

Cationic Gold Clusters with Eight Valence Electrons: Possible Spherical Aromatic Systems with Sigma Holes

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Supporting Information

Complete Gaussian09 Reference.

Tables S1A-S1B: Initial structures and distance matrices for the $[\text{Au}_9]^+$ structures.

Tables S2A-S2B: Initial structures and distance matrices for the $[\text{Au}_{11}]^{3+}$ structures.

Tables S3A-S3B: Initial structures and distance matrices for the $[\text{Au}_{12}]^{4+}$ structures.

Table S4: Orbital energies and HOMO-LUMO gaps for the lowest energy structures.

Complete Gaussian09 Reference.

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1A: Initial polyhedral structures of the $[\text{Au}_9]^+$ clusters.

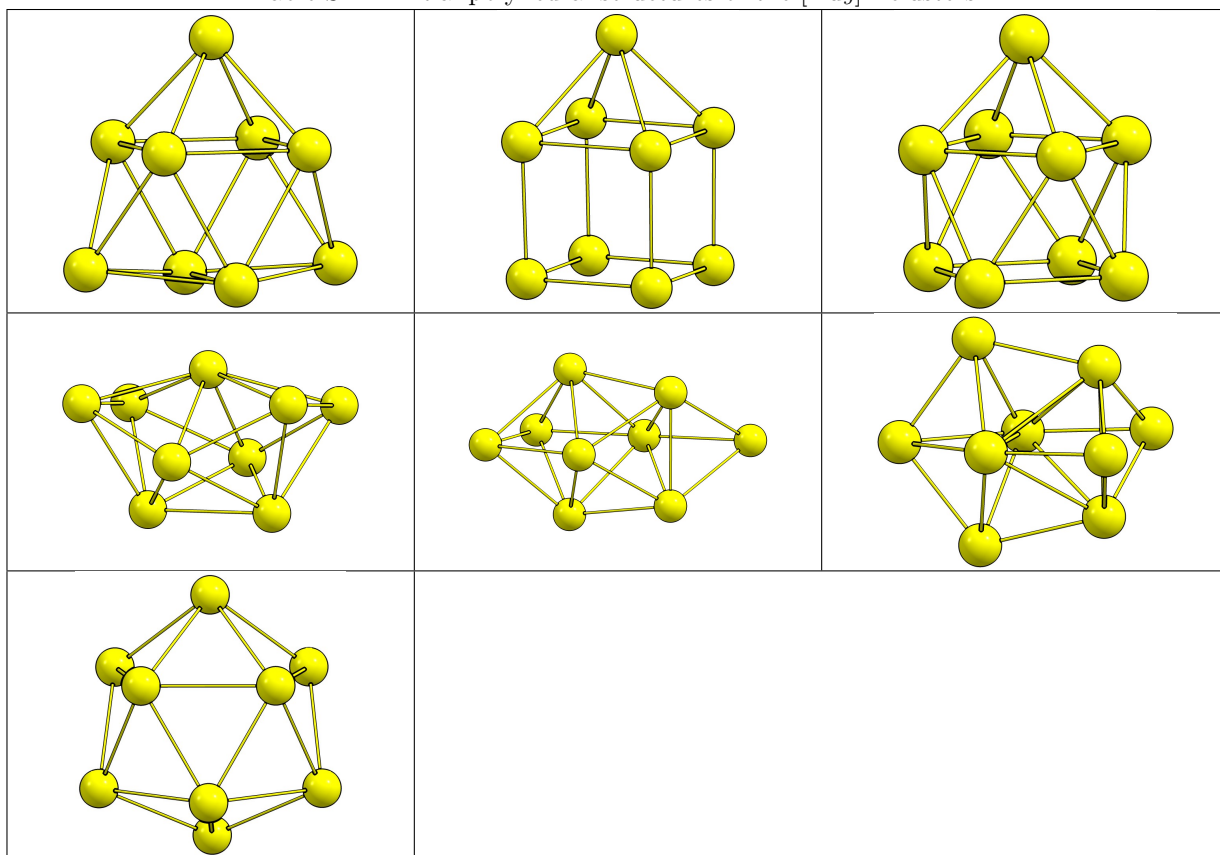
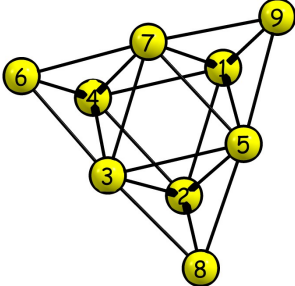
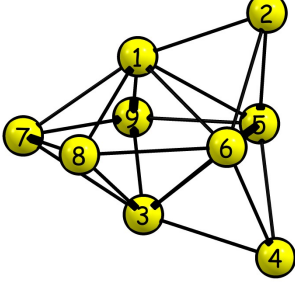
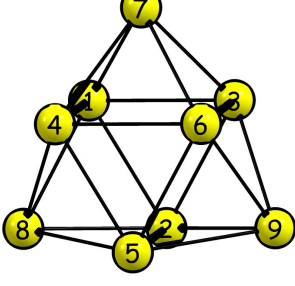


Table S1B: Distance table for the lowest-lying $[\text{Au}_9]^{1+}$ optimized structures obtained at the B3PW91/def2-TZVPD level of theory. Included are the zero-point corrected absolute energy in (a.u.), relative energy in (kcal/mol) and symmetry.

	<table><tr><th></th><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Au</td><td>0.000000</td><td></td><td></td><td></td><td></td><td></td></tr><tr><td>2 Au</td><td>2.741968</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>3 Au</td><td>4.052696</td><td>2.929672</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>4 Au</td><td>2.741307</td><td>2.742312</td><td>2.929886</td><td>0.000000</td><td></td><td></td></tr><tr><td>5 Au</td><td>2.930247</td><td>2.929645</td><td>2.852863</td><td>4.048130</td><td>0.000000</td><td></td></tr><tr><td>6 Au</td><td>4.758443</td><td>4.755274</td><td>2.689064</td><td>2.807359</td><td>4.749132</td><td></td></tr><tr><td>7 Au</td><td>2.935322</td><td>4.051967</td><td>2.852645</td><td>2.929331</td><td>2.851975</td><td></td></tr><tr><td>8 Au</td><td>4.755840</td><td>2.808638</td><td>2.687847</td><td>4.755509</td><td>2.688200</td><td></td></tr><tr><td>9 Au</td><td>2.809407</td><td>4.755616</td><td>4.748736</td><td>4.751734</td><td>2.688412</td><td></td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td>9</td><td></td><td></td></tr><tr><td>6 Au</td><td>0.000000</td><td></td><td></td><td></td><td></td><td></td></tr><tr><td>7 Au</td><td>2.689305</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>8 Au</td><td>5.370982</td><td>4.747663</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>9 Au</td><td>5.371119</td><td>2.687893</td><td>5.370723</td><td>0.000000</td><td></td><td></td></tr></table>			1	2	3	4	5	1 Au	0.000000						2 Au	2.741968	0.000000					3 Au	4.052696	2.929672	0.000000				4 Au	2.741307	2.742312	2.929886	0.000000			5 Au	2.930247	2.929645	2.852863	4.048130	0.000000		6 Au	4.758443	4.755274	2.689064	2.807359	4.749132		7 Au	2.935322	4.051967	2.852645	2.929331	2.851975		8 Au	4.755840	2.808638	2.687847	4.755509	2.688200		9 Au	2.809407	4.755616	4.748736	4.751734	2.688412			6	7	8	9			6 Au	0.000000						7 Au	2.689305	0.000000					8 Au	5.370982	4.747663	0.000000				9 Au	5.371119	2.687893	5.370723	0.000000		
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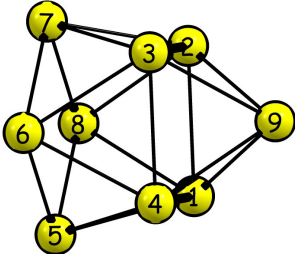
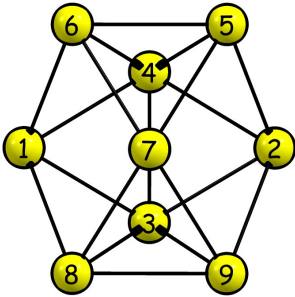
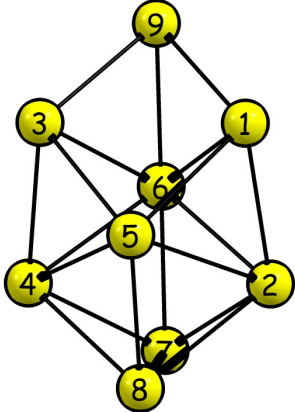
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	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Au</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Au</td><td>4.543825</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Au</td><td>2.789308</td><td>2.789588</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Au</td><td>2.789302</td><td>2.789528</td><td>2.724591</td><td>0.000000</td><td></td></tr><tr><td>5 Au</td><td>4.558282</td><td>2.841272</td><td>4.542381</td><td>2.896847</td><td>0.000000</td></tr><tr><td>6 Au</td><td>2.840839</td><td>4.557770</td><td>4.541676</td><td>2.897470</td><td>2.795884</td></tr><tr><td>7 Au</td><td>3.014658</td><td>3.012126</td><td>3.161919</td><td>3.161948</td><td>2.687501</td></tr><tr><td>8 Au</td><td>2.840901</td><td>4.557822</td><td>2.897435</td><td>4.541703</td><td>5.290346</td></tr><tr><td>9 Au</td><td>4.558284</td><td>2.841274</td><td>2.896747</td><td>4.542322</td><td>4.492979</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th></th></tr><tr><td>6 Au</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Au</td><td>2.687307</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Au</td><td>4.489377</td><td>2.687307</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 Au</td><td>5.290332</td><td>2.687506</td><td>2.795898</td><td>0.000000</td><td></td></tr></table>		1	2	3	4	5	1 Au	0.000000					2 Au	4.543825	0.000000				3 Au	2.789308	2.789588	0.000000			4 Au	2.789302	2.789528	2.724591	0.000000		5 Au	4.558282	2.841272	4.542381	2.896847	0.000000	6 Au	2.840839	4.557770	4.541676	2.897470	2.795884	7 Au	3.014658	3.012126	3.161919	3.161948	2.687501	8 Au	2.840901	4.557822	2.897435	4.541703	5.290346	9 Au	4.558284	2.841274	2.896747	4.542322	4.492979		6	7	8	9		6 Au	0.000000					7 Au	2.687307	0.000000				8 Au	4.489377	2.687307	0.000000			9 Au	5.290332	2.687506	2.795898	0.000000	
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Table S2A: Initial polyhedral structures of the $[\text{Au}_{11}]^{3+}$ clusters.

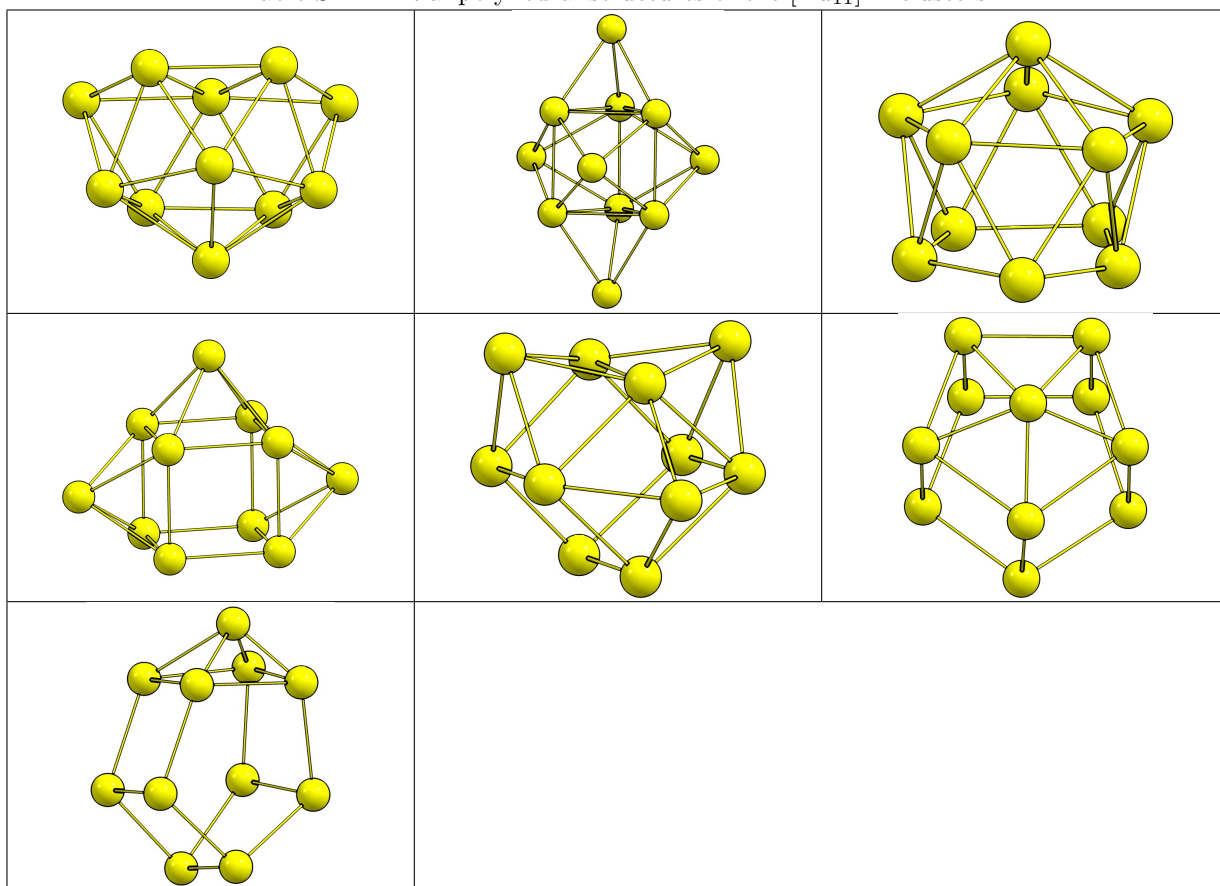
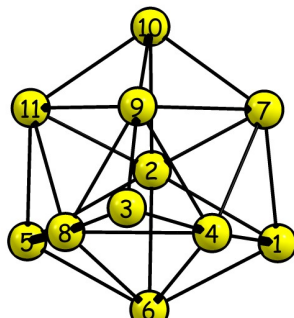
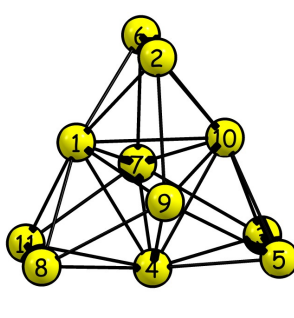


Table S2B: Distance table for the lowest-lying $[\text{Au}_{11}]^{3+}$ optimized structures obtained at the B3PW91/def2-TZVPD level of theory. Included are the zero-point corrected absolute energy in (a.u.), relative energy in (kcal/mol) and symmetry.

 1. -1493.398031 0.0 C_{3v}	1	2	3	4	5
1 Au	0.000000				
2 Au	2.838216	0.000000			
3 Au	5.471223	4.711733	0.000000		
4 Au	2.768587	3.031628	2.733235	0.000000	
5 Au	4.913920	2.836676	5.470162	4.664918	0.000000
6 Au	2.827941	2.737277	4.795929	2.948854	2.826522
7 Au	2.828237	2.737769	4.795275	2.948640	5.521889
8 Au	4.668492	3.033369	2.733765	2.872634	2.767565
9 Au	4.665289	3.029273	2.734375	2.870574	4.663060
10 Au	4.914652	2.836675	5.471501	4.666372	4.912848
11 Au	5.523979	2.738072	4.796867	4.674547	2.826832
	6	7	8	9	10
6 Au	0.000000				
7 Au	4.578957	0.000000			
8 Au	2.950001	4.675437	0.000000		
9 Au	4.671724	2.947882	2.870984	0.000000	
10 Au	5.521729	2.828443	4.667316	2.767515	0.000000
11 Au	4.578999	4.580426	2.949720	2.948211	2.828109
	11				
11 Au	0.000000				
 2. -1493.394963 +1.9 D_{3h}	1	2	3	4	5
1 Au	0.000000				
2 Au	2.768711	0.000000			
3 Au	4.631550	5.495256	0.000000		
4 Au	2.940740	4.636812	2.766820	0.000000	
5 Au	4.634298	4.702037	2.851420	2.766958	0.000000
6 Au	2.768549	2.851102	4.693398	4.633899	5.495325
7 Au	2.931515	4.684064	2.878400	2.932751	4.684036
8 Au	2.769456	4.696506	5.494542	2.770530	4.695017
9 Au	2.933449	2.881601	4.683571	2.934883	2.881175
10 Au	2.940547	2.769233	2.768732	2.941322	2.768995
11 Au	2.765775	5.492432	4.693327	2.765709	5.490460
	6	7	8	9	10
6 Au	0.000000				
7 Au	2.878649	0.000000			
8 Au	5.495564	4.683496	0.000000		
9 Au	4.683633	4.785285	2.875461	0.000000	
10 Au	2.769073	2.937774	4.633817	2.932901	0.000000
11 Au	4.695532	2.875524	2.852030	4.679459	4.633139
	11				
11 Au	0.000000				

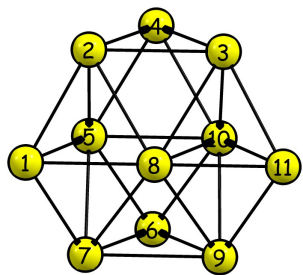
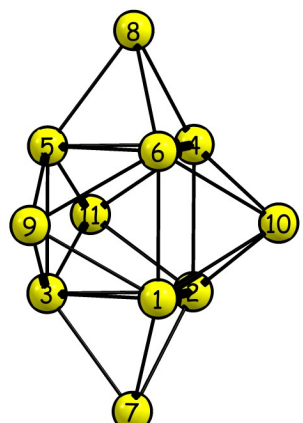
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Table S3A: Initial polyhedral structures of the $[\text{Au}_{12}]^{4+}$ clusters.

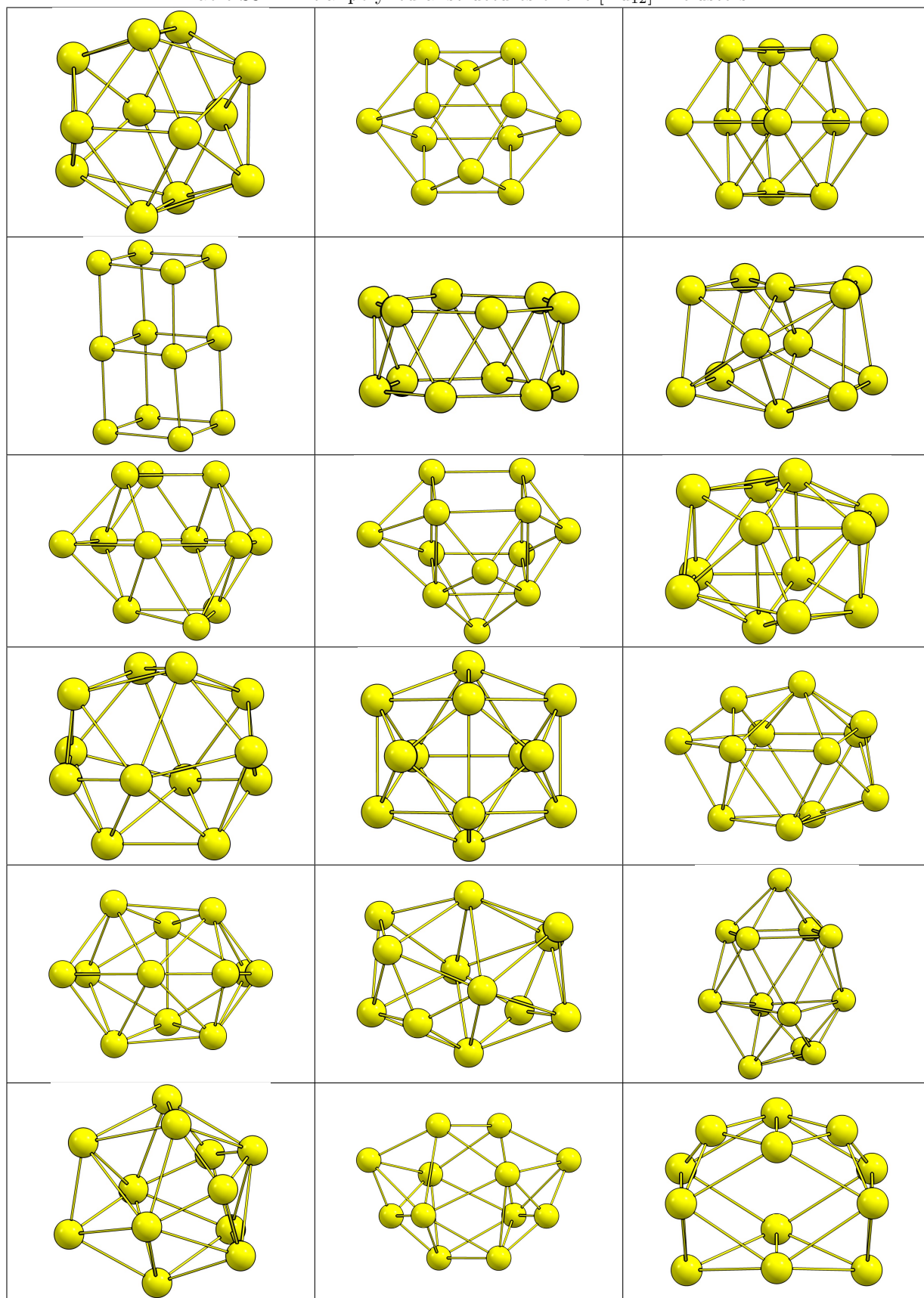
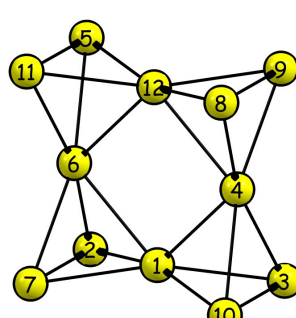
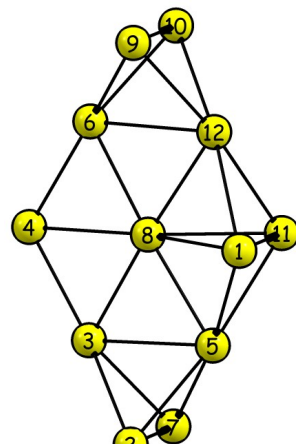
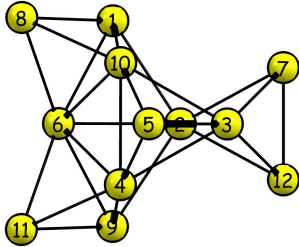
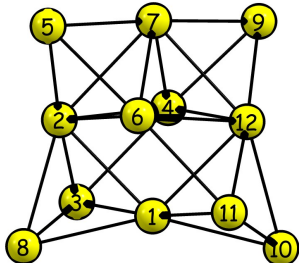
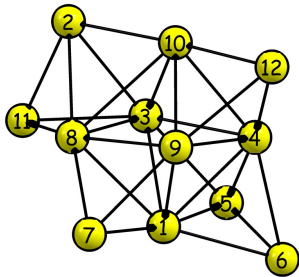
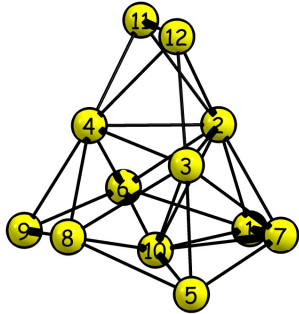
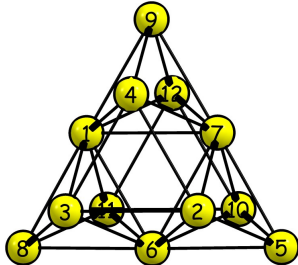
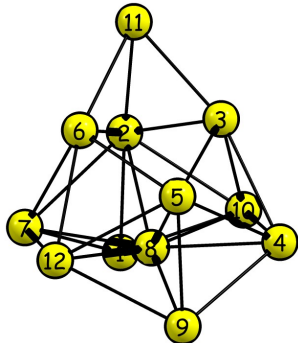


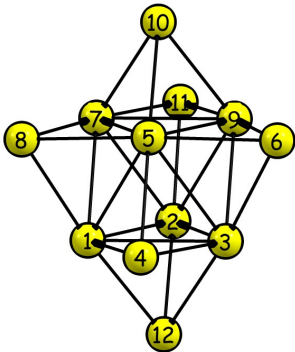
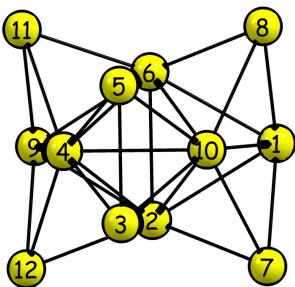
Table S3B: Distance table for the lowest-lying $[\text{Au}_{12}]^{4+}$ optimized structures obtained at the B3PW91/def2-TZVPD level of theory. Included are the zero-point corrected absolute energy in (a.u.), relative energy in (kcal/mol) and symmetry.

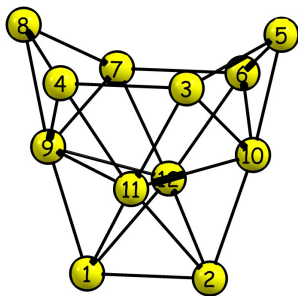
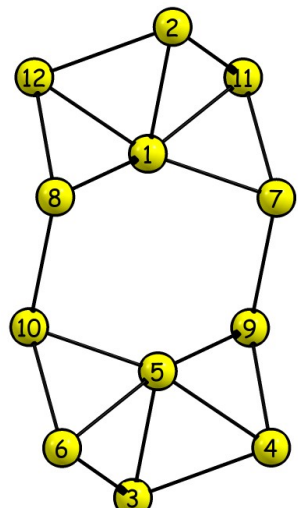
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7 Au	5.699455	2.655716	2.813954	5.414048	2.814605																																																																																																																																			
8 Au	2.918984	4.592735	2.749574	2.742965	2.785430																																																																																																																																			
9 Au	5.042869	8.788937	7.074990	5.412643	7.000665																																																																																																																																			
10 Au	5.698975	9.181705	7.075328	5.413735	7.001137																																																																																																																																			
11 Au	2.652360	5.699422	4.804234	5.506182	2.899057																																																																																																																																			
12 Au	2.899006	7.001685	5.532213	4.857090	4.675734																																																																																																																																			
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7 Au	7.075524	0.000000																																																																																																																																						
8 Au	2.749392	4.592929	0.000000																																																																																																																																					
9 Au	2.813749	9.181344	4.591865	0.000000																																																																																																																																				
10 Au	2.813632	8.789157	4.592394	2.655797	0.000000																																																																																																																																			
11 Au	4.804604	5.043349	2.919456	5.699127	5.043766																																																																																																																																			
12 Au	2.861167	7.001274	2.785418	2.814462	2.814292																																																																																																																																			
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11 Au	4.418902	2.705949	2.788397	5.548995	4.970054																																																																																																																																			
12 Au	4.810607	5.518314	4.841805	2.770725	5.643223																																																																																																																																			
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8 Au	5.554209	2.720075	0.000000																																																																																																																																					
9 Au	4.431329	2.737658	2.868746	0.000000																																																																																																																																				
10 Au	5.517560	4.930215	3.118216	2.844038	0.000000																																																																																																																																			
11 Au	6.769553	5.091696	2.818500	5.489704	4.645093																																																																																																																																			
12 Au	5.043435	5.521869	4.974125	2.794380	2.687265																																																																																																																																			
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9 Au	4.705944	4.863980	2.801076	0.000000																																																																																																																																				
10 Au	4.814407	4.691316	2.772771	4.862659	0.000000																																																																																																																																			
11 Au	2.737151	4.902725	4.700444	6.736550	4.901947																																																																																																																																			
12 Au	2.860314	2.871909	2.803782	2.985774	5.550068																																																																																																																																			
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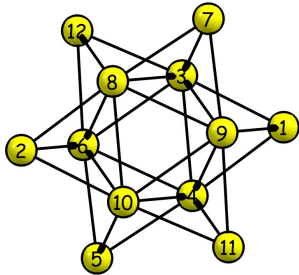
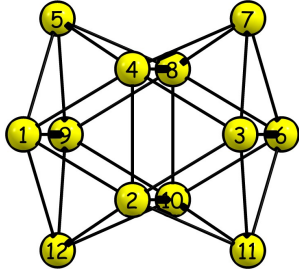
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6 Au	0.000000																																																																																																																																																
7 Au	2.910238	0.000000																																																																																																																																															
8 Au	2.806742	2.795223	0.000000																																																																																																																																														
9 Au	4.860795	5.409944	2.806715	0.000000																																																																																																																																													
10 Au	2.805823	4.663492	2.804267	2.805826	0.000000																																																																																																																																												
11 Au	2.913640	4.973650	4.665539	5.407685	2.794149																																																																																																																																												
12 Au	5.407455	6.557666	4.665366	2.913623	2.793952																																																																																																																																												
	11	12																																																																																																																																															
11 Au	0.000000																																																																																																																																																
12 Au	4.269376	0.000000																																																																																																																																															

Table S4: HOMO-LUMO gaps for the lowest-lying structures.

Structure	HOMO (a.u.)	LUMO (a.u.)	H/L gap (a.u.)	H/L gap (eV)
Au9-1	-0.134490	-0.100856	0.033634	0.92
Au9-2	-0.131993	-0.112147	0.019846	0.54
Au9-3	-0.125641	-0.107958	0.017683	0.48
Au9-4	-0.124639	-0.107801	0.016838	0.46
Au9-5	-0.134311	-0.109572	0.024739	0.67
Au9-6	-0.135678	-0.117950	0.017728	0.48
Au11-1	-0.132807	-0.117497	0.015310	0.42
Au11-2	-0.124665	-0.120051	0.004614	0.13
Au11-3	-0.124629	-0.116453	0.008176	0.22
Au11-4	-0.129579	-0.119546	0.010033	0.27
Au12-1	-0.129806	-0.115094	0.014712	0.40
Au12-2	-0.131754	-0.114870	0.016884	0.46
Au12-3	-0.130477	-0.106807	0.023670	0.64
Au12-4	-0.131573	-0.102064	0.029509	0.80
Au12-5	-0.130293	-0.102502	0.027791	0.76
Au12-6	-0.132533	-0.109249	0.023284	0.63
Au12-7	-0.127498	-0.105175	0.022323	0.61
Au12-8	-0.132581	-0.106674	0.025907	0.70
Au12-9	-0.125787	-0.102473	0.023314	0.63
Au12-10	-0.128499	-0.105781	0.022718	0.62
Au12-11	-0.135003	-0.111431	0.023572	0.64
Au12-12	-0.129360	-0.111978	0.017382	0.47
Au12-13	-0.125972	-0.099224	0.026748	0.73
Au12-14	-0.129735	-0.119169	0.010566	0.29