

Supplementary Information S2

Modulation of the photoelectrochemical behavior of Au nanocluster–TiO₂ electrode by doping

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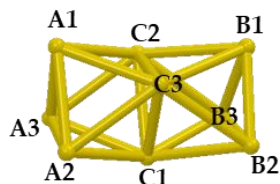
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xyz coordinates of $\text{Au}_{18}(\text{SCH}_3)_{14}$ and five lowest energy isomers of $\text{Au}_{18-x}\text{Ag}_x(\text{SCH}_3)_{14}$ with $1 \leq x \leq 4$ at each x value.

1. $\text{Au}_{18}(\text{SCH}_3)_{14}$



88			
Au	-1.35123	-1.31865	0.486057
Au	1.085413	-2.45128	-1.16965
Au	0.97715	0.198773	0.431214
Au	-1.24084	0.877119	-1.32279
Au	-1.63455	-4.76716	-0.46317
Au	-1.15282	-1.78441	-2.62773
Au	1.169357	-0.16624	-2.71148
Au	1.284511	-2.53609	2.336542
Au	-4.37998	-0.7723	-1.49112
Au	4.184213	-0.37372	-1.15638
Au	-2.95353	1.199049	0.995678
Au	-0.59688	2.730661	0.907507
Au	1.550572	3.283387	-1.7515
Au	-3.00601	3.952806	-0.79288
Au	-0.80221	0.553915	2.729338
Au	0.17356	-4.5646	-3.66974
Au	3.070538	-2.32179	-4.07943
Au	-2.81587	3.658589	2.813612
S	-2.14031	2.78873	-2.68124
S	-2.30458	-3.42624	1.3677
S	-3.48418	-1.81852	-3.43015
S	1.976591	-3.96927	0.560493
S	3.348471	0.876593	0.673653
S	-5.18583	0.300784	0.482298
S	2.194468	1.909836	-3.58354
S	0.842125	4.574009	0.128162
S	0.570064	-1.09999	4.088148
S	-0.90554	-6.14535	-2.25694
S	5.062228	-1.55562	-3.02544
S	-3.75665	5.120322	1.156312
S	-2.03582	2.120272	4.444517

S	1.182794	-3.13223	-5.28324
C	-4.141	-3.34148	1.29552
C	-4.06004	-3.56664	-3.39039
C	0.472746	-7.11895	-1.51163
C	-6.2287	1.715419	-0.06655
C	3.814065	-3.88119	0.498812
C	4.005156	0.077948	2.196183
C	-0.73097	-2.04833	4.983305
C	1.110063	2.437296	-4.97624
C	-3.5861	2.193109	-3.64829
C	1.877596	-4.28141	-6.54828
C	5.668636	-0.21	-4.13303
C	2.296022	4.614935	1.258818
C	-2.68722	6.622166	1.20278
C	-0.60286	2.933749	5.267607
H	-4.53983	-4.32607	1.576729
H	-4.49647	-3.0626	0.295152
H	-4.47502	-2.58588	2.019737
H	-3.81448	-4.05331	-2.43703
H	-3.55995	-4.10062	-4.21045
H	-5.14684	-3.57926	-3.55153
H	0.984826	-7.65998	-2.31907
H	0.028554	-7.83909	-0.81043
H	1.177362	-6.46783	-0.97814
H	-7.12757	1.315397	-0.55574
H	-5.68729	2.376854	-0.75569
H	-6.51852	2.283015	0.828718
H	4.148216	-4.4627	-0.37178
H	4.217757	-4.32986	1.417063
H	4.168123	-2.84628	0.39658
H	5.09443	0.220519	2.220032
H	3.761836	-0.99198	2.23284
H	3.547671	0.577765	3.061289
H	-0.24365	-2.82867	5.584609
H	-1.43995	-2.50928	4.283079
H	-1.26176	-1.3494	5.645292
H	1.205465	1.693	-5.77905
H	1.461208	3.414447	-5.33657
H	0.063208	2.51483	-4.65565
H	-4.29711	1.64048	-3.02003
H	-3.21138	1.524711	-4.43601
H	-4.07996	3.0624	-4.1044
H	1.036514	-4.77021	-7.05949

H	2.530354	-5.03896	-6.09721
H	2.447851	-3.68265	-7.27215
H	5.967627	-0.66442	-5.08755
H	6.544625	0.24846	-3.65366
H	4.89262	0.548675	-4.29841
H	3.035903	5.310257	0.837761
H	2.744347	3.619054	1.367588
H	1.957511	4.989551	2.235095
H	-3.01349	7.289817	0.393383
H	-1.62852	6.364996	1.068754
H	-2.83988	7.117308	2.171621
H	0.084303	3.382072	4.539119
H	-0.0696	2.162032	5.840988
H	-0.97696	3.708756	5.951233

2. $\text{Au}_{17}\text{Ag}(\text{SCH}_3)_{14} : \text{C}_1$

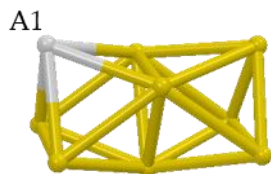


88	C1		
Au	-1.31034	-1.3575	0.59601
Au	1.076744	-2.47443	-1.09398
Au	0.97268	0.173987	0.487414
Ag	-1.25345	0.858067	-1.39039
Au	-1.65384	-4.7969	-0.49621
Au	-1.13027	-1.82977	-2.58221
Au	1.183973	-0.221	-2.66555
Au	1.290927	-2.51957	2.406708
Au	-4.33934	-0.73104	-1.56634
Au	4.195326	-0.37179	-1.18213
Au	-2.92517	1.151173	0.996272
Au	-0.59264	2.686712	0.904696
Au	1.484074	3.244773	-1.7973
Au	-3.01853	3.958017	-0.72618
Au	-0.79683	0.546235	2.747835
Au	0.216947	-4.61283	-3.66972
Au	3.109852	-2.364	-4.08173
Au	-2.78784	3.608147	2.8886
S	-2.21178	2.878657	-2.67855

S	-2.39159	-3.46912	1.316765
S	-3.41843	-1.79031	-3.48426
S	1.987678	-3.97105	0.646027
S	3.346993	0.908909	0.618769
S	-5.15973	0.314739	0.411584
S	2.13832	1.850154	-3.60707
S	0.787139	4.550699	0.073628
S	0.581331	-1.07576	4.15316
S	-0.86571	-6.18685	-2.25516
S	5.091325	-1.57867	-3.02549
S	-3.75159	5.079497	1.259394
S	-1.98788	2.069474	4.511083
S	1.222574	-3.17763	-5.28035
C	-4.21865	-3.34318	1.148587
C	-4.0408	-3.5237	-3.45936
C	0.509194	-7.13178	-1.46756
C	-6.17803	1.755901	-0.11203
C	3.823681	-3.86153	0.571374
C	4.03616	0.162518	2.154106
C	-0.72352	-2.01153	5.056303
C	1.026935	2.317921	-5.00032
C	-3.69231	2.357651	-3.63921
C	1.916321	-4.32095	-6.55114
C	5.695428	-0.24417	-4.1482
C	2.263477	4.62799	1.173272
C	-2.70244	6.594462	1.320566
C	-0.54261	2.879333	5.315956
H	-4.6526	-4.32568	1.38155
H	-4.51389	-3.0313	0.138252
H	-4.57631	-2.5991	1.87341
H	-3.8381	-4.01429	-2.49811
H	-3.52798	-4.07142	-4.2623
H	-5.12172	-3.50902	-3.65583
H	1.044821	-7.67692	-2.2567
H	0.059794	-7.84834	-0.76608
H	1.194701	-6.46517	-0.92849
H	-7.0743	1.379367	-0.62423
H	-5.61804	2.429061	-0.7745
H	-6.47362	2.301859	0.794661
H	4.159498	-4.45754	-0.28879
H	4.23924	-4.28516	1.496144
H	4.163729	-2.82472	0.444279
H	5.125096	0.309788	2.155541

H	3.798823	-0.90678	2.228848
H	3.591345	0.687919	3.010679
H	-0.23978	-2.78392	5.670596
H	-1.43164	-2.48087	4.3611
H	-1.25619	-1.30225	5.7057
H	1.117651	1.547326	-5.77828
H	1.363838	3.285314	-5.39838
H	-0.01548	2.398104	-4.66641
H	-4.36839	1.730637	-3.04196
H	-3.33979	1.773556	-4.50118
H	-4.22441	3.250247	-3.99601
H	1.074943	-4.81033	-7.0612
H	2.57253	-5.07821	-6.10479
H	2.482534	-3.71846	-7.27512
H	6.001594	-0.7094	-5.0952
H	6.566303	0.226311	-3.67117
H	4.915854	0.507389	-4.32795
H	2.979747	5.335403	0.731968
H	2.734418	3.642156	1.278612
H	1.93793	5.002347	2.153975
H	-3.04925	7.272845	0.52878
H	-1.6426	6.354767	1.164952
H	-2.84626	7.069403	2.300811
H	0.128304	3.339462	4.579619
H	0.005397	2.104024	5.870287
H	-0.90679	3.645028	6.015271

3. $\text{Au}_{17}\text{Ag}(\text{SCH}_3)_{14} : \text{A1}$



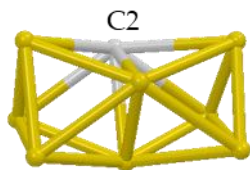
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Au	-1.38224	-1.27468	0.467268
Au	1.068772	-2.40558	-1.22183
Au	0.962663	0.234937	0.414251
Au	-1.23029	0.894614	-1.33912
Au	-1.62408	-4.73193	-0.43712
Au	-1.1711	-1.73548	-2.68072
Au	1.150123	-0.12127	-2.76618

Au	1.291939	-2.55046	2.295783
Au	-4.40179	-0.79303	-1.4472
Au	4.166752	-0.3699	-1.1389
Au	-2.94356	1.219689	0.946367
Au	-0.60889	2.713394	0.874649
Au	1.600413	3.297974	-1.70776
Au	-2.98669	3.949157	-0.88733
Ag	-0.81343	0.534859	2.81046
Au	0.153301	-4.54557	-3.66802
Au	3.052576	-2.3062	-4.07921
Au	-2.83289	3.697134	2.723362
S	-2.13079	2.763647	-2.76395
S	-2.26631	-3.38448	1.400491
S	-3.52611	-1.80748	-3.41308
S	1.954326	-3.95048	0.479804
S	3.338609	0.858731	0.710409
S	-5.18541	0.257392	0.550212
S	2.224245	1.956713	-3.57227
S	0.90136	4.559697	0.196642
S	0.614746	-1.17338	4.101712
S	-0.92896	-6.11338	-2.24154
S	5.039702	-1.53707	-3.01853
S	-3.73603	5.150839	1.037012
S	-2.1017	2.200391	4.407276
S	1.17557	-3.132	-5.29092
C	-4.10561	-3.33315	1.371227
C	-4.06958	-3.56587	-3.37318
C	0.449879	-7.09901	-1.5132
C	-6.26885	1.651421	0.025666
C	3.792507	-3.89389	0.406671
C	3.985412	0.027465	2.218928
C	-0.65327	-2.16863	4.995517
C	1.166444	2.545301	-4.96117
C	-3.58426	2.139229	-3.70164
C	1.884778	-4.29827	-6.5322
C	5.649671	-0.18594	-4.11701
C	2.338209	4.554504	1.34753
C	-2.64701	6.639291	1.074324
C	-0.70808	3.058104	5.255679
H	-4.47796	-4.31836	1.68482
H	-4.48977	-3.08578	0.373339
H	-4.43736	-2.56695	2.085163
H	-3.7976	-4.05301	-2.42728

H	-3.57655	-4.08665	-4.20588
H	-5.15896	-3.59658	-3.51338
H	0.948772	-7.64293	-2.32695
H	0.008217	-7.81661	-0.8078
H	1.164637	-6.45299	-0.98694
H	-7.17677	1.234053	-0.43148
H	-5.76161	2.315931	-0.68584
H	-6.539	2.22074	0.92605
H	4.111228	-4.44951	-0.48642
H	4.193053	-4.3828	1.305636
H	4.16531	-2.86265	0.340179
H	5.076098	0.158862	2.24328
H	3.730404	-1.04023	2.237082
H	3.533988	0.51681	3.093075
H	-0.15325	-2.97948	5.543355
H	-1.38834	-2.5952	4.3001
H	-1.1602	-1.50403	5.709783
H	1.264803	1.827141	-5.78717
H	1.534705	3.529325	-5.28367
H	0.116027	2.624495	-4.65275
H	-4.29126	1.608337	-3.0508
H	-3.21589	1.445745	-4.47031
H	-4.08084	2.994156	-4.18138
H	1.049933	-4.79513	-7.04586
H	2.533236	-5.04872	-6.06349
H	2.462582	-3.70899	-7.25786
H	5.948625	-0.63532	-5.07393
H	6.526357	0.267091	-3.63364
H	4.875723	0.57575	-4.27793
H	3.096451	5.244198	0.950729
H	2.767789	3.54919	1.444171
H	1.991504	4.917303	2.325437
H	-2.94885	7.295092	0.246074
H	-1.58909	6.366552	0.966752
H	-2.81197	7.155592	2.030065
H	0.03107	3.44265	4.541235
H	-0.22391	2.322587	5.91417
H	-1.10173	3.886334	5.861121

4. $\text{Au}_{17}\text{Ag}(\text{SCH}_3)_{14} : \text{C}_2$



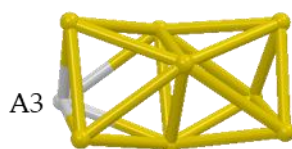
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Au	-1.42466	-1.28831	0.438099
Au	1.044927	-2.45538	-1.1546
Ag	1.006757	0.170211	0.430504
Au	-1.27916	0.876892	-1.33738
Au	-1.61299	-4.76778	-0.44875
Au	-1.1833	-1.78766	-2.61766
Au	1.137701	-0.17038	-2.6951
Au	1.301727	-2.50764	2.323565
Au	-4.41192	-0.76933	-1.49586
Au	4.192967	-0.36634	-1.13597
Au	-2.99158	1.20029	0.975333
Au	-0.62643	2.682562	0.895243
Au	1.572798	3.239318	-1.70903
Au	-3.00384	3.975738	-0.82922
Au	-0.87222	0.511391	2.714055
Au	0.155912	-4.56323	-3.67321
Au	3.042355	-2.31545	-4.08043
Au	-2.86049	3.674363	2.787961
S	-2.12144	2.81969	-2.7139
S	-2.26084	-3.42752	1.389598
S	-3.51152	-1.83108	-3.42501
S	1.985297	-3.9553	0.559443
S	3.428179	0.885167	0.717232
S	-5.23651	0.318657	0.46093
S	2.204225	1.885001	-3.55915
S	0.851456	4.512213	0.17474
S	0.566864	-1.06642	4.059443
S	-0.90616	-6.14677	-2.25109
S	5.031784	-1.55772	-3.02167
S	-3.77423	5.135253	1.114797
S	-2.09141	2.151802	4.434867
S	1.153324	-3.12245	-5.28576
C	-4.10046	-3.37047	1.35771
C	-4.08224	-3.58048	-3.36507
C	0.481166	-7.12018	-1.52259
C	-6.2646	1.735086	-0.11168
C	3.820824	-3.85634	0.466418
C	4.116287	0.063613	2.214902

C	-0.68851	-2.0508	4.981834
C	1.127022	2.446021	-4.94465
C	-3.56254	2.229994	-3.69324
C	1.851039	-4.26618	-6.55437
C	5.652677	-0.22049	-4.13077
C	2.285342	4.546879	1.330253
C	-2.70194	6.634633	1.178832
C	-0.64233	2.961932	5.232665
H	-4.48088	-4.36156	1.641587
H	-4.48127	-3.0905	0.366984
H	-4.42826	-2.62353	2.093767
H	-3.83387	-4.05559	-2.40666
H	-3.58234	-4.12228	-4.1801
H	-5.16932	-3.5977	-3.52389
H	0.984373	-7.66051	-2.33607
H	0.045426	-7.8408	-0.81664
H	1.191643	-6.46919	-0.99697
H	-7.16242	1.337907	-0.60511
H	-5.71204	2.386023	-0.80189
H	-6.55791	2.313141	0.775746
H	4.143506	-4.43373	-0.41116
H	4.240979	-4.30563	1.376909
H	4.16617	-2.8188	0.361477
H	5.209425	0.173463	2.215926
H	3.845851	-0.99977	2.259017
H	3.696798	0.57179	3.094667
H	-0.16537	-2.81158	5.577958
H	-1.39429	-2.53755	4.296004
H	-1.2288	-1.36498	5.64971
H	1.205787	1.706998	-5.75411
H	1.497852	3.418783	-5.29705
H	0.08281	2.542786	-4.62056
H	-4.27294	1.666926	-3.07355
H	-3.18209	1.572782	-4.48766
H	-4.06017	3.101316	-4.14148
H	1.012028	-4.75727	-7.06664
H	2.507613	-5.02194	-6.10597
H	2.4185	-3.66308	-7.27677
H	5.947889	-0.67794	-5.08507
H	6.532789	0.229511	-3.65077
H	4.884591	0.546128	-4.29633
H	3.022973	5.258507	0.933282
H	2.743627	3.554372	1.426936

H	1.926162	4.900025	2.307065
H	-3.01216	7.303088	0.363834
H	-1.64176	6.37464	1.063417
H	-2.86918	7.130663	2.14484
H	0.054825	3.37125	4.49064
H	-0.1248	2.19766	5.830102
H	-0.99638	3.76656	5.892349

5. $\text{Au}_{17}\text{Ag}(\text{SCH}_3)_{14} : \text{A}_3$



88

Au	-1.34672	-1.35346	0.508984
Au	1.052042	-2.48537	-1.17422
Au	0.95113	0.194827	0.464556
Au	-1.26912	0.849649	-1.27103
Au	-1.64893	-4.7948	-0.47427
Au	-1.18524	-1.81371	-2.62176
Au	1.126002	-0.19025	-2.70298
Au	1.323843	-2.52722	2.334963
Au	-4.43934	-0.75497	-1.52755
Au	4.148246	-0.34579	-1.14324
Au	-3.01591	1.105751	1.022205
Ag	-0.61638	2.736156	0.900697
Au	1.519904	3.287666	-1.72239
Au	-2.97194	3.938214	-0.7759
Au	-0.87199	0.503193	2.720709
Au	0.174888	-4.5988	-3.67067
Au	3.061188	-2.3325	-4.05837
Au	-2.80364	3.626028	2.815416
S	-2.10323	2.768692	-2.65395
S	-2.32929	-3.46024	1.358418
S	-3.51381	-1.83171	-3.434
S	1.985474	-3.97476	0.559578
S	3.302185	0.918967	0.674615
S	-5.28127	0.346512	0.415928
S	2.160576	1.889454	-3.54158
S	0.852563	4.636557	0.123021
S	0.636693	-1.07629	4.085772

S	-0.90835	-6.17861	-2.2599
S	5.039907	-1.54204	-2.99604
S	-3.73615	5.096255	1.169018
S	-2.03742	2.067614	4.430902
S	1.190361	-3.16219	-5.27594
C	-4.16312	-3.34501	1.260702
C	-4.10459	-3.57493	-3.3811
C	0.468266	-7.1461	-1.50321
C	-6.24207	1.804262	-0.16718
C	3.820974	-3.87896	0.462
C	3.983204	0.148386	2.201396
C	-0.61113	-2.04409	5.035567
C	1.106171	2.428041	-4.95244
C	-3.54964	2.200539	-3.63795
C	1.90527	-4.30571	-6.53453
C	5.643033	-0.20265	-4.11273
C	2.324482	4.684816	1.231902
C	-2.69737	6.618475	1.228058
C	-0.58484	2.840912	5.259835
H	-4.58262	-4.32962	1.509792
H	-4.49943	-3.03397	0.262942
H	-4.49602	-2.60393	2.000414
H	-3.8674	-4.05478	-2.42217
H	-3.60414	-4.12006	-4.19361
H	-5.19061	-3.58089	-3.54806
H	0.984452	-7.69071	-2.30564
H	0.022889	-7.86326	-0.79973
H	1.170164	-6.49127	-0.97079
H	-7.13587	1.442974	-0.69445
H	-5.64699	2.44558	-0.83056
H	-6.54507	2.380533	0.718093
H	4.140824	-4.45624	-0.41678
H	4.244204	-4.3288	1.370848
H	4.168706	-2.84217	0.356736
H	5.067796	0.323894	2.221159
H	3.77257	-0.92816	2.243662
H	3.512769	0.638488	3.065017
H	-0.08898	-2.81513	5.6193
H	-1.34141	-2.51872	4.367019
H	-1.12757	-1.3532	5.7173
H	1.209829	1.685636	-5.75602
H	1.470979	3.403697	-5.30336
H	0.054504	2.513261	-4.64993

H	-4.2777	1.658803	-3.01982
H	-3.1763	1.527391	-4.42225
H	-4.02187	3.079476	-4.09854
H	1.072874	-4.80052	-7.05413
H	2.559113	-5.05868	-6.07753
H	2.478243	-3.70254	-7.25263
H	5.946656	-0.66327	-5.06285
H	6.515572	0.263855	-3.63478
H	4.863744	0.550858	-4.28569
H	3.078574	5.350136	0.788724
H	2.755085	3.684593	1.37008
H	2.005434	5.096081	2.200531
H	-3.03583	7.281943	0.420388
H	-1.63309	6.384997	1.095569
H	-2.86458	7.105406	2.198474
H	0.0991	3.305747	4.538612
H	-0.05328	2.046922	5.803421
H	-0.94554	3.598195	5.969991

6. $\text{Au}_{17}\text{Ag}(\text{SCH}_3)_{14} : \text{A}_2$



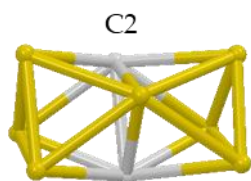
88 A2

Au	-1.36494	-1.29356	0.506237
Au	1.125182	-2.44099	-1.18628
Au	0.980549	0.181565	0.426096
Au	-1.23405	0.89724	-1.27864
Au	-1.6397	-4.74329	-0.4509
Au	-1.12451	-1.75877	-2.61962
Au	1.193907	-0.15295	-2.71618
Au	1.287758	-2.57883	2.325164
Au	-4.37257	-0.75251	-1.44906
Au	4.191547	-0.37516	-1.14903
Ag	-2.97467	1.253402	0.991981
Au	-0.50317	2.733894	0.932372
Au	1.525325	3.322984	-1.79678
Au	-3.00117	3.954058	-0.75216
Au	-0.75775	0.570925	2.715216
Au	0.189594	-4.56573	-3.65657

Au	3.096947	-2.33136	-4.07401
Au	-2.77668	3.66456	2.822898
S	-2.14786	2.788663	-2.64038
S	-2.32544	-3.39927	1.373476
S	-3.45955	-1.78102	-3.39343
S	1.992618	-3.98479	0.532732
S	3.347992	0.870404	0.681983
S	-5.24957	0.295144	0.499888
S	2.182112	1.932198	-3.60889
S	0.823557	4.631698	0.074311
S	0.554562	-1.17158	4.089843
S	-0.90537	-6.12934	-2.23618
S	5.082105	-1.55148	-3.01635
S	-3.73083	5.140415	1.191487
S	-2.0082	2.084192	4.415645
S	1.214001	-3.15287	-5.2779
C	-4.16223	-3.33032	1.299173
C	-4.03507	-3.52938	-3.37406
C	0.463282	-7.11005	-1.48275
C	-6.31366	1.680984	-0.08481
C	3.831053	-3.90517	0.486037
C	3.997211	0.064663	2.203932
C	-0.77739	-2.11831	4.938949
C	1.085902	2.427079	-5.00448
C	-3.59633	2.195829	-3.60563
C	1.911084	-4.31408	-6.53032
C	5.683079	-0.20167	-4.12183
C	2.310325	4.724607	1.159582
C	-2.6439	6.630938	1.215132
C	-0.60397	2.886275	5.298002
H	-4.55151	-4.3223	1.567582
H	-4.51904	-3.04149	0.302176
H	-4.50462	-2.58753	2.032647
H	-3.79104	-4.0258	-2.42526
H	-3.53419	-4.05521	-4.19892
H	-5.12177	-3.53985	-3.53626
H	0.972459	-7.6592	-2.28656
H	0.012209	-7.82318	-0.77879
H	1.171887	-6.46145	-0.95148
H	-7.18447	1.267934	-0.61203
H	-5.76767	2.366336	-0.7469
H	-6.65445	2.233501	0.802415
H	4.169037	-4.47379	-0.39164

H	4.225829	-4.371	1.399603
H	4.191115	-2.87062	0.403677
H	5.087059	0.202109	2.23208
H	3.748678	-1.0042	2.236038
H	3.539003	0.563762	3.069031
H	-0.31709	-2.92437	5.527532
H	-1.48398	-2.54661	4.215763
H	-1.30541	-1.42696	5.611228
H	1.188861	1.674314	-5.79836
H	1.421283	3.404584	-5.37857
H	0.03903	2.493462	-4.68148
H	-4.30735	1.645001	-2.97602
H	-3.22328	1.526286	-4.39303
H	-4.0875	3.066911	-4.06127
H	1.071187	-4.80502	-7.0415
H	2.55982	-5.06962	-6.07038
H	2.486236	-3.72283	-7.25656
H	5.988766	-0.6543	-5.07513
H	6.554082	0.263389	-3.63964
H	4.902568	0.551482	-4.2909
H	3.026763	5.41872	0.697943
H	2.77668	3.738522	1.28201
H	1.995717	5.120085	2.135599
H	-2.98008	7.299709	0.410746
H	-1.59056	6.363382	1.060321
H	-2.77362	7.129696	2.185414
H	0.08835	3.374082	4.600683
H	-0.07011	2.099774	5.849962
H	-1.00531	3.626452	6.004339

7. $\text{Au}_{16}\text{Ag}_2(\text{SCH}_3)_{14}$: C1, C2

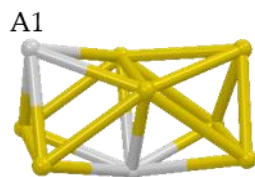


88	C1		
Au	-1.37698	-1.30326	0.540205
Au	1.046222	-2.47171	-1.08332
Ag	1.019097	0.167443	0.459109
Ag	-1.29148	0.87444	-1.41049

Au	-1.62493	-4.79173	-0.49652
Au	-1.16038	-1.82451	-2.56493
Au	1.15642	-0.21926	-2.65109
Au	1.29037	-2.50569	2.3847
Au	-4.37464	-0.74161	-1.54073
Au	4.22213	-0.37077	-1.14023
Au	-2.95685	1.168105	0.974676
Au	-0.61634	2.648613	0.882865
Au	1.517436	3.204897	-1.75919
Au	-3.02918	3.972281	-0.77632
Au	-0.84629	0.522431	2.724886
Au	0.20378	-4.59305	-3.68514
Au	3.094242	-2.34229	-4.07824
Au	-2.81886	3.64473	2.855772
S	-2.22033	2.889482	-2.72661
S	-2.32667	-3.4705	1.332901
S	-3.45121	-1.80639	-3.45548
S	1.984554	-3.96786	0.635018
S	3.444846	0.896908	0.696167
S	-5.2035	0.324589	0.422554
S	2.153977	1.829803	-3.58929
S	0.810925	4.496564	0.11424
S	0.564203	-1.05182	4.112403
S	-0.86959	-6.17624	-2.27442
S	5.074292	-1.57219	-3.01279
S	-3.766	5.100537	1.201411
S	-2.01761	2.134327	4.499427
S	1.203515	-3.14088	-5.28318
C	-4.16121	-3.38109	1.226914
C	-4.05729	-3.5452	-3.42021
C	0.509887	-7.13284	-1.5091
C	-6.22222	1.75729	-0.12437
C	3.819781	-3.85612	0.544666
C	4.132722	0.097201	2.206079
C	-0.71374	-2.00915	5.032323
C	1.045861	2.331987	-4.97358
C	-3.70193	2.354862	-3.67897
C	1.89458	-4.27301	-6.56553
C	5.690239	-0.23805	-4.12893
C	2.262849	4.559246	1.246667
C	-2.71211	6.612699	1.260842
C	-0.55835	2.952236	5.269846
H	-4.56897	-4.37296	1.466947

H	-4.49628	-3.0677	0.229529
H	-4.508	-2.64892	1.969101
H	-3.84571	-4.02947	-2.45766
H	-3.54355	-4.09194	-4.22321
H	-5.13924	-3.54061	-3.61134
H	1.034938	-7.6743	-2.30781
H	0.065135	-7.8526	-0.80795
H	1.203768	-6.47296	-0.97251
H	-7.11871	1.373636	-0.6307
H	-5.66244	2.420845	-0.79656
H	-6.5176	2.316658	0.77421
H	4.148372	-4.44634	-0.32212
H	4.242242	-4.28598	1.463389
H	4.157231	-2.81803	0.421898
H	5.226831	0.19626	2.200296
H	3.851881	-0.96238	2.271778
H	3.722547	0.626286	3.077959
H	-0.20779	-2.76741	5.646221
H	-1.41733	-2.49695	4.34523
H	-1.25425	-1.30671	5.682493
H	1.117553	1.56607	-5.75813
H	1.402275	3.295135	-5.36491
H	0.006694	2.431859	-4.63482
H	-4.37226	1.72817	-3.0751
H	-3.34989	1.768247	-4.53948
H	-4.24043	3.242599	-4.03815
H	1.052692	-4.75889	-7.07809
H	2.552518	-5.03326	-6.12687
H	2.458779	-3.66367	-7.28524
H	5.993957	-0.70025	-5.07827
H	6.564074	0.223177	-3.64824
H	4.916762	0.520608	-4.30518
H	2.983408	5.279061	0.833437
H	2.737459	3.574396	1.343651
H	1.91332	4.913938	2.226381
H	-3.0445	7.284609	0.45748
H	-1.65089	6.367714	1.123906
H	-2.86792	7.098212	2.234102
H	0.124197	3.363623	4.515309
H	-0.02684	2.191526	5.859524
H	-0.9036	3.756597	5.934502

8. $\text{Au}_{16}\text{Ag}_2(\text{SCH}_3)_{14}$: A1, C1

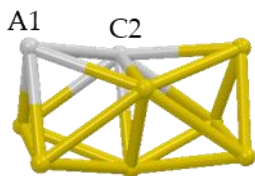


88	C1		
Au	-1.34484	-1.29631	0.56509
Au	1.064471	-2.42046	-1.15035
Au	0.952119	0.222795	0.463846
Ag	-1.24137	0.87943	-1.41326
Au	-1.64065	-4.75688	-0.46633
Au	-1.14684	-1.77987	-2.63643
Au	1.169035	-0.16951	-2.72254
Au	1.287142	-2.53472	2.355422
Au	-4.36249	-0.76611	-1.50894
Au	4.178182	-0.37012	-1.16141
Au	-2.90162	1.168279	0.951768
Au	-0.59682	2.668689	0.872192
Au	1.541857	3.271669	-1.75076
Au	-2.995	3.935184	-0.8305
Ag	-0.79793	0.537756	2.836906
Au	0.191208	-4.58226	-3.67042
Au	3.090142	-2.34126	-4.0831
Au	-2.80045	3.642866	2.794318
S	-2.19838	2.841724	-2.77636
S	-2.33192	-3.42552	1.363421
S	-3.46672	-1.79395	-3.45686
S	1.959954	-3.95233	0.556452
S	3.340578	0.886839	0.662349
S	-5.15554	0.26976	0.488131
S	2.179488	1.907105	-3.59135
S	0.851362	4.546871	0.145234
S	0.61667	-1.15898	4.162537
S	-0.89737	-6.14481	-2.24652
S	5.068994	-1.5577	-3.01982
S	-3.73047	5.094127	1.127075
S	-2.05219	2.163339	4.485604
S	1.206728	-3.15897	-5.28649
C	-4.16686	-3.33972	1.269215
C	-4.0445	-3.54244	-3.42759
C	0.47574	-7.11335	-1.48514

C	-6.20346	1.694634	-0.0235
C	3.797608	-3.87403	0.485213
C	4.003931	0.097331	2.186558
C	-0.6689	-2.14239	5.045328
C	1.103897	2.441839	-4.98856
C	-3.68779	2.280643	-3.70054
C	1.903609	-4.31124	-6.54729
C	5.675793	-0.21576	-4.13183
C	2.308804	4.571588	1.270478
C	-2.6642	6.598208	1.171875
C	-0.64669	3.025358	5.309749
H	-4.56864	-4.3262	1.539621
H	-4.51029	-3.05568	0.266152
H	-4.51054	-2.58861	1.993474
H	-3.808	-4.03223	-2.47364
H	-3.53726	-4.07351	-4.2451
H	-5.12977	-3.5534	-3.59895
H	0.991369	-7.66199	-2.28516
H	0.027133	-7.82694	-0.78013
H	1.178129	-6.45818	-0.95367
H	-7.11156	1.303729	-0.50294
H	-5.67128	2.363407	-0.71263
H	-6.47655	2.250445	0.884322
H	4.124609	-4.44694	-0.39379
H	4.202974	-4.33584	1.396186
H	4.15718	-2.84	0.394073
H	5.09624	0.216323	2.192973
H	3.737572	-0.96632	2.242805
H	3.570729	0.619748	3.050847
H	-0.18057	-2.95263	5.604461
H	-1.39832	-2.56871	4.343847
H	-1.18126	-1.47003	5.748391
H	1.198364	1.696848	-5.79073
H	1.464976	3.41623	-5.34643
H	0.056279	2.527557	-4.6727
H	-4.35391	1.673849	-3.07241
H	-3.34312	1.667572	-4.54535
H	-4.22745	3.158569	-4.08138
H	1.063477	-4.80105	-7.059
H	2.555635	-5.06785	-6.09372
H	2.474937	-3.71393	-7.2715
H	5.980246	-0.67434	-5.08264
H	6.548342	0.247869	-3.65113

H	4.898268	0.539612	-4.30453
H	3.046863	5.274292	0.858646
H	2.758499	3.574475	1.361471
H	1.972604	4.930087	2.253593
H	-2.98852	7.262544	0.359021
H	-1.60442	6.342943	1.042268
H	-2.82062	7.097107	2.138193
H	0.075577	3.418864	4.582819
H	-0.14408	2.290127	5.954631
H	-1.03345	3.848239	5.92691

9. $\text{Au}_{16}\text{Ag}_2(\text{SCH}_3)_{14}$: A1, C2



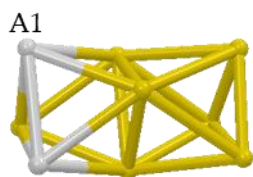
88

Au	-1.46549	-1.24431	0.426311
Au	1.020684	-2.41884	-1.2104
Ag	0.998448	0.174	0.420481
Au	-1.2637	0.887878	-1.35207
Au	-1.60703	-4.7242	-0.41279
Au	-1.2017	-1.73552	-2.67685
Au	1.126572	-0.12674	-2.74154
Au	1.317837	-2.49372	2.280034
Au	-4.44062	-0.7945	-1.45904
Au	4.183426	-0.36035	-1.14725
Au	-2.9921	1.224019	0.910656
Au	-0.63768	2.65675	0.858942
Au	1.63501	3.251808	-1.63752
Au	-2.97961	3.968062	-0.93952
Ag	-0.9106	0.517902	2.805705
Au	0.127021	-4.54302	-3.66916
Au	3.019987	-2.29951	-4.09896
Au	-2.90495	3.703676	2.686541
S	-2.09392	2.789241	-2.80535
S	-2.21862	-3.37539	1.434879
S	-3.55382	-1.82034	-3.41452
S	1.955166	-3.9326	0.488281
S	3.426046	0.860638	0.729984
S	-5.24533	0.271249	0.52096

S	2.250679	1.934304	-3.52099
S	0.916767	4.487299	0.274684
S	0.639267	-1.09177	4.063716
S	-0.94239	-6.10709	-2.22839
S	5.011127	-1.53452	-3.04779
S	-3.75539	5.162456	0.978061
S	-2.20527	2.207406	4.386053
S	1.133376	-3.12567	-5.29764
C	-4.05963	-3.34903	1.454988
C	-4.08492	-3.58215	-3.35553
C	0.440574	-7.10162	-1.52056
C	-6.32044	1.661551	-0.0305
C	3.790653	-3.86442	0.375489
C	4.128065	0.015982	2.208057
C	-0.56472	-2.11982	5.009548
C	1.216559	2.567917	-4.90792
C	-3.5363	2.166386	-3.76245
C	1.835539	-4.28779	-6.54696
C	5.624763	-0.19092	-4.15266
C	2.324138	4.460926	1.460813
C	-2.64958	6.637791	1.042313
C	-0.81625	3.061577	5.245705
H	-4.41307	-4.34036	1.771157
H	-4.47304	-3.09864	0.469665
H	-4.38043	-2.59181	2.183542
H	-3.81207	-4.056	-2.40319
H	-3.58663	-4.10944	-4.18093
H	-5.1738	-3.62162	-3.49736
H	0.924684	-7.64781	-2.34164
H	0.004772	-7.81741	-0.80972
H	1.167054	-6.46111	-1.00382
H	-7.22598	1.242084	-0.49035
H	-5.80475	2.315774	-0.74531
H	-6.59613	2.242435	0.860792
H	4.094729	-4.43252	-0.51466
H	4.212288	-4.33549	1.274262
H	4.152582	-2.83125	0.284383
H	5.220252	0.134501	2.202368
H	3.865076	-1.04977	2.233097
H	3.710986	0.503158	3.100708
H	-0.01782	-2.89828	5.559506
H	-1.29947	-2.58919	4.341788
H	-1.07946	-1.46133	5.723869

H	1.30581	1.860693	-5.7443
H	1.610584	3.547893	-5.21185
H	0.16574	2.666914	-4.60657
H	-4.25062	1.633866	-3.12099
H	-3.15852	1.47475	-4.52835
H	-4.02893	3.020932	-4.24694
H	0.998058	-4.78517	-7.05569
H	2.489351	-5.03764	-6.08479
H	2.406775	-3.6954	-7.27531
H	5.909686	-0.64135	-5.11339
H	6.510774	0.252524	-3.67745
H	4.857419	0.579417	-4.30354
H	3.081029	5.173968	1.104767
H	2.765586	3.458795	1.532951
H	1.948176	4.786319	2.44096
H	-2.92512	7.298584	0.208872
H	-1.5929	6.352468	0.957718
H	-2.82881	7.154462	1.995246
H	-0.06117	3.428719	4.538713
H	-0.35005	2.329965	5.921309
H	-1.20962	3.901747	5.834657

10. $\text{Au}_{16}\text{Ag}_2(\text{SCH}_3)_{14}$: A1, A2

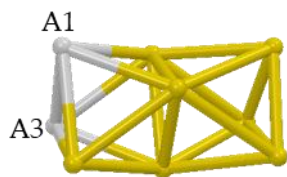


88	A2		
Au	-1.39928	-1.25622	0.493562
Au	1.098682	-2.40495	-1.23553
Au	0.959481	0.212174	0.411799
Au	-1.24785	0.895773	-1.29503
Au	-1.63613	-4.70803	-0.41954
Au	-1.14434	-1.7216	-2.67774
Au	1.167725	-0.11283	-2.76175
Au	1.309302	-2.57988	2.294065
Au	-4.39584	-0.77048	-1.43396
Au	4.169402	-0.3625	-1.14355
Ag	-2.98212	1.254211	0.957506
Au	-0.53731	2.697629	0.886159
Au	1.572137	3.339503	-1.72536

Au	-2.97973	3.945892	-0.85474
Ag	-0.76792	0.518925	2.799182
Au	0.16554	-4.55076	-3.65368
Au	3.07743	-2.31728	-4.0797
Au	-2.80375	3.687853	2.724574
S	-2.13524	2.753448	-2.72695
S	-2.29238	-3.3615	1.416407
S	-3.4983	-1.77878	-3.39627
S	1.970147	-3.96016	0.464417
S	3.329075	0.862696	0.704082
S	-5.2601	0.261676	0.53077
S	2.205497	1.981072	-3.57242
S	0.881967	4.613851	0.17688
S	0.629908	-1.21799	4.110682
S	-0.93827	-6.0961	-2.2181
S	5.057084	-1.52565	-3.01958
S	-3.71235	5.163063	1.06452
S	-2.08589	2.150451	4.374055
S	1.203544	-3.15873	-5.28563
C	-4.1318	-3.31881	1.383577
C	-4.04519	-3.53613	-3.36875
C	0.426199	-7.09585	-1.48256
C	-6.34275	1.63987	-0.03909
C	3.80851	-3.90467	0.394804
C	3.980131	0.038935	2.214939
C	-0.6493	-2.21212	4.989687
C	1.142082	2.543121	-4.96781
C	-3.59087	2.142659	-3.67061
C	1.910622	-4.33621	-6.517
C	5.654638	-0.17093	-4.12047
C	2.343854	4.629763	1.29723
C	-2.60096	6.635937	1.090338
C	-0.70879	2.996683	5.261548
H	-4.4992	-4.31337	1.672427
H	-4.51539	-3.04827	0.391583
H	-4.4688	-2.57284	2.116298
H	-3.78206	-4.02745	-2.42246
H	-3.54643	-4.05472	-4.19935
H	-5.13351	-3.56415	-3.5175
H	0.918944	-7.64983	-2.2933
H	-0.02551	-7.80466	-0.77464
H	1.148734	-6.45669	-0.9586
H	-7.22243	1.219659	-0.54554

H	-5.81461	2.323278	-0.7172
H	-6.66703	2.196255	0.851918
H	4.12777	-4.45516	-0.50122
H	4.208173	-4.39864	1.291355
H	4.18153	-2.87317	0.334485
H	5.069819	0.177853	2.240361
H	3.732574	-1.03046	2.234495
H	3.524606	0.526713	3.087906
H	-0.15911	-3.03456	5.529214
H	-1.38721	-2.62292	4.28761
H	-1.15122	-1.55111	5.710951
H	1.247967	1.816753	-5.78561
H	1.499837	3.527292	-5.30145
H	0.090717	2.614452	-4.66076
H	-4.30694	1.62223	-3.02139
H	-3.22563	1.442232	-4.43443
H	-4.07374	3.002386	-4.15569
H	1.074815	-4.8341	-7.02813
H	2.556039	-5.08539	-6.04211
H	2.491269	-3.75436	-7.24645
H	5.957591	-0.61923	-5.07668
H	6.527182	0.291249	-3.63829
H	4.874027	0.583513	-4.28315
H	3.088662	5.32085	0.877827
H	2.782389	3.628102	1.393567
H	2.016164	4.998706	2.279379
H	-2.90657	7.297388	0.268012
H	-1.54867	6.348628	0.966243
H	-2.74578	7.152338	2.049257
H	0.035499	3.405833	4.566575
H	-0.22787	2.247124	5.906131
H	-1.11844	3.804602	5.883428

11. $\text{Au}_{16}\text{Ag}_2(\text{SCH}_3)_{14}$: A1, A3

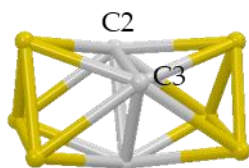


88			
Au	-1.36705	-1.30007	0.483425
Au	1.042252	-2.4394	-1.23327

Au	0.946106	0.235031	0.453103
Au	-1.22298	0.889653	-1.28821
Au	-1.63876	-4.75347	-0.45446
Au	-1.19886	-1.75175	-2.67345
Au	1.120173	-0.14644	-2.76237
Au	1.308286	-2.57378	2.294938
Au	-4.45535	-0.77424	-1.45278
Au	4.135696	-0.33489	-1.11282
Au	-2.9709	1.154221	0.951063
Ag	-0.60337	2.735571	0.894385
Au	1.558615	3.308165	-1.70387
Au	-2.96011	3.932608	-0.86683
Ag	-0.85497	0.461371	2.808973
Au	0.161239	-4.57539	-3.67289
Au	3.055786	-2.3128	-4.05554
Au	-2.81358	3.668508	2.725252
S	-2.08998	2.751817	-2.7348
S	-2.28478	-3.41005	1.385693
S	-3.55638	-1.80404	-3.39912
S	1.958315	-3.96592	0.470584
S	3.300198	0.902581	0.731289
S	-5.25903	0.297051	0.527572
S	2.193201	1.935807	-3.54576
S	0.899671	4.635535	0.161436
S	0.638487	-1.20276	4.108872
S	-0.93761	-6.13901	-2.25402
S	5.023858	-1.51302	-2.97897
S	-3.7278	5.123964	1.053127
S	-2.07348	2.160557	4.390203
S	1.198211	-3.15941	-5.2838
C	-4.12282	-3.33209	1.340573
C	-4.10634	-3.56052	-3.35839
C	0.432116	-7.1298	-1.51527
C	-6.28601	1.723503	-0.02146
C	3.795053	-3.89247	0.380817
C	3.959914	0.083514	2.241407
C	-0.60068	-2.21781	5.021504
C	1.163761	2.518233	-4.95774
C	-3.53858	2.13438	-3.68542
C	1.92475	-4.31894	-6.52086
C	5.630503	-0.16694	-4.08518
C	2.369615	4.66662	1.272534
C	-2.67129	6.635378	1.098646

C	-0.66581	2.993646	5.241092
H	-4.51307	-4.31745	1.63103
H	-4.49431	-3.05891	0.344438
H	-4.44994	-2.57581	2.0673
H	-3.8353	-4.04906	-2.41289
H	-3.61441	-4.08238	-4.19103
H	-5.1957	-3.5887	-3.49892
H	0.931378	-7.67933	-2.32502
H	-0.01609	-7.84268	-0.80921
H	1.148676	-6.48617	-0.9886
H	-7.1955	1.333536	-0.49924
H	-5.74301	2.371327	-0.72183
H	-6.55928	2.302248	0.871906
H	4.110532	-4.43763	-0.51976
H	4.20836	-4.38503	1.271968
H	4.157771	-2.85728	0.320139
H	5.048569	0.231197	2.263712
H	3.721047	-0.98777	2.260697
H	3.502592	0.567365	3.115441
H	-0.0811	-3.02518	5.556058
H	-1.34431	-2.6501	4.338651
H	-1.10229	-1.56341	5.749012
H	1.273162	1.794506	-5.77748
H	1.541655	3.498863	-5.2797
H	0.108534	2.604285	-4.66805
H	-4.25601	1.610031	-3.0408
H	-3.16613	1.436171	-4.44779
H	-4.02323	2.991499	-4.1733
H	1.09714	-4.81826	-7.04383
H	2.572102	-5.0679	-6.04826
H	2.506618	-3.72531	-7.23973
H	5.938088	-0.62215	-5.0366
H	6.501213	0.296577	-3.60098
H	4.851708	0.587531	-4.25653
H	3.128032	5.331691	0.836458
H	2.79384	3.662733	1.40348
H	2.050889	5.071269	2.244024
H	-2.99274	7.290241	0.277131
H	-1.60815	6.387855	0.982796
H	-2.84393	7.139421	2.059432
H	0.074636	3.382381	4.530218
H	-0.18656	2.243957	5.886852
H	-1.0501	3.816493	5.859613

12. $\text{Au}_{15}\text{Ag}_3(\text{SCH}_3)_{14}$: C1, C2, C3

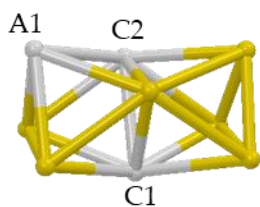


88	C1		
Ag	-1.41438	-1.33251	0.45508
Au	1.052816	-2.43743	-1.09442
Ag	1.017702	0.18352	0.445031
Ag	-1.23214	0.957117	-1.46511
Au	-1.64225	-4.78748	-0.43898
Au	-1.14056	-1.76697	-2.58544
Au	1.188505	-0.18444	-2.65428
Au	1.269548	-2.5136	2.353199
Au	-4.3337	-0.76426	-1.51734
Au	4.239324	-0.37846	-1.15066
Au	-2.8892	1.174146	0.939145
Au	-0.58471	2.670707	0.864383
Au	1.54217	3.240106	-1.76063
Au	-3.03555	4.002349	-0.80806
Au	-0.79328	0.530298	2.681879
Au	0.196515	-4.5789	-3.65942
Au	3.094958	-2.33158	-4.08785
Au	-2.8437	3.653516	2.838016
S	-2.24481	2.935696	-2.77518
S	-2.36232	-3.50153	1.404248
S	-3.4332	-1.79675	-3.45931
S	1.965786	-3.96962	0.600885
S	3.469076	0.877781	0.694021
S	-5.13334	0.285156	0.463215
S	2.188546	1.863008	-3.58736
S	0.838393	4.534199	0.111837
S	0.548351	-1.05568	4.077165
S	-0.88445	-6.14765	-2.24055
S	5.083769	-1.5682	-3.03485
S	-3.76171	5.121046	1.175762
S	-2.07925	2.128336	4.482291
S	1.191685	-3.13431	-5.26953
C	-4.20108	-3.46454	1.308551
C	-4.00249	-3.54798	-3.4264

C	0.485463	-7.12982	-1.49201
C	-6.18003	1.707169	-0.0601
C	3.802238	-3.86532	0.518161
C	4.146839	0.061566	2.199337
C	-0.7508	-1.98761	4.993579
C	1.089412	2.363448	-4.97955
C	-3.73413	2.360115	-3.6909
C	1.87194	-4.27258	-6.55235
C	5.697649	-0.22758	-4.14437
C	2.290941	4.579993	1.244953
C	-2.69591	6.624602	1.240612
C	-0.64283	2.953161	5.28833
H	-4.59056	-4.46668	1.534305
H	-4.55242	-3.1416	0.319807
H	-4.56128	-2.75262	2.064375
H	-3.77602	-4.02979	-2.46607
H	-3.48274	-4.08164	-4.2342
H	-5.08539	-3.56312	-3.61129
H	0.996792	-7.67518	-2.29701
H	0.034247	-7.84654	-0.79181
H	1.19282	-6.48379	-0.95606
H	-7.09017	1.31391	-0.53346
H	-5.64749	2.370196	-0.75444
H	-6.44882	2.269625	0.844851
H	4.1298	-4.44685	-0.35491
H	4.21881	-4.30938	1.432815
H	4.145965	-2.82775	0.409407
H	5.24184	0.149907	2.196668
H	3.85576	-0.99573	2.25827
H	3.740036	0.589292	3.073605
H	-0.25746	-2.74096	5.623495
H	-1.44977	-2.47866	4.304205
H	-1.29157	-1.27007	5.626618
H	1.168148	1.598016	-5.76386
H	1.448434	3.327022	-5.36728
H	0.047439	2.462422	-4.64922
H	-4.37224	1.715797	-3.07089
H	-3.38797	1.783379	-4.56044
H	-4.30583	3.232563	-4.03594
H	1.025405	-4.75447	-7.06093
H	2.526998	-5.03582	-6.11457
H	2.436979	-3.66799	-7.27535
H	5.996617	-0.68367	-5.0981

H	6.574749	0.22786	-3.66406
H	4.925628	0.53459	-4.31179
H	3.017388	5.297247	0.837776
H	2.75814	3.591096	1.336977
H	1.942451	4.930328	2.226564
H	-3.01763	7.298791	0.43487
H	-1.63571	6.371462	1.111124
H	-2.85416	7.112217	2.212449
H	0.074285	3.33702	4.551089
H	-0.1427	2.202273	5.917059
H	-0.99991	3.778438	5.920339

13. $\text{Au}_{15}\text{Ag}_3(\text{SCH}_3)_{14}$: A1, C1, C2

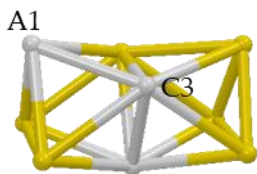


88	C1		
Au	-1.45228	-1.22796	0.489782
Au	1.021115	-2.43274	-1.14093
Ag	0.997329	0.168224	0.449657
Ag	-1.27414	0.910255	-1.44663
Au	-1.60916	-4.74004	-0.4545
Au	-1.17964	-1.76965	-2.62383
Au	1.146833	-0.17425	-2.69892
Au	1.308888	-2.49181	2.331566
Au	-4.40516	-0.7663	-1.49811
Au	4.204039	-0.36879	-1.14697
Au	-2.94976	1.205529	0.90594
Au	-0.6141	2.618371	0.843265
Au	1.586785	3.223686	-1.69796
Au	-3.00809	3.964824	-0.88672
Ag	-0.88745	0.531375	2.818517
Au	0.176854	-4.56868	-3.67849
Au	3.071999	-2.32541	-4.09639
Au	-2.86863	3.666525	2.758411
S	-2.20488	2.872629	-2.83178
S	-2.26429	-3.40378	1.384155
S	-3.4991	-1.79932	-3.43938
S	1.956946	-3.94615	0.555997

S	3.431741	0.867403	0.713249
S	-5.2147	0.293248	0.479164
S	2.198642	1.881856	-3.56301
S	0.888775	4.475881	0.207602
S	0.634843	-1.08199	4.107933
S	-0.9004	-6.13181	-2.24596
S	5.052024	-1.55166	-3.03273
S	-3.74316	5.126204	1.068297
S	-2.15255	2.180312	4.459188
S	1.184528	-3.14232	-5.29591
C	-4.10433	-3.36616	1.355466
C	-4.0641	-3.55159	-3.39947
C	0.478567	-7.10672	-1.50338
C	-6.27092	1.70072	-0.06446
C	3.792253	-3.86365	0.443492
C	4.132124	0.044239	2.204334
C	-0.59274	-2.09024	5.04506
C	1.123258	2.453974	-4.94585
C	-3.69147	2.294762	-3.75115
C	1.882597	-4.29501	-6.55606
C	5.667928	-0.21108	-4.14065
C	2.318639	4.478697	1.367636
C	-2.64597	6.60787	1.126778
C	-0.75361	3.03712	5.299806
H	-4.47213	-4.36248	1.637958
H	-4.49007	-3.08924	0.365804
H	-4.43988	-2.62451	2.093331
H	-3.8217	-4.03431	-2.44342
H	-3.55635	-4.08392	-4.21578
H	-5.14986	-3.57002	-3.5668
H	0.984573	-7.65349	-2.31072
H	0.036059	-7.82191	-0.79611
H	1.188036	-6.45513	-0.97699
H	-7.1752	1.296082	-0.53972
H	-5.74057	2.360272	-0.76363
H	-6.55068	2.271348	0.832129
H	4.101194	-4.44352	-0.43734
H	4.21815	-4.31631	1.349634
H	4.145173	-2.82901	0.335339
H	5.225099	0.154799	2.195342
H	3.861818	-1.01906	2.249045
H	3.719988	0.550454	3.088713
H	-0.0618	-2.87025	5.60834

H	-1.32428	-2.55663	4.371815
H	-1.10969	-1.42	5.746729
H	1.19701	1.716252	-5.75683
H	1.502488	3.424452	-5.29539
H	0.079742	2.558247	-4.62204
H	-4.35882	1.697624	-3.11531
H	-3.34435	1.66884	-4.58547
H	-4.23146	3.165801	-4.14708
H	1.043443	-4.78773	-7.0665
H	2.536774	-5.04902	-6.10135
H	2.452496	-3.69783	-7.28152
H	5.967182	-0.66672	-5.09455
H	6.545004	0.243197	-3.65916
H	4.896337	0.551691	-4.30738
H	3.059465	5.198317	0.991583
H	2.77445	3.483083	1.44174
H	1.955572	4.808466	2.351177
H	-2.94066	7.275284	0.305187
H	-1.58942	6.330006	1.018818
H	-2.80987	7.114057	2.088085
H	-0.00719	3.403636	4.583138
H	-0.27803	2.30744	5.971038
H	-1.13943	3.878497	5.892115

14. $\text{Au}_{15}\text{Ag}_3(\text{SCH}_3)_{14}$: A1, C1, C3

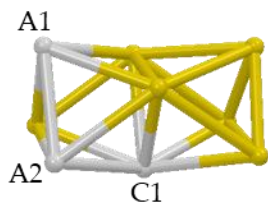


88	C1		
Ag	-1.38734	-1.32997	0.451318
Au	1.077885	-2.37578	-1.16326
Au	0.929233	0.269013	0.431193
Ag	-1.189	0.976124	-1.46848
Au	-1.64335	-4.76922	-0.42967
Au	-1.12622	-1.71681	-2.65456
Au	1.200134	-0.12693	-2.7293
Au	1.245478	-2.53166	2.316555
Au	-4.31234	-0.79722	-1.47468
Au	4.18791	-0.3969	-1.15517
Au	-2.83112	1.184225	0.91089

Au	-0.57304	2.718492	0.838713
Au	1.576638	3.309799	-1.75724
Au	-3.00408	3.98289	-0.86871
Ag	-0.75842	0.59267	2.802336
Au	0.185641	-4.57437	-3.66074
Au	3.084716	-2.33689	-4.08882
Au	-2.80436	3.681147	2.77065
S	-2.23816	2.89298	-2.82976
S	-2.35508	-3.47228	1.410878
S	-3.44716	-1.77887	-3.4585
S	1.924701	-3.95153	0.523523
S	3.360876	0.845396	0.680363
S	-5.07041	0.214877	0.54506
S	2.208717	1.945519	-3.60169
S	0.898693	4.592352	0.13855
S	0.593788	-1.14142	4.1153
S	-0.89732	-6.13341	-2.23173
S	5.069952	-1.56761	-3.02902
S	-3.71696	5.13689	1.098186
S	-2.07827	2.185655	4.457856
S	1.193109	-3.14978	-5.28176
C	-4.19457	-3.45504	1.326371
C	-3.98492	-3.54013	-3.44038
C	0.476722	-7.11261	-1.48696
C	-6.16532	1.614722	0.060153
C	3.764417	-3.89121	0.479926
C	3.996778	0.024702	2.198852
C	-0.70806	-2.09085	5.011046
C	1.1266	2.477922	-4.99524
C	-3.74067	2.284532	-3.70118
C	1.883282	-4.30442	-6.54427
C	5.676859	-0.21587	-4.12905
C	2.351217	4.581075	1.271298
C	-2.6412	6.634257	1.142526
C	-0.70378	3.053709	5.32657
H	-4.56938	-4.45459	1.586104
H	-4.55505	-3.16901	0.329727
H	-4.55931	-2.72346	2.060723
H	-3.72755	-4.03208	-2.49304
H	-3.47503	-4.05216	-4.2682
H	-5.07152	-3.5722	-3.60024
H	0.98559	-7.65888	-2.29292
H	0.029929	-7.82833	-0.78288

H	1.184302	-6.46289	-0.95577
H	-7.08	1.201374	-0.38681
H	-5.67115	2.291202	-0.6493
H	-6.41989	2.168871	0.974314
H	4.097881	-4.46231	-0.39785
H	4.151258	-4.36324	1.393698
H	4.136356	-2.86064	0.400528
H	5.090292	0.130754	2.220765
H	3.717553	-1.03653	2.235522
H	3.55853	0.538215	3.065956
H	-0.23176	-2.90109	5.580405
H	-1.44393	-2.51443	4.314919
H	-1.20787	-1.39967	5.704599
H	1.221878	1.73458	-5.79878
H	1.483423	3.454027	-5.35246
H	0.079163	2.55953	-4.67762
H	-4.37162	1.668227	-3.04668
H	-3.4074	1.671355	-4.55042
H	-4.31451	3.14426	-4.0734
H	1.04056	-4.79511	-7.05082
H	2.536883	-5.06035	-6.09189
H	2.451548	-3.70882	-7.27222
H	5.97861	-0.66539	-5.085
H	6.551264	0.241131	-3.64544
H	4.900694	0.542882	-4.29278
H	3.108069	5.267241	0.8659
H	2.777221	3.573785	1.364461
H	2.017153	4.945291	2.253042
H	-2.96102	7.300092	0.329134
H	-1.58269	6.372896	1.014633
H	-2.79575	7.134181	2.108665
H	0.042358	3.447036	4.623915
H	-0.22122	2.32201	5.990656
H	-1.1114	3.877456	5.928933

15. $\text{Au}_{15}\text{Ag}_3(\text{SCH}_3)_{14}$: A1, A2, C1

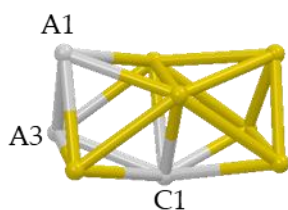


88	A1	A2	C1
Au	-1.3545	-1.26483	0.584433
Au	1.094786	-2.41587	-1.17702
Au	0.959897	0.197683	0.466718
Ag	-1.23097	0.873506	-1.37838
Au	-1.66613	-4.71802	-0.44577
Au	-1.12264	-1.76448	-2.64697
Au	1.186707	-0.15762	-2.73434
Au	1.316885	-2.56179	2.34409
Au	-4.35774	-0.73073	-1.50228
Au	4.185965	-0.3464	-1.16758
Ag	-2.93847	1.208775	0.960153
Au	-0.52506	2.641372	0.896423
Au	1.500567	3.308149	-1.78357
Au	-2.98742	3.920741	-0.78751
Ag	-0.75343	0.517799	2.83471
Au	0.20167	-4.59171	-3.64456
Au	3.117544	-2.35051	-4.07709
Au	-2.77444	3.61619	2.813492
S	-2.19771	2.828747	-2.73269
S	-2.37128	-3.37929	1.374724
S	-3.44279	-1.75104	-3.44918
S	1.981924	-3.95602	0.52636
S	3.337566	0.902593	0.657302
S	-5.22959	0.285988	0.463827
S	2.158393	1.934767	-3.60935
S	0.810537	4.592388	0.108839
S	0.644106	-1.20993	4.168356
S	-0.92191	-6.12237	-2.21222
S	5.087183	-1.53044	-3.02341
S	-3.70316	5.090929	1.169683
S	-2.04938	2.091972	4.471321
S	1.249471	-3.20902	-5.27596
C	-4.20552	-3.29917	1.267994
C	-4.0372	-3.49396	-3.44011
C	0.430202	-7.10655	-1.43365
C	-6.27688	1.697238	-0.08917
C	3.819588	-3.88057	0.450888

C	4.014432	0.120956	2.179907
C	-0.64128	-2.20459	5.038429
C	1.070748	2.436718	-5.00934
C	-3.68491	2.281995	-3.66883
C	1.965299	-4.39258	-6.49635
C	5.673965	-0.18661	-4.14369
C	2.296723	4.661285	1.195606
C	-2.61039	6.576882	1.204988
C	-0.66694	2.937434	5.350832
H	-4.60409	-4.29204	1.518901
H	-4.54232	-2.99917	0.267461
H	-4.55801	-2.56248	2.002769
H	-3.8071	-3.99633	-2.49114
H	-3.53496	-4.02162	-4.26286
H	-5.12242	-3.49189	-3.61223
H	0.940037	-7.67192	-2.22572
H	-0.03391	-7.80538	-0.72388
H	1.141269	-6.45792	-0.90567
H	-7.15752	1.305356	-0.61618
H	-5.72505	2.384822	-0.74392
H	-6.60195	2.239647	0.810048
H	4.142544	-4.4402	-0.43812
H	4.227144	-4.35719	1.353172
H	4.18071	-2.84588	0.374776
H	5.103895	0.263618	2.189192
H	3.771206	-0.94842	2.23089
H	3.568228	0.629905	3.045612
H	-0.15468	-3.02569	5.583141
H	-1.37491	-2.61652	4.332635
H	-1.14921	-1.54234	5.754286
H	1.17826	1.687006	-5.80541
H	1.411484	3.415031	-5.37623
H	0.022101	2.504074	-4.69246
H	-4.37009	1.696171	-3.04158
H	-3.33991	1.650751	-4.49984
H	-4.20189	3.165347	-4.06817
H	1.133254	-4.89647	-7.00759
H	2.610991	-5.13647	-6.01364
H	2.547263	-3.814	-7.22736
H	5.982261	-0.64623	-5.09278
H	6.541521	0.290785	-3.66744
H	4.886764	0.558041	-4.31897
H	3.012691	5.36757	0.752019

H	2.764767	3.673125	1.293649
H	1.980794	5.032303	2.18079
H	-2.93848	7.250371	0.40124
H	-1.55751	6.304676	1.054734
H	-2.74292	7.072929	2.176294
H	0.066907	3.358694	4.651851
H	-0.17325	2.184628	5.981942
H	-1.07366	3.736655	5.98576

16. $\text{Au}_{15}\text{Ag}_3(\text{SCH}_3)_{14}$: A1, A3, C1

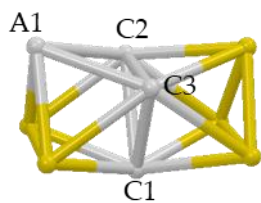


88	C1		
Au	-1.33942	-1.34184	0.597061
Au	1.022685	-2.46015	-1.16797
Au	0.908932	0.217934	0.499827
Ag	-1.2601	0.830078	-1.37299
Au	-1.66673	-4.78721	-0.48768
Au	-1.17926	-1.80767	-2.65454
Au	1.130851	-0.19677	-2.72068
Au	1.310938	-2.55275	2.35285
Au	-4.40131	-0.74087	-1.53979
Au	4.128345	-0.32186	-1.13899
Au	-2.91207	1.091957	0.976478
Ag	-0.59825	2.694727	0.891603
Au	1.495922	3.281641	-1.73429
Au	-2.95733	3.908624	-0.80815
Ag	-0.83084	0.468989	2.848391
Au	0.197438	-4.61774	-3.67452
Au	3.09256	-2.34983	-4.05401
Au	-2.77537	3.604583	2.807583
S	-2.15531	2.812816	-2.74552
S	-2.37061	-3.46692	1.345541
S	-3.50065	-1.79768	-3.46989
S	1.954655	-3.96641	0.542472
S	3.270159	0.948409	0.668855
S	-5.20855	0.317891	0.440384
S	2.138585	1.889012	-3.55648
S	0.845645	4.624524	0.121072

S	0.671842	-1.1752	4.170976
S	-0.91122	-6.17677	-2.26186
S	5.046542	-1.52571	-2.9736
S	-3.70378	5.058988	1.147408
S	-2.03091	2.114506	4.486896
S	1.238006	-3.20035	-5.27966
C	-4.20122	-3.34335	1.215398
C	-4.09946	-3.53888	-3.42523
C	0.452783	-7.14651	-1.48505
C	-6.19265	1.779414	-0.09172
C	3.789746	-3.87017	0.437198
C	3.958568	0.188251	2.197652
C	-0.56663	-2.17769	5.098989
C	1.085523	2.420211	-4.97127
C	-3.64371	2.281392	-3.68927
C	1.965136	-4.35826	-6.51774
C	5.648328	-0.19019	-4.09579
C	2.333056	4.686085	1.207621
C	-2.66315	6.580586	1.201216
C	-0.6087	2.950314	5.310035
H	-4.62855	-4.3282	1.44994
H	-4.51758	-3.02508	0.213489
H	-4.54554	-2.60579	1.953304
H	-3.86143	-4.02579	-2.47018
H	-3.60413	-4.08078	-4.24291
H	-5.18593	-3.53833	-3.58887
H	0.974164	-7.69889	-2.27879
H	-0.00337	-7.85684	-0.78155
H	1.152444	-6.49143	-0.94986
H	-7.09902	1.422209	-0.60005
H	-5.61841	2.433416	-0.76109
H	-6.47344	2.339581	0.811063
H	4.105473	-4.42791	-0.45557
H	4.216581	-4.33976	1.334269
H	4.13711	-2.8313	0.353849
H	5.045393	0.350024	2.204116
H	3.734548	-0.88496	2.254938
H	3.504556	0.694915	3.060544
H	-0.04843	-2.98523	5.63462
H	-1.31958	-2.60901	4.425979
H	-1.05855	-1.51496	5.82555
H	1.190365	1.673456	-5.77047
H	1.452581	3.393577	-5.32585

H	0.033751	2.508132	-4.67024
H	-4.33582	1.697076	-3.0681
H	-3.29938	1.651609	-4.52175
H	-4.15347	3.169321	-4.08767
H	1.137566	-4.85844	-7.03988
H	2.613925	-5.10644	-6.04591
H	2.545456	-3.76366	-7.23704
H	5.965693	-0.65623	-5.03868
H	6.511621	0.288713	-3.61331
H	4.863819	0.554415	-4.28315
H	3.070096	5.366318	0.758564
H	2.77999	3.691135	1.330958
H	2.022699	5.084179	2.184475
H	-3.00672	7.245857	0.397122
H	-1.60012	6.345788	1.060097
H	-2.82229	7.066642	2.173509
H	0.118912	3.335585	4.584148
H	-0.11761	2.203844	5.950574
H	-0.98169	3.776479	5.931006

17. $\text{Au}_{14}\text{Ag}_4(\text{SCH}_3)_{14}$: A1, C1, C2, C3

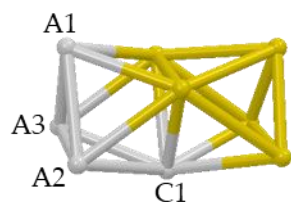


88	C1		
Ag	-1.47093	-1.29382	0.399845
Au	1.035044	-2.39594	-1.14893
Ag	0.976393	0.193594	0.443838
Ag	-1.21882	0.977245	-1.49374
Au	-1.63359	-4.75644	-0.42168
Au	-1.15307	-1.72275	-2.64657
Au	1.180621	-0.14166	-2.70404
Au	1.267812	-2.49089	2.302788
Au	-4.34489	-0.79551	-1.47884
Au	4.205822	-0.38188	-1.14114
Au	-2.86611	1.193762	0.881425
Au	-0.5783	2.652759	0.817755
Au	1.608101	3.260725	-1.71906
Au	-3.0097	3.998628	-0.90684
Ag	-0.83593	0.578626	2.795097

Au	0.171742	-4.56309	-3.66682
Au	3.068702	-2.32353	-4.09561
Au	-2.86266	3.691587	2.749853
S	-2.23523	2.910184	-2.8662
S	-2.32089	-3.46022	1.428441
S	-3.46959	-1.78362	-3.4566
S	1.928344	-3.94602	0.533207
S	3.438991	0.848187	0.72378
S	-5.11833	0.22817	0.528358
S	2.219667	1.911454	-3.58042
S	0.921321	4.521031	0.184355
S	0.611755	-1.07973	4.080864
S	-0.90659	-6.12056	-2.23224
S	5.0515	-1.55701	-3.03387
S	-3.72694	5.152616	1.05683
S	-2.16119	2.195101	4.447665
S	1.174785	-3.13533	-5.28735
C	-4.16262	-3.46758	1.390511
C	-4.00572	-3.54529	-3.43538
C	0.469595	-7.10608	-1.49983
C	-6.21161	1.623435	0.026112
C	3.765948	-3.8716	0.449563
C	4.127895	0.012441	2.212847
C	-0.64518	-2.05631	5.012721
C	1.138485	2.47061	-4.96437
C	-3.73441	2.302827	-3.74497
C	1.865904	-4.28814	-6.55122
C	5.66715	-0.21257	-4.1373
C	2.356719	4.511531	1.338319
C	-2.62802	6.632961	1.115128
C	-0.79349	3.063247	5.326994
H	-4.51863	-4.47199	1.657567
H	-4.55219	-3.18371	0.404318
H	-4.51716	-2.74195	2.135832
H	-3.75024	-4.03479	-2.48629
H	-3.49466	-4.05911	-4.26134
H	-5.09205	-3.57735	-3.59665
H	0.970903	-7.65195	-2.31077
H	0.025237	-7.82207	-0.79454
H	1.183476	-6.46063	-0.9718
H	-7.12443	1.208436	-0.42299
H	-5.71318	2.29539	-0.68453
H	-6.47082	2.183395	0.935504

H	4.085206	-4.44963	-0.42884
H	4.174936	-4.33043	1.36033
H	4.125898	-2.83846	0.351355
H	5.222173	0.109647	2.206739
H	3.844719	-1.04769	2.255043
H	3.720285	0.521319	3.097759
H	-0.13406	-2.84278	5.585139
H	-1.37934	-2.512	4.335388
H	-1.15366	-1.36995	5.704733
H	1.215638	1.729824	-5.77217
H	1.51268	3.441465	-5.31816
H	0.094491	2.571188	-4.64082
H	-4.37287	1.693855	-3.09092
H	-3.39804	1.682836	-4.58803
H	-4.30195	3.162617	-4.1269
H	1.02421	-4.78022	-7.05802
H	2.521621	-5.04275	-6.09966
H	2.432542	-3.6908	-7.27896
H	5.964635	-0.66509	-5.09319
H	6.545461	0.238418	-3.65501
H	4.896522	0.552003	-4.30035
H	3.105687	5.219834	0.957188
H	2.800163	3.510616	1.416938
H	2.000786	4.850308	2.321475
H	-2.92325	7.302005	0.295078
H	-1.57167	6.354819	1.006121
H	-2.79044	7.137934	2.077353
H	-0.03024	3.437195	4.631997
H	-0.33023	2.337647	6.01134
H	-1.20194	3.900823	5.909495

18. $\text{Au}_{14}\text{Ag}_4(\text{SCH}_3)_{14}$: A1, A2, A3, C1

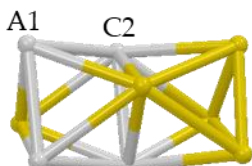


88			
Au	-1.36651	-1.29473	0.601804
Au	1.056636	-2.44478	-1.19729
Au	0.908143	0.208735	0.490197
Ag	-1.25291	0.832383	-1.35289

Au	-1.68725	-4.73964	-0.46587
Au	-1.15435	-1.78951	-2.66872
Au	1.147114	-0.17848	-2.74161
Au	1.334408	-2.57943	2.338733
Au	-4.39293	-0.72522	-1.51788
Au	4.135076	-0.30506	-1.1442
Ag	-2.94426	1.159725	0.973003
Ag	-0.53077	2.687399	0.89808
Au	1.48656	3.316417	-1.75952
Au	-2.94807	3.896262	-0.77708
Ag	-0.78606	0.458681	2.849005
Au	0.2056	-4.61897	-3.65544
Au	3.119548	-2.35396	-4.05164
Au	-2.74718	3.599771	2.810878
S	-2.16183	2.802178	-2.71802
S	-2.39788	-3.41314	1.362084
S	-3.48183	-1.7675	-3.45484
S	1.973157	-3.96529	0.507193
S	3.26565	0.954363	0.666246
S	-5.26683	0.312679	0.437546
S	2.132471	1.919336	-3.57544
S	0.844493	4.665842	0.095944
S	0.687722	-1.23098	4.17522
S	-0.93909	-6.1433	-2.23205
S	5.065663	-1.49938	-2.97912
S	-3.67706	5.06998	1.170485
S	-2.02634	2.071103	4.461544
S	1.278656	-3.24011	-5.27303
C	-4.23057	-3.31534	1.240319
C	-4.08688	-3.50682	-3.42893
C	0.402727	-7.13445	-1.4441
C	-6.28041	1.742631	-0.12886
C	3.80924	-3.8809	0.405868
C	3.954963	0.195635	2.195297
C	-0.5621	-2.244	5.076296
C	1.073139	2.43872	-4.98994
C	-3.65525	2.278475	-3.65818
C	2.023898	-4.42462	-6.47439
C	5.649643	-0.16022	-4.10641
C	2.351644	4.750528	1.154757
C	-2.61149	6.57543	1.209127
C	-0.62682	2.892416	5.33773
H	-4.64097	-4.30883	1.468505

H	-4.5558	-2.993	0.242722
H	-4.58349	-2.58988	1.986095
H	-3.85128	-4.00452	-2.47876
H	-3.59455	-4.04273	-4.25233
H	-5.17343	-3.49977	-3.59207
H	0.913571	-7.70416	-2.23245
H	-0.06939	-7.82934	-0.73573
H	1.11506	-6.48934	-0.91344
H	-7.15983	1.36765	-0.6701
H	-5.70697	2.421436	-0.77416
H	-6.60996	2.289994	0.765685
H	4.121926	-4.42738	-0.49486
H	4.231707	-4.3672	1.296124
H	4.164505	-2.84356	0.338905
H	5.041106	0.361361	2.203801
H	3.734715	-0.87837	2.251794
H	3.497835	0.699848	3.058016
H	-0.05285	-3.06648	5.597685
H	-1.31542	-2.65551	4.391219
H	-1.05251	-1.59343	5.814943
H	1.187722	1.694006	-5.78973
H	1.427184	3.417151	-5.34381
H	0.020013	2.512154	-4.68977
H	-4.34896	1.699172	-3.03438
H	-3.31481	1.645025	-4.48934
H	-4.15919	3.169495	-4.05704
H	1.204695	-4.93799	-6.99695
H	2.66695	-5.16081	-5.9765
H	2.613835	-3.84562	-7.19865
H	5.972053	-0.62566	-5.04795
H	6.507471	0.331083	-3.62662
H	4.856087	0.574166	-4.296
H	3.075995	5.429671	0.683771
H	2.807118	3.759827	1.283037
H	2.056489	5.159168	2.132039
H	-2.9585	7.245646	0.41074
H	-1.55452	6.324757	1.050705
H	-2.74859	7.063448	2.183772
H	0.111518	3.305912	4.638879
H	-0.14307	2.128625	5.963102
H	-1.02027	3.694494	5.97724

19. Au₁₄Ag₄(SCH₃)₁₄ : A1, A2, C1, C2

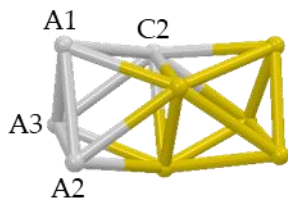


88	A2	C1	
Au	-1.46085	-1.17759	0.520147
Au	1.057376	-2.43566	-1.16004
Ag	1.014803	0.130565	0.45204
Ag	-1.2696	0.902893	-1.4117
Au	-1.62765	-4.69083	-0.43866
Au	-1.15464	-1.76298	-2.61693
Au	1.164026	-0.16909	-2.70503
Au	1.333929	-2.52269	2.328313
Au	-4.39956	-0.73514	-1.48127
Au	4.212198	-0.34782	-1.14562
Ag	-3.00924	1.253807	0.918084
Au	-0.55652	2.563121	0.8583
Au	1.541772	3.253752	-1.72624
Au	-3.00052	3.949811	-0.85225
Ag	-0.85942	0.503086	2.816368
Au	0.189073	-4.56722	-3.66002
Au	3.098934	-2.32695	-4.09143
Au	-2.83316	3.650054	2.770983
S	-2.21114	2.854232	-2.79698
S	-2.29721	-3.35326	1.395161
S	-3.47399	-1.76495	-3.41811
S	1.987229	-3.95294	0.536452
S	3.430393	0.881272	0.716495
S	-5.2986	0.306266	0.45911
S	2.177707	1.903741	-3.57604
S	0.842014	4.506071	0.180546
S	0.645975	-1.1397	4.12104
S	-0.91992	-6.09949	-2.21795
S	5.069956	-1.52468	-3.03104
S	-3.70913	5.128294	1.101594
S	-2.13351	2.127772	4.443179
S	1.22137	-3.17046	-5.28813
C	-4.13685	-3.32517	1.361831
C	-4.0554	-3.51213	-3.39551
C	0.43856	-7.09212	-1.4616

C	-6.35324	1.695495	-0.13591
C	3.822649	-3.86566	0.427153
C	4.140825	0.064268	2.206377
C	-0.58721	-2.16191	5.034867
C	1.095477	2.441582	-4.96717
C	-3.6994	2.289955	-3.72182
C	1.927887	-4.34201	-6.52545
C	5.670141	-0.17983	-4.14231
C	2.300012	4.54736	1.305432
C	-2.58356	6.589684	1.145683
C	-0.74004	2.965889	5.31243
H	-4.49968	-4.32857	1.624724
H	-4.52161	-3.03098	0.376895
H	-4.47854	-2.60009	2.11327
H	-3.82585	-4.00345	-2.44064
H	-3.54598	-4.04419	-4.21097
H	-5.1399	-3.51918	-3.57193
H	0.937354	-7.6542	-2.26295
H	-0.01911	-7.79372	-0.75037
H	1.157796	-6.44892	-0.93805
H	-7.225	1.28499	-0.66351
H	-5.80056	2.373765	-0.79938
H	-6.69212	2.253952	0.748309
H	4.134039	-4.4367	-0.45859
H	4.248631	-4.32539	1.329671
H	4.173161	-2.82923	0.32883
H	5.232391	0.187916	2.197468
H	3.883251	-1.00224	2.249294
H	3.72284	0.56423	3.091567
H	-0.06167	-2.95603	5.583201
H	-1.32026	-2.61053	4.351171
H	-1.10223	-1.50414	5.749769
H	1.184637	1.696436	-5.76977
H	1.456983	3.415146	-5.32683
H	0.049387	2.529629	-4.64685
H	-4.37504	1.700118	-3.0881
H	-3.35395	1.659441	-4.55325
H	-4.228	3.166271	-4.12131
H	1.09248	-4.84023	-7.03686
H	2.576542	-5.09103	-6.05477
H	2.505357	-3.75543	-7.25353
H	5.973984	-0.63455	-5.09521
H	6.542417	0.285289	-3.66243

H	4.890471	0.574226	-4.31097
H	3.019899	5.273943	0.902968
H	2.773934	3.56018	1.381064
H	1.956081	4.883069	2.293828
H	-2.88057	7.263959	0.330641
H	-1.5343	6.292654	1.01876
H	-2.72327	7.096479	2.11045
H	0.011425	3.348037	4.609542
H	-0.27057	2.220615	5.970407
H	-1.13212	3.793148	5.920107

20. $\text{Au}_{14}\text{Ag}_4(\text{SCH}_3)_{14}$: A1, A2, A3, C2

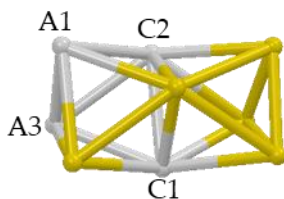


88	A2		
Au	-1.5214	-1.23916	0.45885
Au	1.029387	-2.458	-1.24521
Ag	0.961433	0.103028	0.419264
Au	-1.29103	0.89697	-1.24808
Au	-1.63797	-4.71797	-0.41677
Au	-1.20234	-1.73502	-2.66445
Au	1.10908	-0.14207	-2.73477
Au	1.349856	-2.55054	2.258336
Au	-4.48038	-0.75806	-1.44107
Au	4.146208	-0.31683	-1.11142
Ag	-3.0828	1.236256	0.931573
Ag	-0.58333	2.678465	0.884807
Au	1.571312	3.297384	-1.64692
Au	-2.94206	3.96981	-0.88079
Ag	-0.90495	0.431157	2.763397
Au	0.15752	-4.57571	-3.65738
Au	3.064185	-2.31689	-4.06211
Au	-2.82719	3.694846	2.689591
S	-2.06349	2.783172	-2.73659
S	-2.2814	-3.38211	1.431921
S	-3.55457	-1.78099	-3.38153
S	1.976723	-3.96995	0.451271
S	3.338904	0.904656	0.749703
S	-5.39005	0.297341	0.492051

S	2.196317	1.936507	-3.49827
S	0.912849	4.611043	0.228261
S	0.676274	-1.16194	4.05575
S	-0.95753	-6.11127	-2.21953
S	5.02285	-1.4937	-2.98909
S	-3.70869	5.177904	1.028866
S	-2.11812	2.14206	4.324899
S	1.205919	-3.18076	-5.27852
C	-4.12273	-3.37184	1.434347
C	-4.09651	-3.54006	-3.34185
C	0.39966	-7.12201	-1.48552
C	-6.4512	1.673569	-0.12224
C	3.811174	-3.88618	0.327519
C	4.0574	0.090393	2.237206
C	-0.51726	-2.20281	5.001179
C	1.177582	2.54051	-4.90872
C	-3.50697	2.177912	-3.70449
C	1.928605	-4.35193	-6.50633
C	5.618665	-0.14724	-4.1001
C	2.379898	4.637033	1.343761
C	-2.61083	6.660378	1.081895
C	-0.70678	2.946312	5.198267
H	-4.47092	-4.37797	1.706081
H	-4.52933	-3.08354	0.456533
H	-4.45688	-2.64912	2.19154
H	-3.82914	-4.02478	-2.39334
H	-3.59832	-4.0624	-4.17044
H	-5.18505	-3.57221	-3.48749
H	0.883735	-7.68353	-2.29629
H	-0.05583	-7.8239	-0.77317
H	1.13103	-6.4885	-0.96697
H	-7.32114	1.251789	-0.64406
H	-5.90387	2.345172	-0.79669
H	-6.79384	2.243191	0.753499
H	4.113093	-4.43387	-0.57608
H	4.243336	-4.37122	1.213771
H	4.163895	-2.84837	0.254811
H	5.143958	0.252618	2.241407
H	3.837603	-0.98502	2.26033
H	3.612709	0.560914	3.125335
H	0.033989	-2.99294	5.529761
H	-1.26394	-2.6584	4.33696
H	-1.01964	-1.55651	5.735389

H	1.27863	1.81942	-5.73177
H	1.570571	3.516925	-5.2253
H	0.123045	2.640602	-4.62128
H	-4.23295	1.655011	-3.0685
H	-3.12867	1.479895	-4.46425
H	-3.98306	3.037571	-4.1962
H	1.099862	-4.85555	-7.02336
H	2.576844	-5.09679	-6.02847
H	2.509276	-3.76484	-7.23156
H	5.924341	-0.6012	-5.05277
H	6.489114	0.321098	-3.61991
H	4.835875	0.603874	-4.26789
H	3.129841	5.320196	0.921162
H	2.816446	3.635921	1.453421
H	2.054537	5.018179	2.322465
H	-2.91115	7.324149	0.25959
H	-1.55406	6.384606	0.971011
H	-2.77524	7.168195	2.042078
H	0.046368	3.32974	4.498166
H	-0.2459	2.183014	5.841239
H	-1.0867	3.76831	5.820268

21. $\text{Au}_{14}\text{Ag}_4(\text{SCH}_3)_{14}$: A1, A3, C1, C2



88			
Au	-1.44398	-1.27958	0.517013
Au	0.99958	-2.4797	-1.14781
Ag	0.965551	0.138512	0.459566
Ag	-1.27572	0.86897	-1.38664
Au	-1.6321	-4.77713	-0.47447
Au	-1.20465	-1.80388	-2.61787
Au	1.117995	-0.20896	-2.69005
Au	1.325948	-2.51992	2.328472
Au	-4.44691	-0.74922	-1.51693
Au	4.16556	-0.33707	-1.11501
Au	-2.96871	1.136224	0.926199
Ag	-0.63192	2.65761	0.870224
Au	1.529677	3.226369	-1.6844

Au	-2.97459	3.944115	-0.84747
Ag	-0.90228	0.473097	2.793314
Au	0.18562	-4.59577	-3.68058
Au	3.078201	-2.33128	-4.0631
Au	-2.81609	3.642092	2.775108
S	-2.15771	2.84834	-2.78096
S	-2.30536	-3.45608	1.368276
S	-3.52299	-1.80949	-3.4352
S	1.964658	-3.97511	0.551162
S	3.36502	0.913784	0.726484
S	-5.27732	0.337224	0.438027
S	2.157638	1.858415	-3.52966
S	0.87361	4.555263	0.17585
S	0.664255	-1.10226	4.104567
S	-0.90561	-6.16346	-2.26383
S	5.039888	-1.53106	-2.98236
S	-3.73101	5.094305	1.104315
S	-2.07003	2.152528	4.454756
S	1.207812	-3.16085	-5.28124
C	-4.1437	-3.39031	1.305143
C	-4.10419	-3.55652	-3.3906
C	0.467096	-7.1387	-1.50989
C	-6.27316	1.777804	-0.13079
C	3.798316	-3.87418	0.423129
C	4.076661	0.119802	2.228607
C	-0.55043	-2.11138	5.058166
C	1.105046	2.420315	-4.93334
C	-3.63971	2.291395	-3.72115
C	1.921194	-4.30399	-6.54095
C	5.651462	-0.19307	-4.09579
C	2.337095	4.595417	1.29515
C	-2.68535	6.61246	1.167449
C	-0.64004	2.982811	5.269404
H	-4.53274	-4.3877	1.552969
H	-4.50622	-3.08008	0.316406
H	-4.48258	-2.66431	2.057038
H	-3.86644	-4.03915	-2.43333
H	-3.59991	-4.09528	-4.20487
H	-5.18981	-3.56662	-3.55953
H	0.979561	-7.68525	-2.31336
H	0.018888	-7.8539	-0.80624
H	1.172615	-6.48737	-0.97788
H	-7.17529	1.403085	-0.634

H	-5.70281	2.423272	-0.81149
H	-6.5613	2.354078	0.759561
H	4.105556	-4.44177	-0.46632
H	4.235929	-4.33206	1.321078
H	4.140463	-2.83502	0.323722
H	5.167065	0.253369	2.22042
H	3.828927	-0.94851	2.282754
H	3.652371	0.626058	3.107087
H	-0.01184	-2.89199	5.613088
H	-1.29243	-2.5777	4.396243
H	-1.05776	-1.44246	5.768219
H	1.193815	1.679828	-5.74032
H	1.487204	3.390635	-5.28026
H	0.056343	2.523687	-4.62654
H	-4.31644	1.689495	-3.0998
H	-3.286	1.674084	-4.55911
H	-4.17046	3.170083	-4.11254
H	1.088704	-4.79857	-7.06054
H	2.575543	-5.05706	-6.08497
H	2.493499	-3.70032	-7.25906
H	5.961899	-0.65313	-5.04398
H	6.520597	0.273472	-3.6116
H	4.873456	0.560603	-4.27374
H	3.083223	5.282312	0.871957
H	2.780826	3.598266	1.411334
H	2.004489	4.978908	2.270418
H	-3.00926	7.274243	0.352402
H	-1.62053	6.372764	1.050525
H	-2.86167	7.105563	2.133311
H	0.095331	3.347746	4.540725
H	-0.15967	2.239655	5.92188
H	-1.00279	3.822545	5.878114