

Supporting Information:

## **Structural Predictions of Thiolate-Protected Gold Nanoclusters via Redistribution of the Au-S “Staple” Motifs on the Known Core**

Dongdong Lin,<sup>a,b</sup> Mengke Zheng,<sup>a</sup> and Wen Wu Xu <sup>\*a,b</sup>

<sup>a</sup> Department of Physics, School of Physical Science and Technology, Ningbo University, Ningbo 315211, China

<sup>b</sup> Laboratory of Clean Energy Storage and Conversion, Ningbo University, Ningbo 315211, China

\*Correspondence should be addressed to: \**W. W. Xu* (xuwenwu@nbu.edu.cn)

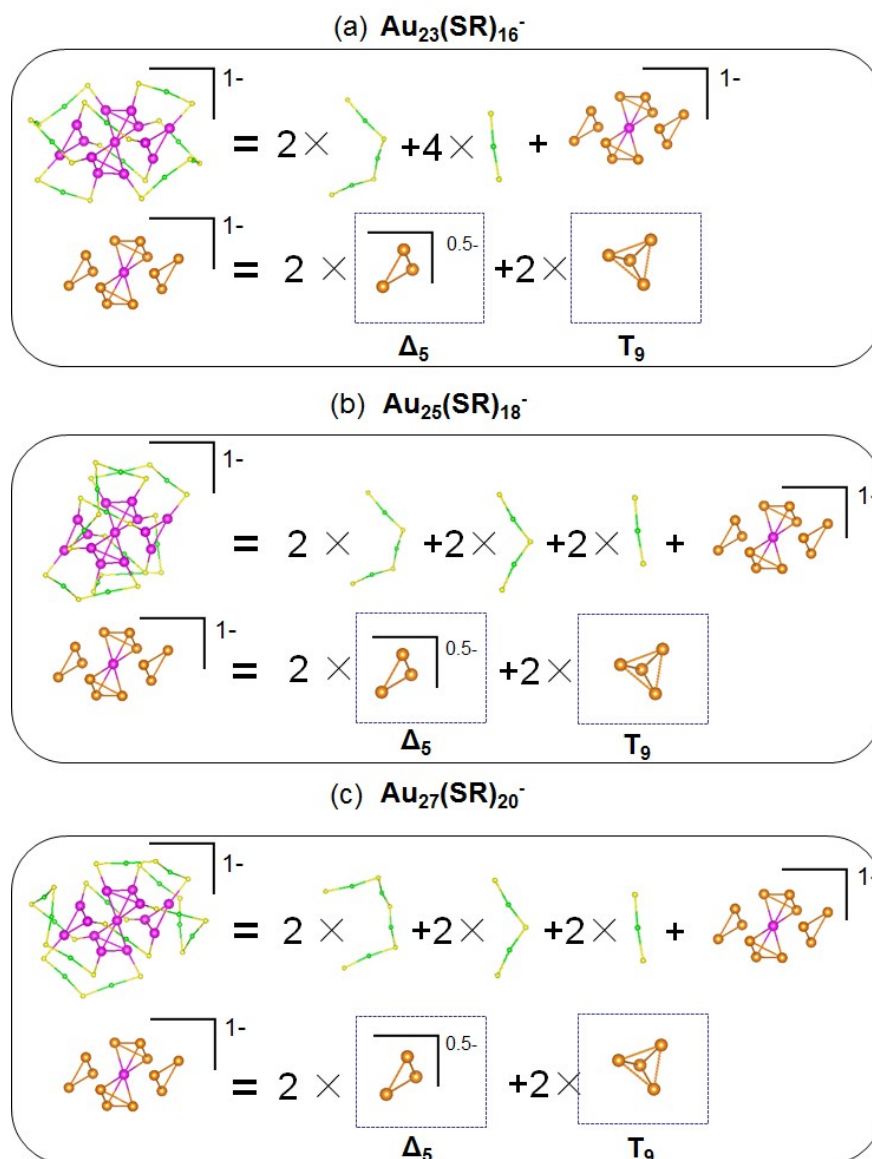


Figure S1. Structural decompositions of  $\text{Au}_{23}(\text{SR})_{16}^-$  (a),  $\text{Au}_{25}(\text{SR})_{18}^-$  (b), and  $\text{Au}_{27}(\text{SR})_{20}^-$  (c). Au atoms with  $1e$  valence electrons are presented in wine and green. Au atoms with  $0.5e$  valence electrons are presented in gold. S is presented in yellow. The R groups were omitted for clarity.

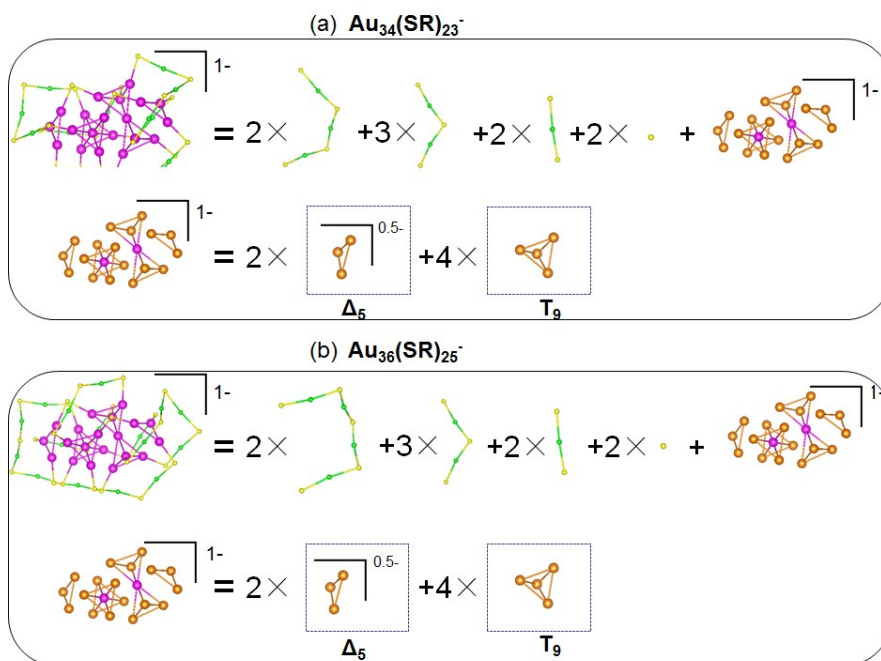


Figure S2. Structural decompositions of  $\text{Au}_{34}(\text{SR})_{21}^-$  (a) and  $\text{Au}_{36}(\text{SR})_{25}^-$  (b). Au atoms with  $1e$  valence electrons are presented in wine and green. Au atoms with  $0.5e$  valence electrons are presented in gold. S is presented in yellow. The R groups were omitted for clarity.

The cartesian coordinates of Au<sub>27</sub>(SH)<sub>20</sub><sup>-</sup>

Au	-0.272920	-2.734178	-0.276342
Au	1.884633	-1.420451	-1.502851
Au	2.414612	1.233199	1.536267
Au	-2.355622	-1.492553	1.349950
Au	1.827162	-1.628694	1.249939
Au	0.021359	-0.266866	3.322675
Au	4.434188	-0.589221	3.142870
Au	4.293514	-0.049119	0.062204
Au	4.954845	-3.508095	-0.353828
Au	-1.580378	5.081813	-0.247674
Au	4.999297	2.695817	1.878591
S	1.308004	1.712060	3.708680
S	3.178944	-2.612389	3.050900
S	0.615865	5.183461	0.667180
S	-1.188564	-2.334537	3.358446
S	3.870567	-5.612558	-0.552390
S	6.264488	-1.543321	-0.112889
S	5.871473	1.277180	3.578590
S	4.301665	4.356657	0.299403
Au	0.284106	2.733345	0.256575
Au	-1.880712	1.412101	1.484991
Au	-2.518871	-1.165909	-1.404628
Au	2.442016	1.447516	-1.243040
Au	-1.885445	1.733701	-1.243182
Au	0.004021	0.211652	-3.269143
Au	-4.535315	0.836004	-2.823378
Au	-4.299258	0.047239	0.235021
Au	-4.824543	3.197641	-0.257857
Au	1.532176	-5.226084	-0.732160
Au	-5.368733	-2.280314	-1.547792
S	-1.441533	-1.672993	-3.580339
S	-2.778360	2.311966	-3.486188
S	-0.837940	-5.100120	-0.801786
S	1.403321	2.156111	-3.369921
S	-3.762814	5.126327	-1.174710
S	-6.242315	1.531009	0.687133
S	-6.515961	-0.512342	-2.665575
S	-4.510107	-4.217651	-0.433222
Au	-0.009150	0.006591	-0.017938
S	-3.076050	2.118263	3.528908
Au	-4.296755	0.077164	3.380940
Au	-4.983092	-2.907485	1.522925
S	-5.681440	-1.868417	3.551702
S	3.122422	-2.042075	-3.526942
Au	5.149126	2.780860	-1.296511
Au	4.576888	-0.209999	-3.093784
S	6.248587	1.494153	-2.968678
H	-6.488448	-0.994461	-3.932404
H	-5.658318	-4.943732	-0.430098
H	-6.787439	-1.270686	3.043894
H	-3.447278	3.459772	-3.206292
H	-3.989101	2.874223	2.867906

H	-6.937379	1.284726	-0.451770
H	-4.330104	6.060292	-0.372502
H	1.284651	5.447179	-0.480427
H	-2.138583	-1.932019	4.241422
H	0.407389	2.594209	3.205064
H	-2.359123	-1.028859	-4.345261
H	0.492809	2.991979	-2.808513
H	-0.951334	-4.855106	-2.130434
H	4.127126	-5.814786	-1.867882
H	6.489879	-1.677913	1.219072
H	4.027552	-3.250606	2.197639
H	6.929282	0.814309	2.867344
H	5.401315	5.151372	0.363739
H	3.904788	-2.965715	-2.905571
H	7.053546	0.804937	-2.122084

The cartesian coordinates of  $\text{Au}_{32}(\text{SH})_{21}^-$

Au	1.692327	-1.440391	4.960355
Au	4.358390	2.796671	-2.813554
Au	4.778820	-2.358872	-0.406242
Au	2.493119	-3.772878	-0.531558
Au	2.918118	-1.753123	-2.306005
Au	0.315294	-3.092855	-2.339509
Au	2.624729	-1.836073	1.744499
Au	0.266217	-3.956122	1.804925
Au	5.740078	-0.464667	1.946573
Au	3.239224	0.204557	-0.089740
Au	0.771990	-1.249091	-0.244352
Au	-1.563602	-2.732085	-0.309260
Au	-1.233162	-0.785581	-2.281560
Au	1.209954	0.957338	-2.226002
Au	1.294782	0.620173	1.899847
Au	-1.291486	-0.739462	1.871092
Au	1.559902	2.762337	-0.125952
Au	-0.776324	1.269548	-0.152365
Au	-3.246754	-0.188289	-0.077791
Au	-4.014973	-2.668953	1.741151
Au	-2.607132	1.726191	1.882711
Au	-0.336455	3.262958	-2.107798
Au	-0.262831	3.832128	2.090154
Au	-2.944213	1.928091	-2.140353
Au	-4.783504	2.399682	-0.179539
Au	-2.499242	3.820830	-0.236981
Au	1.466750	4.780430	-3.999165
S	0.032786	-0.340152	6.281469
S	3.311599	-2.831125	3.902825
S	5.218315	1.170860	-1.326064
S	7.007636	-1.886211	0.503426
S	1.309541	-5.670544	0.492382
S	-0.839804	-2.614738	3.424927
S	3.318011	4.363582	0.578492
S	2.320653	-0.200634	-4.107895

S	0.846110	2.369256	3.601123
S	-3.333996	-4.386979	0.231710
S	-2.363180	0.513685	-4.055511
S	-1.294123	5.639897	0.896231
S	-7.006616	1.868405	0.711530
S	-0.856160	5.151958	-3.644980
S	3.778248	4.455151	-4.425689
Au	-1.594844	0.905835	5.040103
S	-3.213268	2.426260	4.173526
H	7.276843	-0.932401	-0.423993
H	4.089162	4.100088	-0.513747
H	2.075365	2.957818	3.488918
H	-2.260217	5.884639	1.815936
H	-0.712484	6.105299	-2.691358
H	3.457740	0.545483	-4.046968
H	3.628534	3.605150	-5.471150
H	5.613432	2.022159	-0.344133
H	-3.501488	-0.233868	-4.047357
H	-7.296870	1.000656	-0.290680
H	-4.095465	-4.017479	-0.839470
H	2.282887	-5.960701	1.390831
H	-2.069987	-3.194315	3.286144
H	4.379498	-2.010895	4.074435
H	0.761953	0.748649	6.627084
H	-4.290286	1.605858	4.271186
S	4.753015	0.958707	3.580268
Au	4.017609	2.528278	1.933746
Au	-5.737066	0.320462	2.015293
S	-4.741585	-1.239976	3.513727
S	0.815965	-4.904224	-3.979665
S	-5.239192	-1.053338	-1.366071
Au	-1.497122	-4.470205	-4.318084
Au	-4.369099	-2.548924	-2.978621
S	-3.777969	-4.007270	-4.769589
H	-5.618067	-1.983548	-0.451172
H	-4.296612	-5.138820	-4.232337
H	0.657204	-5.894581	-3.067041
H	-5.878642	-1.906407	3.839693
H	5.891501	1.598964	3.951041

The cartesian coordinates of  $\text{Au}_{34}(\text{SH})_{23}^-$

Au	-6.617837	-2.824056	-0.773118
Au	-5.153146	-2.639047	2.379696
Au	-5.360120	-0.304749	0.355901
Au	-4.027178	-0.258223	-2.037507
Au	-3.518890	-2.215596	-0.197962
Au	-1.834757	-2.104011	-2.614325
Au	-3.207640	1.888257	-0.161592
Au	-2.170667	2.187681	-3.126190
Au	-2.156813	1.821725	4.319174
Au	-2.749537	-0.080492	1.781927
Au	-1.329173	-0.094505	-0.687757

Au	-0.027981	-0.031672	-3.129155
Au	0.641073	-2.098767	-1.365974
Au	-0.649359	-2.186713	1.300761
Au	-0.812185	1.905987	1.325471
Au	0.769285	1.997885	-1.115511
Au	0.043080	-0.248734	3.186138
Au	1.318301	-0.121887	0.746935
Au	2.730105	0.065773	-1.730228
Au	5.170423	2.227605	-2.364049
Au	3.188653	1.894501	0.325922
Au	1.848407	-2.265490	2.503112
Au	2.114648	2.008290	3.291290
Au	3.534305	-2.218422	0.076811
Au	5.359055	-0.269664	-0.376578
Au	4.037331	-0.370475	2.023145
Au	4.952913	-3.018872	3.138063
Au	6.719439	-2.790376	0.570930
S	-6.547426	-4.177172	1.198223
S	-7.086627	-1.800472	-2.903664
S	-3.762601	-1.289645	3.739606
S	-7.084724	0.949030	1.583291
S	-4.012872	1.039616	-4.130776
S	-0.457148	3.688410	-2.454238
S	-0.710027	0.313552	5.469276
S	-2.141155	-4.065774	0.717609
S	0.330597	3.501727	2.816677
S	0.643748	0.656008	-5.425307
S	2.089011	-4.032156	-0.830141
S	4.002403	0.822162	4.167355
S	7.070200	1.000876	-1.609743
S	2.934518	-4.188160	3.607807
S	7.083830	-1.955938	2.798062
S	6.752952	-3.933031	-1.531690
Au	5.129904	-2.492174	-2.530091
S	3.597944	-1.160959	-3.754747
S	3.540193	3.727419	-3.233699
Au	2.150934	2.055588	-4.212753
Au	-4.947955	-2.772441	-3.410184
S	-2.910266	-3.855488	-3.988303
S	-3.565346	3.540268	3.453105
Au	-5.207173	2.122491	2.474744
S	-4.043083	4.196199	-0.504369
S	4.086487	4.169089	0.761139
Au	-1.944042	5.235161	-0.108588
Au	2.023566	5.251569	0.249758
S	0.041078	6.576860	0.024537
H	-5.522850	-4.969086	0.794455
H	-7.870658	-2.797368	-3.390305
H	-2.719106	-3.228252	-5.175034
H	-4.662724	-0.306471	3.995737
H	-1.596376	-0.712267	5.534741
H	-4.253363	3.821589	4.588879
H	-7.217170	0.041381	2.582247

H	-1.487329	-4.366278	-0.432197
H	2.711819	-4.119220	-2.033036
H	1.524705	-0.354248	-5.635515
H	4.226530	4.087627	-4.348264
H	7.132514	0.140472	-2.656255
H	2.568846	-2.046880	-3.726378
H	5.873773	-4.903558	-1.180401
H	7.876202	-2.974391	3.223026
H	2.943308	-4.951729	2.486716
H	4.914941	1.757669	3.806095
H	0.990860	4.214698	1.831823
H	4.657092	4.309766	-0.462966
H	0.122292	6.759331	-1.315513
H	-4.550101	4.344008	0.746390
H	0.322083	3.526052	-3.569411
H	-4.952814	1.932679	-3.733802

The cartesian coordinates of Au<sub>36</sub>(SH)<sub>25</sub><sup>-</sup>

Au	7.084926	0.595381	-2.161466
Au	-1.144056	5.004830	1.579069
Au	-5.484235	-0.215900	-0.542211
Au	-4.159188	-0.087524	1.822906
Au	-3.644562	1.745933	-0.218115
Au	-2.033093	1.891836	2.220089
Au	-3.232044	-2.257170	0.023778
Au	-2.196540	-2.500758	2.952802
Au	-5.008819	-2.662668	-2.635603
Au	-2.653637	-0.416951	-1.974464
Au	-1.391416	-0.218826	0.565151
Au	-0.280151	-0.167892	3.079567
Au	0.599699	1.844401	1.328990
Au	-0.596653	1.803959	-1.382771
Au	-0.732799	-2.322055	-1.251826
Au	0.725121	-2.290801	1.290096
Au	0.278844	-0.249405	-3.093417
Au	1.384541	-0.232913	-0.576543
Au	2.643706	-0.366642	1.967046
Au	1.816702	-2.401715	4.225202
Au	3.227825	-2.254898	0.017920
Au	2.029060	1.824983	-2.296198
Au	2.208896	-2.561870	-2.908153
Au	3.640790	1.759698	0.155114
Au	5.476751	-0.193813	0.556748
Au	4.172487	-0.126371	-1.822986
Au	1.123577	4.953640	-1.721477
S	8.289590	-1.426291	-1.809122
S	6.151956	2.759948	-2.637579
S	-3.570517	0.692275	-4.026799
S	-6.976607	-1.398159	-2.129705
S	-3.762343	-1.069991	4.066971
S	-0.726251	-4.157216	2.058491
S	-0.383962	-1.009651	-5.351572



S	-2.325045	3.549919	-1.277339
S	0.726428	-4.194208	-1.990677
S	0.363327	-0.881780	5.360492
S	2.337026	3.587254	1.194141
S	3.791739	-1.164596	-4.041919
S	6.956360	-1.338812	2.184228
S	2.473270	3.958160	-3.412571
S	-0.096466	6.274831	-0.149429
Au	6.322302	-2.656977	-1.226366
S	4.576613	-4.190782	-0.733304
H	-6.856428	-0.483386	-3.127367
H	-1.308557	-0.032513	-5.535998
H	0.045747	-4.445052	-3.139293
H	4.839286	-2.023785	-3.955908
H	3.670950	4.202265	-2.825502
H	-2.811552	3.349492	-2.530964
H	0.990812	6.651613	0.567362
H	-4.339038	-0.360020	-4.405657
H	2.837847	3.390014	2.443723
H	6.824666	-0.404188	3.162134
H	1.297037	0.089493	5.530733
H	-4.816102	-1.924134	4.009869
H	-0.042722	-4.392189	3.208748
H	7.301261	3.399778	-2.977031
H	8.649696	-1.152801	-0.530021
H	5.043868	-4.539155	0.493884
S	-3.285802	-4.181545	-3.280105
Au	-1.841057	-2.497592	-4.181049
Au	4.987090	-2.598171	2.696790
S	3.262887	-4.106079	3.365160
S	-2.407962	4.044405	3.354961
S	3.548942	0.773265	4.009802
Au	6.416547	2.922869	-0.254144
Au	5.254408	1.965607	2.870812
S	7.003701	3.350411	2.017286
H	4.316224	-0.273297	4.406954
H	7.990168	2.423042	2.093478
H	-1.362498	3.878186	4.203026
H	3.821921	-4.491967	4.540928
H	-3.848305	-4.591087	-4.446218
S	-4.590233	-4.165433	0.824404
Au	-6.317060	-2.610939	1.324781
Au	-5.273506	1.897913	-2.894962
S	-8.264038	-1.357520	1.926486
S	-7.027649	3.283954	-2.053399
Au	-7.048322	0.671655	2.201913
Au	-6.397406	2.935241	0.220373
S	-6.067518	2.829322	2.596831
H	-5.079425	-4.524996	-0.391149
H	-8.659300	-1.117417	0.651356
H	-7.204914	3.485089	2.948516
H	-7.999185	2.338283	-2.081683