

Supporting Information:

Two-Dimensional Growth Mode of Thiolate-Protected Gold Nanoclusters

$\text{Au}_{28+4n}(\text{SR})_{20+2n}$  ( $n = 0 - 8$ ): Compared with their One-Dimensional Growth

Mode

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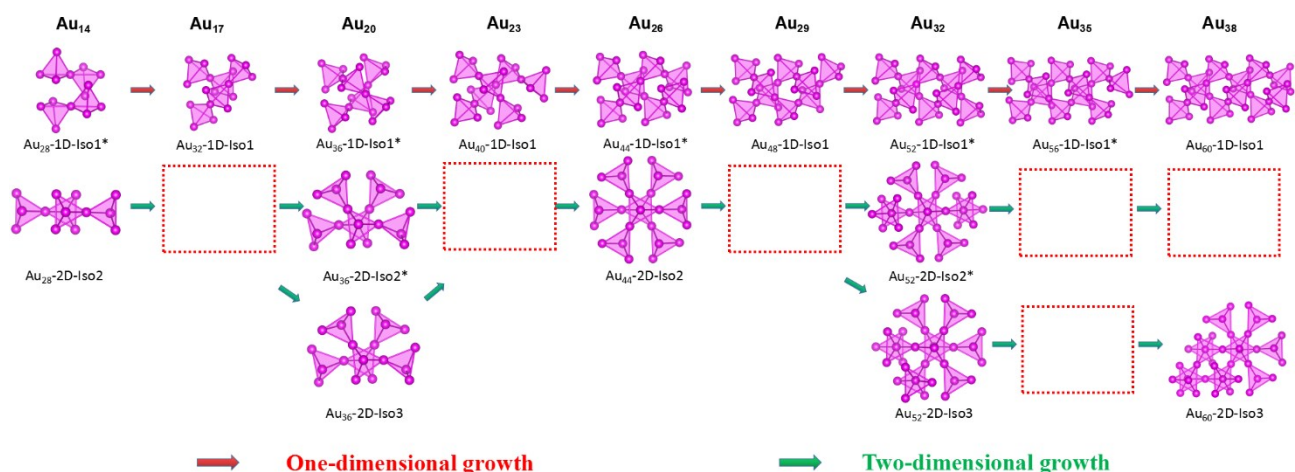
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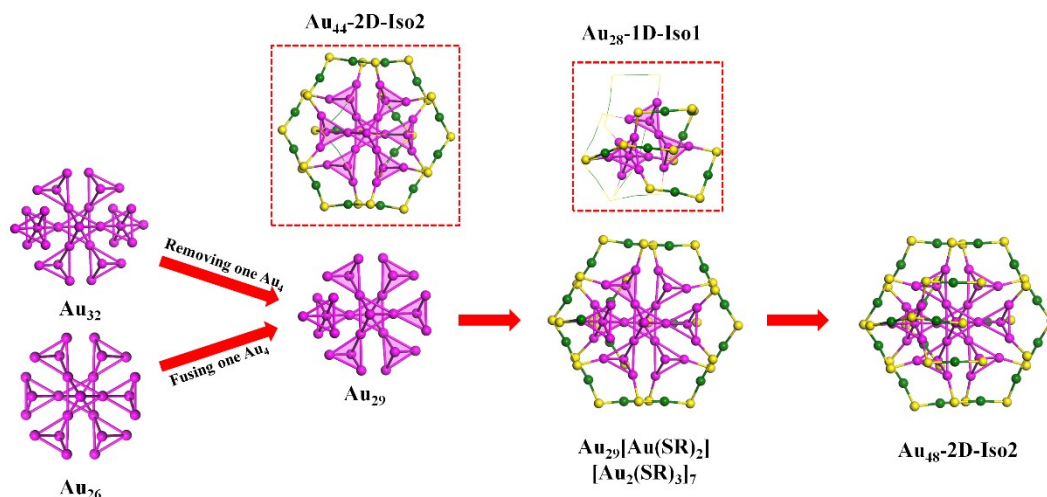
AUTHOR INFORMATION

**Corresponding Author**

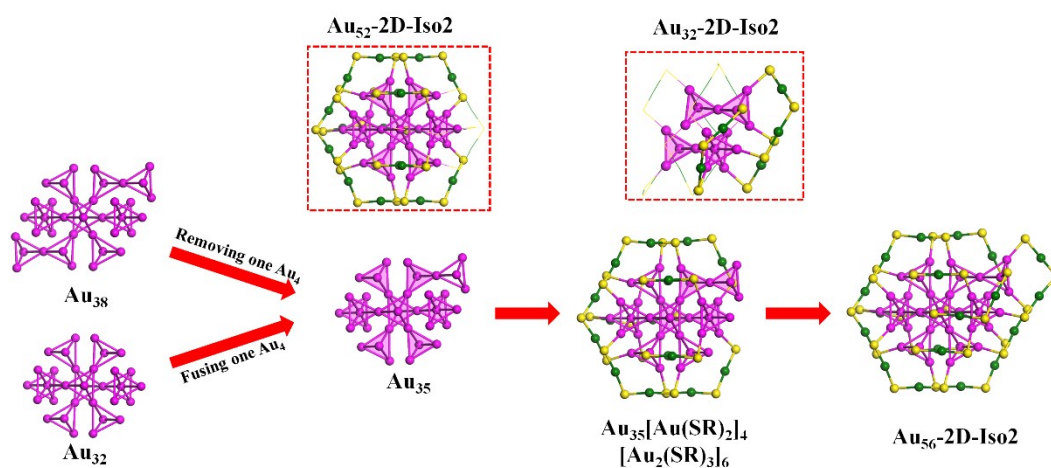
\*W. W. Xu (xuwenwu@nbu.edu.cn)



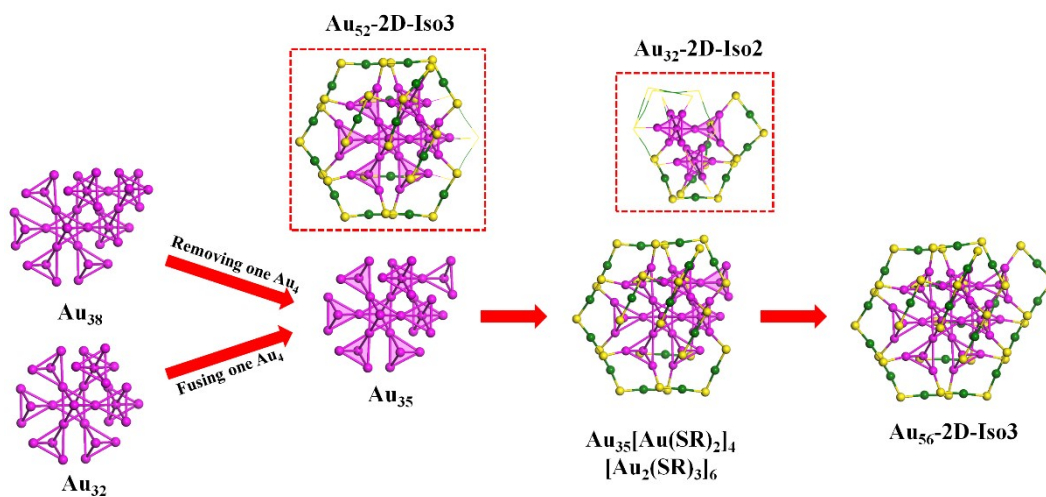
**Figure S1.** The one-dimensional (red arrow) of the cores of  $\text{Au}_{28+4n}(\text{SR})_{20+2n}$  ( $n = 0 - 8$ ) nanoclusters and two-dimensional (green arrow) growth of the cores of  $\text{Au}_{28+4n}(\text{SR})_{20+2n}$  ( $n = 0, 2, 4, 6, \text{ and } 8$ ) nanoclusters. The dotted squares in red denote several “missing” gold nanoclusters. Au atoms are presented in wine. S is presented in yellow. The R groups are omitted for clarity. \* denotes the experimentally crystallized structure.



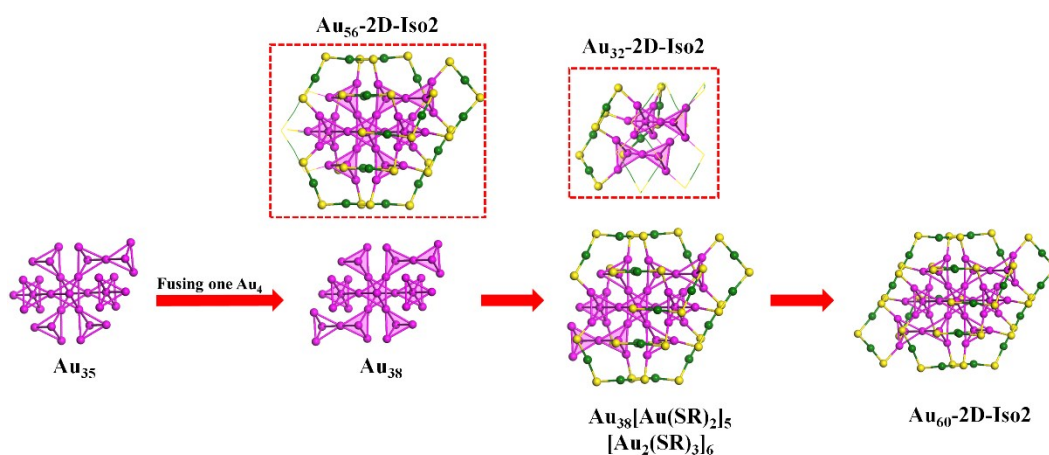
**Figure S2.** The structural prediction of  $\text{Au}_{48}\text{-2D-Iso2}$ . Au atoms are presented in wine, blue, and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.



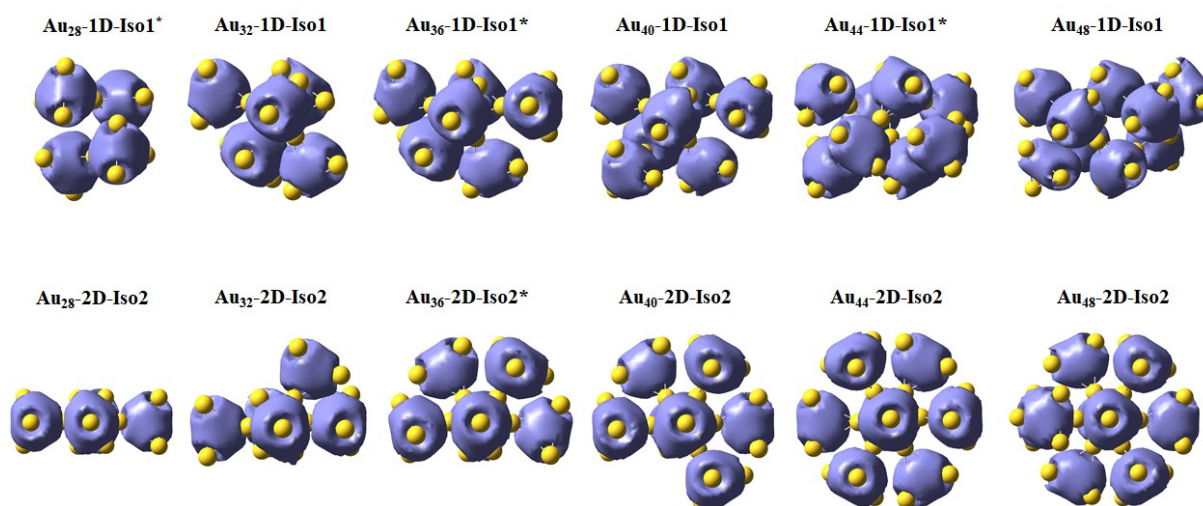
**Figure S3.** The structural prediction of  $\text{Au}_{56}\text{-2D-Iso2}$ . Au atoms are presented in wine, blue, and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.



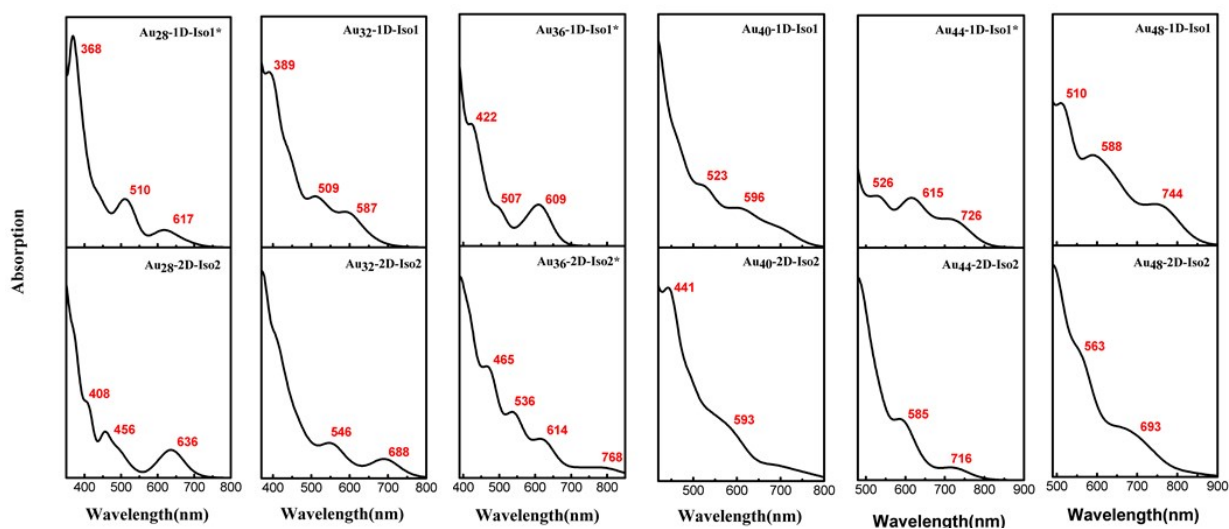
**Figure S4.** The structural prediction of  $\text{Au}_{56}\text{-2D-Iso3}$ . Au atoms are presented in wine, blue, and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.



**Figure S5.** The structural prediction of Au<sub>60</sub>-2D-Iso2. Au atoms are presented in wine, blue, and dark green, respectively. S is presented in yellow. The R groups are omitted for clarity.



**Figure S6.** Visualization of the valence electron distributions in the Au<sub>14+3n</sub><sup>(6+n)+</sup> of Au<sub>28+4n</sub>(SR)<sub>20+2n</sub> (n = 0 - 5) nanoclusters. Au atoms are presented in yellow. \* denotes the experimentally crystallized structure.



**Figure S7** Computed absorption spectra of  $\text{Au}_{28+4n}(\text{SR})_{20+2n}$  ( $n = 0 - 5$ ) isomers. The prominent absorption peaks for three clusters are highlighted in red. The R groups are simplified by H atoms. \* denotes the experimentally crystallized structure.

The cartesian coordinates of Au<sub>32</sub>-2D-Iso2

Au	-0.350927	-0.929434	1.971630
Au	0.138659	1.366680	0.355693
Au	-2.375688	0.008308	0.238244
Au	-1.759296	1.480905	2.470013
Au	-4.817150	-1.318655	0.364985
Au	-3.231248	-1.474157	-1.968823
Au	2.075205	1.478553	-1.731902
Au	0.721762	3.780334	-0.937063
Au	2.654334	2.638291	0.741694
Au	-4.505322	0.955813	-1.274736
Au	1.776730	-1.263275	-0.279552
Au	2.595722	-0.022094	2.139208
Au	3.874563	-2.351066	1.177170
Au	4.231274	0.112199	-0.155338
Au	1.277352	-2.660725	-2.607389
Au	-0.316387	-0.395962	-2.087278
Au	-0.662091	-2.689260	-0.518312
S	0.521280	6.103219	-1.721431
S	2.818404	0.738114	-3.961144
S	6.215546	1.261164	-0.985259
S	-1.354496	1.321014	-3.519009
S	4.068457	3.709288	2.408194
S	-5.874704	2.595195	-2.464024
S	-2.742485	4.327229	-0.085075
S	-3.394651	-2.850492	-3.974578
S	-6.639360	-2.647131	1.316238
S	1.950283	-5.617235	-0.164217
S	-2.359701	-4.288140	0.274359
S	-3.343109	-1.792984	4.211440
S	2.559898	0.673453	4.492724
S	5.507263	-3.737111	2.373890
S	1.156350	-4.006664	-4.684418
S	-1.663303	2.840182	4.546696
Au	5.692873	2.021770	2.765834
Au	6.461450	-1.598708	2.795070
Au	5.236431	2.963857	-2.301894
Au	1.331079	-4.042537	1.519382
Au	2.546893	5.389640	-2.767267
Au	-1.998175	2.703343	-1.678365
Au	-7.750152	1.679224	-1.354594
Au	-8.139681	-0.982558	0.565916
Au	-2.852929	-2.916795	2.162743
Au	3.926245	-1.160293	-3.049576
Au	3.521771	-4.181743	-1.235016
S	5.268178	-2.994135	-2.337585
S	7.461626	0.503158	3.209668
S	4.539923	4.664877	-3.813258
S	-9.581262	0.764807	-0.148701
S	0.668631	-2.710969	3.379993
Au	-4.173629	2.909131	1.164390
Au	-4.474494	0.029254	3.191362

S	-5.860748	1.791860	2.412177
Au	0.477081	1.783724	4.552682
Au	-1.136521	-3.426676	-4.362068
H	-1.255357	3.995036	3.944043
H	2.097902	-0.526159	4.956120
H	4.794666	4.456275	1.526089
H	7.324999	0.496469	4.567768
H	6.275910	-4.032606	1.284887
H	-0.490122	-3.396225	3.630201
H	-1.491704	-5.117068	0.929001
H	-2.137213	-1.161633	4.344320
H	-5.747218	2.568679	3.530964
H	-1.654860	4.256489	0.738928
H	-0.205121	2.011444	-3.783076
H	1.132096	6.664807	-0.636663
H	3.936552	3.817628	-4.698536
H	6.394632	1.987616	0.164214
H	1.665302	0.087194	-4.302686
H	5.202309	-3.697820	-3.506558
H	0.914440	-5.358918	-1.018052
H	1.460725	-2.983883	-5.535179
H	-3.727063	-4.000305	-3.318137
H	-10.140822	0.091935	-1.196797
H	-6.774235	-3.474428	0.238049
H	-5.991266	1.856366	-3.606577

The cartesian coordinates of Au<sub>40</sub>-2D-Iso2

Au	0.042778	1.015336	-1.365764
Au	1.137148	-1.689131	-1.113273
Au	-1.746659	-1.323546	-0.779969
Au	-0.638853	-1.024604	-3.240816
Au	-1.005592	3.732027	-1.633418
Au	1.731515	3.304373	-1.849474
Au	0.475622	3.155071	0.644049
Au	-2.941656	1.531315	-0.917212
Au	-2.527533	3.369185	1.128026
Au	-4.543117	-0.986782	-0.635514
Au	-3.166742	-1.814173	1.673860
Au	2.702322	-2.474472	1.138857
Au	2.333786	-4.262822	-0.986254
Au	4.016216	-2.093443	-1.292391
Au	-3.407223	-3.555292	-0.554292
Au	-4.068804	1.074863	1.603865
Au	1.697617	0.415324	1.058427
Au	3.157599	0.724400	-1.465638
Au	3.467064	2.582920	0.643971
Au	4.500762	-0.016980	0.937694
Au	0.525712	0.266376	3.533114
Au	-0.124953	-1.780283	1.734672
Au	-1.248389	0.798267	1.351226
S	2.841038	-6.632816	-1.422220
S	2.995430	-2.956163	3.534131

S	6.549163	-0.862120	1.983885
S	-0.548287	-4.239588	1.776568
S	6.187475	-1.961264	-2.411406
S	-4.489983	-5.767630	-0.497485
S	-0.536837	-4.919798	-2.961444
S	-3.338986	-2.621929	3.990432
S	-5.739025	0.637262	3.340582
S	-6.760517	-0.140170	-1.250744
S	-2.535129	5.617808	2.098789
S	0.633355	4.012890	2.969129
S	-2.583613	5.130997	-2.882843
S	-3.404717	1.653083	-3.355618
S	4.284701	4.845218	1.146203
S	3.713407	0.411603	-3.892485
S	3.444314	4.297675	-3.305280
S	-0.209914	0.376743	5.904034
S	-0.411342	-0.974960	-5.736185
Au	6.592458	0.239958	-1.618851
Au	5.221191	3.346951	-2.047987
Au	6.306713	-3.197676	1.703291
Au	2.434285	5.872296	0.076501
Au	4.577897	-6.076299	0.113172
Au	-0.566595	-4.420520	-0.611465
Au	-6.142614	-4.514336	0.662459
Au	-6.708756	-1.345565	2.471345
Au	-6.282463	2.042647	-0.456903
Au	-4.268791	4.685944	-1.271468
Au	-0.923559	6.299072	0.493979
Au	3.495818	-0.679607	3.986524
Au	2.418444	2.632923	3.679549
S	4.294587	1.479803	4.577242
S	7.114092	2.452756	-0.919217
S	6.311880	-5.573343	1.640329
S	-7.863607	-3.275566	1.710123
S	-6.058978	4.307074	0.252315
S	0.718141	7.104401	-1.028501
Au	-2.526623	-3.752551	-3.492137
Au	-3.896264	-0.628565	-3.680972
S	-4.613334	-2.841060	-4.171451
Au	1.704109	-0.267066	-4.894939
Au	-1.808954	-1.134339	4.989590
H	-0.096797	-2.295148	-5.880170
H	3.661188	1.721044	-4.270244
H	6.840858	-2.634787	-1.417864
H	8.032281	2.716742	-1.895673
H	3.431928	5.525663	-2.707386
H	3.801890	4.908591	2.424700
H	0.954221	8.302548	-0.416053
H	-3.651010	6.027447	1.426564
H	-2.134377	6.307869	-2.354565
H	-7.060669	4.817588	-0.523914
H	-7.370118	-0.571569	-0.102220
H	-2.103048	1.615043	-3.767035



H	-4.335762	-2.802480	-5.508480
H	0.344453	-3.933505	-3.308461
H	0.752967	-4.636375	1.912350
H	3.583969	-6.403689	-2.544791
H	5.571438	-5.745139	2.774550
H	7.341382	-0.635047	0.889998
H	1.670045	-2.895596	3.865844
H	3.858842	1.478141	5.871751
H	-0.380922	3.271982	3.505272
H	0.663301	-0.563569	6.369068
H	-4.491719	-1.968452	4.324425
H	-7.871839	-3.941725	2.901310
H	-6.691960	1.497620	2.876782
H	-3.811741	-6.182154	0.612873

The cartesian coordinates of Au<sub>48</sub>-2D-Iso2

Au	-4.216593	-0.049641	-0.599550
Au	-4.099224	2.900643	-0.763076
Au	-4.434705	1.323709	1.842328
Au	-4.406962	-1.439810	1.835444
Au	-4.032229	-3.020409	-0.753825
Au	-1.650997	1.465856	-1.308177
Au	-1.612380	-1.493834	-1.316967
Au	1.410273	-1.638349	-5.081843
Au	-1.073439	0.003514	-3.682869
Au	1.334697	1.723131	-5.067513
Au	0.851978	3.101050	-1.734015
Au	0.925879	0.024375	-1.836906
Au	0.929746	-3.048617	-1.765297
Au	0.703608	-4.380656	0.711801
Au	-1.951157	-6.524338	1.224691
Au	-4.829717	-4.779707	2.018346
Au	-4.935892	4.659138	2.088644
Au	-2.096880	6.488163	1.284958
Au	0.591073	4.389072	0.767788
Au	-7.180668	1.664956	0.203167
Au	-7.133534	-1.813594	0.168007
Au	-3.901945	-0.088652	-4.458451
S	0.364281	-6.586551	1.734360
S	-4.265233	-6.671899	0.698428
S	-5.524402	-2.972167	3.390716
S	-8.067125	-0.100550	1.525639
S	-5.580053	2.808963	3.426742
S	-4.419698	6.577862	0.787555
S	0.220848	6.595929	1.776522
S	-6.448124	3.539121	-1.061778
S	0.181850	3.539837	-4.100996
S	-2.091506	-0.062034	-6.004609
S	0.313625	-3.499732	-4.139083
S	2.614667	0.074969	-6.209936

S	-6.364071	-3.580042	-1.223728
S	-5.506035	-0.227650	-2.755753
Au	3.164933	0.044062	0.027018
Au	3.061379	-3.035789	0.047820
Au	3.348724	-1.337832	-2.457478
Au	3.313740	1.455450	-2.440572
Au	2.987215	3.130934	0.074147
Au	3.075495	1.424771	2.525082
Au	3.131120	-1.350805	2.530220
Au	0.639308	-1.514321	0.720009
Au	0.600685	1.531073	0.727688
Au	0.574879	3.269631	3.723467
Au	0.324710	-0.012708	3.052492
Au	0.662336	-3.270204	3.661045
Au	-1.958020	-3.032886	1.142111
Au	-1.921418	-0.029767	1.288493
Au	-2.030674	2.971583	1.159991
Au	-1.808735	4.389518	-1.235179
Au	0.654027	6.628708	-1.858506
Au	3.621599	4.958899	-2.476663
Au	3.774994	-4.831716	-2.501274
Au	0.844082	-6.576330	-1.902363
Au	-1.693218	-4.413617	-1.271190
Au	5.409723	0.082030	1.667622
Au	6.145377	-1.677536	-0.642905
Au	6.092727	1.866335	-0.652236
Au	2.593659	-0.093831	6.015155
Au	6.134279	-0.042889	4.792156
S	-1.632441	6.496342	-2.479365
S	2.934050	6.888587	-1.266759
S	4.533973	3.164972	-3.730045
S	7.042653	0.104877	-1.943306
S	4.643180	-3.002626	-3.735278
S	3.129481	-6.786038	-1.308274
S	-1.442905	-6.502082	-2.532059
S	5.417659	-3.625517	0.510003
S	3.023284	-3.360843	3.943371
S	-1.704407	-3.275220	3.609512
S	0.286128	0.122517	5.521422
S	-1.788050	3.253368	3.617840
S	2.927586	3.339938	4.054507
S	5.323759	3.788379	0.517262
S	7.536820	0.268639	2.901203
S	4.837361	-0.382481	6.741383
H	0.290599	-6.131438	3.022261
H	-4.582413	-7.623089	1.626603
H	-4.475793	-3.029592	4.266238
H	-1.984045	4.605607	3.572657
H	2.944221	2.576563	5.191974
H	-4.524921	2.873876	4.294186
H	-4.750672	7.513247	1.726747
H	0.162757	6.148431	3.067826
H	-6.654928	3.027860	-2.312848

H	-6.462789	-2.873793	-2.389958
H	-9.313262	-0.110868	0.965735
H	-5.942753	1.061657	-2.811191
H	-2.057963	1.289750	-6.189100
H	-1.398352	5.926407	-3.699997
H	3.253473	7.804174	-2.229108
H	3.647691	3.210486	-4.772886
H	5.404694	3.260468	1.775468
H	8.274726	0.129167	-1.353589
H	5.453137	-3.103746	1.773061
H	7.914693	-1.036385	2.770315
H	5.008495	0.852427	7.296654
H	-0.034855	-1.189066	5.737242
H	-1.882371	-4.630369	3.602568
H	3.056531	-2.688518	5.135774
H	-1.221458	-5.916860	-3.747717
H	3.771798	-3.072811	-4.789017
H	3.471214	-7.686781	-2.276903
H	1.875516	0.059108	-7.358454
H	-0.933189	-2.943188	-4.078741
H	-1.039070	2.933254	-3.997857

The cartesian coordinates of Au<sub>56</sub>-2D-Iso2

Au	-2.931426	1.045951	-0.416772
Au	-3.827744	-1.867395	-0.267575
Au	-2.908385	-0.504525	-2.834887
Au	-2.291091	2.176056	-2.908987
Au	-2.038108	3.971683	-0.526608
Au	-3.067165	2.649390	1.968505
Au	-3.826619	-0.015307	2.143266
Au	-1.132957	-0.939893	0.876455
Au	-0.281296	1.979477	0.718862
Au	-0.474080	4.056180	3.439677
Au	-0.921727	0.700738	3.127210
Au	-2.053049	-2.409915	3.939670
Au	0.831574	-3.016500	1.934890
Au	1.549603	-0.054998	1.924315
Au	2.454714	2.853864	1.704507
Au	3.071676	3.969720	-0.827402
Au	1.287426	6.602655	-2.215774
Au	-1.710303	5.454283	-3.582498
Au	-4.052918	-3.817149	-3.072642
Au	-1.892464	-6.221076	-1.656264
Au	0.743523	-4.491662	-0.456017
Au	-5.453355	1.802811	0.705658
Au	-5.605406	-0.117407	-1.621671
Au	-5.091470	3.292953	-2.005228
Au	-3.723859	1.767045	5.010108
Au	-6.895238	0.769140	3.693406
S	3.585412	6.058271	-2.019247
S	-0.958110	7.356293	-2.378374
S	-2.567235	3.650335	-4.861965

S	-6.179916	1.588217	-3.271367
S	-4.220206	-5.820857	-1.777561
S	0.404996	-6.728630	-1.442832
S	-4.340711	-1.872708	3.729742
S	0.189998	-2.999437	4.342941
S	-1.519054	1.034875	5.507095
S	1.724940	3.409380	4.019626
S	-2.687983	4.845854	3.057979
S	-4.155592	5.164294	-0.869257
S	-8.005538	-1.067257	2.677889
S	-5.931033	2.652428	4.780294
Au	4.050923	-0.786804	0.554664
Au	4.828756	2.174521	0.385876
Au	4.171518	0.690730	2.939597
Au	3.465018	-1.976450	3.026859
Au	3.213706	-3.768898	0.631912
Au	4.213959	-2.372649	-1.800093
Au	4.975390	0.291601	-1.943515
Au	2.260591	1.233844	-0.721439
Au	1.424105	-1.726667	-0.585604
Au	1.678380	-3.701807	-3.391592
Au	2.110581	-0.411983	-2.976695
Au	3.420106	2.604139	-3.679690
Au	0.332153	3.266828	-1.864622
Au	-0.364390	0.311460	-1.762447
Au	-1.329170	-2.605882	-1.509402
Au	-2.004744	-3.604713	1.006057
Au	-0.267579	-6.347528	2.183601
Au	2.880158	-5.347602	3.498487
Au	5.397910	3.856814	3.211650
Au	3.366186	6.230615	1.647952
Au	0.423118	4.744261	0.535135
Au	6.540291	-1.516275	-0.428990
Au	7.217729	0.226997	1.915825
Au	6.299865	-3.202654	2.042934
Au	4.903163	-1.148296	-5.311353
Au	7.959474	-1.873775	-3.287139
S	-2.560892	-5.750897	2.066624
S	1.959137	-7.171368	2.288102
S	3.890543	-3.635289	4.798433
S	7.357407	-1.593341	3.446592
S	5.254601	2.018779	4.705550
S	5.686157	5.745302	1.801392
S	1.109304	6.924268	1.446982
S	7.283939	2.165275	0.538891
S	5.736388	2.148754	-3.371433
S	1.175293	3.133152	-4.204579
S	2.561470	-0.800716	-5.378178
S	-0.576714	-3.147592	-3.827426
S	3.954188	-4.377426	-3.199727
S	5.338461	-4.991500	0.806434
S	8.775547	-2.312234	-1.100883
S	7.254675	-1.437827	-5.502155

H	3.746523	5.470134	-3.244077
H	-0.778219	8.181616	-3.451783
H	-1.378432	3.286292	-5.430610
H	-1.068625	-4.423290	-3.790680
H	4.390018	-3.776858	-4.350722
H	-4.491144	-6.660193	-2.820878
H	0.791378	-6.354859	-2.701496
H	-4.685791	4.884422	0.358433
H	-7.436641	1.807280	-2.770057
H	-7.408155	-2.039262	3.429339
H	-5.673260	3.338908	3.626811
H	-1.814571	-0.284401	5.726614
H	-4.419108	-1.062514	4.828672
H	0.002590	-4.351966	4.410229
H	-2.680900	-5.236835	3.328309
H	1.776251	-8.008536	3.351730
H	2.777077	-3.320929	5.526848
H	5.827795	-4.635187	-0.419047
H	8.641843	-1.946800	3.142933
H	7.494322	1.523087	-0.649173
H	9.430445	-1.126010	-0.936703
H	7.244232	-2.725423	-5.954664
H	2.617148	0.517264	-5.738871
H	1.338453	4.484112	-4.337131
H	5.894112	1.404172	-4.508288
H	0.716471	6.658374	2.729777
H	5.977459	6.648307	2.784039
H	2.281288	4.657746	3.993932
H	-3.168668	4.501482	4.291585
Au	-6.231344	-2.833924	-1.333522
Au	-6.358345	-1.145536	0.874910
S	-3.885956	-1.967521	-4.566585
S	-7.681067	2.831805	0.623571
S	-8.061048	-4.276395	-2.095043
Au	-8.960167	1.204051	-0.527485
Au	-9.243922	-2.221346	-1.910291
S	-10.489796	-0.230466	-1.640383
H	-8.060723	2.443721	1.882573
H	-10.296878	0.261324	-2.899106
H	-7.771324	-4.179510	-3.425498
H	-5.166399	-1.515818	-4.420409
H	4.077102	2.390912	5.292160

The cartesian coordinates of Au<sub>56</sub>-2D-Iso3

Au	0.129360	-0.051742	1.697396
Au	-1.608399	1.870638	0.200438
Au	-2.721721	-0.724997	1.205438
Au	-1.957989	1.390980	2.938855
Au	-0.094791	-0.304731	5.144397
Au	1.880432	-1.852608	3.068584
Au	2.938068	0.548539	2.165666
Au	2.310394	-1.534171	0.266592

Au	-0.960523	-2.744768	2.620870
Au	1.074236	-4.126790	1.258541
Au	0.985685	-4.912742	4.520239
Au	-2.338904	-5.620782	4.025046
Au	-3.875281	-3.228380	2.129012
Au	-4.836561	-5.892176	0.557143
Au	-6.805205	-3.705326	-1.293720
Au	-3.537035	-2.864058	-0.628166
Au	-1.116978	-4.977574	-2.333168
Au	-5.162248	-0.892999	-2.217105
Au	-7.896867	0.365261	-0.839549
Au	-6.655755	3.313413	-2.051077
Au	-4.190243	1.541144	-3.105514
Au	-1.346790	2.386570	-2.652917
Au	-3.316975	3.738886	-1.123488
Au	-3.452355	4.491139	-4.617142
Au	-0.094770	5.314244	-3.958394
Au	-0.608139	4.432828	-0.920663
Au	-5.518889	-1.473106	0.763670
Au	2.480250	5.889781	-0.408511
Au	-1.593421	-4.718261	0.711400
S	-2.698856	-6.914149	0.568199
S	-5.331921	5.128752	-1.289038
S	4.767202	5.247876	-0.402470
S	0.252497	6.705266	-0.453570
S	-2.199996	6.423711	-4.041974
S	-4.784133	2.629941	-5.233163
S	-1.126579	1.667794	-5.024613
S	-8.124108	1.616850	-2.846368
S	-6.726103	-2.435610	-3.297010
S	-3.276889	-4.110477	-2.777202
S	1.018613	-5.971933	-2.007856
S	-0.302093	-6.841315	3.987598
S	-4.398859	-4.461632	4.181425
S	-7.058740	-5.045328	0.655385
S	-7.829730	-0.817121	1.217356
S	-2.958270	1.934689	5.132198
S	-1.695200	-2.022677	4.871927
S	2.336702	-3.072878	5.170744
Au	0.558652	0.379782	-1.243266
Au	1.333617	2.588802	0.603506
Au	3.434250	1.123978	-0.773952
Au	1.657908	2.759824	-2.210531
Au	1.057441	0.840839	-4.737132
Au	-0.225581	-1.663755	-2.992517
Au	-2.356518	-0.291676	-1.739745
Au	-0.574953	-2.224540	-0.258987
Au	2.816072	-1.238730	-2.583849
Au	1.800508	-3.649895	-1.644755
Au	2.006476	-3.650323	-4.876318
Au	5.419863	-2.936084	-4.332072
Au	5.641352	-0.320920	-2.095957
Au	8.187151	-2.616413	-0.596631

Au	9.101519	0.974560	-0.343804
Au	5.226809	-0.567206	0.644535
Au	4.414177	-3.635275	1.980045
Au	4.579528	3.587321	1.324521
Au	0.957588	2.344638	3.438873
Au	2.031399	4.697687	2.326498
Au	1.138116	6.167106	5.024616
Au	-1.731666	3.868043	5.739295
Au	-0.686318	4.091758	2.042154
Au	6.122679	1.853143	-0.447565
Au	-3.977367	3.830298	1.925437
Au	-4.536962	1.116422	-0.365963
Au	4.463921	-2.950908	-1.054171
S	6.530491	-4.270996	-0.963632
S	-5.558155	2.086576	1.684546
S	-2.535613	5.678803	2.325084
S	-0.667182	5.844916	6.519469
S	2.971098	6.597041	3.576435
S	1.415447	1.451517	5.671444
S	4.588218	2.106150	3.196758
S	8.198782	3.163285	-0.581011
S	5.930769	-1.893287	2.583185
S	3.084317	-5.535952	1.445677
S	4.060553	-4.845401	-4.694173
S	6.828133	-1.041440	-4.109470
S	10.053233	-1.187682	-0.225729
S	2.104763	4.417279	-4.001603
S	3.253910	-0.007097	-4.702516
S	-0.090773	-2.612711	-5.272272
H	-0.377604	-7.340725	5.256890
H	-5.174221	-5.412705	3.580552
H	3.528896	-3.602512	4.758293
H	7.032323	-2.435541	1.975594
H	2.831171	-5.929909	2.732378
H	-2.543284	-7.056105	-0.783296
H	-7.678372	-6.108352	0.062085
H	-5.754626	-3.176588	-3.910658
H	-8.393816	-1.974589	0.760286
H	-9.290757	2.244094	-2.510609
H	-5.054126	5.635457	-2.529671
H	-6.511469	2.810062	1.025003
H	-2.558482	5.585205	3.691340
H	-4.049173	2.594104	4.637332
H	0.043488	5.270748	7.533655
H	2.351948	7.565042	2.838789
H	0.493138	2.244752	6.302407
H	-1.017341	-3.005023	5.539580
H	8.235557	3.516489	0.736772
H	10.070204	-1.291125	1.135227
H	6.689185	-4.344118	-2.322574
H	7.844822	-1.643580	-3.421608
H	4.301693	-4.974127	-6.032235
H	-0.850357	-3.714226	-4.985930

H	1.366618	-6.032141	-3.328780
H	-3.990469	-5.201156	-2.365691
H	-3.818973	1.993116	-5.962456
H	-2.082597	6.941056	-5.300463
H	2.632382	5.359543	-3.157979
H	-0.774741	2.903415	-5.492328
H	3.834936	1.085289	-4.124161
H	4.706602	4.371368	-1.448054
H	0.262640	7.122169	-1.755963
H	5.698781	1.398195	2.831305

The cartesian coordinates of Au<sub>60</sub>-2D-Iso2

Au	3.442182	-1.183436	-0.406164
Au	4.567638	1.652929	-0.200549
Au	3.600770	0.384889	-2.807904
Au	2.796102	-2.243152	-2.922893
Au	2.328582	-4.049190	-0.589976
Au	3.403448	-2.826640	1.943336
Au	4.349482	-0.223799	2.183713
Au	1.775832	0.914501	0.859644
Au	0.679656	-1.930947	0.622831
Au	0.726216	-4.061573	3.287388
Au	1.380920	-0.743928	3.070898
Au	2.720429	2.229633	4.005062
Au	-0.045886	3.102295	1.959829
Au	-0.984013	0.225639	1.818666
Au	-2.162801	-2.601290	1.491886
Au	-2.853235	-3.509271	-1.055881
Au	-1.284131	-6.317894	-2.359193
Au	1.962569	-5.515156	-3.585760
Au	5.000313	3.609413	-2.944607
Au	3.033779	6.153796	-1.469054
Au	0.237768	4.620019	-0.380235
Au	5.879848	-2.141005	0.763206
Au	6.229787	-0.213948	-1.530346
Au	5.506608	-3.576619	-1.951315
Au	4.039905	-2.049971	5.027834
Au	7.322596	-1.248959	3.815362
S	-3.527811	-5.558566	-2.232506
S	0.874065	-7.307059	-2.473941
S	3.137353	-3.830412	-4.777526
S	6.757793	-1.947093	-3.164003
S	5.319019	5.563640	-1.603932
S	0.794359	6.867862	-1.237094
S	4.973380	1.559117	3.815768
S	0.509516	2.943192	4.382463
S	1.871031	-1.183789	5.458978
S	-1.439665	-3.271466	3.794008
S	2.884987	-5.024229	2.983009
S	4.373951	-5.372664	-0.875473
S	8.586479	0.511962	2.846723
S	6.192532	-3.069658	4.846672



Au	-3.449484	1.180249	0.404483
Au	-4.564695	-1.652234	0.214855
Au	-3.601759	-0.381796	2.822561
Au	-2.800091	2.248568	2.918277
Au	-2.323581	4.043395	0.582158
Au	-3.393207	2.809796	-1.954923
Au	-4.354568	0.208689	-2.185842
Au	-1.780301	-0.922024	-0.854936
Au	-0.681941	1.921872	-0.625713
Au	-0.676806	4.013609	-3.296407
Au	-1.389446	0.729725	-3.073003
Au	-2.734312	-2.246056	-3.997445
Au	0.042790	-3.107469	-1.963762
Au	0.975700	-0.229419	-1.818099
Au	2.163358	2.601105	-1.478717
Au	2.851719	3.500281	1.071661
Au	1.290348	6.316181	2.354237
Au	-1.963782	5.530626	3.560404
Au	-4.983009	-3.583245	2.992372
Au	-3.031558	-6.148416	1.485136
Au	-0.233030	-4.627490	0.373418
Au	-5.876201	2.142843	-0.781550
Au	-6.218017	0.239786	1.532192
Au	-5.502969	3.607776	1.915931
Au	-4.084996	2.039625	-5.002795
Au	-7.355773	1.223655	-3.787876
S	3.531502	5.546325	2.252382
S	-0.864916	7.314066	2.445297
S	-3.147689	3.854637	4.755262
S	-6.759761	1.990100	3.140468
S	-4.790359	-1.746820	4.503105
S	-5.307825	-5.534049	1.647950
S	-0.799541	-6.876576	1.221501
S	-4.990517	-1.594273	-3.790545
S	-0.519082	-2.941171	-4.383278
S	-1.915028	1.176403	-5.449477
S	1.484141	3.208959	-3.806174
S	-2.832425	4.989404	-3.003960
S	-4.360186	5.393061	0.826766
S	-8.604743	-0.538820	-2.808027
S	-6.243737	3.043794	-4.834780
H	-3.593018	-4.974794	-3.467934
H	0.644820	-8.079443	-3.576949
H	2.070636	-3.387051	-5.508477
H	2.114908	4.421947	-3.787474
H	-3.296290	4.684592	-4.254297
H	5.659102	6.402809	-2.626926
H	0.386036	6.613534	-2.517817
H	4.876771	-5.147757	0.374860
H	7.976077	-2.241838	-2.610286
H	8.039742	1.518961	3.590610
H	5.922860	-3.719875	3.675002
H	2.248730	0.104381	5.731051

H	4.985796	0.723880	4.898523
H	0.781179	4.275836	4.519685
H	3.581785	4.964225	3.489193
H	-0.641707	8.092761	3.545084
H	-2.085397	3.416852	5.496110
H	-4.829510	5.146296	-0.432651
H	-7.969637	2.269649	2.561964
H	-8.055212	-1.546366	-3.549555
H	-6.005107	3.715787	-3.669464
H	-2.293220	-0.111179	-5.723313
H	-0.781277	-4.275048	-4.526960
H	-5.025411	-0.765281	-4.877231
H	-0.374224	-6.637765	2.499664
H	-5.652649	-6.374222	2.668377
H	-2.071656	-4.483393	3.744093
H	3.343296	-4.727007	4.237125
Au	7.071502	2.434370	-1.190778
Au	6.997624	0.719653	1.002339
S	4.722354	1.809541	-4.483078
S	8.028753	-3.328724	0.745459
S	9.021837	3.742282	-1.890390
Au	9.484695	-1.782963	-0.304714
Au	10.065875	1.620386	-1.638818
S	11.171861	-0.441543	-1.297885
H	8.381772	-2.993595	2.027579
H	11.039578	-0.918225	-2.570134
H	8.778905	3.648488	-3.230367
H	5.963170	1.262340	-4.320703
H	-3.643866	-2.177178	5.111030
Au	-6.996789	-0.731385	-0.983828
Au	-7.064039	-2.410892	1.233633
S	-9.006048	-3.669718	2.033423
S	-8.030133	3.320804	-0.884063
Au	-10.063258	-1.577891	1.627683
Au	-9.490763	1.799695	0.195359
S	-11.189374	0.445555	1.149568
H	-8.749824	-3.463877	3.358579
H	-11.128158	0.966359	2.409885
H	-7.800715	4.121544	0.201112