

Theoretical Study on A Novel $\text{Au}_{99+31n}(\text{SR})_{40+10n}$ Cluster Sequence with D_5 Symmetry

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I. Computational methods and details

The geometric optimizations of $\text{Au}_{99+31n}(\text{SR})_{40+10n}$ ($n = 0, 1, 2, 3$) cluster series are implemented in CP2K Code¹ based on the level of PBE^{2,3}(D3BJ)^{4,5}/DZVP-MOLOPT-SR-GTH. To ensure the rationality of structural optimization, the sizes of cells of these clusters are set to $26.25870000^3 \text{ \AA}^3$, $29.05660000^3 \text{ \AA}^3$, $32.14064023^3 \text{ \AA}^3$ and $34.93894883^3 \text{ \AA}^3$, respectively. The convergence threshold of density matrix of inner SCF is $1.0\text{E-}06$. The maximum geometry change, RMS geometry change, Maximum force and RMS force is set to $3\text{E-}3$, $1.5\text{E-}3$, $4.5\text{E-}4$ and $3\text{E-}4$, respectively. The single-point energy and sTDA⁶ calculations of $\text{Au}_{99+31n}(\text{SR})_{40+10n}$ ($n = 0, 1, 2, 3$) cluster series are implemented using the ORCA 5.0.4 program system^{7, 8} at theoretical level of PBE0⁹(D3BJ)/Def2-TZVP¹⁰ and PBE0(D3BJ)⁹/Def2-SV(P)¹⁰, respectively. The convergence criteria were maintained at their default settings throughout the computational procedures. Note that the Def2 basis set family incorporates relativistic pseudopotentials for elements beyond the fourth period, thereby effectively accounting for scalar relativistic effects in these heavy metal-containing systems.

In sTDA calculations, the energy threshold is set to 4 eV, which is sufficient to ensure that the computed spectra cover the wavelength range of interest. Additionally, the parameters of PThresh and PTLimit are set to 1.0×10^{-4} and 30, respectively, to control the range of configuration functions, with negligible sacrifice in accuracy. All R ligands were simplified to methyl substituent groups in all calculations. Finally, the wavefunction analyses and electronic structure characterizations were conducted using the Multiwfn software package (version 3.8_dev)^{11, 12}, with all molecular orbital isosurfaces visualized through integration with the VMD 1.9.3 software.

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II. Supporting tables and figures

Table S1. The 50 experimentally characterized thiolate-protected gold nanoclusters (RS-AuNCs) and their corresponding literature sources.

Size	Item	RS-AuNCs	Reference	Size	Item	RS-AuNCs	Reference
		Au S				Au S	
Small size	1	10 10	<i>J. Phys. Chem. Lett.</i> 2017 , 8, 1979	26*	42 26		<i>Chem. Sci.</i> , 2018 , 9, 2437–2442
	2	16 12	<i>J. Am. Chem. Soc.</i> 2018 , 140, 10988	27*	42 26		<i>Angew. Chem. Int. Ed.</i> 2019 , 58, 4510
	3	18 14	<i>Angew. Chem. Int. Ed.</i> 2015 , 54, 3140	28	42 32		<i>J. Am. Chem. Soc.</i> 2022 , 42, 19243
	4	20 16	<i>J. Am. Chem. Soc.</i> 2014 , 136, 11922	29	43 25		<i>J. Phys. Chem. Lett.</i> 2017 , 8, 5338
	5*	21 15	<i>J. Phys. Chem. C</i> 2018 , 122, 14898	30	44 28		<i>J. Am. Chem. Soc.</i> 2016 , 138, 3950
	6*	21 15	<i>J. Am. Chem. Soc.</i> 2016 , 138, 10754	31	44 26		<i>J. Am. Chem. Soc.</i> 2016 , 138, 10425
	7	22 16	<i>J. Am. Chem. Soc.</i> 2020 , 142, 20426	32	46 26		<i>Angew. Chem. Int. Ed.</i> 2021 , 60, 8668
	8	23 16	<i>J. Am. Chem. Soc.</i> 2013 , 135, 18264	33	48 28		<i>Angew. Chem.</i> 2018 , 130, 15676
	9	24 16	<i>J. Am. Chem. Soc.</i> 2014 , 136, 14933	34*	48 26		<i>Acta Chim. Sinica</i> 2020 , 78, 407
	10	24 20	<i>Nanoscale</i> 2014 , 6, 6458	35*	48 26		<i>Angew. Chem. Int. Ed.</i> 2021 , 60, 8668
	11	25 18	<i>JACS</i> 2008 , 130, 5883; 3754	36	49 27		<i>Angew. Chem.</i> 2017 , 129, 12818
	12*	28 20	<i>J. Am. Chem. Soc.</i> 2016 , 138, 1482	37*	52 32		<i>Nanoscale</i> 2017 , 9, 14809
	13*	28 20	<i>J. Am. Chem. Soc.</i> 2013 , 135, 10011	38*	52 32		<i>Sci. Adv.</i> 2015 , 1, e1500425
	14	28 22	<i>Angew. Chem. Int. Ed.</i> 2021 , 133, 18076	39	56 34		<i>Angew. Chem. Int. Ed.</i> 2020 , 59, 731
	15	29 19	<i>Nature</i> 2021 , 594, 380	40	67 35		<i>Angew. Chem. Int. Ed.</i> 2021 , 60, 11184
	16*	30 18	<i>Angew. Chem.</i> 2016 , 128, 6806	41	92 44		<i>J. Am. Chem. Soc.</i> 2016 , 138, 8710
	17*	30 18	<i>Nature</i> 2021 , 594, 380	42	102 44		<i>Science</i> 2007 , 318, 430
	18	32 24	<i>Angew. Chem. Int. Ed.</i> 2021 , 60, 12253	43	130 50		<i>J. Am. Chem. Soc.</i> 2015 , 137, 10076
	19	34 22	<i>Nanoscale</i> 2017 , 9, 3742	44	133 52		<i>Sci. Adv.</i> 2015 , 1, e1500045
	20*	36 24	<i>Angew. Chem. Int. Ed.</i> 2012 , 51, 13114	45	138 48		<i>Nat. Commun.</i> , 2023 , 14, 2397
	21*	36 24	<i>Nat. Commun.</i> 2020 , 11, 3349	46	144 60		<i>Sci. Adv.</i> 2018 , 4, eaat7259
	22	37 23	<i>Acta Chim. Sinica</i> 2020 , 78, 407	47	146 57		<i>J. Phys. Chem. Lett.</i> 2017 , 8, 5523
	23*	38 24	<i>J. Am. Chem. Soc.</i> 2010 , 132, 8280	48	191 66		<i>J. Am. Chem. Soc.</i> 2020 , 142, 15799
	24*	38 24	<i>ACS Nano</i> 2009 , 3, 3795	49	246 80		<i>Science</i> 2016 , 354, 1580
	25	40 24	<i>Sci. Adv.</i> 2015 , 1, e1500425	50	279 84		<i>J. Am. Chem. Soc.</i> 2017 , 139, 15450
*indicates that the systems share the same number of gold (Au) and sulfur (S) atoms.							

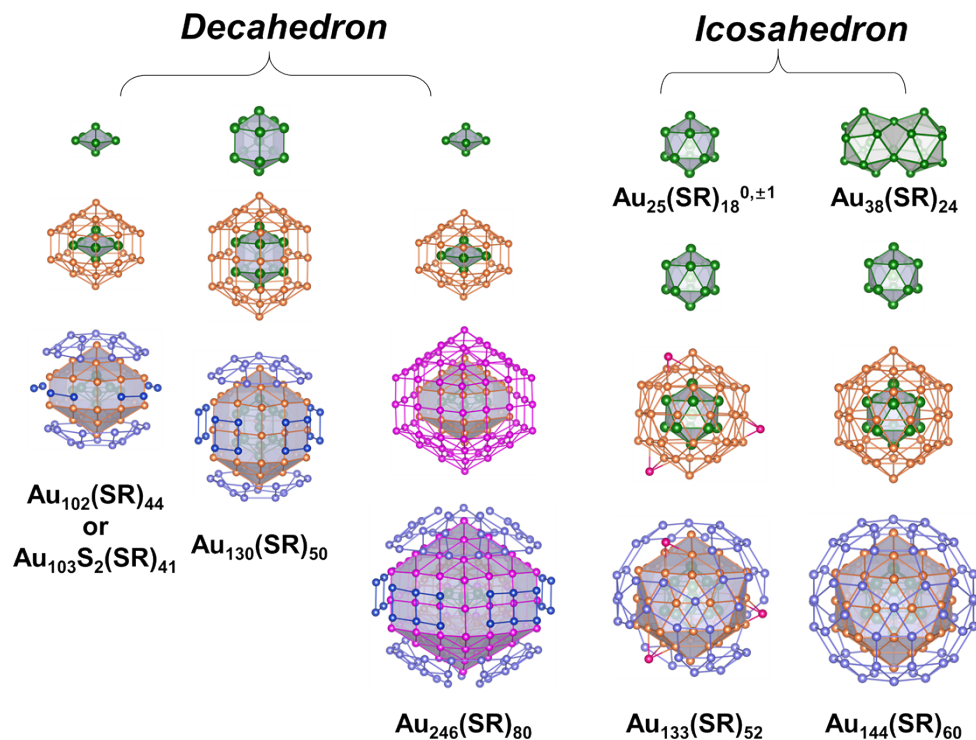


Figure S1. The core-shell structure of large-sized RS-AuNCs.

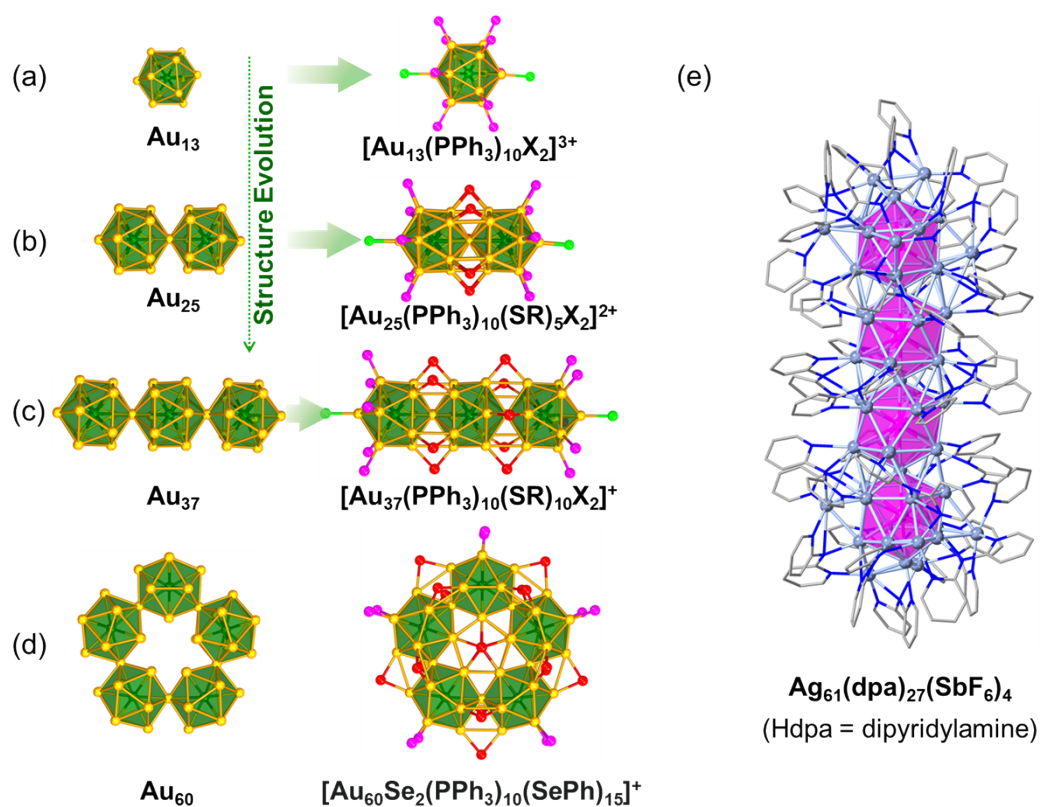


Figure S2. Some representative clusters constructed via vertex-sharing of icosahedral Au_{13} building blocks.

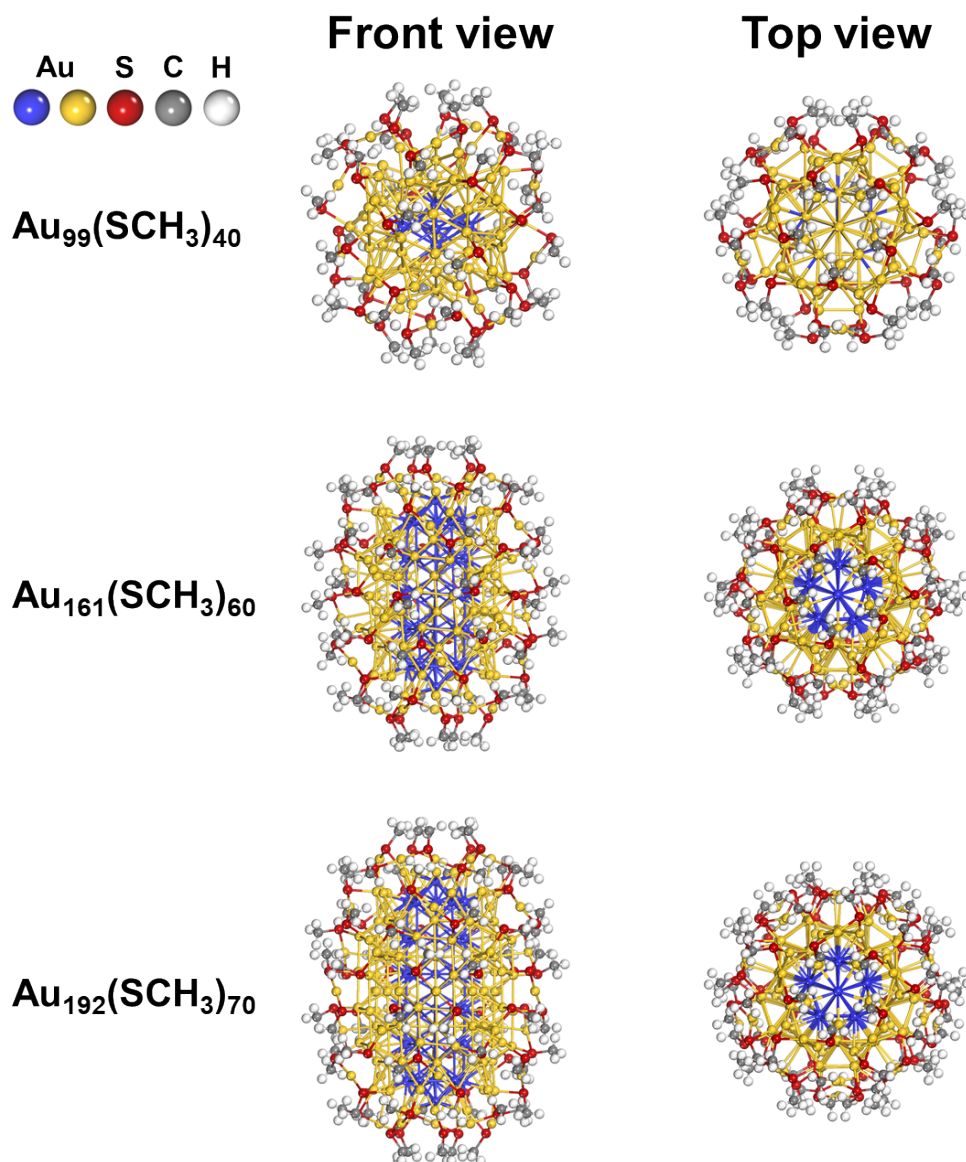


Figure S3. Structural configurations of $\text{Au}_{99}(\text{SCH}_3)_{40}$, $\text{Au}_{161}(\text{SR})_{60}$ and $\text{Au}_{192}(\text{SR})_{70}$ clusters constructed based on ‘divide-and-protect’ approach.

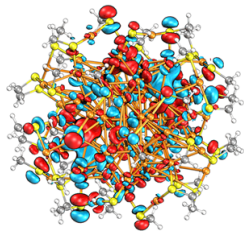
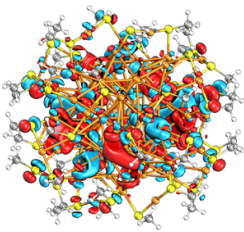
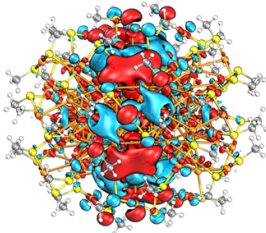
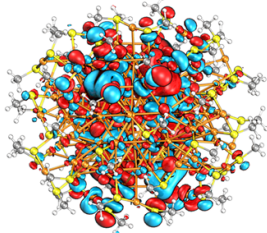
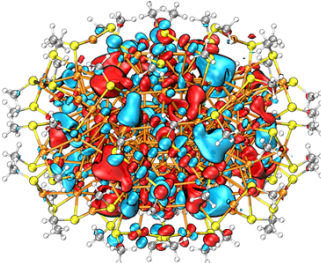
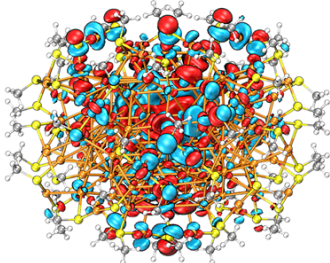
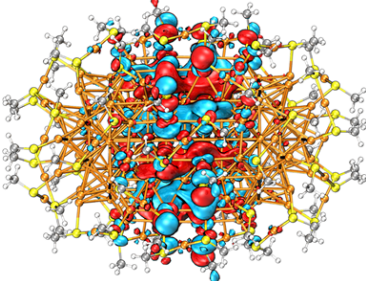
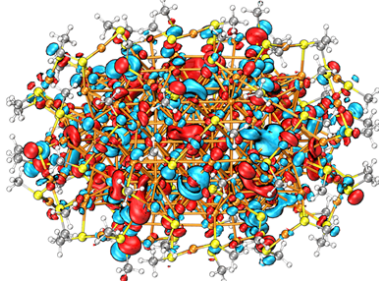
Clusters	HOMO	LUMO	H-L gap/eV
$\text{Au}_{99}(\text{SR})_{40}$			<i>Alpha:</i> 0.022 <i>Beta:</i> 0.479
$\text{Au}_{130}(\text{SR})_{50}$			0.308
$\text{Au}_{161}(\text{SR})_{60}$			<i>Alpha:</i> 0.030 <i>Beta:</i> 0.038
$\text{Au}_{192}(\text{SR})_{70}$			0.011

Figure S4. Molecular Orbital Diagrams of $\text{Au}_{99+31n}(\text{SR})_{40+10n}$ cluster sequence. It is worth mentioning that in the energy calculations, the unrestricted open-shell method was adopted for $\text{Au}_{99}(\text{SR})_{40}$ and $\text{Au}_{161}(\text{SR})_{50}$, where only their alpha orbital isosurface plots are presented here. This is sufficient to demonstrate the fact that both their HOMO and LUMO are predominantly contributed by the atomic orbitals of Au. In the orbital isosurfaces, cyan and red colors represent the positive and negative phases of the orbitals, respectively. The atomic color codes: orange, yellow, gray, and white correspond to Cu, S, C, and H atoms, respectively.

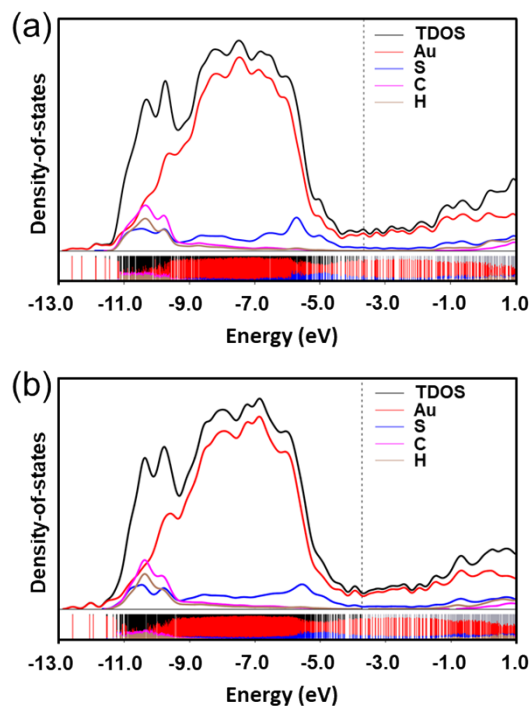


Figure S5. The comparison of PDOS between $\text{Au}_{192}(\text{SCH}_3)_{70}$ and $\text{Au}_{191}(\text{SCH}_3)_{66}$ clusters.

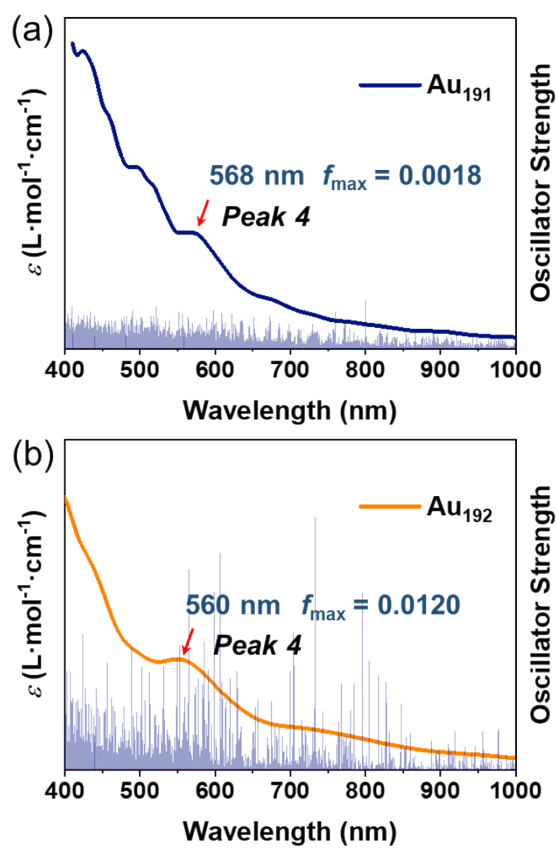


Figure S6. The comparison of calculated UV-Vis between $\text{Au}_{192}(\text{SCH}_3)_{70}$ and $\text{Au}_{191}(\text{SCH}_3)_{66}$ clusters.

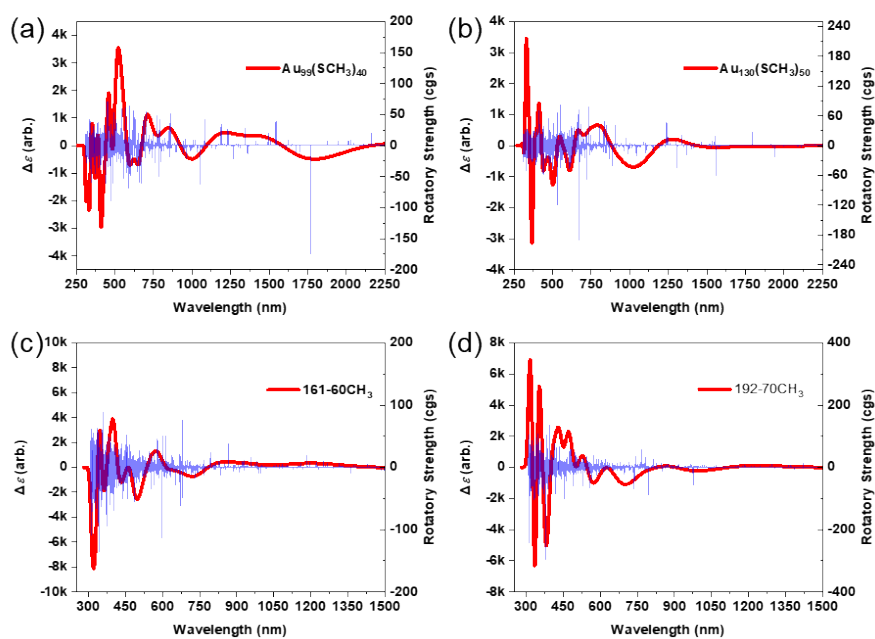


Figure S7. Simulated ECD spectra of the $\text{Au}_{99+31n}(\text{SR})_{40+10n}$ cluster sequence.

Table S2. The Cartesian coordinates of Au₉₉(SR)₄₀.

Atoms	x	y	z	Atoms	x	y	z
Au	5.4707	0.9359	2.5654	C	-1.8246	6.1731	5.8854
Au	3.8725	3.2552	3.6633	C	-5.6485	-6.5281	4.0095
Au	3.7707	0.5336	5.0576	C	-1.8293	-3.6075	7.6996
Au	3.7707	-4.6425	2.0905	C	-5.5948	-5.8764	-4.9726
Au	5.4927	-2.1261	1.7089	C	-1.7567	-8.4521	-1.1186
Au	3.8564	-2.4693	4.2513	C	-5.6628	2.8913	-7.0792
Au	3.9011	-0.4657	-4.8580	C	-1.7581	-1.5847	-8.3735
Au	3.7853	2.5566	-4.3950	C	-5.6434	7.6507	0.5587
Au	5.4903	0.7885	-2.5916	C	-1.7946	7.4598	-4.0999
Au	3.8604	4.4999	-1.9719	C	-8.9406	3.2870	0.2168
Au	3.7743	4.9746	1.0497	C	-5.3412	6.1512	4.8785
Au	5.5008	2.7124	-0.1252	C	-8.9066	0.7100	2.9615
Au	3.8713	-4.7936	-1.0385	C	-5.3701	-2.7040	7.3286
Au	3.8037	-3.3924	-3.7649	C	-5.2674	-7.8693	-0.2950
Au	5.4995	-2.2745	-1.4725	C	-8.9044	-2.7360	1.5907
Au	-5.5014	1.1498	2.4357	C	-5.3037	-2.0926	-7.5846
Au	-3.9016	0.2694	4.8716	C	-8.9051	-2.5737	-2.1106
Au	-3.7979	3.1865	3.9479	C	-5.3135	6.4953	-4.3760
Au	-3.7847	4.7461	-1.7921	C	-8.8673	1.1633	-2.7850
Au	-5.5097	2.6864	-0.2931	C	8.8908	0.2849	-3.0142
Au	-3.8719	4.7423	1.2658	C	5.3772	-3.7743	-6.8287
Au	-3.8481	-3.1014	-3.8225	C	8.9141	-2.9446	-1.1608
Au	-3.7527	-4.9234	-1.3564	C	5.2817	-7.7171	1.5398
Au	-5.4839	-2.3849	-1.3603	C	5.3088	-0.8919	7.8108
Au	-3.8570	-4.5824	1.7640	C	8.9154	-2.2067	2.4775
Au	-3.7921	-2.7836	4.2437	C	5.2942	7.0929	3.3401
Au	-5.4886	-2.0320	1.8115	C	8.8693	1.5931	2.5680
Au	-3.8779	2.6471	-4.1243	C	5.3176	5.3626	-5.7495
Au	-3.7671	-0.2622	-5.0835	C	8.9358	3.2800	-0.6955
Au	-5.4699	0.5156	-2.6852	H	6.3343	7.1204	-2.4728
Au	4.6514	-0.0005	0.0106	H	5.8954	7.1129	-0.7335
Au	3.0602	1.8534	-1.6269	H	5.6159	8.5947	-1.7216
Au	3.0767	2.1309	1.2540	H	2.5471	8.7767	3.0218
Au	3.0588	-0.5342	2.4136	H	2.1921	7.0072	3.0483
Au	3.0810	-2.4534	0.2510	H	0.9723	8.1759	3.6506
Au	3.0930	-0.9767	-2.2527	H	5.7159	1.0454	-8.6274
Au	1.5541	0.9460	-3.9328	H	6.4222	-0.1473	-7.4739
Au	1.4238	3.7436	-3.2798	H	5.9649	1.4921	-6.9011
Au	1.5356	4.0333	-0.3252	H	2.2369	5.0515	-5.7603
Au	1.4248	4.2702	2.5470	H	1.0082	5.9630	-6.6963
Au	1.5370	1.5586	3.7382	H	2.5777	5.5378	-7.4649

Au	1.4125	-1.0911	4.8600	H	5.6705	-7.9252	-3.6459
Au	1.5375	-3.0662	2.6446	H	6.3682	-7.2142	-2.1423
Au	1.4321	-4.9417	0.4602	H	5.9529	-6.1497	-3.5272
Au	1.5616	-3.4377	-2.1062	H	2.6341	-5.2812	-7.5901
Au	1.4573	-1.9451	-4.5713	H	2.2503	-3.8397	-6.5739
Au	-4.6533	-0.0144	-0.0163	H	1.0541	-4.4412	-7.7668
Au	-3.0889	1.9100	-1.5656	H	5.6052	-5.9317	6.4495
Au	-3.0537	-0.9073	-2.3022	H	6.3313	-4.2988	6.2112
Au	-3.0753	-2.4706	0.1266	H	5.8867	-5.2956	4.7861
Au	-3.0893	-0.6246	2.3725	H	0.9700	-8.7203	1.8607
Au	-3.0701	2.0727	1.3263	H	2.5188	-8.8877	2.7603
Au	-1.5453	4.0248	-0.2870	H	2.2304	-7.4557	1.6991
Au	-1.4401	3.8215	-3.1658	H	6.3577	4.5632	5.9542
Au	-1.5421	0.9607	-3.9307	H	5.9288	2.8997	6.4770
Au	-1.4046	-1.8276	-4.6365	H	5.6665	4.2885	7.5974
Au	-1.5261	-3.4385	-2.1423	H	2.5319	-0.1494	9.2988
Au	-1.4200	-4.9570	0.3060	H	2.2098	-0.7159	7.6160
Au	-1.5504	-3.0738	2.6090	H	0.9648	-0.9305	8.8898
Au	-1.4518	-1.2240	4.8172	H	-6.4215	0.9674	7.4181
Au	-1.5605	1.5308	3.7465	H	-5.9761	2.5013	6.5976
Au	-1.4341	4.1967	2.6700	H	-5.7197	2.3276	8.3713
Au	0.1918	5.8727	-1.9231	H	-2.2536	5.8712	4.9196
Au	-0.2164	6.1027	0.9962	H	-1.0312	6.9167	5.7122
Au	-0.2057	2.8446	-5.4900	H	-2.6025	6.6069	6.5309
Au	0.1922	3.6534	4.9921	H	-5.9397	-5.5520	4.4210
Au	-0.2208	0.9461	6.1124	H	-5.6580	-7.2897	4.8046
Au	0.2213	-0.0011	-6.1839	H	-6.3495	-6.8116	3.2088
Au	-0.1706	-4.3390	-4.4006	H	-1.0445	-3.2061	8.3589
Au	0.2291	-5.8702	-1.8984	H	-2.6235	-4.0651	8.3085
Au	0.1829	-3.6111	5.0154	H	-2.2399	-2.7925	7.0875
Au	-0.2157	-5.5089	2.7796	H	-5.8682	-5.9821	-3.9139
Au	2.5348	7.3783	-0.3786	H	-5.5880	-6.8645	-5.4603
S	3.9523	6.9228	-2.2291	H	-6.3197	-5.2164	-5.4732
S	1.0027	8.1905	1.2483	H	-0.9639	-8.9114	-0.5082
Au	2.5860	1.8873	-7.1213	H	-2.5072	-9.2116	-1.3836
S	4.0358	0.0065	-7.2417	H	-2.2239	-7.6366	-0.5490
S	1.0392	3.6691	-7.4079	H	-5.9356	1.8521	-6.8492
Au	2.5862	-6.1760	-4.0294	H	-5.6798	3.0528	-8.1690
S	3.9881	-6.9004	-2.2528	H	-6.3719	3.5740	-6.5860
S	1.0689	-5.8670	-5.8339	H	-2.1975	-1.8867	-7.4123
Au	2.5243	-5.7232	4.6715	H	-0.9540	-2.2868	-8.6420
S	3.9483	-4.2666	5.8952	H	-2.5265	-1.5860	-9.1608
S	0.9955	-7.3362	3.8247	H	-5.9214	7.1154	-0.3595

Au	2.5585	2.6449	6.8906	H	-5.6472	8.7371	0.3772
S	3.9742	4.2633	5.8764	H	-6.3576	7.3999	1.3577
S	1.0135	1.3620	8.1673	H	-2.2358	6.4539	-4.0768
Au	-2.6008	2.9487	6.7511	H	-0.9988	7.4892	-4.8597
S	-4.0365	1.0976	7.1561	H	-2.5639	8.2092	-4.3413
S	-1.0584	4.7563	6.7607	H	-9.6375	3.7589	0.9257
Au	-2.5721	-5.4925	4.9284	H	-8.7735	2.2400	0.4940
S	-3.9700	-6.4829	3.2805	H	-9.3596	3.3423	-0.7991
S	-1.0549	-4.9065	6.6625	H	-4.6449	6.4913	4.1004
Au	-2.5049	-6.3777	-3.7457	H	-4.8689	6.2322	5.8685
S	-3.9359	-5.1285	-5.1729	H	-6.2551	6.7652	4.8560
S	-0.9743	-7.8391	-2.6588	H	-9.6260	0.1301	3.5596
Au	-2.5672	1.5473	-7.2205	H	-8.6407	0.1575	2.0519
S	-3.9864	3.2993	-6.4669	H	-9.3534	1.6793	2.6942
S	-1.0136	0.0886	-8.2781	H	-4.6782	-1.8540	7.4041
Au	-2.5582	7.3445	-0.7551	H	-4.8979	-3.6119	7.7333
S	-3.9754	7.1748	1.1431	H	-6.2912	-2.4880	7.8909
S	-1.0295	7.8966	-2.4916	H	-4.7830	-8.5327	-1.0268
S	-7.3718	4.2315	0.2011	H	-6.1810	-8.3502	0.0884
Au	-6.5839	4.2830	2.4137	H	-4.5798	-7.6595	0.5359
S	-5.8175	4.3988	4.6363	H	-9.6080	-3.5104	1.2507
S	-7.4232	1.0683	3.9753	H	-8.6701	-2.0532	0.7655
Au	-6.6045	-0.9983	4.7367	H	-9.3540	-2.1774	2.4240
S	-5.8267	-3.0524	5.5888	H	-6.2145	-2.5924	-7.9496
S	-5.7540	-6.3363	-1.1723	H	-4.6177	-2.8343	-7.1547
Au	-6.5505	-4.9025	0.5175	H	-4.8140	-1.5659	-8.4170
S	-7.3926	-3.5400	2.2397	H	-8.7353	-1.5781	-1.6845
S	-5.7932	-0.8315	-6.3494	H	-9.3225	-3.2411	-1.3426
Au	-6.5605	-2.0540	-4.4906	H	-9.6057	-2.5075	-2.9573
S	-7.3378	-3.3309	-2.6801	H	-4.6208	5.8464	-4.9281
S	-5.7972	5.7585	-2.7705	H	-4.8361	7.4635	-4.1638
Au	-6.5794	3.5962	-3.2838	H	-6.2255	6.6574	-4.9704
S	-7.4135	1.4718	-3.8551	H	-8.5791	1.1019	-1.7278
S	7.4181	0.4695	-4.0881	H	-9.3059	0.2074	-3.1076
Au	6.6080	-1.6921	-4.5253	H	-9.6035	1.9682	-2.9299
S	5.8366	-3.8534	-5.0573	H	9.3243	1.2888	-2.8913
S	7.3999	-3.8326	-1.6798	H	9.6236	-0.3711	-3.5085
Au	6.5686	-4.9303	0.2259	H	8.6172	-0.1259	-2.0342
S	5.7797	-6.0579	2.1353	H	4.9068	-4.7343	-7.0900
S	5.7966	0.1649	6.3963	H	6.2970	-3.6445	-7.4188
Au	6.5699	-1.3277	4.7503	H	4.6831	-2.9473	-7.0319
S	7.3465	-2.8654	3.1548	H	9.3345	-2.4740	-2.0611
S	5.7836	6.1276	1.8616	H	9.6368	-3.6688	-0.7562

Au	6.5762	4.0704	2.6918	H	8.6894	-2.1767	-0.4105
S	7.4138	2.0584	3.5775	H	4.7944	-8.2374	2.3774
S	5.8002	3.6660	-5.2535	H	6.1901	-8.2655	1.2449
Au	6.5775	3.8836	-3.0419	H	4.5931	-7.6500	0.6863
S	7.3500	4.1828	-0.8442	H	6.2203	-1.3287	8.2476
Au	1.4712	-0.0010	0.0025	H	4.6226	-1.6910	7.5009
Au	-1.4699	-0.0034	-0.0042	H	4.8201	-0.2436	8.5532
Au	-0.0053	1.8884	-1.6086	H	9.3338	-2.9861	1.8239
Au	0.0002	2.1082	1.3038	H	9.6147	-2.0094	3.3046
Au	-0.0079	-0.5825	2.4169	H	8.7469	-1.2900	1.9004
Au	0.0048	-2.4683	0.1892	H	6.2044	7.3444	3.9054
Au	0.0126	-0.9452	-2.2997	H	4.6026	6.5303	3.9812
C	5.6171	7.4933	-1.7259	H	4.8137	8.0169	2.9858
C	1.7659	8.0098	2.9060	H	9.3064	0.6954	3.0299
C	5.7028	0.6780	-7.5891	H	9.6062	2.4100	2.5943
C	1.8032	5.2039	-6.7586	H	8.5831	1.3758	1.5311
C	5.6637	-7.0535	-2.9734	H	4.8495	5.2962	-6.7425
C	1.8400	-4.7382	-7.0556	H	6.2291	5.9773	-5.8137
C	5.6101	-5.0305	5.8156	H	4.6172	5.8090	-5.0315
C	1.7673	-8.1751	2.3891	H	8.7921	2.1986	-0.8000
C	5.6510	3.9606	6.5457	H	9.3425	3.5070	0.3015
C	1.7660	-0.2732	8.5188	H	9.6313	3.6448	-1.4663
C	-5.7068	1.8046	7.4019				

Table S3. The Cartesian coordinates of Au₁₆₁(SCH₃)₆₀.

Atoms	x	y	z	Atoms	x	y	z
Au	1.4664	1.3524	3.8823	C	-8.6430	-6.9184	2.9483
Au	1.4231	-1.4510	4.8659	C	-5.0342	-4.9643	7.0241
Au	1.4728	-3.3790	-2.3403	C	-8.3286	-7.6780	-1.3072
Au	1.4121	-1.6985	-4.7846	C	-8.3181	-1.1676	-7.6580
Au	1.4751	1.1824	-3.9386	H	-0.0781	4.5957	8.7513
Au	1.4395	4.0327	-3.0765	H	-1.7528	4.4611	8.1213
Au	1.4781	4.1088	-0.0898	H	-1.1133	6.0578	8.6388
Au	7.6439	0.0043	-0.0026	H	-2.3084	8.9172	3.3552
Au	5.9443	-0.5823	2.3758	H	-3.5247	9.3149	4.6155
Au	5.9464	-2.4326	0.1703	H	-4.0278	9.1885	2.8934
Au	5.9301	-0.9166	-2.2760	H	-0.0423	9.7637	-1.6761
Au	5.9560	1.8643	-1.5737	H	-1.7136	9.1130	-1.7270
Au	5.9263	2.0766	1.3045	H	-1.0904	10.0982	-3.0939
Au	4.4300	1.4422	3.7753	H	-3.9902	5.5968	-7.8429
Au	4.3014	-1.2160	4.8553	H	-2.2686	5.9416	-7.4415
Au	4.4484	-3.1361	2.5373	H	-3.4774	7.2697	-7.4273
Au	4.3176	-4.9856	0.3395	H	-4.0290	-5.7524	-7.7295
Au	4.4407	-3.3850	-2.2042	H	-2.3090	-5.2617	-7.9380
Au	4.2859	-1.8782	-4.6440	H	-3.5198	-4.8481	-9.1984
Au	4.4372	1.0454	-3.8974	H	-0.0671	1.3869	-9.7944
Au	4.3216	3.8340	-3.2036	H	-1.7447	1.1302	-9.2104
Au	4.4422	4.0298	-0.2042	H	-1.0987	0.1310	-10.556
Au	4.2860	4.2452	2.6579	H	-3.9935	-9.1285	3.0763
Au	1.4813	-3.2745	2.4923	H	-2.2749	-9.1798	2.5401
Au	1.4116	4.1803	2.8779	H	-3.4909	-	1.7624
						10.2486	
Au	1.4322	-5.0727	0.1251	H	-1.0982	-9.9874	-3.4281
Au	-1.4697	-3.3935	2.3248	H	-0.0692	-8.8677	-4.3811
Au	-1.4260	-1.7186	4.7770	H	-1.7421	-8.3909	-3.9415
Au	-1.4822	1.1576	3.9481	H	-2.3025	-0.4315	9.5168
Au	-1.4358	4.0106	3.1044	H	-3.5141	-1.5124	10.2841
Au	-1.4711	4.1058	0.1159	H	-4.0237	0.0853	9.6345
Au	-1.4069	4.2006	-2.8494	H	-1.0897	-6.3450	8.4458
Au	-1.4709	1.3761	-3.8734	H	-0.0586	-6.9024	7.0862
Au	-1.4346	-1.4295	-4.8695	H	-1.7359	-6.3493	6.7696
Au	-1.4796	-3.2598	-2.5077	H	3.9916	5.5372	7.8791
Au	-1.4170	-5.0751	-0.1569	H	2.2725	5.8956	7.4794
Au	-7.6437	0.0060	-0.0066	H	3.4887	7.2172	7.4807
Au	-5.9445	-0.9355	2.2583	H	1.7266	9.1003	1.7928
Au	-5.9476	1.8608	1.5769	H	1.0847	10.0791	3.1557
Au	-5.9252	2.0895	-1.2947	H	0.0523	9.7421	1.7270

Au	-5.9540	-0.5663	-2.3742	H	4.0373	9.2087	-2.8319
Au	-5.9309	-2.4412	-0.1813	H	2.3177	8.9402	-3.2938
Au	-4.4359	-3.3995	2.1845	H	3.5327	9.3463	-4.5526
Au	-4.3042	-1.8989	4.6295	H	0.0724	4.6584	-8.7135
Au	-4.4480	1.0215	3.9009	H	1.7517	4.5284	-8.0937
Au	-4.3194	3.8141	3.2265	H	1.0995	6.1257	-8.5935
Au	-4.4366	4.0317	0.2278	H	4.0036	0.1345	-9.6305
Au	-4.2783	4.2654	-2.6306	H	2.2822	-0.3822	-9.5141
Au	-4.4318	1.4655	-3.7631	H	3.4929	-1.4596	- 10.2882
Au	-4.3170	-1.1919	-4.8546	H	0.0806	-8.8946	4.3258
Au	-4.4465	-3.1259	-2.5530	H	1.7535	-8.4071	3.8967
Au	-4.2945	-4.9933	-0.3715	H	1.1189	-10.002	3.3678
Au	-1.4397	-0.0026	0.0005	H	3.5154	- 10.2383	-1.8114
Au	-4.3685	0.0003	-0.0012	H	4.0175	-9.1133	-3.1217
Au	-2.8984	-0.8820	2.3496	H	2.2991	-9.1675	-2.5861
Au	-2.8943	-2.5082	-0.1083	H	1.7333	1.0811	9.2221
Au	-2.9004	-0.6706	-2.4178	H	1.0850	0.0781	10.5640
Au	-2.8897	2.0908	-1.3854	H	0.0561	1.3381	9.8056
Au	-2.9000	1.9597	1.5631	H	3.5095	-4.8994	9.1704
Au	1.4394	-0.0024	0.0005	H	4.0207	-5.7929	7.6959
Au	-0.0009	-0.7951	2.4171	H	2.2993	-5.3077	7.9078
Au	0.0020	-2.5420	-0.0053	H	0.0539	-6.8777	-7.1260
Au	-0.0031	-0.7796	-2.4190	H	1.7256	-6.3231	-6.7827
Au	0.0055	2.0577	-1.4878	H	1.1023	-6.3107	-8.4676
Au	-0.0039	2.0472	1.5012	H	9.4065	-4.1753	5.9210
Au	8.3590	-2.1855	-1.6618	H	8.8671	-5.2041	4.5604
Au	6.7867	-4.7032	-1.1296	H	8.7695	-5.8284	6.2394
Au	6.6595	-3.3317	-3.8816	H	4.3543	-8.8699	1.9524
Au	6.6781	2.6259	-4.3541	H	5.8680	-8.8177	2.9253
Au	8.3836	0.8134	-2.6087	H	5.4747	-7.4921	1.7685
Au	6.7544	-0.4020	-4.8549	H	9.3589	4.3689	5.8679
Au	6.7538	3.1654	3.6941	H	8.8177	2.7591	6.4269
Au	6.6668	0.4303	5.0824	H	8.6837	4.1724	7.5250
Au	8.3778	0.8464	2.5995	H	4.3194	-0.8809	9.0444
Au	6.7756	-2.5157	4.1489	H	5.8278	0.0658	9.3063
Au	6.6853	-4.6857	1.9684	H	5.4444	-0.6185	7.6831
Au	8.3639	-2.2053	1.6148	H	8.8650	6.8914	-0.5932
Au	6.7876	4.4678	-1.8449	H	8.7843	8.3716	-1.6030
Au	6.6574	4.9735	1.1880	H	9.4150	6.8344	-2.2951
Au	8.3487	2.7533	0.0643	H	5.8055	8.8948	2.8173
Au	3.0636	-5.8779	-2.1463	H	5.4207	7.1410	2.9811

Au	2.7735	-4.3368	-4.5813	H	4.2836	8.3612	3.6166
Au	3.0652	-3.8650	4.9210	H	9.3717	-0.0835	-7.3143
Au	2.8005	-5.6961	2.6943	H	8.8287	1.5434	-6.8092
Au	2.7780	0.8026	6.2524	H	8.6977	1.0580	-8.5320
Au	3.0422	3.4892	5.1939	H	5.8629	5.4056	-7.5547
Au	2.7764	6.2006	1.1615	H	5.4673	5.0122	-5.8406
Au	3.0767	6.0210	-1.7130	H	4.3561	6.0325	-6.7956
Au	3.0489	0.2267	-6.2528	H	9.4114	-6.9028	-2.1682
Au	2.7994	3.0214	-5.5240	H	8.8542	-5.9480	-3.5744
Au	4.3687	-0.0005	-0.0001	H	8.7605	-7.7390	-3.6232
Au	2.8967	-0.6849	2.4147	H	5.8071	-5.5620	-7.4883
Au	2.8994	-2.5074	0.0969	H	5.4209	-4.0425	-6.5981
Au	2.8932	-0.8666	-2.3552	H	4.2871	-4.6601	-7.8308
Au	2.9018	1.9695	-1.5514	H	-8.8745	-5.1857	-4.5665
Au	2.8915	2.0817	1.3984	H	-8.7902	-5.7844	-6.2552
Au	-2.7830	-5.6844	-2.7333	H	-9.4173	-4.1335	-5.9079
Au	-3.0743	-3.8380	-4.9441	H	-5.4438	-7.4991	-1.8165
Au	0.1783	-5.8482	-2.5132	H	-4.3130	-8.8657	-2.0184
Au	-0.1891	-4.1805	-4.8091	H	-5.8327	-8.8183	-2.9821
Au	-2.7832	-4.3534	4.5600	H	-8.6802	4.2101	-7.5090
Au	-3.0475	-5.8896	2.1162	H	-9.3568	4.4114	-5.8532
Au	0.1774	-4.2007	4.7865	H	-8.8174	2.7994	-6.4080
Au	-0.1611	-5.8587	2.4795	H	-5.4615	-0.5804	-7.6720
Au	-3.0673	0.1930	6.2552	H	-4.3496	-0.8415	-9.0445
Au	-2.8031	2.9880	5.5448	H	-5.8553	0.1144	-9.2880
Au	-0.1798	0.5419	6.3460	H	-8.7553	8.3857	1.6545
Au	0.1569	3.2450	5.4672	H	-9.4066	6.8507	2.3321
Au	-3.0670	6.0074	1.7543	H	-8.8480	6.9134	0.6338
Au	-2.7663	6.2077	-1.1199	H	-5.4015	7.1746	-2.9285
Au	-0.1843	6.2016	1.4379	H	-4.2611	8.3992	-3.5499
Au	0.1935	6.2160	-1.3988	H	-5.7833	8.9274	-2.7474
Au	-2.7911	0.8357	-6.2420	H	-8.8617	1.4995	6.7603
Au	-3.0412	3.5192	-5.1733	H	-8.7637	1.0077	8.4829
Au	0.1634	0.5773	-6.3346	H	-9.4070	-0.1330	7.2481
Au	-0.1563	3.2793	-5.4452	H	-4.3534	5.9879	6.8322
Au	-8.3517	-2.2425	-1.5864	H	-5.8664	5.3679	7.5844
Au	-6.7891	-2.4986	-4.1376	H	-5.4727	4.9862	5.8672
Au	-6.6682	-4.7019	-1.9881	H	-8.8322	-6.0180	3.5425
Au	-6.6714	-3.3562	3.8380	H	-8.7053	-7.8077	3.5856
Au	-8.3805	-2.2097	1.5973	H	-9.3785	-6.9785	2.1367
Au	-6.7660	-4.7313	1.0976	H	-4.3227	-4.6685	7.8056
Au	-6.7833	4.4626	1.8699	H	-5.8333	-5.5805	7.4501
Au	-6.6507	4.9890	-1.1586	H	-5.4462	-4.0631	6.5569

Au	-8.3544	2.7538	-0.0540	H	-9.2656	-8.1411	-0.9787
Au	-6.7455	3.2035	-3.6782	H	-7.6360	-7.5948	-0.4618
Au	-6.6740	0.4656	-5.0671	H	-7.8802	-8.2813	-2.1033
Au	-8.3809	0.8968	-2.5873	H	-7.6152	-1.9277	-7.2984
Au	-6.7759	-0.4290	4.8334	H	-7.8816	-0.6190	-8.4990
Au	-6.6841	2.6082	4.3617	H	-9.2522	-1.6441	-7.9755
Au	-8.3664	0.8220	2.6056	S	-	-3.8044	1.8483
					10.2324		
S	-0.1845	5.4257	6.5058	Au	-9.4854	-4.8219	-0.1321
Au	-1.9897	6.0798	5.1360	S	-	-2.7716	-2.9330
					10.3258		
S	-3.7578	7.0267	3.8814	Au	-9.4941	-1.3026	-4.5690
S	-0.1493	7.8789	-3.1518	S	-8.6860	6.0975	-1.9488
Au	-1.9526	6.7698	-4.1930	Au	-9.4641	4.0251	-2.7567
S	-3.7174	5.8619	-5.4810	S	-	2.0372	-3.7511
					10.2233		
S	-3.7610	-3.4206	-7.2658	S	-8.7423	3.6799	5.1343
Au	-1.9891	-1.9213	-7.7254	Au	-9.4990	3.7667	2.9014
S	-0.1794	-0.5925	-8.4483	S	-	4.0671	0.7046
					10.2764		
S	-3.7295	-7.9702	1.0000	S	-8.7098	-3.7792	5.1253
Au	-1.9654	-7.9443	-0.5764	Au	-9.4921	-1.6390	4.5163
S	-0.1649	-8.2240	-2.0746	S	-	0.5265	4.0876
					10.2998		
S	-3.7487	-1.5190	7.8810	C	-	-2.9365	1.4814
					11.7991		
Au	-1.9796	-3.0070	7.3731	C	-	-1.9089	-2.1212
					11.7205		
S	-0.1708	-4.5102	7.1812	C	-8.2629	7.0106	-3.4785
S	3.7234	5.8282	5.5199	C	-	1.5829	-2.9599
					11.8079		
Au	1.9584	6.7422	4.2371	C	-8.3493	5.4256	5.5201
S	0.1555	7.8548	3.2000	C	-	2.9979	0.4864
					11.7446		
S	3.7664	7.0531	-3.8339	C	-8.3009	-3.5943	6.8999
Au	1.9956	6.1149	-5.0922	C	-	0.3454	3.0066
					11.7639		
S	0.1866	5.4700	-6.4616	H	-	-2.1481	0.7389
					11.6509		
Au	1.9657	-2.9749	-7.3863	H	-	-2.4960	2.4240
					12.1452		
S	3.7298	-1.4790	-7.8858	H	-	-3.6637	1.1205
					12.5352		

S	0.1833	-8.2310	2.0253	H	- 11.3851	-0.9805	-1.6503
Au	1.9866	-7.9443	0.5324	H	- 12.1182	-2.5920	-1.3629
S	3.7525	-7.9620	-1.0417	H	- 12.4952	-1.6982	-2.8665
S	0.1664	-0.6378	8.4536	H	-7.8131	7.9649	-3.1860
Au	1.9753	-1.9625	7.7187	H	-9.1905	7.1959	-4.0312
S	3.7466	-3.4592	7.2464	H	-7.5647	6.4397	-4.1013
S	0.1618	-4.4851	-7.2047	H	- 12.5340	2.3846	-3.1340
Au	5.5861	-5.6823	4.6191	H	- 11.6838	1.4122	-1.8878
S	7.0088	-4.2364	5.8331	H	- 12.1510	0.6614	-3.4443
S	4.1557	-7.3784	3.8180	H	-7.6510	5.8468	4.7878
Au	5.5394	2.6475	6.8444	H	-7.9075	5.4561	6.5216
S	6.9610	4.2513	5.8472	H	-9.2858	5.9943	5.5137
S	4.1144	1.3567	8.2104	H	- 12.5138	3.2890	1.2103
Au	5.5761	7.3236	-0.3901	H	- 11.4846	1.9434	0.6120
S	7.0173	6.8492	-2.2039	H	- 12.1125	3.1727	-0.5309
S	4.1194	8.2312	1.2293	H	-7.8595	-4.5359	7.2426
Au	5.5534	1.8796	-7.0908	H	-9.2326	-3.4057	7.4449
S	6.9735	-0.0035	-7.2322	H	-7.5997	-2.7678	7.0629
S	4.1347	3.7321	-7.4318	H	- 12.5313	-0.2309	3.5352
Au	5.5680	-6.1622	-3.9712	H	- 11.5000	-0.1490	2.0677
S	7.0126	-6.8468	-2.2282	H	- 12.1361	1.3557	2.8036
S	4.1150	-5.9489	-5.8178	S	10.2216	1.9866	3.7568
Au	-5.5853	-5.6622	-4.6475	Au	9.4715	3.9791	2.7651
S	-7.0200	-4.2056	-5.8359	S	8.7040	6.0621	1.9733
S	-4.1375	-7.3567	-3.8720	S	10.3192	3.9816	-0.7081
Au	-5.5424	2.6856	-6.8296	Au	9.4922	3.7616	-2.8977
S	-6.9591	4.2908	-5.8298	S	8.7209	3.7256	-5.1279
S	-4.1264	1.3910	-8.2006	S	8.6984	-3.7536	-5.1703
Au	-5.5603	7.3235	0.4450	Au	9.4745	-1.6052	-4.5908
S	-7.0078	6.8412	2.2521	S	10.2355	0.5844	-4.2102
S	-4.1006	8.2437	-1.1642	S	8.7472	-6.0018	1.9647

Au	-5.5828	1.8401	7.0904	Au	9.5046	-4.7535	0.1120
S	-7.0087	-0.0411	7.2102	S	10.2776	-3.6982	-1.8394
S	-4.1524	3.6808	7.4497	S	8.7061	0.0121	6.3705
Au	-5.5516	-6.1877	3.9382	Au	9.4904	-1.3460	4.6086
S	-6.9801	-6.8817	2.1871	S	10.3058	-2.8298	2.9782
S	-4.1209	-5.9653	5.8001	C	11.7940	1.5138	2.9530
S	-8.7232	-6.0322	-2.0054	C	8.2944	6.9682	3.5108
S	-8.7169	0.0436	-6.3448	C	11.7163	2.8092	-0.5612
C	-0.8628	5.0978	8.1737	C	8.3197	5.4783	-5.4707
C	-3.3521	8.7985	3.6645	C	8.2825	-3.5834	-6.9453
C	-0.8298	9.3629	-2.3246	C	11.8140	0.4775	-3.2933
C	-3.3109	6.2044	-7.2326	C	8.3603	-7.6403	1.2466
C	-3.3520	-4.9849	-8.1242	C	11.7546	-2.7155	-1.3935
C	-0.8525	0.6427	-9.6188	C	8.3019	-1.1923	7.6883
C	-3.3191	-9.2692	2.2228	C	11.7569	-2.0251	2.2089
C	-0.8500	-8.9367	-3.6149	H	12.1413	0.6001	3.4497
C	-3.3451	-0.7659	9.4999	H	12.5262	2.3158	3.0994
C	-0.8438	-6.1996	7.3879	H	11.6516	1.3217	1.8865
C	3.3164	6.1550	7.2744	H	9.2264	7.1495	4.0573
C	0.8357	9.3442	2.3822	H	7.5998	6.3952	4.1356
C	3.3611	8.8237	-3.6050	H	7.8432	7.9243	3.2262
C	0.8574	5.1600	-8.1357	H	12.1133	2.9139	0.4542
C	3.3247	-0.7171	-9.5001	H	12.4909	3.0801	-1.2869
C	0.8650	-8.9539	3.5623	H	11.3828	1.7811	-0.7290
C	3.3432	-9.2574	-2.2686	H	9.2529	6.0515	-5.4417
C	0.8403	0.5931	9.6284	H	7.6138	5.8773	-4.7333
C	3.3417	-5.0296	8.0954	H	7.8859	5.5329	-6.4746
C	0.8419	-6.1716	-7.4125	H	7.8354	-4.5261	-7.2772
C	8.6830	-4.9378	5.6067	H	9.2125	-3.4042	-7.4962
C	5.0663	-8.2205	2.4777	H	7.5842	-2.7553	-7.1123
C	8.6245	3.8356	6.4839	H	11.6830	-0.0213	-2.3299
C	5.0302	-0.1754	8.5954	H	12.1583	1.5059	-3.1342
C	8.6904	7.2799	-1.6022	H	12.5429	-0.0660	-3.9047
C	5.0086	8.1434	2.8220	H	7.9159	-8.2556	2.0359
C	8.6371	0.7109	-7.4944	H	9.2991	-8.0947	0.9107
C	5.0596	5.1917	-6.8415	H	7.6657	-7.5501	0.4035
C	8.6787	-6.8532	-2.9834	H	12.1206	-2.2596	-2.3205
C	5.0093	-4.9484	-7.0562	H	12.5219	-3.3818	-0.9838
C	-8.6956	-4.9041	-5.6097	H	11.5034	-1.9357	-0.6695
C	-5.0336	-8.2181	-2.5342	H	7.8598	-0.6399	8.5240
C	-8.6227	3.8754	-6.4673	H	9.2352	-1.6654	8.0137
C	-5.0527	-0.1349	-8.5856	H	7.6023	-1.9557	7.3289
C	-8.6736	7.2931	1.6461	H	12.1362	-2.7145	1.4465

C	-4.9879	8.1747	-2.7587	H	12.5247	-1.8629	2.9735
C	-8.6800	0.6646	7.4455	H	11.4785	-1.0745	1.7456
C	-5.0645	5.1529	6.8701				

Table S4. The Cartesian coordinates of Au₁₉₂(SCH₃)₇₀.

Atoms	x	y	z	Atoms	x	y	z
S	-1.6475	-3.7405	7.9914	C	-3.0672	-2.8200	-8.7740
Au	-0.0054	-2.0774	8.3178	H	-1.3917	-9.5644	2.9621
S	1.6371	-0.4570	8.8121	H	-3.0756	-8.9555	3.1104
S	-1.6487	-8.7548	-1.0956	H	-2.2248	-9.5961	4.5556
Au	-0.0083	-8.5509	0.5884	H	-3.8761	-5.5626	8.0830
S	1.6350	-8.5233	2.2815	H	-5.1681	-6.7903	7.9044
S	-1.6343	-1.6859	-8.6630	H	-5.6029	-5.1032	8.3275
Au	0.0097	-3.2194	-7.9461	H	-1.3858	-0.1365	10.0106
S	1.6516	-4.8208	-7.3910	H	-3.0689	0.1992	9.4782
Au	1.6190	3.7618	-5.1422	H	-2.2129	1.3719	10.5344
Au	1.3289	5.7074	-2.8973	H	-5.5507	6.3704	7.4308
Au	4.5315	3.6181	-5.1136	H	-3.8244	5.9780	7.7735
Au	4.2269	5.5420	-2.9572	H	-5.1092	5.4457	8.9023
Au	1.6209	-3.7268	-5.1680	H	-5.6110	9.0176	-3.7510
Au	1.3364	-0.9886	-6.3234	H	-3.8839	9.2507	-3.2863
Au	4.5344	-3.7419	-5.0212	H	-5.1767	10.1378	-2.4203
Au	4.2341	-1.0943	-6.1832	H	-1.3943	9.4836	3.2074
Au	1.3307	-6.3165	-1.0182	H	-3.0782	9.0886	2.7211
Au	1.6142	-6.0680	1.9467	H	-2.2138	10.4502	1.9315
Au	4.2282	-6.2183	-0.8712	H	-5.5600	-0.7805	-9.7521
Au	4.5254	-5.9331	2.0075	H	-3.8321	-0.2648	-9.7971
Au	1.3267	-2.9180	5.6938	H	-5.1144	0.8316	-
							10.3975
Au	1.6205	-0.0241	6.3726	H	-2.2268	5.0936	-9.3272
Au	4.2220	-2.7458	5.6483	H	-1.4028	6.0046	-8.0136
Au	4.5313	0.0784	6.2655	H	-3.0843	5.4156	-7.7828
Au	1.6167	6.0551	1.9852	H	-3.8869	-9.4053	-2.7959
Au	1.3307	4.5166	4.5293	H	-5.1821	-9.6096	-4.0162
Au	4.5280	5.9812	1.8606	H	-5.6132	-9.4882	-2.2801
Au	4.2269	4.5205	4.3568	H	-2.2183	-7.3044	-7.7195
Au	-4.2290	3.8655	-4.9497	H	-1.3883	-5.7773	-8.1819
Au	-4.5338	5.6592	-2.6851	H	-3.0730	-5.7337	-7.5597
Au	-1.3317	3.8356	-5.1219	H	5.5621	-9.1036	3.5700
Au	-1.6207	5.7168	-2.8198	H	3.8325	-8.9247	4.0497
Au	-4.2269	-3.5123	-5.2072	H	5.1119	-8.9851	5.3014
Au	-4.5259	-0.8009	-6.2132	H	3.0727	-4.6282	8.2779
Au	-1.3285	-3.6853	-5.2319	H	2.2109	-6.1564	8.6609
Au	-1.6136	-0.9131	-6.3088	H	1.3905	-4.5749	8.9066
Au	-4.5298	-6.1530	-1.1590	H	5.5563	0.5964	9.7700
Au	-4.2304	-6.0349	1.7296	H	3.9950	-0.9828	8.9562
Au	-1.6182	-6.2771	-1.0816	H	5.1036	2.2815	10.1828

Au	-1.3340	-6.1135	1.8855	H	1.3882	7.0623	7.0939
Au	-4.5327	-3.0030	5.4974	H	3.0717	6.4509	6.9523
Au	-4.2231	-0.2210	6.2761	H	2.2092	6.3434	8.5233
Au	-1.6217	-2.9644	5.6383	H	5.5857	9.4662	2.4364
Au	-1.3274	-0.0926	6.3966	H	3.8567	9.6105	1.9434
Au	-4.2273	5.9012	2.1445	H	5.1406	10.3794	0.9591
Au	-4.5284	4.3014	4.5547	H	1.4013	-1.5432	-9.8975
Au	-1.3312	6.0595	2.0594	H	3.0845	-1.1380	-9.4168
Au	-1.6175	4.4499	4.5587	H	2.2308	-0.1244	- 10.6277
Au	-0.0007	-4.1446	0.2891	H	5.1655	4.1210	-9.5725
Au	0.0014	-4.3323	-2.7077	H	5.5975	5.2437	-8.2432
Au	0.0002	3.1820	-2.6743	H	3.8717	4.8166	-8.5477
Au	-0.0018	5.0974	-0.3629	H	3.0814	-9.3056	-1.8424
Au	-0.0008	3.5263	2.1965	H	2.2246	- 10.1385	-3.1824
Au	0.0019	1.9170	4.7345	H	1.3977	-9.8863	-1.6055
Au	-0.0005	-1.0030	4.0304	H	5.1690	-7.8265	-6.8822
Au	2.8939	-4.0900	0.3505	H	5.6048	-6.2152	-7.5371
Au	2.8431	-4.3256	-2.6171	H	3.8779	-6.6346	-7.2295
Au	2.8990	-1.5970	-3.7813	H	1.3983	8.9319	-4.5319
Au	2.8436	1.1507	-4.9245	H	3.0809	8.5988	-3.9965
Au	2.8963	3.1013	-2.6889	H	2.2282	10.0655	-3.4090
Au	2.8384	5.0390	-0.4305	H	- 12.9907	-0.1597	-2.1652
Au	2.8941	3.5159	2.1181	H	- 13.6094	-1.7049	-2.8261
Au	2.8411	1.9621	4.6602	H	- 13.9466	-0.1689	-3.6847
Au	2.8937	-0.9289	3.9971	H	-9.0228	2.0321	-7.3083
Au	2.8364	-3.8262	3.3067	H	-9.2712	3.7765	-7.6530
Au	9.0639	-0.0002	0.0048	H	- 10.6500	2.6395	-7.7618
Au	7.3828	-2.1391	-1.1856	H	- 12.9184	1.9554	-0.7083
Au	7.3817	0.4719	-2.3978	H	- 13.6031	2.0601	-2.3604
Au	7.3764	2.4322	-0.2915	H	- 13.9376	3.3584	-1.1728
Au	7.3796	1.0305	2.2209	H	-9.0027	7.5660	-0.3349
Au	7.3730	-1.7959	1.6695	H	-9.2733	8.4532	1.2023
Au	5.8651	-4.0289	0.3946	H	- 10.6376	8.1823	0.0752

Au	5.7552	-4.3450	-2.4644	H	-9.2474	1.4623	8.4247
Au	5.8709	-1.6182	-3.7073	H	- 10.6218	2.4487	7.8381
Au	5.7570	1.0027	-4.8943	H	-8.9945	2.6602	7.1112
Au	5.8678	3.0286	-2.6861	H	- 13.9410	2.2906	2.9314
Au	5.7486	4.9680	-0.5619	H	- 12.9945	1.3787	1.7092
Au	5.8648	3.4902	2.0509	H	- 13.6231	3.0101	1.3214
Au	5.7528	2.0666	4.5519	H	-8.9824	-5.9094	4.7289
Au	5.8641	-0.8717	3.9553	H	-9.2425	-7.5356	4.0138
Au	5.7455	-3.6909	3.3757	H	- 10.6107	-6.6624	4.7694
Au	0.0026	-1.5579	-3.8539	H	- 13.9293	-2.0543	2.9685
Au	-0.0034	-3.9129	3.2836	H	- 12.9364	-1.1669	1.7646
Au	0.0019	1.2338	-4.9608	H	- 13.6176	-0.3033	3.1787
Au	-2.8935	-1.4799	-3.8308	H	-9.2496	-6.1421	-5.9404
Au	-2.8398	-4.2484	-2.7403	H	- 10.6199	-6.5913	-4.8793
Au	-2.8962	-4.0967	0.2237	H	-8.9916	-6.3275	-4.1732
Au	-2.8429	-3.9167	3.1955	H	- 13.9448	-3.5435	-1.0223
Au	-2.8952	-1.0513	3.9654	H	- 12.9846	-2.0942	-0.5765
Au	-2.8371	1.8314	4.7135	H	- 13.6245	-3.1743	0.7011
Au	-2.8952	3.4484	2.2243	H	13.6198	-3.3307	-0.2553
Au	-2.8430	5.0486	-0.2863	H	13.9446	-3.4462	1.5033
Au	-2.8962	3.1839	-2.5925	H	13.0173	-2.0561	0.8485
Au	-2.8387	1.2909	-4.8906	H	10.6351	-5.8174	5.8017
Au	-9.0634	-0.0024	0.0016	H	9.0096	-5.6768	5.0527
Au	-7.3789	-2.0101	-1.3984	H	9.2544	-5.2178	6.7711
Au	-7.3817	-1.9500	1.4790	H	13.5989	-1.2282	2.9086
Au	-7.3751	0.8051	2.3148	H	13.9316	0.4141	3.5399
Au	-7.3814	2.4450	-0.0470	H	12.9143	0.2027	2.0756
Au	-7.3761	0.7065	-2.3427	H	10.6276	3.6571	7.3245
Au	-5.8666	-1.4160	-3.7943	H	8.9931	3.0198	6.9460
Au	-5.7524	-4.1225	-2.8239	H	9.2648	4.7901	7.0697
Au	-5.8668	-4.0416	0.1749	H	9.2481	8.2104	-2.3768

Au	-5.7542	-3.9572	3.0511	H	10.6190	8.1139	-1.2293
Au	-5.8651	-1.0811	3.9011	H	8.9904	7.5521	-0.7264
Au	-5.7457	1.6799	4.7109	H	12.9880	2.1311	0.4880
Au	-5.8651	3.3758	2.2355	H	13.6164	2.4903	2.1260
Au	-5.7553	4.9948	-0.1426	H	13.9431	3.6231	0.7769
Au	-5.8697	3.1677	-2.5195	H	9.2686	0.2708	-8.5264
Au	-5.7517	1.4091	-4.7969	H	10.6443	1.3264	-8.0796
S	-1.4029	-7.4008	3.9980	H	9.0161	1.6406	-7.3933
Au	-3.2305	-6.2430	4.9119	H	13.6201	2.7616	-1.6711
S	-5.1267	-5.3421	5.9854	H	13.9376	1.7957	-3.1457
S	-1.3917	1.5178	8.2737	H	12.9557	1.1041	-1.8114
Au	-3.2141	2.7515	7.4548	H	9.2598	-8.0335	-2.9029
S	-5.1043	4.0618	6.9366	H	10.6337	-7.2754	-3.7650
S	-5.1294	7.8407	-1.7130	H	9.0049	-6.5270	-3.8456
Au	-3.2296	7.9401	-0.3203	H	13.6253	-0.7510	-3.0634
S	-1.4018	8.3397	1.0989	H	13.9397	-2.4603	-2.6309
S	-5.1116	0.7943	-7.9938	H	12.9426	-1.4292	-1.5521
Au	-3.2242	2.1635	-7.6467	H	-3.0278	-3.0177	9.8395
S	-1.4026	3.6440	-7.5880	H	-4.0057	-3.3432	8.3644
S	-5.1297	-7.3371	-3.2328	H	-3.0790	-1.8367	8.4874
Au	-3.2321	-6.5999	-4.4221	H	3.8268	1.1069	9.7384
S	-1.4021	-6.0922	-5.8038	H	3.0694	-2.3678	8.3492
S	5.1057	-6.8370	4.2220	H	3.0160	-1.9682	10.0997
Au	3.2134	-5.9275	5.2940	H	3.9919	-8.8329	1.8243
S	1.3918	-5.2217	6.5968	H	3.0687	-8.6532	0.3217
S	5.1072	1.9085	7.8079	H	3.0035	- 10.2087	1.2175
Au	3.2172	3.2104	7.2682	H	-3.0805	-8.6366	0.8678
S	1.3941	4.6656	6.9981	H	-3.0297	- 10.2883	0.1637
Au	3.2279	7.9035	-0.8157	H	-4.0069	-8.9865	-0.6028
S	5.1194	8.0044	0.5879	H	3.0374	-4.3594	-9.3172
S	1.4086	0.3395	-8.4106	H	4.0105	-4.4777	-7.8087
Au	3.2351	1.6688	-7.7685	H	3.0843	-3.0028	-8.1402
S	5.1282	3.0327	-7.4292	H	-3.0704	-3.5030	-7.9213
S	1.4059	-7.8865	-2.9304	H	-3.0007	-3.3825	-9.7119
Au	3.2335	-6.8668	-3.9955	H	-3.9909	-2.2321	-8.7458
S	5.1302	-6.1254	-5.1837	S	-1.6424	7.7198	-4.2783
S	1.4036	8.1025	-2.2810	Au	-0.0009	6.5632	-5.5179
S	-11.6993	-0.9843	-4.0694	S	1.6397	5.5376	-6.8695
Au	-10.9054	1.1423	-4.6805	S	-1.6409	6.4550	6.0137
S	-10.1417	3.2228	-5.4819	Au	0.0004	7.2776	4.5317
S	-11.7281	3.5291	-2.1495	S	1.6452	8.2457	3.1443

Au	-10.9063	4.7915	-0.3439	C	3.0770	6.5894	-6.4461
S	-10.1339	6.2149	1.3691	C	-3.0798	7.4792	-5.3864
S	-10.1246	0.6229	6.3499	C	3.0789	8.1610	4.2800
Au	-10.8937	1.8291	4.4777	C	-3.0791	7.4357	5.4462
S	-11.6991	3.1810	2.7315	H	3.9984	6.0468	-6.6836
S	-10.1240	-5.8349	2.5611	H	3.0770	6.8115	-5.3764
Au	-10.8962	-3.6766	3.1107	H	3.0187	7.5164	-7.0275
S	-11.7160	-1.5959	3.8374	H	-3.0814	6.4609	-5.7823
S	-10.1273	-4.2373	-4.7637	H	-3.0201	8.2058	-6.2044
Au	-10.8983	-4.1055	-2.5403	H	-4.0008	7.6256	-4.8119
S	-11.7088	-4.1647	-0.3339	H	3.0189	8.9963	4.9867
S	11.6894	-4.1070	0.9229	H	4.0021	8.2222	3.6938
Au	10.8944	-3.7150	3.0999	H	3.0764	7.2091	4.8164
S	10.1296	-3.5134	5.3194	H	-3.0649	7.5288	4.3580
S	11.7212	-0.3860	4.1254	H	-3.0369	8.4258	5.9140
Au	10.9017	1.7922	4.4621	H	-4.0000	6.9163	5.7333
S	10.1303	3.9571	4.9875	Au	-6.9601	5.7353	-4.6045
S	10.1261	5.9775	-2.2233	S	-8.3849	6.5934	-2.9221
Au	10.8957	4.8227	-0.3187	S	-5.5338	5.2885	-6.4404
S	11.7014	3.8454	1.6621	Au	-6.9448	6.1566	4.0342
S	10.1395	-0.2731	-6.3526	S	-8.3687	4.8261	5.3746
Au	10.9058	1.1779	-4.6605	S	-5.5232	7.7652	3.0363
S	11.7145	2.7556	-3.1159	Au	-6.9471	-1.9267	7.1047
S	10.1298	-6.1406	-1.7022	S	-8.3726	-3.6088	6.2486
Au	10.9029	-4.0819	-2.5506	S	-5.5181	-0.4877	8.3261
S	11.7279	-2.1226	-3.5556	Au	-6.9459	-7.3534	0.3515
Au	9.8138	2.1490	-1.6851	S	-8.3755	-7.0596	-1.5092
Au	8.2147	2.3617	-4.2262	S	-5.5192	-8.0734	2.0976
Au	8.1032	4.6113	-2.1744	Au	-6.9483	-2.5998	-6.8855
Au	8.1038	3.4935	3.7080	S	-8.3765	-0.7374	-7.1812
Au	9.8149	2.2797	1.5074	S	-5.5236	-4.4847	-7.0303
Au	8.2036	4.7607	0.9386	C	-	6.5609	-3.6677
					10.0549		
Au	8.2027	-4.4023	2.0439	C	-6.4446	4.1379	-7.5233
Au	8.1056	-5.0066	-0.9418	C	-	5.5356	5.1166
					10.0348		
Au	9.8185	-2.7279	0.1264	C	-6.4424	8.4368	1.6114
Au	8.2148	-3.2953	-3.5477	C	-	-3.1465	6.8403
					10.0405		
Au	8.1097	-0.6452	-5.0491	C	-6.4246	1.0820	8.5273
Au	9.8155	-0.9509	-2.5564	C	-	-7.4823	-0.8781
					10.0395		
Au	8.2098	0.5757	4.8117	C	-6.4356	-7.7891	3.6484

Au	8.0989	-2.4535	4.4735	C	- 10.0417	-1.4650	-7.3898
Au	9.8053	-0.7493	2.6362	C	-6.4419	-5.8699	-6.2798
Au	-9.8088	2.0353	-1.8210	H	- 10.2519	5.6045	-4.1643
Au	-8.2144	4.5729	-1.5915	H	- 10.1252	7.3808	-4.3914
Au	-8.1072	2.9355	-4.1632	H	- 10.7801	6.7041	-2.8569
Au	-8.1048	-3.0499	-4.0840	H	-6.8757	3.3158	-6.9417
Au	-9.8146	-1.1008	-2.5002	H	-5.7267	3.7259	-8.2430
Au	-8.2097	-0.1010	-4.8464	H	-7.2284	4.6977	-8.0449
Au	-8.2094	-2.7584	3.9827	H	- 10.0956	6.4794	5.6702
Au	-8.0998	0.0743	5.1002	H	- 10.7636	4.8155	5.5088
Au	-9.8109	-0.5722	2.6763	H	- 10.2352	5.7101	4.0538
Au	-8.2031	2.9331	3.8667	H	-6.8732	7.6284	1.0107
Au	-8.1062	4.8632	1.5115	H	-5.7295	8.9966	0.9941
Au	-9.8168	2.3496	1.3890	H	-7.2270	9.1031	1.9859
Au	-8.2081	-4.6419	-1.3996	H	- 10.1046	-3.3837	7.9082
Au	-8.1034	-4.8239	1.6386	H	- 10.7672	-3.7417	6.2733
Au	-9.8169	-2.7197	0.2690	H	- 10.2406	-2.0816	6.6798
Au	-2.9178	0.0012	-0.0015	H	-6.8601	1.4038	7.5753
Au	-5.8138	0.0001	-0.0001	H	-5.7029	1.8375	8.8611
Au	-4.3472	-2.1042	-1.3666	H	-7.2042	0.9397	9.2836
Au	-4.3467	0.6479	-2.4265	H	- 10.2366	-6.9988	0.0849
Au	-4.3493	2.5063	-0.1354	H	- 10.1000	-8.5712	-0.7707
Au	-4.3466	0.9025	2.3414	H	- 10.7710	-7.1302	-1.6161
Au	-4.3486	-1.9479	1.5804	H	-5.7196	-7.8764	4.4745
Au	-0.0002	0.0008	-0.0014	H	-7.2155	-8.5530	3.7372
Au	-1.4312	-2.1258	-1.3583	H	-6.8718	-6.7843	3.6627
Au	-1.4309	0.6334	-2.4443	H	- 10.2408	-2.2316	-6.6330
Au	-1.4330	2.5186	-0.1558	H	- 10.1029	-1.9026	-8.3927

Au	-1.4314	0.9249	2.3464	H	- 10.7715	-0.6528	-7.2825
Au	-1.4331	-1.9465	1.6020	H	-5.7283	-6.6856	-6.1124
Au	2.9178	0.0007	0.0000	H	-7.2257	-6.1863	-6.9763
Au	1.4334	-2.1518	-1.3168	H	-6.8735	-5.5734	-5.3175
Au	1.4336	0.5859	-2.4554	Au	6.9590	-2.9126	-6.7542
Au	1.4320	2.5156	-0.2031	S	8.3854	-4.4568	-5.6701
Au	1.4322	0.9692	2.3284	S	5.5350	-1.6578	-8.1686
Au	1.4309	-1.9161	1.6392	Au	6.9431	-7.3287	0.6861
Au	5.8140	0.0002	0.0018	S	8.3653	-6.7806	2.4951
Au	4.3489	-2.1506	-1.2911	S	5.5248	-8.2831	-0.9512
Au	4.3495	0.5645	-2.4448	Au	6.9479	-1.6206	7.1807
Au	4.3473	2.5007	-0.2193	S	8.3710	0.2690	7.2124
Au	4.3476	0.9816	2.3106	S	5.5207	-3.4665	7.5828
Au	4.3449	-1.8942	1.6478	Au	6.9452	6.3280	3.7599
C	-2.1073	-9.0465	3.6150	S	8.3687	6.9476	1.9756
C	-4.9082	-5.7351	7.7606	S	5.5222	6.1389	5.6422
C	-2.0988	0.6472	9.7205	Au	6.9530	5.5263	-4.8601
C	-4.8594	5.6293	7.8509	S	8.3839	4.0187	-5.9894
C	-4.9152	9.1990	-2.9224	S	5.5241	7.2575	-4.1088
C	-2.1057	9.4521	2.3711	C	10.0533	-4.0759	-6.3172
C	-4.8669	0.0642	-9.6550	C	6.4527	-0.1389	-8.5891
C	-2.1136	5.1989	-8.2423	C	10.0298	-7.2925	1.9353
C	-4.9183	-9.1476	-3.0577	C	6.4456	-8.2102	-2.5235
C	-2.1038	-6.2394	-7.4882	C	10.0403	-0.4131	7.5188
C	4.8659	-8.6509	4.2868	C	6.4294	-4.9458	7.0243
C	2.1008	-5.1340	8.2823	C	10.0355	7.0282	2.7248
C	4.8607	1.4168	9.5543	C	6.4371	5.1513	6.8725
C	2.0997	6.2977	7.4338	C	10.0498	4.7571	-5.8291
C	4.8892	9.5193	1.5904	C	6.4356	8.1321	-2.7935
C	2.1151	-0.7274	-9.7199	H	10.7807	-4.5825	-5.6705
C	4.9050	4.4546	-8.5613	H	10.2497	-2.9983	-6.3067
C	2.1112	-9.4642	-2.3261	H	10.1215	-4.4600	-7.3412
C	4.9101	-6.7612	-6.8868	H	5.7380	0.5660	-9.0309
C	2.1118	9.0158	-3.7007	H	7.2338	-0.3937	-9.3137
C	-13.2140	-0.7149	-3.0796	H	6.8879	0.3132	-7.6914
C	-9.7214	2.8730	-7.2289	H	10.7605	-6.8401	2.6172
C	-13.1940	2.6328	-1.5209	H	10.2305	-6.9515	0.9138
C	-9.7116	7.7578	0.4788	H	10.0876	-8.3857	1.9848
C	-9.6960	1.9397	7.5474	H	5.7331	-8.4142	-3.3318
C	-13.2173	2.3697	2.1125	H	7.2291	-8.9754	-2.5044
C	-9.6882	-6.5510	4.1889	H	6.8779	-7.2150	-2.6746
C	-13.1987	-1.2510	2.8225	H	10.2413	-1.2799	6.8798

C	-9.6957	-6.0068	-4.9498	H	10.1060	-0.7015	8.5741
C	-13.2173	-3.1297	-0.3150	H	10.7656	0.3789	7.2938
C	13.2221	-3.1246	0.7447	H	7.2089	-5.1737	7.7593
C	9.7069	-5.2357	5.7743	H	6.8657	-4.7825	6.0329
C	13.1888	-0.2215	3.0451	H	5.7090	-5.7707	6.9642
C	9.7032	3.8346	6.7636	H	10.7634	7.0650	1.9048
C	9.6944	7.6297	-1.5630	H	10.2368	6.1500	3.3480
C	13.2145	2.9251	1.2041	H	10.0967	7.9400	3.3296
C	9.7168	0.8647	-7.7231	H	7.2216	5.7787	7.3091
C	13.2070	2.0159	-2.3593	H	6.8675	4.2563	6.4098
C	9.7066	-7.0834	-3.2135	H	5.7218	4.8430	7.6444
C	13.2073	-1.6463	-2.5902	H	10.7793	3.9873	-6.1099
C	-3.0834	-2.8967	8.7519	H	10.2452	5.0830	-4.8017
C	3.0728	-1.5598	9.0846	H	10.1151	5.6114	-6.5123
C	3.0680	-9.1188	1.3101	H	7.2170	8.7430	-3.2586
C	-3.0849	-9.2165	-0.0581	H	6.8694	7.4204	-2.0830
C	3.0895	-4.0891	-8.2565	H	5.7174	8.7700	-2.2641