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Formation of the Me_2SAuCl complex in the reaction of $HAuCl_4$ with quercetin in dimethyl sulfoxide

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Figure S1 shows changes in the optical density of the reaction mixture $HAuCl_4$ ($1*10^{-1}$ M) + quercetin ($1*10^{-1}$ M) in DMSO/H_2O (4:1), recorded using a Specord-M-40 spectrophotometer ("Carl Zeiss", Germany). It shows that the characteristic absorption peak of quercetin in the region of 380 nm practically disappears after 24 hours. At the same time, a peak λ_{max} = 292 nm with a shoulder of ~ 320-326 nm is formed.

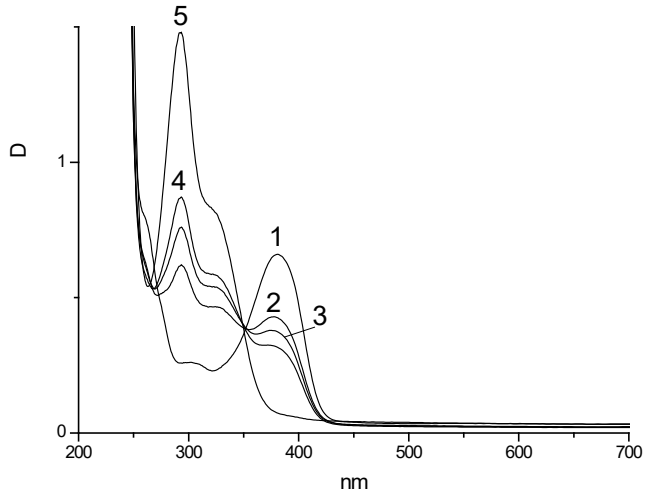

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Figure S1 Spectra of the initial solution of quercetin (*1*) and after adding $HAuCl_4$ in DMSO/H_2O (4:1): after 10 min (*2*), 60 min (*3*), 120 min (*4*), 1 day (*5*). [**Qc**]=$1*10^{-4}$ M, [Au]= $1*10^{-4}$ M

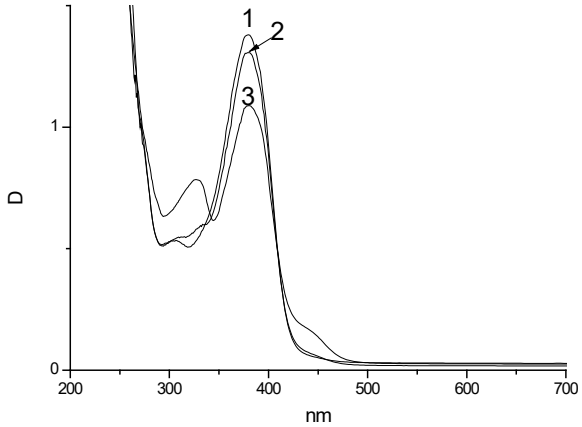
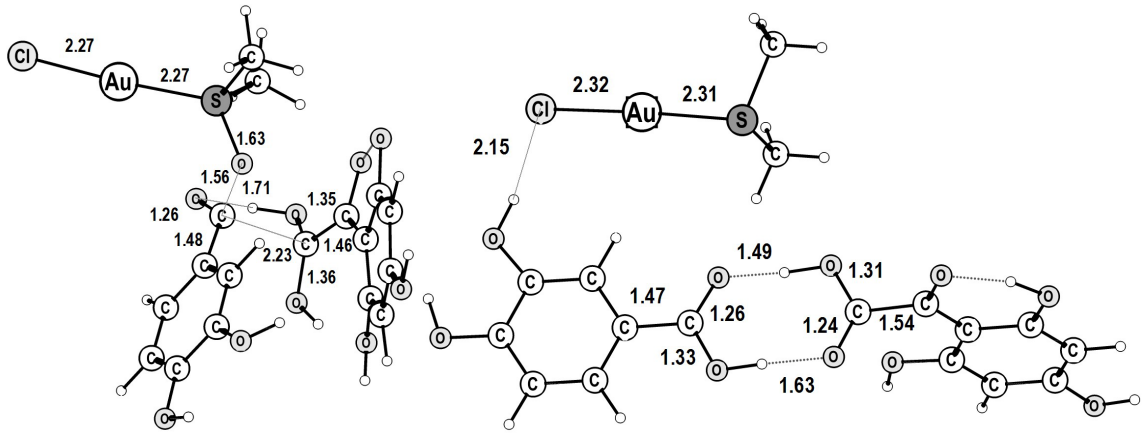


Figure S2 Spectra of the initial solution of quercetin ($2.5*10^{-4}$ M) in DMSO/H_2O (4:1) (*1*) and after its storage in an inert atmosphere: 1 day (*2*), 1 month (*3*)

A solution of quercetin in DMSO/H_2O (4:1) is quite stable under anaerobic conditions. From the spectra in Figure S2 it is clear that after 24 hours there is only a slight decrease in the height of the peak with λ_{max} = 380 nm. After 1 month of storage, the relative decrease in peak height was ~20%. In this case, the formation of an absorption band with λ_{max} = 326 nm and a shoulder at ~445 nm was recorded.

The results of a theoretical study of the mechanism of formation of the Me_2SAuCl complex are reflected in Figures S3 and S4, which show the structure of intermediate and final products in the interaction of the initial complex $(Me_2SO)AuCl$ with ketal **C** and its protonated form, respectively



(*a*) (*b*)

Figure S3. Structure of the transition state of the O atom transfer from the $(Me_2SO)AuCl$ complex to ketal **C** (*a*) and the resulting product (*b*).

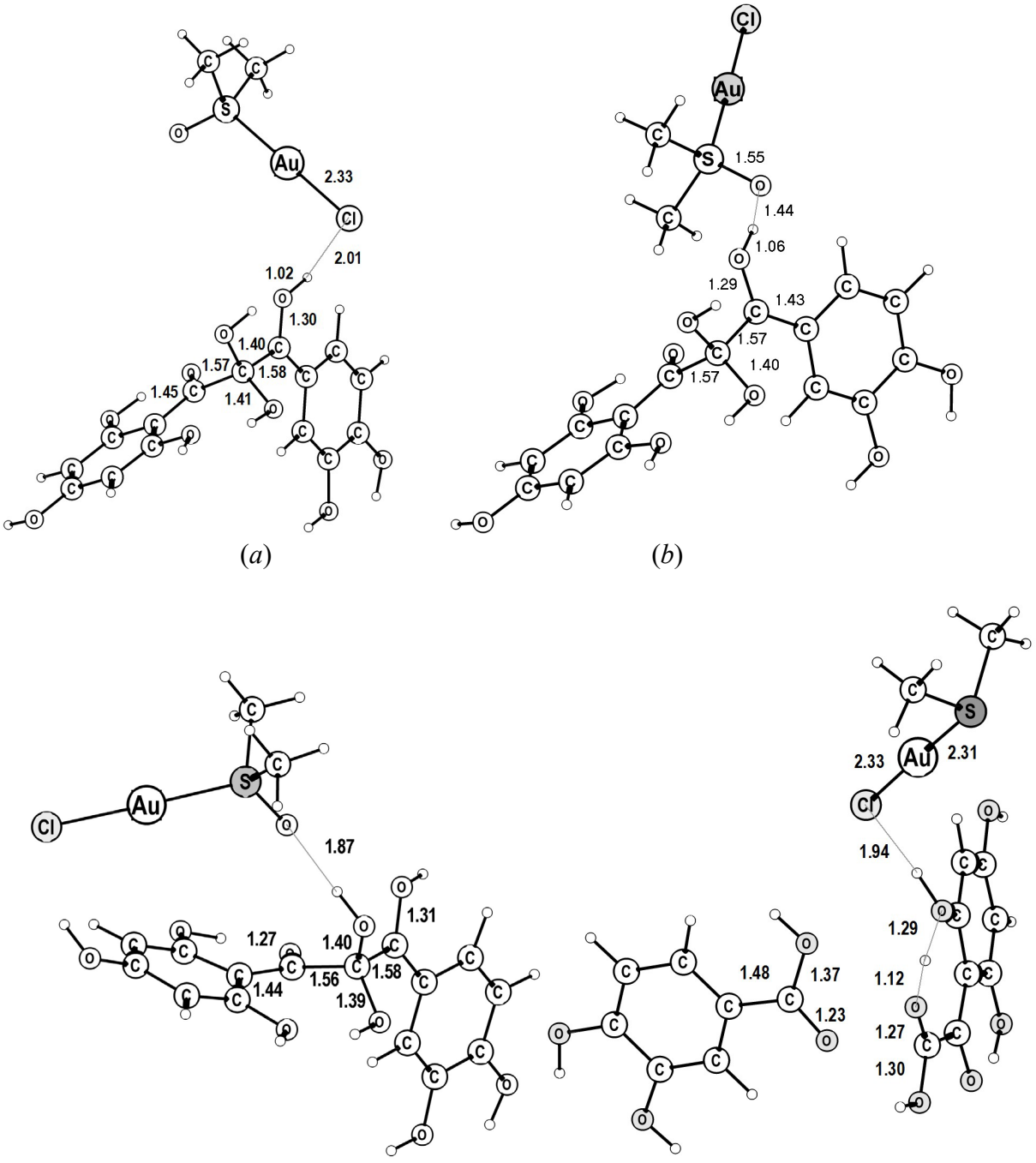


Figure S4 Structure of the pre-reaction complex between (Me_2SO)AuCl and protonated ketal **C** with AuCl…HO hydrogen bond (*a*) , the isomer complexes with SO…HO hydrogen bond including the same (*b*) or adjacent (*c*) OH group and the resulting product (*d*).

When the ketal **C** is protonated, the charge on the carbonyl group increases from -0.05 to 0.30. In the complexes (*a*) (*b*) with a hydrogen bond, the fragment (Me_2SO)AuCl acquires a close charge of 0.268 and 0.263, respectively. However, the charges on the carbonyl group differs significantly: 0.15 for (*a*) and 0.27 for (*b*). It can be noted that it is for the pre-reaction complex the charge on the carbonyl group is much closer to its value 0.13 for the adduct formed.
So, indeed there is resemblance of the electronic structure of the pre-reaction complex and the adduct.

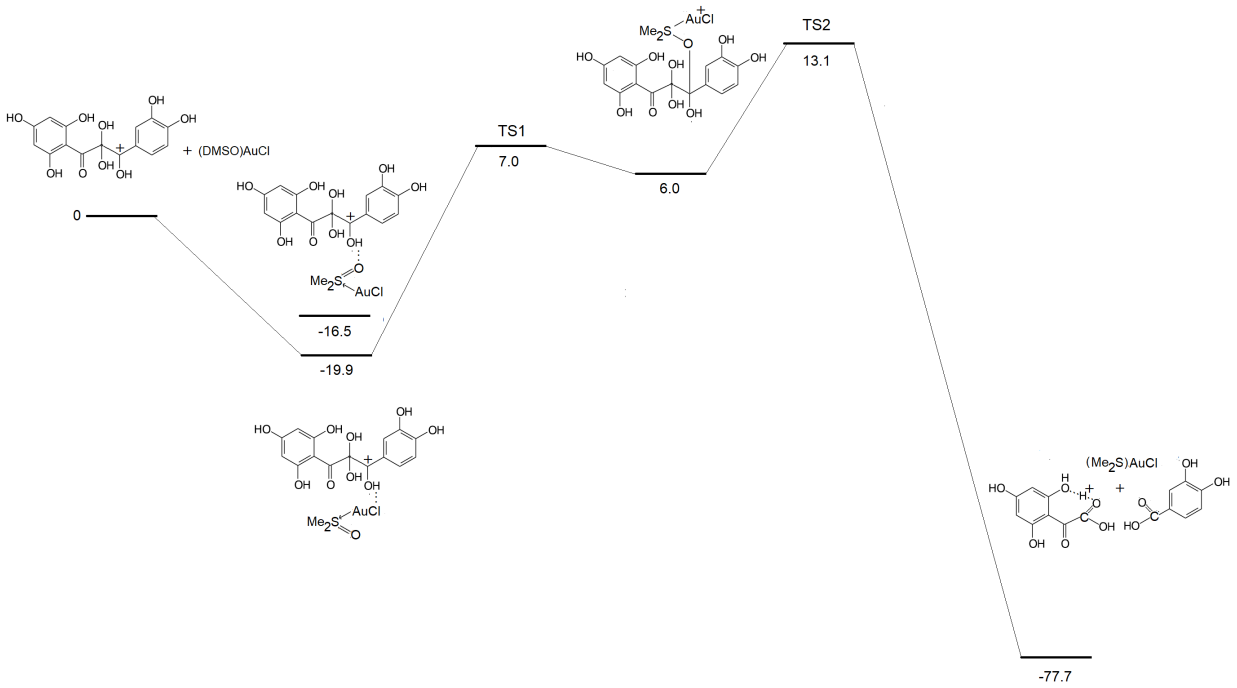


Figure S5. The energy diagram of the oxidation reaction between $(Me_2SO)AuCl$ and the protonated ketal C

Due to the importance of relativistic effects for the gold atom, additional calculations were carried out using a scalar relativistic approximation based on the Dirac equation with spin-orbit effects excluded [K.G. Dyall, *J. Chem. Phys*., 100 (1994) 2118]. This approach leads to four-component one-electron wave functions. An energy-optimized extended Gaussian basis for large components and a corresponding kinetically balanced basis for small components: Au [33s31p28d25f22g19h16i10k/21s20p19d17f14g7h4i1k] S,Cl [18s17p15d11f9g/11s9p7d4f2g], C [12s10p9d6f4g/7s6p5d3f1g] and H[8s6p3d/3s2d1f] [D.N. Laikov, *Chem. Phys. Lett*., 416 (2005) 116.] were used. The geometric parameters of the complexes $[(Me_2S)AuCl]_2$ and $[(Me_2S)AuCl]_3$ in this approach change slightly, within 0.01-0.05 Å, and the calculated energies of aurophilic interaction, equal to 10.2 kcal/mol, differ little from data based on the SBK pseudopotential

According to X-ray diffraction data, Me_2SAuCl complexes form infinite chains (see Fig. S5) with short Au-Au contacts 3.1873 Å

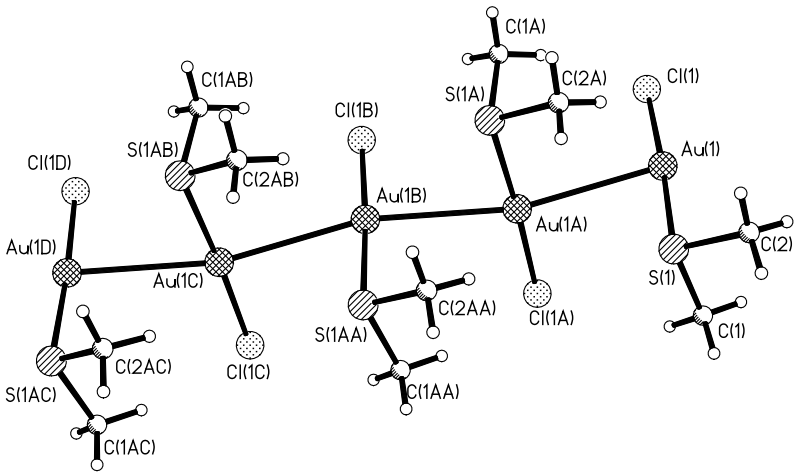


Figure S6 Structure of a one-dimensional chain of Me_2SAuCl complexes according to X-ray diffraction data. Valence distances: Au(1)-S(1) 2.273(2), Au(1)-Cl(1) 2.288(2), Au(1)-Au(1)#1 3.1873(2), Au(1)-Au(1)#2 3.1874(2), S(1)-C(2) 1.798(9), S(1)-C(1) 1.797(8), and angles: S(1)-Au(1)-Cl(1) 176.80(7), S(1)-Au(1)-Au(1)#1 93.27(5), Cl(1)-Au(1)-Au(1)#1 89.90(5), S(1)-Au(1)-Au(1)#2 76.94(5), Cl(1)-Au(1)-Au(1)# 2 99.98(5), Au(1)#1-Au(1)-Au(1)#2 167.61(2), C(2)-S(1)-C(1) 100.8(4), C(2)-S(1)-Au(1) 107.7(3), C(1)-S(1)-Au(1) 105.6(3)

The resulting Me_2SAuCl crystals, dried after washing, were placed on the substrate of a Perkin-Elmer-spectrum-100 IR spectrometer to record IR spectra. In Figure S3, the experimental spectrum is compared with the calculated spectra of Me_2S, Me_2SAuCl and the trimer $(Me_2SAuCl)_3$ as well.

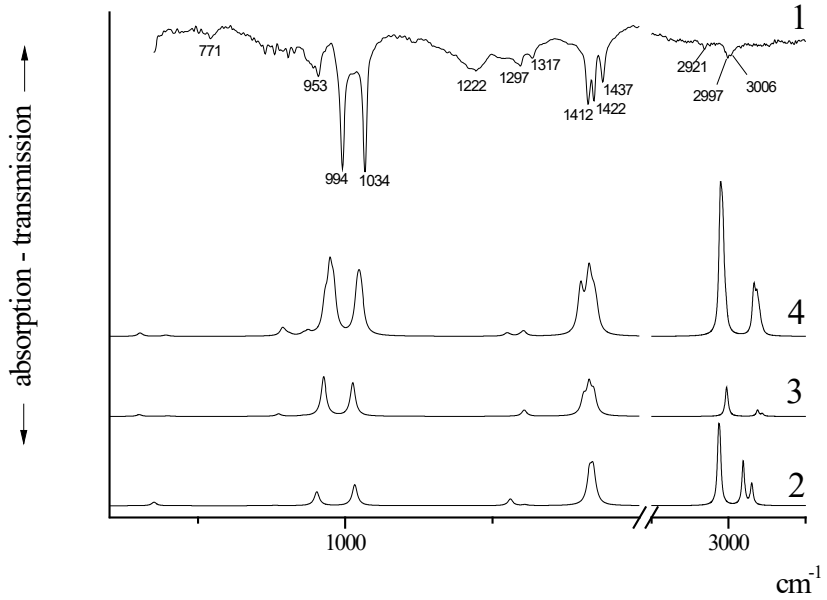


Figure S7 IR spectra: experimental for the Me_2SAuCl complex (*1*) and theoretical spectra for Me_2S (*2*), Me_2SAuCl (*3*) and its trimer – $(Me_2SAuCl)_3$ (*4*).

The split band at 3091, 3074 cm^{-1} in the theoretical IR spectrum of Me_2SAuCl corresponds to asymmetric C-H vibrations of methyl groups, and the band at 2978 cm^{-1} corresponds to symmetric C-H vibrations of methyl groups. The band at 1415 cm^{-1} and the low-intensity band at 1305 cm^{-1} are due to the near-scissor vibrations and umbrella C-H bending vibrations of the methyl groups, respectively. In the trimer, there is a visible splitting of this band into two bands, corresponding to symmetric 1310 cm^{-1} and antisymmetric 1284 cm^{-1} vibrations of each pair of Me groups. The bands at 1011, 960, 881 cm^{-1} (respective effective masses are 1.26, 1.19, 1.17) correspond to various mixed-type deformation vibrations, including scissor, waggind and rocking vibrations of the Me-S-Me unit and deformation vibrations of CH_2 groups. Low-intensity bands at 698, 653 cm^{-1} (reduced masses 6.47, 5.35) correspond to symmetric and antisymmetric S-C vibrations

Cartesian coordinates of calculated structures and their energies E and E_0, the last contains ZPVE contribution

quercetin

8	0.86984534	0.32771859	0.02774925
6	1.65362787	-0.05271773	-1.02412757
6	-0.44697928	-0.06353802	0.15156148
6	-1.00001402	-0.87245565	-0.82426391
6	-0.22626434	-1.31257621	-1.96505105
6	-1.08379134	0.46546672	1.35514954
6	-0.35506750	1.29599599	2.23747398
6	-3.01121467	0.68265327	2.82098458
1	0.68195645	1.54052313	2.01731925
6	-0.94585328	1.81036047	3.39097609
6	-2.43268058	0.16530291	1.66908615
1	-0.38346921	2.45095784	4.07093852
1	-3.02018711	-0.47194974	1.00935022
6	-2.27699398	1.51130855	3.69664382
6	2.97139363	0.40365586	-1.04494154
6	3.77837591	0.01440092	-2.12344791
6	1.13372607	-0.87803078	-2.04420501
6	3.29961452	-0.80816044	-3.16261575
1	3.94340477	-1.10056206	-3.99427565
6	1.97927185	-1.25801104	-3.13015432
1	3.36524252	1.03971728	-0.25513161
8	5.06583498	0.47390028	-2.12196191
1	5.51828479	0.13785485	-2.91412315
8	1.49199438	-2.04414703	-4.10665230
1	0.53249021	-2.23020840	-3.85919508
8	-0.79511803	-2.05675624	-2.82975198
8	-2.28361271	-1.32514776	-0.81961218
1	-2.31756873	-1.86034089	-1.65541259
8	-2.86037463	2.01110595	4.82254498
1	-3.77977534	1.68253769	4.83971560
8	-4.31556445	0.44580580	3.20957046
1	-4.75053409	-0.12466413	2.55585960

E = -203.268634 E_0 = -203.044559

Structure A

6	3.37931022	1.04214154	1.72211015
6	3.68377609	-0.23144081	1.19571850
6	2.71862146	-1.24415005	0.97332377
6	1.41135372	-0.92974878	1.32066601
6	1.08170504	0.33034494	1.84599304
6	2.05426060	1.33217708	2.04996206
1	4.17288065	1.77476030	1.85755975
8	4.99704418	-0.45143782	0.89787389
1	5.09353738	-1.35277238	0.54577210
8	0.32730552	-1.74450455	1.17912110
6	-1.99787999	-1.17937328	0.64662390
6	-0.86676119	-1.03470237	1.73320061
6	-0.32465752	0.39772662	2.07355413
8	1.67548190	2.53038214	2.54309035
8	-0.98848544	1.35268205	2.49019715
8	-1.30280936	-1.64609234	2.87776069
1	2.99144668	-2.21709641	0.56343079
6	-1.93514937	-0.54261273	-0.67942534
6	-0.85826377	0.26819094	-1.09590727
6	-0.86156539	0.84534694	-2.36288223
6	-1.95532328	0.61623497	-3.22745845
6	-3.02853811	-0.18559347	-2.82188678
6	-3.01943862	-0.76376827	-1.55572191
1	-0.00357511	0.46958034	-0.45187285
8	0.18279322	1.62711995	-2.76517978
8	-1.86675134	1.23164815	-4.45101291
1	-3.86885942	-0.35165637	-3.50095259
1	-3.84642922	-1.38971524	-1.22315418
1	-0.01569252	1.94372818	-3.66614852
1	0.69573874	2.48522628	2.67833297
1	-2.66078472	1.03987109	-4.97644441
8	-2.94355132	-1.89157042	0.99327770
1	-2.12073970	-2.13092621	2.59047856

E = -219.270664 E0 = -219.043488

Structure B

8	-3.59494697	1.55701726	0.79905132
8	-3.56876228	3.65965658	-0.51094608
6	-1.58409065	4.85875655	-0.81583267
6	-0.21836790	5.02380131	-0.55112833
6	0.47980912	4.14222605	0.28373333
6	-0.17113636	3.05444057	0.86331989
6	-1.57426196	2.80510293	0.58795555
6	-2.26393316	3.78278904	-0.24721714
8	0.48933607	6.06054208	-1.07767014
1	-0.10456042	6.59781109	-1.62997075
1	-2.13927149	5.55251899	-1.44844903
1	1.53061398	4.31332471	0.50908676
8	0.58101950	2.30302236	1.68282766
6	-2.55598791	-0.87840461	1.32807117

6	-1.83726415	0.41932986	1.73691782
6	-2.34622471	1.66030810	0.99390607
6	-3.37846818	-1.64842096	2.26187516
6	-3.65707386	-1.16178013	3.55871257
6	-4.45507915	-1.90673114	4.41540909
6	-4.99219773	-3.14712593	3.99486046
6	-4.71764508	-3.62734217	2.70630166
6	-3.91610613	-2.88341362	1.84647179
8	-4.79840046	-1.54310295	5.70073766
8	-5.77167671	-3.86790029	4.84020306
1	-3.24738509	-0.20524767	3.89147438
1	-5.14447264	-4.58402433	2.40403815
1	-3.69293242	-3.23999631	0.84069322
1	-4.38395798	-0.69581299	5.92904885
1	-5.83953697	-3.36547220	5.67580070
1	-3.87280635	2.81809517	-0.02314400
8	-2.25232517	-1.21245919	0.18153803
8	-0.91399195	0.38939826	2.55196376
1	0.04370671	1.59002767	2.13508254

E = -219.263723 E0 = -219.038377

Structure C

8	-3.54680631	-0.05011574	0.65962414
8	-5.99837943	0.07618338	0.65501104
6	-7.09955091	2.08018557	1.13992266
6	-7.05832890	3.42524097	1.49710067
6	-5.82914957	4.08240821	1.68209182
6	-4.64119880	3.38613854	1.49492439
6	-4.60953309	2.00991450	1.11023721
6	-5.90162950	1.36892010	0.96585416
8	-8.18401528	4.16914415	1.69368397
1	-8.96216748	3.60425109	1.54739170
1	-8.04114017	1.54470824	1.01019712
1	-5.82587490	5.13130853	1.98294901
8	-3.45478453	4.04642632	1.71321622
6	-0.99667890	0.56268726	0.27479503
6	-1.94661159	1.68126333	0.87723018
6	-3.42035214	1.18407590	0.87565445
6	-1.03465398	0.17236729	-1.14321096
6	-1.87661199	0.80153975	-2.08736308
6	-1.86578779	0.38205947	-3.40991083
6	-1.02564798	-0.67639987	-3.82436487
6	-0.19063988	-1.30312461	-2.89051243
6	-0.19455892	-0.87966535	-1.56460956
8	-2.63616444	0.93135747	-4.41748002
8	-1.02928705	-1.07792745	-5.12372573
1	-2.50924615	1.63796492	-1.78657298
1	0.45021180	-2.11922347	-3.22546869
1	0.44838538	-1.36031380	-0.82776325
1	-3.18197565	1.64722580	-4.05528571
1	-1.67378114	-0.51660222	-5.59711406
8	-1.58790170	1.83509324	2.22139739

1	-5.02501834	-0.25646789	0.61631834
8	-0.18448941	0.08998652	1.07331139
8	-1.71614796	2.83836993	0.09927665
1	-2.14292385	3.56628571	0.59992956
1	-0.82044222	1.20869517	2.31734993
1	-3.64946168	4.95102704	2.01169956

E = -236.489963 E0 = -236.237750

Structure of protonated form of C, CH^+

8	-3.67634506	0.00032834	0.33004811
8	-6.12143630	0.06842262	0.87001303
6	-7.10177512	2.03248327	1.66556721
6	-6.99930774	3.38002881	2.01358946
6	-5.77600683	4.07507590	1.88237416
6	-4.65498402	3.40712852	1.43000502
6	-4.68099819	2.01177914	1.09122661
6	-5.97350691	1.35225576	1.19739656
8	-8.04407279	4.10406663	2.46927254
1	-8.84017312	3.54532808	2.52326348
1	-8.04185353	1.48560270	1.74505579
1	-5.74532910	5.13768175	2.12740071
8	-3.47980487	4.10280700	1.26132300
6	-1.31149017	0.35438977	0.17775037
6	-2.05612705	1.63543228	0.72338300
6	-3.55555599	1.20567155	0.70615888
6	-1.02875859	0.04048640	-1.18332747
6	-1.69029469	0.71633993	-2.25191811
6	-1.43799230	0.35553959	-3.56024253
6	-0.50595445	-0.68276806	-3.85407068
6	0.16740511	-1.34456551	-2.80855849
6	-0.09508066	-0.99117475	-1.49904997
8	-2.00836447	0.90534712	-4.67119550
8	-0.26130934	-1.02830215	-5.11927364
1	-2.39826757	1.51277036	-2.03076701
1	0.89320395	-2.11762328	-3.05926487
1	0.48245185	-1.50108462	-0.72311995
1	-2.63650772	1.61009726	-4.44055504
1	-0.80511559	-0.46727975	-5.71250204
8	-1.72435946	1.88400491	2.05795443
1	-5.21645255	-0.25911729	0.56564775
8	-0.85044002	-0.37045534	1.16877341
8	-1.70978326	2.68537816	-0.13897498
1	-2.21432053	3.46095482	0.20629079
1	-0.79859498	2.19026635	2.09783815
1	-3.59934243	5.01819837	1.56946020
1	-0.44470362	-1.19999792	0.84165243

E = -236.840022 E_0 = -236.575396

Pre-reaction complex between **C** and [(dmso)AuCl]

8	0.95887646	1.27334433	1.69234023
8	3.25927473	0.35023825	1.57517935
6	3.62359531	-1.93420369	1.90769790
6	3.13368016	-3.20906530	2.19625366
6	1.76477969	-3.42483921	2.42995391
6	0.88052867	-2.35427365	2.36989374
6	1.31619642	-1.02190628	2.06746144
6	2.73976267	-0.85105348	1.84681150
8	3.94390349	-4.29975844	2.27093781
1	4.86024389	-4.02608102	2.09235410
1	4.68405388	-1.75018879	1.73101446
1	1.41426391	-4.43057712	2.66492249
8	-0.44108512	-2.54413966	2.60237704
6	-2.11751716	-0.80232595	1.55283252
6	-1.09178886	0.20317625	2.21495209
6	0.45838652	0.13495094	1.95330066
6	-2.08805308	-1.13590350	0.12379105
6	-1.15888631	-0.56095746	-0.77413162
6	-1.19614860	-0.89534133	-2.12469138
6	-2.14429348	-1.83963586	-2.59379081
6	-3.05515164	-2.42490060	-1.70489732
6	-3.03242265	-2.06717568	-0.35963418
8	-0.37886768	-0.38269572	-3.09383843
8	-2.16047080	-2.15545259	-3.91310339
1	-0.42100706	0.16548034	-0.43527226
1	-3.77778728	-3.14483239	-2.09042818
1	-3.74538297	-2.49961098	0.34211395
1	0.10286165	0.41952489	-2.76336674
1	-1.46098535	-1.61261934	-4.33302934
8	-1.53389438	1.46968926	1.73148049
1	2.46881143	0.98615765	1.57748165
8	-2.99327126	-1.20780480	2.32077167
16	0.14172106	3.25209458	-1.98631417
6	-1.57085840	3.05393706	-1.38634376
6	0.93058764	4.02511319	-0.53786334
8	0.77863120	1.87657543	-2.13350762
1	-1.55518795	2.46273071	-0.45889140
1	-2.11350013	2.53450797	-2.18512534
1	-1.98457974	4.05963228	-1.23650938
1	0.42196231	4.97525225	-0.33194284
1	1.97605367	4.19644807	-0.81828238
1	0.85365359	3.30954284	0.29163995
79	0.17168842	4.68693986	-3.75998443
17	0.18626932	6.14533060	-5.51123413
8	-1.22375482	0.08598311	3.59967922
1	-2.07527211	-0.41474926	3.69804436
1	-0.73977128	2.03789255	1.85328511
1	-0.61542807	-3.49066792	2.74229986

E = -428.702040 E_0 = -428.368111

Transition state of O atom transfer from [(dmso)AuCl] to C

8	0.52592325	1.73330536	2.30652824
8	2.69506604	1.06862151	1.52686175
6	3.21769052	-1.17730035	1.07968282
6	2.85517290	-2.52227351	1.06318559
6	1.56680928	-2.91458356	1.46203105
6	0.64618537	-1.93733063	1.85390961
6	0.92094661	-0.54753415	1.81856443
6	2.28731992	-0.20176149	1.48295548
8	3.71739940	-3.51912083	0.69146912
1	4.57825990	-3.12220712	0.47533948
1	4.22493084	-0.84990765	0.81653934
1	1.33265580	-3.97686480	1.55395686
8	-0.57582710	-2.36084227	2.34583852
6	-1.33617343	1.01695276	-0.44141099
6	-1.45018531	0.61353918	1.74909786
6	-0.01987646	0.59246996	2.02793528
6	-1.43895585	-0.30997373	-1.07769350
6	-0.33442700	-1.18035413	-1.18256004
6	-0.51469609	-2.47747483	-1.64803494
6	-1.78771403	-2.92256310	-2.06600087
6	-2.87889537	-2.04985849	-1.99015066
6	-2.70985918	-0.75961718	-1.48360346
8	0.50377447	-3.41327437	-1.73321022
8	-1.94467702	-4.20026745	-2.52091425
1	0.66163302	-0.85305586	-0.88600031
1	-3.85905556	-2.40342474	-2.31189484
1	-3.56174330	-0.08595974	-1.39731683
1	1.16724058	-3.21402141	-1.04489091
1	-1.06644688	-4.62487051	-2.45890131
8	-2.08633847	1.77234634	2.04105974
1	1.83460562	1.55747324	1.95520957
8	-2.20403533	1.92443180	-0.49648104
16	0.14766283	3.12873510	-1.04232907
6	-0.29271779	4.07275488	0.44751180
6	1.95562094	3.26832929	-1.08119140
8	0.11603419	1.55422743	-0.62549132
1	-0.02695114	3.42616461	1.30659189
1	-1.36943215	4.25406431	0.39373080
1	0.28357120	5.00633936	0.40249543
1	2.19791485	4.33233463	-1.18937058
1	2.29019177	2.70213388	-1.95711505
1	2.34099386	2.83125656	-0.14978988
79	-0.79774445	3.90412961	-2.95781637
17	-1.63935604	4.78858157	-4.87423184
8	-2.28651540	-0.45931193	1.77786061
1	-1.76488420	-1.28407768	1.91277923
1	-2.50661554	2.05980004	1.17852894
1	-0.66839639	-3.31629321	2.18839105

E = -428.619032 E_0 = -428.289332

Product of reaction between **C** and [(dmso)AuCl]

8	-1.27017597	-0.60115847	4.00671803
8	-3.36881920	-1.49127280	5.06362143
6	-4.88490023	-2.76226062	3.78562330
6	-5.23494441	-3.33340666	2.55927342
6	-4.42283146	-3.18774583	1.41782494
6	-3.23835026	-2.46778866	1.51473664
6	-2.82365340	-1.87856535	2.74775440
6	-3.69240651	-2.03437158	3.88695352
8	-6.38100739	-4.05191976	2.39657851
1	-6.85503049	-4.08547071	3.24538012
1	-5.51425398	-2.86752854	4.67044395
1	-4.74261984	-3.63398025	0.47532895
8	-2.43434876	-2.27976780	0.43009513
6	2.16920659	-0.61165584	-0.79511760
6	-0.52420449	-1.04813832	1.82300124
6	-1.59063654	-1.15054128	2.92331149
6	3.20811009	-0.44684125	-1.82303945
6	3.28968011	0.77375565	-2.53196561
6	4.27035275	0.94523184	-3.50207236
6	5.17757331	-0.11161301	-3.78107412
6	5.09228132	-1.32124379	-3.08400330
6	4.11328883	-1.48854745	-2.10511054
8	4.47177219	2.05978814	-4.26456434
8	6.12827151	0.07761021	-4.73154047
1	2.58653306	1.57791301	-2.30805722
1	5.80312156	-2.11459038	-3.31638219
1	4.04552947	-2.42521833	-1.55430311
1	3.93602578	2.83936800	-3.96456058
1	6.00319473	0.99329715	-5.05830401
8	0.31243674	-1.94837435	1.70040951
1	-2.47893706	-1.01706833	4.90881386
8	2.19585458	-1.76949312	-0.14296858
16	0.28234447	3.65759926	0.02976266
6	-1.15130484	2.79214272	-0.73081595
6	-0.54734111	5.20497496	0.57893531
8	1.31625855	0.28031503	-0.55290560
1	-1.84214951	2.51777824	0.07599299
1	-0.74608359	1.88884521	-1.20010196
1	-1.62925922	3.43382969	-1.47900416
1	-1.02378590	5.71160469	-0.26723308
1	0.23083335	5.84249198	1.01411224
1	-1.28246190	4.93463700	1.34794722
79	1.63383550	4.24724650	-1.75425917
17	3.03050744	4.73620791	-3.53470399
8	-0.54396651	0.08646968	1.16362837
1	0.25479493	0.12077977	0.47675032
1	1.46372967	-1.81221633	0.56101942
1	-2.79206392	-2.78110783	-0.32192958

E = -428.805956 E_0 = -428.472897

Pre-reaction complex between CH+ and [(dmso)AuCl]

8	1.10816143	-0.87519297	0.34001484
8	3.15096893	-2.06766364	1.08421707
6	3.06833027	-3.58902317	2.85066142
6	2.34725278	-4.25775486	3.83842685
6	0.95973191	-4.04885763	3.98715892
6	0.30205522	-3.17035005	3.14499785
6	0.97947971	-2.45267626	2.10256795
6	2.41111560	-2.69279398	1.99905493
8	2.91441176	-5.13095843	4.70299431
1	3.86943702	-5.19788948	4.52534897
1	4.14259115	-3.72822128	2.72476863
1	0.42767002	-4.58258308	4.77610049
8	-1.04847618	-2.97020276	3.32299916
6	-1.28106670	-0.32864085	-0.27561931
6	-1.10570565	-1.08618679	1.09444501
6	0.40185267	-1.49920057	1.17939193
6	-1.21146071	-0.94479729	-1.56082048
6	-1.04711358	-2.35838156	-1.68116521
6	-0.95352640	-2.94010619	-2.92865406
6	-1.00391808	-2.13715766	-4.10405808
6	-1.15428433	-0.74323928	-3.99584666
6	-1.25944045	-0.15733179	-2.74744556
8	-0.81366689	-4.27736147	-3.18293349
8	-0.90820372	-2.70726249	-5.31103356
1	-1.04197255	-2.98058618	-0.78706575
1	-1.18118896	-0.14658443	-4.90721799
1	-1.36071058	0.92723741	-2.69838944
1	-0.79328569	-4.79149155	-2.35894124
1	-0.81123008	-3.67542880	-5.19126843
8	-1.28064821	-0.22911910	2.18659972
1	2.51905280	-1.44029407	0.59425102
8	-1.57005582	0.91914960	-0.06783228
16	0.51795368	6.40907509	-0.72930741
6	-0.26595489	7.51950515	0.49045383
6	0.72466998	7.54763216	-2.14228588
8	1.86463833	5.98044577	-0.22721796
1	0.43448256	8.34380605	0.67769351
1	-0.41680757	6.92131064	1.39627584
1	-1.22431875	7.87008699	0.08675310
1	-0.26467556	7.89546582	-2.46572874
1	1.21513278	6.96856616	-2.93301539
1	1.36690276	8.37153101	-1.80487821
79	-0.97750349	4.76577461	-1.31283270
17	-2.48024459	3.09084731	-1.91454593
8	-2.05749140	-2.12068391	1.03955161
1	-1.98663823	-2.57024957	1.91550942
1	-2.06112241	0.33485411	2.03131494
1	-1.34947160	-3.48555247	4.09161517
1	-1.81570831	1.51853575	-0.85506272

E = -429.061931 E_0 = -428.717352

Complex between CH+ and [(dmso)AuCl] with SO..HO hydrogen bond

8	0.64660132	0.59042998	0.57342173
8	1.90142617	1.85798209	2.29872483
6	1.99905622	1.09722708	4.50316681
6	1.69201789	0.13544712	5.46592325
6	0.97355903	-1.02938491	5.12110334
6	0.54531672	-1.21491333	3.81980935
6	0.79254053	-0.24826813	2.78489874
6	1.57521185	0.91372902	3.18337011
8	2.06760899	0.24016335	6.75944885
1	2.56220801	1.06769518	6.89774017
1	2.56962711	1.99465786	4.74432922
1	0.78318196	-1.77736092	5.89221687
8	-0.11312253	-2.37771728	3.49906336
6	-0.87695581	-0.95732217	-0.67607694
6	-0.70270203	-1.33567423	0.84176158
6	0.30654647	-0.28454349	1.42529549
6	-0.08012897	-1.47138696	-1.74756432
6	1.19782166	-2.06135312	-1.51469063
6	1.94813318	-2.52398739	-2.57692774
6	1.44192042	-2.44306367	-3.90659786
6	0.17240709	-1.88599803	-4.14425169
6	-0.57161061	-1.39887651	-3.08468819
8	3.19283801	-3.08640944	-2.49760171
8	2.16820405	-2.90699379	-4.92984219
1	1.58707745	-2.13722253	-0.50121330
1	-0.20638328	-1.86124903	-5.16570111
1	-1.56425770	-1.00190752	-3.28875351
1	3.48918147	-3.16041030	-1.57543982
1	3.00920031	-3.26828911	-4.57866751
8	-1.89732695	-1.13476402	1.55124508
1	1.51394814	1.54807263	1.41336594
8	-1.88680460	-0.17458729	-0.85921514
16	-2.11443249	2.86122202	-2.53536183
6	-3.38236521	3.13777202	-1.25433050
6	-0.59230908	3.27996879	-1.62396051
8	-2.07560432	1.34343708	-2.82589746
1	-3.13818042	2.51502276	-0.38385834
1	-4.33847547	2.84665379	-1.70483446
1	-3.38278602	4.20780409	-1.00987863
1	-0.65332064	4.33994468	-1.34521183
1	0.23543882	3.11620915	-2.32366208
1	-0.51559543	2.62224833	-0.74758517
79	-2.41320578	4.22525623	-4.32081951
17	-2.69761888	5.61733955	-6.07968221
8	-0.26059981	-2.66594861	0.86848094
1	-0.17521675	-2.88305569	1.82683155
1	-2.57572561	-1.73722318	1.19299536
1	-0.22634714	-2.91741172	4.30092677
1	-1.92999733	0.38703959	-1.76180517

E = -429.056553 E_0 = -428.711902

Complex between CH+ and [(dmso)AuCl] with SO..HO hydrogen bond, which is higher in energy

8	1.59639470	-0.53193783	0.09055480
8	1.15009508	-1.74453238	2.25981844
6	-0.95479891	-2.69502722	2.64894915
6	-2.23343795	-3.04198804	2.19034778
6	-2.59854351	-2.82435208	0.83970851
6	-1.73578569	-2.14824985	-0.00022430
6	-0.45427615	-1.68006463	0.44188820
6	-0.06000581	-2.05779162	1.78632942
8	-3.16287414	-3.59868630	2.98325624
1	-2.96187242	-3.39115021	3.93166668
1	-0.63878081	-2.91756010	3.66693087
1	-3.57157822	-3.17776945	0.49473513
8	-2.08404735	-1.94615887	-1.31735022
6	1.18840995	1.12342215	-1.62211100
6	-0.06430490	0.19028715	-1.40349635
6	0.39695441	-0.75818707	-0.25621248
6	2.24630693	0.94285263	-2.56159482
6	2.51696804	-0.33624913	-3.12985711
6	3.58455248	-0.49685257	-3.99083316
6	4.40812487	0.61422379	-4.33260647
6	4.13617639	1.88695575	-3.79493276
6	3.07767847	2.04443302	-2.91970468
8	3.96694566	-1.66467844	-4.58627537
8	5.43581880	0.45614829	-5.17194554
1	1.88685690	-1.18437979	-2.86915670
1	4.76115177	2.72722874	-4.09587055
1	2.86500261	3.05790654	-2.56871129
1	3.37788612	-2.39797584	-4.34187237
1	5.47001480	-0.48251523	-5.45395299
8	-1.18350789	0.95151940	-1.05211865
1	1.63788419	-1.27314588	1.51611364
8	1.09167046	2.21659429	-0.90275954
16	-2.09433871	1.68454046	2.99234066
6	-1.38997592	3.02848865	4.00350895
6	-3.70354353	2.41171496	2.53050721
8	-1.24623315	1.56100560	1.74072658
1	-1.32547565	3.92335831	3.37142134
1	-0.39569313	2.68797329	4.31430939
1	-2.03723857	3.17992368	4.87680105
1	-4.28653021	2.57018709	3.44684917
1	-4.19670255	1.67966969	1.88078899
1	-3.50589678	3.34876898	1.99418729
79	-2.44024849	-0.15215404	4.31607646
17	-2.81356693	-1.97859976	5.67252378
8	-0.29910960	-0.44039066	-2.62454548
1	-1.07614066	-1.02200040	-2.45353374
1	-1.18660145	1.15154335	-0.08667031
1	-2.99460855	-2.25676465	-1.46169396
1	1.90082501	2.76041623	-0.99230990

E = -429.054187 E_0 = -428.708223

Transition state of formation of adduct between CH+ and [(dmso)AuCl

8	1.33527460	-0.67384795	-0.06118173
8	3.37310702	-1.52125021	1.05265090
6	3.24552429	-2.54668286	3.14066727
6	2.49625576	-3.02265029	4.21497878
6	1.09192113	-2.90259483	4.21766298
6	0.44985942	-2.28036373	3.16164107
6	1.15968329	-1.72041558	2.04586987
6	2.60050636	-1.93150501	2.06144658
8	3.04677755	-3.63846576	5.28669465
1	4.01330977	-3.68739845	5.17971393
1	4.32978175	-2.65522992	3.09876814
1	0.52802034	-3.33238580	5.04702091
8	-0.92688445	-2.24795160	3.16805219
6	-1.26547316	0.49917918	-0.34060070
6	-0.83960980	-0.37160441	0.92763949
6	0.62004244	-0.94655564	0.93472568
6	-1.38630396	-0.03843168	-1.71915245
6	-0.27097814	-0.38046362	-2.51571159
6	-0.46193294	-0.88032891	-3.79646069
6	-1.76788288	-1.05727423	-4.32235617
6	-2.87316192	-0.73429191	-3.52979500
6	-2.68573261	-0.22839155	-2.24447732
8	0.54539522	-1.23028586	-4.66015482
8	-1.94305980	-1.54627960	-5.56773072
1	0.73315969	-0.25024732	-2.11637870
1	-3.87436306	-0.90196701	-3.92582068
1	-3.57286783	-0.06610266	-1.62933039
1	1.40457765	-1.22226869	-4.20759925
1	-1.06289909	-1.73605267	-5.94914488
8	-0.94247883	0.42045888	2.08944790
1	2.73332321	-1.13962376	0.36473612
8	-2.32303763	1.23816652	0.06828810
16	-0.19841927	3.15371318	-0.67208361
6	-0.37982179	3.96241123	0.94794019
6	1.41455936	3.76021275	-1.24465020
8	0.12273897	1.63916251	-0.37584855
1	0.49422870	3.69539502	1.55475178
1	-1.30433631	3.56621254	1.38281398
1	-0.45997587	5.04340928	0.77389085
1	1.33570897	4.84946487	-1.35468218
1	1.59569349	3.28128119	-2.21333111
1	2.16397237	3.46688128	-0.49950081
79	-1.87790630	3.67526915	-2.11877274
17	-3.55235757	4.21374971	-3.53445127
8	-1.80660331	-1.38525478	0.85171803
1	-1.69726380	-1.92028734	1.67467409
1	-1.88821697	0.63942964	2.19453965
1	-1.25516680	-2.72634503	3.94913725
1	-2.84300339	1.50820336	-0.72127011

E = -429.019596 E_0 = -428.674623

Adduct between CH+ and [(dmso)AuCl]

8	1.46911231	-0.54311286	0.32533120
8	3.51514994	-1.51151490	1.31305518
6	3.44255894	-2.61185099	3.36598504
6	2.72366756	-3.09544614	4.45748043
6	1.32707478	-2.91856177	4.53179636
6	0.66234556	-2.23928011	3.52637026
6	1.34167586	-1.67849160	2.39208819
6	2.77461069	-1.93385511	2.33963031
8	3.29697297	-3.76703028	5.48276905
1	4.25510959	-3.84833872	5.32988485
1	4.51944267	-2.75648317	3.27270967
1	0.78643291	-3.34459119	5.37839894
8	-0.70831179	-2.13482326	3.60864281
6	-1.06316500	0.54261491	0.02367204
6	-0.68881692	-0.31032333	1.33178821
6	0.77584940	-0.86775821	1.32451426
6	-1.18920567	-0.16342718	-1.30810461
6	-0.11988634	-0.23264416	-2.22375573
6	-0.29598922	-0.86510370	-3.45173657
6	-1.54423062	-1.43568257	-3.80023934
6	-2.59726560	-1.38280530	-2.88336424
6	-2.42041848	-0.75764219	-1.64703816
8	0.67401879	-0.98590803	-4.41660525
8	-1.71262599	-2.04385029	-4.99707406
1	0.85518003	0.17452183	-1.95617475
1	-3.54632403	-1.85064285	-3.14425953
1	-3.23711438	-0.80562814	-0.92313730
1	1.54219390	-0.72925195	-4.06633377
1	-0.86633096	-2.00086771	-5.48344632
8	-0.79062314	0.53009065	2.46109013
1	2.86033836	-1.06831022	0.67539724
8	-2.25023813	1.21897794	0.36034696
16	-0.43094908	3.05215181	-0.63040007
6	-0.95687744	4.02389814	0.81613325
6	1.24070025	3.68298574	-0.93681029
8	0.02366459	1.60087003	-0.02815307
1	-0.23527265	3.83600951	1.62125182
1	-1.96052937	3.67422159	1.07695688
1	-0.96960645	5.07568203	0.49960120
1	1.13645185	4.73864613	-1.21805656
1	1.64610318	3.09687017	-1.76874244
1	1.82776762	3.54938136	-0.02021351
79	-1.78125652	3.17477240	-2.43887141
17	-3.09670435	3.41887275	-4.25156667
8	-1.65557427	-1.31893826	1.30015576
1	-1.53625302	-1.82844916	2.13666829
1	-1.73728185	0.75862997	2.53965631
1	-1.01702268	-2.60755309	4.40113635
1	-2.89440739	1.04101877	-0.35485479

E = -429.021840 E_0 = -428.676224

Transition state of decay of adduct between CH+ and [(dmso)AuCl

8	1.69586277	0.89632063	1.43522980
8	3.00786852	-0.95606120	0.39297522
6	2.50940128	-3.17737627	0.94801007
6	1.75128041	-4.11004198	1.66102418
6	0.70014030	-3.68755405	2.50083914
6	0.39268291	-2.34171004	2.57965821
6	1.08692968	-1.34217757	1.83339756
6	2.21956671	-1.81567593	1.06505896
8	1.99094479	-5.43899316	1.62678729
1	2.74682109	-5.63017198	1.04337517
1	3.36189652	-3.47832855	0.33802991
1	0.17192743	-4.42992964	3.10082131
8	-0.57968061	-1.92301550	3.47301807
6	-1.09397547	1.34984494	0.24108980
6	-0.61269399	0.74026933	1.92253989
6	0.80003131	0.09093338	1.76364515
6	-0.98597212	0.21613293	-0.74335275
6	0.28967709	-0.08407315	-1.26410014
6	0.47700602	-1.18277102	-2.09197189
6	-0.63099943	-1.97350482	-2.48468304
6	-1.90744944	-1.65515127	-2.00024347
6	-2.07962354	-0.58444713	-1.12121340
8	1.69635634	-1.57953792	-2.58312660
8	-0.45785143	-3.03506983	-3.30436531
1	1.14448211	0.53781815	-1.00040559
1	-2.75393436	-2.26437732	-2.31728763
1	-3.08542267	-0.37512283	-0.75549947
1	2.40636716	-1.22691810	-2.01427041
1	0.49299910	-3.09094673	-3.52636680
8	-0.50931679	1.81992682	2.75860220
1	2.75408234	-0.03984161	0.74523926
8	-2.38625293	1.83881735	0.47630770
16	-0.62478193	3.55778444	-1.46115154
6	-1.67151382	4.78851873	-0.62658326
6	1.03296593	4.29108640	-1.36765228
8	-0.24111139	2.37068768	0.08272529
1	-1.28267776	4.91128758	0.39165617
1	-2.68596351	4.37640569	-0.61563359
1	-1.62580316	5.72005659	-1.20524612
1	1.01355894	5.24501435	-1.90863903
1	1.71628766	3.58490912	-1.85141763
1	1.27774674	4.41645970	-0.30593595
79	-1.29002111	3.01926559	-3.55433116
17	-1.92745726	2.64224245	-5.68722382
8	-1.71801203	-0.03330788	2.17055360
1	-1.45962843	-0.81892432	2.72880513
1	-1.41671841	2.05201200	3.03466963
1	-0.97702187	-2.69677443	3.91173155
1	-2.95052588	1.08801200	0.74154285

E = -429.008377 E_0 = -428.664933

Product of reaction between CH+ and [(dmso)AuCl]

8	1.61881569	-1.48765650	3.74054098
8	-0.11776640	-3.23661322	3.62205879
6	-2.02290080	-2.95099993	2.31594457
6	-2.80408669	-2.16903382	1.46913372
6	-2.40689775	-0.85848473	1.11992199
6	-1.21590423	-0.35874796	1.60186633
6	-0.33670330	-1.11509425	2.44930263
6	-0.81690877	-2.44518055	2.81640847
8	-3.98011374	-2.58925837	0.95192164
1	-4.17468933	-3.49202583	1.26173508
1	-2.32050689	-3.95636367	2.61573264
1	-3.05478908	-0.24994468	0.49099366
8	-0.90791800	0.95915605	1.29277706
6	2.23201705	-0.90101071	-0.60863570
6	1.77504453	0.50033922	2.54156641
6	0.98303003	-0.76598117	2.94141801
6	2.95449052	-1.58528780	-1.70040975
6	3.99508334	-2.46862790	-1.33633775
6	4.70693101	-3.14314961	-2.31743166
6	4.40424727	-2.94232828	-3.68891456
6	3.38322087	-2.05544230	-4.05103980
6	2.66414438	-1.38260380	-3.06394145
8	5.72768904	-4.03168608	-2.08991995
8	5.10061779	-3.59942707	-4.64290779
1	4.21855246	-2.61055629	-0.27704562
1	3.17562346	-1.90007765	-5.10951140
1	1.90254333	-0.66947486	-3.39149276
1	5.89465206	-4.12569230	-1.13791296
1	5.76719434	-4.16046042	-4.19898666
8	2.97428671	0.53481160	3.04998662
1	0.71817507	-2.71570929	3.87866742
8	1.07514931	-0.24336797	-0.91746436
16	-4.25679516	5.76214165	-0.34511427
6	-6.01086360	5.44012893	-0.80014657
6	-3.80761199	6.97634859	-1.65345866
8	2.60610563	-0.89388313	0.56258062
1	-6.56549045	6.37596496	-0.65518450
1	-6.38149449	4.67636288	-0.10702761
1	-6.08524627	5.08809371	-1.83423330
1	-3.99462941	6.56049794	-2.64891121
1	-2.74210357	7.19888130	-1.52536235
1	-4.40248910	7.88208001	-1.47979179
79	-3.10191317	3.82351717	-0.86160119
17	-1.91550370	1.87128025	-1.33978290
8	1.34113825	1.50660441	1.90895529
1	0.30393035	1.31039270	1.54976448
1	3.42213617	1.35694144	2.75679300
1	-1.29502382	1.26022310	0.39133100
1	0.85582435	-0.38910628	-1.85669680

E = -429.142576 E_0 = -428.800051

Ion pair $[AuCl_4]^-H^+$

79	0.44190996	-0.00619535	-0.24434889
17	-1.91641876	0.47419976	-0.56998901
17	-0.54792213	-0.43909790	1.93080463
17	2.60470703	-0.52529895	0.34031242
17	1.11068224	0.47238396	-2.39201923
1	-1.69295834	0.02400847	0.93524008

E = -196.475227 E_0 = -196.465424

$[AuCl_4]^-$

79	-0.00000086	-0.00000504	0.00000690
17	0.00000863	0.00000010	2.35576843
17	0.00000746	-0.00000512	-2.35576621
17	0.05340445	-2.35515475	-0.00000560
17	-0.05341968	2.35516482	-0.00000352

E = -196.037061 E_0 = -196.032782

[(dmso)AuCl

6	0.16152968	1.51834758	-2.28533977
79	1.77201332	2.45737041	0.50543792
17	2.61010778	1.88809815	2.55174167
1	0.99893157	0.84744598	-2.50783320
1	-0.52145085	1.05892390	-1.55974711
1	-0.35084471	1.82744747	-3.20559494
16	0.90034233	3.01500384	-1.53282683
6	-0.61435609	4.01008556	-1.27009734
1	-0.27887227	4.96040808	-0.83970524
1	-1.08395771	4.16613933	-2.24991816
1	-1.27065297	3.47761164	-0.57032498
8	1.75148300	3.70210862	-2.56627454

E = -192.190466 E_0 = -192.110327

isomer form of [(dmso)AuCl

6	1.26358790	2.74204587	-4.39281650
79	3.59562919	4.11145825	-2.13738632
17	5.69138352	4.91315677	-2.49551959
1	1.40070148	1.67128695	-4.20136620
1	0.55929516	2.89819433	-5.22153437
1	2.23060404	3.23598353	-4.56690093
16	0.53166323	3.45105565	-2.87174869
6	0.49879325	5.20214850	-3.40488008
1	0.12127235	5.77906724	-2.55241563
1	1.52749741	5.50013187	-3.65480755
1	-0.18254880	5.29097562	-4.26219838
8	1.64436359	3.35426997	-1.76862015

E = -192.182211 E_0 = -192.102907

dimer $[(Me_2S)AuCl]_2$

6	-0.32924231	2.14021838	-2.80348718
79	1.96897720	2.08338201	-0.33555019
17	3.43846509	1.05916326	1.13579261
1	0.33179387	1.44926009	-3.33946743
1	-0.97275227	1.60316034	-2.09572723
1	-0.91924599	2.72796342	-3.51912084
16	0.75868096	3.30861750	-1.89014172
6	-0.51743951	4.22746865	-0.93568738
1	0.02170330	4.92731477	-0.28673852
1	-1.13720436	4.77974208	-1.65438601
1	-1.11381403	3.52013787	-0.34590903
6	1.74528909	-1.48226248	2.91212419
79	-0.36430159	-0.18561906	0.68746139
17	-2.17742341	1.19181158	0.24503981
1	2.22834345	-0.49911774	2.95679948
1	0.84460383	-1.51266141	3.53490572
1	2.45715914	-2.26825567	3.19623723
16	1.31284213	-1.73397826	1.14311336
6	0.41112016	-3.33458871	1.29364438
1	0.04477852	-3.58719135	0.29184913
1	1.12647675	-4.09618035	1.63143432
1	-0.42969231	-3.24589255	1.99022838

$E =$ -352.443741 $E_0 =$ -352.289765

trimer $[(Me_2S)AuCl]_3$

6	0.26850586	-8.37482015	-0.45288431
79	-2.75663153	-7.00897743	-0.22469998
17	-4.80280150	-6.90755283	0.87090322
1	0.35738178	-8.24517999	0.63208356
1	-0.31663717	-9.27109900	-0.69679326
1	1.26602697	-8.40299904	-0.91064631
16	-0.60080943	-6.88510353	-1.09266728
6	-0.68883542	-7.34264824	-2.87114668
1	-1.28173844	-6.56569268	-3.36786160
1	0.33537188	-7.34612682	-3.26674487
1	-1.16827285	-8.32326864	-2.97859615
6	-5.99725053	-8.30216719	-4.70995682
79	-3.90812743	-9.25408568	-2.29478106
17	-2.24573611	-10.78652648	-1.67130827
1	-5.15668972	-8.41049886	-5.40512678
1	-6.46259067	-9.27311550	-4.49813505
1	-6.72488827	-7.58276075	-5.10853758
16	-5.31636275	-7.59875989	-3.15293278
6	-6.83791355	-7.57412334	-2.12584924
1	-6.51186330	-7.29820522	-1.11420768
1	-7.50076782	-6.80435998	-2.54256289
1	-7.30464578	-8.56630640	-2.14348965
6	-4.12409199	-10.56436699	1.47433816
79	-6.03201963	-11.47800865	-1.18925576
17	-7.42143716	-11.16361117	-3.02285651
1	-3.30112897	-10.26895667	0.81286180

1	-4.86425991	-9.75972017	1.53856613
1	-3.73886817	-10.84440775	2.46402448
16	-4.84274348	-12.07688928	0.71988801
6	-6.15621949	-12.42745677	1.96214684
1	-6.71425770	-13.29836785	1.59982880
1	-5.66542116	-12.66573808	2.91518957
1	-6.82535758	-11.56674708	2.06841558

E = -528.673581 E_0 = -528.442579

dimer $[(Me_2S)AuCl]_2$, relativistic calculations

6	-0.25352111	2.29925958	-2.86843438
79	2.02820506	2.08944363	-0.46051339
17	3.49116661	0.93380789	0.84768871
1	0.43524013	1.70170926	-3.47540811
1	-0.87829610	1.65519995	-2.23821246
1	-0.86836692	2.93411915	-3.51897355
16	0.77044314	3.39171074	-1.82822303
6	-0.53424394	4.15098112	-0.80568622
1	-0.03035242	4.79167670	-0.07392386
1	-1.16559661	4.76178317	-1.46337839
1	-1.12023863	3.37131462	-0.30440645
6	1.72358215	-1.38647659	2.84003502
79	-0.44201712	-0.36923058	0.57106103
17	-2.19928593	0.95930601	-0.01476537
1	2.21869862	-0.41111545	2.77225000
1	0.85035058	-1.34397856	3.49936380
1	2.43892320	-2.14603657	3.17981408
16	1.22702226	-1.80793535	1.13845413
6	0.37805503	-3.39155979	1.46832091
1	-0.03446599	-3.74032615	0.51548215
1	1.12255929	-4.10989481	1.83456691
1	-0.42874358	-3.26126558	2.19730293

E = -39928.849117 E_0 = -39928.695476

trimer $[(Me_2S)AuCl]_3$, relativistic calculations

6	4.18440679	0.78269101	0.71942070
79	1.09105568	1.81261849	1.14800432
17	-0.91943439	1.56393890	2.21815060
1	4.26096053	0.72885549	1.81088942
1	3.70310561	-0.11806060	0.31720313
1	5.18001865	0.93550237	0.28405311
16	3.17236761	2.24840613	0.33233394
6	3.12139888	2.10007829	-1.48260395
1	2.46933020	2.89967024	-1.85060240
1	4.14095339	2.24482736	-1.86165140
1	2.72268223	1.11936019	-1.76845010
6	-1.95893152	0.89204635	-3.48957647
79	0.15924643	-0.20009854	-1.23666189
17	1.92534972	-1.63852207	-0.89908040
1	-1.10388704	0.97698804	-4.16903295
1	-2.32554561	-0.14116543	-3.45808013
1	-2.74848060	1.59081356	-3.79400744
16	-1.37927134	1.38593866	-1.83339886
6	-2.90716754	1.11983243	-0.88338200
1	-2.64654316	1.29004619	0.16837313
1	-3.64117302	1.86278563	-1.22027888
1	-3.26743997	0.09678597	-1.04214448
6	0.38195730	-2.15355455	2.31949376
79	-1.88519072	-2.56582739	-0.14242208
17	-2.80519274	-2.42217570	-2.22979350
1	1.09774679	-2.52023669	1.57561272
1	0.26922227	-1.06804572	2.22009877
1	0.69459105	-2.42888408	3.33473457
16	-1.20607725	-2.97772582	1.98791784
6	-2.28680024	-1.98638338	3.07295900
1	-3.31407912	-2.32593036	2.90339727
1	-1.99511393	-2.18330378	4.11224795
1	-2.18406491	-0.92127116	2.83627668

E = -59893.282422 E_0 = -59893.051515