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

Supporting Information
On the Structure of $Au_{11}(SR)_9$ and $Au_{13}(SR)_{11}$ clusters

C. Emilio Cárdenas,[a] Alfredo Tlahuice-Flores[a*]

[a] Universidad Autonoma de Nuevo León, CICFIM,-Facultad de Ciencias Físico-Matemáticas, San Nicolás de los Garza, Nuevo León, 66455, México; tlahuicef@gmail.com

TABLE S1. Relative energies (eV) of of $Au_{11}(SCH_3)_9$ cluster the isomers and calculated HOMO-LUMO gap values.

Isomer	Configuration	Relative energy, eV	HOMO-LUMO gap, eV
Iso 1	$Au_3+Au_2(SCH_3)_3+Au_6(SCH_3)_6$	0.000	1.994
Iso2	$Au_4+Au_2(SCH_3)_3+Au_5(SCH_3)_6$	0.190	1.312
Iso3	$Au_4+Au_3(SCH_3)_4+Au_4(SCH_3)_5$	0.338	1.964
Iso4	$Au_4+Au(SCH_3)_2+Au_6(SCH_3)_7$	0.482	2.1431

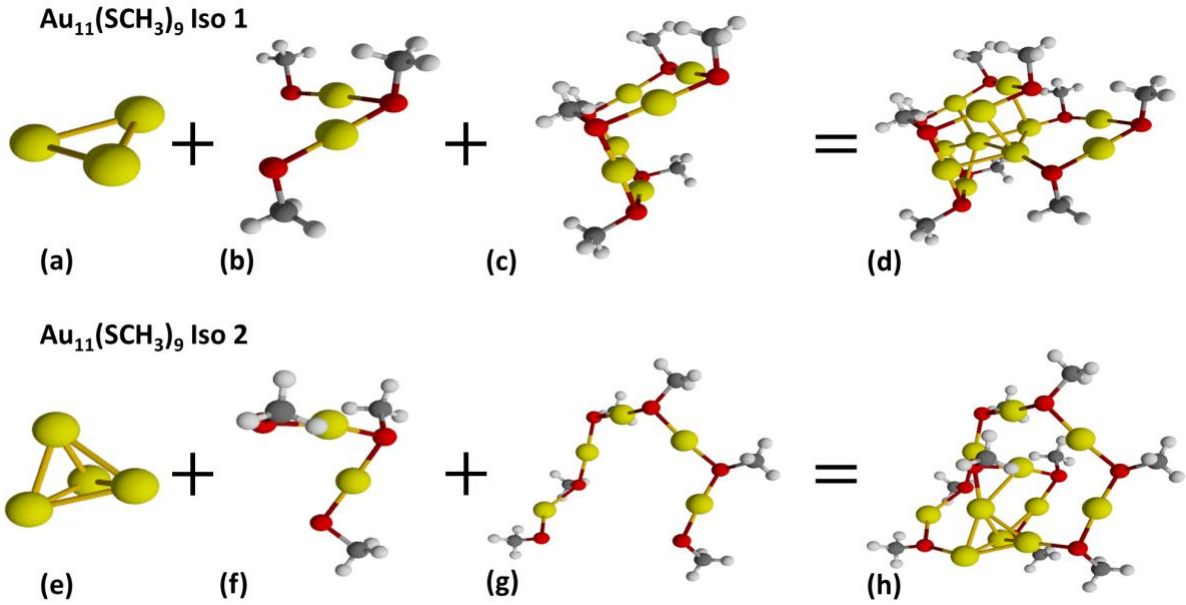

FIG. S1. Lowest energy isomers of $Au_{11}(SCH_3)_9$ clusters. (a) Triangular core (Au_3), (b) Dimer motif ($Au_2(SCH_3)_3$), (c) Cyclomer ($Au_6(SCH_3)_6$), (d) Iso 1 of $Au_{11}(SCH_3)_9$ cluster, (e) Tetrahedral core (Au_4), (f) Dimer motif ($Au_2(SCH_3)_3$), (g) Pentamer motif ($Au_5(SCH_3)_6$), (h) Iso 2 of $Au_{11}(SCH_3)_9$ cluster. Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

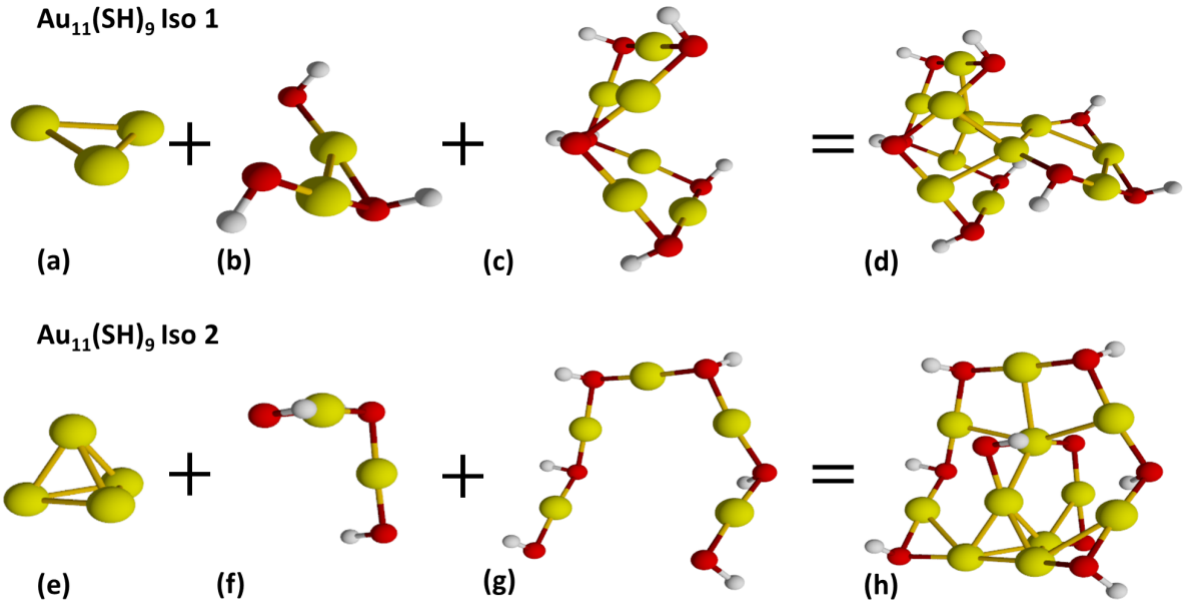

FIG. S2. Lowest energy isomers of $Au_{11}(SH)_9$ clusters. (a) Triangular core (Au_3), (b) Dimer motif ($Au_2(SH)_3$), (c) Cyclomer ($Au_6(SH)_6$), (d) Iso 1 of $Au_{11}(SH)_9$ cluster, (e) Tetrahedral core (Au_4), (f) Dimer motif ($Au_2(SH)_3$), (g) Pentamer motif ($Au_5(SH)_6$), (h) Iso 2 of $Au_{11}(SH)_9$ cluster. Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

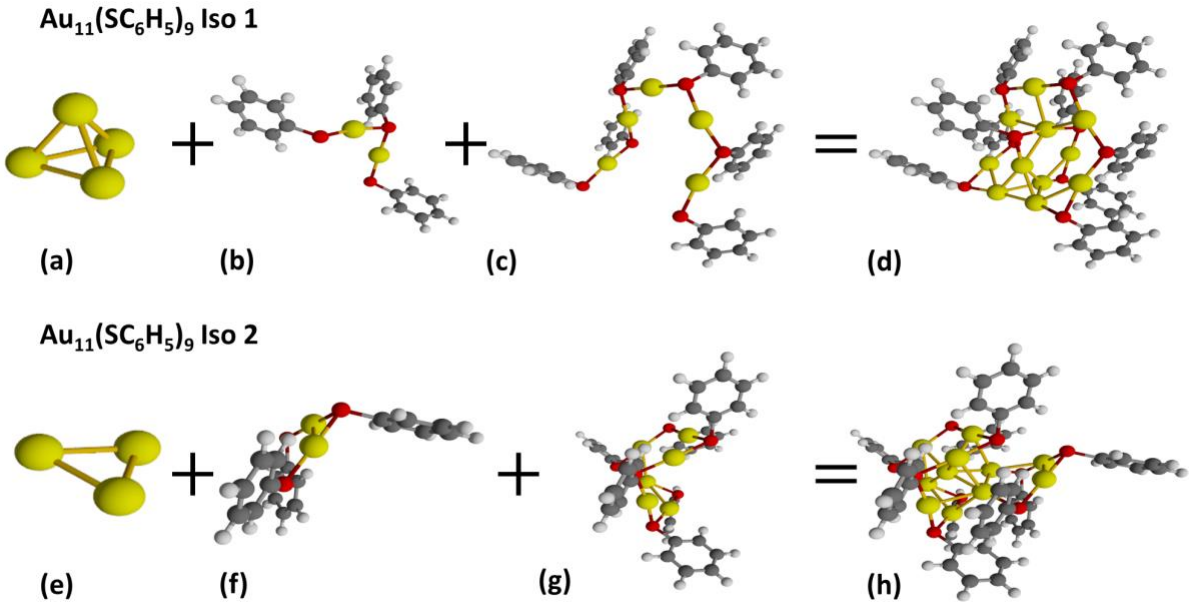

FIG. S3. Lowest energy isomers of $Au_{11}(SPh)_9$ clusters. (a) Tetrahedral core (Au_4), (b) Dimer motif ($Au_2(SPh)_3$), (c) Pentamer motif $Au_5(SPh)_6$, (d) Iso 1 of $Au_{11}(SPh)_9$ cluster, (e) Triangular core (Au_3), (f) Dimer motif ($Au_2(SPh)_3$), (g) cyclomer motif ($Au_6(SPh)_6$), (h) Iso 2 of $Au_{11}(SPh)_9$ cluster. Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

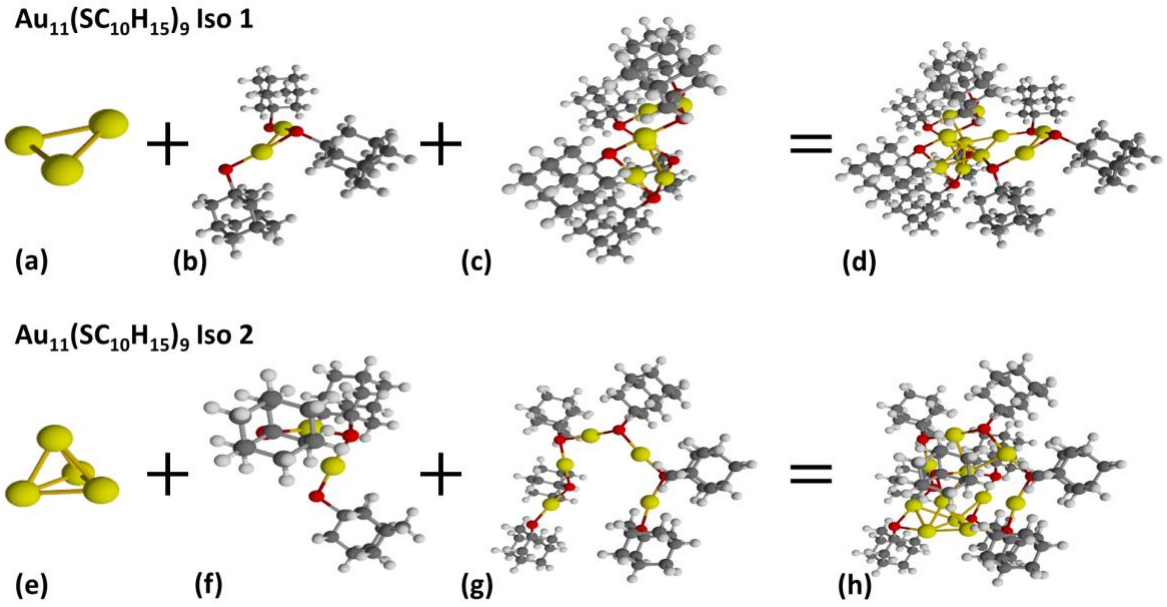

FIG. S4. Lowest energy isomers of $Au_{11}(SR)_9$ clusters with R= adamantly ($SC_{10}H_{15}$). (a) Triangular core (Au_3), (b) Dimer motif ($Au_2(SC_{10}H_{15})_3$), (c) cyclomer motif $Au_6(SC_{10}H_{15})_6$, (d) Iso 1 of $Au_{11}(SC_{10}H_{15})_9$ cluster, (e) Tetrahedral core (Au_4), (f) Dimer motif ($Au_2(SC_{10}H_{15})_3$), (g) pentamer motif motif ($Au_5(SC_{10}H_{15})_6$), (h) Iso 2 of $Au_{11}(SC_{10}H_{15})_9$ cluster. Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

TABLE S2. Relative energies (eV) of $Au_{13}(SCH_3)_{11}$ cluster isomers and calculated HOMO-LUMO gap values.

Isomer	**Configuración**	**Relative energy, (Relative energy w/correction) eV**	**HOMO-LUMO gap, eV**
-	$Au_4+Au_6(SCH_3)_6+Au_2(SCH_3)_3+Au(SCH_3)_2$	- (0.000)	1.9996
Iso1	$Au_4+Au_2(SCH_3)_3+Au_7(SCH_3)_8$	0.000 (0.52)	2.4075
Iso2	$Au_4+Au_4(SCH_3)_5+Au_5(SCH_3)_6$	0.013	1.1432
Iso3	$Au_3+Au_4(SCH_3)_5+Au_6(SCH_3)_6$	0.170	1.9728
Iso4	$Au_4+Au_3(SCH_3)_4+Au_6(SCH_3)_7$	0.187	0.8575
Iso5	$Au_6+3[Au_2(SCH_3)_3]+Au(SCH_3)_2$	0.990	0.1868

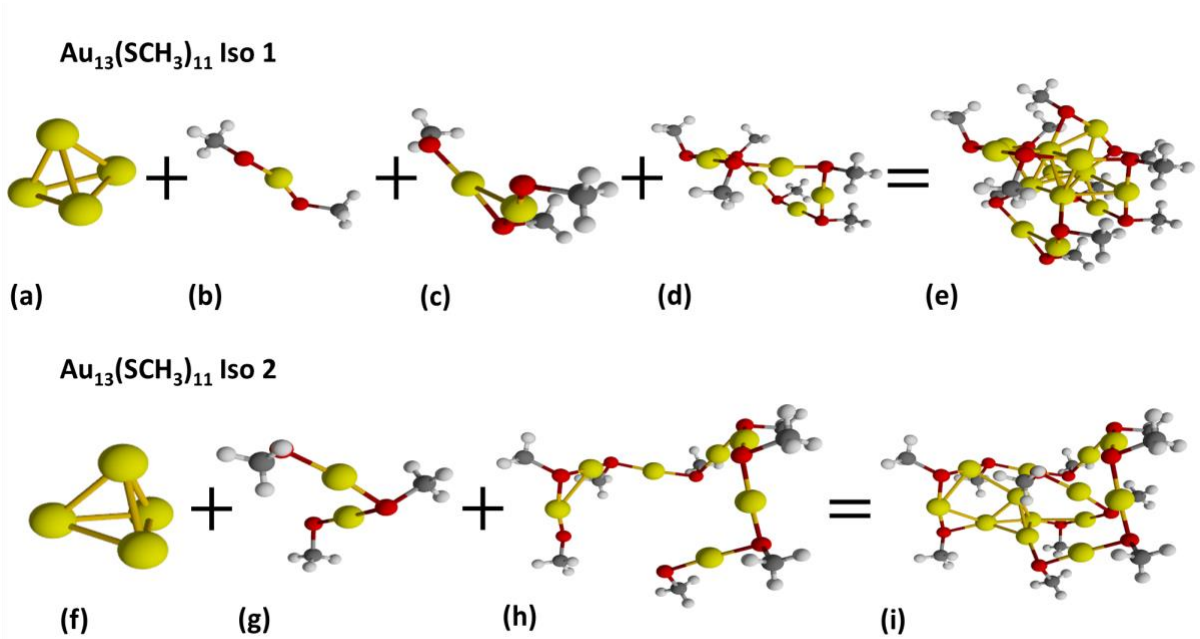

FIG. S5. Lowest energy isomers of $Au_{13}(SR)_{11}$ clusters with R= Methyl. (a) Tetrahedral core (Au_4), (b) monomer motif ($Au(SCH_3)_2$), (c) dimer motif $Au_2(SCH_3)_3$, (d) cyclomer ($Au_6(SCH_3)_6$), cluster, (e) Iso 1 of $Au_{13}(SCH_3)_{11}$ cluster, (f) Tetrahedral core (Au_4), (g) dimer motif ($Au_2(SCH_3)_3$), (h) heptamer motif ($Au_7(SCH_3)_8$), (i) Iso 2 of $Au_{13}(SCH_3)_{11}$ cluster . Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

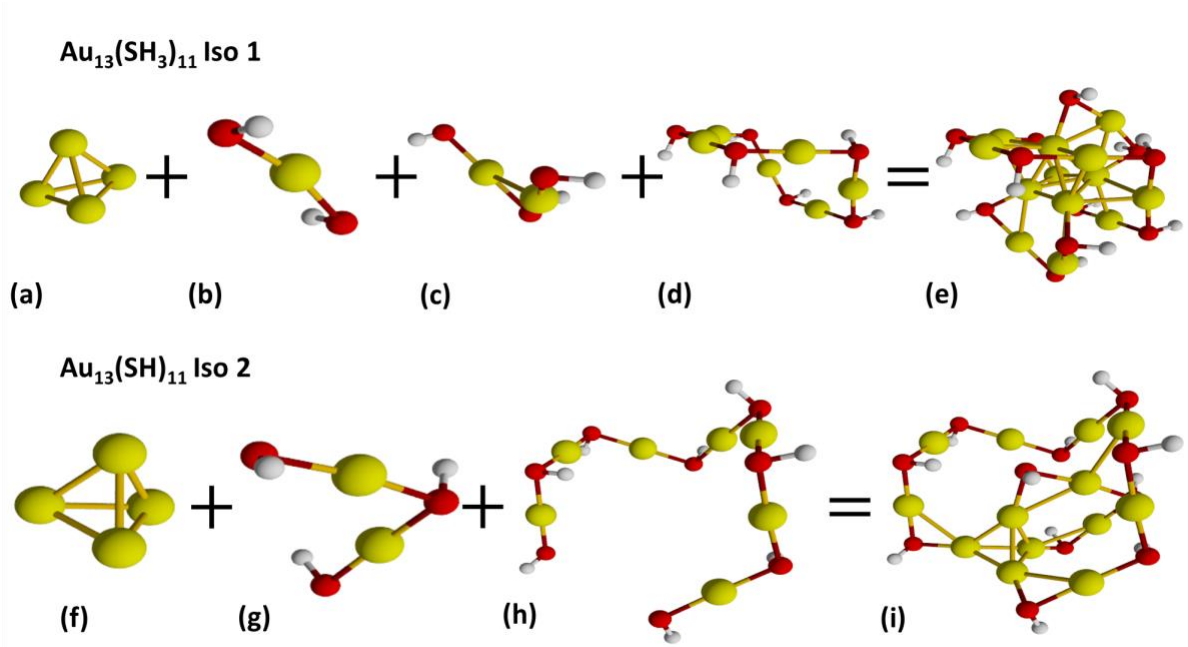

FIG. S6. Lowest energy isomers of $Au_{13}(SR)_{11}$ clusters with R= H. (a) Tetrahedral core (Au_4), (b) monomer motif ($Au(SH)_2$), (c) dimer motif $Au_2(SH)_3$, (d) cyclomer ($Au_6(SH)_6$), cluster, (e) Iso 1 of $Au_{13}(SH)_{11}$ cluster, (f) Tetrahedral core (Au_4), (g) dimer motif ($Au_2(SH)_3$), (h) heptamer motif ($Au_7(SH)_8$), (i) Iso 2 of $Au_{13}(SH)_{11}$ cluster . Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

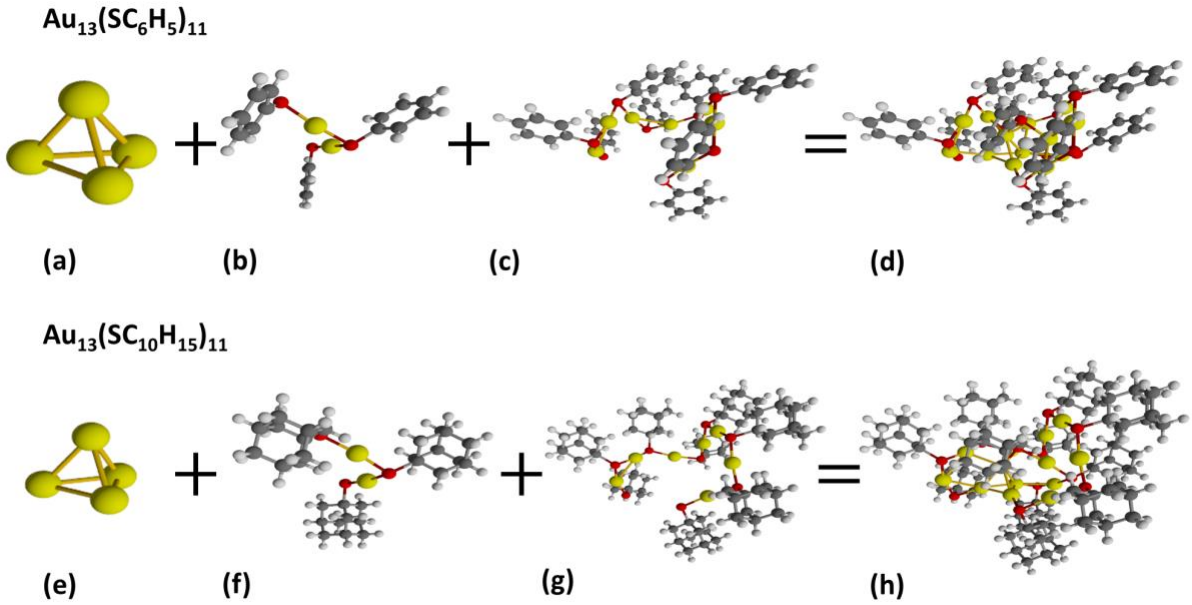

FIG. S7. Lowest energy isomers of $Au_{13}(SR)_{11}$ clusters with R= Ph, adamantyl. (a) Tetrahedral core (Au_4), (b) dimer motif ($Au_2(SPh)_3$), (c) heptamer motif $Au_7(SPh)_8$, (d) $Au_{13}(SC_6H_5)_{11}$ cluster, (e) Tetrahedral core (Au_4) cluster, (f) dimer motif ($Au_2(SC_{10}H_{15})_3$), (g) heptamer motif ($Au_7(SC_{10}H_{15})_8$), (h) $Au_{13}(SC_{10}H_{15})_{11}$ cluster. Color code: Gold atoms are shown in yellow, Sulphur atoms are red balls, Carbon atoms are displayed in gray, and Hydrogen atoms in white.

Lowest energy $Au_{13}(SCH_3)_{11}$ cluster

Au	-3.07362	-0.32455	-1.55762
Au	0.00013	-1.56694	1.27244
Au	-0.14492	-0.79978	-1.44721
Au	-1.30040	0.72907	0.61153
Au	0.51994	2.70071	1.93982
Au	2.14958	-3.31521	0.79888
Au	-1.25100	-3.43467	-0.70811
Au	-1.39476	2.96525	-1.08288
Au	1.50803	0.56914	0.19071
Au	0.72877	0.80788	-4.02945
Au	2.22585	-0.38652	2.91760
Au	2.58033	2.42370	-2.18754
Au	-2.27462	-0.66853	3.00533
S	-3.40233	-2.58404	-1.05162
S	0.16374	-1.41793	-3.72476
S	0.19773	4.16162	0.13926
S	3.62234	1.53408	-0.32286
S	3.54314	-2.22097	2.31442
S	0.90848	1.33775	3.79842
S	1.65196	2.93916	-4.26365
S	0.81501	-4.53658	-0.67087
S	-3.05375	1.88876	-2.32953
S	-0.83152	-2.44412	3.44187
S	-3.32349	1.16360	2.00529
C	3.96886	2.85522	0.89350
C	0.31570	4.16459	-4.00984
C	-1.48811	-1.69527	-4.46545

C	-4.57146	2.54380	-1.53288
C	-0.76262	5.55831	0.84331
C	2.03670	2.30621	4.87152
C	4.91096	-1.54423	1.30357
C	0.48670	-6.09468	0.23865
C	-4.21920	-2.57827	0.58371
C	-1.71910	-4.00136	3.06551
C	-2.99584	2.63940	3.03469
H	3.10297	3.51180	1.02554
H	4.21082	2.36733	1.84593
H	4.83156	3.43080	0.53837
H	-0.32569	3.89205	-3.16169
H	-0.27994	4.20570	-4.92904
H	0.78294	5.13844	-3.82477
H	-1.37274	-1.72497	-5.55510
H	-1.85304	-2.66329	-4.10165
H	-2.19171	-0.90726	-4.17916
H	-5.43186	2.04088	-1.98740
H	-4.62309	3.62085	-1.72818
H	-4.55057	2.35139	-0.45438
H	-1.04777	6.22207	0.01950
H	-1.65585	5.20283	1.36377
H	-0.11203	6.09317	1.54440
H	2.92826	2.62876	4.32695
H	2.32532	1.66648	5.71295
H	1.48754	3.18021	5.23922
H	4.53629	-0.88412	0.51507
H	5.45595	-2.38995	0.87013

H	5.57141	-0.98216	1.97401
H	0.04926	-5.89506	1.22020
H	-0.20512	-6.69376	-0.36394
H	1.43842	-6.62524	0.35481
H	-4.39356	-3.62038	0.87473
H	-5.17655	-2.05668	0.48080
H	-3.60137	-2.07060	1.33637
H	-2.53742	-4.13551	3.78122
H	-0.99562	-4.81894	3.17715
H	-2.10721	-3.99771	2.04105
H	-1.93887	2.69707	3.31735
H	-3.62266	2.59324	3.93169
H	-3.26614	3.52124	2.44020

Lowest energy $Au_{11}(SCH_3)_9$ cluster

Au	0.437350	1.556385	3.186755
Au	-1.209997	-0.643088	1.868135
Au	-0.553976	3.434415	1.570606
Au	-0.163033	3.885199	4.293973
Au	-1.385049	7.058258	3.898777
Au	-1.793725	6.396676	0.824962
Au	2.092391	-0.634745	2.474136
Au	3.248718	1.778996	4.267928
Au	-3.301565	2.260655	2.372778
Au	0.570300	1.907010	6.519415
Au	-2.684387	2.523097	5.473938
S	-0.307431	5.872425	5.568026
S	-2.464994	8.182235	2.164515
S	-0.964131	4.622955	-0.415048

S	0.339222	-2.136478	2.771969
S	3.920995	0.795377	2.259148
S	-2.840613	0.617698	0.784071
S	2.741413	2.735848	6.324234
S	-3.876754	3.861365	3.975935
S	-1.578425	1.132838	6.974262
C	-4.254994	7.902249	2.478810
C	-2.421479	3.862371	-1.229756
C	3.476066	2.002881	0.948227
C	-4.330608	-0.458731	0.790309
C	0.572761	-3.391661	1.448323
C	3.746002	1.819172	7.557516
C	1.409048	6.525666	5.589952
C	-1.678236	-0.534128	6.206998
C	-5.650503	3.557371	4.355608
H	-4.801837	8.156074	1.563480
H	-4.560653	8.573250	3.289452
H	-4.451053	6.863533	2.760111
H	-2.741124	4.532619	-2.036274
H	-3.239065	3.702651	-0.521038
H	-2.106102	2.899419	-1.646167
H	3.531305	1.487690	-0.017154
H	4.215275	2.810958	0.981395
H	2.469265	2.404902	1.108024
H	-4.127019	-1.323225	0.148135
H	-5.161723	0.121742	0.373092
H	-4.581006	-0.793430	1.800249
H	-0.330354	-4.011432	1.413879

H	1.435695	-4.010111	1.720314
H	0.739322	-2.922817	0.474856
H	4.796761	2.094537	7.409149
H	3.623427	0.737533	7.452419
H	3.417068	2.136996	8.553592
H	1.384584	7.516607	6.057652
H	1.822571	6.596120	4.580558
H	2.015480	5.840809	6.193929
H	-2.714844	-0.879032	6.297327
H	-1.014863	-1.202976	6.766097
H	-1.385389	-0.508132	5.152975
H	-6.246703	3.947097	3.522318
H	-5.893480	4.107639	5.271904
H	-5.856515	2.493376	4.496605