000	0.000000
H	-1.103736	0.000000	5.491440
H	1.103736	0.000000	5.491440
H	0.000000	5.491440	-1.103736
H	0.000000	5.491440	1.103736
H	-1.103736	0.000000	-5.491440
H	1.103736	0.000000	-5.491440
H	0.000000	-5.491440	1.103736
H	0.000000	-5.491440	-1.103736
H	5.491440	1.103736	0.000000
H	5.491440	-1.103736	0.000000
H	-5.491440	-1.103736	0.000000
H	-5.491440	1.103736	0.000000
Br	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(O)(S_2PH_2)_6]^{2+}$ (*T*)
BP86/Def2TZVP
E= -48514.5859741 a. u.

Ag	1.359998	1.359998	1.359998
Ag	1.651374	-1.651374	1.651374
Ag	-1.359998	-1.359998	1.359998
Ag	-1.651374	1.651374	1.651374
Ag	1.651374	1.651374	-1.651374
Ag	1.359998	-1.359998	-1.359998
Ag	-1.651374	-1.651374	-1.651374
Ag	-1.359998	1.359998	-1.359998
S	0.033907	1.800223	3.656253
S	3.656253	0.033907	1.800223
S	-0.033907	-1.800223	3.656253
S	-3.656253	-0.033907	1.800223
S	-0.033907	1.800223	-3.656253
S	3.656253	-0.033907	-1.800223
S	0.033907	-1.800223	-3.656253
S	-3.656253	0.033907	-1.800223
S	1.800223	3.656253	0.033907
S	1.800223	-3.656253	-0.033907
S	-1.800223	-3.656253	0.033907
S	-1.800223	3.656253	-0.033907
P	0.000000	4.589786	0.000000
P	4.589786	0.000000	0.000000
P	0.000000	-4.589786	0.000000
P	-4.589786	0.000000	0.000000
P	0.000000	0.000000	4.589786
P	0.000000	0.000000	-4.589786
H	0.003204	5.491960	-1.095756
H	-0.003204	5.491960	1.095756
H	5.491960	-1.095756	0.003204
H	5.491960	1.095756	-0.003204
H	-0.003204	-5.491960	-1.095756
H	0.003204	-5.491960	1.095756
H	-5.491960	1.095756	0.003204
H	-5.491960	-1.095756	-0.003204
H	1.095756	-0.003204	5.491960
H	-1.095756	0.003204	5.491960
H	-1.095756	-0.003204	-5.491960
H	1.095756	0.003204	-5.491960
O	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(S)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -48837.6482363 a. u.

Ag	1.582623	1.582623	1.582623
Ag	-1.582623	1.582623	1.582623
Ag	-1.582623	1.582623	-1.582623
Ag	1.582623	1.582623	-1.582623
Ag	1.582623	-1.582623	1.582623
Ag	-1.582623	-1.582623	1.582623
Ag	-1.582623	-1.582623	-1.582623
Ag	1.582623	-1.582623	-1.582623
S	1.812461	3.721245	0.000000
S	0.000000	1.812461	3.721245
S	-1.812461	3.721245	0.000000
S	0.000000	1.812461	-3.721245
S	1.812461	-3.721245	0.000000
S	0.000000	-1.812461	3.721245
S	-1.812461	-3.721245	0.000000
S	0.000000	-1.812461	-3.721245
S	3.721245	0.000000	1.812461
S	-3.721245	0.000000	1.812461
S	-3.721245	0.000000	-1.812461
S	3.721245	0.000000	-1.812461
P	4.636451	0.000000	0.000000
P	0.000000	0.000000	4.636451
P	-4.636451	0.000000	0.000000
P	0.000000	0.000000	-4.636451
P	0.000000	4.636451	0.000000
P	0.000000	-4.636451	0.000000
H	5.536605	-1.096925	0.000000
H	5.536605	1.096925	0.000000
H	-1.096925	0.000000	5.536605
H	1.096925	0.000000	5.536605
H	-5.536605	-1.096925	0.000000
H	-5.536605	1.096925	0.000000
H	1.096925	0.000000	-5.536605
H	-1.096925	0.000000	-5.536605
H	0.000000	5.536605	1.096925
H	0.000000	5.536605	-1.096925
H	0.000000	-5.536605	-1.096925
H	0.000000	-5.536605	1.096925
S	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Se)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -50841.2405264 a. u.

Ag	1.621442	1.621442	1.621442
Ag	-1.621442	1.621442	1.621442
Ag	-1.621442	1.621442	-1.621442
Ag	1.621442	1.621442	-1.621442
Ag	1.621442	-1.621442	1.621442
Ag	-1.621442	-1.621442	1.621442
Ag	-1.621442	-1.621442	-1.621442
Ag	1.621442	-1.621442	-1.621442
S	1.817752	3.742205	0.000000
S	0.000000	1.817752	3.742205
S	-1.817752	3.742205	0.000000
S	0.000000	1.817752	-3.742205
S	1.817752	-3.742205	0.000000
S	0.000000	-1.817752	3.742205
S	-1.817752	-3.742205	0.000000
S	0.000000	-1.817752	-3.742205
S	3.742205	0.000000	1.817752
S	-3.742205	0.000000	1.817752
S	-3.742205	0.000000	-1.817752
S	3.742205	0.000000	-1.817752
P	4.649630	0.000000	0.000000
P	0.000000	0.000000	4.649630
P	-4.649630	0.000000	0.000000
P	0.000000	0.000000	-4.649630
P	0.000000	4.649630	0.000000
P	0.000000	-4.649630	0.000000
H	5.548976	-1.097384	0.000000
H	5.548976	1.097384	0.000000
H	-1.097384	0.000000	5.548976
H	1.097384	0.000000	5.548976
H	-5.548976	-1.097384	0.000000
H	-5.548976	1.097384	0.000000
H	1.097384	0.000000	-5.548976
H	-1.097384	0.000000	-5.548976
H	0.000000	5.548976	1.097384
H	0.000000	5.548976	-1.097384
H	0.000000	-5.548976	-1.097384
H	0.000000	-5.548976	1.097384
Se	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(N)(S_2PH_2)_6]^{2+}$ (S_6)
BP86/Def2TZVP
E= -48494.1651034 a. u.

Ag	0.000000	0.000000	3.780423
Ag	-0.033889	1.823762	1.233804
Ag	1.562480	0.941230	-1.233804
Ag	1.596369	-0.882532	1.233804
Ag	-1.562480	-0.941230	1.233804
Ag	-1.596369	0.882532	-1.233804
Ag	0.000000	0.000000	-3.780423
Ag	0.033889	-1.823762	-1.233804
S	1.742656	1.837647	4.408712
S	-2.462777	0.590361	4.408712
S	0.000000	4.042832	2.296979
S	3.501195	2.021416	-2.296979
S	0.000000	-4.042832	-2.296979
S	-3.501195	-2.021416	2.296979
S	-1.742656	-1.837647	-4.408712
S	2.462777	-0.590361	-4.408712
S	0.720121	-2.428008	4.408712
S	-3.501195	2.021416	-2.296979
S	-0.720121	2.428008	-4.408712
S	3.501195	-2.021416	2.296979
P	2.688734	-2.126350	4.149387
P	-3.185840	-1.265337	4.149387
P	-2.688734	2.126350	-4.149387
P	3.185840	1.265337	-4.149387
P	0.497107	3.391687	4.149387
P	-0.497107	-3.391687	-4.149387
H	3.397110	-3.153651	4.833356
H	3.101684	-0.991347	4.901294
H	-4.429697	-1.365158	4.833356
H	-2.409374	-2.190464	4.901294
H	-3.101684	0.991347	-4.901294
H	-3.397110	3.153651	-4.833356
H	4.429697	1.365158	-4.833356
H	2.409374	2.190464	-4.901294
H	-0.692310	3.181811	4.901294
H	1.032587	4.518809	4.833356
H	0.692310	-3.181811	-4.901294
H	-1.032587	-4.518809	-4.833356
N	0.000000	0.000000	0.000000
XX	0.192897	0.552268	-0.811043

Computed optimized structure of $[Ag_8(N)(S_2PH_2)_6]^{2+}$ (C_3)
BP86/Def2TZVP
E= -48494.1290515 a. u.

Ag	0.000000	0.000000	3.279436
Ag	-1.822553	0.000000	0.950935
Ag	-1.188772	2.094331	-1.023581
Ag	0.911276	1.578377	0.950935
Ag	0.911276	-1.578377	0.950935
Ag	-1.219358	-2.076672	-1.023581
Ag	0.000000	0.000000	-2.886562
Ag	2.408130	-0.017659	-1.023581
S	0.104262	2.644573	3.276012
S	-2.342398	-1.231993	3.276012
S	-2.872474	2.614837	1.232266
S	0.823956	3.849505	-1.186038
S	2.921791	-2.638319	-1.186038
S	-0.828278	-3.795054	1.232266
S	0.024145	-2.670417	-3.326507
S	2.300576	1.356119	-3.326507
S	2.238136	-1.412580	3.276012
S	-3.745747	-1.211186	-1.186038
S	-2.324721	1.314298	-3.326507
S	3.700752	1.180217	1.232266
P	3.742653	-0.120328	2.756834
P	-1.975534	-3.181069	2.756834
P	-3.732536	-0.073620	-2.841840
P	1.802511	3.269281	-2.841840
P	-1.767119	3.301397	2.756834
P	1.930025	-3.195661	-2.841840
H	4.889590	-0.950867	2.631462
H	4.077907	0.594732	3.940030
H	-3.268270	-3.759076	2.631462
H	-1.523901	-3.828937	3.940030
H	-3.856428	-0.914899	-3.982630
H	-4.982408	0.603453	-2.896130
H	3.013810	4.013165	-2.896130
H	1.135888	3.797214	-3.982630
H	-2.554007	3.234205	3.940030
H	-1.621320	4.709943	2.631462
H	2.720540	-2.882315	-3.982630
H	1.968598	-4.616618	-2.896130
N	0.000000	0.000000	-0.467169

Computed optimized structure of $[Ag_8(P)(S_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E= -48780.8423359 a. u.

Ag	1.525553	1.525553	1.525553
Ag	1.526013	-1.526013	1.526013
Ag	-1.525553	-1.525553	1.525553
Ag	-1.526013	1.526013	1.526013
Ag	1.526013	1.526013	-1.526013
Ag	1.525553	-1.525553	-1.525553
Ag	-1.526013	-1.526013	-1.526013
Ag	-1.525553	1.525553	-1.525553
S	0.000057	1.818255	3.810952
S	3.810952	0.000057	1.818255
S	-0.000057	-1.818255	3.810952
S	-3.810952	-0.000057	1.818255
S	-0.000057	1.818255	-3.810952
S	3.810952	-0.000057	-1.818255
S	0.000057	-1.818255	-3.810952
S	-3.810952	0.000057	-1.818255
S	1.818255	3.810952	0.000057
S	1.818255	-3.810952	-0.000057
S	-1.818255	-3.810952	0.000057
S	-1.818255	3.810952	-0.000057
P	0.000000	4.704870	0.000000
P	4.704870	0.000000	0.000000
P	0.000000	-4.704870	0.000000
P	-4.704870	0.000000	0.000000
P	0.000000	0.000000	4.704870
P	0.000000	0.000000	-4.704870
H	0.000011	5.615570	-1.091588
H	-0.000011	5.615570	1.091588
H	5.615570	-1.091588	0.000011
H	5.615570	1.091588	-0.000011
H	-0.000011	-5.615570	-1.091588
H	0.000011	-5.615570	1.091588
H	-5.615570	1.091588	0.000011
H	-5.615570	-1.091588	-0.000011
H	1.091588	-0.000011	5.615570
H	-1.091588	0.000011	5.615570
H	-1.091588	-0.000011	-5.615570
H	1.091588	0.000011	-5.615570
P	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(C)(S_2PH_2)_6]^{2+}$ (S_6)
BP86/Def2TZVP
E= -48477.4823739 a. u.

Ag	0.000000	0.000000	3.684875
Ag	1.536749	0.977816	1.207274
Ag	1.615188	-0.841956	-1.207274
Ag	0.078439	-1.819772	1.207274
Ag	-1.615188	0.841956	1.207274
Ag	-0.078439	1.819772	-1.207274
Ag	0.000000	0.000000	-3.684875
Ag	-1.536749	-0.977816	-1.207274
S	2.430930	-0.072964	4.813558
S	-1.152276	2.141729	4.813558
S	3.447494	2.173302	2.296057
S	3.605882	-1.898966	-2.296057
S	-3.447494	-2.173302	-2.296057
S	-3.605882	1.898966	2.296057
S	-2.430930	0.072964	-4.813558
S	1.152276	-2.141729	-4.813558
S	-1.278654	-2.068765	4.813558
S	-0.158388	4.072269	-2.296057
S	1.278654	2.068765	-4.813558
S	0.158388	-4.072269	2.296057
P	0.045942	-3.445828	4.214571
P	-3.007146	1.683127	4.214571
P	-0.045942	3.445828	-4.214571
P	3.007146	-1.683127	-4.214571
P	2.961204	1.762701	4.214571
P	-2.961204	-1.762701	-4.214571
H	-0.138054	-4.622124	5.001165
H	1.348285	-3.069437	4.649415
H	-3.933850	2.430620	5.001165
H	-3.332353	0.367069	4.649415
H	-1.348285	3.069437	-4.649415
H	0.138054	4.622124	-5.001165
H	3.933850	-2.430620	-5.001165
H	3.332353	-0.367069	-4.649415
H	1.984067	2.702368	4.649415
H	4.071903	2.191504	5.001165
H	-1.984067	-2.702368	-4.649415
H	-4.071903	-2.191504	-5.001165
C	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(\square)(Se_2PH_2)_6]^{2+}$ (T_h)
BP86/Def2TZVP
E = -72481.9035453 a. u.

Ag	1.809103	1.809103	1.809103
Ag	1.809103	1.809103	-1.809103
Ag	1.809103	-1.809103	-1.809103
Ag	1.809103	-1.809103	1.809103
Ag	-1.809103	1.809103	1.809103
Ag	-1.809103	1.809103	-1.809103
Ag	-1.809103	-1.809103	-1.809103
Ag	-1.809103	-1.809103	1.809103
Se	3.756900	0.000000	1.970242
Se	1.970242	3.756900	0.000000
Se	3.756900	0.000000	-1.970242
Se	1.970242	-3.756900	0.000000
Se	-3.756900	0.000000	1.970242
Se	-1.970242	3.756900	0.000000
Se	-3.756900	0.000000	-1.970242
Se	-1.970242	-3.756900	0.000000
Se	0.000000	1.970242	3.756900
Se	0.000000	1.970242	-3.756900
Se	0.000000	-1.970242	-3.756900
Se	0.000000	-1.970242	3.756900
P	0.000000	0.000000	4.759605
P	0.000000	4.759605	0.000000
P	0.000000	0.000000	-4.759605
P	0.000000	-4.759605	0.000000
P	4.759605	0.000000	0.000000
P	-4.759605	0.000000	0.000000
H	-1.101830	0.000000	5.649381
H	1.101830	0.000000	5.649381
H	0.000000	5.649381	-1.101830
H	0.000000	5.649381	1.101830
H	-1.101830	0.000000	-5.649381
H	1.101830	0.000000	-5.649381
H	0.000000	-5.649381	1.101830
H	0.000000	-5.649381	-1.101830
H	5.649381	1.101830	0.000000
H	5.649381	-1.101830	0.000000
H	-5.649381	-1.101830	0.000000
H	-5.649381	1.101830	0.000000

Computed optimized structure of $[Ag_8(H)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E = -72482.8006685 a. u.

Ag	1.145243	1.145243	1.145243
Ag	1.841585	-1.841585	1.841585
Ag	-1.145243	-1.145243	1.145243
Ag	-1.841585	1.841585	1.841585
Ag	1.841585	1.841585	-1.841585
Ag	1.145243	-1.145243	-1.145243
Ag	-1.841585	-1.841585	-1.841585
Ag	-1.145243	1.145243	-1.145243
Se	0.154086	1.935197	3.651300
Se	3.651300	0.154086	1.935197
Se	-0.154086	-1.935197	3.651300
Se	-3.651300	-0.154086	1.935197
Se	-0.154086	1.935197	-3.651300
Se	3.651300	-0.154086	-1.935197
Se	0.154086	-1.935197	-3.651300
Se	-3.651300	0.154086	-1.935197
Se	1.935197	3.651300	0.154086
Se	1.935197	-3.651300	-0.154086
Se	-1.935197	-3.651300	0.154086
Se	-1.935197	3.651300	-0.154086
P	0.000000	4.687595	0.000000
P	4.687595	0.000000	0.000000
P	0.000000	-4.687595	0.000000
P	-4.687595	0.000000	0.000000
P	0.000000	0.000000	4.687595
P	0.000000	0.000000	-4.687595
H	0.051541	5.587449	-1.094091
H	-0.051541	5.587449	1.094091
H	5.587449	-1.094091	0.051541
H	5.587449	1.094091	-0.051541
H	-0.051541	-5.587449	-1.094091
H	0.051541	-5.587449	1.094091
H	-5.587449	1.094091	0.051541
H	-5.587449	-1.094091	-0.051541
H	1.094091	-0.051541	5.587449
H	-1.094091	0.051541	5.587449
H	-1.094091	-0.051541	-5.587449
H	1.094091	0.051541	-5.587449
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(F)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E = -72582.1181297 a. u.

Ag	1.462365	1.462365	1.462365
Ag	1.775345	-1.775345	1.775345
Ag	-1.462365	-1.462365	1.462365
Ag	-1.775345	1.775345	1.775345
Ag	1.775345	1.775345	-1.775345
Ag	1.462365	-1.462365	-1.462365
Ag	-1.775345	-1.775345	-1.775345
Ag	-1.462365	1.462365	-1.462365
Se	0.044588	1.954365	3.739229
Se	3.739229	0.044588	1.954365
Se	-0.044588	-1.954365	3.739229
Se	-3.739229	-0.044588	1.954365
Se	-0.044588	1.954365	-3.739229
Se	3.739229	-0.044588	-1.954365
Se	0.044588	-1.954365	-3.739229
Se	-3.739229	0.044588	-1.954365
Se	1.954365	3.739229	0.044588
Se	1.954365	-3.739229	-0.044588
Se	-1.954365	-3.739229	0.044588
Se	-1.954365	3.739229	-0.044588
P	0.000000	4.749348	0.000000
P	4.749348	0.000000	0.000000
P	0.000000	-4.749348	0.000000
P	-4.749348	0.000000	0.000000
P	0.000000	0.000000	4.749348
P	0.000000	0.000000	-4.749348
H	0.006618	5.649467	-1.095188
H	-0.006618	5.649467	1.095188
H	5.649467	-1.095188	0.006618
H	5.649467	1.095188	-0.006618
H	-0.006618	-5.649467	-1.095188
H	0.006618	-5.649467	1.095188
H	-5.649467	1.095188	0.006618
H	-5.649467	-1.095188	-0.006618
H	1.095188	-0.006618	5.649467
H	-1.095188	0.006618	5.649467
H	-1.095188	-0.006618	-5.649467
H	1.095188	0.006618	-5.649467
F	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Cl)(Se_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E = -72942.5151396 a. u.

Ag	1.721620	1.721620	1.721620
Ag	1.721620	1.721620	-1.721620
Ag	1.721620	-1.721620	-1.721620
Ag	1.721620	-1.721620	1.721620
Ag	-1.721620	1.721620	1.721620
Ag	-1.721620	1.721620	-1.721620
Ag	-1.721620	-1.721620	-1.721620
Ag	-1.721620	-1.721620	1.721620
Se	3.790253	0.000000	1.971947
Se	1.971947	3.790253	0.000000
Se	3.790253	0.000000	-1.971947
Se	1.971947	-3.790253	0.000000
Se	-3.790253	0.000000	1.971947
Se	-1.971947	3.790253	0.000000
Se	-3.790253	0.000000	-1.971947
Se	-1.971947	-3.790253	0.000000
Se	0.000000	1.971947	3.790253
Se	0.000000	1.971947	-3.790253
Se	0.000000	-1.971947	-3.790253
Se	0.000000	-1.971947	3.790253
P	0.000000	0.000000	4.773309
P	0.000000	4.773309	0.000000
P	0.000000	0.000000	-4.773309
P	0.000000	-4.773309	0.000000
P	4.773309	0.000000	0.000000
P	-4.773309	0.000000	0.000000
H	-1.096138	0.000000	5.671670
H	1.096138	0.000000	5.671670
H	0.000000	5.671670	-1.096138
H	0.000000	5.671670	1.096138
H	-1.096138	0.000000	-5.671670
H	1.096138	0.000000	-5.671670
H	0.000000	-5.671670	1.096138
H	0.000000	-5.671670	-1.096138
H	5.671670	1.096138	0.000000
H	5.671670	-1.096138	0.000000
H	-5.671670	-1.096138	0.000000
H	-5.671670	1.096138	0.000000
Cl	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Br)(Se_2PH_2)_6]^+$ (T_h)
BP86/Def2TZVP
E = -75056.6912847

Ag	1.759936	1.759936	1.759936
Ag	1.759936	1.759936	-1.759936
Ag	1.759936	-1.759936	-1.759936
Ag	1.759936	-1.759936	1.759936
Ag	-1.759936	1.759936	1.759936
Ag	-1.759936	1.759936	-1.759936
Ag	-1.759936	-1.759936	-1.759936
Ag	-1.759936	-1.759936	1.759936
Se	3.806297	0.000000	1.979282
Se	1.979282	3.806297	0.000000
Se	3.806297	0.000000	-1.979282
Se	1.979282	-3.806297	0.000000
Se	-3.806297	0.000000	1.979282
Se	-1.979282	3.806297	0.000000
Se	-3.806297	0.000000	-1.979282
Se	-1.979282	-3.806297	0.000000
Se	0.000000	1.979282	3.806297
Se	0.000000	1.979282	-3.806297
Se	0.000000	-1.979282	-3.806297
Se	0.000000	-1.979282	3.806297
P	0.000000	0.000000	4.777708
P	0.000000	4.777708	0.000000
P	0.000000	0.000000	-4.777708
P	0.000000	-4.777708	0.000000
P	4.777708	0.000000	0.000000
P	-4.777708	0.000000	0.000000
H	-1.096511	0.000000	5.675338
H	1.096511	0.000000	5.675338
H	0.000000	5.675338	-1.096511
H	0.000000	5.675338	1.096511
H	-1.096511	0.000000	-5.675338
H	1.096511	0.000000	-5.675338
H	0.000000	-5.675338	1.096511
H	0.000000	-5.675338	-1.096511
H	5.675338	1.096511	0.000000
H	5.675338	-1.096511	0.000000
H	-5.675338	-1.096511	0.000000
H	-5.675338	1.096511	0.000000
Br	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(O)(Se_2PH_2)_6]$ (*T*)
BP86/Def2TZVP
E = -72557.6425719

Ag	1.344496	1.344496	1.344496
Ag	1.693914	-1.693914	1.693914
Ag	-1.344496	-1.344496	1.344496
Ag	-1.693914	1.693914	1.693914
Ag	1.693914	1.693914	-1.693914
Ag	1.344496	-1.344496	-1.344496
Ag	-1.693914	-1.693914	-1.693914
Ag	-1.344496	1.344496	-1.344496
Se	0.064295	1.952931	3.758211
Se	3.758211	0.064295	1.952931
Se	-0.064295	-1.952931	3.758211
Se	-3.758211	-0.064295	1.952931
Se	-0.064295	1.952931	-3.758211
Se	3.758211	-0.064295	-1.952931
Se	0.064295	-1.952931	-3.758211
Se	-3.758211	0.064295	-1.952931
Se	1.952931	3.758211	0.064295
Se	1.952931	-3.758211	-0.064295
Se	-1.952931	-3.758211	0.064295
Se	-1.952931	3.758211	-0.064295
P	0.000000	4.754370	0.000000
P	4.754370	0.000000	0.000000
P	0.000000	-4.754370	0.000000
P	-4.754370	0.000000	0.000000
P	0.000000	0.000000	4.754370
P	0.000000	0.000000	-4.754370
H	0.012768	5.663704	-1.089501
H	-0.012768	5.663704	1.089501
H	5.663704	-1.089501	0.012768
H	5.663704	1.089501	-0.012768
H	-0.012768	-5.663704	-1.089501
H	0.012768	-5.663704	1.089501
H	-5.663704	1.089501	0.012768
H	-5.663704	-1.089501	-0.012768
H	1.089501	-0.012768	5.663704
H	-1.089501	0.012768	5.663704
H	-1.089501	-0.012768	-5.663704
H	1.089501	0.012768	-5.663704
O	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(S)(Se_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E = -72880.6944484

Ag	1.592242	1.592242	1.592242
Ag	1.592242	1.592242	-1.592242
Ag	1.592242	-1.592242	-1.592242
Ag	1.592242	-1.592242	1.592242
Ag	-1.592242	1.592242	1.592242
Ag	-1.592242	1.592242	-1.592242
Ag	-1.592242	-1.592242	-1.592242
Ag	-1.592242	-1.592242	1.592242
Se	3.823446	0.000000	1.970742
Se	1.970742	3.823446	0.000000
Se	3.823446	0.000000	-1.970742
Se	1.970742	-3.823446	0.000000
Se	-3.823446	0.000000	1.970742
Se	-1.970742	3.823446	0.000000
Se	-3.823446	0.000000	-1.970742
Se	-1.970742	-3.823446	0.000000
Se	0.000000	1.970742	3.823446
Se	0.000000	1.970742	-3.823446
Se	0.000000	-1.970742	-3.823446
Se	0.000000	-1.970742	3.823446
P	0.000000	0.000000	4.792317
P	0.000000	4.792317	0.000000
P	0.000000	0.000000	-4.792317
P	0.000000	-4.792317	0.000000
P	4.792317	0.000000	0.000000
P	-4.792317	0.000000	0.000000
H	-1.090550	0.000000	5.699786
H	1.090550	0.000000	5.699786
H	0.000000	5.699786	-1.090550
H	0.000000	5.699786	1.090550
H	-1.090550	0.000000	-5.699786
H	1.090550	0.000000	-5.699786
H	0.000000	-5.699786	1.090550
H	0.000000	-5.699786	-1.090550
H	5.699786	1.090550	0.000000
H	5.699786	-1.090550	0.000000
H	-5.699786	-1.090550	0.000000
H	-5.699786	1.090550	0.000000
S	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(Se)(Se_2PH_2)_6]$ (T_h)
BP86/Def2TZVP
E = -74884.2889372 a. u.

Ag	1.63146	1.63146	1.63146
Ag	1.63146	1.63146	-1.63146
Ag	1.63146	-1.63146	-1.63146
Ag	1.63146	-1.63146	1.63146
Ag	-1.63146	1.63146	1.63146
Ag	-1.63146	1.63146	-1.63146
Ag	-1.63146	-1.63146	-1.63146
Ag	-1.63146	-1.63146	1.63146
Se	3.84428	0.00000	1.97755
Se	1.97755	3.84428	0.00000
Se	3.84428	0.00000	-1.97755
Se	1.97755	-3.84428	0.00000
Se	-3.84428	0.00000	1.97755
Se	-1.97755	3.84428	0.00000
Se	-3.84428	0.00000	-1.97755
Se	-1.97755	-3.84428	0.00000
Se	0.00000	1.97755	3.84428
Se	0.00000	1.97755	-3.84428
Se	0.00000	-1.97755	-3.84428
Se	0.00000	-1.97755	3.84428
P	0.00000	0.00000	4.80322
P	0.00000	4.80322	0.00000
P	0.00000	0.00000	-4.80322
P	0.00000	-4.80322	0.00000
P	4.80322	0.00000	0.00000
P	-4.80322	0.00000	0.00000
H	-1.09111	0.00000	5.70959
H	1.09111	0.00000	5.70959
H	0.00000	5.70959	-1.09111
H	0.00000	5.70959	1.09111
H	-1.09111	0.00000	-5.70959
H	1.09111	0.00000	-5.70959
H	0.00000	-5.70959	1.09111
H	0.00000	-5.70959	-1.09111
H	5.70959	1.09111	0.00000
H	5.70959	-1.09111	0.00000
H	-5.70959	-1.09111	0.00000
H	-5.70959	1.09111	0.00000
Se	0.00000	0.00000	0.00000

Computed optimized structure of $[Ag_8(N)(Se_2PH_2)_6]^-$ (S_6)
BP86/Def2TZVP
E = -72537.1923087 a. u.

Ag	0.000000	0.000000	3.743424
Ag	0.000000	1.840090	1.227040
Ag	1.593565	0.920045	-1.227040
Ag	1.593565	-0.920045	1.227040
Ag	-1.593565	-0.920045	1.227040
Ag	-1.593565	0.920045	-1.227040
Ag	0.000000	0.000000	-3.743424
Ag	0.000000	-1.840090	-1.227040
Se	2.081851	1.649572	4.327354
Se	-2.469497	0.978150	4.327354
Se	0.128344	4.187179	2.290547
Se	3.690376	1.982440	-2.290547
Se	-0.128344	-4.187179	-2.290547
Se	-3.690376	-1.982440	2.290547
Se	-2.081851	-1.649572	-4.327354
Se	2.469497	-0.978150	-4.327354
Se	0.387646	-2.627722	4.327354
Se	-3.562032	2.204739	-2.290547
Se	-0.387646	2.627722	-4.327354
Se	3.562032	-2.204739	2.290547
P	2.542399	-2.387734	4.215631
P	-3.339038	-1.007915	4.215631
P	-2.542399	2.387734	-4.215631
P	3.339038	1.007915	-4.215631
P	0.796639	3.395649	4.215631
P	-0.796639	-3.395649	-4.215631
H	3.156657	-3.473320	4.899636
H	2.939051	-1.312615	5.058006
H	-4.586312	-0.997086	4.899636
H	-2.606284	-1.888986	5.058006
H	-2.939051	1.312615	-5.058006
H	-3.156657	3.473320	-4.899636
H	4.586312	0.997086	-4.899636
H	2.606284	1.888986	-5.058006
H	-0.332768	3.201601	5.058006
H	1.429654	4.470405	4.899636
H	0.332768	-3.201601	-5.058006
H	-1.429654	-4.470405	-4.899636
N	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(N)(Se_2PH_2)_6]^-$ (C_3)
BP86/Def2TZVP
E = -72537.1780136 a. u.

Ag	0.000000	0.000000	3.319425
Ag	0.000000	1.821471	0.955004
Ag	2.120290	1.201888	-1.009195
Ag	1.577440	-0.910735	0.955004
Ag	-1.577440	-0.910735	0.955004
Ag	-2.101010	1.235281	-1.009195
Ag	0.000000	0.000000	-2.876619
Ag	-0.019280	-2.437169	-1.009195
Se	2.736991	-0.175276	3.365389
Se	-1.216702	2.457942	3.365389
Se	2.637739	3.072941	1.159751
Se	3.994483	-0.854424	-1.097048
Se	-2.737195	-3.032112	-1.097048
Se	-3.980114	0.747879	1.159751
Se	-2.748759	0.085740	-3.457002
Se	1.300126	-2.423365	-3.457002
Se	-1.520289	-2.282666	3.365389
Se	-1.257289	3.886536	-1.097048
Se	1.448633	2.337625	-3.457002
Se	1.342375	-3.820820	1.159751
P	-0.069401	-3.869934	2.806589
P	-3.316761	1.995070	2.806589
P	-0.096898	3.816298	-2.932428
P	3.353460	-1.824233	-2.932428
P	3.386162	1.874864	2.806589
P	-3.256562	-1.992065	-2.932428
H	-0.870027	-5.038532	2.700452
H	0.654368	-4.183360	3.988784
H	-3.928483	3.272731	2.700452
H	-3.950080	1.524981	3.988784
H	-0.985895	3.854879	-4.040755
H	0.522165	5.086751	-3.081283
H	4.144173	-2.995584	-3.081283
H	3.831370	-1.073629	-4.040755
H	3.295712	2.658379	3.988784
H	4.798510	1.765801	2.700452
H	-2.845475	-2.781250	-4.040755
H	-4.666338	-2.091167	-3.081283
N	0.000000	0.000000	-0.465839

Computed optimized structure of $[Ag_8(P)(Se_2PH_2)_6]^-$ (T_h)
BP86/Def2TZVP
E = -72823.8802208 a. u.

Ag	1.497288	1.497288	1.497288
Ag	1.497288	1.497288	-1.497288
Ag	1.497288	-1.497288	-1.497288
Ag	1.497288	-1.497288	1.497288
Ag	-1.497288	1.497288	1.497288
Ag	-1.497288	1.497288	-1.497288
Ag	-1.497288	-1.497288	-1.497288
Ag	-1.497288	-1.497288	1.497288
Se	3.770087	0.000000	1.952464
Se	1.952464	3.770087	0.000000
Se	3.770087	0.000000	-1.952464
Se	1.952464	-3.770087	0.000000
Se	-3.770087	0.000000	1.952464
Se	-1.952464	3.770087	0.000000
Se	-3.770087	0.000000	-1.952464
Se	-1.952464	-3.770087	0.000000
Se	0.000000	1.952464	3.770087
Se	0.000000	1.952464	-3.770087
Se	0.000000	-1.952464	-3.770087
Se	0.000000	-1.952464	3.770087
P	0.000000	0.000000	4.766963
P	0.000000	4.766963	0.000000
P	0.000000	0.000000	-4.766963
P	0.000000	-4.766963	0.000000
P	4.766963	0.000000	0.000000
P	-4.766963	0.000000	0.000000
H	-1.089542	0.000000	5.676369
H	1.089542	0.000000	5.676369
H	0.000000	5.676369	-1.089542
H	0.000000	5.676369	1.089542
H	-1.089542	0.000000	-5.676369
H	1.089542	0.000000	-5.676369
H	0.000000	-5.676369	1.089542
H	0.000000	-5.676369	-1.089542
H	5.676369	1.089542	0.000000
H	5.676369	-1.089542	0.000000
H	-5.676369	-1.089542	0.000000
H	-5.676369	1.089542	0.000000
P	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_8(C)(Se_2PH_2)_6]^{2-}$ (S_6)
BP86/Def2TZVP
E = -72520.521988 a. u.

Ag	0.000000	0.000000	3.676565
Ag	-0.010090	1.829550	1.204858
Ag	1.579392	0.923513	-1.204858
Ag	1.589482	-0.906037	1.204858
Ag	-1.579392	-0.923513	1.204858
Ag	-1.589482	0.906037	-1.204858
Ag	0.000000	0.000000	-3.676565
Ag	0.010090	-1.829550	-1.204858
Se	1.733522	1.885393	4.800881
Se	-2.499559	0.558577	4.800881
Se	0.028326	4.203139	2.303473
Se	3.654188	2.077039	-2.303473
Se	-0.028326	-4.203139	-2.303473
Se	-3.654188	-2.077039	2.303473
Se	-1.733522	-1.885393	-4.800881
Se	2.499559	-0.558577	-4.800881
Se	0.766037	-2.443971	4.800881
Se	-3.625863	2.126100	-2.303473
Se	-0.766037	2.443971	-4.800881
Se	3.625863	-2.126100	2.303473
P	2.834951	-2.013521	4.334311
P	-3.161236	-1.448379	4.334311
P	-2.834951	2.013521	-4.334311
P	3.161236	1.448379	-4.334311
P	0.326285	3.461900	4.334311
P	-0.326285	-3.461900	-4.334311
H	3.664640	-2.851331	5.135064
H	3.178886	-0.748028	4.888055
H	-4.301645	-1.748006	5.135064
H	-2.237254	-2.378982	4.888055
H	-3.178886	0.748028	-4.888055
H	-3.664640	2.851331	-5.135064
H	4.301645	1.748006	-5.135064
H	2.237254	2.378982	-4.888055
H	-0.941632	3.127010	4.888055
H	0.637005	4.599337	5.135064
H	0.941632	-3.127010	-4.888055
H	-0.637005	-4.599337	-5.135064
C	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(\square)(Se_2PH_2)_6]^{2+}$ (*T*)
BP86/Def2TZVP
E = -58243.1420932 a. u.

Ag	1.662037	1.662037	1.662037
Cu	1.782213	-1.782213	1.782213
Ag	-1.662037	-1.662037	1.662037
Cu	-1.782213	1.782213	1.782213
Cu	1.782213	1.782213	-1.782213
Ag	1.662037	-1.662037	-1.662037
Cu	-1.782213	-1.782213	-1.782213
Ag	-1.662037	1.662037	-1.662037
Se	-0.183510	1.962192	3.548492
Se	3.548492	-0.183510	1.962192
Se	0.183510	-1.962192	3.548492
Se	-3.548492	0.183510	1.962192
Se	0.183510	1.962192	-3.548492
Se	3.548492	0.183510	-1.962192
Se	-0.183510	-1.962192	-3.548492
Se	-3.548492	-0.183510	-1.962192
Se	1.962192	3.548492	-0.183510
Se	1.962192	-3.548492	0.183510
Se	-1.962192	-3.548492	-0.183510
Se	-1.962192	3.548492	0.183510
P	0.000000	4.582602	0.000000
P	4.582602	0.000000	0.000000
P	0.000000	-4.582602	0.000000
P	-4.582602	0.000000	0.000000
P	0.000000	0.000000	4.582602
P	0.000000	0.000000	-4.582602
H	-0.131746	5.472154	-1.094780
H	0.131746	5.472154	1.094780
H	5.472154	-1.094780	-0.131746
H	5.472154	1.094780	0.131746
H	0.131746	-5.472154	-1.094780
H	-0.131746	-5.472154	1.094780
H	-5.472154	1.094780	-0.131746
H	-5.472154	-1.094780	0.131746
H	1.094780	0.131746	5.472154
H	-1.094780	-0.131746	5.472154
H	-1.094780	0.131746	-5.472154
H	1.094780	-0.131746	-5.472154

Computed optimized structure of $[Cu_4Ag_4(H)(Se_2PH_2)_6]^+$ (*T*) - *T(Cu$_4$)*-BP86/Def2TZVP
E = -58244.0267965 a. u.

Cu	1.030373	1.030373	1.030373
Ag	1.704593	-1.704593	1.704593
Cu	-1.030373	-1.030373	1.030373
Ag	-1.704593	1.704593	1.704593
Ag	1.704593	1.704593	-1.704593
Cu	1.030373	-1.030373	-1.030373
Ag	-1.704593	-1.704593	-1.704593
Cu	-1.030373	1.030373	-1.030373
Se	0.374990	1.863497	3.398001
Se	3.398001	0.374990	1.863497
Se	-0.374990	-1.863497	3.398001
Se	-3.398001	-0.374990	1.863497
Se	-0.374990	1.863497	-3.398001
Se	3.398001	-0.374990	-1.863497
Se	0.374990	-1.863497	-3.398001
Se	-3.398001	0.374990	-1.863497
Se	1.863497	3.398001	0.374990
Se	1.863497	-3.398001	-0.374990
Se	-1.863497	-3.398001	0.374990
Se	-1.863497	3.398001	-0.374990
P	0.000000	4.515889	0.000000
P	4.515889	0.000000	0.000000
P	0.000000	-4.515889	0.000000
P	-4.515889	0.000000	0.000000
P	0.000000	0.000000	4.515889
P	0.000000	0.000000	-4.515889
H	0.183149	5.416614	-1.079997
H	-0.183149	5.416614	1.079997
H	5.416614	-1.079997	0.183149
H	5.416614	1.079997	-0.183149
H	-0.183149	-5.416614	-1.079997
H	0.183149	-5.416614	1.079997
H	-5.416614	1.079997	0.183149
H	-5.416614	-1.079997	-0.183149
H	1.079997	-0.183149	5.416614
H	-1.079997	0.183149	5.416614
H	-1.079997	-0.183149	-5.416614
H	1.079997	0.183149	-5.416614
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Ag_4Cu_4(H)(Se_2PH_2)_6]^+$ (*T*) - *T(Ag4)*-BP86/Def2TZVP
E = -58244.0267965 a. u.

Ag	1.136747	1.136747	1.136747
Cu	1.721221	-1.721221	1.721221
Ag	-1.136747	-1.136747	1.136747
Cu	-1.721221	1.721221	1.721221
Cu	1.721221	1.721221	-1.721221
Ag	1.136747	-1.136747	-1.136747
Cu	-1.721221	-1.721221	-1.721221
Ag	-1.136747	1.136747	-1.136747
Se	-0.110594	1.949954	3.499324
Se	3.499324	-0.110594	1.949954
Se	0.110594	-1.949954	3.499324
Se	-3.499324	0.110594	1.949954
Se	0.110594	1.949954	-3.499324
Se	3.499324	0.110594	-1.949954
Se	-0.110594	-1.949954	-3.499324
Se	-3.499324	-0.110594	-1.949954
Se	1.949954	3.499324	-0.110594
Se	1.949954	-3.499324	0.110594
Se	-1.949954	-3.499324	-0.110594
Se	-1.949954	3.499324	0.110594
P	0.000000	4.543208	0.000000
P	4.543208	0.000000	0.000000
P	0.000000	-4.543208	0.000000
P	-4.543208	0.000000	0.000000
P	0.000000	0.000000	4.543208
P	0.000000	0.000000	-4.543208
H	-0.107077	5.442033	-1.091201
H	0.107077	5.442033	1.091201
H	5.442033	-1.091201	-0.107077
H	5.442033	1.091201	0.107077
H	0.107077	-5.442033	-1.091201
H	-0.107077	-5.442033	1.091201
H	-5.442033	1.091201	-0.107077
H	-5.442033	-1.091201	0.107077
H	1.091201	0.107077	5.442033
H	-1.091201	-0.107077	5.442033
H	-1.091201	0.107077	-5.442033
H	1.091201	-0.107077	-5.442033
H	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(F)(Se_2PH_2)_6]^+$ (*T*) - *T(Ag$_4$)*-BP86/Def2TZVP
E = -58343.3546439 a. u.

Ag	1.421174	1.421174	1.421174
Cu	1.763946	-1.763946	1.763946
Ag	-1.421174	-1.421174	1.421174
Cu	-1.763946	1.763946	1.763946
Cu	1.763946	1.763946	-1.763946
Ag	1.421174	-1.421174	-1.421174
Cu	-1.763946	-1.763946	-1.763946
Ag	-1.421174	1.421174	-1.421174
Se	-0.172607	1.957901	3.549914
Se	3.549914	-0.172607	1.957901
Se	0.172607	-1.957901	3.549914
Se	-3.549914	0.172607	1.957901
Se	0.172607	1.957901	-3.549914
Se	3.549914	0.172607	-1.957901
Se	-0.172607	-1.957901	-3.549914
Se	-3.549914	-0.172607	-1.957901
Se	1.957901	3.549914	-0.172607
Se	1.957901	-3.549914	0.172607
Se	-1.957901	-3.549914	-0.172607
Se	-1.957901	3.549914	0.172607
P	0.000000	4.574327	0.000000
P	4.574327	0.000000	0.000000
P	0.000000	-4.574327	0.000000
P	-4.574327	0.000000	0.000000
P	0.000000	0.000000	4.574327
P	0.000000	0.000000	-4.574327
H	-0.136849	5.473300	-1.087956
H	0.136849	5.473300	1.087956
H	5.473300	-1.087956	-0.136849
H	5.473300	1.087956	0.136849
H	0.136849	-5.473300	-1.087956
H	-0.136849	-5.473300	1.087956
H	-5.473300	1.087956	-0.136849
H	-5.473300	-1.087956	0.136849
H	1.087956	0.136849	5.473300
H	-1.087956	-0.136849	5.473300
H	-1.087956	0.136849	-5.473300
H	1.087956	-0.136849	-5.473300
F	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(Cl)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E = -58703.7438784 a. u.

Cu	1.727771	1.727771	1.727771
Ag	1.643842	-1.643842	1.643842
Cu	-1.727771	-1.727771	1.727771
Ag	-1.643842	1.643842	1.643842
Ag	1.643842	1.643842	-1.643842
Cu	1.727771	-1.727771	-1.727771
Ag	-1.643842	-1.643842	-1.643842
Cu	-1.727771	1.727771	-1.727771
Se	0.201852	1.968340	3.582367
Se	3.582367	0.201852	1.968340
Se	-0.201852	-1.968340	3.582367
Se	-3.582367	-0.201852	1.968340
Se	-0.201852	1.968340	-3.582367
Se	3.582367	-0.201852	-1.968340
Se	0.201852	-1.968340	-3.582367
Se	-3.582367	0.201852	-1.968340
Se	1.968340	3.582367	0.201852
Se	1.968340	-3.582367	-0.201852
Se	-1.968340	-3.582367	0.201852
Se	-1.968340	3.582367	-0.201852
P	0.000000	4.584591	0.000000
P	4.584591	0.000000	0.000000
P	0.000000	-4.584591	0.000000
P	-4.584591	0.000000	0.000000
P	0.000000	0.000000	4.584591
P	0.000000	0.000000	-4.584591
H	0.138781	5.482733	-1.088148
H	-0.138781	5.482733	1.088148
H	5.482733	-1.088148	0.138781
H	5.482733	1.088148	-0.138781
H	-0.138781	-5.482733	-1.088148
H	0.138781	-5.482733	1.088148
H	-5.482733	1.088148	0.138781
H	-5.482733	-1.088148	-0.138781
H	1.088148	-0.138781	5.482733
H	-1.088148	0.138781	5.482733
H	-1.088148	-0.138781	-5.482733
H	1.088148	0.138781	-5.482733
Cl	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(Br)(Se_2PH_2)_6]^+$ (*T*)
BP86/Def2TZVP
E = -60817.9190975 a. u.

Cu	1.665384	1.665384	1.665384
Ag	1.744243	-1.744243	1.744243
Cu	-1.665384	-1.665384	1.665384
Ag	-1.744243	1.744243	1.744243
Ag	1.744243	1.744243	-1.744243
Cu	1.665384	-1.665384	-1.665384
Ag	-1.744243	-1.744243	-1.744243
Cu	-1.665384	1.665384	-1.665384
Se	0.210553	1.968600	3.585751
Se	3.585751	0.210553	1.968600
Se	-0.210553	-1.968600	3.585751
Se	-3.585751	-0.210553	1.968600
Se	-0.210553	1.968600	-3.585751
Se	3.585751	-0.210553	-1.968600
Se	0.210553	-1.968600	-3.585751
Se	-3.585751	0.210553	-1.968600
Se	1.968600	3.585751	0.210553
Se	1.968600	-3.585751	-0.210553
Se	-1.968600	-3.585751	0.210553
Se	-1.968600	3.585751	-0.210553
P	0.000000	4.584320	0.000000
P	4.584320	0.000000	0.000000
P	0.000000	-4.584320	0.000000
P	-4.584320	0.000000	0.000000
P	0.000000	0.000000	4.584320
P	0.000000	0.000000	-4.584320
H	0.134840	5.482393	-1.088595
H	-0.134840	5.482393	1.088595
H	5.482393	-1.088595	0.134840
H	5.482393	1.088595	-0.134840
H	-0.134840	-5.482393	-1.088595
H	0.134840	-5.482393	1.088595
H	-5.482393	1.088595	0.134840
H	-5.482393	-1.088595	-0.134840
H	1.088595	-0.134840	5.482393
H	-1.088595	0.134840	5.482393
H	-1.088595	-0.134840	-5.482393
H	1.088595	0.134840	-5.482393
Br	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(O)(Se_2PH_2)_6]$ (*T*) - *T(Cu₄)*-BP86/Def2TZVP
E = -58318.8790952 a. u.

Cu	1.171007	1.171007	1.171007
Ag	1.673239	-1.673239	1.673239
Cu	-1.171007	-1.171007	1.171007
Ag	-1.673239	1.673239	1.673239
Ag	1.673239	1.673239	-1.673239
Cu	1.171007	-1.171007	-1.171007
Ag	-1.673239	-1.673239	-1.673239
Cu	-1.171007	1.171007	-1.171007
Se	0.335176	1.894148	3.483436
Se	3.483436	0.335176	1.894148
Se	-0.335176	-1.894148	3.483436
Se	-3.483436	-0.335176	1.894148
Se	-0.335176	1.894148	-3.483436
Se	3.483436	-0.335176	-1.894148
Se	0.335176	-1.894148	-3.483436
Se	-3.483436	0.335176	-1.894148
Se	1.894148	3.483436	0.335176
Se	1.894148	-3.483436	-0.335176
Se	-1.894148	-3.483436	0.335176
Se	-1.894148	3.483436	-0.335176
P	0.000000	4.549935	0.000000
P	4.549935	0.000000	0.000000
P	0.000000	-4.549935	0.000000
P	-4.549935	0.000000	0.000000
P	0.000000	0.000000	4.549935
P	0.000000	0.000000	-4.549935
H	0.161555	5.460675	-1.077694
H	-0.161555	5.460675	1.077694
H	5.460675	-1.077694	0.161555
H	5.460675	1.077694	-0.161555
H	-0.161555	-5.460675	-1.077694
H	0.161555	-5.460675	1.077694
H	-5.460675	1.077694	0.161555
H	-5.460675	-1.077694	-0.161555
H	1.077694	-0.161555	5.460675
H	-1.077694	0.161555	5.460675
H	-1.077694	-0.161555	-5.460675
H	1.077694	0.161555	-5.460675
O	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(S)(Se_2PH_2)_6]$ (*T*)
BP86/Def2TZVP
E = -58641.9347209 a. u.

Ag	1.658948	1.658948	1.658948
Cu	1.360536	-1.360536	1.360536
Ag	-1.658948	-1.658948	1.658948
Cu	-1.360536	1.360536	1.360536
Cu	1.360536	1.360536	-1.360536
Ag	1.658948	-1.658948	-1.658948
Cu	-1.360536	-1.360536	-1.360536
Ag	-1.658948	1.658948	-1.658948
Se	-0.284804	1.935363	3.570061
Se	3.570061	-0.284804	1.935363
Se	0.284804	-1.935363	3.570061
Se	-3.570061	0.284804	1.935363
Se	0.284804	1.935363	-3.570061
Se	3.570061	0.284804	-1.935363
Se	-0.284804	-1.935363	-3.570061
Se	-3.570061	-0.284804	-1.935363
Se	1.935363	3.570061	-0.284804
Se	1.935363	-3.570061	0.284804
Se	-1.935363	-3.570061	-0.284804
Se	-1.935363	3.570061	0.284804
P	0.000000	4.583437	0.000000
P	4.583437	0.000000	0.000000
P	0.000000	-4.583437	0.000000
P	-4.583437	0.000000	0.000000
P	0.000000	0.000000	4.583437
P	0.000000	0.000000	-4.583437
H	-0.153468	5.492188	-1.079648
H	0.153468	5.492188	1.079648
H	5.492188	-1.079648	-0.153468
H	5.492188	1.079648	0.153468
H	0.153468	-5.492188	-1.079648
H	-0.153468	-5.492188	1.079648
H	-5.492188	1.079648	-0.153468
H	-5.492188	-1.079648	0.153468
H	1.079648	0.153468	5.492188
H	-1.079648	-0.153468	5.492188
H	-1.079648	0.153468	-5.492188
H	1.079648	-0.153468	-5.492188
S	0.000000	0.000000	0.000000

Computed optimized structure of $[Cu_4Ag_4(Se)(Se_2PH_2)_6]$ (*T*)
BP86/Def2TZVP
E = -60645.5225314 a. u.

Ag	1.666505	1.666505	1.666505
Cu	1.448015	-1.448015	1.448015
Ag	-1.666505	-1.666505	1.666505
Cu	-1.448015	1.448015	1.448015
Cu	1.448015	1.448015	-1.448015
Ag	1.666505	-1.666505	-1.666505
Cu	-1.448015	-1.448015	-1.448015
Ag	-1.666505	1.666505	-1.666505
Se	-0.265038	1.952165	3.599061
Se	3.599061	-0.265038	1.952165
Se	0.265038	-1.952165	3.599061
Se	-3.599061	0.265038	1.952165
Se	0.265038	1.952165	-3.599061
Se	3.599061	0.265038	-1.952165
Se	-0.265038	-1.952165	-3.599061
Se	-3.599061	-0.265038	-1.952165
Se	1.952165	3.599061	-0.265038
Se	1.952165	-3.599061	0.265038
Se	-1.952165	-3.599061	-0.265038
Se	-1.952165	3.599061	0.265038
P	0.000000	4.592422	0.000000
P	4.592422	0.000000	0.000000
P	0.000000	-4.592422	0.000000
P	-4.592422	0.000000	0.000000
P	0.000000	0.000000	4.592422
P	0.000000	0.000000	-4.592422
H	-0.149849	5.500186	-1.080594
H	0.149849	5.500186	1.080594
H	5.500186	-1.080594	-0.149849
H	5.500186	1.080594	0.149849
H	0.149849	-5.500186	-1.080594
H	-0.149849	-5.500186	1.080594
H	-5.500186	1.080594	-0.149849
H	-5.500186	-1.080594	0.149849
H	1.080594	0.149849	5.500186
H	-1.080594	-0.149849	5.500186
H	-1.080594	0.149849	-5.500186
H	1.080594	-0.149849	-5.500186
Se	0.000000	0.000000	0.000000