

Electronic Supplementary Materials

Unraveling a Generic Growth Pattern in Structure Evolution of Thiolate-Protected Gold Nanoclusters

Wen Wu Xu,¹ Yadong Li,^{1,3} Yi Gao*,^{1,2,4} Xiao Cheng Zeng*^{4,5}

¹*Division of Interfacial Water and Key Laboratory of Interfacial Physics and Technology, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China.*

²*Shanghai Science Research Center, Chinese Academy of Sciences, Shanghai 201204, China*

³*University of Chinese Academy of Sciences, Beijing 100049, China*

⁴*Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, USA*

⁵*Collaborative Innovation Center of Chemistry for Energy Materials, University of Science and Technology of China, Hefei, Anhui 230026, China*

Correspondence Email: gaoyi@sinap.ac.cn, xzengl@unl.edu

Fig. S1. Optimized structures of Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, Au₅₂(SR)₃₂, Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. Red and yellow denote S and Au atoms, respectively. Methyl groups are omitted for clarity.

Fig. S2. The structures of Au₂₈(S-c-C₆H₁₁)₂₀ (a), Au₂₈(TBBT)₂₀ (c), and their Au₂₀ kernels (b and d). Red and yellow denote S and Au atoms in the staple, respectively. The Au₂₀ kernels are in olive. Ligands are omitted for clarity.

Fig. S3. Computed nucleus-independent chemical shift (NICS) grid for Au₂₀(SR)₁₆, Au₂₈(SR)₂₀, Au₃₆(SR)₂₄, Au₄₄(SR)₂₈, and Au₅₂(SR)₃₂ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au₄ units are in red. The green (0) and blue (1-10) balls denote the centers of total structure and the tetrahedron Au₄ unit, respectively.

Fig. S4. The double-helix structures of Au₃₈ in Au₆₀(SR)₃₆, Au₄₄ in Au₆₈(SR)₄₀, and Au₅₀ in Au₇₆(SR)₄₄. The Au atoms are in olive and wine, respectively.

Fig. S5. Computed (red line) and experimental (black line) (a) XRD and (b) optical absorption spectra.

Fig. S6. Computed nucleus-independent chemical shift (NICS) grid for Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au₄ units are in red. The green (0) and blue (1-16) balls denote the centers of total structure and the tetrahedron Au₄ unit, respectively.

Table S1. Computed nucleus-independent chemical shift (NICS) values of Au₆₀(SR)₃₆, Au₆₈(SR)₄₀, and Au₇₆(SR)₄₄. “0” denotes the NICS values at the center of the total structures. “1-16” denote the NICS values at the centers of tetrahedron Au₄ units of these clusters (ESI Fig. S6).

Coordinates file of optimized structure of Au₆₀(SCH₃)₃₆

Coordinates file of optimized structure of Au₆₈(SCH₃)₄₀

Coordinates file of optimized structure of Au₇₆(SCH₃)₄₄

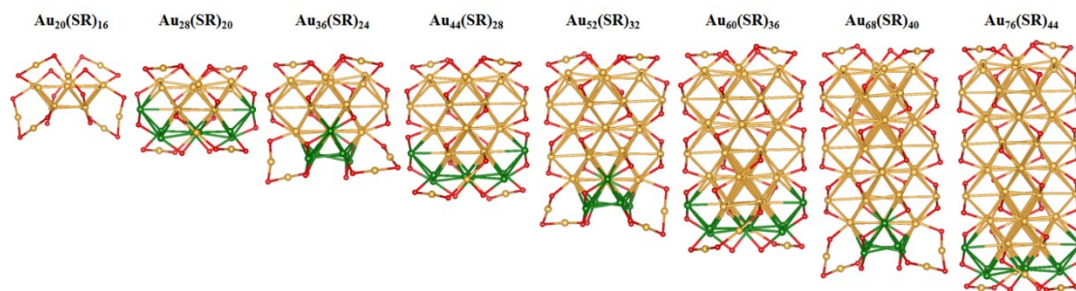


Fig. S1. Optimized structures of $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, $\text{Au}_{52}(\text{SR})_{32}$, $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$. Red and yellow denote S and Au atoms, respectively. Methyl groups are omitted for clarity.

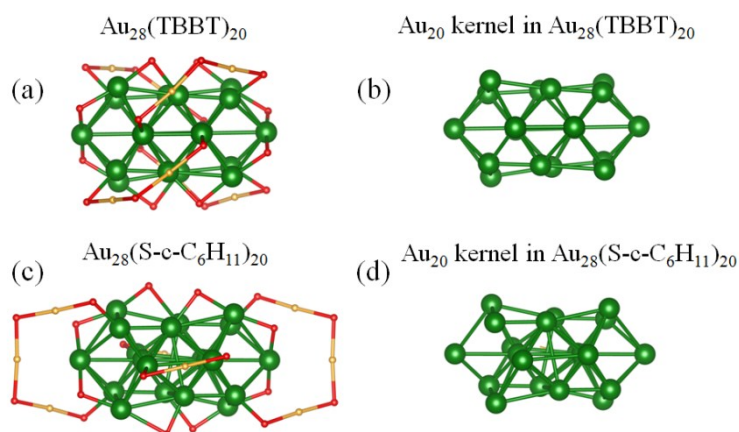


Fig. S2. The structures of $\text{Au}_{28}(\text{S-c-C}_6\text{H}_{11})_{20}$ (a), $\text{Au}_{28}(\text{TBBT})_{20}$ (c), and their Au_{20} kernels (b and d). Red and yellow denote S and Au atoms in the staple, respectively. The Au_{20} kernels are in olive. Ligands are omitted for clarity.

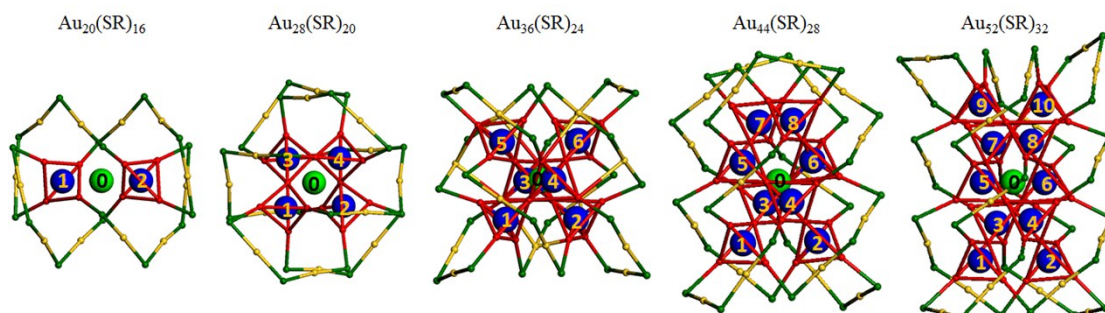


Fig. S3. Computed nucleus-independent chemical shift (NICS) grid for $\text{Au}_{20}(\text{SR})_{16}$, $\text{Au}_{28}(\text{SR})_{20}$, $\text{Au}_{36}(\text{SR})_{24}$, $\text{Au}_{44}(\text{SR})_{28}$, and $\text{Au}_{52}(\text{SR})_{32}$ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au_4 units are in red. The green (0) and blue (1-10) balls denote the centers of total structure and the tetrahedron Au_4 unit, respectively.

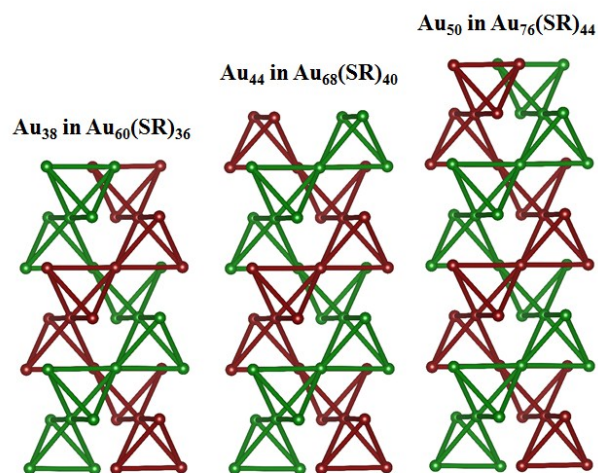


Fig. S4. The double-helix structures of Au₃₈ in Au₆₀(SR)₃₆, Au₄₄ in Au₆₈(SR)₄₀, and Au₅₀ in Au₇₆(SR)₄₄. The Au atoms are in olive and wine, respectively.

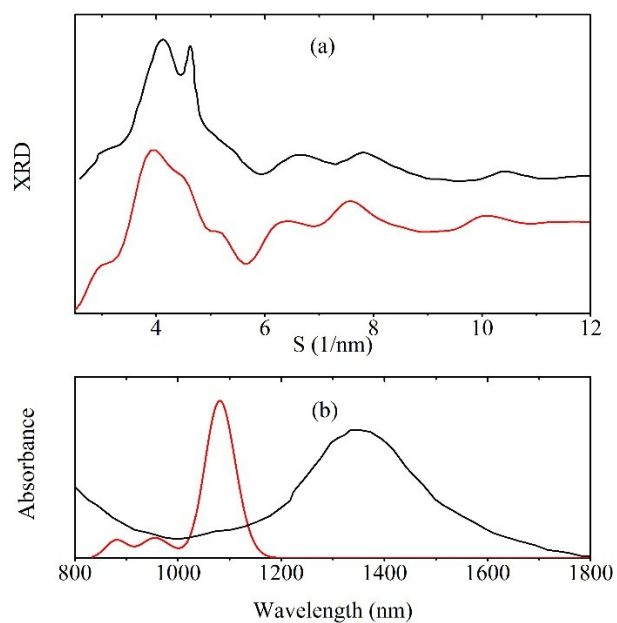


Fig. S5. Computed (red line) and experimental (black line) (a) XRD and (b) optical absorption spectra.

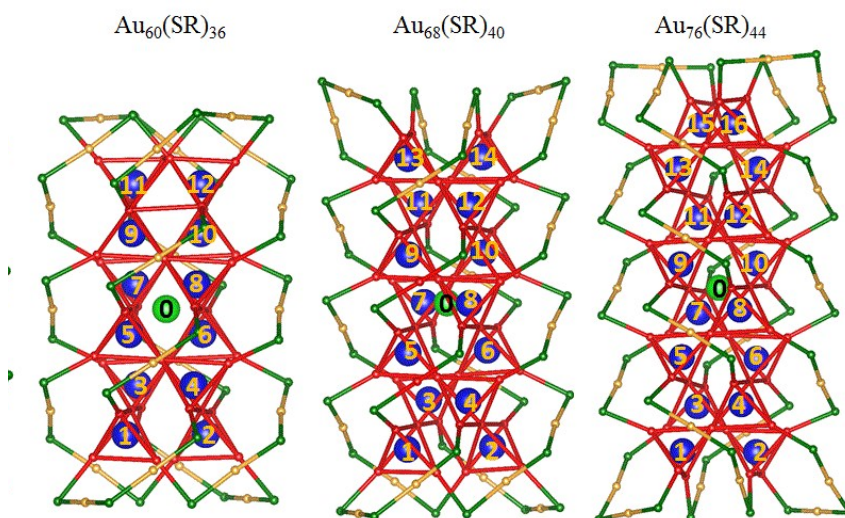


Fig. S6. Computed nucleus-independent chemical shift (NICS) grid for $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$ clusters. Olive and yellow denote S and Au atoms, respectively. The tetrahedron Au_4 units are in red. The green (0) and blue (1-16) balls denote the centers of total structure and the tetrahedron Au_4 unit, respectively.

Table S1. Computed nucleus-independent chemical shift (NICS) values of $\text{Au}_{60}(\text{SR})_{36}$, $\text{Au}_{68}(\text{SR})_{40}$, and $\text{Au}_{76}(\text{SR})_{44}$. “0” denotes the NICS values at the center of the total structures. “1-16” denote the NICS values at the centers of tetrahedron Au_4 units of these clusters (ESI Fig. S6).

	$\text{Au}_{60}(\text{SR})_{36}$	$\text{Au}_{68}(\text{SR})_{40}$	$\text{Au}_{76}(\text{SR})_{44}$
0	-15.6	-9.7	-15.1
1	-25.5	-23.4	-24.5
2	-24.0	-22.0	-21.1
3	-23.9	-22.1	-20.8
4	-22.0	-24.0	-24.0
5	-21.3	-24.1	-22.7
6	-25.2	-24.2	-19.2
7	-26.5	-26.7	-21.4
8	-22.6	-25.1	-27.9
9	-23.7	-23.1	-26.9
10	-24.0	-20.8	-23.1
11	-22.4	-23.5	-21.8
12	-25.8	-23.1	-21.1
13		-24.5	-18.8
14		-25.8	-22.0
15			-24.0
16			-26.6

Coordinates of the optimized structure of Au₆₀(SCH₃)₃₆

Au	17.122707048	4.404385117	25.201650990
Au	14.486219184	3.471272597	26.314130598
Au	16.326299973	1.452006454	24.891069256
Au	14.833251322	3.443896836	23.292916987
Au	16.931743602	4.338248168	28.105233061
Au	15.887734923	1.555299472	27.833564944
Au	12.315527616	2.453256387	24.249125914
Au	16.731513588	1.411276358	21.905771177
Au	15.052150645	6.297644304	26.620923421
Au	17.235840616	1.587450055	19.118350560
Au	13.070383233	2.812941121	18.082714115
Au	19.736041069	2.386332135	20.714158594
Au	14.089709735	0.547265915	23.002085600
Au	17.220117822	-3.832557345	23.451820410
Au	12.756621450	2.607989455	21.485827123
Au	11.468271780	7.947492382	27.788657227
Au	12.939436545	5.562273061	24.984701542
Au	20.121637195	5.441429358	24.042320289
Au	13.880421864	0.670626879	26.100089090
Au	18.613015792	2.517181901	26.863394470
Au	13.261704620	8.923055167	24.732875197
Au	13.118156416	5.649261554	21.539005008
Au	15.604210876	6.208594809	23.658162368
Au	14.108967085	3.397278071	29.753431261
Au	18.858390635	2.209097923	23.648012010
Au	17.324714079	4.435326756	22.342855120
Au	17.959353140	7.707644225	25.552974208
Au	12.776883876	5.161004860	27.784283216
Au	11.194250970	-0.375320525	24.292578277
Au	15.421335464	-1.538283650	24.496215616
Au	14.537766056	0.581686327	19.935342963
Au	19.238206692	5.281909957	26.843263888
Au	15.416017792	3.362648951	20.277415762
Au	18.071636173	-0.478864813	23.634711751
Au	15.799877493	-1.529392805	21.633258526
Au	11.474100796	2.496901000	27.575836144
Au	13.237936017	-2.163942699	22.864454894
Au	17.976436244	-0.732851244	26.678207677
Au	18.678102935	1.804787870	30.293106977
Au	20.803633075	4.700684158	29.452277517
S	20.970115188	3.274362939	24.359074176

S	20.543048850	0.183019244	20.392186036
S	19.293724451	4.703766977	20.913993965
S	15.224116824	-5.100633700	23.544094465
S	11.508412710	9.614215299	26.151921485
S	10.416954161	3.233867306	25.613739080
S	10.123445154	0.295148984	22.285977006
S	16.013040279	-2.029888901	26.840624462
S	19.978684877	0.518056785	26.587034621
S	16.860709207	0.420687048	29.776041790
S	14.869431102	2.855566693	16.546870455
S	11.382673865	5.714870470	23.139258116
S	12.378755992	1.782774351	29.648261940
S	11.918954586	-0.743186015	26.516671446
S	11.236583268	2.785899706	19.571122027
S	14.508910589	5.560422644	19.637578141
S	14.761164743	8.412502586	23.004865416
S	19.255171543	-2.633206429	23.403795248
S	21.047041460	6.507305272	27.967051461
S	20.703202968	2.860408393	30.889225932
S	11.251896424	6.238228095	29.388498210
S	19.439623542	7.683085591	23.708380568
Au	18.320477278	-0.815690304	20.577180890
Au	11.935970107	-0.463057873	20.830420198
Au	16.367937206	-1.482188959	18.624411700
Au	13.661005674	-2.335315525	19.668247283
Au	12.450833901	-0.356791679	18.072401813
Au	15.209129576	0.490668812	16.940064416
Au	17.539951809	-3.484703245	20.242756303
Au	14.813172145	-4.500631764	21.222878165
Au	15.307329569	-4.410559096	18.489972314
Au	14.373257324	-2.184602938	16.639343153
Au	16.963577647	-1.469770843	15.868177725
Au	12.704804686	-4.945303484	19.365149171
S	11.200218383	0.608718871	16.206111135
S	17.816666216	-1.642502703	13.592398691
Au	12.352851865	-0.127978247	14.307805332
Au	15.593165718	-1.155885775	12.991331231
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S	11.474664584	-7.030952360	19.006174677
S	18.692940803	-5.574877254	20.797716185
Au	13.556883655	-7.976993167	19.555415680
Au	17.060899149	-7.197271580	20.362670180
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S	18.487516674	1.630813769	16.992887531

S	16.516281046	-5.114513070	16.497128822
Au	19.343289484	-0.529475605	17.346204866
Au	18.389811242	-3.829262600	17.114292659
S	20.388643594	-2.644997516	17.539272866
S	12.633371117	-3.447668311	15.495358527
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Au	10.676593293	-3.414589593	20.859736532
Au	11.208717472	-3.182132085	17.348207950
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C	20.419761360	3.562106475	32.560224154
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C	22.303352883	3.138666586	23.104067604
C	18.801344304	5.280892486	19.248877355
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C	21.518601416	-0.250711288	21.879950856
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C	20.901722322	0.119530164	28.120314150
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C	15.721912721	0.574162098	31.203639768
C	12.113420603	11.128034657	26.993389492
C	12.318661226	6.765653851	30.786972045
C	10.635188808	7.382874572	22.996286264
C	8.964946799	2.133520171	25.405368877
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C	21.300006785	-2.787801189	15.948758822
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C	20.003844170	-5.894196301	19.558936857
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H	20.245788771	0.109041063	29.000705785
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H	13.063783828	10.955527363	27.508524307
H	11.347319342	11.436611357	27.715216998
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H	11.823244151	7.595321399	31.306807706
H	9.961288095	7.520642286	23.852051825
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H	9.224545456	1.080634258	25.574307479
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H	11.603683436	2.387841582	31.859695941
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H	13.108326361	-2.518238043	27.601056795
H	8.974506693	-1.870255042	22.145358061
H	8.200762369	-0.598968833	21.155341582
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H	9.653845504	-1.287329956	15.993244913
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H	16.529672585	-7.098673084	22.937626316
H	14.858036993	-7.478097423	23.468814275
H	16.103353419	-7.034434558	24.685103354
H	10.288938867	-8.352436593	20.652942682
H	9.573114094	-6.714641479	20.458296360
H	11.063288814	-6.919055821	21.424942741
H	16.200611006	-9.465989479	17.925178864
H	15.349563474	-10.836898636	18.711515516
H	17.059365497	-10.486433669	19.127606660
H	19.613241370	-5.834218864	18.534298989
H	20.430585107	-6.887248215	19.755507883
H	20.771442012	-5.120781193	19.690932384
H	15.215948638	9.655225575	26.339932522
H	16.539002831	10.382818046	27.335581914
H	15.079162084	9.693328413	28.125212177
H	17.531650994	5.336657188	31.613486538
H	17.142243774	3.601380787	31.389007613
H	16.079026613	4.644888550	32.416298427

Coordinates file of optimized structure of Au₆₈(SCH₃)₄₀

Au	16.934049356	4.480996238	25.254217901
Au	14.393569619	3.474283331	26.408604898
Au	16.265033364	1.497309120	24.946649020
Au	14.743963327	3.455632067	23.337117550
Au	16.652384914	4.465900112	28.263833666
Au	15.913909126	1.424952510	27.787265363
Au	12.253156810	2.411699124	24.320028414
Au	16.652228296	1.476222336	21.922749449
Au	15.001784693	6.403038922	26.663639009
Au	16.522731505	4.436869149	31.052728087
Au	17.142122883	1.650130445	19.126681893
Au	13.223415965	8.680015919	24.786194318
Au	12.939244397	2.775223608	18.119669340
Au	19.196482386	5.661473009	30.422604547
Au	15.468737680	9.151357798	26.738485147
Au	19.634050418	2.513249395	20.720245521
Au	12.946955934	8.722520500	28.288773262
Au	14.040340595	0.543095747	23.030220182
Au	17.274421342	-3.758111332	23.437541424

Au	12.661716709	2.563259274	21.543449532
Au	11.706408768	5.391237047	31.395921060
Au	12.883286307	5.561194349	25.020702825
Au	19.804491238	5.617599725	24.066164660
Au	13.835318391	0.627408419	26.103908749
Au	18.443284060	2.697740184	26.989833100
Au	14.619107798	4.707500813	33.524674112
Au	12.965763135	5.587081703	21.555414559
Au	15.388374469	6.240714045	23.551854281
Au	14.254179252	3.517243717	29.589230128
Au	18.740110678	2.342547964	23.694965806
Au	17.193132783	4.492585734	22.346082655
Au	17.370615356	7.468999949	25.504171448
Au	12.648022339	5.410855278	27.806560245
Au	11.168513313	-0.460232075	24.325538669
Au	15.438182084	-1.511799946	24.486865017
Au	14.472437936	0.582518535	19.952479868
Au	19.043031374	5.442333817	26.997774498
Au	15.289921298	3.381302921	20.291364900
Au	18.048864856	-0.372124190	23.639191715
Au	15.792298767	-1.499014788	21.639362961
Au	14.779930752	6.224572939	29.795332762
Au	11.652647743	2.368090112	27.732520253
Au	13.249579174	-2.195687471	22.880834794
Au	18.287637218	2.222738624	30.141902966
Au	17.937388997	-0.634484554	26.692166949
Au	17.115044111	7.483157787	28.322405535
Au	17.905763111	11.250423874	27.349203909
Au	20.582262285	8.755486919	27.803969271
S	20.790279353	3.505038804	24.422823553
S	20.234702030	3.536640479	30.426812584
S	16.844860165	3.962740238	33.437015391
S	20.491888590	0.329507665	20.413855424
S	19.145583265	4.820329570	20.908662972
S	15.320180086	-5.092359253	23.543053547
S	12.433887529	5.517805176	33.632827703
S	15.660787200	11.574860013	26.723774198
S	10.464209945	3.128693738	25.839848417
S	10.081920686	0.214136204	22.332705730
S	16.053495179	-2.059748568	26.820275274
S	19.870729268	0.722387948	26.681307629
S	16.410342175	0.803591575	30.120537122
S	11.547761844	9.026588173	26.421740520
S	14.727722378	2.868294087	16.571605053

S	11.262698810	5.616414086	23.196064944
S	12.781322567	1.588931081	29.661002454
S	11.918541416	-0.855082125	26.534442674
S	18.514864313	7.907904383	30.271107266
S	11.125365986	2.693843728	19.629824927
S	14.307230160	5.533414631	19.613558567
S	14.528324242	8.439371560	22.849238638
S	14.278227855	8.582152117	30.216906833
S	19.273780918	-2.497630310	23.394045936
S	21.121886597	6.478430836	27.784482463
S	20.122546102	11.048326816	28.070013254
S	10.701052559	5.357758324	29.283893100
S	18.889901915	7.757780666	23.634054853
Au	18.290581968	-0.716334213	20.583788797
Au	11.906661140	-0.512673599	20.869066172
Au	16.344820973	-1.430099235	18.634262732
Au	13.659640803	-2.359932617	19.691260069
Au	12.402579934	-0.407581425	18.102409514
Au	15.126082000	0.512667565	16.955776218
Au	17.573280583	-3.407997421	20.228052557
Au	14.874595904	-4.501198628	21.226206721
Au	15.351015849	-4.396086181	18.496032969
Au	14.367043913	-2.188964383	16.660235385
Au	16.929108161	-1.395117235	15.873098627
Au	12.761885740	-4.984327437	19.383318087
S	11.115180772	0.538566384	16.250365001
S	17.761719549	-1.560077200	13.587304723
Au	12.274919162	-0.156352113	14.339514707
Au	15.521595828	-1.126032017	13.005006550
S	13.349685208	-0.607537726	12.295547856
S	11.559166376	-7.081571377	19.010542205
S	18.762907942	-5.478207221	20.781687504
Au	13.661403651	-7.980025438	19.563133073
Au	17.159369637	-7.131726534	20.354606657
S	15.666605286	-8.955231294	20.255804573
S	18.387494806	1.732706135	16.997065944
S	16.574480860	-5.056294342	16.497937739
Au	19.292650053	-0.408411549	17.350954228
Au	18.414680190	-3.721492599	17.116062770
S	20.389202021	-2.496522506	17.541844492
S	12.642897308	-3.475880630	15.523587133
S	11.752045406	-4.177762342	22.875096862
Au	10.706654768	-3.486344199	20.883327941
Au	11.216813273	-3.241723501	17.380482060

C	22.382647453	6.287488221	26.468268384
C	21.112381171	11.901160986	26.779493743
C	15.830128216	9.726195681	22.936176751
C	20.126578864	8.991377498	24.184382989
C	22.129243645	3.409621314	23.169976941
C	18.624802324	5.378462833	19.245834961
C	15.501144345	6.913377754	19.762007074
C	21.474809326	-0.058495085	21.909610498
C	20.146380064	-2.844675967	24.967124502
C	20.721240022	0.359880960	28.263679066
C	16.700430174	-3.771417974	26.902072185
C	20.665438413	3.207526897	32.181237857
C	17.097231946	-0.893800250	30.171646692
C	17.461546329	8.248316716	31.731287998
C	17.803289970	5.343384416	34.184871453
C	11.483399274	4.209868227	34.506109852
C	9.838466122	6.971907942	29.183520944
C	13.112658899	8.695355931	31.626679024
C	11.284310559	10.844029728	26.341701010
C	10.490343775	7.272097628	23.040044244
C	9.019527000	2.011859411	25.672625697
C	11.613775271	1.786445160	31.060677103
C	12.512408900	-2.578380784	26.695538998
C	8.652248061	-0.917745398	22.165940002
C	10.335546564	4.347339624	19.572239942
C	13.986445505	3.060831885	14.906050300
C	9.491594883	-0.305619983	16.126954485
C	12.655444334	-2.230471283	11.783468381
C	17.944812583	-3.358825123	13.257453579
C	19.872174780	2.810245538	17.078108144
C	21.302911430	-2.615924115	15.950431840
C	17.096910052	-6.795490892	16.736073446
C	13.098601269	-5.251190673	15.472125157
C	8.423698162	-4.417381637	18.639589658
C	10.423955799	-4.007779961	24.130406798
C	14.873793540	12.144891746	28.284840438
C	15.894833452	-6.829457856	23.668805872
C	10.593123942	-7.352351190	20.553424513
C	16.235640279	-10.004401953	18.862046321
C	20.078380142	-5.774703250	19.541486415
S	9.471310315	-2.939473279	18.947832955
H	22.027456356	6.678324964	25.506048658
H	22.582132188	5.212928981	26.366544127
H	23.291641957	6.813620122	26.789980594

H	20.933163337	11.476070589	25.785709114
H	22.171731003	11.792969079	27.046026100
H	20.833086418	12.962367569	26.788648483
H	15.350551404	10.699289850	22.766765626
H	16.557399629	9.516099757	22.140671854
H	16.333226056	9.713946611	23.910668976
H	20.970407483	8.975514697	23.481495304
H	20.469776317	8.782579261	25.209259435
H	19.640821964	9.976724885	24.163710927
H	21.739640850	3.508072461	22.148418776
H	22.621078914	2.435912774	23.292513133
H	22.847979848	4.213172335	23.381529627
H	17.800090472	4.767999978	18.856408039
H	19.496612775	5.321439283	18.582177025
H	18.312015256	6.425458262	19.342435088
H	16.067129877	6.951416880	18.821925696
H	16.174572540	6.764192995	20.615403180
H	14.933202939	7.841974036	19.895864067
H	22.432951938	0.471841515	21.827040955
H	21.644516245	-1.143155321	21.915648486
H	20.945661998	0.238895190	22.823712386
H	20.473859644	-3.892803377	24.952564148
H	19.501803465	-2.649855284	25.835455479
H	21.019202379	-2.178551307	25.013449226
H	21.148951498	-0.649908419	28.204558459
H	20.030958555	0.438588265	29.115392152
H	21.522355268	1.101403865	28.383982834
H	17.387719904	-3.979898722	26.069562933
H	15.839792408	-4.450901698	26.831384415
H	17.205299826	-3.906643188	27.868409940
H	21.394884932	3.961262404	32.502715896
H	21.119780403	2.209330294	32.230173134
H	19.774321252	3.238316261	32.819549304
H	17.867904604	-1.040611207	29.402648072
H	16.266574163	-1.587013637	29.981370270
H	17.510367639	-1.064195548	31.175404454
H	16.973429126	9.216995573	31.566744345
H	18.121230467	8.302886290	32.607763780
H	16.702559291	7.467820692	31.863893984
H	18.803323454	5.355761348	33.731602337
H	17.881065384	5.153073863	35.263657068
H	17.314085633	6.306821652	34.014428051
H	11.616382869	3.233562709	34.028549685
H	10.424691519	4.497853096	34.487994633

H	11.839801282	4.173008496	35.542606427
H	9.022439100	6.972585770	29.917425646
H	9.433509696	7.061977663	28.167498404
H	10.527664650	7.807140030	29.369094731
H	12.278696019	7.989170247	31.513231005
H	12.739839546	9.726016942	31.684565676
H	13.669930770	8.448676938	32.539532603
H	10.681860793	11.143777194	27.209210018
H	10.735710192	11.060863356	25.416798145
H	12.241236206	11.378026885	26.338791155
H	9.821807621	7.409383298	23.900301157
H	9.908397188	7.282658842	22.107792103
H	11.240565323	8.072301557	23.029027549
H	9.298952757	0.959786420	25.812848954
H	8.607718446	2.152532944	24.664104673
H	8.281653410	2.315736698	26.426867206
H	10.836706423	1.017062970	30.961202479
H	11.158627908	2.785334405	31.073809496
H	12.181325772	1.624417065	31.986218294
H	13.178800831	-2.609282037	27.567633030
H	13.058162189	-2.905147116	25.801401883
H	11.637059250	-3.216993232	26.871998782
H	8.968846516	-1.970259822	22.182222917
H	8.171556768	-0.706084877	21.201648707
H	7.953495848	-0.712373325	22.988856687
H	9.678260146	4.430277530	20.448094427
H	9.742043999	4.396061618	18.648946272
H	11.079447668	5.152823464	19.591904256
H	14.780846983	2.879718860	14.169574635
H	13.621844346	4.092794967	14.817104908
H	13.162734249	2.353944323	14.739911849
H	9.610594184	-1.382282182	15.954677594
H	8.937390725	0.158325426	15.300829291
H	8.963655333	-0.140697311	17.074268445
H	12.679806888	-2.947333109	12.612098526
H	13.247378144	-2.597398675	10.934835387
H	11.618038698	-2.060541124	11.466815358
H	17.952488793	-3.510943051	12.169929126
H	17.134188060	-3.932262664	13.719846860
H	18.903245819	-3.682518416	13.685792577
H	19.545243747	3.830605082	16.841593144
H	20.579732792	2.468589938	16.312599590
H	20.341521051	2.782725554	18.070815937
H	20.670626721	-2.303187211	15.111384062

H	21.631076241	-3.655065354	15.816079602
H	22.179375351	-1.957865904	16.018089774
H	17.882280835	-7.031374956	16.005597895
H	16.215681965	-7.424728006	16.553554655
H	17.456688240	-6.964076547	17.762593111
H	13.421091652	-5.606424973	16.457424671
H	13.919863509	-5.362219914	14.751875297
H	12.218789629	-5.815000183	15.133956308
H	9.036431591	-5.323531317	18.572133918
H	7.894094911	-4.258295353	17.691481552
H	7.697661812	-4.505061379	19.458306155
H	10.801480048	-4.443614965	25.064535348
H	9.547240102	-4.575667848	23.792309130
H	10.162422929	-2.951567457	24.295335835
H	15.096268885	11.462059903	29.112548459
H	13.788031525	12.176190491	28.122982446
H	15.246300354	13.153375680	28.506924307
H	16.263172147	-6.989381091	24.691835144
H	16.689052735	-7.049926697	22.943515509
H	15.031438711	-7.480715005	23.479441221
H	11.176054340	-7.073524892	21.437890718
H	10.308355581	-8.411600512	20.597027095
H	9.693979787	-6.723865892	20.503042627
H	16.337575755	-9.431051050	17.935536418
H	15.499629371	-10.807274089	18.727614408
H	17.204435070	-10.435308969	19.145824690
H	19.684729345	-5.724633737	18.517707027
H	20.524596567	-6.758824517	19.739304698
H	20.830489527	-4.985699832	19.670637907

Coordinates of the optimized structure of Au₇₆(SCH₃)₄₄

Au	16.784098294	4.277115656	25.195007697
Au	14.406185599	3.161392825	26.611765110
Au	16.267022236	1.306532022	25.014326831
Au	14.429355704	3.127339129	23.551895135
Au	17.354323962	7.228243372	28.446990288
Au	16.711863804	4.252383225	28.265162552
Au	17.206874769	7.287837304	31.526295277
Au	17.988844947	10.212800088	31.696725906
Au	17.549551746	10.142966759	34.879284801
Au	16.179862350	1.466979727	28.236948931
Au	12.200812909	2.118502199	25.112689191
Au	16.268917019	1.350923173	21.945858687

Au	14.931056809	6.286308874	29.841486577
Au	14.991213593	6.173777592	26.759805097
Au	15.570208500	9.247019317	29.984027988
Au	15.399990706	9.301243007	32.953598466
Au	16.360714689	12.203557448	33.029922912
Au	16.374231031	1.451647392	18.417569803
Au	17.985352587	-0.217700192	20.402031844
Au	19.097032396	2.554531147	20.173863342
Au	13.917302320	0.140532050	23.451985645
Au	11.990023479	1.747700933	21.915365448
Au	12.693619979	4.873363675	25.034254710
Au	13.116680922	8.228759616	25.143388214
Au	19.449562748	5.422307669	23.582607007
Au	20.076821460	8.290523253	26.889329635
Au	13.806437306	11.410359811	28.313178513
Au	20.811782677	11.331720500	30.197062941
Au	14.058653576	0.114969175	26.337428264
Au	18.463837098	2.414989268	26.513967140
Au	12.384901174	5.120404382	21.984621489
Au	15.071027229	6.195921400	23.878044224
Au	18.932503746	5.335060488	29.853241083
Au	14.399035572	3.181616739	29.549043670
Au	14.807855740	6.282254439	32.704571785
Au	19.327605377	8.161960081	33.177367038
Au	14.957738024	9.362997252	35.689233494
Au	18.552138439	2.538288490	23.704600964
Au	16.626253536	4.182651565	22.072583324
Au	13.290638059	8.009043460	28.209603563
Au	17.274005641	7.122344363	25.353484294
Au	17.951163915	10.033385252	28.607204493
Au	13.922556539	11.181365588	31.367502518
Au	18.778302534	12.898672513	31.721207232
Au	16.451216943	4.453647714	31.342210220
Au	12.739578898	5.271709647	28.262945839
Au	13.166560761	8.472627101	31.426787551
Au	16.837868729	7.478690257	34.707690368
Au	13.387596986	11.737066518	34.620677702
Au	11.107300604	-1.269856112	24.957968050
Au	15.764150747	-1.535832125	24.848971966
Au	13.762926016	0.160683812	20.504256296
Au	15.728086621	9.232388056	27.116463883
Au	19.060366188	5.408800715	27.046024331
Au	19.669228978	8.339569860	30.400010380
Au	16.522975698	12.186625242	30.215612552

Au	20.515202763	11.509665116	33.745781843
Au	14.482054918	3.064127361	20.619633433
Au	18.070827070	-0.426318452	23.223205622
Au	15.885340502	-1.510332430	21.781826452
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