

Supplementary Materials for Unraveling structures of protection ligands on gold nanoparticle $\text{Au}_{68}(\text{SH})_{32}$

Wen Wu Xu, Yi Gao, Xiao Cheng Zeng

Published 24 April 2015, *Sci. Adv.* **1**, e1400211 (2015)

DOI: 10.1126/sciadv.1400211

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Fig. S1. MO energy level diagram for **Iso1**, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes.

Fig. S2. MO energy level diagram for **Iso2**, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes.

Fig. S3. MO energy level diagram for **Iso3**, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes.

Fig. S4. MO energy level diagram for **Iso4**, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes.

Table S1. Bond CNA signatures for **Iso1** to **Iso4**.

Coordinate files

Supplementary Materials

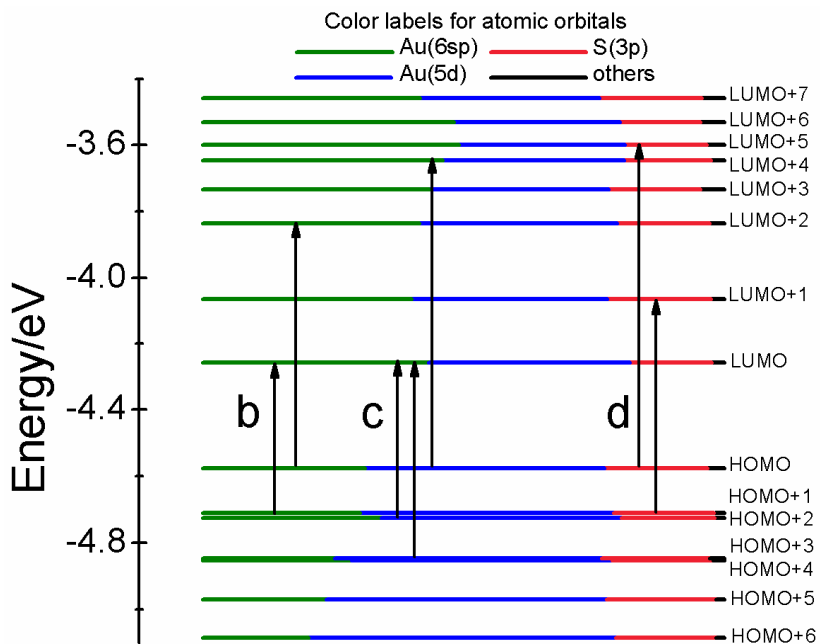


Fig. S1. MO energy level diagram for Iso1, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes. The energies are in eV. Various colors are used to mark relative contributions (line length with color labels) of different orbitals. The major orbital contributions, i.e., those from the Au(6sp), Au(5d), and S(3p) are in olive, blue, and pink, respectively.

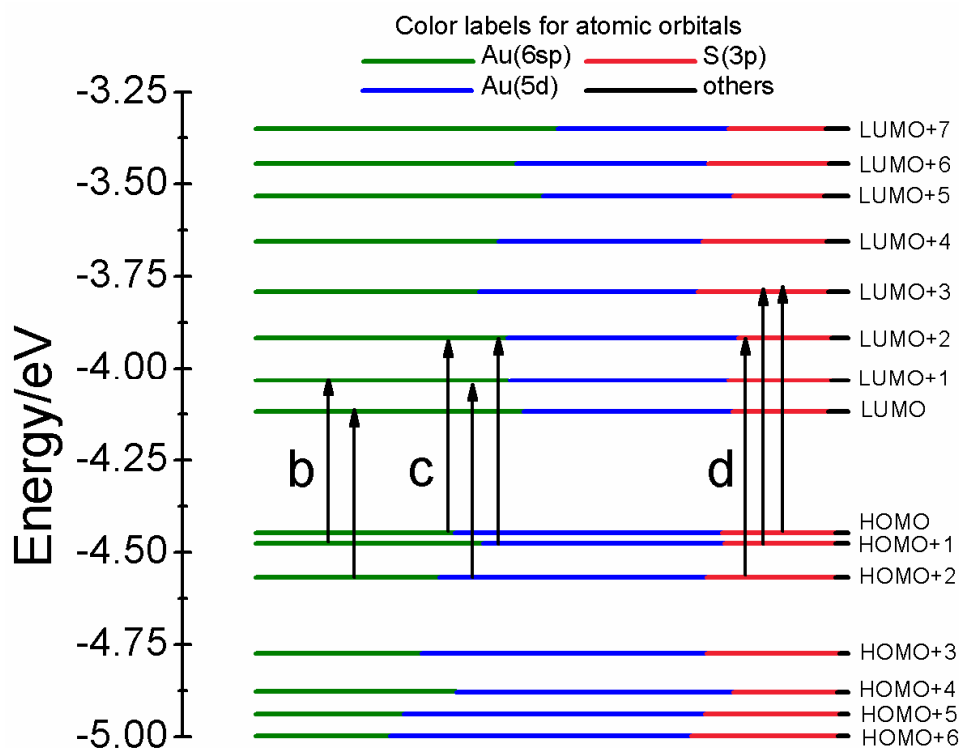


Fig. S2. MO energy level diagram for Iso2, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes. The energies are in eV. Various colors are used to mark relative contributions (line length with color labels) of different orbitals. The major orbital contributions, ie., those from the Au(6sp), Au(5d), and S(3p) are in olive, blue, and pink, respectively.

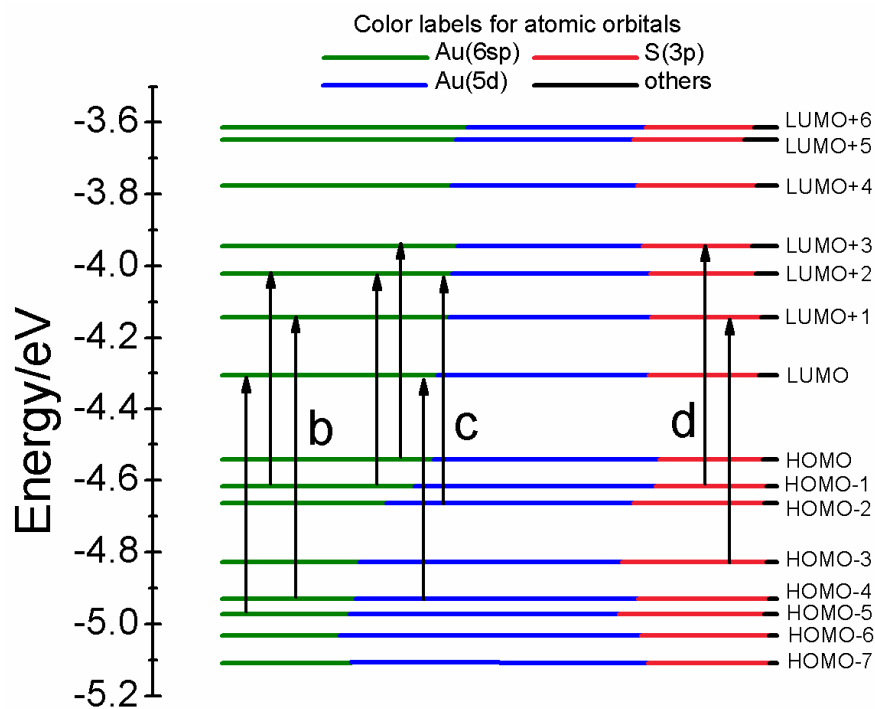


Fig. S3. MO energy level diagram for Iso3, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes. The energies are in eV. Various colors are used to mark relative contributions (line length with color labels) of different orbitals. The major orbital contributions, ie., thoes from the Au(6sp), Au(5d), and S(3p) are in olive, blue, and pink, respectively.

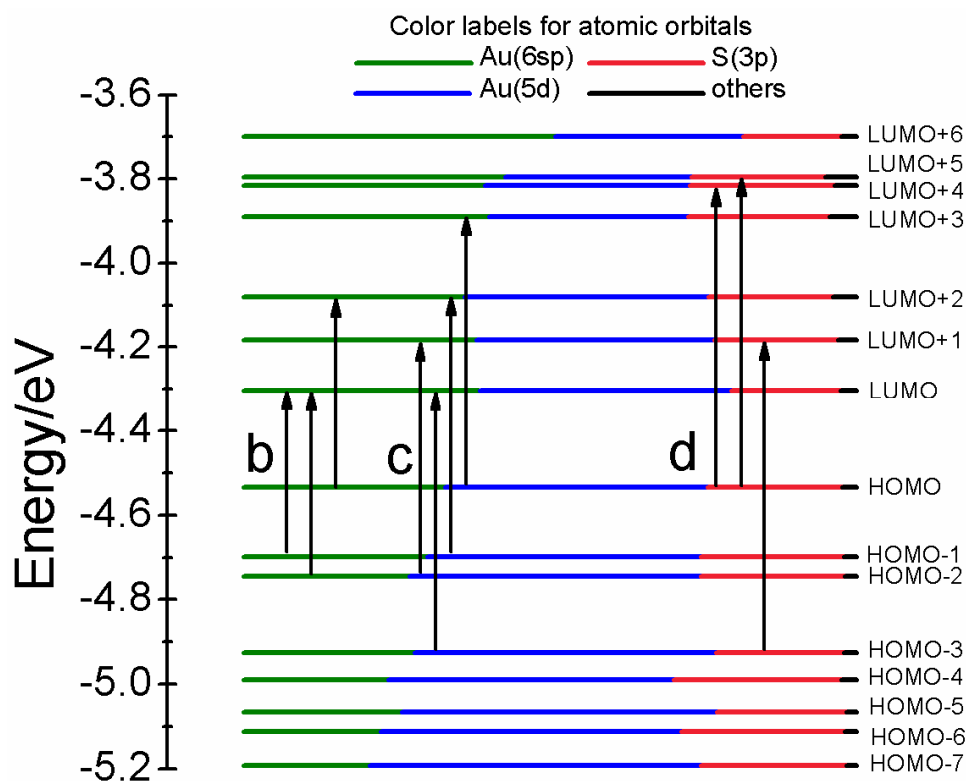


Fig. S4. MO energy level diagram for Iso4, with the three peaks b, c, and d in Fig. 4 being assigned to various excitation modes. The energies are in eV. Various colors are used to mark relative contributions (line length with color labels) of different orbitals. The major orbital contributions, ie., thoes from the Au(6sp), Au(5d), and S(3p) are in olive, blue, and pink, respectively.

	421	311	211
Iso1	22	40	23
Iso2	10	33	21
Iso3	35	54	22
Iso4	24	41	25

Table S1. Bond CNA signatures for Iso1 to Iso4.

Coordinates file of optimized structure of Iso1

Au	-0.228674602	0.331167340	0.093032677
Au	-1.908934334	0.494822667	-2.480654149
Au	-1.429921488	2.389602383	1.927271813
Au	0.669607632	1.376761501	-2.936177153
Au	-2.602373546	-1.704890332	1.084017666
Au	-0.960738313	-0.183302183	3.084615607
Au	-3.768564590	0.364206074	2.952556782
Au	-3.162522624	0.904797259	0.079109052
Au	1.374080411	1.602459782	2.223340786
Au	0.294484202	-2.191326792	1.383018819
Au	-1.593052926	-4.156219001	2.112191039
Au	2.171250601	2.221324182	-0.483189213
Au	-1.001143817	2.828597163	-1.031095599
Au	-1.071908939	-2.068154545	-1.387038941
Au	0.794168092	4.265121831	0.939299142
Au	-2.676163804	-3.300305753	-3.420658712
Au	-1.520774367	1.269775520	-5.219997543
Au	1.557112921	-1.064142556	-1.824406476
Au	1.147969840	4.561918580	-1.808247585
Au	4.000947860	0.522444844	-1.744955900
Au	1.808939946	-0.876063934	3.497290076
Au	2.581282686	-0.559236205	0.806826640
Au	-2.903325384	-2.324648931	3.939447711
Au	-0.154594641	-2.672717856	4.401098874
Au	-1.643277993	-0.498805575	5.738513348
Au	0.503306062	1.289083955	5.036750590
Au	-2.507315117	2.164321279	4.581911970
Au	2.986224733	2.848137377	-3.297338723
Au	2.797267974	0.099601441	-4.292571036
Au	1.252650706	2.121055756	-5.548250873
Au	-0.339656793	-1.258299076	-4.128370534
Au	-0.660838857	3.656412412	-3.825134479
Au	-3.461118800	-0.752831631	-4.449788320
Au	-3.949061576	-1.506948570	-1.627600866
Au	-5.307255837	-0.768299236	0.873132503
Au	-4.671105898	1.074714023	-2.535958301
Au	4.525520681	1.471854307	0.877054287
Au	3.351443083	3.472353893	2.819087582
Au	3.971716072	0.925022155	3.676894249
Au	4.832949700	-1.757146697	-0.255859933
Au	-2.056751831	4.834150774	0.752237333
Au	-3.916163129	3.317945745	-1.025098320
Au	-4.067564319	3.086201131	1.950676302
Au	0.385924440	3.811572429	3.647592692
Au	0.945985850	-3.715475611	-2.766859191
Au	2.483354178	-3.244699203	-0.199778989
Au	-0.167837260	-4.510726874	-0.349308226
Au	-3.041581699	-4.033690245	-0.606616858
Au	0.422486597	7.116999592	-0.438681763
Au	3.633957287	6.062420413	-2.000227222
Au	-1.135282746	2.889990560	-7.688694304
Au	-3.841689565	0.991970253	-7.086252582
Au	5.777251198	-1.388221164	-3.211527311
Au	1.836629765	-3.879099648	-5.463029101
Au	-3.244780877	5.536692422	-3.416913646
Au	6.347294441	2.848750626	3.396616543
Au	3.841271670	2.847071550	6.029783622
Au	3.347223344	-2.480503245	5.176435706

Au	1.514709843	6.495349891	2.992701763
Au	-4.459813087	0.690560294	6.602940676
Au	-6.640861443	0.375791038	3.803401433
Au	-7.098877181	-0.331121253	-1.717379418
Au	-4.570463074	-4.806125773	2.151955835
Au	-0.283542238	-7.148424320	0.756419459
Au	-1.431871031	5.648956331	4.855492695
Au	-7.084581258	2.759953591	0.282406046
Au	-0.706388053	-6.306379370	-2.767323359
Au	3.417869299	-5.362044711	-2.535212981
S	2.689285571	7.770951747	-0.685771421
S	-1.930948133	7.088208269	-0.173857146
S	4.793095520	4.489184717	-3.318285149
S	-3.466045425	3.266270738	-7.620283252
S	1.211671043	2.679736388	-7.899371356
S	-4.404366842	-1.262013589	-6.673915862
S	7.060589090	-1.809257682	-1.253637199
S	4.571696874	-1.277147652	-5.235767355
S	0.194192527	-2.406191238	-6.258277132
S	3.582060319	-5.357263644	-4.885959035
S	-1.349527071	5.824793894	-4.739019681
S	-5.168032245	5.160373842	-2.088578545
S	6.036197982	3.641760719	5.599186618
S	6.878207043	2.141301355	1.204172769
S	1.753049323	2.240314081	6.915253540
S	3.452846173	-5.534893919	-0.177343911
S	5.103341229	-0.933178595	4.919001751
S	3.784593240	5.892577315	2.708634296
S	-0.621919348	7.397600912	3.504837060
S	-6.250684207	1.848873798	5.608186741
S	-2.818519198	-0.500409215	7.851056447
S	-7.432106204	-1.044193113	2.089092225
S	-6.313458245	-2.530622572	-1.983662670
S	-8.097769430	1.815063668	-1.595894101
S	-6.348455585	3.866547199	2.227776886
S	-2.439982496	4.019058420	6.207506779
S	0.379995553	-7.915443094	-1.373303281
S	1.597231178	-4.043348897	5.463957665
S	-0.961223242	-6.454773310	2.900317617
S	-4.979194562	-3.620238445	4.141240209
S	-4.375711604	-5.971363337	0.099939218
S	-2.023409135	-5.360052044	-4.509505295
H	-5.498668980	2.737484121	4.909860245
H	-3.368371432	-1.728219272	7.681394506
H	-7.095288004	-2.220828560	2.676349430
H	-9.234749608	1.406110218	-0.978404072
H	-6.213006127	-2.472582284	-3.334360523
H	-3.252072679	-1.783596043	-7.161229175
H	-3.680985244	3.186371351	-8.957378898
H	1.210236382	1.395579311	-8.339315007
H	5.467249138	3.913784003	-2.292270159
H	2.486817777	8.635897846	-1.710553852
H	-2.245990176	6.670123003	-1.442220432
H	-0.216152208	8.212364745	4.511315692
H	3.827002591	5.959508040	1.355495482
H	1.228175941	3.488979242	6.837163200
H	6.698776547	2.645585145	6.238114120
H	6.756067043	3.361591819	0.628165700
H	7.336808173	-0.518256537	-0.941489278
H	5.275947432	-0.260487476	-5.792695176
H	-0.836233245	-3.287118067	-6.199821036

H	4.557804166	-4.412901009	-4.946231707
H	-3.303376119	-6.735144470	0.436534338
H	-2.207902548	-6.985517210	2.854644545
H	4.749792860	-5.168288164	-0.026517775
H	4.964927156	-0.362054602	6.140217518
H	1.891143664	-4.796524524	4.375888018
H	1.623734572	-7.362442256	-1.380928527
H	-1.327726155	3.605497808	6.860729441
H	-6.151428623	5.076676562	1.647952885
H	-4.907588622	6.093744969	-1.140831885
H	-1.894485292	5.353582326	-5.889713728
H	-4.515089395	-4.570846395	4.989231233
H	-3.155417313	-6.055588965	-4.237549897

Coordinates file of optimized structure of Iso2

Au	-0.010986348	0.671377356	0.476724584
Au	-1.332846811	-0.130418642	-1.913269499
Au	-1.148383373	2.943643171	2.007373744
Au	0.863045765	1.454230212	-2.757661830
Au	-2.425252593	-0.603616300	1.440703619
Au	-0.813815201	0.623693348	3.591239216
Au	-3.580322906	1.637635835	2.735073748
Au	-2.608232625	1.819512952	-0.276896539
Au	2.079009273	1.088050533	2.413672113
Au	0.621578517	-1.576945309	2.214159022
Au	-1.733275213	-2.925334890	2.917997982
Au	2.575124735	2.192846552	-0.374457464
Au	2.087587252	3.302437395	4.188018077
Au	-0.257593174	3.205876218	-0.827363782
Au	-0.729904540	-2.242089323	-0.131748433
Au	1.475138256	4.036627428	1.440167109
Au	-0.804186151	-2.766288059	-3.014320653
Au	-1.804353237	1.707745581	-4.128894822
Au	1.616204788	-1.255534502	-2.419445360
Au	1.920243210	4.889099988	-1.229188859
Au	3.942761690	0.489453335	-2.155589446
Au	2.687548886	-1.336139319	3.983872124
Au	2.492059644	-0.659714419	0.230274271
Au	-3.313489320	-0.783675511	4.179529924
Au	-0.027349702	-1.719354550	5.117420463
Au	-1.384744311	0.406818108	6.417474682
Au	1.321252879	0.773236232	5.361508778
Au	-0.458028236	2.938918173	5.388284731
Au	3.046300854	3.087365913	-3.187838588
Au	2.640321227	0.462315399	-4.685948225
Au	0.556374110	2.007545408	-5.777143670
Au	-0.130164887	-0.549691681	-4.753576816
Au	0.178922788	4.032968477	-3.518832005
Au	-2.962798581	-1.127378583	-3.969189662
Au	-3.342601323	-1.963034491	-1.094297043
Au	-4.936751184	0.399679984	0.195631931
Au	-4.240454965	1.317541388	-2.536034420
Au	4.961168788	0.799608918	0.479393059
Au	4.137479755	3.053778608	2.238015738
Au	4.714935346	0.570202508	3.445836275
Au	4.558881912	-2.054405256	-0.849161829
Au	-1.010916415	5.444188351	0.703100559
Au	-2.647311786	3.832995197	-2.414794076
Au	-5.001703069	3.166071510	-0.501698896
Au	-0.237216947	5.072847420	3.472198247

Au	1.335090011	-3.844570555	-1.203131867
Au	2.975422593	-3.168093706	1.224227429
Au	0.072108259	-4.459613073	1.271935020
Au	-1.443893465	-4.786717600	-1.196024909
Au	0.933475876	7.682416256	-1.033653534
Au	4.013996530	6.369246773	-2.498445452
S	3.203951907	8.260930532	-1.338241855
S	-1.376244790	7.481293355	-0.586444279
S	4.909450416	4.598197018	-3.742017136
Au	-2.031250466	3.590904143	-6.688498882
Au	-4.040320920	0.968934805	-6.241021540
S	-4.340065324	3.309941795	-6.272240697
S	0.227376619	3.815660466	-7.397889383
S	-3.902964468	-1.390289069	-6.240547683
Au	5.583849743	-1.192885784	-3.942911889
S	6.548235132	-2.437960585	-2.180084661
S	4.676041385	-0.181977275	-5.861514716
Au	1.654537386	-3.534909452	-4.579714897
S	0.619917139	-2.332834594	-6.341431556
S	2.729090136	-4.879385309	-2.963224527
Au	-2.299117981	6.116735869	-4.381537426
S	0.046491619	6.208966528	-4.618593675
S	-4.628424991	6.433126970	-4.442966304
Au	6.956236081	2.444007320	2.932519800
Au	4.731040909	2.405791512	5.831970662
S	6.589974456	3.612308320	4.961524114
S	7.354890677	1.298969919	0.903837265
S	3.147690168	1.126894096	7.015963250
Au	4.978029265	-3.025449338	3.704737821
S	3.800554344	-4.873160214	2.813284126
S	6.185654577	-1.161528515	4.472047515
Au	2.860302228	6.125197292	3.194661805
S	4.799931454	5.449118352	2.011750840
S	0.976979968	7.043120108	4.320153988
Au	-4.584988192	0.974126495	6.613789699
Au	-6.169756255	0.235919337	3.348560143
S	-6.349097375	1.673355890	5.218269622
S	-2.976759554	0.452750840	8.258311730
S	-6.442003137	-1.086058060	1.424254951
Au	-5.865049562	-1.321135392	-2.722292436
S	-5.393582365	-3.300490423	-1.526594444
S	-6.340406059	0.726750986	-3.803893508
Au	-3.051777051	4.347924074	4.793773177
S	-1.718242689	4.589337262	6.753508503
S	-4.475381763	3.984833313	2.954444449
Au	-0.227438198	-5.045953267	4.467271906
S	0.380934813	-6.428418649	2.661229835
S	-0.579981933	-3.760097567	6.409558646
Au	-3.844861777	-4.452183621	4.198204469
Au	-3.320580530	-6.440433377	0.853688675
S	-3.653487755	-6.560262859	3.167190599
S	-4.296150991	-2.581461274	5.545290369
S	-3.061267839	-6.574069128	-1.480704506
H	-7.306643833	0.971910809	5.876597626
H	-3.207496089	-0.881921049	8.304312782
H	-5.504601029	-2.029049049	1.696438233
H	-7.154018089	1.204568722	-2.827468745
H	-4.853060251	-4.010471493	-2.546373967
H	-2.694716412	-1.428469595	-6.855450566
H	-4.722127136	3.447929345	-7.567952510
H	0.088445511	3.018382942	-8.486748960

H	5.744145458	4.135047784	-2.779710670
H	3.018939982	9.035270208	-2.437400735
H	-1.734935212	6.830818249	-1.731665051
H	1.241880848	6.511434296	5.538057128
H	4.251805842	5.584909781	0.776912239
H	2.543198182	2.147159460	7.671783933
H	7.538220631	2.982291378	5.698089503
H	7.384004793	2.397108088	0.1111106676
H	7.235957449	-1.419016318	-1.606296778
H	-5.534634200	5.807454378	0.548410983
H	5.283212476	1.020387577	-5.707904872
H	-0.511846929	-3.079555316	-6.326262780
H	3.816850975	-4.090824951	-2.765783674
H	-2.156166863	-7.584092564	-1.493402839
H	-4.979918156	-6.838086702	3.122611411
H	4.804900863	-5.302765927	2.010084146
H	5.665853166	-1.107642954	5.722838536
H	0.652739042	-3.942775842	6.941775727
H	-0.836059899	-6.979867182	2.416111168
H	-3.603417152	4.470241838	2.029891285
H	-2.397647152	3.673317249	7.487343959
H	-4.624165695	7.754052117	-4.129466044
H	0.312915266	6.902078137	-3.469873131
H	-3.225722651	-2.740870849	6.365046894
S	-6.364552303	5.151644075	-0.300246441
Au	-5.278527419	5.709582928	-2.316119879

Coordinates file of optimized structure of Iso3

Au	0.147103128	0.015446466	-0.285573016
Au	-1.565690539	-0.650867473	-2.519634923
Au	-0.310241797	2.588141231	1.168300675
Au	1.184648297	0.239327546	-3.081769574
Au	-2.747898913	-0.915193238	0.160843105
Au	-0.764586135	-0.228554201	2.519511519
Au	-2.202286734	1.667578310	-1.005735461
Au	1.921622164	0.997123151	1.841990004
Au	-0.141147042	-2.580444438	0.927970144
Au	2.891366868	1.040973329	-0.840852530
Au	2.609539172	-1.564007213	0.749945478
Au	0.358216131	2.621117720	-1.654701934
Au	-1.773209671	-3.313599708	-1.388456292
Au	0.832101194	-2.381089219	-1.836085744
Au	-1.224659536	1.791460017	-3.970470179
Au	-3.555184631	-0.975334493	3.161848600
Au	-3.000022122	1.513919296	1.803816501
Au	-4.149554219	0.493684800	-2.750485351
Au	0.136710779	-0.010186078	-5.714034640
Au	-2.842862895	-3.433454307	1.544688395
Au	3.794207554	-0.598850860	3.188201512
Au	1.537269885	3.505707974	3.236054858
Au	-2.675455897	-0.465634678	-5.180254639
Au	-4.491781076	-3.689408163	-1.059512326
Au	-1.540812447	-0.093322339	5.226823521
Au	-5.268866050	-1.972988939	1.183619530
Au	1.344240307	-1.949442800	3.323603300
Au	1.430791024	0.739460579	4.566768873
Au	-1.099450451	2.278262969	3.897529068
Au	-5.151848887	0.662022539	0.134203333
Au	2.325571485	3.630041087	0.461240448
Au	2.880185282	3.425942034	-2.506003123

Au	-0.551547298	4.513608040	-3.643473668
Au	0.086684080	5.448288995	1.330119245
Au	3.499678218	-1.480648435	-2.043687672
Au	1.994142781	-2.037295931	-4.474631364
Au	1.354095344	2.564241693	-4.862266029
Au	-2.563414308	4.352368004	1.876498013
Au	-0.919810080	-2.643826811	-4.291445901
Au	-3.326799861	3.427368432	-2.984496834
Au	-2.559240002	-5.678666047	-0.019276340
Au	-0.790154429	5.177887220	3.912073821
Au	-0.740329478	-5.167724880	2.053745363
Au	-3.701573813	-2.390819289	-3.384705432
Au	1.100617590	5.369284692	-1.438184675
Au	2.074412056	-4.173932477	-0.080356703
Au	3.870029684	0.989876241	-3.606109460
Au	-4.311389868	3.318165915	-0.166399804
Au	-1.247651449	-2.869970428	3.871118213
Au	-1.694656781	4.619222747	-0.859948019
Au	-6.550382103	3.100222649	-2.250438212
Au	-4.963319543	5.967537922	-0.983699993
S	-7.155102975	5.107578102	-1.121998943
S	-6.396092418	1.116309978	-3.535922857
S	-2.821226450	6.928078255	-0.943034089
Au	-4.708227127	-3.779774462	3.911142523
S	-2.840486912	-4.205694400	5.271391229
S	-6.679435514	-3.443150415	2.652123504
Au	2.855697706	-5.350240591	2.506578500
Au	5.038642730	-3.443389762	0.285290926
S	4.895669944	-4.180060366	2.518958555
S	0.955071722	-6.731964854	2.753041219
S	5.560702770	-2.817277788	-1.935092800
Au	0.364508073	7.848675252	-2.553772172
S	2.728371476	3.936859287	-6.417122049
S	-0.367573043	6.817561310	-4.548951207
Au	2.480738458	-5.124113808	-3.331812931
S	3.034661957	-4.065760121	-5.368337020
S	1.949191435	-6.285798643	-1.352049252
Au	-1.751749090	-5.908823220	-3.433643481
S	-2.769688447	-7.283747743	-1.807041116
S	-0.765140599	-4.852686397	-5.304660130
Au	-3.753246622	2.530238997	-6.108166982
S	-4.238784556	4.558550922	-5.002658971
S	-3.515857279	0.499656821	-7.281767391
Au	2.385253463	7.191641419	0.321978795
S	1.024370808	8.941359480	-0.550022799
S	3.916800136	5.564431868	1.096522688
Au	5.683411007	3.033152661	-1.774426962
S	6.229337513	4.722129151	-3.350320076
S	5.342318250	1.372284543	-0.151478750
Au	4.500225591	2.292937798	4.429235871
S	5.818569346	0.334114478	4.183810887
S	3.332410680	4.310606344	4.764989665
Au	0.111316661	3.215051131	6.521247330
S	1.638313486	1.458555728	6.917443081
S	-1.192975673	5.177175295	6.314544609
Au	-4.628616370	2.518772025	4.035550302
S	-4.945614270	0.319095120	4.836318217
S	-4.560609205	4.772697522	3.305921316
Au	0.255823120	-2.277822577	6.423981244
S	2.127502192	-3.261258247	5.389550346
S	-1.589285352	-1.142443708	7.424150060

Au	3.235992360	-0.181599108	-6.615102426
S	5.271886101	0.271851178	-5.491445662
S	1.249746599	-0.591586534	-7.837269192
Au	-7.265234275	-1.773575192	-0.875310458
S	-6.884117697	-4.010820298	-1.530998398
S	-7.627508788	0.437069807	-0.147271745
H	-3.899691824	5.305372426	4.363755366
H	-6.136836586	0.123562290	4.217127895
H	-7.175322830	-2.456880271	3.438189098
H	-2.532109722	-5.412047627	4.735847295
H	-6.771441019	-3.775965224	-2.861788039
H	-7.907076092	0.110367940	1.138983815
H	-3.076619348	5.180120519	-5.326324892
H	-2.284379599	0.747721894	-7.792906613
H	3.290095562	2.859199186	-7.023559125
H	0.857430326	6.655765809	-5.104650451
H	1.155269809	0.652417592	-8.369092815
H	5.489245702	1.493741760	-6.037997779
H	4.303591945	-3.733205965	-5.023026372
H	0.601213525	-6.200455964	-1.513237465
H	6.374443807	-1.788136811	-1.592646463
H	4.404206590	-2.992697053	3.011477217
H	1.067503461	-7.346662703	1.549891588
H	3.015596242	-2.315300650	5.785171221
H	-2.520566388	-2.093232906	7.165277906
H	5.600794566	-0.116794282	5.443735091
H	4.017392433	5.021987613	3.833757926
H	0.759782142	0.589780490	7.473858412
H	-2.396998799	4.554840195	6.245394590
H	5.109329708	2.192032179	0.904608079
H	7.174197972	4.007571165	-4.010794657
H	-0.104121507	8.617103399	0.133213958
H	4.671029583	5.546577247	-0.030779538
H	-7.227117944	4.590823209	0.130879388
H	-5.934711240	1.695370234	-4.679353036
H	-2.718872231	7.028662085	-2.290667278
H	-1.676994510	-8.033987580	-1.519805543
H	-1.917206967	-4.758335523	-6.014736136
Au	4.444804815	4.261148959	-4.834880607

Coordinates file of optimized structure of Iso4

Au	0.225918848	0.377516693	-0.192369066
Au	-1.305406097	-0.517576857	-2.548344852
Au	-0.519629723	2.754123035	1.419592014
Au	1.308747136	0.564147867	-3.067150440
Au	-2.396927426	-0.784679078	0.250752741
Au	-0.698599220	-0.234474531	2.651969557
Au	-2.137399517	1.834309830	-1.026449465
Au	1.847829764	1.217475378	2.037692055
Au	0.026771934	-2.471186271	1.044713949
Au	2.846697673	1.789361646	-0.521960576
Au	2.562646608	-1.305927692	0.913895098
Au	0.473601167	3.048557703	-1.458957150
Au	-1.540140305	-3.144662220	-1.334724831
Au	1.117081130	-2.004077373	-1.662072601
Au	-1.071092816	2.099962227	-3.757609169
Au	-3.481977237	-1.045971827	3.105819574
Au	-3.155027884	1.490697053	1.777379119
Au	-4.114217160	-0.305936586	-1.984996541
Au	-0.176051750	-0.086008805	-5.436654617

Au	-2.683313461	-3.419883233	1.406179940
Au	3.745824561	-0.288674370	3.394824252
Au	1.210034278	3.519869740	3.637117133
Au	-2.977870930	-0.006180349	-4.747926274
Au	-4.279942740	-3.634289400	-1.297419286
Au	-1.749985991	-0.327588671	5.329809822
Au	-4.996164219	-1.861928222	0.877104563
Au	1.439921519	-2.095968314	3.517323977
Au	1.244857278	0.688857011	4.697708474
Au	-1.376785285	2.091795320	4.090417518
Au	-5.466686233	0.910315569	0.340216542
Au	1.960416525	4.076626881	0.911132145
Au	2.924011450	2.912904486	-3.114227894
Au	-0.322279899	5.031427339	-3.114840665
Au	-0.320607084	5.612148929	2.083973273
Au	3.691596044	-0.508264320	-1.930465864
Au	2.279537749	-1.833234270	-4.278431599
Au	1.140705687	2.425982337	-5.439510409
Au	-2.805015896	4.337626762	2.252732537
Au	-0.400139472	-2.771735238	-4.021814724
Au	4.819426384	0.207670956	0.771635840
Au	-3.103355391	3.823001562	-2.840529374
Au	-2.388689133	-5.651471477	-0.211874342
Au	-1.429697636	4.868836938	4.583996721
Au	-0.606558181	-5.188179640	1.875900753
Au	-3.211699043	-2.583404718	-3.632961128
Au	2.209813748	5.223668754	-1.694257732
Au	2.248325557	-3.942351354	-0.045144098
Au	3.736309755	0.646438082	-4.603198913
Au	-4.241788829	3.391783299	-0.038549553
Au	-1.267227291	-2.937261058	3.843341830
Au	-1.644675629	4.768463187	-0.469656122
Au	-6.252198765	2.773397425	-2.250221610
Au	-4.754700850	5.976412941	-1.085041947
S	-6.846279043	4.977157598	-1.559180884
S	-6.125098231	0.617203121	-3.212281636
S	-2.714624823	7.051832521	-0.609755634
Au	-4.568891551	-4.025430560	3.609379740
S	-2.762048699	-4.575996161	5.027443706
S	-6.417950555	-3.517070535	2.249145651
Au	3.052489939	-4.822971305	2.616974861
Au	5.097437125	-2.853639910	0.310625499
S	5.079509934	-3.613583387	2.547252685
S	1.269762258	-6.366330581	2.855811378
S	5.438886599	-2.287479032	-1.962304466
Au	0.917544472	5.502391254	-5.880905159
S	2.320396729	3.962467615	-6.982922554
S	-0.564750262	6.905495358	-4.690872950
Au	2.722287963	-4.927449174	-3.246193814
S	3.304619479	-3.848550541	-5.257378111
S	2.234512333	-6.089908275	-1.257106047
Au	-1.912470525	-5.748825850	-3.692508413
S	-2.999058255	-7.080668521	-2.059300762
S	-0.666653970	-4.759961196	-5.441179208
Au	-4.006620814	2.765545348	-5.885626452
S	-4.256494908	4.837437873	-4.802940386
S	-3.929410701	0.643443937	-6.915879442
Au	2.492578967	7.084938468	0.795392966
S	3.952068040	6.837655561	-1.051973222
S	1.007756884	7.616962267	2.528954841
Au	5.823401435	2.583659066	-1.474672469

S	5.243371277	3.737867266	-3.460609132
S	6.764067264	1.617043451	0.466305039
Au	4.119405334	2.322846453	5.133020800
S	5.344911570	0.288658330	5.171110733
S	2.999316822	4.395806665	5.112693703
Au	-0.092487895	2.837147014	6.956926652
S	1.405735763	1.026717602	7.137599658
S	-1.324409322	4.847740547	6.984382591
Au	-5.044828956	2.213872616	3.936018949
S	-5.294056053	-0.045388124	4.561614714
S	-5.001594976	4.519125670	3.409770824
Au	0.024987374	-2.493000695	6.552004508
S	2.087521960	-3.218675562	5.669731032
S	-1.957431433	-1.522176865	7.456321334
Au	2.491807196	-0.560776722	-7.195732353
S	4.707881578	0.192147732	-6.791156683
S	0.265807576	-1.251398558	-7.573342046
Au	-7.279433497	-1.775142586	-0.859567724
S	-6.699233934	-3.894672659	-1.727764473
S	-7.864227596	0.326243920	0.067378720
H	-4.506763411	4.973971776	4.588011317
H	-6.326184851	-0.293680735	3.719041427
H	-6.946297923	-2.585126527	3.078401350
H	-2.360626952	-5.662962253	4.322941327
H	-6.601060798	-3.508815233	-3.023399241
H	-8.104722209	-0.126895106	1.321915165
H	-3.146469900	5.423463115	-5.314636812
H	-2.715545035	0.803356028	-7.498001084
H	3.378849201	4.154584704	-6.154792490
H	0.388929195	7.694494593	-4.138353209
H	-0.055681146	-0.205686128	-8.375186062
H	4.510816192	1.427557945	-7.314996356
H	4.577031879	-3.545582907	-4.897352830
H	0.883567620	-6.068888625	-1.396771025
H	6.494625853	-1.465457366	-1.747386013
H	4.620440775	-2.441805291	3.106157742
H	1.580011480	-7.089530961	1.751518041
H	2.800418404	-2.158854824	6.122630596
H	-2.822736853	-2.472232784	7.024363960
H	4.658323753	-0.239817979	6.214084953
H	3.734165183	4.920895355	4.100399633
H	0.499545187	0.081084839	7.500120056
H	-2.542014898	4.274269314	7.152734058
H	7.553548066	0.732794767	-0.191228527
H	5.631518838	2.741469915	-4.300883503
H	3.468541698	7.913911930	-1.720450856
H	1.712212086	7.068038457	3.549559834
H	-7.196260129	4.661461559	-0.287036227
H	-5.349816455	1.034461346	-4.255748951
H	-2.353166990	7.206398212	-1.908505695
H	-2.003604928	-7.994879717	-1.944916833
H	-1.719878036	-4.286246996	-6.151415511