

Kernel-Differentiated Fusion Strategy Redefines Critical Size Thresholds in Giant Twinned-FCC RS-AuNCs: Unlocking Size Adaptability and Birth of Metallicity

Youqiong Fang[†], Yong Pei^{*,‡} and Lin Xiong^{*,†}

[†]School of Food and Chemical Engineering, Shaoyang University, Shaoyang 422000, People's Republic of China

[‡]Department of Chemistry, Key Laboratory for Green Organic Synthesis and Application of Hunan Province, Key Laboratory of Environmentally Friendly Chemistry and Applications of Ministry of Education, Xiangtan University, Hunan Province 411105, China

*Corresponding author: ypei2@xtu.edu.cn (Y. P.); linxiong@hnsyu.edu.cn (L. X.).

Contents

I. Computational methods and details

II. Supporting figures and tables

Figure S1. The O-symmetric Au₁₂₇-o (a) and experimentally determined Au₂₇₉(SR)₈₄ (b) clusters share a consistent shell-core structure, with both clusters containing an O_h-symmetric Au₁₃ gold core in their innermost layer.

Figure S2. (a) Structure of the D-symmetric Au₁₃ core with twinned-FCC features in the Au₁₄₆(SR)₅₇ cluster; (b) The structural transformation between O_h-symmetry Au₁₃ and D_{3h}-symmetry Au₁₃.

Figure S3. Comparison of the structures and relative energies of three Au₁₂₇(SR)₄₈ isomers.

Figure S4. Comparison of the relative energies between isomers of RS-AuNCs that have been experimentally determined.

Figure S5. The structure of the experimentally determined Au₁₉₁(SR)₆₆ cluster can be obtained using Au₂₆ (generated through a '*kernel-differentiated fusion*' strategy) as the starting nucleus, followed by a layer-by-layer growth pattern.

Table S1. The Cartesian coordinates of Au₁₂₇(SCH₃)₄₈.

Table S2. The Cartesian coordinates of Au₁₆₄(SCH₃)₆₀.

Table S3. The Cartesian coordinates of Au₁₈₂(SCH₃)₆₆.

Table S4. The Cartesian coordinates of Au₁₈₈(SCH₃)₆₆.

I. Computational methods and details

The geometric optimizations of Au₁₂₇(SR)₄₈, Au₁₆₄(SR)₆₀, Au₁₈₂(SR)₆₆, Au₁₈₈(SR)₆₆ and other related clusters are implemented in CP2K Code¹ based on the level of PBE², ³(D3BJ)⁴, ⁵/DZVP-MOLOPT-SR-GTH. To ensure the rationality of structural optimization, the sizes of cells of these clusters are set by Multiwfn software (version 3.8_dev)^{6, 7}. The convergence threshold of density matrix of inner SCF is 1.0E-06. The maximum geometry change, RMS geometry change, Maximum force and RMS force is set to 3E-3, 1.5E-3, 4.5E-4 and 3E-4, respectively. The single-point energy calculations of all clusters are implemented using the ORCA 5.0.4 program system^{8, 9} at theoretical level of PBE (D3BJ)/Def2-TZVP. All electronic excitation calculations were performed using the sTDA approach implemented in the ORCA 5.0.4 program system software at the PBE(D3BJ)/Def2-SVP¹⁰ level. 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.

It is noted that the energy threshold is set to 4 eV in sTDA calculations, 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 H in sTDA calculations.

II. Supporting figures and tables

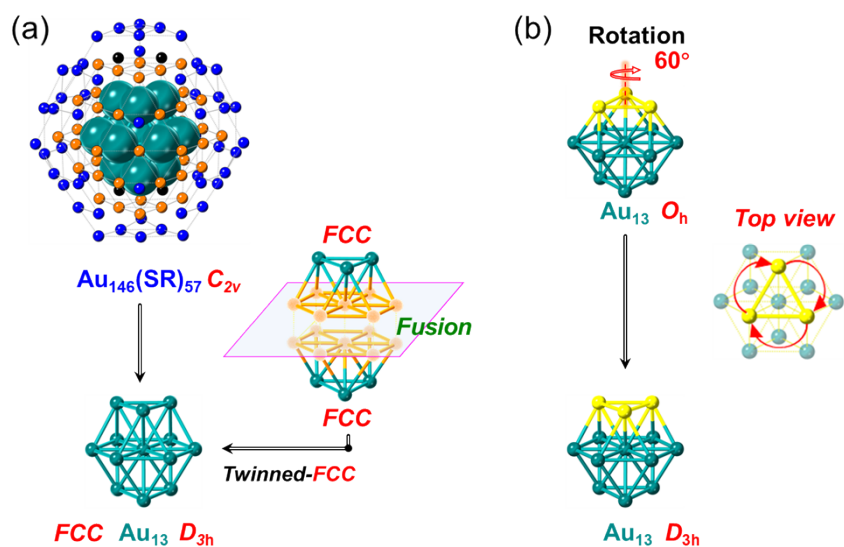
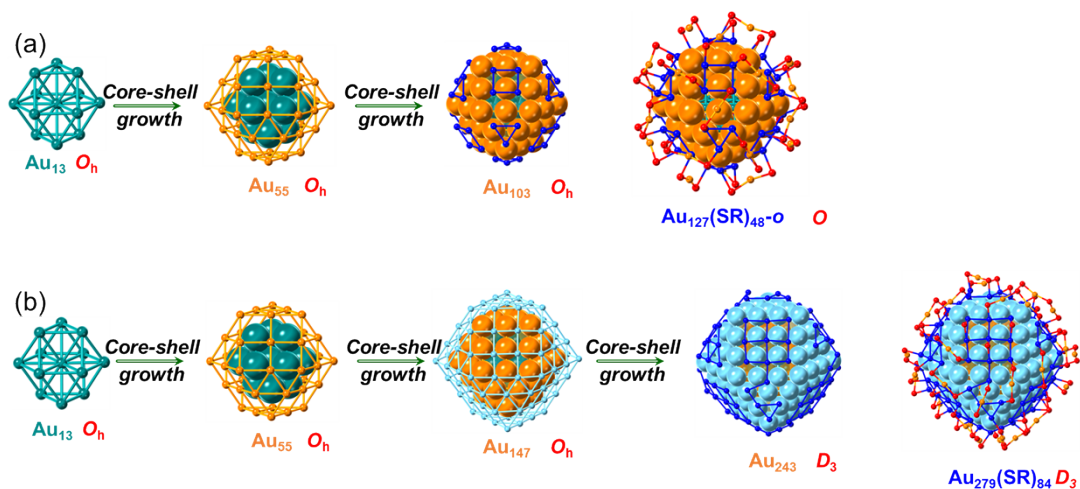


Figure S2. (a) Structure of the D -symmetric Au_{13} core with twinned-FCC features in the $\text{Au}_{146}(\text{SR})_{57}$ cluster; (b) The structural transformation between O_h -symmetry Au_{13} and D_{3h} -symmetry Au_{13} .

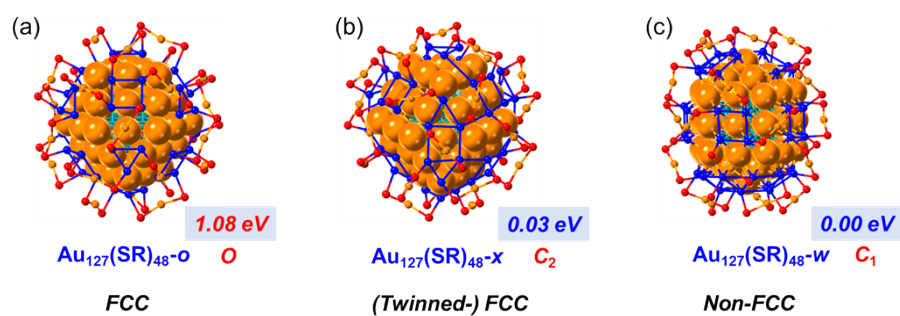


Figure S3. Comparison of the structures and relative energies of three $\text{Au}_{127}(\text{SR})_{48}$ isomers: (a) $\text{Au}_{127}\text{-o}$; (b) $\text{Au}_{127}\text{-x}$ and (c) $\text{Au}_{127}\text{-w}$. The red spheres represent S atoms, the rest are Au atoms. All R groups are omitted for clarity.

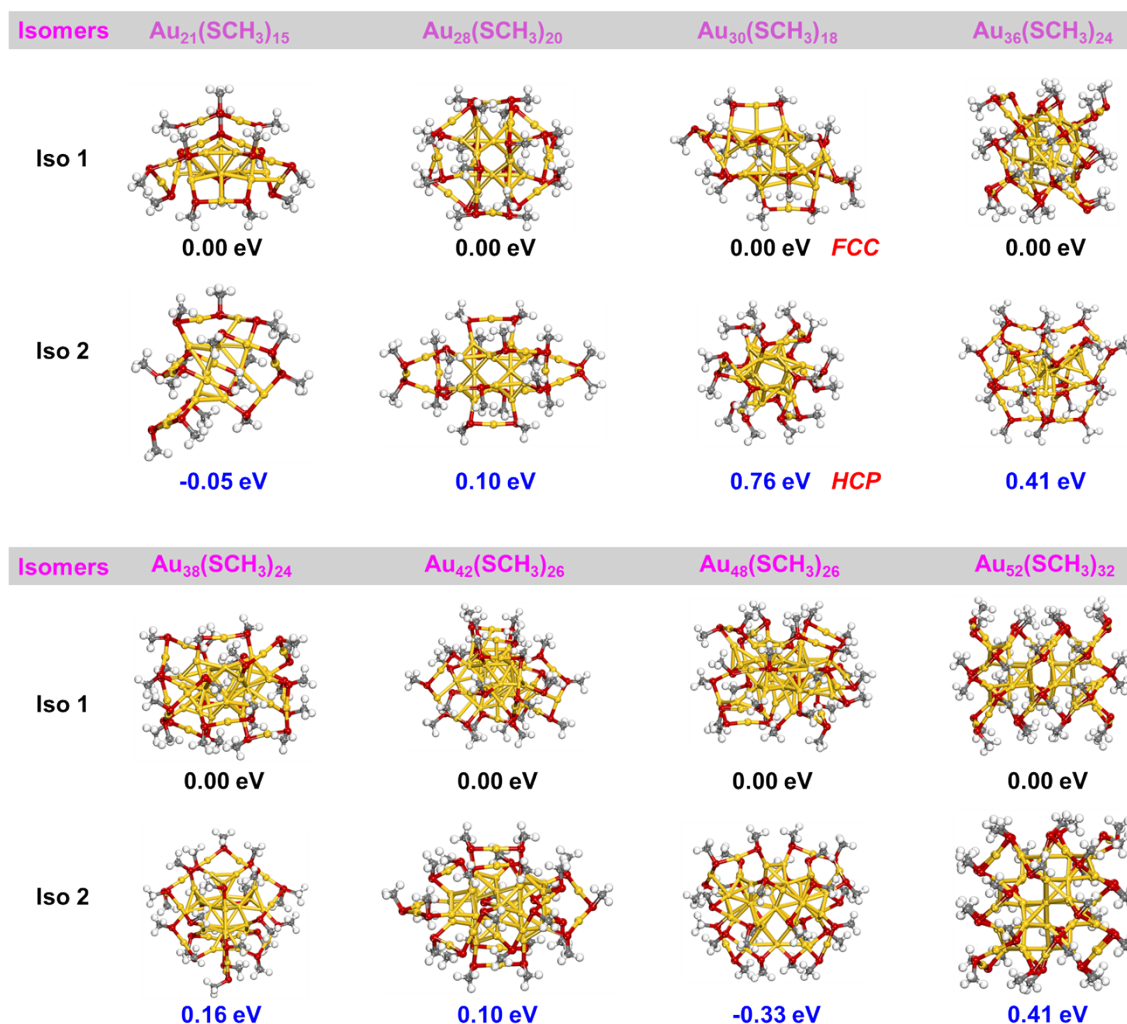


Figure S4. Comparison of the relative energies between isomers of RS-AuNCs that have been experimentally determined. Red balls, S; white balls, H; yellow balls, Au.

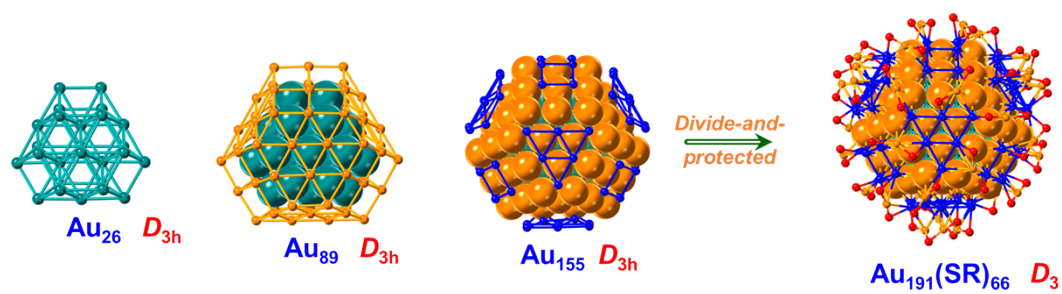


Figure S5. The structure of the experimentally determined $\text{Au}_{191}(\text{SR})_{66}$ cluster can be obtained using Au_{26} (generated through a ‘*kernel-differentiated fusion*’ strategy) as the starting nucleus, followed by a layer-by-layer growth pattern.

Table S1. The Cartesian coordinates of Au₁₂₇(SR)₄₈, R = CH₃.

Atoms	x	y	z	Atoms	x	y	z
Au	-1.496893	2.3299588	5.8590772	S	3.9501029	-6.883523	-3.815118
Au	1.4705497	-2.32256	5.8600875	S	-1.10699	-9.055253	2.2677644
Au	-2.02722	4.6853786	4.1948813	S	1.715027	-6.824526	5.3083811
Au	1.4084225	2.4630779	5.8866894	S	8.9078101	-1.971639	1.3999428
Au	1.997735	-4.677151	4.192921	S	6.7081523	-5.631933	-0.61386
Au	1.0603919	4.8247978	4.1881715	S	6.2721812	2.2550631	-5.518699
Au	-1.437383	-2.455975	5.8794842	S	8.0830906	-0.900436	-2.498592
Au	-1.085195	-4.815979	4.1807844	S	5.2118174	-3.050756	-6.393632
Au	5.6963813	-3.504139	2.777243	S	1.2986654	-5.550382	-7.337281
Au	-1.861925	6.9835733	1.0828457	S	-2.582631	-3.037526	-8.475063
Au	-6.904284	0.8735516	2.1079427	S	-3.26965	-6.335548	-5.172446
Au	6.8758705	-0.861754	2.1248063	S	-8.102313	0.9248029	-2.514934
Au	6.6895346	2.0637844	2.0762903	S	-6.277784	-2.223775	-5.53457
Au	5.3470094	-1.26548	4.8096549	S	-7.693021	-4.006578	-1.46933
Au	4.9205324	4.1947724	3.2762952	S	-6.795692	-5.701897	2.8609488
Au	-5.716053	3.5103612	2.7572184	S	-5.5751	-2.865467	6.8357869
Au	-5.223635	-1.646096	4.7661515	S	-2.42978	-6.186948	5.7019635
Au	-4.947557	-4.190703	3.2740146	S	1.6090396	1.7162586	8.2248991
Au	-6.714365	-2.053183	2.061486	S	-1.642416	-1.711915	8.2201987
Au	-0.563791	7.0616545	-1.679036	S	2.9733712	-3.349052	7.4862982
Au	1.0945787	7.1346016	0.7931767	S	6.5771105	-4.709703	4.6895742
Au	5.199925	1.6563425	4.7756204	S	2.5837617	3.0381448	-8.461424
Au	-5.372182	1.2813009	4.7951382	S	3.2615593	6.3365613	-5.156085
Au	1.8533807	-6.967925	1.0732099	S	7.6818622	4.0215342	-1.45124
Au	-1.108213	-7.129824	0.7898034	S	6.768035	5.7105851	2.8781004
Au	0.5571569	-7.046098	-1.689661	S	5.557426	2.8775482	6.8436763
Au	4.5594777	-2.171722	-4.198244	S	2.412001	6.1943578	5.7041696
Au	6.0089998	-1.965652	-1.670409	S	-2.998796	3.3460696	7.4924951
Au	4.6001275	-4.446877	-0.926225	S	-6.567974	4.7369637	4.6667084
Au	3.0938321	-4.608828	-3.542683	S	-8.932502	1.9943261	1.3917961
Au	-2.687888	-4.902716	-3.286892	S	-6.718484	5.6541136	-0.609429
Au	-4.155849	-2.617607	-4.375737	S	-5.226443	3.0807792	-6.386836
Au	-4.153198	-5.055442	-0.675869	S	-1.304977	5.5678672	-7.330605
Au	-5.597751	-2.794022	-1.806261	S	-7.538131	1.3145389	5.9703251
Au	5.7567952	0.4782473	-0.131705	S	-8.815462	-2.362824	3.3102575
Au	2.7364692	2.5424432	3.3968143	S	8.7918359	2.3718706	3.3269826
Au	3.1190439	-2.239852	3.3772698	S	7.5119185	-1.302291	5.9888635
Au	2.826246	0.0880374	5.0564779	S	-1.591227	1.7760616	-9.410633
Au	-3.286348	4.5884615	1.6597717	S	1.5181771	-1.761404	-9.422885
Au	-4.54013	2.0688655	0.7689243	H	3.4776762	9.294281	2.3136433

Au	-2.979465	-0.051003	-5.048529	H	2.954323	7.9592924	3.403989
Au	-3.138058	2.249448	3.3614893	H	2.7490847	9.6676699	3.9209004
Au	2.7808821	2.5722213	-1.69715	H	-4.02943	7.2573409	5.8334365
Au	-1.803373	4.7375056	-0.867636	H	-3.634529	7.8136575	4.1663853
Au	3.0771604	-2.212698	-1.759238	H	-3.103351	8.784628	5.582997
Au	4.3592209	0.2738115	2.5057759	H	0.0150365	10.083112	-0.1501
Au	-3.091502	2.2187411	-1.752069	H	-1.163715	10.598656	-1.405741
Au	-0.011731	0.0030812	-5.102036	H	0.481954	11.331875	-1.357671
Au	-1.577469	2.3497621	-4.235134	H	5.9010223	8.5922776	-2.612924
Au	-0.184672	2.3996818	3.3545427	H	5.251119	7.0419323	-3.256744
Au	3.2735064	-4.57316	1.6652069	H	6.6597399	7.0295533	-2.132704
Au	-2.763733	-2.537538	3.3869619	H	-5.13539	7.3986846	1.2312802
Au	-0.245813	4.7866193	-3.33434	H	-5.700032	9.0319506	0.7427812
Au	4.525822	-2.068797	0.7805459	H	-4.839052	8.814197	2.3052132
Au	1.1944292	4.8941774	-0.812829	H	-2.957119	7.4437046	-5.925085
Au	2.9583631	0.0742577	-5.053192	H	-1.744654	7.5890592	-4.60924
Au	0.1597282	-2.399877	3.3479941	H	-2.991151	8.8692253	-4.818443
Au	4.2277136	2.6697045	0.8570295	H	1.1710238	-10.58245	-1.406806
Au	-2.853539	-0.068513	5.0469376	H	-0.472752	-11.3181	-1.35027
Au	1.7824513	-4.715443	-0.871881	H	-0.004949	-10.06181	-0.151182
Au	4.3822931	0.2761903	-2.613417	H	-5.907144	-8.601523	-2.624326
Au	-5.764382	-0.461872	-0.143132	H	-5.254927	-7.052144	-3.267798
Au	-4.254882	-2.682495	0.8577759	H	-6.664342	-7.03769	-2.145185
Au	2.6058781	4.9403072	1.7509538	H	5.7056916	-8.98484	0.7403616
Au	-4.39359	-0.267425	2.4944356	H	4.8371051	-8.787357	2.3015559
Au	-0.350448	4.7913905	1.7169848	H	5.1227424	-7.361133	1.2386891
Au	-1.209534	-4.898826	-0.822517	H	2.9834018	-8.853109	-4.823729
Au	-1.369577	-2.442929	-4.261253	H	2.9478283	-7.4297	-5.932984
Au	0.331525	-4.781878	1.7057625	H	1.7365617	-7.572974	-4.616189
Au	1.5681693	-2.337747	-4.249079	H	-2.774165	-9.64612	3.9198943
Au	-2.786008	-2.583384	-1.702492	H	-3.499132	-9.279216	2.3093291
Au	1.3492055	2.453919	-4.248585	H	-2.973391	-7.939782	3.3932121
Au	-4.398378	-0.261461	-2.611954	H	3.6248153	-7.74351	4.0994789
Au	0.2310024	-4.771666	-3.353525	H	3.1373905	-8.766978	5.4949695
Au	-0.012728	0.0038145	5.0583387	H	4.0372229	-7.229196	5.7757589
Au	-2.63097	-4.934615	1.7451531	H	10.094188	-1.848271	3.4876201
Au	-0.001208	0.0209183	-0.034891	H	10.481355	-3.36677	2.5948323
Au	-1.304063	-2.471205	0.8244032	H	8.9416539	-3.221715	3.5219374
Au	1.2858273	2.4769045	0.8449364	H	7.1916117	-4.802678	-2.872289
Au	-0.144791	2.4035342	-1.686621	H	6.8981985	-6.570801	-2.817577
Au	-1.622239	2.2950267	0.7911193	H	8.4778903	-5.906491	-2.256741
Au	0.1297456	-2.404313	-1.697453	H	6.6612073	4.59048	-5.911159
Au	1.4398646	0.0842401	-2.547399	H	8.209279	3.69968	-5.670563

Au	-1.451951	-0.085474	-2.546141	H	7.1951374	4.1515203	-4.250923
Au	2.8749974	0.1723011	-0.037412	H	8.0580703	-2.466931	-4.380871
Au	-1.477924	-0.075067	2.484733	H	9.1621947	-2.975083	-3.052816
Au	1.5952214	-2.299507	0.7992561	H	9.6531357	-1.659843	-4.18104
Au	1.4353433	0.0646913	2.4954578	H	6.5130581	-4.999856	-7.006434
Au	-2.886027	-0.19072	-0.044155	H	5.9598152	-5.124595	-5.299499
Au	4.1392634	2.6311262	-4.376716	H	7.3200344	-4.029319	-5.731086
Au	-4.618853	4.4528387	-0.926069	H	1.5727318	-5.924949	-9.709149
Au	-3.108524	4.6239705	-3.534029	H	0.9056443	-4.280185	-9.401414
Au	-4.57129	2.1960907	-4.193892	H	-0.154419	-5.721894	-9.235402
Au	2.6688884	4.9047524	-3.273894	H	-4.910471	-3.309995	-9.058054
Au	-6.033235	1.9882095	-1.673261	H	-4.269356	-1.722361	-9.590572
Au	4.136501	5.0473298	-0.664037	H	-4.720014	-1.982259	-7.862799
Au	5.5930759	2.8016727	-1.80115	H	-1.95194	-7.895687	-6.466417
Au	1.4377545	1.4188379	-7.043046	H	-2.025058	-8.342733	-4.723126
Au	0.0069456	3.9854786	-6.062122	H	-0.917216	-7.037903	-5.269603
Au	-1.475081	-1.405058	-7.041496	H	-9.664541	1.6864812	-4.203968
Au	-0.019778	-3.965435	-6.077295	H	-8.068945	2.4939717	-4.394609
Au	1.5728181	-1.589356	-6.965804	H	-9.179407	3.0003949	-3.071237
Au	-1.591966	1.61641	-6.9535	H	-7.215288	-4.117017	-4.273824
Au	-0.344395	7.8317386	3.6974963	H	-6.681503	-4.555854	-5.933575
Au	2.5299563	8.2651896	-1.562481	H	-8.224635	-3.655524	-5.693986
Au	-3.514537	7.7645771	-1.660094	H	-9.874341	-3.203795	-0.79581
Au	-2.53222	-8.266837	-1.570432	H	-9.206312	-2.286374	-2.196496
Au	3.5113399	-7.739456	-1.667226	H	-8.621505	-1.932034	-0.540815
Au	0.3284589	-7.826869	3.6915995	H	-6.73279	-8.03925	2.2443573
Au	7.7017484	-3.742605	0.3948453	H	-5.587963	-7.651269	3.5810042
Au	7.0649005	0.7170812	-3.902662	H	-5.165778	-7.242834	1.8786424
Au	3.1793871	-4.186381	-6.825655	H	-7.262501	-4.476514	7.4800996
Au	-2.86308	-4.595822	-6.714919	H	-7.258349	-4.252163	5.693124
Au	-7.075453	-0.687064	-3.919627	H	-7.979038	-2.993138	6.7490079
Au	-7.10488	-4.770793	0.6936879	H	-0.802278	-5.487966	7.4002832
Au	-3.936846	-4.441006	6.1768969	H	-0.744616	-7.242349	7.0502695
Au	-0.016642	0.0018245	8.0675095	H	-2.07539	-6.576965	8.0709238
Au	4.6606239	-4.017495	5.9465154	H	0.6573046	2.6464574	10.248783
Au	2.8592992	4.5913629	-6.694893	H	-0.156511	3.3346162	8.7960662
Au	7.0874226	4.7835819	0.7105123	H	1.4963893	3.8852079	9.2500107
Au	3.918146	4.4495898	6.1811537	H	0.1222809	-3.331968	8.7899989
Au	-4.668259	4.0251155	5.9377366	H	-1.531043	-3.882679	9.2414648
Au	-7.721769	3.7658708	0.3922677	H	-0.692502	-2.64595	10.243204
Au	-3.191836	4.2126897	-6.817474	H	4.0244703	-1.136879	7.6896715
Au	-8.128827	-0.518299	4.6091457	H	4.5036432	-2.2582	9.0193734
Au	8.1025654	0.5292874	4.6266107	H	2.8706001	-1.491252	9.011508

Au	-0.039054	0.0051238	-9.396384	H	5.434596	-6.59559	3.6384371
C	2.7360259	8.9782232	3.0621606	H	6.4930944	-7.120227	5.0001472
C	-3.284345	7.7666454	5.203025	H	7.2110604	-6.641247	3.4183978
C	-0.100763	10.412989	-1.190747	H	4.2759816	1.7349757	-9.584648
C	5.7135382	7.5306318	-2.38907	H	4.6661323	1.891101	-7.828783
C	-4.907278	8.4715462	1.2616295	H	4.941675	3.2719808	-8.940928
C	-2.785328	7.7906657	-4.895822	H	0.91	7.0419607	-5.26146
C	0.1082839	-10.3968	-1.190259	H	1.9489815	7.8938325	-6.459206
C	-5.718479	-7.539958	-2.400304	H	2.0184404	8.3471209	-4.716976
C	4.9057977	-8.43677	1.2607668	H	9.2111263	2.3131271	-2.174741
C	2.7770709	-7.774767	-4.903013	H	8.6116233	1.9458831	-0.527102
C	-2.757879	-8.961347	3.0574533	H	9.8601793	3.2249129	-0.761328
C	3.2917247	-7.734625	5.1430965	H	5.5586316	7.6587972	3.5982445
C	9.6751325	-2.684145	2.9060981	H	5.1441599	7.2559204	1.8926572
C	7.3932561	-5.725869	-2.315352	H	6.7103514	8.0493317	2.268333
C	7.1799985	3.8331781	-5.30215	H	7.237805	4.2637634	5.696381
C	8.8052014	-2.124682	-3.655368	H	7.9611555	3.0098461	6.7565185
C	6.3594592	-4.448317	-6.06631	H	7.2412919	4.4937503	7.482683
C	0.8679909	-5.335624	-9.101921	H	0.7981358	5.5017988	7.417222
C	-4.295045	-2.445582	-8.762851	H	0.7332652	7.2538648	7.0575391
C	-1.891385	-7.515277	-5.43573	H	2.0736362	6.5977706	8.0723963
C	-8.819512	2.1507548	-3.673135	H	-2.913699	1.4780268	9.0075757
C	-7.196791	-3.796273	-5.324245	H	-4.056376	1.1348576	7.6731233
C	-8.976003	-2.723991	-1.212808	H	-4.544437	2.2494403	9.0050755
C	-5.981303	-7.321502	2.6076482	H	-6.453382	7.1533329	4.9329007
C	-7.178339	-3.74334	6.6623834	H	-7.126699	6.6537339	3.3380015
C	-1.410232	-6.381996	7.2159114	H	-5.3591	6.581781	3.6175815
C	0.8069515	3.0271449	9.2261583	H	-10.11515	1.8648576	3.4812588
C	-0.84141	-3.024755	9.2198507	H	-10.50633	3.3842814	2.5917639
C	3.6734582	-1.91043	8.3848513	H	-8.964787	3.2401261	3.5159482
C	6.3980561	-6.444523	4.1356861	H	-7.216495	4.8324183	-2.86725
C	4.2903708	2.4129772	-8.718368	H	-6.908765	6.5985685	-2.81123
C	1.8850927	7.517542	-5.427185	H	-8.491229	5.9459017	-2.245508
C	8.9687172	2.7437517	-1.190866	H	-7.333432	4.0642024	-5.726612
C	5.9562771	7.33139	2.6258469	H	-6.523054	5.0320723	-7.001738
C	7.1585749	3.7579258	6.6673073	H	-5.97072	5.1567118	-5.294533
C	1.4023837	6.3962938	7.22353	H	-1.567981	5.9305317	-9.705386
C	-3.709276	1.9033457	8.3760687	H	-0.916339	4.2824135	-9.38601
C	-6.341614	6.458492	4.0856711	H	0.1561811	5.716104	-9.224995
C	-9.698656	2.7024795	2.9004758	H	-6.794996	1.3727892	8.2552551
C	-7.40819	5.7565022	-2.308501	H	-6.546395	-0.272901	7.5709633
C	-6.371625	4.4807178	-6.061056	H	-8.196827	0.2666106	8.0494691
C	-0.869831	5.3392123	-9.092628	H	-10.4019	-2.496981	1.5128492

C	-7.232129	0.5846194	7.6239571	H	-9.837233	-0.798287	1.7058441
C	-10.14996	-1.708011	2.2367215	H	-11.02941	-1.494032	2.8636739
C	10.122875	1.7098572	2.2541278	H	10.403862	2.5085172	1.5515145
C	7.2044249	-0.570924	7.6415972	H	9.7926924	0.8223627	1.6963005
C	-3.242664	1.1022675	-9.825988	H	10.989568	1.455374	2.8836641
C	3.1512306	-1.084911	-9.898532	H	6.7639006	-1.357405	8.27272
S	1.0862272	9.0625046	2.2703722	H	6.5210296	0.2883789	7.5867455
S	-1.720814	6.8250064	5.318893	H	8.169067	-0.254856	8.0687855
S	0.4806412	9.1398179	-2.375848	H	-3.493893	0.2617444	-9.169916
S	4.6336145	7.4306004	-0.911371	H	-3.252165	0.7839786	-10.87977
S	-3.301259	8.8293024	0.4515901	H	-3.970038	1.9142163	-9.667814
S	-3.957939	6.9028612	-3.804464	H	3.1348433	-0.804662	-10.96324
S	-0.478072	-9.13222	-2.381152	H	3.8928439	-1.881155	-9.727531
S	-4.639964	-7.440198	-0.921295	H	3.404812	-0.216951	-9.280785
S	3.3047318	-8.806028	0.4440664				

Table S2. The Cartesian coordinates of Au₁₆₄(SR)₆₀, R = CH₃.

Atoms	x	y	z	Atoms	x	y	z
Au	-0.00166	1.4297348	-0.116842	C	1.3355099	11.147775	-0.602616
Au	2.419354	0.031683	-0.98632	C	6.4435516	8.891451	1.6053995
Au	-2.38898	2.8476312	-0.995014	C	-3.378235	8.8736394	5.11546
Au	-2.42574	1.3905403	1.5599929	C	2.8762083	9.8523515	3.8908913
Au	-2.396582	-0.053132	-0.970448	C	1.5848049	6.9706251	7.2229851
Au	2.4054105	1.432663	1.6068968	C	6.8992269	2.8977134	6.8972574
Au	-0.031133	2.8708052	2.3906646	C	-2.660423	3.0669911	-9.433057
Au	0.0242179	-0.025193	2.431598	C	3.5041084	1.2071083	-9.254689
Au	-0.020114	4.3243492	-0.070922	C	2.2106852	5.3486477	-8.442806
Au	0.004349	-0.004531	-2.687423	C	7.023084	7.3653141	-4.235932
Au	2.3743278	2.9254688	-0.890166	C	-1.995139	5.8069663	8.5372093
Au	0.0122445	2.8640212	-2.625459	C	-7.623295	4.8242327	5.240375
Au	0.0268779	-1.448888	-0.131157	C	-2.205406	10.479897	0.9534037
Au	2.4087646	-2.871172	-1.027506	C	-7.137321	7.5800707	-2.678627
Au	-2.365631	-1.471351	1.6131069	C	-1.388725	7.2751413	-8.170686
Au	-2.353485	-2.948874	-0.89133	C	-7.069431	5.157221	-5.8016
Au	2.4602015	-1.426588	1.5390398	C	-3.160112	10.769928	-4.124595
Au	0.0756949	-2.913578	2.3752438	C	2.9179547	9.8768502	-5.988275
Au	-0.001265	-2.877656	-2.639223	C	-3.55261	0.8481356	9.7557934
Au	0.0463558	-4.351714	-0.097053	C	2.5945491	3.2991526	10.246031
Au	-2.467813	0.0098975	-6.075692	C	-8.536793	-5.944256	-1.303923
Au	2.4787041	2.9582613	-5.945376	C	-6.445053	-6.972924	4.5366401
Au	-4.817088	-0.21799	-4.402486	C	-10.45586	-1.27246	-0.822229
Au	-2.304024	2.9435862	-6.003392	C	-7.508478	-3.351971	-6.358823
Au	4.816385	3.1779665	-4.215395	C	10.245674	-3.205487	-2.488302
Au	-4.785892	2.8370786	-4.38958	C	6.5147605	-0.761271	-7.243945
Au	2.4541024	0.0004732	-6.094738	C	10.464621	-2.064078	1.1612811
Au	4.8158287	0.2129554	-4.439197	C	7.2984403	-7.751716	1.9464673
Au	3.9032041	6.903155	-2.87902	C	1.3758306	-7.257995	-8.231184
Au	-7.205908	-0.090171	-0.873004	C	7.0557652	-5.151165	-5.878986
Au	1.2828045	8.2429889	-2.297225	C	-3.566411	-1.182267	-9.228808
Au	-1.73322	8.2457741	-2.154516	C	2.599517	-3.048612	-9.469603
Au	1.6376414	6.7407105	-4.879291	C	2.0806983	-5.89165	8.4728799
Au	-3.955446	6.5751079	-3.430077	C	7.6899975	-4.870414	5.1323887
Au	-7.126913	1.4241099	1.5882249	C	-2.829551	-9.891012	3.8634507
Au	-7.08644	2.8893748	-0.934469	C	3.4411889	-8.934136	5.0373233
Au	-1.348705	6.7999979	-4.797791	C	2.2768501	-10.52879	0.8954319
Au	7.0285597	2.9761432	-0.833622	C	7.1405334	-7.598944	-2.783869
Au	7.2302361	0.060824	-0.93958	C	-2.249892	-5.328013	-8.461016
Au	7.1257189	1.6586269	1.7890394	C	-7.028525	-7.363609	-4.234937

Au	2.2993844	5.8741499	4.0824925	C	-1.293745	-11.16514	-0.651337
Au	2.2965099	7.3836332	1.5503906	C	-6.411423	-8.91662	1.5994314
Au	4.7197945	5.8468795	0.9495045	C	-1.495272	-7.027634	7.186658
Au	4.6752003	4.2860344	3.4834005	C	-6.847473	-2.961863	6.9660247
Au	-2.48817	5.6799393	4.1843385	C	-2.479412	-3.366695	10.242054
Au	-4.889387	4.2962181	3.1100032	C	3.6669481	-0.938786	9.6905079
Au	-4.850306	5.8052336	0.5003859	C	-2.932578	-9.850425	-6.046335
Au	-2.527453	7.1557351	1.640199	C	3.1598433	-10.77136	-4.215529
Au	-1.579417	2.8807402	6.7973354	C	-9.417585	-2.493405	4.2490962
Au	-4.059323	1.4317881	6.019309	C	-6.782687	0.696872	8.1395077
Au	1.59433	-0.02786	7.023557	C	6.8740867	-0.767581	8.0803768
Au	3.9256865	1.4219603	6.1071219	C	9.482064	2.4384511	4.2083021
Au	1.4764017	2.9918141	6.9185115	H	-10.33196	2.1350278	-2.129932
Au	-1.554537	-0.037277	7.025148	H	-10.84247	3.4095837	-3.291759
Au	-2.492638	-2.95201	-5.942514	H	-10.56344	3.8348997	-1.563441
Au	-4.818001	-3.183783	-4.199298	H	-7.431609	1.228154	-7.646597
Au	2.2895085	-2.931555	-6.035861	H	-6.205515	-0.083044	-7.791219
Au	4.7813844	-2.84007	-4.436551	H	-5.731854	1.5278581	-7.1467
Au	-7.003889	-3.00275	-0.806483	H	-10.80486	1.1247628	1.6576339
Au	-1.266729	-8.255581	-2.339819	H	-10.05674	1.9409581	0.243509
Au	-3.898243	-6.915017	-2.888666	H	-11.23981	2.8302114	1.2703931
Au	1.3410159	-6.800716	-4.848202	H	-8.253547	8.0388183	2.2363807
Au	3.9544805	-6.582281	-3.494313	H	-6.600302	8.6005838	1.7831093
Au	1.7458461	-8.266717	-2.21147	H	-6.796094	7.2815732	2.9868204
Au	-7.090234	-1.685796	1.8228505	H	7.5163132	6.2354632	-1.351728
Au	-1.650588	-6.737894	-4.911966	H	8.8952961	5.5781674	-2.304172
Au	7.1045653	-2.912175	-1.007434	H	9.1889197	6.7681967	-0.978183
Au	7.1670884	-1.45229	1.5203018	H	7.425483	7.5089822	4.4353871
Au	4.9383354	-4.343699	3.0451191	H	6.1656397	6.9039208	5.5664904
Au	2.5437621	-5.733441	4.1346978	H	5.7138202	7.3322909	3.8859197
Au	4.8810178	-5.842731	0.4328255	H	11.198348	1.8781461	-1.509775
Au	2.5653559	-7.198857	1.5850883	H	11.067599	0.4513587	-0.423688
Au	-4.687522	-5.881149	0.9496219	H	9.9598327	1.8499907	-0.207628
Au	-4.625824	-4.335464	3.4908075	H	6.8785477	4.082973	-6.982975
Au	-2.245834	-5.929536	4.0615287	H	7.2041338	2.3434618	-6.631148
Au	-2.25787	-7.419558	1.5244653	H	8.5536791	3.5338475	-6.600321
Au	-3.869223	-1.509322	6.1153701	H	1.0048886	10.440436	0.1658768
Au	1.6635278	-2.950438	6.7632625	H	0.469446	11.54552	-1.152865
Au	4.1366698	-1.509869	5.9746042	H	1.8905359	11.971106	-0.127135
Au	-1.406099	-3.06435	6.9054369	H	6.7727297	9.8693439	1.2216875
Au	-0.140603	7.2395939	0.013252	H	7.2925214	8.3705444	2.0720881
Au	-2.375345	4.3284375	-3.533685	H	5.6416259	9.0311771	2.3408693
Au	2.3985795	4.4598884	-3.393387	H	-4.235692	8.4023367	5.619452

Au	0.0997327	4.3052975	-5.128735	H	-3.606405	9.0040787	4.0487552
Au	-4.812467	-1.569409	-1.761537	H	-3.159155	9.8492303	5.5771153
Au	0.0590994	-1.48082	4.9932513	H	3.7473178	10.189907	3.3079378
Au	-2.472966	-1.522021	-3.494035	H	3.1539015	8.9868616	4.5088307
Au	-2.47636	4.3310703	1.540892	H	2.5227377	10.674403	4.5330176
Au	-4.86345	-0.062649	0.7234755	H	0.8756546	6.1471201	7.0657522
Au	2.3730594	4.3949506	1.6805302	H	1.1252911	7.9176258	6.8988508
Au	-0.028507	5.8177948	-2.584157	H	1.8622001	7.0220345	8.286406
Au	0.004231	1.4189569	5.000809	H	6.8081561	3.0699227	5.8205752
Au	-2.354513	-0.015473	4.2141301	H	7.4468099	1.9598523	7.0724933
Au	-2.428005	1.3940703	-3.576612	H	7.4336866	3.738487	7.3650398
Au	4.7394131	4.4733589	-1.622144	H	-2.909324	2.0029906	-9.319723
Au	2.431303	-1.398696	-3.601259	H	-2.257419	3.253425	-10.44123
Au	-4.831119	1.3821717	3.2543494	H	-3.550651	3.69036	-9.258777
Au	2.3435783	5.9028244	-0.841273	H	3.2414416	1.5118258	-10.27947
Au	-4.798311	2.8433906	0.6574848	H	4.3167745	0.4660389	-9.293139
Au	-0.036817	4.3728277	4.8929346	H	3.8257661	2.0809104	-8.671368
Au	2.478094	1.5134113	-3.503893	H	1.7701945	4.6187517	-9.139116
Au	-2.452389	5.8075001	-0.999331	H	2.6410933	6.1945761	-8.999437
Au	-0.059927	-1.417483	-5.245702	H	1.4366393	5.7071754	-7.753463
Au	4.7759809	2.9242588	0.8855678	H	7.6603916	7.6657205	-5.08361
Au	-0.087237	5.8366819	2.4636773	H	7.1281489	6.288839	-4.056589
Au	-4.767466	4.2711649	-1.912745	H	7.3052426	7.9346284	-3.337814
Au	-4.82011	1.3327974	-1.888515	H	-1.612069	6.2641135	7.6161178
Au	4.8961932	0.0284738	0.6920513	H	-1.161451	5.4866681	9.180194
Au	2.4107123	-0.042523	4.2013542	H	-2.626375	6.5349336	9.0720606
Au	4.828802	1.5498692	-1.786444	H	-7.524181	3.7342153	5.309079
Au	2.3364654	2.8955257	4.1940581	H	-8.339568	5.0873223	4.4467546
Au	-2.459188	2.8644599	4.0702165	H	-7.966352	5.2309912	6.2045365
Au	4.7624519	1.3930476	3.36093	H	-1.464582	10.0333	0.2783579
Au	0.0514319	1.4259913	-5.238512	H	-1.737281	10.695525	1.9264471
Au	4.8344051	-1.351014	-1.930186	H	-2.604719	11.403625	0.5068885
Au	-4.723416	-4.491313	-1.615086	H	-7.035034	6.6149449	-2.169046
Au	-2.322879	-5.925387	-0.859132	H	-7.613093	7.4378431	-3.660888
Au	0.0966142	-4.433545	4.8643656	H	-7.751538	8.2536058	-2.06335
Au	-2.392913	-4.46894	-3.403391	H	-1.951811	7.4439171	-9.102259
Au	-4.74394	-2.95887	0.9025324	H	-1.056814	6.2303647	-8.127236
Au	-2.332771	-4.435908	1.6700226	H	-0.523202	7.953627	-8.124992
Au	-2.280719	-2.954626	4.1906561	H	-7.936042	4.4786278	-5.819091
Au	2.3774442	-4.336178	-3.574509	H	-7.218427	5.9798128	-6.518117
Au	-4.714065	-1.446818	3.3822842	H	-6.938691	5.5524295	-4.788141
Au	-0.105886	-4.302912	-5.151635	H	-3.382632	9.8974432	-4.751886
Au	0.1684858	-7.269975	-0.0288	H	-2.993886	11.653558	-4.759797

Au	2.4717867	-5.833489	-1.049669	H	-3.997047	10.955198	-3.434842
Au	0.0378258	-5.83139	-2.618975	H	2.6418234	10.896516	-6.301015
Au	4.8319078	-2.873522	0.6067159	H	3.7302106	9.4990398	-6.626915
Au	2.5179475	-2.92098	4.0334992	H	3.2414325	9.8874284	-4.939667
Au	2.5167507	-4.372733	1.4967439	H	-4.259568	0.0367532	9.5315355
Au	0.13132	-5.879641	2.4259443	H	-3.758037	1.7188403	9.1201444
Au	4.8879308	-1.435111	3.2114591	H	-3.636182	1.1346145	10.816304
Au	4.7793178	-4.29005	-1.969559	H	3.4123624	3.9992578	10.017357
Au	-7.645987	1.9005855	-4.15034	H	2.9019461	2.2704003	10.018343
Au	-8.101096	4.5412816	1.4402997	H	2.3169034	3.3790684	11.308864
Au	7.6511405	5.0063945	1.8537652	H	-8.852017	-5.577924	-2.291654
Au	8.2484559	2.0823549	-3.350908	H	-9.172778	-6.787568	-0.990047
Au	4.0230805	9.0247967	-0.674977	H	-7.490074	-6.267558	-1.335193
Au	-0.203117	8.4791602	3.944369	H	-6.13791	-6.966167	5.5938499
Au	4.0513286	4.6570781	6.8652889	H	-5.625152	-7.373541	3.9274879
Au	0.3502178	1.9797846	-8.215199	H	-7.354254	-7.579431	4.4147494
Au	4.3749397	6.0991937	-6.00667	H	-10.10272	-2.284351	-0.587412
Au	-4.471301	4.923531	6.4389855	H	-11.46058	-1.319012	-1.27117
Au	-4.462945	8.7071342	-0.862572	H	-10.48387	-0.673821	0.0983307
Au	-3.946524	5.860232	-6.443837	H	-6.901028	-4.04323	-6.962373
Au	-0.09166	9.6154111	-4.651911	H	-7.242988	-2.310441	-6.585503
Au	-0.404546	2.0157547	9.4131662	H	-8.57862	-3.514404	-6.560344
Au	-7.606284	-5.054597	1.8749113	H	10.851693	-3.42963	-3.380312
Au	-8.261923	-2.092339	-3.30042	H	10.572988	-3.834858	-1.646096
Au	7.6448097	-1.901437	-4.217239	H	10.346143	-2.141245	-2.233041
Au	8.1519927	-4.550981	1.3447164	H	7.4150288	-1.183361	-7.715647
Au	3.9292286	-5.837447	-6.508562	H	6.1570934	0.1011572	-7.82683
Au	-0.40103	-1.964889	-8.221933	H	5.7285149	-1.52546	-7.194561
Au	4.5501844	-4.996155	6.3667537	H	10.075845	-1.941159	0.1439171
Au	0.2568584	-8.530547	3.8943802	H	11.294662	-2.786889	1.1671348
Au	4.4925156	-8.732012	-0.944442	H	10.807777	-1.091569	1.5459963
Au	-4.392636	-6.086305	-6.008679	H	8.3577915	-7.978618	2.1439176
Au	-3.98823	-9.052935	-0.68638	H	6.7787691	-8.665489	1.618481
Au	-3.985162	-4.725798	6.8754579	H	6.8217014	-7.356372	2.8542763
Au	0.5108259	-2.10539	9.3877977	H	0.5082508	-7.934009	-8.183387
Au	0.0873378	-9.607985	-4.718726	H	1.9380351	-7.435294	-9.161953
Au	-7.375317	0.1643901	4.8630596	H	1.0483057	-6.211173	-8.193974
Au	7.4330364	-0.22347	4.8012232	H	7.1958819	-5.969319	-6.602635
S	-8.494255	3.6259604	-2.768638	H	6.9296397	-5.553668	-4.867962
S	-6.965483	0.1288808	-5.534487	H	7.9260984	-4.477666	-5.899217
S	-9.093631	2.6265945	2.3910935	H	-3.894385	-2.046759	-8.634696
S	-7.171196	6.5533435	0.6702941	H	-3.309459	-1.504876	-10.24939
S	8.7948023	4.529132	-0.152878	H	-4.371635	-0.433741	-9.273696

S	6.8613362	5.1740255	4.0686375	H	2.1854137	-3.236995	-10.4731
S	9.3677768	0.4063434	-2.117851	H	3.4913059	-3.672418	-9.305126
S	7.1673629	3.7347965	-4.626769	H	2.8490517	-1.984398	-9.360197
S	2.4333313	10.33946	-1.825517	H	2.7105874	-6.622606	9.0053476
S	5.8845865	7.8791563	0.1878715	H	1.6961151	-6.344779	7.5508854
S	-1.939421	7.769409	5.3710089	H	1.2477288	-5.572205	9.1173932
S	1.5554088	9.4351743	2.6908524	H	8.3990683	-5.130873	4.3310917
S	3.1009055	6.7301624	6.2231217	H	8.0464008	-5.268249	6.0951053
S	5.244577	2.7524743	7.6660242	H	7.5835431	-3.780993	5.1957522
S	-1.408278	3.5634621	-8.197491	H	-2.473665	-10.71436	4.5026322
S	2.0549055	0.3726799	-8.507272	H	-3.70346	-10.23024	3.2852781
S	3.5574399	4.4978968	-7.533941	H	-3.104372	-9.02496	4.481174
S	5.2976708	7.8107327	-4.640428	H	3.6559108	-9.063008	3.9678747
S	-3.008457	4.3297497	8.1710642	H	3.2296408	-9.909908	5.5020763
S	-6.02609	5.619531	4.8189713	H	4.3047624	-8.462428	5.530744
S	-3.592059	9.3210383	1.2602716	H	2.699876	-11.47811	0.5319356
S	-5.514433	8.372898	-2.975164	H	1.5677724	-10.13116	0.1594147
S	-2.484901	7.6836288	-6.761492	H	1.7623544	-10.684	1.8560997
S	-5.594246	4.1995653	-6.3172	H	7.6096392	-7.457283	-3.769653
S	-1.650419	10.501332	-3.122965	H	7.7582333	-8.274128	-2.174133
S	1.4563736	8.803141	-6.22969	H	7.0450681	-6.633288	-2.274269
S	-1.871643	0.1826111	9.476631	H	-1.8216	-4.598392	-9.164848
S	1.1463937	3.78333	9.2364345	H	-2.68419	-6.178467	-9.007889
S	-8.761023	-4.567079	-0.123956	H	-1.464479	-5.683296	-7.782273
S	-6.805105	-5.232961	4.0860674	H	-7.312014	-7.944543	-3.344761
S	-9.350746	-0.425767	-2.02324	H	-7.66623	-7.649674	-5.087236
S	-7.176536	-3.724348	-4.600005	H	-7.13223	-6.289287	-4.042106
S	8.5040302	-3.634319	-2.852753	H	-0.430344	-11.55551	-1.210973
S	6.9583921	-0.119809	-5.584708	H	-1.840836	-11.99561	-0.178868
S	9.1510513	-2.641999	2.3013156	H	-0.962666	-10.46132	0.120127
S	7.2148744	-6.555307	0.5638138	H	-6.756605	-9.889692	1.2168719
S	2.4736682	-7.664103	-6.822737	H	-7.252388	-8.385499	2.0693976
S	5.5833317	-4.182669	-6.378491	H	-5.607332	-9.066138	2.3302403
S	-2.106623	-0.355367	-8.495598	H	-0.789172	-6.202519	7.0208005
S	1.3611072	-3.544693	-8.219763	H	-1.039136	-7.972972	6.8535833
S	3.0972494	-4.415192	8.1135355	H	-1.753949	-7.081273	8.254985
S	6.0944347	-5.678711	4.7303307	H	-6.794227	-3.355632	5.9462318
S	-1.516649	-9.476808	2.653526	H	-7.306337	-1.961798	6.9477904
S	2.0043174	-7.831733	5.3127948	H	-7.445911	-3.640217	7.5936031
S	3.6486762	-9.349206	1.1873091	H	-3.301693	-4.069702	10.038236
S	5.5131394	-8.386889	-3.069011	H	-2.793719	-2.343426	9.9995968
S	-3.586529	-4.48085	-7.534874	H	-2.18403	-3.421697	11.301231
S	-5.304654	-7.80606	-4.646462	H	3.8887997	-1.737319	8.9712158

S	-2.407462	-10.3555	-1.860392	H	3.7539257	-1.32558	10.717781
S	-5.848943	-7.910116	0.1787718	H	4.3620703	-0.100108	9.5428013
S	-3.025354	-6.786859	6.2108482	H	-2.67002	-10.86514	-6.382454
S	-5.173748	-2.825618	7.6943723	H	-3.752379	-9.451664	-6.662007
S	-1.048836	-3.863185	9.215627	H	-3.242419	-9.87706	-4.994029
S	1.9784023	-0.272439	9.4614302	H	3.3863116	-9.891816	-4.831399
S	-1.46715	-8.782274	-6.28432	H	2.9880527	-11.64485	-4.863842
S	1.6541237	-10.50971	-3.206597	H	3.99631	-10.97226	-3.529604
S	-8.825052	-0.999284	3.3672921	H	-8.588525	-3.119587	4.5974786
S	-6.441196	1.541356	6.5529295	H	-10.03159	-3.073136	3.5426463
S	6.5219803	-1.610648	6.4961591	H	-10.03304	-2.169195	5.1036688
S	8.8737128	0.9597903	3.3123189	H	-6.467415	1.3774552	8.9454378
C	-10.23487	3.1962539	-2.39824	H	-6.234257	-0.250462	8.224215
C	-6.534329	0.7802813	-7.192808	H	-7.866288	0.518763	8.2156896
C	-10.4322	2.0825746	1.2636276	H	6.3257347	0.1792084	8.169928
C	-7.208128	7.7308624	2.0723722	H	7.958404	-0.590601	8.1496354
C	8.5661656	5.9230723	-1.312952	H	6.5646454	-1.448752	8.8881551
C	6.5045523	6.9124884	4.5194046	H	10.095162	3.0230154	3.5052856
C	10.50458	1.2420167	-0.94107	H	10.10236	2.0983454	5.0532556
C	7.4837686	3.3784397	-6.392141	H	8.6608384	3.0657268	4.5732015

Table S3. The Cartesian coordinates of Au₁₈₂(SR)₆₆, R = CH₃.

Atoms	x	y	z	Atoms	x	y	z
Au	5.9098628	1.6282078	-2.347717	C	-8.950406	7.5706396	-3.162217
Au	5.8469543	3.3758536	0.0113385	C	-5.317703	6.3746661	-7.033331
Au	4.4538669	4.1901178	-2.437084	C	-1.171989	9.9350091	3.5442962
Au	2.9578583	-0.110281	-4.783448	C	-3.167328	10.150142	-2.534021
Au	4.4926913	2.4118324	-4.738979	C	-10.40467	-2.391954	2.4914981
Au	1.5482848	2.4714664	-4.827961	C	-9.199249	-4.063345	-3.540162
Au	1.4945068	4.2278794	-2.44064	C	-10.62853	-0.193761	-2.400138
Au	-1.446516	4.2778861	-2.415758	C	-8.009345	3.7858332	-7.036594
Au	-2.907803	0.0433713	-4.840403	C	-5.215138	9.2468002	2.377093
Au	0.0199737	-0.017419	-4.924838	C	-7.327451	4.9561185	7.0133285
Au	-1.3656	2.5576555	-4.796619	C	-11.07289	3.9148073	3.1255394
Au	-5.855857	1.715453	-2.451824	C	-8.292279	1.2695307	7.0128884
Au	-4.328796	2.6273314	-4.750461	C	-8.687016	8.4798661	1.1692862
Au	-4.35597	4.2531319	-2.364996	C	-11.71082	3.1981879	-1.208376
Au	-5.845097	3.3426996	-0.01495	C	1.2911055	-4.567698	10.189405
Au	5.8803794	-1.715724	0.0479511	C	6.5627163	-4.70871	6.3625196
Au	2.9560006	-3.419488	-2.424652	C	-1.138074	-1.906391	10.543537
Au	4.4683061	-0.900026	-2.39249	C	-4.531501	-6.504528	7.4353597
Au	-0.104194	-5.105785	-4.733498	C	-1.224837	-4.627597	-10.17151
Au	1.4253725	-2.588544	-4.81912	C	-6.527167	-4.727816	-6.355771
Au	-2.985248	-3.430855	-2.411954	C	1.1684825	-1.949141	-10.53388
Au	-1.53138	-2.518184	-4.78969	C	4.5976519	-6.510767	-7.399928
Au	-5.849841	-1.750719	-0.040705	C	-2.027069	-11.57114	-3.16985
Au	-4.406839	-0.864181	-2.444459	C	-2.916981	-7.844604	-7.031525
Au	-7.228969	0.7542735	-0.13818	C	-8.106654	-6.003646	3.4615412
Au	1.4428584	-5.959854	-2.428091	C	-7.207229	-7.872437	-2.546199
Au	-2.903034	-6.667655	0.125981	C	7.2596025	-7.808655	2.6116883
Au	0.022228	-6.747855	0.0057492	C	8.150591	-5.978256	-3.432097
Au	-1.507216	-5.930574	-2.348637	C	5.490381	-9.138276	-2.316842
Au	-4.400564	-4.231127	0.0307024	C	0.7551937	-8.887219	-6.996367
Au	-5.892338	1.5950148	2.3382246	C	-5.438915	-9.147485	2.3768746
Au	-4.457577	4.1667147	2.4304916	C	-0.690104	-8.861667	7.0356689
Au	-4.310981	5.8329847	0.1119282	C	2.1107425	-11.54625	3.1928092
Au	-1.444222	5.9094879	0.0244637	C	2.9190975	-7.800168	7.0520858
Au	-2.932224	-0.119476	4.7864754	C	-3.027343	-11.77811	1.1852329
Au	-4.481029	2.3962489	4.7230393	C	3.0834828	-11.77123	-1.148019
Au	-1.528765	2.4750819	4.8206147	C	3.2840244	3.3913123	10.195448
Au	-1.491573	4.2190665	2.4278005	C	0.8562801	8.0258157	6.3206106
Au	1.4468006	4.2922562	2.4100854	C	2.1957054	-0.018275	10.544249
Au	1.4362433	5.9145165	-0.03751	C	7.8997756	-0.671935	7.4317368

Au	4.2992123	5.8597712	-0.121582	C	4.6634544	1.179444	-10.1497
Au	2.9338933	0.069518	4.8355429	C	7.3941949	-3.314585	-6.289321
Au	0.0001695	-0.009285	4.9335748	C	1.1226094	1.8633529	-10.53506
Au	1.3801321	2.5805315	4.7923849	C	3.3443335	7.1553144	-7.451388
Au	5.8706668	1.7575581	2.4536407	C	11.068666	3.9568005	-3.132741
Au	4.3422052	2.6601699	4.7492424	C	8.2643714	1.363887	-6.995197
Au	4.3561473	4.2836264	2.3607147	C	9.2261332	-3.985936	3.5612865
Au	-2.917603	-3.426938	2.4420624	C	10.422775	-2.354112	-2.495547
Au	-4.44823	-0.922513	2.400701	C	3.111478	10.168798	2.5602676
Au	0.1587664	-5.0934	4.7555571	C	1.1012082	9.9970266	-3.464428
Au	-1.382331	-2.582924	4.8349581	C	5.1555453	9.2875993	-2.371831
Au	3.0202158	-3.404314	2.4199668	C	7.3174268	5.0259718	-7.017503
Au	1.5645741	-2.496326	4.8005068	C	10.656689	-0.120734	2.3685502
Au	4.433177	-0.831805	2.4487853	C	8.0537879	3.8319406	7.0276533
Au	7.2461934	0.8051066	0.1363093	C	8.9372761	7.6357565	3.128784
Au	-1.389942	-5.961167	2.450362	C	5.3476981	6.346374	7.0164414
Au	2.9531121	-6.658468	-0.109164	C	11.714064	3.2776187	1.1903961
Au	1.559021	-5.922251	2.3710973	C	8.6479045	8.5418013	-1.19034
Au	4.4479226	-4.213335	-0.016559	H	-4.256304	2.1801704	10.479463
Au	1.4610213	0.8272662	0.0068988	H	-3.951027	0.400934	10.362936
Au	1.4856851	-0.871216	-2.409835	H	-5.613882	1.0156935	10.67145
Au	-0.002263	1.685545	2.4128058	H	-7.372952	-4.465852	6.0973887
Au	2.8988365	1.6991116	2.4037064	H	-7.565065	-2.800972	5.4504583
Au	1.4890449	-0.847264	2.4231078	H	-7.992209	-3.152041	7.1626859
Au	2.9355754	1.6442978	-2.39398	H	-0.354826	1.4067683	11.123408
Au	2.887788	3.3268297	-0.008698	H	-1.746497	1.1483797	10.01751
Au	4.3452328	0.8301116	0.014917	H	-1.77333	2.5027708	11.203717
Au	0.0009072	3.3808993	-0.003607	H	-2.30092	7.4246982	7.1167457
Au	-1.435055	0.814398	-0.006405	H	-3.515944	7.4266386	8.4468557
Au	2.9521739	-1.699818	0.0073309	H	-4.033479	7.7695207	6.7551606
Au	-0.004694	-3.373006	-2.39348	H	-3.609262	4.2598323	-10.73435
Au	-1.459308	-0.876512	2.4235317	H	-3.96002	2.5058698	-10.52907
Au	0.0413534	-3.371403	2.4049318	H	-2.26513	3.1182299	-10.38221
Au	-1.422396	-4.174304	0.0133134	H	-1.486437	7.8946326	-5.534039
Au	-2.925246	-1.713624	-0.00132	H	-1.246065	8.4683893	-7.221174
Au	1.4711565	-4.170592	0.0038868	H	0.105773	8.5621981	-6.033491
Au	-1.458329	-0.868703	-2.415825	H	-3.001765	0.1524644	-11.24413
Au	-2.91933	1.6292618	2.3873213	H	-1.330216	-0.485658	-11.10951
Au	0.0210228	1.6831504	-2.419402	H	-1.858861	0.8612557	-10.04585
Au	-2.883397	3.307854	0.0003081	H	-7.569122	-1.742214	-7.149239
Au	-2.880609	1.6723553	-2.403553	H	-8.128233	-0.704281	-8.508361
Au	-4.326588	0.8033706	-0.016392	H	-8.724877	-0.391415	-6.836306
Au	0.0176494	-1.688739	0.004992	H	-9.010755	6.6137954	-3.697156

Au	-4.358203	-2.671867	4.7767069	H	-9.065846	8.4053502	-3.872028
Au	-2.735512	-5.159306	4.8116667	H	-9.744838	7.6136071	-2.402053
Au	-4.343913	-5.891166	2.4667216	H	-5.642741	5.3503299	-6.823352
Au	-5.907879	-3.397571	2.4410297	H	-4.748283	6.3908143	-7.974786
Au	-5.905728	-0.109338	4.7558228	H	-6.188287	7.0442369	-7.104982
Au	-7.358148	-0.831499	2.2818426	H	-1.938395	9.2700654	3.9657424
Au	-0.069837	1.7182247	7.2245205	H	-1.628535	10.893446	3.2517634
Au	2.8914174	1.747284	7.0760268	H	-0.384629	10.117399	4.2921748
Au	1.5245218	-0.808558	7.2297392	H	-3.812524	10.001283	-3.413513
Au	-1.466423	-0.919668	7.2261472	H	-2.109492	10.039059	-2.81043
Au	0.072291	-3.385036	7.0824719	H	-3.340986	11.148739	-2.102252
Au	-2.973184	1.630423	7.0606385	H	-9.792039	-3.262429	2.7650848
Au	-4.460357	-2.486105	-4.787178	H	-11.36173	-2.726664	2.0608561
Au	-5.814858	0.159014	-4.809073	H	-10.5886	-1.759311	3.3732742
Au	-7.260532	-0.87554	-2.475707	H	-8.934042	-4.807136	-4.30644
Au	-5.862914	-3.47061	-2.449895	H	-9.059262	-3.048302	-3.937933
Au	-2.984907	-5.082946	-4.778635	H	-10.25091	-4.204477	-3.245273
Au	-4.340179	-5.990192	-2.299857	H	-10.8595	-1.205305	-2.031848
Au	1.4917352	-0.939906	-7.217283	H	-11.52493	0.2553542	-2.853987
Au	2.9878725	1.6176463	-7.07135	H	-10.27781	0.42166	-1.560762
Au	0.0904177	1.6987998	-7.228323	H	-7.833964	4.782635	-7.47017
Au	-1.496123	-0.841278	-7.22463	H	-8.809097	3.280767	-7.599613
Au	-2.873329	1.7196443	-7.079749	H	-7.094328	3.1825813	-7.08491
Au	-0.028333	-3.409977	-7.065405	H	-5.567494	8.6393977	1.5323261
Au	-0.037011	6.7865021	-2.451356	H	-4.455236	9.9575055	2.0179287
Au	-2.990269	6.7321315	-2.311747	H	-6.054198	9.7945337	2.8314949
Au	-2.863792	5.1003453	-4.786947	H	-7.318284	5.8928937	7.5935088
Au	0.1203139	5.0790331	-4.785461	H	-6.331622	4.4964931	7.0482409
Au	2.9076804	6.6979306	-2.465207	H	-8.079143	4.2730184	7.4365096
Au	3.0763803	4.9477393	-4.80647	H	-11.83119	3.5903035	3.8546613
Au	6.9599775	3.6365452	-3.875587	H	-11.5353	4.5688608	2.3697026
Au	6.7270928	5.6698029	-1.661802	H	-10.27082	4.4613798	3.6374066
Au	8.2950371	3.0591466	-1.268594	H	-7.601884	2.0993552	6.8245987
Au	6.6256625	4.2142952	3.8854973	H	-7.99367	0.7515911	7.9367297
Au	6.7720766	5.6706139	1.2781068	H	-9.323188	1.643542	7.1055266
Au	8.2720565	3.0261254	1.6689789	H	-8.036746	8.4830922	0.2827021
Au	4.4935913	-2.451396	4.7978185	H	-8.236182	9.0860529	1.9690449
Au	5.8374882	0.1923934	4.8127007	H	-9.674477	8.8919351	0.90947
Au	7.2875913	-0.821767	2.4780509	H	-11.37976	2.6230368	-0.33231
Au	5.8972983	-3.428735	2.4578935	H	-12.0162	2.5144209	-2.014043
Au	3.0365088	-5.047395	4.7913208	H	-12.56277	3.839461	-0.930911
Au	4.3854305	-5.962596	2.3115577	H	1.5983855	-3.528862	10.374853
Au	4.3941703	-2.660428	-4.765968	H	1.9681784	-5.254174	10.722102

Au	2.7929948	-5.153657	-4.788451	H	0.2564653	-4.73145	10.527916
Au	4.3993891	-5.880993	-2.44238	H	6.1972794	-5.177779	5.4383734
Au	5.9433249	-3.372915	-2.421828	H	6.6065061	-5.456028	7.1677747
Au	5.9144548	-0.099096	-4.750837	H	7.5636429	-4.284423	6.1884522
Au	7.3768716	-0.796696	-2.278919	H	-0.18313	-2.069937	10.032354
Au	-6.619542	4.1745151	-3.889811	H	-1.351672	-2.744169	11.224027
Au	-8.26427	2.96939	-1.679885	H	-1.09393	-0.970775	11.120085
Au	-6.793894	5.6314198	-1.276656	H	-4.671952	-7.414246	6.833793
Au	-6.973232	3.583773	3.8690949	H	-5.263889	-5.740626	7.1436182
Au	-8.298625	3.0055062	1.2577298	H	-4.646051	-6.739748	8.5052297
Au	-6.745883	5.6222092	1.6599107	H	-0.187332	-4.784304	-10.50427
Au	-0.112854	5.0893725	4.7818812	H	-1.541895	-3.593784	-10.36895
Au	-3.069196	4.9282142	4.7905216	H	-1.891673	-5.32682	-10.70101
Au	-2.925405	6.6812913	2.453925	H	-6.150702	-5.222176	-5.449849
Au	0.0239167	6.783725	2.4322121	H	-6.610904	-5.458978	-7.17303
Au	2.866924	5.1334831	4.776699	H	-7.513282	-4.283012	-6.150424
Au	2.9753032	6.754643	2.3041492	H	1.3792711	-2.799723	-11.19861
Au	-0.288112	-7.855069	-3.862567	H	1.1343317	-1.023184	-11.12639
Au	1.561346	-8.672096	-1.646621	H	0.210764	-2.097962	-10.02331
Au	-1.479093	-8.724766	-1.255301	H	4.7223565	-6.720412	-8.473797
Au	0.3455141	-7.841249	3.8941023	H	4.7288665	-7.436505	-6.819958
Au	1.529077	-8.713579	1.2781712	H	5.3280017	-5.755249	-7.081544
Au	-1.513172	-8.671977	1.6744767	H	-2.674955	-12.06541	-3.911895
Au	-5.346682	-0.859324	7.5642276	H	-1.696669	-12.30175	-2.416502
Au	-2.027612	4.1898147	8.2259578	H	-1.15076	-11.13941	-3.668546
Au	-1.922848	5.0098642	-7.615134	H	-3.21779	-7.346009	-7.965228
Au	-4.603049	-0.395386	-8.243027	H	-3.085264	-8.929288	-7.111447
Au	-5.735916	7.1983154	-3.93314	H	-1.860186	-7.638291	-6.832653
Au	-2.010802	8.8899942	0.4100331	H	-7.166313	-6.402218	3.8679868
Au	-8.707892	-2.789819	-0.43184	H	-8.759899	-6.833123	3.1489716
Au	-8.878517	1.8358342	-4.411431	H	-8.618691	-5.40206	4.2285359
Au	-6.097986	6.7110516	4.3895709	H	-7.970994	-8.542271	-2.120941
Au	-9.165133	1.3035626	3.8964757	H	-6.74449	-8.34089	-3.4285
Au	-9.608125	5.5024986	-0.019197	H	-7.660876	-6.908631	-2.817211
Au	3.4186748	-4.153226	7.5928344	H	8.0201468	-8.502235	2.2210296
Au	-2.627363	-3.837321	8.2406984	H	6.7872165	-8.239812	3.5072664
Au	-3.383038	-4.236156	-7.603735	H	7.7200206	-6.838769	2.8450985
Au	2.6742525	-3.858338	-8.218119	H	8.8443632	-6.776107	-3.125025
Au	-3.356574	-8.618274	-3.929042	H	8.6242229	-5.365475	-4.214288
Au	-6.709631	-6.20993	0.3830158	H	7.2192535	-6.419878	-3.814104
Au	6.7661977	-6.1837	-0.344229	H	5.5629921	-10.1434	-2.758784
Au	2.8718193	-8.653901	-4.352255	H	4.7710044	-9.138296	-1.48735
Au	-2.812537	-8.636464	4.3962456	H	6.4746145	-8.823341	-1.936953

Au	3.4039824	-8.58227	3.9533484	H	0.864723	-7.7972	-7.055572
Au	0.0265565	-11.09894	0.0240911	H	-0.214634	-9.197962	-7.411871
Au	1.887455	5.0258709	7.5869856	H	1.5665439	-9.368728	-7.564663
Au	4.6372783	-0.344473	8.241469	H	-5.515126	-10.14784	2.8295876
Au	5.3344703	-0.897314	-7.561355	H	-4.717524	-9.156615	1.5496526
Au	2.0234793	4.156727	-8.246228	H	-6.421294	-8.833097	1.9920144
Au	9.1595726	1.3462109	-3.883694	H	-1.515411	-9.31959	7.6022687
Au	8.7409329	-2.736767	0.440765	H	-0.771955	-7.7689	7.0931179
Au	1.9622594	8.9049097	-0.378221	H	0.2696776	-9.195697	7.4575421
Au	6.0585983	6.7690331	-4.3921	H	2.7644974	-12.03222	3.9347328
Au	8.913391	1.9024724	4.3926141	H	1.7849202	-12.28068	2.4410383
Au	5.7381049	7.2372353	3.9295128	H	1.2307476	-11.12195	3.6916007
Au	9.589084	5.5688329	-0.007569	H	3.0815956	-8.885102	7.138516
S	-5.011687	1.3386397	8.3616838	H	1.8663933	-7.589601	6.8381044
S	-5.576941	-3.093406	6.8740423	H	3.2091726	-7.298404	7.9873475
S	-0.309022	3.0068185	9.3305965	H	-2.883587	-12.83606	0.9141705
S	-3.691405	5.4188525	7.1116305	H	-3.352369	-11.20888	0.3029362
S	-3.643617	3.6053696	-8.416439	H	-3.780683	-11.70365	1.9829731
S	-0.131011	6.3404313	-6.88238	H	3.8281962	-11.69837	-1.95416
S	-2.716261	-1.317322	-9.329351	H	2.9485748	-12.82784	-0.867633
S	-6.49969	0.4549351	-7.14747	H	3.4148706	-11.19275	-0.273936
S	-7.341994	7.7651526	-2.301845	H	3.9313759	2.5702559	10.539413
S	-4.222207	6.9906873	-5.700973	H	2.2268233	3.1506693	10.374992
S	-0.35814	9.2037212	2.0723288	H	3.5487681	4.3190096	10.727352
S	-3.646153	8.8841515	-1.301305	H	0.917126	8.0690765	5.224332
S	-9.537779	-1.353549	1.2579235	H	1.8616292	8.1602245	6.7402256
S	-8.136808	-4.386102	-2.083241	H	0.1799055	8.8129014	6.6894565
S	-9.33987	-0.358933	-3.68959	H	1.349364	-0.450419	11.097387
S	-8.583051	4.0210826	-5.314099	H	1.8749419	0.8987362	10.037083
S	-4.430932	8.2072309	3.663517	H	3.014968	0.2012678	11.245484
S	-7.833781	5.3483618	5.2977351	H	8.7599491	-0.329746	6.8356103
S	-10.43586	2.4269611	2.2612766	H	7.6073614	-1.687004	7.1300873
S	-8.237036	0.0559928	5.6410386	H	8.1573057	-0.662087	8.5028167
S	-8.91862	6.7890096	1.8302448	H	5.6083919	0.9842758	-10.68098
S	-10.37156	4.2568923	-1.867561	H	4.2500756	2.1472301	-10.47091
S	1.3588253	-4.970311	8.4084318	H	3.9515462	0.3670915	-10.35577
S	5.4962703	-3.310112	6.8818182	H	8.0721593	-3.019039	-7.103383
S	-2.502177	-1.741089	9.3270403	H	7.5208001	-4.384127	-6.063866
S	-2.82857	-5.908435	7.1440689	H	7.6120444	-2.721061	-5.391621
S	-1.295017	-5.014998	-8.387282	H	0.3359584	1.3371018	-11.09458
S	-5.437478	-3.348748	-6.879444	H	1.7532238	1.1352403	-10.01253
S	2.5292084	-1.772089	-9.314717	H	1.7290083	2.4600632	-11.23222
S	2.8913832	-5.919578	-7.112691	H	2.3102364	7.4003306	-7.174046

S	-3.015305	-10.28954	-2.307363	H	3.5019748	7.3635595	-8.521005
S	-3.971043	-7.196577	-5.678689	H	4.050555	7.7436639	-6.846229
S	-7.822832	-4.911124	2.0169473	H	10.264709	4.4983666	-3.646765
S	-5.878958	-7.640735	-1.308467	H	11.825736	3.6299635	-3.862727
S	5.9439773	-7.612504	1.3540296	H	11.530889	4.6179009	-2.382636
S	7.8565577	-4.884273	-1.991318	H	7.5757176	2.1881919	-6.779033
S	5.000629	-7.954725	-3.623883	H	7.9519215	0.8632149	-7.924262
S	0.8353935	-9.489677	-5.269749	H	9.2932921	1.7409343	-7.097193
S	-4.947103	-7.951688	3.6729717	H	10.282285	-4.093257	3.2686403
S	-0.776433	-9.466225	5.3102997	H	8.9801532	-4.743725	4.3200563
S	3.0848839	-10.256	2.3275283	H	9.0545443	-2.978942	3.9673721
S	3.9945381	-7.163167	5.7130803	H	10.609608	-1.720558	-3.376243
S	-1.451538	-11.13557	1.8596718	H	9.8091925	-3.223136	-2.770739
S	1.4990121	-11.14123	-1.813208	H	11.378498	-2.690456	-2.063495
S	3.6132528	3.6460359	8.4163948	H	2.0534083	10.046396	2.8294879
S	0.1375735	6.4131948	6.8485595	H	3.2783585	11.17174	2.1358606
S	2.7554338	-1.273213	9.329497	H	3.7529775	10.020229	3.4425783
S	6.531738	0.5073316	7.1446915	H	0.3345268	10.119251	-4.244547
S	5.0301738	1.3000957	-8.363283	H	1.9370899	9.3970217	-3.851273
S	5.6557339	-3.107739	-6.835488	H	1.4666863	10.98702	-3.153134
S	0.2929868	2.9804484	-9.339182	H	5.9902247	9.8470712	-2.820125
S	3.6937395	5.3865746	-7.141918	H	5.5125943	8.6739003	-1.533761
S	10.438336	2.4749144	-2.255905	H	4.3909616	9.9887491	-2.00392
S	8.2349575	0.1230524	-5.647537	H	8.0949531	4.3756234	-7.444797
S	8.1768921	-4.328474	2.0980367	H	7.2774579	5.9689206	-7.585125
S	9.557275	-1.312898	-1.264022	H	6.3386057	4.5319285	-7.064551
S	3.6097801	8.9171292	1.3204171	H	10.298854	0.4892608	1.5281693
S	0.2928059	9.2002741	-2.025085	H	10.892536	-1.13242	2.0045096
S	4.3777326	8.2559442	-3.669678	H	11.552219	0.3351116	2.817059
S	7.8010681	5.4139349	-5.293856	H	7.141325	3.2247601	7.0848734
S	9.37624	-0.288375	3.6653842	H	7.882597	4.8238835	7.4727402
S	8.5993861	4.0825795	5.2971691	H	8.8640976	3.3245417	7.5732862
S	7.3209844	7.8146383	2.2790517	H	9.7265922	7.6876384	2.3638482
S	4.2398869	6.9991322	5.7117156	H	9.0105546	6.679184	3.6624354
S	10.363622	4.3255972	1.8397068	H	9.0486557	8.4707042	3.8388277
S	8.8840613	6.853663	-1.856351	H	6.2256328	7.0065108	7.0900743
C	-4.662456	1.2116742	10.152119	H	5.661037	5.3237548	6.781421
C	-7.305425	-3.393805	6.3375678	H	4.7918776	6.3469974	7.9659826
C	-1.1411	1.9015986	10.534495	H	11.392824	2.6975283	0.3136258
C	-3.340154	7.1922032	7.3852592	H	12.020476	2.598565	1.9999823
C	-3.324864	3.3413376	-10.19675	H	12.561448	3.925705	0.916985
C	-0.767729	7.9781819	-6.360323	H	8.0251915	8.5378452	-0.284286
C	-2.175117	-0.059621	-10.54939	H	8.1658374	9.1418027	-1.976479

C	-7.86594	-0.72516	-7.438887	H	9.6381988	8.9670272	-0.962624
---	----------	----------	-----------	---	-----------	-----------	-----------

Table S4. The Cartesian coordinates of Au₁₈₈(SR)₆₆, R = CH₃.

Atoms	x	y	z	Atoms	x	y	z
Au	-1.413237	0.8456376	-7.233016	S	-5.565824	5.7984744	6.0292066
Au	2.9827125	-1.722681	-7.026066	S	-0.322354	10.440131	1.7482176
Au	-1.576318	0.8728474	7.1990271	S	-3.817157	10.149657	-1.389665
Au	0.0717878	3.3451819	-7.077338	S	4.4842684	9.0724719	-2.905586
Au	1.5533779	0.8047537	-7.212807	S	5.5744975	5.7452108	-6.06538
Au	-2.872102	-1.719326	-7.078713	S	9.3674571	3.5955776	1.8262844
Au	-0.069725	-1.681132	7.2253292	S	7.8366246	6.2967784	-1.70319
Au	-0.079882	3.4083911	7.0358022	S	6.6868579	7.0312875	3.3826545
Au	0.0454609	-1.745329	-7.207032	S	2.6242617	8.6217013	5.1956978
Au	2.8483668	-1.66979	7.0906346	S	3.8127336	10.143577	1.2915133
Au	1.3899478	0.8984137	7.2259428	S	0.3250933	10.426812	-1.859291
Au	-3.003343	-1.663914	7.0354118	S	-1.598009	-9.933291	1.7601354
Au	-3.048078	7.8110618	-1.627108	S	1.5365922	-9.952678	-1.742879
Au	-6.935163	-3.995422	-1.711036	S	-2.747491	-9.342688	-3.344055
Au	-1.73952	6.979728	3.9953788	S	-6.11187	-6.630844	-5.25716
Au	1.7238364	6.9415579	-4.063251	S	-5.692902	-8.405251	2.8998493
Au	-1.329247	6.9573367	-4.036946	S	-2.32958	-7.622447	6.1194856
Au	3.0299435	7.817566	1.5453822	S	-8.929522	-5.499089	1.7660595
Au	-2.973409	7.7597988	1.4403162	S	-6.903079	-8.394921	-1.345675
Au	-0.039759	7.9863995	1.6033772	S	-10.0919	-0.707064	-3.016921
Au	6.7579987	-2.338331	-3.919411	S	-7.712983	1.8555434	-6.181961
Au	0.0273892	7.9716178	-1.682428	S	-9.51944	2.3125749	3.2215564
Au	2.9568838	7.7408276	-1.515181	S	-8.867869	-1.967241	5.1289156
Au	-5.345535	-4.686478	-4.034423	S	-10.75198	-1.77538	1.2123154
Au	-5.283754	-6.439033	1.4892529	S	-9.20592	-4.966672	-1.88184
Au	-5.263392	-6.558864	-1.593125	S	9.4944751	2.269753	-3.261959
Au	-6.866415	-2.035675	-4.108522	S	8.8284627	-2.014647	-5.134862
Au	5.2087085	-6.571903	1.629404	S	10.062364	-0.714588	3.0146445
Au	-6.94951	-4.016599	1.6070836	S	7.6829867	1.8750063	6.1603288
Au	5.2099189	-4.979184	-3.982352	S	9.1656415	-4.971749	1.9196483
Au	6.831341	-2.019742	4.1181449	S	10.710468	-1.804434	-1.202383
Au	5.2987924	-4.676594	4.0634603	S	5.6425376	-8.436098	-2.832948
Au	8.3105667	-1.296702	-1.476068	S	2.2876476	-7.674606	-6.060002
Au	5.2369801	-6.460778	-1.436155	S	2.679135	-9.340041	3.3997095
Au	6.9140778	-4.036608	-1.582128	S	6.0688332	-6.623278	5.280866
Au	1.3246271	6.9932299	3.9600817	S	6.8472044	-8.410669	1.3867326

Au	6.8943229	-3.999902	1.7298357	S	8.8930661	-5.51798	-1.726278
Au	8.1717425	-1.345361	1.583397	S	-0.174804	-2.749784	9.4446007
Au	-6.789519	-2.298368	3.9344212	S	1.9684131	-6.254873	7.1623216
Au	-8.206153	-1.331894	-1.578574	S	4.3219487	-2.443257	8.8684699
Au	-8.341096	-1.269155	1.4851952	S	7.8981053	-3.200016	5.9620564
Au	-5.242762	-4.948389	4.0260876	S	2.4812047	1.3835102	9.3660821
Au	-4.445012	2.5011987	2.3842423	S	4.4390047	4.999482	7.1078064
Au	-0.038736	-5.06974	-2.417865	S	-0.170695	5.0971277	8.785933
Au	0.0680275	5.1425334	-2.389446	S	-1.26788	8.5293485	5.8143544
Au	-0.087368	5.1638804	2.3370268	S	-2.563378	1.6034671	9.3141691
Au	2.9920179	1.6202507	-4.853871	S	-6.657393	1.4534514	7.0202954
Au	2.8669797	5.1012248	2.4040377	S	-4.4133	-2.567466	8.8015914
Au	2.9542205	5.0121365	-2.407435	S	-6.834354	-5.250165	5.8452306
Au	-4.354115	2.5524816	-2.485833	S	2.4886659	1.4262866	-9.395327
Au	-4.493014	-4.256158	-0.054838	S	6.5561273	1.3524233	-7.0523
Au	4.3916357	5.7889326	0.0407496	S	4.4104172	-2.647726	-8.765874
Au	4.4308959	2.4739582	-2.408199	S	6.8038586	-5.337947	-5.789585
Au	-2.975368	-5.075095	-2.413275	S	0.1266286	-2.842229	-9.418571
Au	1.4408098	5.969955	0.0163351	S	-2.01415	-6.322286	-7.101164
Au	4.4165524	-0.939381	-4.71874	S	-4.361549	-2.508001	-8.838203
Au	-1.461461	5.9769913	-0.078047	S	-7.947221	-3.225837	-5.941421
Au	-1.359807	4.2122413	-4.796892	S	-2.496874	1.2973213	-9.384848
Au	-1.555845	4.2281119	4.7655366	S	-4.452668	4.9379632	-7.159245
Au	-4.49763	-2.55087	-2.397921	S	0.1940379	5.0061388	-8.84872
Au	-5.824425	0.0140093	-2.465271	S	1.2595258	8.4720292	-5.900876
Au	-5.871638	3.3711713	-0.070488	H	-9.196528	5.0388209	3.2477795
Au	1.5421142	4.1801363	-4.800414	H	-10.01738	6.5417469	2.6825174
Au	-0.012096	-3.394156	-4.864538	H	-8.661305	6.6418571	3.8648994
Au	-2.886725	5.0919097	-2.460722	H	-10.63545	5.3289694	-3.023777
Au	-4.364077	-0.833253	-4.836734	H	-9.96111	4.1000398	-4.15746
Au	-2.970175	5.0364876	2.3603187	H	-8.896234	5.3884149	-3.495576
Au	-4.411932	5.7975915	-0.096167	H	-7.997843	7.761656	-1.567965
Au	-7.250751	0.9042727	-0.044133	H	-7.165679	9.1405639	-2.384859
Au	-2.949157	-3.352453	-4.778225	H	-6.250898	8.0618884	-1.278282
Au	-2.869054	1.7056035	-4.906651	H	-2.771041	7.0080343	-7.162381
Au	4.4682533	-2.538618	2.4160966	H	-1.709227	8.424988	-7.491363
Au	4.4597213	-2.645622	-2.31294	H	-3.503783	8.606148	-7.527011
Au	2.8445904	1.7436071	4.8949944	H	-6.328823	8.5063109	1.3225509
Au	5.8824492	-0.065192	-2.349616	H	-5.618487	10.127859	0.9869459
Au	5.7992227	0.0210026	2.4628137	H	-6.728039	9.8966889	2.3901206
Au	-5.938701	-1.747978	-0.020515	H	-3.386402	6.1123371	7.1234781
Au	7.2293639	0.8871086	0.0371189	H	-4.570136	5.1997544	8.116543
Au	4.3342203	2.5670899	2.4624912	H	-4.717598	6.9886473	7.9711445

Au	-5.91183	-0.036153	2.3495533	H	-2.051951	10.369239	3.4823184
Au	5.9052856	-1.760795	0.0265393	H	-1.256482	11.97564	3.3401843
Au	1.349211	4.2601837	4.7516604	H	-0.39643	10.608965	4.148548
Au	4.4477048	-4.263668	0.0872981	H	-3.91218	10.96879	-3.649447
Au	2.9195664	-3.321226	4.7981937	H	-2.20672	10.857727	-3.091475
Au	2.9322492	-3.418561	-4.756899	H	-3.247182	12.207035	-2.514939
Au	-4.4918	-2.625238	2.3313765	H	6.7156901	9.8839053	-2.467167
Au	-2.939842	-5.055489	2.4017959	H	6.3248817	8.4926116	-1.397792
Au	-0.02218	-6.770284	0.0247399	H	5.6062129	10.110731	-1.062856
Au	4.3381311	-0.803721	4.8453783	H	4.7536068	6.9377641	-8.017974
Au	2.9284523	-5.056062	2.449804	H	4.5986266	5.1510819	-8.163962
Au	-2.967235	-3.378804	4.7858701	H	3.4083634	6.0680005	-7.182325
Au	2.8991194	-5.070617	-2.367575	H	10.612479	5.3583739	2.9149193
Au	2.8073918	-6.721537	0.0767026	H	9.9897489	4.1304548	4.0796789
Au	-2.855267	-6.717112	-0.027027	H	8.8854192	5.3938173	3.4327441
Au	-4.441798	-0.896898	4.7224659	H	8.6257642	6.5908032	-3.946888
Au	5.8468899	3.3560144	0.0371686	H	9.1694532	4.9981839	-3.313613
Au	-3.012125	1.6634479	4.8410571	H	9.9918866	6.5091417	-2.773428
Au	-0.016839	-3.360643	4.8877474	H	7.9869076	7.7414411	1.4864093
Au	-0.00676	-5.059103	2.451456	H	7.1611801	9.1378521	2.2804188
Au	-1.453591	0.8180149	-0.01914	H	6.2419474	8.0439888	1.1918674
Au	0.0100081	-0.008943	-2.43884	H	3.4918749	8.6701824	7.4451552
Au	-0.014888	-1.669111	0.0037311	H	2.7546162	7.0721386	7.0937503
Au	-0.038061	0.0012668	2.4329672	H	1.6963546	8.4952917	7.4046481
Au	1.4346998	0.8242095	0.0082629	H	2.2063022	10.879322	2.9843712
Au	1.4846083	2.495419	-2.403674	H	3.2609736	12.214795	2.4016804
Au	-0.010786	3.4067609	-0.017372	H	3.9097852	10.976726	3.5467497
Au	2.9297591	-0.037867	-2.373835	H	0.4020564	10.554755	-4.260539
Au	-2.898504	-0.00113	-2.429692	H	2.0566561	10.333578	-3.588381
Au	-2.918409	3.3245888	-0.033183	H	1.2552664	11.939685	-3.475402
Au	-1.434911	2.5336051	-2.417466	H	0.1746428	-10.41583	3.3947504
Au	-4.34612	0.8399352	-0.042632	H	-0.683766	-11.89811	2.8336818
Au	-2.965696	-0.024408	2.3685199	H	-1.479074	-10.77679	4.0012699
Au	-1.420751	-0.837165	-4.842614	H	0.6176216	-11.88874	-2.862684
Au	-1.503847	2.5176897	2.3833716	H	1.4407268	-10.75555	-3.998667
Au	2.8952029	3.3178236	0.0109094	H	-0.218973	-10.3891	-3.40957
Au	0.0600716	1.6501407	-4.840903	H	-2.766007	-10.81176	-1.440133
Au	1.4761935	-0.866021	-4.814662	H	-4.3761	-10.77382	-2.258754
Au	2.8731581	0.0094714	2.4370582	H	-3.880438	-9.431806	-1.170815
Au	2.9541821	-1.719502	0.0352323	H	-6.424232	-5.801349	-7.486818
Au	1.3987962	2.5412361	2.4057098	H	-5.709184	-7.456841	-7.485064
Au	-1.486829	-2.519263	2.407413	H	-4.668081	-6.031386	-7.151342
Au	1.4157643	-4.185407	0.0244038	H	-6.004915	-9.923082	1.0762189

Au	1.4451969	-2.513449	2.4158204	H	-5.220462	-10.7378	2.4827629
Au	-1.456764	-4.181588	0.0081892	H	-4.247785	-9.687862	1.397325
Au	-1.476174	-2.542126	-2.397462	H	-3.78153	-7.492813	8.0624206
Au	-1.499689	-0.838678	4.8225044	H	-3.746514	-5.914834	7.1844451
Au	1.4500443	-2.543964	-2.385976	H	-2.343752	-6.41634	8.1844199
Au	4.3277257	0.8323869	0.0407334	H	-8.003875	-6.949117	3.5103387
Au	1.3981569	-0.807968	4.8500391	H	-9.794145	-7.056702	3.3743515
Au	-0.077388	1.6839512	4.8265216	H	-9.031711	-5.625748	4.168781
Au	-2.986086	-1.720173	-0.023123	H	-8.948115	-8.975898	-2.48562
Au	4.4330479	4.0458545	-4.761585	H	-7.543195	-8.87903	-3.612934
Au	5.7898329	5.1113315	-2.372398	H	-8.342528	-7.374669	-3.040962
Au	-4.237261	4.2937314	-4.828873	H	-11.60516	-0.241563	-1.22118
Au	-7.275098	2.5754631	2.3104591	H	-11.88346	0.8660604	-2.619652
Au	4.215263	4.3326499	4.7852216	H	-10.51303	1.1658132	-1.497821
Au	5.8150013	4.9784146	2.4156191	H	-6.930537	-0.209485	-7.266435
Au	-5.809295	5.137754	2.3270267	H	-6.642605	1.2712111	-8.239191
Au	-5.690178	1.7399851	-4.845441	H	-8.297835	0.5670868	-8.155014
Au	-4.447636	4.0846947	4.7241308	H	-10.1131	1.3814973	1.0299613
Au	-7.32341	2.4158018	-2.48605	H	-10.75231	3.0389839	1.2888911
Au	-5.836645	4.9681452	-2.4618	H	-11.5467	1.6244672	2.0846595
Au	-1.579232	-5.867748	-4.756417	H	-7.630696	-1.034299	7.0342898
Au	5.6633585	1.7717055	4.8215827	H	-8.319911	-2.66818	7.3557466
Au	7.3027375	2.4255004	2.4616283	H	-9.387107	-1.214655	7.3598723
Au	1.5464114	-5.832597	4.806456	H	-10.59219	-3.529933	2.9111523
Au	-1.400807	-7.557539	-2.376662	H	-12.27627	-3.277284	2.3285929
Au	5.9204094	1.5052611	-4.715655	H	-11.5211	-2.096898	3.4679061
Au	7.263026	2.5458582	-2.333131	H	-10.96676	-4.957102	-3.510538
Au	1.5595817	-7.570057	-2.364027	H	-9.336335	-4.989695	-4.285096
Au	-1.400525	-5.807973	4.7963465	H	-9.998125	-3.445982	-3.633095
Au	1.3634513	-5.849638	-4.753162	H	11.529021	1.5932941	-2.131384
Au	-1.601233	-7.560233	2.423458	H	10.102453	1.3604657	-1.064061
Au	1.3572537	-7.536703	2.4376064	H	10.739559	3.0150863	-1.345413
Au	-5.941093	1.5487084	4.7066283	H	8.2681148	-2.731217	-7.353575
Au	-8.490255	4.8877671	-0.127147	H	9.3460055	-1.285228	-7.372193
Au	-4.597556	7.6932877	-4.294941	H	7.5911175	-1.090111	-7.044753
Au	-5.004654	7.3392627	4.3162773	H	11.578366	-0.253999	1.2194328
Au	-2.100909	10.297741	0.2213622	H	11.860587	0.8495362	2.6199411
Au	5.0075804	7.3094763	-4.377558	H	10.493144	1.1580548	1.4975483
Au	8.4725299	4.8678633	0.0575136	H	6.8732293	-0.173559	7.2556302
Au	4.5909465	7.7279929	4.2207309	H	6.587221	1.3165418	8.2116103
Au	2.1016774	10.303739	-0.327109	H	8.2379836	0.5991656	8.1521193
Au	-0.040025	-9.791379	-0.001091	H	9.9554121	-3.448111	3.6687995
Au	-4.383407	-7.893006	-4.238799	H	10.916518	-4.96444	3.5588446

Au	-3.930646	-7.931879	4.3957975	H	9.2815637	-4.987279	4.3236897
Au	-7.904465	-6.979714	0.2540503	H	11.462771	-2.130252	-3.463221
Au	-8.79664	0.6008639	-4.48872	H	10.552636	-3.569807	-2.889915
Au	-9.078876	0.1640837	4.1110822	H	12.239447	-3.296394	-2.324244
Au	-9.986714	-3.343647	-0.373233	H	5.9562616	-9.939941	-0.996993
Au	9.0425359	0.1217204	-4.134003	H	5.1592996	-10.76336	-2.391609
Au	8.7705986	0.6039895	4.4814821	H	4.198998	-9.697896	-1.311372
Au	9.9711302	-3.366131	0.4040526	H	2.3090704	-6.494693	-8.139148
Au	3.8823928	-7.985021	-4.333646	H	3.7460208	-7.567761	-7.999607
Au	4.3258228	-7.890359	4.2879511	H	3.7065442	-5.978105	-7.13943
Au	7.8544389	-6.964839	-0.186378	H	2.7065526	-10.87837	1.5555415
Au	0.8575763	-4.471073	8.193744	H	4.3451565	-10.71694	2.2981453
Au	6.0812638	-2.707417	7.3468924	H	3.7288673	-9.449615	1.1853285
Au	3.4650596	3.1591913	8.1721308	H	5.7517303	-7.423924	7.5304966
Au	-0.803915	6.71406	7.2141863	H	4.6124138	-6.077462	7.1811212
Au	-4.599877	1.5950095	8.1260955	H	6.3527699	-5.724575	7.4887559
Au	-5.490285	-3.927686	7.2303695	H	8.8823169	-9.012788	2.5346521
Au	4.4834146	1.4288775	-8.12769	H	7.4781929	-8.892993	3.6592435
Au	5.4898362	-4.019454	-7.204606	H	8.2953094	-7.40127	3.0822955
Au	-0.899091	-4.551035	-8.147483	H	9.7447683	-7.131514	-3.285367
Au	-6.120847	-2.744566	-7.314733	H	9.0060958	-5.712429	-4.123373
Au	-3.485834	3.0824439	-8.204218	H	7.9573766	-7.003917	-3.435841
Au	0.7956727	6.6467544	-7.285658	H	1.6139541	-1.176927	10.028139
C	-9.057727	6.0988963	2.9928961	H	1.8176441	-2.753233	10.865986
C	-9.748097	4.7288784	-3.279124	H	0.5515304	-1.598628	11.414717
C	-7.055773	8.1072167	-2.021913	H	1.6300483	-8.619975	7.0480357
C	-2.658459	8.0919268	-7.044307	H	0.0506245	-7.790522	7.2489016
C	-5.944323	9.4297279	1.7725477	H	1.1625231	-7.968745	8.660885
C	-4.437477	6.0625362	7.4458419	H	5.0515092	-0.131617	9.2900128
C	-1.093661	10.885608	3.3453453	H	5.8244677	-1.329046	10.391129
C	-3.226784	11.145498	-2.806943	H	4.1129731	-0.824086	10.642699
C	5.9349917	9.4136252	-1.848109	H	10.190882	-2.478112	5.9526548
C	4.4624251	6.0140047	-7.494142	H	9.5553486	-2.635344	7.632163
C	9.7425093	4.7463417	3.2009934	H	9.1552598	-1.188444	6.6244602
C	9.0307482	6.0610503	-3.071049	H	0.5875752	1.2541552	10.836966
C	7.0468699	8.0987843	1.9350441	H	0.6019185	2.8336816	9.9842972
C	2.646078	8.1550891	6.9645924	H	1.7341505	2.5451936	11.351933
C	3.2296853	11.155542	2.7008144	H	6.6542303	5.8689907	6.8955276
C	1.0967005	10.849234	-3.46175	H	6.7246224	4.0951223	7.1701132
C	-0.803029	-10.84489	3.1341873	H	6.3677724	5.2108762	8.5471455
C	0.750982	-10.83161	-3.143304	H	-1.507031	4.1469761	10.557312
C	-3.528451	-10.16648	-1.90496	H	-2.547233	4.5889379	9.1751892
C	-5.671299	-6.457268	-7.023698	H	-1.911173	5.879141	10.261337

C	-5.233892	-9.832006	1.8557366	H	-3.65815	8.6229747	6.4036722
C	-3.145582	-6.774365	7.5211449	H	-3.017638	10.175422	5.7950363
C	-8.928319	-6.375075	3.3714393	H	-2.626759	9.6536763	7.4741023
C	-8.054379	-8.397448	-2.766724	H	-1.555924	-0.032491	10.753669
C	-11.1212	0.39138	-1.981253	H	-3.047963	-0.697138	10.011217
C	-7.366369	0.746508	-7.596215	H	-3.172323	0.4839249	11.363061
C	-10.58877	2.0545794	1.7545037	H	-7.887588	3.0119069	8.3937405
C	-8.503752	-1.683759	6.8989885	H	-8.527911	2.9143899	6.71212
C	-11.33912	-2.779425	2.6243055	H	-7.051184	3.8786425	7.0474532
C	-9.949982	-4.533703	-3.495278	H	-2.691929	-4.287442	9.1594923
C	10.572622	2.0258214	-1.799591	H	-4.132902	-4.507855	10.218292
C	8.4602776	-1.744239	-6.905246	H	-2.920941	-3.224219	10.576968
C	11.096508	0.3793467	1.9804858	H	-7.45386	-7.569255	5.9081578
C	7.3145805	0.7811527	7.5816246	H	-7.071495	-6.949533	7.5582095
C	9.9019377	-4.535973	3.5367406	H	-5.749445	-7.385956	6.4064184
C	11.294692	-2.810059	-2.614776	H	2.3030404	0.2802023	-11.49854
C	5.1817392	-9.852228	-1.773103	H	1.7612242	-0.778227	-10.13979
C	3.1091271	-6.84293	-7.468302	H	3.5097261	-0.542371	-10.44623
C	3.4499272	-10.17436	1.9598556	H	7.6844759	2.8970014	-8.52742
C	5.6401095	-6.438655	7.0500842	H	8.4508275	2.8031628	-6.898821
C	7.994508	-8.421991	2.8108962	H	6.958377	3.7764655	-7.126607
C	8.8884745	-6.438654	-3.306337	H	4.1144143	-4.58235	-10.18493
C	1.0928726	-1.995061	10.540441	H	2.909157	-3.292632	-10.53681
C	1.0999031	-7.810169	7.57358	H	2.6806733	-4.358271	-9.119128
C	4.8887623	-1.032113	9.8919749	H	7.3282105	-7.682568	-5.754632
C	9.337294	-2.27144	6.6163601	H	7.1610918	-7.070184	-7.439333
C	1.2207106	2.0860345	10.493504	H	5.6982506	-7.439335	-6.443239
C	6.2315178	5.0299114	7.4701407	H	-1.860803	-2.862199	-10.84376
C	-1.69594	4.9090507	9.7872156	H	-0.60043	-1.700518	-11.39346
C	-2.803365	9.3112464	6.4426796	H	-1.667528	-1.280232	-10.01126
C	-2.595936	0.1874972	10.472654	H	-1.204463	-8.04556	-8.586532
C	-7.616764	2.9799306	7.3269791	H	-1.677522	-8.68675	-6.970828
C	-3.438089	-3.775712	9.7789871	H	-0.097652	-7.859495	-7.17234
C	-6.756344	-6.959785	6.5038294	H	-5.867154	-1.40092	-10.3622
C	2.5231446	-0.061379	-10.47409	H	-4.155197	-0.908532	-10.63136
C	7.4954731	2.8721302	-7.442772	H	-5.080707	-0.196744	-9.278864
C	3.4254459	-3.847505	-9.740713	H	-10.25082	-2.543821	-5.971769
C	6.7255658	-7.055102	-6.428559	H	-9.560986	-2.59492	-7.636192
C	-1.14186	-2.098022	-10.51937	H	-9.217108	-1.201709	-6.537578
C	-1.145937	-7.880417	-7.499606	H	-1.745439	2.2991288	-11.44927
C	-4.926131	-1.104606	-9.872069	H	-0.507594	1.2001206	-10.73193
C	-9.380336	-2.286438	-6.59464	H	-0.731782	2.8541718	-10.07084
C	-1.239086	1.9936716	-10.51946	H	-6.742424	4.0482612	-7.232509

C	-6.242289	4.9793625	-7.532425	H	-6.369801	5.156462	-8.611165
C	1.7578615	4.7607117	-9.773786	H	-6.664119	5.8223927	-6.962969
C	2.7975196	9.2519456	-6.52566	H	2.0313007	5.7145501	-10.25113
S	-7.853181	6.3204689	1.63239	H	1.5817745	3.992815	-10.54105
S	-9.391482	3.5992459	-1.882681	H	2.5664569	4.4237922	-9.11528
S	-6.701427	7.0163048	-3.452887	H	2.6156281	9.616795	-7.548466
S	-2.628806	8.5744199	-5.280079	H	3.026593	10.099066	-5.861489
S	-4.492068	9.09731	2.8306482	H	3.645686	8.5551332	-6.507952

Refs.

1. T. D. Kühne, M. Iannuzzi, M. Del Ben, V. V. Rybkin, P. Seewald, F. Stein, T. Laino, R. Z. Khaliullin, O. Schütt, F. Schiffmann, D. Golze, J. Wilhelm, S. Chulkov, M. H. Bani-Hashemian, V. Weber, U. Borštnik, M. Taillefumier, A. S. Jakobovits, A. Lazzaro, H. Pabst, T. Müller, R. Schade, M. Guidon, S. Andermatt, N. Holmberg, G. K. Schenter, A. Hehn, A. Bussy, F. Belleflamme, G. Tabacchi, A. Glöß, M. Lass, I. Bethune, C. J. Mundy, C. Plessl, M. Watkins, J. VandeVondele, M. Krack and J. Hutter, *J. Chem. Phys.*, 2020, **152**, 194103.
2. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
3. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396-1396.
4. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
5. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
6. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.
7. T. Lu, *J. Chem. Phys.*, 2024, **161**, 082503.
8. F. Neese, *WIREs Computational Molecular Science*, 2018, **8**, e1327.
9. F. Neese, *WIREs Computational Molecular Science*, 2012, **2**, 73-78.
10. F. Weigend and R. Ahlrichs, *Physical Chemistry Chemical Physics*, 2005, **7**, 3297-3305.