Supporting Information for

The Golden Pathway to Thiolate-Stabilized Nanoparticles: Following the Formation of Gold(I) Thiolate from Gold(III) Chloride

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Table S1. Acid/Base Reactions for the Removal of the First Thiol Proton

Bases	Reaction Energies (eV)
Cl^-	-0.14
SCH_3^-	-1.03
CH_3O^-	-1.78
$HSCH_3$	1.76
CH_3OH	0.72

Cl^- is a better base for removal of the thiol proton than either the free thiol ($HSCH_3$) or the solvent (CH_3OH). However, basic conditions in which the conjugate base of the thiol or solvent (SCH_3^- and CH_3O^-, respectively) is present would favorably lead to proton dissociation. The reaction energies reported in Table S1 do not contain zero-point energies; however, these corrections are typically on the order of hundredths of an eV for the systems examined here.

Optimized BP86/TZP Coordinates for Gold-Containing Species

$AuCl_4^-$

Au	0.000000	0.000000	0.000000
Cl	2.348411	0.000000	0.000000
Cl	0.000000	2.348411	0.000000
Cl	-2.348411	0.000000	0.000000
Cl	0.000000	-2.348411	0.000000

$AuCl_3(HSCH_3)$

Au	-0.427964	0.018826	-0.952522
Cl	-0.231014	2.310031	-0.493768
Cl	-0.739763	-0.448864	1.337270

Cl	-0.575167	-2.267872	-1.469824
S	-0.209147	0.475215	-3.271735
C	1.385919	-0.269429	-3.764267
H	2.171301	-0.006753	-3.052034
H	1.219777	-1.349496	-3.806255
H	1.598560	0.129417	-4.762162
H	0.233700	1.756201	-3.119135

$AuCl_3(SCH_3)^-$

Au	-0.317609	0.088425	-0.872068
Cl	-0.826642	2.366225	-0.522649
Cl	-1.096599	-0.447287	1.367557
Cl	0.193807	-2.165031	-1.237658
S	0.395243	0.802150	-3.010326
C	0.980350	-0.624244	-3.992301
H	1.858939	-1.099184	-3.544932
H	0.186502	-1.357616	-4.164614
H	1.263411	-0.164350	-4.950997

$AuCl_4^-$ + $HSCH_3$ Transition State

Au	-0.38575500	0.25654700	0.25390700
Cl	1.92182696	0.20305800	0.69153702
Cl	-0.42429999	2.66411591	0.69384700
Cl	-2.66953897	0.31376201	-0.26062399
Cl	-0.75513500	-1.86075306	1.75350904
S	0.21782200	-1.17237306	-1.93373501
C	-1.06048799	-0.85242301	-3.20614791
H	-1.35250902	0.20105501	-3.20188904
H	-0.64532697	-1.14529502	-4.17592001
H	-1.91485703	-1.48649597	-2.95192504
H	1.10714805	-0.23919000	-2.36535406

$AuCl_4^-$ + SCH_3^- Transition State

Au	-0.38575500	0.25654700	0.25390700
Cl	1.92182696	0.20305800	0.69153702
Cl	-0.42429999	2.66411591	0.69384700
Cl	-2.66953897	0.31376201	-0.26062399
Cl	-0.75513500	-1.86075306	1.75350904
S	0.21782200	-1.17237306	-1.93373501
C	-1.06048799	-0.85242301	-3.20614791
H	-1.35250902	0.20105501	-3.20188904
H	-0.64532697	-1.14529502	-4.17592001
H	-1.91485703	-1.48649597	-2.95192504

$AuCl_3HSCH_3$ + Cl^- Proton Dissociation

Au	-0.40730301	-0.04932200	-0.91588098

Cl	-0.48102301	2.25022101	-0.46657100
Cl	-0.59796202	-0.49976400	1.43679404
Cl	-0.50136000	-2.35049295	-1.39292598
S	-0.25006601	0.38972700	-3.24146199
C	1.33662999	-0.36218500	-3.75307393
H	2.16984510	0.07485200	-3.19446206
H	1.27644706	-1.44446099	-3.60722494
H	1.43261600	-0.12854600	-4.82118893
H	0.24187601	1.87523103	-3.43262410
Cl	0.80495203	3.33525300	-4.01208687

$AuCl_3(SCH_3)^-$ + $HSCH_3$ Disulfide Formation

Au	-0.04683800	0.35245001	0.33101699
Cl	1.93705499	-0.94809699	0.54133803
S	-1.06437600	-3.81761599	-2.29766393
Cl	-2.05793691	1.57374597	0.17923300
Cl	1.00736403	2.23931408	1.91498804
S	-0.73177302	-1.57999694	-1.18847895
C	-2.27700305	-1.00997996	-2.03547192
H	-2.48676991	-0.00023500	-1.66920197
H	-2.11480403	-0.97927302	-3.11847591
H	-3.11092091	-1.67405999	-1.78402996
C	-0.25245801	-3.74816298	-3.93756008
H	-0.09011900	-4.77437305	-4.28501511
H	-0.95323700	-3.23470402	-4.60418510
H	0.69049799	-3.19858003	-3.86659193
H	-0.02046800	-4.35996008	-1.61646605

$AuCl_3(SCH_3)^-$ + $HSCH_3$

Au	-0.79522783	-0.06639688	0.81510395
Cl	1.54129124	-0.06749187	0.51919109
S	-0.63309985	2.76245213	0.72811806
Cl	-3.13017368	-0.05993484	1.06535673
Cl	-0.46071687	0.45336425	3.50115108
S	-0.99989182	-1.87314117	-0.74014020
C	-0.04910986	-3.23844385	0.02086817
H	1.00343859	-2.96628499	0.15465018
H	-0.49584380	-3.56263494	0.96745265
H	-0.12211789	-4.05953360	-0.70815623
C	-2.32830572	3.45878696	0.66976005
H	-3.03769350	2.76091599	1.12710965
H	-2.33687353	4.42687607	1.18016958
H	-2.56550860	3.59462762	-0.39064682
H	-0.52334487	2.67794704	2.08393645

$AuCl_2^-$

Au	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	2.319288
Cl	0.000000	0.000000	-2.319288

$AuCl_2(HSCH_3)_2^+$ *trans*

Au	0.000000	0.000000	-0.667961
S	2.327932	-0.567981	-0.742605
Cl	0.520475	2.282468	-0.634203
S	-2.327932	0.567981	-0.742605
Cl	-0.520475	-2.282468	-0.634203
C	-2.710284	1.117003	0.960075
C	2.710284	-1.117003	0.960075
H	3.800182	-1.221815	0.996887
H	2.355242	-0.386881	1.690938
H	2.227076	-2.090166	1.087399
H	-3.800182	1.221815	0.996887
H	-2.355242	0.386881	1.690938
H	-2.227076	2.090166	1.087399
H	2.782920	0.711555	-0.619934
H	-2.782920	-0.711555	-0.619934

$AuCl_2(HSCH_3)_2^+ + Cl^-$ Proton Dissociation *trans*

Au	0.06603700	0.24277300	-0.31619501
S	2.10848188	-0.86285901	-0.87332702
Cl	0.61750501	2.03362298	-1.73251498
S	-1.91090906	1.56224000	0.26581201
Cl	-0.53581399	-1.55765498	1.04936802
C	-3.16603088	0.52092701	1.08995700
C	2.85660791	-1.35170197	0.72320098
H	3.83221412	-1.77577901	0.45117900
H	2.99776196	-0.47958401	1.36942899
H	2.23566794	-2.11150289	1.20408404
H	-4.09530592	1.10085201	1.06469595
H	-3.27581310	-0.43836001	0.57942998
H	-2.82807302	0.38403600	2.12023497
H	3.21615505	0.36012200	-1.11637104
H	-2.45598412	1.52351296	-0.98019701
Cl	4.45099020	1.31166303	-1.27306497

$AuCl_2(HSCH_3)(SCH_3)$ *trans*

Au	0.025328	-0.080786	-0.458154
S	2.472694	-0.248448	-0.579871
Cl	0.210654	1.963693	0.657970
S	-2.346946	-0.122177	-0.473088
Cl	-0.099848	-2.155104	-1.576446
C	-2.994623	1.372115	0.357810

C	2.907541	-1.431472	0.751758
H	3.998118	-1.412837	0.846646
H	2.420555	-1.150861	1.689065
H	2.570624	-2.415185	0.410618
H	-4.085054	1.250721	0.281794
H	-2.708011	1.410306	1.413397
H	-2.697532	2.289187	-0.160294
H	2.741829	0.894012	0.110662

$AuCl_2(SCH_3)_2^-$ *trans*

Au	0.000000	0.000000	0.138571
S	2.414284	0.167606	0.137296
Cl	0.035709	2.351699	0.139376
S	-2.414284	-0.167606	0.137296
Cl	-0.035709	-2.351699	0.139376
C	-3.159156	1.511128	0.131413
C	3.159156	-1.511128	0.131413
H	4.243450	-1.333833	0.123771
H	2.891807	-2.076562	1.030310
H	2.879310	-2.075705	-0.764163
H	-4.243450	1.333833	0.123771
H	-2.891807	2.076562	1.030310
H	-2.879310	2.075705	-0.764163

$AuCl_2(SCH_3)_2^-$ *cis*

Au	0.173563	0.063818	-0.005804
S	2.524336	0.168481	-0.008300
S	0.039119	2.424406	-0.014284
Cl	-2.267836	0.168822	-0.009974
Cl	0.043119	-2.347556	-0.003420
C	1.703511	3.183190	-0.000519
C	3.203174	-1.532033	-0.031179
H	1.495458	4.262362	0.003967
H	2.267200	2.924447	0.902947
H	2.278286	2.933480	-0.899463
H	4.290988	-1.370885	-0.038799
H	2.924590	-2.096085	0.864028
H	2.910211	-2.076458	-0.933966

$AuCl_2(HSCH_3)(SCH_3)$ + $HSCH_3$ *trans* Transition State

Au	-0.583954	0.067933	0.039068
Cl	1.726338	0.642740	-0.515609
S	-1.028995	2.204639	1.178258
Cl	-2.843464	0.507999	-1.084076
S	-0.325602	-2.048994	-0.995242
C	-0.110579	-1.643864	-2.763170

H	0.805901	-1.066095	-2.926050
H	-0.019431	-2.617953	-3.265698
H	-0.986252	-1.114518	-3.154941
C	0.479375	2.688096	2.095484
H	1.363117	2.529894	1.470426
H	0.360815	3.739008	2.377909
H	0.512904	2.057168	2.989539
H	-0.828686	2.998941	0.092934
S	-1.375895	-1.223302	2.248027
C	-2.858891	-2.162253	1.722011
H	-2.694021	-2.591707	0.728656
H	-3.056945	-2.937535	2.468696
H	-3.680437	-1.439959	1.696101
H	-0.478982	-2.238879	2.136651

$AuCl_2(SCH_3)_2^-$ + $HSCH_3$ *trans* Transition State

Au	-0.039361	0.964156	-0.212470
Cl	2.353312	1.467085	-0.310846
S	-0.407569	2.838734	1.264667
Cl	-2.147264	1.564633	-1.568169
S	0.292711	-1.040356	-1.533687
C	0.644696	-0.376241	-3.207975
H	1.562836	0.223792	-3.201535
H	0.784721	-1.243328	-3.867903
H	-0.199057	0.223899	-3.569019
C	0.026789	4.287106	0.224730
H	-0.635962	4.350944	-0.646548
H	-0.113684	5.177217	0.853056
H	1.073763	4.232631	-0.096465
S	-1.341319	-0.738093	1.432532
C	-1.690610	0.068161	3.041864
H	-1.856651	1.142768	2.905352
H	-2.566944	-0.410777	3.489884
H	-0.808588	-0.105340	3.666553
H	-2.524379	-0.436929	0.834336

$AuCl_2(HSCH_3)(SCH_3)$ + Cl^- Proton Dissociation *trans*

Au	1.724599	-0.393128	0.525800
Cl	-2.680220	-0.091940	0.035941
Cl	2.540783	1.849065	0.159081
S	1.112952	-2.672121	0.735295
C	-0.306662	-2.864544	1.872516
H	-0.082804	-2.502126	2.882232
H	-1.221722	-2.407317	1.478506
H	-0.446873	-3.954368	1.914086
Cl	3.494316	-1.241610	-0.847580

S	-0.047146	0.264248	1.942235
C	-0.194760	2.083377	1.949092
H	0.674065	2.506478	2.459588
H	-0.286174	2.474976	0.932927
H	-1.108041	2.278617	2.525844
H	-1.235366	0.033325	1.010353

$AuCl_3$

Au	0.000000	0.000000	0.000000
Cl	1.155045	2.000597	0.000000
Cl	-2.310090	0.000000	0.000000
Cl	1.155045	-2.000597	0.000000

$AuCl(HSCH_3)$

Au	-0.070696	-0.314971	-0.446369
S	-0.437425	1.954261	-0.294526
C	1.213162	2.769017	-0.225242
H	1.877896	2.359028	-0.988648
H	1.604857	2.576230	0.777793
H	1.045647	3.840928	-0.369369
Cl	0.228109	-2.611735	-0.593967
H	-0.688621	2.208934	-1.608494

$AuCl(HSCH_3) + HSCH_3$ Transition State

Au	-0.12244900	0.31443399	0.23218000
Cl	1.50445294	1.52014196	1.66661406
S	-0.55438602	-1.77277803	-0.71549797
C	-1.56808102	-1.58378196	-2.24215794
H	-1.15157104	-0.80783802	-2.88855600
H	-1.58684599	-2.55554008	-2.74647307
H	-2.57483006	-1.31293905	-1.90912700
H	0.62765700	-1.99502003	-1.35058999
S	-1.63886499	2.52122688	0.24328400
C	-2.70111108	2.68265605	-1.25258696
H	-3.07191801	3.71014500	-1.32068706
H	-2.14521599	2.40526795	-2.15240598
H	-3.54027891	1.99600804	-1.10229099
H	-0.65092999	3.36036706	-0.16324900

$AuCl(SCH_3)^-$

Au	-0.089182	-0.056624	-0.446853
S	-0.454297	2.211333	-0.383421
C	1.202270	2.987750	-0.074456
H	1.893192	2.786243	-0.900349
H	1.635918	2.633894	0.867135
H	1.025868	4.068796	-0.006814

Cl	0.200245	-2.405919	-0.519514

$Au_2(SCH_3)_2Cl^-$

Au	1.198797	1.603953	0.101937
S	-1.018303	1.397412	0.713908
Au	-1.720474	0.347045	-1.269708
S	-2.502467	-0.595473	-3.241184
Cl	3.439122	1.876790	-0.540418
C	-1.053700	0.104637	2.045016
C	-1.002042	-1.272330	-4.101249
H	-0.286798	-0.474743	-4.329233
H	-0.515255	-2.043801	-3.495022
H	-2.108152	-0.099193	2.262080
H	-0.546806	-0.808953	1.723784
H	-0.564356	0.525826	2.929893
H	-1.354941	-1.719486	-5.039030

$Au_2(SCH_3)_2Cl_2^-$ Transition State

Au	-0.16285001	1.03538299	1.97999597
Cl	0.82258701	0.96112800	4.12684917
S	-1.24241400	1.12440205	-0.04829000
C	-0.29733801	2.36161304	-1.05320299
H	-0.45837799	3.36845803	-0.65260899
H	0.77136600	2.12551594	-1.06140900
H	-0.69348198	2.29095697	-2.07332110
Au	-1.02195299	-1.25700903	-1.28808606
Cl	-1.22874200	-0.15597500	-3.59026098
S	-0.81893098	-3.30734992	-0.19911000
C	-0.98111397	-2.94098091	1.61488998
H	-0.35401699	-2.08548498	1.89592302
H	-2.02337503	-2.72220993	1.87533903
H	-0.65248799	-3.83422089	2.16269708

$AuCl(HSCH_3)(SCH_3)_2 + HSCH_3$ Transition State

Au	1.025755	-0.052601	2.269805
Cl	-0.938325	1.153782	2.985515
S	1.373606	1.078617	0.224184
C	0.212610	2.499698	0.159821
H	-0.831152	2.171355	0.142692
H	0.380230	3.197683	0.986321
H	0.456986	2.995689	-0.790368
S	0.907804	-1.288989	4.376980
C	-0.461514	-2.488571	4.144509
H	-1.386910	-1.904983	4.170392
H	-0.353234	-3.012928	3.191574
H	-0.423867	-3.183157	4.989725

S	2.904088	-1.341996	1.601948
C	4.311292	-0.353973	2.247267
H	5.208591	-0.920870	1.964467
H	4.342187	0.633669	1.774075
H	4.273308	-0.260371	3.338121
H	1.932998	-2.139108	4.074120

$AuCl(HSCH_3)(SCH_3)_2$ + $HSCH_3$ Transition State

Au	0.88582897	-0.36521900	1.94819903
Cl	-0.00002200	1.60461497	3.29454994
S	1.00680995	0.75800699	-0.20998400
C	0.59121197	2.52714801	0.04008500
H	-0.45919099	2.65396905	0.32238999
H	1.23810899	2.98478198	0.79535598
H	0.76979101	3.00554109	-0.93283701
S	0.94105601	-1.72750103	3.95813608
C	-0.81693298	-1.78922403	4.48511314
H	-1.18764102	-0.77912098	4.69199705
H	-1.44750404	-2.27918911	3.73266006
H	-0.83689898	-2.38599706	5.40701485
S	3.53091192	0.09128800	2.35529494
C	3.62596202	1.88909900	2.70648909
H	4.50282812	2.07904696	3.33311105
H	3.74808192	2.38098407	1.73627102
H	2.70209503	2.22157001	3.19204903
H	3.52945590	-0.32369000	3.65157294
S	-0.03877800	-2.27597904	0.78067100
C	1.30038404	-2.91469693	-0.29478100
H	0.94875097	-3.86553311	-0.70947599
H	1.43121898	-2.18064189	-1.09673297
H	2.22347593	-3.04306006	0.27607799
H	0.17623800	-3.12894011	1.83091295

$Au(HSCH_3)_2^+$

Au	0.000000	0.000000	0.444569
S	2.331178	0.148895	0.390875
S	-2.331178	-0.148895	0.390875
C	-2.964483	1.563838	0.632226
C	2.964483	-1.563838	0.632226
H	4.037779	-1.478580	0.826934
H	2.444184	-2.057653	1.455357
H	2.789076	-2.085575	-0.312953
H	-4.037779	1.478580	0.826934
H	-2.444184	2.057653	1.455357
H	-2.789076	2.085575	-0.312953
H	-2.520178	-0.580566	1.668537

H	2.520178	0.580566	1.668537

$Au(HSCH_3)(SCH_3)$

Au	2.119669	-0.106463	-0.467010
S	0.692209	1.288826	-1.712652
C	0.458469	2.876585	-0.807041
H	-0.227766	2.655488	0.015878
H	1.410982	3.253331	-0.427134
H	-0.002624	3.582927	-1.504606
H	1.591338	1.752840	-2.623462
S	3.430327	-1.601473	0.709697
C	5.137343	-0.869896	0.683596
H	5.779626	-1.575576	1.224769
H	5.504832	-0.761937	-0.342444
H	5.159126	0.099978	1.191533

$Au(SCH_3)_2^-$

Au	0.000000	0.000000	-0.440243
S	2.335169	0.148543	-0.492988
S	-2.335169	-0.148543	-0.492988
C	-2.983021	1.436420	0.230474
C	2.983021	-1.436420	0.230474
H	4.077298	-1.355063	0.245745
H	2.618997	-1.585538	1.253462
H	2.696449	-2.293407	-0.389939
H	-4.077298	1.355063	0.245745
H	-2.618997	1.585538	1.253462
H	-2.696449	2.293407	-0.389939

$Au(HSCH_3)(SCH_3)_3$

Au	0.007780	0.022688	0.319427
S	2.427298	0.106621	0.348916
S	-0.101949	2.390618	0.365757
S	-2.411542	-0.069873	0.339634
S	0.071135	-2.424620	0.150180
C	1.584943	3.099492	0.339871
C	-3.127054	1.616852	0.392970
C	-1.584961	-3.174459	0.343562
C	3.113403	-1.597289	0.425211
H	1.411900	4.184598	0.349269
H	2.162259	2.821173	1.228531
H	2.131487	2.831668	-0.571216
H	4.201511	-1.460555	0.375060
H	2.871840	-2.099616	1.369386
H	2.803016	-2.211870	-0.427832
H	-1.416793	-4.239166	0.534084

H	-2.137217	-2.703225	1.161112
H	-2.102083	-3.037466	-0.610405
H	-4.213553	1.459323	0.389389
H	-2.843112	2.149370	1.307582
H	-2.847071	2.204290	-0.488903
H	0.501564	-2.663121	1.418238

$Au(HSCH_3)_2(SCH_3)_2^+$

Au	0.000000	0.000000	0.435437
S	2.392595	0.085191	0.313300
S	-0.082014	2.422068	0.487353
S	-2.392595	-0.085191	0.313300
S	0.082014	-2.422068	0.487353
C	1.609659	3.125528	0.554328
C	-3.133677	1.562483	0.561892
C	-1.609659	-3.125528	0.554328
C	3.133677	-1.562483	0.561892
H	1.453587	4.210972	0.499881
H	2.116340	2.894238	1.498133
H	2.219509	2.821415	-0.304329
H	4.192222	-1.371190	0.768215
H	2.653397	-2.091215	1.389529
H	3.021132	-2.103217	-0.381765
H	-1.453587	-4.210972	0.499881
H	-2.116340	-2.894238	1.498133
H	-2.219509	-2.821415	-0.304329
H	-4.192222	1.371190	0.768215
H	-2.653397	2.091215	1.389529
H	-3.021132	2.103217	-0.381765
H	-2.580314	-0.539416	1.582574
H	2.580314	0.539416	1.582574

$Au(HSCH_3)(SCH_3)^{2+}$

Au	0.008451	-0.003697	0.493389
S	2.400975	0.103518	0.270151
S	-0.085936	2.371568	0.572967
S	-2.409965	-0.060621	0.596095
S	0.061495	-2.486354	0.397440
C	1.586510	3.095578	0.561373
C	-3.142432	1.605550	0.577347
C	-1.621265	-3.197416	0.473840
C	3.142544	-1.538176	0.568170
H	1.380867	4.174448	0.502634
H	2.135802	2.897185	1.487919
H	2.161926	2.809274	-0.326190
H	4.221015	-1.350300	0.618127

H	2.785031	-1.977258	1.502194
H	2.910690	-2.158748	-0.300773
H	-1.474191	-4.277049	0.577186
H	-2.186053	-2.804345	1.322558
H	-2.105069	-2.970935	-0.479685
H	-4.179455	1.455615	0.897545
H	-2.613940	2.278839	1.258758
H	-3.104104	1.953500	-0.458018
H	-2.451682	-0.246372	1.944962
H	0.372360	-2.659371	1.711178
H	2.628371	0.607036	1.514654

$Au(HSCH_3)_4^{3+}$

Au	0.000000	0.000000	0.477836
S	2.423671	0.079282	0.404102
S	-0.073094	2.424422	0.435872
S	-2.423671	-0.079282	0.404102
S	0.073094	-2.424422	0.435872
C	1.588075	3.146993	0.631330
C	-3.145557	1.592292	0.474992
C	-1.588075	-3.146993	0.631330
C	3.145557	-1.592292	0.474992
H	1.396433	4.220996	0.743735
H	2.094179	2.756214	1.516915
H	2.137292	2.958846	-0.294566
H	4.224397	-1.411273	0.547980
H	2.794103	-2.146654	1.348063
H	2.912002	-2.089349	-0.469772
H	-1.396433	-4.220996	0.743735
H	-2.094179	-2.756214	1.516915
H	-2.137292	-2.958846	-0.294566
H	-4.224397	1.411273	0.547980
H	-2.794103	2.146654	1.348063
H	-2.912002	2.089349	-0.469772
H	-0.450242	2.529402	1.740841
H	-2.565693	-0.376276	1.726498
H	0.450242	-2.529402	1.740841
H	2.565693	0.376276	1.726498

$Au_4(SCH_3)_4Cl^-$ Linear Chain

Au	2.730108	4.593097	-1.219426
S	0.831823	4.535953	-2.587635
C	1.379346	5.196929	-4.233383
H	1.589604	6.264732	-4.109135
H	2.266736	4.671272	-4.595500
H	0.544385	5.059843	-4.929328

Au	0.716203	2.197846	-2.820342
S	0.471309	-0.098677	-3.047632
C	2.107777	-0.826917	-2.558610
H	2.348626	-0.586039	-1.517637
H	2.009733	-1.914641	-2.663513
H	2.909091	-0.471981	-3.215474
Au	3.842049	3.182130	1.803457
S	4.632902	4.633580	0.146998
C	4.663516	6.314876	0.931754
H	3.703083	6.553410	1.395647
H	5.461833	6.309183	1.681536
H	4.897349	7.036606	0.141887
Au	2.274781	3.257937	4.895961
Cl	1.444914	4.859683	6.389592
S	3.032776	1.670766	3.398528
C	4.529670	0.909569	4.187267
H	5.238999	1.674119	4.513593
H	4.180986	0.317657	5.040198
H	4.987988	0.254132	3.438722

$Au_4(SCH_3)_4Cl^-$ Intermediate

Au	3.109270	3.847406	-1.016732
S	1.146285	4.238432	-2.229597
C	1.634253	5.389742	-3.601410
H	1.843048	6.367897	-3.154896
H	2.511656	5.017826	-4.136923
H	0.777195	5.464216	-4.279478
Au	1.080804	2.073792	-3.150178
S	1.035008	-0.095522	-3.975720
C	-0.542932	-0.237900	-4.944696
H	-0.557840	0.470169	-5.780327
H	-0.575988	-1.261206	-5.339225
H	-1.415007	-0.071452	-4.303013
Au	4.934329	1.144385	0.296844
S	5.089631	3.476595	0.179682
C	4.774749	4.099911	1.898124
H	3.854902	3.678118	2.310866
H	5.636709	3.813234	2.510020
H	4.704230	5.191323	1.839394
Au	6.440563	-1.623670	-1.225139
Cl	8.083477	-2.083000	-2.831169
S	4.872498	-1.192374	0.413869
C	3.234899	-1.681430	-0.307747
H	3.056106	-1.184397	-1.264964
H	3.246136	-2.769116	-0.434333
H	2.468613	-1.395885	0.420990

$Au_4(SCH_3)_4Cl^-$ Transition State

Au	2.72298503	3.93323207	-1.08586204
S	0.49747100	4.16124201	-1.79656005
C	0.50606501	5.39996576	-3.17697811
H	0.62868100	6.39134121	-2.72775698
H	1.31308401	5.19939089	-3.88611507
H	-0.46674100	5.33405113	-3.67635798
Au	0.75316298	2.02935410	-2.78793502
S	0.92125303	-0.14898200	-3.59149289
C	1.44715595	0.00988200	-5.36038589
H	2.36589193	0.59848499	-5.44638777
H	1.62632203	-1.01037002	-5.72008181
H	0.64470202	0.47584701	-5.94281578
Au	4.75543308	1.29384601	-0.61853200
S	4.95444107	3.63111997	-0.43927801
C	5.05330086	4.01182985	1.37240803
H	4.26662397	3.49835896	1.93080497
H	6.04133320	3.68849802	1.71763599
H	4.95609999	5.09725285	1.48200297
Au	3.00366402	-1.40406704	-2.50118494
Cl	2.40054202	-3.43602800	-3.95880699
S	4.65748787	-1.03433001	-0.85485601
C	3.86922503	-1.61674905	0.72099102
H	2.90758801	-1.12428904	0.88912600
H	3.72954512	-2.69988894	0.63200301
H	4.56027412	-1.39542902	1.54196799

$Au_4(SCH_3)_4$ Cyclic Cluster

Au	2.557167	4.141032	-0.826691
S	0.739108	4.456769	-2.281445
C	1.395632	5.454369	-3.700781
H	1.549814	6.475036	-3.335077
H	2.332148	5.038355	-4.080324
H	0.628540	5.448709	-4.482465
Au	0.824686	2.210029	-2.964067
S	0.863189	-0.091365	-3.439623
C	1.143477	-0.245549	-5.265968
H	1.982524	0.373045	-5.593780
H	1.341608	-1.302278	-5.474586
H	0.218681	0.067024	-5.762559
Au	4.704443	1.581816	-0.269170
S	4.384719	3.743008	0.595654
C	3.665835	3.516611	2.290349
H	2.827981	2.815135	2.277173
H	4.468829	3.143511	2.934849

H	3.335625	4.501896	2.636085
Au	2.953890	-0.364370	-2.410654
S	5.034046	-0.488946	-1.331486
C	4.874888	-1.783292	-0.013338
H	3.974862	-1.631184	0.587454
H	4.839875	-2.755174	-0.516822
H	5.770713	-1.718246	0.613424