

巯基保护的中空金纳米球

许文武，高崑*

中国科学院上海应用物理研究所水科学与技术研究室，微观界面物理与探测重点实验室，上海 201800

Thiolate-Protected Hollow Gold Nanospheres

XU Wenwu, GAO Yi*

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

*Corresponding author. Email: gaoyi@sinap.ac.cn

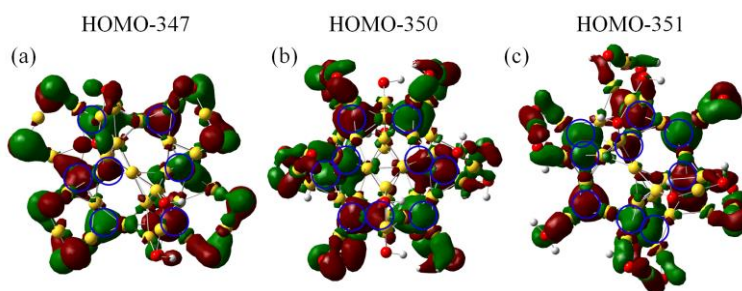


Fig. S1 The HOMO-347, HOMO-350, and HOMO-351 of hollow $\text{Au}_{60}(\text{SH})_{20}$ sphere.

The circle in blue denotes the local orbital across the tetrahedral Au_4 units. Au, yellow; S, red; H, white.

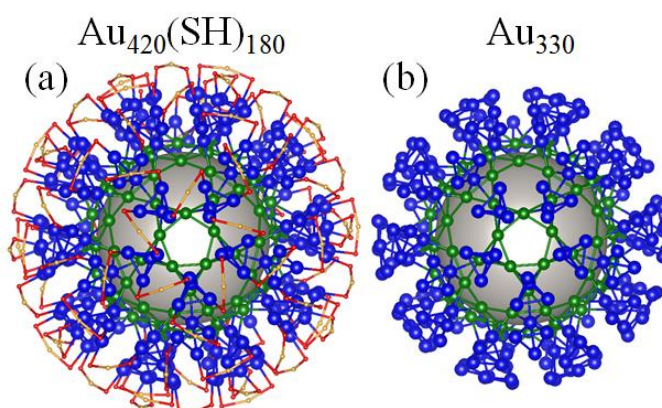


Fig. S2 The sketch map of bilayer $\text{Au}_{420}(\text{SH})_{180}$ constructed by fusing one layer tetrahedral Au_4 on the Au_{150} fullerene cage of $\text{Au}_{180}(\text{SR})_{60}$. The second layer is in blue. Au, olive, blue, and yellow; S, red. The H atoms are omitted for clarity.

The spherical hollow characteristic are indicated by gray balls.

Harmonic frequencies (IR intensity in parenthesis) of $\text{Au}_{60}(\text{SH})_{20}$ with PBE/LANL2DZ implemented in Gaussian09 program package.

8.4822	(0.0862)	8.8456	(0.0023)	9.1147	(0.0356)
9.6644	(0.0350)	10.2330	(0.0220)	10.4987	(0.0239)
11.3193	(0.0927)	12.4744	(0.0040)	12.6657	(0.0136)
12.7169	(0.0473)	13.5640	(0.0386)	13.7994	(0.0206)
14.3013	(0.0167)	14.8598	(0.0255)	15.3039	(0.0499)
15.9979	(0.0424)	16.5963	(0.0110)	16.9309	(0.0105)
17.0283	(0.0142)	17.3913	(0.1292)	17.9213	(0.0101)
18.4117	(0.0109)	18.8895	(0.0354)	19.5316	(0.0216)
21.1382	(0.0024)	21.1993	(0.0144)	21.7082	(0.0491)
22.4401	(0.0218)	22.6447	(0.0118)	23.0041	(0.0071)
24.3023	(0.0275)	24.5390	(0.0180)	24.7847	(0.0771)
25.2659	(0.0022)	25.4530	(0.0174)	25.4567	(0.0114)
25.7992	(0.0547)	27.0883	(0.1632)	27.3848	(0.0402)
27.5393	(0.0305)	28.0879	(0.0210)	30.6735	(0.1766)
31.8145	(0.2513)	32.2209	(0.0754)	32.7267	(0.1867)
32.7640	(0.0409)	32.9771	(0.0736)	33.1255	(0.0132)
33.5650	(0.1035)	34.2917	(0.0823)	34.4886	(0.0175)
34.7635	(0.0151)	35.8915	(0.1076)	36.0986	(0.0847)
36.9527	(0.0537)	37.1949	(0.1441)	38.0950	(0.0368)
38.4941	(0.0363)	38.6262	(0.0413)	38.9524	(0.0348)

39.6796	(0.0662)	40.9678	(0.2261)	41.4471	(0.3076)
41.6567	(0.0970)	44.0391	(0.0070)	45.1067	(0.0183)
45.2163	(0.0124)	45.5993	(0.2248)	45.7614	(0.0198)
45.9460	(0.0131)	46.1786	(0.1005)	46.3575	(0.0398)
47.8581	(0.0445)	48.2419	(0.0235)	48.8689	(0.2132)
48.9779	(0.0399)	49.1147	(0.1296)	49.5894	(0.1239)
49.6446	(0.0350)	49.7845	(0.0537)	49.8716	(0.0980)
49.9509	(0.1598)	50.0943	(0.0565)	51.1535	(0.0394)
51.6920	(0.0744)	52.9605	(0.2560)	53.1694	(0.2673)
53.7544	(0.0132)	54.7500	(0.0066)	56.7932	(0.1300)
57.0875	(0.0365)	58.1453	(0.0375)	58.2445	(0.0513)
59.4730	(0.0157)	59.5867	(0.0161)	59.6888	(0.0123)
59.8463	(0.0012)	61.2009	(0.0617)	62.5127	(0.0124)
62.7172	(0.0031)	62.8649	(0.0146)	64.6243	(0.0569)
64.8482	(0.0610)	66.4590	(0.0001)	68.0976	(0.0017)
68.1417	(0.0041)	68.2340	(0.0042)	68.3120	(0.0042)
68.7166	(0.4165)	70.9418	(0.0101)	71.1301	(0.0049)
71.5166	(0.0020)	71.6357	(0.0044)	74.3982	(0.0050)
74.5605	(0.0050)	75.9779	(0.0122)	76.6725	(0.0027)
76.7834	(0.0028)	77.8982	(0.0002)	78.3404	(0.0030)
78.4837	(0.0010)	79.9050	(0.0202)	79.9983	(0.0110)
81.9251	(0.0515)	82.1306	(0.3875)	82.2363	(0.3619)
87.7178	(0.0748)	87.8946	(0.0286)	89.1650	(0.0600)
89.1741	(0.1000)	90.1178	(0.0327)	90.3558	(0.0140)
91.0394	(0.1308)	91.4546	(0.1753)	91.6739	(0.1268)
91.8139	(1.4915)	92.1683	(0.6013)	92.7719	(0.2861)
93.5286	(1.0784)	93.7437	(0.5886)	93.9781	(0.0745)
94.4053	(0.4778)	94.4353	(0.2914)	94.8259	(0.1532)
95.0418	(0.0948)	95.1705	(0.1141)	95.2048	(0.0202)
95.2435	(0.1919)	95.4500	(0.3238)	95.7087	(0.3670)
97.0044	(0.1650)	103.7657	(0.0158)	103.8668	(0.0018)
107.3093	(0.0149)	107.6312	(0.0028)	107.8349	(0.0052)
108.8361	(0.0001)	108.9665	(0.0261)	109.0649	(0.0009)
109.1993	(0.0003)	111.9188	(0.0029)	112.2244	(0.0235)
112.6826	(0.0021)	112.7038	(0.0035)	112.9277	(0.0056)
112.9887	(0.0039)	113.1745	(0.0006)	113.2644	(0.0006)
118.0289	(0.7223)	118.3607	(0.9608)	118.4795	(1.0396)
120.8823	(0.0184)	121.1749	(0.0032)	121.4195	(0.0020)
123.0620	(0.0002)	138.5302	(0.5982)	138.5746	(0.6796)
139.9218	(0.8323)	153.2546	(0.0002)	153.3011	(0.0003)
153.7839	(0.0002)	154.0585	(0.0008)	154.1238	(0.0012)
164.5000	(0.0005)	164.6107	(0.0018)	165.7840	(0.0001)
166.2368	(0.0009)	188.8017	(0.0003)	189.0656	(0.0002)
189.3129	(0.0001)	189.4104	(0.0001)	191.4758	(0.0001)
191.8661	(0.0005)	192.7067	(0.1163)	247.2890	(0.0916)
247.4574	(0.1255)	247.6378	(0.3329)	247.7638	(0.1130)
247.8999	(0.1357)	248.0891	(0.3444)	248.2649	(0.1957)
248.6434	(0.0384)	248.8712	(0.2599)	249.1574	(0.2275)
256.5273	(10.3772)	256.6619	(2.1290)	256.9289	(6.4316)
257.0754	(4.3002)	257.1107	(27.1407)	257.3154	(21.0176)
257.5042	(5.4363)	257.6035	(18.3741)	257.9162	(23.2108)
258.3468	(7.0773)	287.4927	(4.7566)	288.1478	(2.6074)
288.4287	(10.8333)	288.4968	(0.1079)	289.5729	(4.5008)
289.7776	(3.4251)	289.9027	(5.8621)	290.2929	(4.0264)

290.5259	(7.3195)	290.8997	(3.9905)	297.1119	(2.2537)
297.4326	(1.9844)	297.6862	(3.2163)	297.7759	(7.5749)
299.1258	(2.9877)	299.3837	(1.5585)	299.5920	(0.2394)
299.6494	(6.7374)	299.9314	(5.5320)	299.9770	(6.7180)
557.0663	(0.2424)	558.2546	(0.1403)	559.9718	(0.4628)
560.3044	(1.2018)	560.5927	(0.1187)	562.0953	(0.7143)
562.6310	(1.8803)	564.3395	(0.9253)	564.5095	(0.4578)
566.0120	(1.4206)	569.4341	(3.9577)	571.3893	(4.0696)
571.7012	(4.6365)	572.7725	(4.2231)	573.7123	(11.3760)
574.2368	(0.7728)	574.4159	(5.0930)	575.5097	(2.1680)
576.8544	(3.7152)	577.5569	(4.3703)	601.7880	(2.2331)
603.0194	(2.9700)	605.5535	(3.3612)	606.4944	(1.9753)
607.1720	(2.6716)	607.5937	(0.5020)	609.4884	(2.8326)
610.2206	(1.9529)	610.4299	(1.1111)	612.8567	(1.4329)
640.9075	(4.0248)	643.8945	(4.5442)	646.1059	(5.1730)
646.6289	(4.5444)	647.7432	(2.1445)	649.5555	(3.9590)
651.0815	(4.4863)	652.1162	(3.7921)	652.7302	(3.5664)
654.1186	(4.1134)	2580.2342	(0.1688)	2580.6151	(0.1629)
2582.2358	(0.1470)	2582.8586	(0.1708)	2582.8680	(0.1434)
2582.9129	(0.2055)	2583.0326	(0.2310)	2583.4339	(0.2116)
2583.4691	(0.2012)	2583.5465	(0.0681)	2583.6916	(0.0836)
2583.7561	(0.1049)	2584.0395	(0.1748)	2584.4912	(0.2209)
2584.6743	(0.0941)	2584.8760	(0.2715)	2584.9162	(0.1907)
2585.8480	(0.1191)	2586.1996	(0.0679)	2586.3204	(0.1470)

Harmonic frequencies (IR intensity in parenthesis) of Au₆₀(SH)₂₀ with B3LYP/LANL2DZ implemented in Gaussian09 program package.

9.5573	(0.0180)	9.7771	(0.0710)	10.0275	(0.0181)
10.1952	(0.0365)	10.7921	(0.0223)	11.1658	(0.0257)
11.5681	(0.0545)	12.9077	(0.0564)	13.2422	(0.0020)
13.5487	(0.0048)	13.7441	(0.0176)	14.0173	(0.0100)
14.2411	(0.0041)	15.7534	(0.0353)	16.0830	(0.0366)
16.4230	(0.0295)	17.1058	(0.0302)	18.3085	(0.1112)
18.6462	(0.0027)	18.7592	(0.0198)	18.9008	(0.0013)
19.0445	(0.0161)	20.4767	(0.0288)	20.6078	(0.0261)
21.4060	(0.0129)	21.7498	(0.0038)	21.8857	(0.0114)
21.9683	(0.0040)	22.1991	(0.0078)	22.3660	(0.0151)
24.2385	(0.0001)	25.7463	(0.0423)	26.1958	(0.0294)
26.2499	(0.0084)	26.5526	(0.0034)	26.5814	(0.0648)
26.9665	(0.0738)	27.7001	(0.1067)	27.8150	(0.0209)
27.9933	(0.0322)	28.4001	(0.0090)	33.5120	(0.0191)
33.6328	(0.0067)	34.0092	(0.0132)	34.0538	(0.0579)
34.2595	(0.0375)	34.5885	(0.1096)	34.8833	(0.4902)
35.2833	(0.0564)	35.3741	(0.0377)	35.5288	(0.0169)
35.7059	(0.0175)	36.6906	(0.0412)	37.6234	(0.0347)
37.7314	(0.0497)	38.2691	(0.2328)	38.5772	(0.1142)
38.7667	(0.0045)	39.2466	(0.0211)	39.7941	(0.0465)
40.2811	(0.0575)	41.8498	(0.0278)	41.9171	(0.1631)
42.6932	(0.0089)	43.0826	(0.2333)	43.9593	(0.1453)
44.0435	(0.0671)	44.1160	(0.0462)	44.2180	(0.0095)
44.9840	(0.0889)	45.1356	(0.0130)	45.3103	(0.0306)
47.9226	(0.0265)	47.9952	(0.0435)	48.0957	(0.0790)
48.1316	(0.0045)	48.3957	(0.0512)	48.8226	(0.1590)
49.3827	(0.0487)	49.6635	(0.0579)	49.8177	(0.1388)

50.2096	(0.2327)	50.4181	(0.3123)	50.9255	(0.1553)
51.5556	(0.0753)	52.0705	(0.0624)	52.2503	(0.1157)
52.9858	(0.0115)	53.4808	(0.0054)	54.9758	(0.0842)
55.1345	(0.0962)	55.2983	(0.0806)	55.5228	(0.0681)
57.9256	(0.0140)	57.9661	(0.0288)	58.4541	(0.0763)
58.6783	(0.0002)	58.8316	(0.0020)	59.5860	(0.0104)
60.9977	(0.0155)	61.1597	(0.0046)	62.6040	(0.0857)
62.6659	(0.1092)	63.5594	(0.0002)	65.5237	(0.0012)
65.5554	(0.0067)	65.7672	(0.0044)	65.9255	(0.0030)
66.4058	(0.4231)	66.7600	(0.0432)	66.9140	(0.0048)
67.6916	(0.0020)	67.7283	(0.0064)	70.1918	(0.0045)
70.3411	(0.0052)	72.2703	(0.0080)	73.8458	(0.0030)
73.9743	(0.0080)	74.0134	(0.0022)	74.0323	(0.0015)
74.2064	(0.0004)	74.9918	(0.0018)	75.1226	(0.0020)
77.0736	(0.0749)	78.7757	(0.4837)	78.8905	(0.4391)
80.5318	(0.0177)	80.5785	(0.0022)	82.1125	(0.0108)
82.2574	(0.0071)	83.8590	(0.0816)	84.5005	(0.0030)
84.7055	(0.0027)	85.5069	(0.0003)	87.0754	(0.0076)
87.1025	(0.0028)	87.2598	(0.0008)	87.3757	(0.0009)
87.4952	(0.0026)	87.6041	(0.0006)	89.6568	(0.0404)
90.6754	(0.6576)	91.5068	(0.1530)	92.0487	(0.5793)
92.3653	(1.7253)	92.7445	(0.0969)	92.9346	(0.7357)
93.3323	(0.3084)	93.6746	(0.2252)	93.9067	(0.1107)
94.2786	(0.8667)	94.9597	(0.1988)	95.2320	(0.2247)
95.3726	(0.0785)	95.4214	(0.0647)	95.8352	(0.1725)
97.5212	(0.3675)	98.8539	(0.0463)	99.0641	(0.0220)
99.3175	(0.0417)	99.6053	(0.0297)	99.8743	(0.0062)
100.3927	(0.0123)	100.6335	(0.0192)	103.4082	(0.0091)
103.6662	(0.0077)	103.9162	(0.0011)	104.1018	(0.0003)
105.9671	(0.0010)	106.2171	(0.0065)	107.1208	(0.0657)
108.4737	(4.7831)	108.6556	(5.1862)	108.8583	(5.9501)
113.9305	(0.0006)	126.1834	(2.2339)	126.1975	(2.4640)
127.3415	(3.0792)	140.2923	(0.0001)	140.4375	(0.0005)
140.5918	(0.0002)	140.7591	(0.0002)	140.9898	(0.0030)
150.6183	(0.0027)	150.7444	(0.0029)	152.3051	(0.0004)
152.7077	(0.0009)	173.7962	(0.0004)	174.0481	(0.0002)
174.1107	(0.0001)	174.3394	(0.0001)	176.3158	(0.0003)
176.7222	(0.0007)	177.3349	(0.1306)	239.9975	(0.2175)
240.1211	(0.1936)	240.6491	(0.2007)	241.0971	(0.0921)
241.2338	(0.2854)	241.4893	(0.6232)	241.7863	(0.3239)
242.1377	(0.4173)	242.4913	(0.6515)	242.6205	(0.2226)
251.8282	(19.0121)	252.0173	(5.7277)	252.4491	(18.9490)
252.9507	(23.6275)	253.0160	(20.7090)	253.4868	(10.1399)
253.6847	(5.4886)	253.9248	(58.0024)	254.0580	(62.7546)
254.8268	(3.1098)	279.5116	(4.9691)	280.1776	(2.6577)
280.3640	(10.7276)	280.4476	(1.8733)	281.8100	(3.4223)
281.9722	(4.0230)	282.0427	(6.3478)	282.2437	(6.3299)
282.4526	(8.8952)	282.7636	(4.4483)	290.9742	(2.6081)
291.2846	(1.3302)	291.3804	(6.7740)	291.5526	(13.3752)
292.8321	(3.4562)	292.9165	(0.5960)	293.0604	(0.4945)
293.2235	(13.1671)	293.3743	(19.3235)	293.4118	(3.2879)
575.6502	(0.7838)	576.1847	(2.1212)	578.2843	(1.8441)
579.5875	(1.5609)	580.3682	(2.0968)	582.4815	(1.1201)
582.8438	(1.4704)	583.4771	(0.2603)	583.8870	(0.5621)

584.4168	(2.1652)	585.7041	(4.5829)	586.2195	(8.7680)
590.1284	(7.0269)	591.2825	(2.6809)	592.1905	(8.9234)
592.7415	(0.7315)	593.3679	(10.5498)	593.7088	(7.4142)
593.7801	(2.7756)	594.9498	(6.3287)	617.6782	(2.1353)
618.3712	(2.7173)	619.4414	(0.3822)	619.7768	(3.6243)
620.2948	(1.4162)	620.4730	(1.9013)	620.9381	(1.5990)
625.2213	(0.6990)	626.5742	(0.8479)	627.4589	(0.8634)
652.7220	(2.7103)	657.4142	(2.7624)	659.2812	(3.9752)
660.3340	(1.8831)	661.3000	(3.1130)	661.6775	(1.5905)
663.1796	(0.9399)	663.5205	(3.3690)	664.0739	(2.7598)
664.2780	(2.2536)	2652.8574	(0.3738)	2653.2030	(0.1217)
2654.1537	(0.2206)	2657.1298	(0.2942)	2657.6194	(0.3055)
2658.0454	(0.3574)	2658.2053	(0.2720)	2660.2528	(0.3740)
2660.3328	(0.2697)	2660.3379	(0.3174)	2660.9126	(0.1869)
2661.6542	(0.3201)	2661.7316	(0.1482)	2661.9072	(0.2962)
2661.9239	(0.2132)	2662.0164	(0.3911)	2662.5602	(0.4426)
2663.1591	(0.4209)	2663.5025	(0.1234)	2663.7113	(0.1926)

Cartesian coordinates of Au₆₀(SH)₂₀ with PBE/LANL2DZ implemented in Gaussian09 program package.

Au	-1.501923	-0.510990	-1.171441
Au	-0.390018	1.295319	0.642352
Au	-3.125317	1.369350	0.082583
Au	-2.049698	-0.736203	1.558501
Au	-6.215220	3.124744	-3.777466
Au	-0.755640	-1.356716	3.940573
Au	-3.529039	-1.554675	3.771948
Au	-5.139161	-0.687086	5.886268
Au	-5.981830	-2.775872	4.248591
Au	-5.911550	-0.167124	3.265893
Au	-5.602972	1.773974	1.284504
Au	-8.098292	0.616786	1.716385
Au	-7.018945	2.359280	3.613601
Au	-4.331858	3.878676	-0.046009
Au	-5.393645	1.760046	-1.496981
Au	-0.581107	-5.818042	2.158623
Au	-1.889353	-4.700562	-0.026331
Au	-3.374912	-5.751388	2.106484
Au	-1.930415	-3.398106	2.435310
Au	-5.891926	-5.359391	3.219213
Au	-7.638314	-4.768194	5.303047
Au	-8.131903	-3.772652	2.753690
Au	-4.841034	-7.941858	3.000627
Au	-5.635930	-6.581260	0.708693
Au	-9.553043	-1.742446	1.473252
Au	-9.155462	-0.121187	-0.759708
Au	-10.852630	0.720878	1.273400
Au	-9.526281	-4.305741	0.395165
Au	-10.911379	-3.802715	2.770059
Au	-7.906050	-6.184076	-0.867554
Au	-8.985955	-4.074395	-2.335675
Au	-10.640922	-6.111197	-1.417220
Au	-5.429852	-6.591011	-2.072206
Au	-6.696195	-8.696922	-0.746117
Au	-0.183137	-5.535274	-2.057457

Au	-2.932814	-5.438213	-2.506313
Au	-1.487847	-3.072667	-2.255621
Au	-4.021686	-7.173360	-4.407304
Au	-5.120393	-4.645973	-4.049551
Au	-0.117078	-1.016344	-3.544996
Au	-2.897075	-1.030060	-3.531025
Au	-7.655420	0.915929	-2.888614
Au	-9.129273	-1.420570	-3.224827
Au	-10.447470	1.016922	-2.943700
Au	-7.495699	-3.245219	-4.542877
Au	-10.265300	-3.483128	-4.732235
Au	-5.040123	-2.035720	-5.026199
Au	-5.901414	-4.115842	-6.666125
Au	-3.382075	-0.051916	-6.088127
Au	-5.138832	0.553742	-4.013764
S	-2.043141	0.713416	-7.958921
S	1.620091	-0.322048	-5.085537
S	1.612038	2.414404	1.428537
S	1.938333	-6.698456	-2.197153
S	1.382906	-7.193692	2.516663
S	-4.956921	-10.224806	3.811344
S	-6.995772	-11.081166	-0.417282
S	-3.604254	-8.665893	-6.272589
S	-5.751905	-5.243757	-8.808330
S	-4.118384	6.276069	-0.336102
S	-6.142891	5.413627	-4.571323
S	1.257947	-0.630997	5.082444
S	-7.450923	3.857320	5.469233
S	-12.913106	1.989403	1.421414
S	-5.315325	0.443017	8.025573
S	-8.965504	-5.470641	7.205836
S	-12.637194	-4.523840	4.311362
S	-12.650024	-7.225849	-2.187362
S	-12.163536	-4.355801	-5.965720
Au	-5.941303	-10.673631	1.685490
Au	-10.812339	-5.004334	5.770499
Au	-12.420231	-5.799193	-4.084448
S	-12.386831	2.430257	-3.299805
Au	1.675985	-6.954552	0.161031
Au	-6.343926	2.180861	6.755579
Au	-12.686679	2.183047	-0.945459
Au	-4.716574	-6.983740	-7.548067
Au	-0.197958	0.157908	-6.552985
Au	-5.132350	5.859718	-2.457360
Au	1.424389	0.927277	3.283795
H	-13.053629	-3.407142	-5.551355
H	-12.016369	-8.305615	-2.732044
H	-5.861396	-11.452721	-1.080609
H	-3.680307	-10.558975	3.460062
H	-4.703047	-9.449663	-6.066060
H	-7.014728	-5.761593	-8.774243
H	1.417578	-7.912347	-2.542989
H	2.209733	-6.169521	2.879503

H	1.877234	-1.574020	-5.566287
H	-2.077865	-0.471687	-8.636157
H	0.960011	3.462097	2.013383
H	0.630557	0.210720	5.955428
H	-2.827680	6.249511	-0.781431
H	-7.417325	5.732439	-4.198355
H	-13.228935	1.420078	-3.666275
H	-13.737935	0.901067	1.401314
H	-6.353473	4.643172	5.263272
H	-4.055673	0.969112	8.005087
H	-8.899627	-6.808185	6.938704
H	-12.905353	-3.282783	4.814040

Cartesian coordinates of Au₆₀(SH)₂₀ with B3LYP/LANL2DZ implemented in Gaussian09 program package.

Au	-1.45070000	-0.46910000	-1.19120000
Au	-0.31460000	1.37290000	0.62940000
Au	-3.09360000	1.43300000	0.10110000
Au	-1.96540000	-0.69480000	1.59370000
Au	-6.23570000	3.18840000	-3.85540000
Au	-0.68930000	-1.35760000	4.01860000
Au	-3.49590000	-1.53710000	3.81930000
Au	-5.10850000	-0.68200000	5.98610000
Au	-5.98800000	-2.77100000	4.30840000
Au	-5.91730000	-0.10740000	3.34760000
Au	-5.61770000	1.84080000	1.30600000
Au	-8.14150000	0.65010000	1.75580000
Au	-7.06270000	2.44830000	3.65610000
Au	-4.31050000	3.97840000	-0.01560000
Au	-5.38730000	1.85510000	-1.51990000
Au	-0.51760000	-5.87160000	2.22320000
Au	-1.80060000	-4.75300000	-0.02430000
Au	-3.34840000	-5.79500000	2.13360000
Au	-1.87040000	-3.41140000	2.46600000
Au	-5.90220000	-5.39390000	3.26570000
Au	-7.63860000	-4.80010000	5.40350000
Au	-8.19510000	-3.79800000	2.82740000
Au	-4.81910000	-8.00600000	3.07780000
Au	-5.64110000	-6.67620000	0.73150000
Au	-9.62550000	-1.74070000	1.49540000
Au	-9.24280000	-0.07100000	-0.76110000
Au	-10.93640000	0.76090000	1.32970000
Au	-9.57940000	-4.34940000	0.41400000
Au	-11.01150000	-3.82720000	2.80100000
Au	-7.93780000	-6.24820000	-0.88600000
Au	-9.07090000	-4.11840000	-2.37250000
Au	-10.71620000	-6.19180000	-1.40510000
Au	-5.41540000	-6.66060000	-2.09350000
Au	-6.71660000	-8.79760000	-0.77460000
Au	-0.10070000	-5.57780000	-2.11520000
Au	-2.89010000	-5.47140000	-2.54410000
Au	-1.41530000	-3.07530000	-2.27770000
Au	-3.97600000	-7.26370000	-4.44840000
Au	-5.11580000	-4.70850000	-4.13120000
Au	-0.01810000	-0.99270000	-3.57680000

Au	-2.83560000	-1.00880000	-3.60620000
Au	-7.68420000	0.96280000	-2.91350000
Au	-9.18080000	-1.41080000	-3.25470000
Au	-10.51260000	1.06230000	-3.00840000
Au	-7.52950000	-3.26980000	-4.59530000
Au	-10.33430000	-3.47860000	-4.80960000
Au	-5.03600000	-2.04240000	-5.08770000
Au	-5.92810000	-4.12570000	-6.76730000
Au	-3.38550000	-0.02120000	-6.18880000
Au	-5.13240000	0.58460000	-4.05820000
S	-1.99690000	0.75700000	-8.04960000
S	1.69930000	-0.27000000	-5.16480000
S	1.71580000	2.46730000	1.45410000
S	2.02930000	-6.78040000	-2.21290000
S	1.46220000	-7.28120000	2.52870000
S	-4.96680000	-10.32070000	3.86760000
S	-7.00910000	-11.19930000	-0.38890000
S	-3.56180000	-8.73140000	-6.36560000
S	-5.72810000	-5.28870000	-8.91510000
S	-4.12200000	6.39660000	-0.35400000
S	-6.13240000	5.51050000	-4.62440000
S	1.34920000	-0.58560000	5.13930000
S	-7.48310000	3.91870000	5.56730000
S	-12.99470000	2.08230000	1.43710000
S	-5.31210000	0.48870000	8.12970000
S	-9.01830000	-5.50450000	7.29920000
S	-12.72050000	-4.56910000	4.39000000
S	-12.75260000	-7.27980000	-2.21870000
S	-12.25230000	-4.40170000	-6.02600000
Au	-5.95740000	-10.83220000	1.74130000
Au	-10.91360000	-5.05700000	5.89490000
Au	-12.56000000	-5.87040000	-4.15240000
S	-12.48020000	2.49000000	-3.31870000
Au	1.80510000	-7.06730000	0.16170000
Au	-6.36550000	2.26240000	6.89930000
Au	-12.81790000	2.28890000	-0.94900000
Au	-4.67690000	-7.06750000	-7.69150000
Au	-0.10240000	0.21960000	-6.67520000
Au	-5.12540000	6.01980000	-2.50560000
Au	1.56500000	0.99950000	3.34810000
H	-13.15110000	-3.46150000	-5.65220000
H	-12.15120000	-8.37150000	-2.74660000
H	-5.89750000	-11.59800000	-1.05070000
H	-3.69910000	-10.67300000	3.54960000
H	-4.63320000	-9.53650000	-6.17570000
H	-6.97760000	-5.80860000	-8.92450000
H	1.52040000	-7.98090000	-2.57630000
H	2.30490000	-6.29370000	2.91170000
H	1.98890000	-1.50260000	-5.64330000
H	-2.02670000	-0.40130000	-8.74940000
H	1.09690000	3.52980000	2.02000000
H	0.74000000	0.24010000	6.02210000
H	-2.83440000	6.39830000	-0.77230000
H	-7.40070000	5.84450000	-4.28910000

H	-13.33010000	1.50490000	-3.69160000
H	-13.84870000	1.03200000	1.44620000
H	-6.41500000	4.72730000	5.37390000
H	-4.06460000	1.01360000	8.13730000
H	-8.94550000	-6.83510000	7.06070000
H	-13.01950000	-3.34490000	4.88430000

Cartesian coordinates of Au₁₄₀(SH)₆₀ with PBE method implemented in Dmol³ code.

Au	-1.383031750	-0.552682876	-1.184026454
Au	-0.122562748	1.383158412	0.408146699
Au	-2.902074426	1.358415931	0.170386146
Au	-1.623338518	-0.672688591	1.604180753
Au	-6.030373953	3.017909239	-3.920565064
Au	-0.626755639	-1.578780524	4.073072360
Au	-3.388974218	-1.495631200	3.613130310
Au	-4.862139526	-0.763547923	5.880372834
Au	-5.897819678	-2.647106402	4.086884956
Au	-5.719374456	0.043707825	3.351030129
Au	-5.431305198	1.862163789	1.260716502
Au	-7.928510832	0.713438626	1.772011721
Au	-6.862347872	2.606267850	3.556059494
Au	-3.950050029	3.947064192	0.116868945
Au	-5.061556735	1.970691473	-1.506588892
Au	-0.614256684	-5.919368753	2.306633778
Au	-1.634615973	-4.873031859	-0.078304601
Au	-3.378196475	-5.689214538	1.939191278
Au	-1.819630148	-3.383315060	2.279507909
Au	-5.882457752	-5.260727904	3.091487122
Au	-7.359549038	-4.658452665	5.388606331
Au	-8.192822901	-3.694446941	2.890813895
Au	-4.720051831	-7.805258565	3.193662657
Au	-5.659760416	-6.786812668	0.751798229
Au	-9.444439372	-1.622750943	1.485476554
Au	-9.132082768	0.121713511	-0.678672005
Au	-10.719930603	0.866183215	1.501936410
Au	-9.423442385	-4.207471510	0.431568519
Au	-10.983295048	-3.625947086	2.695954298
Au	-7.835503531	-6.106071560	-0.865308260
Au	-9.112845178	-4.112283308	-2.353454174
Au	-10.615539528	-6.171676416	-1.168658969
Au	-5.334177187	-6.596909284	-2.020483212
Au	-6.813254057	-8.711880034	-0.938865467
Au	-0.053722787	-5.658960277	-2.245921192
Au	-2.836978754	-5.442473187	-2.541590760
Au	-1.283203143	-3.138093711	-2.238223911
Au	-3.876132892	-7.372651315	-4.283554282
Au	-5.039778247	-4.825007072	-4.157458241
Au	0.266109663	-1.105588277	-3.382904807
Au	-2.522378011	-1.082695447	-3.683934674
Au	-7.343205421	0.873490203	-2.687239514
Au	-8.940013185	-1.396746662	-3.012807198
Au	-10.093644935	1.165046521	-3.096378229
Au	-7.360347328	-3.267203323	-4.375984441
Au	-10.124117083	-3.191261469	-4.802659216

Au	-4.842472892	-2.125893028	-4.853696994
Au	-5.908463797	-3.965311113	-6.673150343
Au	-3.386080855	-0.121388063	-6.169706449
Au	-4.839799795	0.481262144	-3.857658566
Au	-7.493559491	5.346725405	-4.257912860
Au	-6.444345244	4.039236444	-6.473650911
Au	-4.744012664	5.352986035	-4.704710927
Au	-2.364058565	2.115178162	-7.456337503
Au	-4.092116042	0.406539637	-8.806266154
Au	-1.508894897	-0.435822099	-8.190784759
Au	-4.496392334	-4.172607961	-9.055593957
Au	-6.519165773	-5.993689018	-8.472945079
Au	-7.153988707	-3.349412343	-9.076305000
Au	-11.032928372	-4.740655648	-6.919419241
Au	-12.851625823	-3.618835680	-5.130442238
Au	-11.477867805	-1.997461504	-6.922695177
Au	-12.769566804	1.193913538	-3.833457244
Au	-11.581069182	3.488277692	-2.793901004
Au	-10.887720959	2.598720627	-5.336298341
Au	2.082929888	-2.056849860	-5.247216339
Au	1.621695869	0.685550117	-5.016842522
Au	1.657322452	3.064422014	-0.899249818
Au	-7.862760176	5.207997658	3.660137774
Au	-8.465474320	3.398349304	5.689902740
Au	-11.700431883	3.414733044	2.019008443
Au	-13.358850441	1.491608261	0.877424296
Au	-12.576638600	1.243907101	3.533152520
Au	-4.436351298	-1.674860831	8.466928692
Au	-3.454888759	0.813116754	7.680166256
Au	-6.191525072	0.439896472	8.001397418
Au	-12.345651817	-3.387425758	5.104659160
Au	-13.712989804	-3.176377017	2.686846533
Au	-12.708835211	-5.643449653	3.521388513
Au	-9.217291120	-6.328125488	6.607627275
Au	-6.649835523	-6.088267432	7.660553410
Au	-8.445454162	-3.967581039	7.853565715
Au	-3.401754581	-9.026188633	5.312594965
Au	-6.066453347	-9.638478434	4.787002212
Au	-4.066444946	-10.510109967	3.062248157
Au	-11.866672902	-8.516932208	-0.352106915
Au	-12.065956415	-7.673073567	-2.999252193
Au	-13.384798011	-6.271313278	-0.983358811
Au	0.269699902	-8.516337270	2.740944019
Au	-7.901273075	-10.886500880	0.403564155
Au	-8.401764083	-10.517357176	-2.309769639
Au	1.396351848	-7.987602718	-1.780802149
Au	-4.926044531	-9.568921600	-5.617378942
Au	-2.804403529	-8.139558042	-6.726146366
Au	1.303563081	-6.887962162	-4.338545041
Au	-2.393281769	-9.711302554	-4.463170509
Au	-5.860715024	-11.274438163	-1.451799658
Au	2.111646495	-6.450589745	2.420135851
Au	0.561090851	-6.582117935	4.724603888
Au	2.010649648	-2.184045899	4.716539537

Au	0.953557665	0.319312390	5.335446118
Au	0.109001709	-1.941727329	6.732003473
Au	-5.879920980	4.400002878	5.449576184
Au	-3.289831727	5.844843375	2.035585468
Au	-2.147674453	5.968447461	-0.497729510
Au	-4.842020973	6.566457533	-0.150583702
Au	0.971436891	3.548676332	1.759275738
Au	2.562195923	1.351109155	1.099480591
Au	2.721850301	-5.607456974	-2.306957567
Au	2.981125894	-0.660948954	-3.001112095
S	-1.577158779	2.153524006	8.397552163
S	-4.350528830	-3.401272390	10.154041208
S	-7.997572025	1.712407581	8.998593744
S	-0.237708971	-2.342403814	9.083886782
S	2.034555551	2.446117113	5.669990747
S	4.075015949	-3.420846113	4.693911071
S	4.491422800	0.390296019	2.184267543
S	0.940986385	5.620333911	3.012830742
S	2.867872431	4.010830816	-2.763427116
S	-0.097779507	6.868776773	-1.426514920
S	-3.174863387	6.681513418	4.292513267
S	-6.234668206	8.226777699	-1.200242103
S	-7.645265800	7.501905556	2.919118956
S	-4.821930138	4.932026347	7.554492034
S	-10.674691405	3.584860500	6.637800251
S	-8.971014299	-2.456138065	9.655789324
S	-11.242676470	-7.636577551	6.822577126
S	-5.224767944	-7.564925628	8.944168120
S	-12.547320984	-3.133091686	7.501634500
S	-13.704050589	-7.836501377	3.470662237
S	-15.731327211	-1.993812401	2.110722606
S	-15.309280598	1.676644293	-0.547639240
S	-13.769876059	0.634629010	5.537489509
S	-11.468588463	5.757258313	2.495866194
S	-12.547323898	5.364067225	-1.621054740
S	-14.850602753	0.119114788	-4.405944421
S	-10.589498065	3.802008640	-7.418110422
S	-12.224834382	-0.190520925	-8.330899994
S	-15.059910970	-4.225344444	-4.361953920
S	-10.801124079	-6.336444619	-8.712363551
S	-12.820388530	-8.318269811	-5.193374697
S	-15.572783057	-5.561298968	-0.238797707
S	-12.021402350	-10.729416885	0.629445478
S	-10.217932883	-11.315467236	-3.703821191
S	-8.445639969	-12.133195336	2.394607974
S	-4.372575183	-12.948333647	-2.335060370
S	-3.763679171	-12.590159525	1.881404403
S	-7.845877406	-10.409235097	6.215385610
S	-1.636753475	-9.324680684	6.940426696
S	4.365879482	-6.507590852	1.539486784
S	1.030814353	-6.177892715	7.055413516
S	0.076533351	-10.923434056	2.836409723
S	1.841901905	2.539198174	-6.546738155
S	5.020777995	-0.096491587	-1.818081745

S	3.114358067	-3.740314660	-6.633405707
S	4.865462555	-4.500269111	-2.292245634
S	1.404323446	-7.844869831	-6.555700009
S	2.059506755	-10.019096212	-0.634179536
S	-2.174693044	-7.831923291	-9.029925225
S	-0.587287108	-11.198395447	-3.863068343
S	-6.587469271	-11.228440586	-6.157635362
S	-8.898448010	-2.351756399	-10.424757977
S	-2.637990592	-3.750058719	-10.545749024
S	-6.889521876	-8.289953849	-9.133527653
S	-5.343375958	0.126028280	-10.846223521
S	-1.917425692	4.474706532	-7.745380293
S	0.548519650	-1.164973575	-9.204882356
S	-9.373603425	6.858860259	-4.015235349
S	-3.078158159	7.080241692	-4.550992336
S	-6.477494448	3.916641803	-8.881663510
Au	-4.183029828	4.279157097	-8.425818171
Au	-3.995528746	-1.821096440	-10.811598811
Au	1.223919026	0.746045949	-7.967634173
Au	4.089522113	-4.129859122	-4.502996168
Au	4.075293180	2.023957308	-2.310179589
Au	0.513436353	6.352485147	0.801335303
Au	3.369521419	1.466113034	3.971218932
Au	2.648315374	-4.851994480	5.936162545
Au	-0.860232721	-0.069781116	8.836105274
Au	-6.477333039	3.396174955	8.287394856
Au	-6.671243424	-2.917833398	10.003270133
Au	-5.437295679	7.112133509	3.704129420
Au	-10.977698989	4.773669103	4.601840643
Au	-4.648768041	7.739741299	-2.899009067
Au	-10.049885477	5.434619410	-5.785520437
Au	-13.638467103	0.028224108	-6.438967486
Au	-14.053445401	3.607148891	-1.111113689
Au	-14.837949296	-0.670629251	3.868235314
Au	-11.988740806	-5.425853642	7.257001125
Au	-6.572413194	-9.057139060	7.685551081
Au	-0.691876870	-10.249792022	4.975025760
Au	3.333788142	-8.352478898	0.465846553
Au	0.489839984	-9.601403019	-5.251326778
Au	-4.526074794	-8.099111205	-9.186046408
Au	-5.497268646	-12.180685075	-4.278224487
Au	-6.114865267	-12.516976369	2.174586266
Au	-11.212136905	-11.158154415	-1.557777658
Au	-14.735495329	-6.774108565	1.620141226
Au	-14.033853070	-6.319061699	-4.789929684
Au	-9.879147544	-4.375637811	-9.673455129
H	-0.961450317	2.230113441	7.188031175
H	-1.507570611	-2.820755197	8.990864932
H	-4.400316751	-4.460554939	9.302518437
H	-8.766447242	-1.306527546	8.958308142
H	-2.657886891	7.880780776	3.921416347
H	-10.969017378	-8.013102553	8.097240568
H	-7.528585398	1.567870082	10.264387897
H	-13.899161500	-3.252795859	7.499296227

H	-12.729164184	-8.443619921	2.742900835
H	-13.350934051	-10.846052242	0.383176289
H	-9.812140825	-12.609593228	-3.652518861
H	-8.898885640	-13.216500182	1.715142019
H	-8.742452546	-9.437602702	5.896983677
H	-5.987412821	-7.500680786	10.064409272
H	-2.164656558	-10.461502398	7.459684635
H	1.383849333	-11.125181965	3.138924937
H	-3.441340728	-13.296029912	2.994759863
H	-3.291009995	-12.142223734	-2.502346797
H	-7.601529645	-10.673664008	-5.441976027
H	-7.152762892	-7.984492814	-10.429251802
H	-2.201101615	-6.473226106	-9.026003223
H	-0.251450384	-10.583964233	-2.697260989
H	2.716542744	-8.179481487	-6.470007572
H	2.150225352	-4.689250025	-6.490056722
H	4.417935298	-3.310942515	-1.808987171
H	5.807384118	-0.225907118	-2.916376904
H	3.580281352	4.870270915	-1.992010339
H	0.581809884	3.025290664	-6.391513533
H	0.913815591	-2.045864470	-8.235618939
H	-6.433286451	-0.464984836	-10.285752337
H	-3.143389230	-4.497048647	-11.559381449
H	-8.398404031	-2.807850840	-11.600483074
H	-9.601162570	-6.853168174	-8.333040277
H	-11.834422806	-7.699886081	-5.896398038
H	-14.772120176	-4.206343445	-3.034265027
H	-15.519057424	1.281771624	-4.613577148
H	-11.314341953	0.731423271	-7.917315191
H	-11.907779768	4.089688862	-7.559348257
H	-6.851807846	5.210404001	-9.045993561
H	-1.326892153	4.313076191	-8.956289264
H	-0.466234485	8.161249247	-1.241615838
H	2.290400492	5.762043595	3.018247274
H	-8.174888565	8.021876440	4.054402969
H	-7.182399779	7.369835972	-1.665605271
H	-2.251471847	6.430119483	-3.689563864
H	-8.802174574	7.841414658	-4.756114953
H	-10.182699538	5.899088598	2.076832127
H	-13.159207682	5.860233440	-2.725822807
H	-16.084935614	2.224107207	0.421805962
H	-15.197752995	-1.240035244	1.113309619
H	-12.914660851	-0.345160601	5.934419455
H	-10.364458359	4.628124336	7.447096070
H	-3.834844703	3.997794047	7.497516951
H	1.767600450	-7.305084935	7.222930715
H	3.888163328	-4.048514946	3.502424794
H	4.876213205	-7.158263758	2.615793404
H	2.962911309	-10.374424530	-1.583404909
H	1.269512121	3.171235175	4.808947956
H	5.328154932	1.398758258	1.835321067
H	-16.225804486	-6.569137865	-0.870848829

Cartesian coordinates of Au₁₈₀(SH)₆₀ with PBE method implemented in Dmol³ code.

Au	3.019707660	-1.425539915	-6.345983810
Au	4.685963084	2.763871775	-3.558578702
Au	0.620647729	4.773277991	-6.208116746
Au	5.713598173	-2.544716499	-2.040692796
Au	5.896117805	4.662023583	-1.909275221
Au	-0.878360567	6.950082552	-1.701967844
Au	7.364936120	-0.510787827	-1.109296012
Au	6.897150976	2.065095976	-2.029576414
Au	4.506321489	6.846424483	-0.863531886
Au	2.681817700	8.389082217	0.564176352
Au	-1.808018665	8.150692725	0.638999817
Au	-3.443428872	6.409035023	-0.790265534
Au	3.305879533	-7.131736845	-2.177957457
Au	5.526891120	-7.670349379	1.224842568
Au	7.128287897	-2.855715043	0.339762437
Au	8.326390945	4.040057911	1.806514526
Au	7.139750084	6.160881159	3.184490094
Au	2.896194932	8.779293907	3.315815016
Au	0.425580439	9.053519198	2.067103123
Au	-8.000590930	5.586743559	1.693365638
Au	3.629556882	-8.478322883	4.689201373
Au	8.576188517	-0.878482070	4.291483455
Au	8.455437423	1.443257853	5.830401427
Au	5.110557080	7.581025082	4.465880087
Au	2.902227743	8.253494704	6.034230045
Au	-4.020542399	7.164505787	4.638749838
Au	-1.814531410	8.013786222	6.122421174
Au	2.779822620	-4.794320182	8.100251294
Au	7.392086208	-2.883301196	5.808642967
Au	-5.213557433	5.098780488	6.068292263
Au	0.592251690	7.761850489	7.496563367
Au	3.025829563	6.775962627	8.386494990
Au	7.229162279	3.501219187	7.266780555
Au	5.406342712	5.323969237	8.318313999
Au	1.407912172	-3.131941540	9.855270613
Au	-1.584965337	4.274338505	10.080713852
Au	7.238090252	0.927660998	8.287746359
Au	0.957357764	3.430533895	10.866316854
Au	3.354107844	4.589475175	10.060177761
Au	5.136611433	0.021291929	9.859337274
Au	1.304614229	-2.460865853	12.565541029
Au	-1.157387733	1.618340617	10.807814696
Au	-6.823505030	0.636423553	3.320472260
Au	-6.725938040	3.129075534	2.080135214
Au	-6.533645838	0.812128887	0.557897604
Au	-8.973915188	1.472516415	1.752932185
Au	-5.219664965	1.357356309	-1.833006593
Au	-5.329797667	-1.240704154	-0.889258008
Au	-7.651919268	-0.022632061	-1.866827248
Au	-6.415328964	0.544605780	6.068140175
Au	-6.405617077	-1.808551965	4.583900762
Au	-8.808640165	-0.420958592	4.973603061

Au	-4.882260652	-3.668570024	5.995023434
Au	-5.204147925	-3.931974257	3.232664705
Au	-7.358440317	-4.415205018	4.933308228
Au	-4.774250491	-3.557886668	0.516051338
Au	-3.236264830	-5.393778467	1.911326162
Au	-5.939412849	-5.931813980	1.418440734
Au	-3.485867334	-3.047061434	-1.904131604
Au	-6.218322264	-3.698331976	-1.872941375
Au	-4.533284161	4.055137067	-1.806601170
Au	-5.819002307	2.961955373	-4.046056081
Au	-3.175657433	2.280327239	-3.471051107
Au	-0.690152143	3.074096103	-4.415323287
Au	-2.611128661	2.098775668	-6.199885726
Au	-1.355780397	0.371705840	-4.394863752
Au	-1.382567265	-2.288270271	-3.561480739
Au	0.982740331	-1.142323408	-4.442050855
Au	-1.063475121	-1.687864824	-6.270396740
Au	-1.166143308	-4.591038386	-2.029887964
Au	-2.922621111	-4.521648322	-4.212295198
Au	-1.003865976	-6.525328767	3.086251315
Au	-1.015867573	-6.031676776	0.349846755
Au	-2.621206233	-8.073316180	1.410078320
Au	1.292819230	-5.523603368	-1.121166090
Au	-0.601536491	-7.329448141	-2.094247108
Au	-5.483067041	2.741436233	7.508713566
Au	-7.584547313	1.206522339	8.525446144
Au	-4.995673218	0.169191755	8.428323833
Au	-3.976954536	-2.418012406	8.311350207
Au	-5.132583952	-4.970800239	8.454155594
Au	-2.611959903	-4.621500272	7.293396327
Au	-5.205115328	-1.502601063	10.662399903
Au	-2.728563733	-0.486262432	9.884725244
Au	0.002457452	-4.872523413	8.197397883
Au	-1.707479148	-7.079237773	8.290187220
Au	-0.783016730	-6.118250526	5.828112266
Au	1.476638437	-6.737260349	4.315579194
Au	-0.468053128	-8.691525406	4.755509209
Au	3.852810488	-6.286276595	2.971109711
Au	3.735094421	-5.876268805	5.720705527
Au	3.719861046	-5.773749204	0.237075817
Au	5.942416182	-4.951967819	1.722114320
Au	3.588320562	-4.345841933	-2.156862265
Au	5.275031705	-4.055905900	7.164662781
Au	4.893683550	-6.639425720	8.155457648
Au	1.499348206	-5.883075915	10.337331183
Au	2.652440961	-0.808072197	10.757859598
Au	-0.116784368	-0.954827746	10.678127510
Au	-2.059458444	-0.354531585	12.597039469
Au	-5.766907632	5.412901377	3.360639581
Au	-5.476272632	5.123144113	0.594663164
Au	-6.047680117	6.409250579	-1.814621133
Au	-3.811925984	4.753488134	8.454952347
Au	-6.595011258	5.103028561	8.498561842

Au	-6.757033031	7.273028230	5.209173353
Au	3.118341903	0.640753696	-4.452262464
Au	3.506282121	-2.000684903	-3.660973043
Au	5.280344812	-4.039774308	-4.360525586
Au	0.564075736	5.380080413	-3.485866425
Au	2.085887845	3.226511799	-4.397287463
Au	4.045488625	2.556953331	-6.275414649
Au	0.369902605	8.140054405	-3.903747029
Au	1.893776619	7.127052409	-1.781168743
Au	-2.851784615	8.930082261	-1.843455555
Au	-1.973092342	8.573954853	3.392696941
Au	-3.675752013	9.882031624	5.181440789
Au	-1.751657382	10.751513131	1.657691973
Au	-1.689838378	6.561602182	8.506851641
Au	-3.369370012	6.323244547	10.729478787
Au	-1.087573096	3.636507668	12.755442723
Au	-1.439084207	9.346820882	8.559176283
Au	3.313264234	1.905871074	10.813324288
Au	4.561227043	0.124567484	12.588033401
Au	2.975360185	3.903347580	12.742469027
Au	6.484379975	-1.759011234	8.181498861
Au	7.847224757	-4.206376643	8.238292900
Au	7.740550391	-0.760542337	10.466949870
Au	7.663337834	-3.207175426	3.049321767
Au	8.678218146	-5.038277016	1.181355888
Au	9.922079010	-3.295380751	4.689490150
Au	8.506764787	-2.872545981	-2.088694364
Au	8.332209910	1.682519118	0.320623170
Au	9.474461968	1.001624672	-2.146076587
Au	7.186830905	3.778688649	-4.230774637
Au	8.796063701	1.605669781	3.067691194
Au	10.731516166	2.673569421	1.360947465
Au	6.785769347	5.906020662	0.422006009
Au	7.017536147	7.230324489	-2.028918736
Au	9.276942298	6.643137072	1.456695077
Au	3.656663847	9.299303392	-1.901341897
Au	10.884716467	0.660267765	4.663807600
Au	2.416768933	10.961574660	1.639942025
Au	6.745593678	5.879926418	5.931510839
Au	7.781277179	8.275616247	4.903691853
Au	4.568494268	10.268542683	5.003479155
Au	2.512701843	9.524578387	8.502444325
Au	9.618641719	2.408008314	8.190849843
Au	8.152853497	5.889459038	8.361699060
Au	4.802727003	6.934778850	10.529179197
S	3.805332676	-9.254931637	-3.174413126
S	6.563962780	-9.748494544	0.628869556
S	-1.092797678	-9.398008466	-3.199806650
S	-3.396364108	-10.263326963	0.828493799
S	-4.105001553	-5.772647367	-5.878718472
S	-7.836054569	-4.970591485	-3.098570810
S	-1.729923598	-2.277441884	-8.496319064
S	-3.476961933	2.109289262	-8.432466762

S	3.514108376	-1.810434395	-8.656234112
S	4.798763743	2.734443602	-8.542172455
S	6.519292780	-5.004894616	-6.175038413
S	10.194036216	-3.957363432	-3.400398177
Au	8.364129645	-4.525999947	-4.784391339
Au	5.200903479	-9.513918392	-1.288693748
Au	-2.205670664	-9.874723898	-1.173133324
Au	-5.973564152	-5.428157543	-4.478194955
Au	-2.660315586	-0.105834975	-8.474438575
Au	4.125341591	0.469216303	-8.630383924
S	-7.538503874	-7.690449778	1.104872959
S	-9.289085491	-5.832447100	5.080907624
S	-0.880537107	-10.993573502	5.280340690
S	-2.195565463	-9.132329765	9.422845267
S	4.365454346	-10.687616315	5.263252681
S	5.850597583	-8.564887307	9.213244083
S	10.699517879	-6.256868037	0.752466656
S	11.986174731	-4.488993675	4.941844554
S	11.599968950	0.941017395	-3.253273246
S	13.065466880	2.811811090	0.829682597
S	8.630843046	4.555624358	-5.977400193
S	8.308453816	8.582120021	-3.531543197
S	0.582494891	5.851950914	-8.352158267
S	0.255113225	9.739106424	-5.685292326
S	-7.478674425	3.518036933	-5.682177751
S	-7.698607055	7.506893477	-3.161461167
S	-9.809892907	-0.415532563	-2.827613493
S	-11.320762285	1.322879566	1.297511696
S	-3.656352218	10.876208937	-2.983944500
S	-2.521140115	12.954805038	1.102807937
S	4.231137491	11.337743669	-3.019589886
S	3.137752368	13.201168541	1.181325319
S	11.231353944	8.029654863	1.276986821
S	9.349300470	10.080157195	5.098364430
S	13.236878963	0.753438047	5.108863478
S	11.796775858	2.876477204	9.077191801
S	9.376396125	-5.432204643	9.620338427
S	9.228717484	-1.479748021	12.204857910
S	1.574804179	-7.444709344	12.153134065
S	1.239654017	-3.495149161	14.726547184
S	-6.454121805	-6.289830938	9.957476856
S	-6.617830040	-2.273525212	12.436855374
S	-11.161604082	-0.491344310	5.431007842
S	-9.725000694	1.186198296	9.607839637
S	-10.070679392	6.785370833	1.490608114
S	-8.698378812	8.621359425	5.622296490
S	-4.739052666	11.926798583	5.843652657
S	-1.943700180	11.438675133	9.618636782
S	-8.323579510	6.122522742	9.806380101
S	-4.631382570	7.450432501	12.432162926
S	-2.770251456	-0.628847119	14.865020298
S	-1.716552107	3.970597373	15.041983858
S	5.384898655	0.013543412	14.840107561

S	3.398189760	4.298158734	15.071142025
S	2.981152001	11.589443925	9.623288677
S	5.901952133	8.471078522	12.005605069
S	9.775376603	6.971981974	9.759541563
S	5.403488291	12.415246017	5.653656014
Au	0.454655305	7.809401322	-7.036229418
Au	-7.637013762	5.505200575	-4.413567922
Au	-10.579457289	0.411195106	-0.754106266
Au	-8.405214044	-6.806801092	3.118560969
Au	-1.538948739	-10.083826456	7.361710068
Au	5.136420858	-9.636127641	7.232136075
Au	11.374238909	-5.354092590	2.830408496
Au	12.359587516	1.834807142	-1.203629738
Au	8.517942703	6.568391412	-4.750085237
Au	3.691290279	12.291633679	-0.926956637
Au	-3.054001332	11.941593624	-0.964124128
Au	-9.386147764	7.737502183	3.539540380
Au	-10.467324908	0.387869678	7.513456984
Au	-6.587569153	-4.281176420	11.191390566
Au	1.357631627	-5.484480158	13.458025895
Au	9.287281445	-3.478242862	10.946132096
Au	12.529011654	1.840011774	7.085371713
Au	10.287253985	9.076089837	3.173918885
Au	7.851352929	7.694238764	10.924629705
Au	4.413423900	2.168282325	14.941049821
Au	-2.307271111	1.686559705	14.961790488
Au	-6.488171603	6.846022376	11.105881482
Au	-3.385796091	11.678660005	7.764648683
Au	4.222477853	12.004037416	7.658083413
H	1.574945777	10.051583176	-5.659657373
H	1.930087780	5.881314496	-8.510109000
H	9.486016952	8.469751317	-2.866814721
H	5.569824597	11.244223097	-2.816868838
H	1.930041014	13.699664211	0.816479009
H	-2.496499991	11.127284838	-3.644178772
H	-1.311527783	13.435396486	0.719686329
H	9.778181910	4.093197249	-5.420168189
H	3.638324081	3.237156383	-9.034902718
H	2.242746321	-1.622937806	-9.091801221
H	10.189092915	-5.107891419	-2.680482989
H	6.377998120	-6.298276474	-5.790894331
H	-2.847148590	-2.947035345	-8.116057250
H	-4.752871117	1.805770953	-8.081957206
H	-8.755348038	7.153948335	-2.386605485
H	-8.490944269	2.854976908	-5.067328158
H	-9.573454906	7.775780683	0.707100640
H	-8.187644859	9.775631439	5.124348917
H	-5.841591645	11.338582970	6.373249137
H	-2.879940263	10.956516742	10.474251707
H	-8.433395718	7.230381596	9.029459696
H	-4.478355311	8.695846295	11.918090706
H	-4.096946161	-0.535541748	14.595334181
H	-2.951607275	4.460557102	14.766792063

H	-9.998692967	2.497071654	9.387129337
H	-11.427511670	0.707362927	4.851649541
H	-8.742501444	-6.730309851	5.939294190
H	-6.765178572	-8.658447448	1.658178385
H	-11.495865429	0.131629886	1.924537992
H	-9.845716088	-1.733550863	-2.506585744
H	-7.732514048	-6.072486625	-2.312899894
H	-3.764737490	-6.997059073	-5.402351235
H	0.083262238	-10.004203770	-2.898343046
H	-2.414556098	-10.928745907	1.488096874
H	0.398963242	-11.286082367	5.624647428
H	-3.529070404	-9.117573570	9.175617215
H	-7.630960442	-6.135402220	9.299316298
H	-7.768878907	-1.775603699	11.919026595
H	0.253148954	-7.748109919	12.109364021
H	-0.112504452	-3.466765060	14.842514076
H	7.118455611	-8.329301630	8.788995887
H	5.544365029	-10.617379638	4.595432716
H	5.700598822	-10.540444043	1.314088726
H	4.766039164	-8.818633839	-4.026861410
H	8.416980518	-6.106525696	10.304532070
H	8.240884257	-1.874266367	13.048901681
H	6.638789989	0.444028277	14.548015963
H	4.543837807	5.004979064	14.897589015
H	11.846063528	4.146925458	8.598618038
H	13.460398015	1.888725203	4.397829688
H	12.787786474	-3.498582681	4.475001970
H	11.260913586	-5.281472993	-0.005648049
H	11.858713057	-0.360360081	-2.967969036
H	13.402404269	1.644362647	1.435017896
H	10.714691777	8.897833047	0.370429043
H	8.588885683	10.974603764	4.416751575
H	10.015830777	5.882486166	10.533505124
H	5.968265173	7.646000659	13.080014314
H	4.014456432	11.108489849	10.359862667
H	6.594565164	11.958278485	6.118298628

Reference 46:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.