

Supporting Information

From Endohedral to Hollow Thiolate-Protected Gold Clusters. Role of Endohedral atoms in Electronic and Optical Properties of $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Au}_{38}(\text{SR})_{20}$.

Alvaro Muñoz-Castro

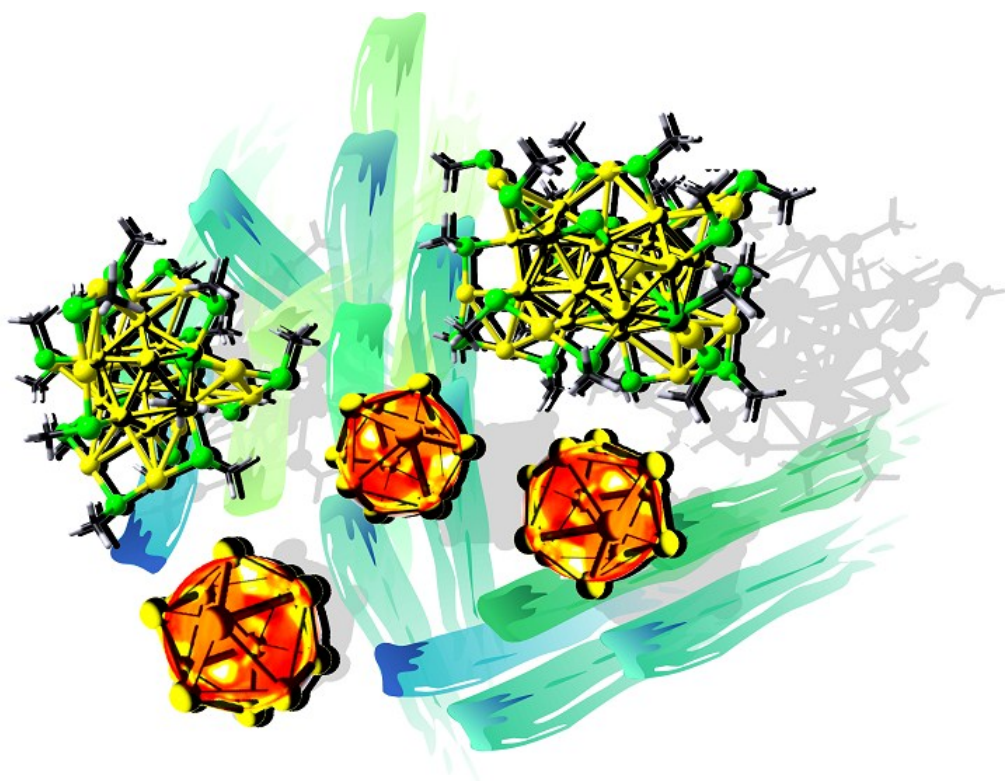


Figure S1. Structural variation of the hollow counterparts in comparison to their parent clusters.

Figure S2. Comparison between superatomic shells for endohedral and hollow isoelectronic counterparts of $[\text{Au}_{25}(\text{SR})_{18}]^-$ cluster. (R=Methyl)

Table S1. Optimized coordinates of the studied compounds.

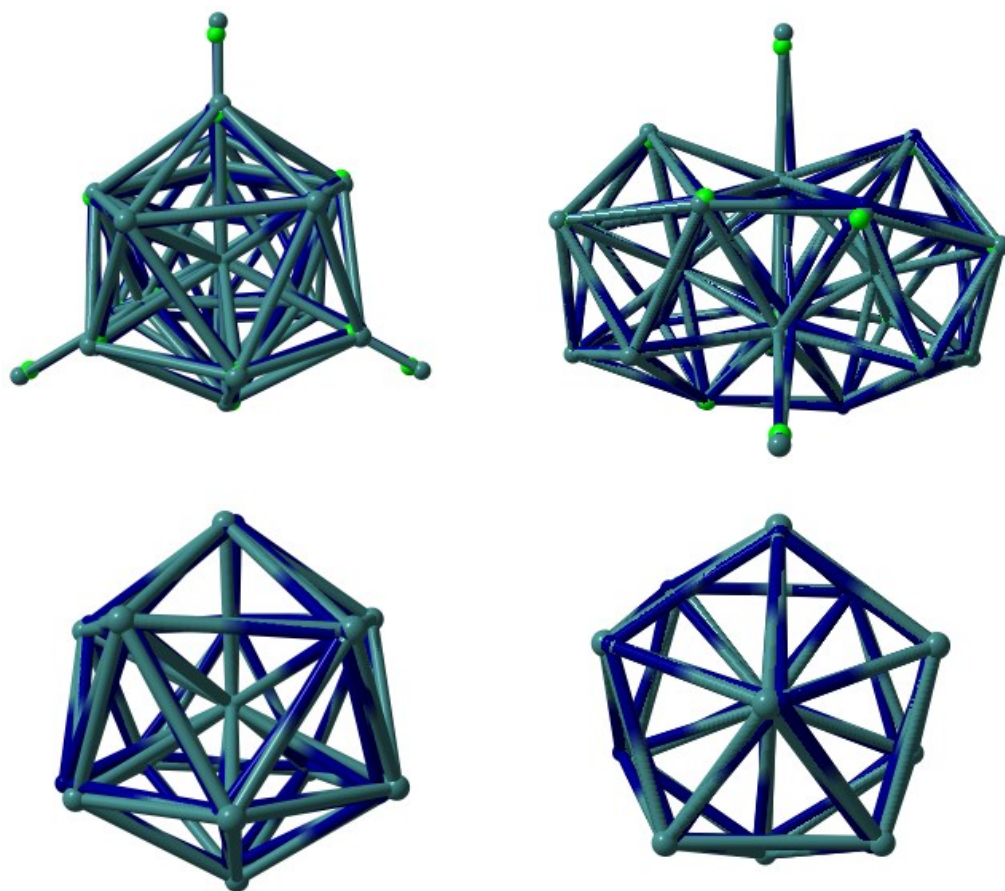


Figure S1. Two views of the structural variation of the hollow counterparts in comparison to their parent clusters. Up, core of $[\text{Au}_{38}(\text{SMe})_{24}]$ derivatives; bottom, core of $[\text{Au}_{25}(\text{SMe})_{18}]^-$. Grey: Endohedral counterpart. Blue, hollow structure. Green, Bi-hollow structure.

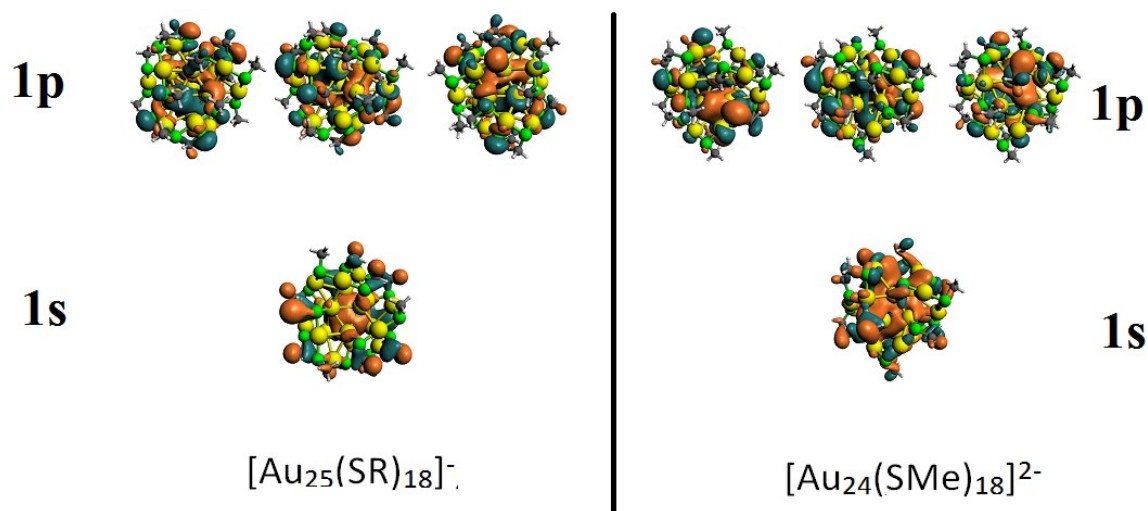


Figure S2. Comparison between superatomic shells for endohedral and hollow isoelectronic counterparts of $[Au_{25}(SR)_{18}]^-$ cluster. (R=Methyl)

Table S1. Optimized coordinates of the studied compounds.

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[Au₂₅C₁₈H₅₄S₁₈]-

Au	0.000000000	-0.000000000	0.000000000
Au	-1.989561550	1.623103305	-1.219689407
Au	-0.663847415	-2.450936564	1.302593275
Au	0.752975143	2.442233481	-1.278493170
Au	2.027333864	-1.595288337	1.251165701
Au	-2.186175467	-1.389660358	-1.222447433
Au	2.556486482	0.022381287	-1.283277626
Au	-2.549431705	-0.008448595	1.251419264
Au	2.205314965	1.426440505	1.135389648
Au	-0.051561922	-0.073968164	-2.843914079
Au	-0.673615204	2.380656908	1.412599336
Au	0.677271092	-2.397373173	-1.401130444
Au	0.000000000	0.000000000	2.850374263
Au	4.085557779	3.007804874	-0.962210489
S	6.050899129	1.915490864	-0.262558464
Au	5.081631878	0.000000000	0.708751360
C	6.842239084	1.326440903	-1.824078564
H	7.682680323	0.676419613	-1.549931311
H	6.122249391	0.778854232	-2.444605524
H	7.211610536	2.207259777	-2.364195304
Au	-4.986067907	0.067898396	-0.867102445
S	-5.991166017	-1.870382571	0.024044905
Au	-4.077115365	-2.939477543	0.891896415
C	-6.956152586	-1.240026665	1.466045753
H	-7.823109033	-0.695244987	1.071559728
H	-6.345789616	-0.567373481	2.080419832
H	-7.292308926	-2.103046366	2.054464817
Au	-2.347801569	1.807818654	4.128737754
S	-0.893953926	3.323398291	5.196792259
Au	1.096817822	2.829088845	4.040720254
C	-0.581473059	2.648942729	6.888014849
H	0.137295133	3.313999027	7.383292290
H	-0.167405829	1.636351874	6.837185935
H	-1.530813080	2.647150625	7.438479793
Au	-1.159602099	-3.007436911	-4.037519875
S	0.725279623	-3.181165723	-5.438379223
Au	2.256222208	-1.937334418	-4.150266363
C	0.317121556	-2.106902231	-6.884209991
H	1.221380029	-2.007604466	-7.498017921
H	-0.031711668	-1.121200899	-6.552769225
H	-0.471645785	-2.607672981	-7.459839160
Au	1.564328070	-4.781759112	0.889880627
S	1.648879125	-5.163468648	3.212094926
Au	1.170359269	-2.998502005	4.000609674
C	3.450152348	-5.398247364	3.551394916
H	3.595790805	-5.412700547	4.638892161
H	4.037589665	-4.592424694	3.096314328
H	3.745302439	-6.362618506	3.119149364
Au	-0.925437690	3.102650540	-3.893404167
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H	-3.924176439	4.616745357	-3.097081005
H	-3.421310711	5.436373201	-4.623453689
S	-3.083644429	-3.132852993	-2.691214105
S	-4.047288878	0.524864664	3.118794897
S	4.018381553	-0.824122044	-3.055692824
S	3.217509009	2.464755442	3.099309982
S	-4.297270320	2.059027232	-1.929566282
S	-2.260284149	-4.268357742	1.580591915
S	2.250017673	4.359585805	-1.551929683
S	4.381907735	-1.940629892	1.847704106
S	1.530550967	-4.690861463	-1.459546383
S	0.695678917	-0.925353447	5.017881740
S	-0.272997568	1.111533106	-4.972913674
S	-1.503677976	4.677157189	1.561390125

C	-0.786944285	-1.283379220	6.062631527
H	-1.447684762	-2.008974959	5.578589824
H	-0.441137968	-1.686593146	7.023668230
H	-1.332183956	-0.342248847	6.217253436
C	0.109222972	-5.787405018	-1.899281279
H	-0.781909099	-5.529426728	-1.316902873
H	0.402971137	-6.825932657	-1.700763033
H	-0.096674427	-5.647733014	-2.968843182
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H	-0.341141083	6.791693473	1.830982055
H	0.223880527	5.551684885	3.009876778
C	1.467897237	1.463688267	-5.483898383
H	2.063756272	1.774560374	-4.618812023
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H	3.110145669	4.682996026	2.028820224
H	4.056611808	4.696919401	3.557808655
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H	4.271848325	-2.902558282	-1.763064666
H	5.474718063	-2.768168149	-3.092058562
H	5.670709556	-1.798608022	-1.582733449
C	-4.087716959	-1.023704409	4.120306915
H	-3.076311474	-1.425966207	4.232451570
H	-4.521136184	-0.802745556	5.104621979
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C	-4.446864938	-2.456185205	-3.737221769
H	-4.164971478	-1.504223671	-4.198336969
H	-4.680911512	-3.193362430	-4.516117723
H	-5.318090574	-2.305586558	-3.086201410
C	4.539155311	-1.420199152	3.614385320
H	4.087489503	-0.434895215	3.775818193
H	5.605984870	-1.390709856	3.871085716
H	4.017514369	-2.166813248	4.229795383
C	-2.504889903	-4.591756737	3.381176833
H	-2.712601846	-3.666832532	3.929112403
H	-3.343017799	-5.290972961	3.498469359
H	-1.580651348	-5.045900449	3.761520684
C	2.510576518	4.788848894	-3.329796178
H	2.713349705	3.897043671	-3.931390808
H	3.355695289	5.485981344	-3.396885946
H	1.592832240	5.273514714	-3.687909459
C	-4.323311110	1.599315520	-3.719533177
H	-3.752347884	0.680542009	-3.890633546
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[Au24C18H54S18]2-

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Au	2.092335642	1.387931150	1.131262673
Au	-0.301344368	0.073932927	-2.859599481
Au	-0.778795647	2.272271998	1.439528734
Au	0.592001296	-2.206702847	-1.424823241
Au	0.000000000	0.000000000	2.757991755
Au	-2.054654146	1.561757158	-1.091517417
Au	-0.682792452	-2.419508489	1.154461068
Au	0.482365396	2.451160378	-1.357919641
Au	1.999541159	-1.503076039	0.991575958
Au	-2.717899383	1.341193356	4.395129387
S	-1.399900540	2.980009762	5.457097541
Au	0.559755567	2.801345050	4.137157535
C	-2.138228922	4.591843433	4.933401734
H	-1.502254341	5.394961252	5.328681765
H	-2.191635174	4.661328085	3.839786485
H	-3.142942108	4.660452468	5.369752705
Au	-1.354240614	-2.585228092	-4.208394979
S	0.503806849	-3.010578504	-5.605962623

Au	1.976235619	-1.617392745	-4.401591841
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H	0.182592898	-5.409016793	-5.635122946
H	1.088705107	-4.916326096	-4.161532571
H	1.921219877	-4.968671950	-5.758476129
Au	1.553261899	-4.778817741	0.661104599
S	1.271516554	-5.418272265	2.912664114
Au	1.099954680	-3.217910188	3.734032469
C	2.922187579	-6.007359650	3.505327784
H	2.834095570	-6.234535570	4.575840230
H	3.692903415	-5.243915774	3.358314214
H	3.183097623	-6.918118541	2.950099854
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S	-2.224716506	5.050287363	-3.391775475
Au	-1.698769861	4.694471934	-1.110271524
C	-4.043245660	4.739891445	-3.496649674
H	-4.556609466	5.574702218	-3.001109111
H	-4.309912359	3.794219338	-3.008653879
H	-4.320284229	4.708572327	-4.558417484
Au	4.003032856	2.870705607	-0.936237432
S	5.968929311	1.848932097	-0.116497847
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H	5.622853310	3.191853516	1.913969629
H	6.836174189	3.914654255	0.809463038
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S	-6.040485416	-2.328216831	0.308504118
Au	-4.001408700	-3.302440074	0.945420837
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H	-6.811822561	-4.195866371	-1.025096304
H	-5.691188462	-3.161805788	-1.976541377
H	-7.388168017	-2.625074003	-1.686372935
S	-0.085788722	1.235278957	-5.097525915
S	1.696782877	-4.463320844	-1.657364099
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S	-3.403357349	-2.334239667	-3.085506194
S	3.426124142	-0.019202643	-3.496168097
S	-3.973005360	-0.398450330	3.447866486
S	2.665398635	2.829292792	3.080439979
S	2.238190520	4.140216402	-1.819121897
S	4.234617674	-1.884990062	2.152871918
S	-4.516070762	1.873145137	-1.094273139
S	-2.124669556	-4.361506720	1.853031844
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H	6.152212497	-3.361053805	1.834402155
H	4.584610005	-4.217064563	1.592482113
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H	3.365065141	4.663907635	-3.911399937
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H	1.066414495	5.169076062	0.710888914
H	0.147157141	6.652878839	1.130415125
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C	3.473875977	-4.104120347	-1.987830945
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H	4.085628948	-4.984121094	-1.747574231
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H	-2.193204129	0.247952093	-5.923622030
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C	3.683486479	1.732762323	4.165742190
H	3.161423087	0.789844921	4.367790302
H	3.887434458	2.258965414	5.107954990
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C	5.057543317	-0.843265370	-3.227287148
H	4.949503346	-1.759732263	-2.638923184
H	5.503837276	-1.073616500	-4.203874496
H	5.693334297	-0.133352904	-2.682329710
C	-5.717862338	0.211456610	3.371550362
H	-5.787194382	1.138498386	2.793753512
H	-6.089556670	0.377361873	4.391512956
H	-6.313101739	-0.566924897	2.875978479
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H	-5.103238210	-0.648511559	-3.385308339

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[Au38C24H72S24]

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Au	0.007542000	1.703336000	-13.781161000
Au	0.000000000	0.000000000	-10.843889000
Au	-1.501792000	-0.059795000	-15.598146000
Au	-1.500839000	2.452797000	-11.463138000
Au	1.520375000	2.378289000	-11.351870000
Au	1.500839000	-2.452797000	-11.463138000
Au	1.501792000	0.059795000	-15.598146000
Au	-1.520375000	-2.378289000	-11.351870000
Au	-2.762340000	-2.484822000	-14.204485000
Au	-2.743253000	2.449217000	-14.280496000
Au	2.759561000	-0.063117000	-9.957185000
Au	2.743253000	-2.449217000	-14.280496000
Au	2.762340000	2.484822000	-14.204485000
Au	-2.759561000	0.063117000	-9.957185000
Au	-4.278517000	-0.142051000	-14.633041000
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Au	4.277314000	-1.678320000	-12.031339000
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Au	-4.290140000	-1.469763000	-11.775616000
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S	2.155830000	4.840919000	-14.509178000
S	-2.142169000	0.963570000	-7.761600000
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C	3.023786000	-0.048541000	-6.420175000
C	3.016111000	-5.520447000	-16.025084000
C	3.037000000	5.541550000	-15.974196000
C	-3.023786000	0.048541000	-6.420175000
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H	-2.953365000	5.917706000	-15.006809000
H	2.968467000	1.033552000	-6.575992000
H	2.953365000	-5.917706000	-15.006809000
H	2.968468000	4.868399000	-16.834782000
H	-2.964867000	-1.033552000	-6.575992000
H	-4.087789000	-5.678291000	-15.689803000
H	-4.065422000	5.347658000	-16.294959000
H	4.072147000	-0.371995000	-6.437404000

H	4.065422000	-5.347658000	-16.294959000
H	4.087789000	5.678291000	-15.689803000
H	-4.072147000	0.371995000	-6.437404000
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S	2.019379000	0.576766000	-17.930874000
S	-2.036780000	-4.132365000	-9.732602000
S	-6.203599000	-2.897559000	-12.221658000
S	-6.192280000	0.982835000	-15.617969000
S	6.194275000	-1.985244000	-10.568854000
S	6.192280000	-0.982835000	-15.617969000
S	6.203599000	2.897559000	-12.221658000
S	-6.194275000	1.985244000	-10.568854000
Au	-3.884889000	-1.843190000	-17.265415000
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Au	3.894092000	2.918589000	-8.959036000
Au	3.867887000	-4.811225000	-12.162690000
Au	3.884889000	1.843190000	-17.265415000
Au	-3.894092000	-2.918589000	-8.959036000
S	-5.748444000	-3.220650000	-16.871834000
S	-5.722205000	5.165367000	-13.561307000
S	5.751306000	1.880232000	-7.964926000
S	5.722205000	-5.165367000	-13.561307000
S	5.748444000	3.220650000	-16.871834000
S	-5.751306000	-1.880232000	-7.964926000
Au	-5.827797000	-2.935057000	-14.538852000
Au	-5.805914000	3.002062000	-14.482059000
Au	5.827797000	0.007818000	-9.384751000
Au	5.805914000	-3.002062000	-14.482059000
Au	5.827797000	2.935057000	-14.538852000
Au	-5.827797000	-0.007818000	-9.384751000
C	-5.683036000	-4.596806000	-11.710408000
C	-5.683959000	1.399284000	-17.347168000
C	5.682018000	-3.270176000	-9.341084000
C	5.683959000	-1.399284000	-17.347168000
C	5.683036000	4.596806000	-11.710408000
C	-5.682018000	3.270176000	-9.341084000
H	-6.427936000	-5.306833000	-12.088084000
H	-6.429402000	2.086858000	-17.763741000
H	6.432571000	-3.293304000	-8.542637000
H	6.429402000	-2.086858000	-17.763741000
H	6.427936000	5.306833000	-12.088084000
H	-6.432571000	3.293304000	-8.542637000
H	-5.657720000	-4.621855000	-10.613114000
H	-5.667099000	0.465134000	-17.923392000
H	5.652801000	-4.236150000	-9.861942000
H	5.667099000	-0.465134000	-17.923392000
H	5.657720000	4.621855000	-10.613114000
H	-5.652801000	4.236150000	-9.861942000
H	-4.690277000	-4.833240000	-12.108134000
H	-4.689529000	1.858331000	-17.357115000
H	4.692283000	-3.040494000	-8.932126000
H	4.689529000	-1.858331000	-17.357115000
H	4.690277000	4.833240000	-12.108134000
H	-4.692283000	3.040494000	-8.932126000
C	-0.822138000	-1.867436000	-18.492038000
C	-0.797949000	5.857532000	-11.559409000
C	0.831356000	3.975083000	-8.341013000
C	0.797949000	-5.857532000	-11.559409000
C	0.822138000	1.867436000	-18.492038000
C	-0.831356000	-3.975083000	-8.341013000
H	-0.686084000	-2.630677000	-17.717259000
H	-0.665245000	5.577030000	-12.610423000

H	0.691724000	2.922767000	-8.068483000
H	0.665245000	-5.577030000	-12.610423000
H	0.686084000	2.630677000	-17.717259000
H	-0.691724000	-2.922767000	-8.068483000
H	-1.210002000	-2.315348000	-19.414214000
H	-1.176534000	6.882811000	-11.475708000
H	1.216007000	4.548778000	-7.489936000
H	1.176534000	-6.882811000	-11.475708000
H	1.210002000	2.315348000	-19.414214000
H	-1.216007000	-4.548778000	-7.489936000
H	0.134914000	-1.366905000	-18.685871000
H	0.158518000	5.761632000	-11.030421000
H	-0.123092000	4.395086000	-8.682299000
H	-0.158518000	-5.761632000	-11.030421000
H	-0.134914000	1.366905000	-18.685871000
H	0.123092000	-4.395086000	-8.682299000
C	-7.215031000	-2.291252000	-17.501824000
C	-7.194176000	5.251724000	-12.448477000
C	7.219529000	2.891698000	-8.450812000
C	7.194176000	-5.251724000	-12.448477000
C	7.215031000	2.291252000	-17.501824000
C	-7.219529000	-2.891698000	-8.450812000
H	-8.106120000	-2.875098000	-17.244714000
H	-8.082200000	5.322397000	-13.086925000
H	8.110262000	2.372420000	-8.079495000
H	8.082200000	-5.322397000	-13.086925000
H	8.106120000	2.875098000	-17.244714000
H	-8.110262000	-2.372420000	-8.079495000
H	-7.117496000	-2.212947000	-18.590629000
H	-7.097067000	6.156052000	-11.837234000
H	7.124197000	3.869826000	-7.966142000
H	7.097067000	-6.156052000	-11.837234000
H	7.117496000	2.212947000	-18.590629000
H	-7.124197000	-3.869826000	-7.966142000
H	-7.272051000	-1.296960000	-17.045917000
H	-7.256090000	4.360503000	-11.814607000
H	7.274067000	3.001778000	-9.539145000
H	7.256090000	-4.360503000	-11.814607000
H	7.272051000	1.296960000	-17.045917000
H	-7.274067000	-3.001778000	-9.539145000

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[Au37C24H72S24]-

Au	-1.990196000	0.001898000	-12.799908000
Au	0.276266000	-1.534877000	-13.631875000
Au	0.295887000	1.477476000	-13.709473000
Au	0.295495000	0.049027000	-11.078610000
Au	-1.412962000	-0.189612000	-15.577296000
Au	-1.417362000	2.505748000	-11.592210000
Au	1.495181000	2.554504000	-11.442643000
Au	1.478832000	-2.462024000	-11.270605000
Au	1.499029000	-0.103806000	-15.686587000
Au	-1.425211000	-2.296929000	-11.236387000
Au	-2.652298000	-2.480672000	-14.054085000
Au	-2.644511000	2.329262000	-14.334445000
Au	2.800765000	-0.095249000	-9.872710000
Au	2.791520000	-2.505476000	-14.334806000
Au	2.818415000	2.566506000	-14.191798000
Au	-2.641090000	0.163710000	-10.017703000
Au	-4.229168000	-0.204511000	-14.590034000
Au	-4.224095000	1.644111000	-12.092664000
Au	4.110677000	1.358602000	-11.756391000
Au	4.096580000	-1.621028000	-12.128295000
Au	4.115336000	0.200732000	-14.496418000
Au	-4.229223000	-1.433550000	-11.714856000
Au	0.000597000	-4.277984000	-15.241102000
Au	0.017477000	4.256063000	-15.308753000
Au	0.010537000	0.058114000	-7.862331000
S	-2.087609000	-4.833359000	-14.325736000
S	-2.083665000	3.758086000	-16.225483000
S	2.085629000	-1.024866000	-7.691619000
S	2.078129000	-3.889178000	-16.263150000

S	2.107564000	4.925394000	-14.476048000
S	-2.075199000	1.130210000	-7.856243000
C	-3.046771000	-5.531179000	-15.743908000
C	-3.028316000	5.341474000	-16.097332000
C	2.976902000	-0.145231000	-6.330124000
C	2.954140000	-5.516835000	-16.213151000
C	2.987043000	5.664966000	-15.925746000
C	-3.038816000	0.274772000	-6.531821000
H	-3.014949000	-4.857231000	-16.606212000
H	-2.982408000	5.743617000	-15.079632000
H	3.010115000	0.933279000	-6.517695000
H	2.974637000	-5.919397000	-15.194596000
H	3.010278000	4.964661000	-16.767659000
H	-3.012167000	-0.811489000	-6.666461000
H	-4.084231000	-5.657731000	-15.409265000
H	-4.070918000	5.126510000	-16.364725000
H	3.996588000	-0.548354000	-6.292759000
H	3.979040000	-5.348490000	-16.567571000
H	4.011013000	5.896222000	-15.605949000
H	-4.074661000	0.631796000	-6.595767000
H	-2.616738000	-6.505478000	-16.004581000
H	-2.600195000	6.056678000	-16.809806000
H	2.460836000	-0.349983000	-5.384517000
H	2.438388000	-6.212718000	-16.885762000
H	2.470993000	6.588454000	-16.214501000
H	-2.609207000	0.548844000	-5.560867000
S	-1.997870000	-0.634539000	-17.918952000
S	-2.001494000	4.760476000	-10.819201000
S	2.100158000	4.107627000	-9.658369000
S	2.051725000	-4.795845000	-10.827856000
S	2.098012000	0.682127000	-17.924010000
S	-2.012529000	-4.095406000	-9.669875000
S	-6.156613000	-2.871564000	-12.172163000
S	-6.150899000	0.910596000	-15.622823000
S	6.027184000	-1.963537000	-10.614332000
S	6.035221000	-0.956519000	-15.548481000
S	6.062923000	2.814066000	-12.226348000
S	-6.141865000	1.989303000	-10.609378000
Au	-3.853493000	-1.909795000	-17.252292000
Au	-3.868808000	4.822275000	-12.243944000
Au	3.916124000	2.852256000	-8.889563000
Au	3.871980000	-4.858085000	-12.293055000
Au	3.925454000	1.966875000	-17.239769000
Au	-3.883683000	-2.897315000	-8.908565000
S	-5.733821000	-3.259157000	-16.826525000
S	-5.752359000	5.130522000	-13.619522000
S	5.787174000	1.831295000	-7.895443000
S	5.745769000	-5.225559000	-13.666791000
S	5.812048000	3.320883000	-16.864434000
S	-5.759181000	-1.853197000	-7.947350000
Au	-5.817792000	-2.925955000	-14.496820000
Au	-5.830138000	2.951254000	-14.505107000
Au	5.781106000	-0.011230000	-9.355606000
Au	5.760760000	-3.033019000	-14.515000000
Au	5.800589000	2.959045000	-14.542216000
Au	-5.832751000	-0.003149000	-9.402293000
C	-5.633326000	-4.574361000	-11.674518000
C	-5.612502000	1.333513000	-17.341504000
C	5.514197000	-3.268610000	-9.409800000
C	5.528580000	-1.315893000	-17.289152000
C	5.588282000	4.513650000	-11.677540000
C	-5.584818000	3.262099000	-9.388307000
H	-6.373407000	-5.288056000	-12.055521000
H	-6.349192000	2.020925000	-17.773874000
H	6.264536000	-3.318971000	-8.612680000
H	6.277475000	-1.978560000	-17.738802000
H	6.348444000	5.218978000	-12.033550000
H	-6.310038000	3.293577000	-8.566592000
H	-5.603308000	-4.606712000	-10.577163000
H	-5.579391000	0.400457000	-17.919864000
H	5.473909000	-4.222261000	-9.952301000

H	5.496287000	-0.359330000	-17.828065000
H	5.557839000	4.512589000	-10.579407000
H	-5.555578000	4.229713000	-9.907152000
H	-4.638885000	-4.800912000	-12.075162000
H	-4.617760000	1.793043000	-17.328112000
H	4.526315000	-3.038315000	-8.995381000
H	4.537558000	-1.784154000	-17.310079000
H	4.601334000	4.781086000	-12.072282000
H	-4.585429000	3.016873000	-9.011309000
C	-0.793255000	-1.884100000	-18.552720000
C	-0.799407000	5.928525000	-11.596453000
C	0.826362000	3.893055000	-8.338489000
C	0.768073000	-5.805963000	-11.688900000
C	0.824581000	1.940540000	-18.377032000
C	-0.814514000	-3.994351000	-8.266881000
H	-0.654156000	-2.688033000	-17.821959000
H	-0.659343000	5.687082000	-12.656191000
H	0.681308000	2.828631000	-8.117002000
H	0.634921000	-5.457174000	-12.720302000
H	0.689057000	2.658981000	-17.559146000
H	-0.679468000	-2.953639000	-7.951987000
H	-1.170894000	-2.282327000	-19.501874000
H	-1.178550000	6.950603000	-11.476805000
H	1.159459000	4.434523000	-7.445261000
H	1.085395000	-6.855339000	-11.671363000
H	1.150847000	2.449842000	-19.291540000
H	-1.193824000	-4.604697000	-7.438619000
H	0.161624000	-1.366434000	-18.710568000
H	0.156437000	5.812861000	-11.067803000
H	-0.112550000	4.317967000	-8.716320000
H	-0.172386000	-5.680888000	-11.137324000
H	-0.118454000	1.406555000	-18.551620000
H	0.142931000	-4.393207000	-8.626342000
C	-7.182178000	-2.328136000	-17.494758000
C	-7.199436000	5.236909000	-12.476421000
C	7.243507000	2.844520000	-8.415785000
C	7.191260000	-5.292583000	-12.516624000
C	7.253006000	2.345576000	-17.492806000
C	-7.213704000	-2.891792000	-8.416684000
H	-8.085560000	-2.887963000	-17.226697000
H	-8.104414000	5.282323000	-13.093396000
H	8.145314000	2.320114000	-8.080254000
H	8.098637000	-5.325169000	-13.131050000
H	8.163456000	2.884868000	-17.207513000
H	-8.113741000	-2.374542000	-8.064758000
H	-7.077758000	-2.282265000	-18.584664000
H	-7.097296000	6.158188000	-11.891479000
H	7.167831000	3.818270000	-7.918950000
H	7.105321000	-6.211091000	-11.924301000
H	7.171165000	2.296718000	-18.584710000
H	-7.112331000	-3.858076000	-7.909300000
H	-7.224432000	-1.320033000	-17.068540000
H	-7.237176000	4.363358000	-11.816403000
H	7.263576000	2.967244000	-9.504112000
H	7.209986000	-4.412890000	-11.863516000
H	7.260142000	1.339215000	-17.059875000
H	-7.258371000	-3.028094000	-9.502596000

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[Au36C24H72S24]2-

Au	-0.006051000	-1.430625000	-13.642614000
Au	0.006051000	1.430625000	-13.642614000
Au	0.000000000	0.000000000	-11.174787000
Au	-1.424592000	-0.163210000	-15.629468000
Au	-1.422721000	2.500443000	-11.542067000
Au	1.432563000	2.337629000	-11.259642000
Au	1.422721000	-2.500443000	-11.542067000
Au	1.424592000	0.163210000	-15.629468000
Au	-1.432563000	-2.337629000	-11.259642000
Au	-2.743920000	-2.333957000	-14.148071000
Au	-2.731464000	2.329710000	-14.170189000
Au	2.730858000	-0.030281000	-10.101701000

Au	2.731464000	-2.329710000	-14.170189000
Au	2.743920000	2.333957000	-14.148071000
Au	-2.730858000	0.030281000	-10.101701000
Au	-4.207471000	-0.144754000	-14.600896000
Au	-4.215252000	1.609258000	-12.061929000
Au	4.205611000	1.438166000	-11.782063000
Au	4.215252000	-1.609258000	-12.061929000
Au	4.207471000	0.144754000	-14.600896000
Au	-4.205611000	-1.438166000	-11.782063000
Au	-0.022399000	-4.091503000	-15.123168000
Au	0.022399000	4.091503000	-15.123168000
Au	0.000000000	0.000000000	-8.095682000
S	-2.095319000	-4.709798000	-14.214752000
S	-2.044882000	3.637863000	-16.136833000
S	2.061798000	-1.116643000	-7.994763000
S	2.044882000	-3.637863000	-16.136833000
S	2.095319000	4.709798000	-14.214752000
S	-2.061798000	1.116643000	-7.994763000
C	-3.056648000	-5.406107000	-15.634243000
C	-3.003778000	5.215174000	-16.006446000
C	3.023887000	-0.231635000	-6.684905000
C	3.003778000	-5.215174000	-16.006446000
C	3.056648000	5.406107000	-15.634243000
C	-3.023887000	0.231635000	-6.684905000
H	-3.006226000	-4.740214000	-16.502374000
H	-2.971788000	5.606440000	-14.983849000
H	2.996072000	0.851321000	-6.846331000
H	2.971788000	-5.606440000	-14.983849000
H	3.006226000	4.740214000	-16.502374000
H	-2.996072000	-0.851321000	-6.846331000
H	-4.100155000	-5.504400000	-15.307857000
H	-4.042900000	4.992635000	-16.282065000
H	4.061785000	-0.584846000	-6.743051000
H	4.042900000	-4.992635000	-16.282065000
H	4.100155000	5.504400000	-15.307857000
H	-4.061785000	0.584846000	-6.743051000
H	-2.649282000	-6.392590000	-15.887241000
H	-2.578733000	5.944658000	-16.706761000
H	2.598418000	-0.481317000	-5.705222000
H	2.578733000	-5.944658000	-16.706761000
H	2.649282000	6.392590000	-15.887241000
H	-2.598418000	0.481317000	-5.705222000
S	-2.153659000	-0.437144000	-17.985897000
S	-2.150773000	4.680809000	-10.603724000
S	2.175756000	4.257376000	-9.867087000
S	2.150773000	-4.680809000	-10.603724000
S	2.153659000	0.437144000	-17.985897000
S	-2.175756000	-4.257376000	-9.867087000
S	-6.148612000	-2.836196000	-12.407010000
S	-6.125731000	1.123690000	-15.519854000
S	6.142033000	-1.786438000	-10.513977000
S	6.125731000	-1.123690000	-15.519854000
S	6.148612000	2.836196000	-12.407010000
S	-6.142033000	1.786438000	-10.513977000
Au	-4.051650000	-1.684668000	-17.426986000
Au	-4.045717000	4.849494000	-11.961117000
Au	4.059078000	3.144521000	-9.040136000
Au	4.045717000	-4.849494000	-11.961117000
Au	4.051650000	1.684668000	-17.426986000
Au	-4.059078000	-3.144521000	-9.040136000
S	-5.948741000	-3.028273000	-17.080314000
S	-5.934477000	5.240429000	-13.302906000
S	5.938397000	2.168833000	-8.018648000
S	5.934477000	-5.240429000	-13.302906000
S	5.948741000	3.028273000	-17.080314000
S	-5.938397000	-2.168833000	-8.018648000
Au	-5.907616000	-2.789423000	-14.735553000
Au	-5.890802000	3.102219000	-14.291774000
Au	5.907405000	0.253896000	-9.391536000
Au	5.890802000	-3.102219000	-14.291774000
Au	5.907616000	2.789423000	-14.735553000

Au	-5.907405000	-0.253896000	-9.391536000
C	-5.662638000	-4.572413000	-11.998577000
C	-5.593821000	1.646015000	-17.211531000
C	5.627652000	-3.004047000	-9.221747000
C	5.593821000	-1.646015000	-17.211531000
C	5.662638000	4.572413000	-11.998577000
C	-5.627652000	3.004047000	-9.221747000
H	-6.412582000	-5.255596000	-12.414735000
H	-6.331979000	2.351000000	-17.611999000
H	6.368514000	-2.994379000	-8.413370000
H	6.331979000	-2.351000000	-17.611999000
H	6.412582000	5.255596000	-12.414735000
H	-6.368514000	2.994379000	-8.413370000
H	-5.635028000	-4.657715000	-10.903356000
H	-5.552195000	0.743180000	-17.836168000
H	5.594728000	-3.994709000	-9.695850000
H	5.552195000	-0.743180000	-17.836168000
H	5.635028000	4.657715000	-10.903356000
H	-5.594728000	3.994709000	-9.695850000
H	-4.669215000	-4.794236000	-12.406120000
H	-4.600125000	2.107300000	-17.170453000
H	4.632722000	-2.750725000	-8.837234000
H	4.600125000	-2.107300000	-17.170453000
H	4.669215000	4.794236000	-12.406120000
H	-4.632722000	2.750725000	-8.837234000
C	-0.985387000	-1.721958000	-18.623581000
C	-0.980316000	5.879387000	-11.387253000
C	1.006866000	4.189427000	-8.434344000
C	0.980316000	-5.879387000	-11.387253000
C	0.985387000	1.721958000	-18.623581000
C	-1.006866000	-4.189427000	-8.434344000
H	-0.920745000	-2.558154000	-17.919262000
H	-0.915725000	5.696757000	-12.465240000
H	0.927732000	3.163510000	-8.058227000
H	0.915725000	-5.696757000	-12.465240000
H	0.920745000	2.558154000	-17.919262000
H	-0.927732000	-3.163510000	-8.058227000
H	-1.336998000	-2.066173000	-19.603403000
H	-1.329910000	6.899024000	-11.186845000
H	1.368411000	4.863679000	-7.648689000
H	1.329910000	-6.899024000	-11.186845000
H	1.336998000	2.066173000	-19.603403000
H	-1.368411000	-4.863679000	-7.648689000
H	0.003127000	-1.253856000	-18.714332000
H	0.008527000	5.719402000	-10.938709000
H	0.021926000	4.515113000	-8.792741000
H	-0.008527000	-5.719402000	-10.938709000
H	-0.003127000	1.253856000	-18.714332000
H	-0.021926000	-4.515113000	-8.792741000
C	-7.385893000	-2.011322000	-17.646775000
C	-7.381064000	5.214873000	-12.151411000
C	7.391269000	3.153641000	-8.601618000
C	7.381064000	-5.214873000	-12.151411000
C	7.385893000	2.011322000	-17.646775000
C	-7.391269000	-3.153641000	-8.601618000
H	-8.301483000	-2.547028000	-17.369979000
H	-8.290750000	5.257670000	-12.761579000
H	8.297947000	2.644150000	-8.254680000
H	8.290750000	-5.257670000	-12.761579000
H	8.301483000	2.547028000	-17.369979000
H	-8.297947000	-2.644150000	-8.254680000
H	-7.320567000	-1.915937000	-18.736857000
H	-7.315600000	6.102126000	-11.510949000
H	7.324465000	4.150839000	-8.151517000
H	7.315600000	-6.102126000	-11.510949000
H	7.320567000	1.915937000	-18.736857000
H	-7.324465000	-4.150839000	-8.151517000
H	-7.368613000	-1.024189000	-17.172094000
H	-7.375083000	4.301667000	-11.546596000
H	7.393980000	3.223939000	-9.694587000
H	7.375083000	-4.301667000	-11.546596000

H	7.368613000	1.024189000	-17.172094000
H	-7.393980000	-3.223939000	-9.694587000