

## Electronic Supporting Information

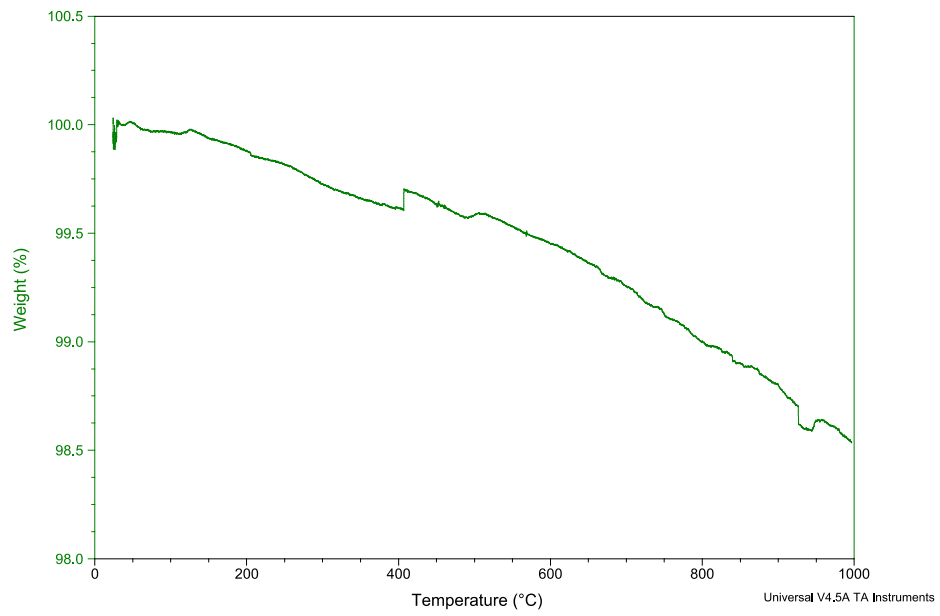
### Capturing Volatile Organic Compounds using Ag and Au nanoparticles: Regium- $\pi$ and C-H $\cdots$ Ag/Au interactions at work.

María de las Nieves Piña,<sup>a</sup> Jeroni Morey,<sup>\*,a</sup> Antonio Frontera<sup>a</sup> and Antonio

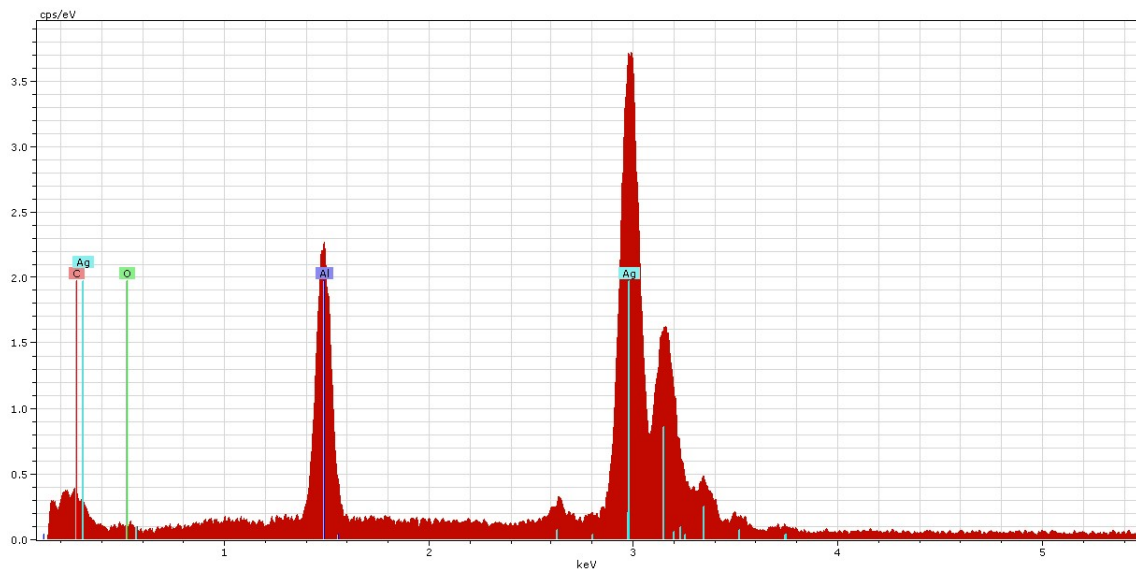
Bauzá<sup>\*,a</sup>

<sup>a</sup>Department of Chemistry, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma (Balears), SPAIN; Fax: (+) 34 971 173426; E-mail: [jeroni.morey@uib.es](mailto:jeroni.morey@uib.es), [antonio.bauza@uib.es](mailto:antonio.bauza@uib.es)

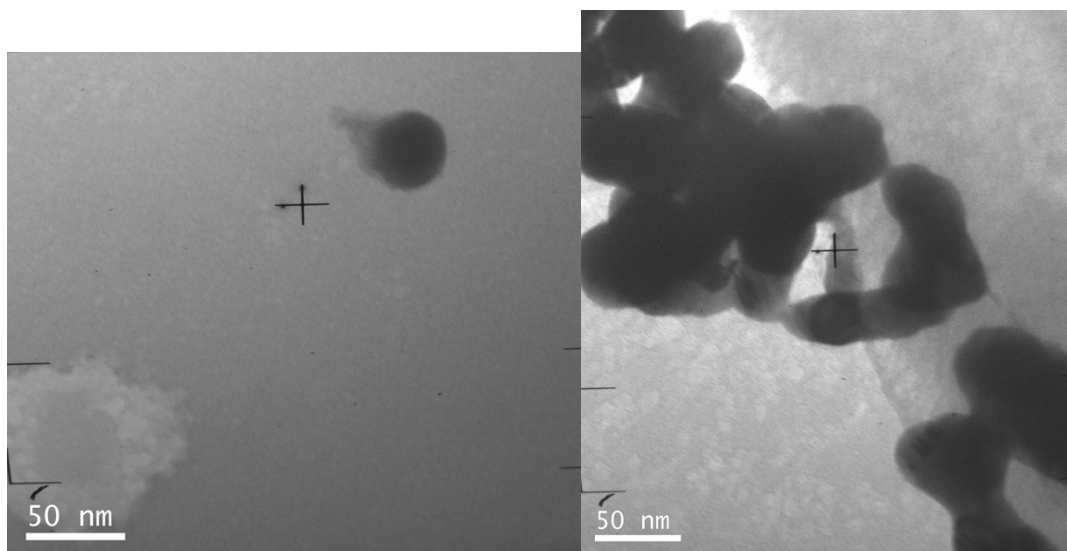
<b>Figure S1</b>	page 2
<b>Figure S2</b>	page 2
<b>Figure S3</b>	page 3
<b>Figure S4</b>	page 3
<b>Figure S5</b>	page 4
<b>Figure S6</b>	page 5
Cartesian coordinates of complexes <b>1</b> to <b>16</b>	page 6



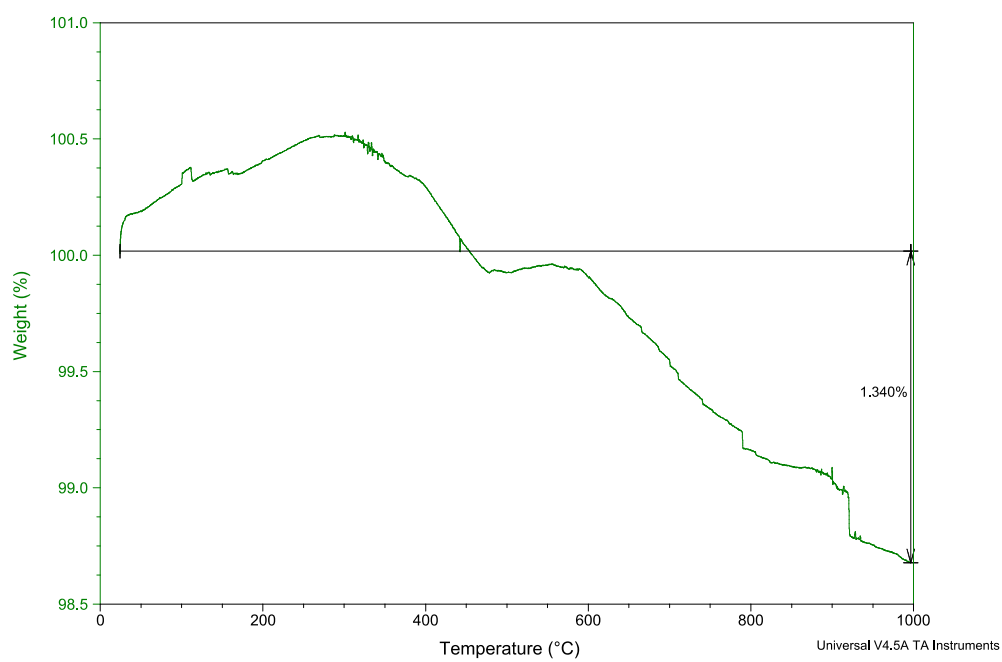
**Figure S1.** Thermogravimetric analysis (TGA) of Ag nanoparticles.



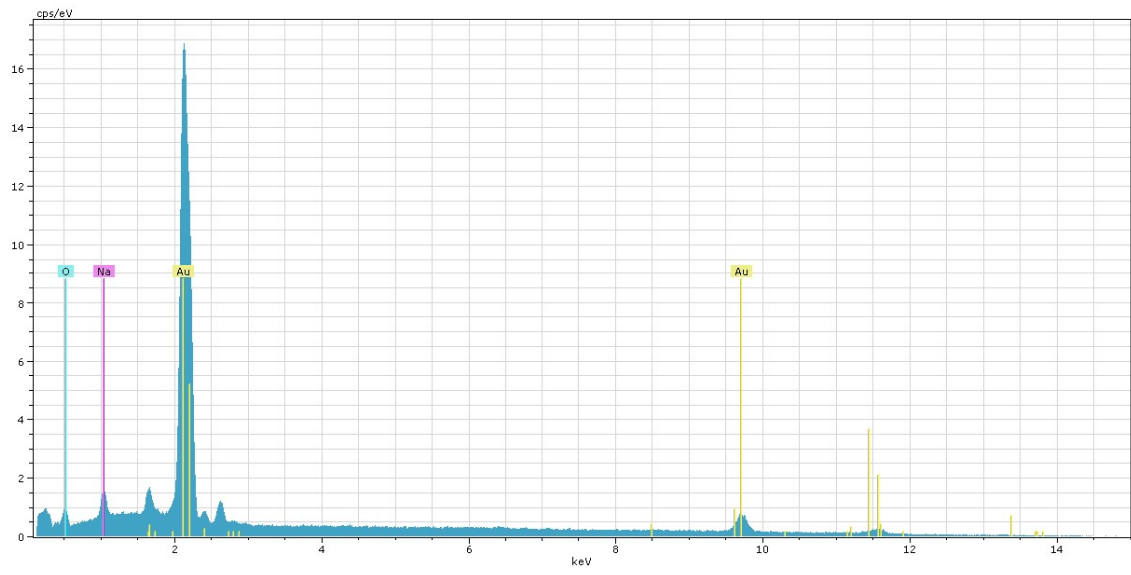
**Figure S2.** SEM-EDX of Ag nanoparticles.



**Figure S3.** TEM micrographs of Ag nanoparticles.



**Figure S4.** Thermogravimetric analysis (TGA) of Au nanoparticles.



**Figure S5.** SEM-EDX of Au nanoparticles.

### Sample Details

### AuNPs Size aver

Record Number: 4 File Name: JeroniPrueba.dts  
Temperature (°C): 25.0 Meas Date & Time: Tuesday, November 23, 2021 12:14:56 PM  
Derived Count Rate (kcps... 345.7 Solvent: Water  
Intercept: 0.806 Measurement quality: **Good**

### Hydrodynamic Radius

Z-Average (± SD) (r.nm): 87.68 ± 56.92

Polydispersity Index: 0.421

Estimated MW (± SD) (KDa): 1.18e5 ± 7.68e+04

%Polydispersity: 64.9

Sample Polydispersity: Polydisperse

### Distribution Results

	Mode ± SD (nm)	%Pd	Est. MW (KDa) (Mean ± SD)*	% Intensity	% Mass	Peak Polydispersity
Peak 1:	82.09 ± 34.23	37.3	1.32e+5 ± 4.91e+4	98.0	64.8	Polydisperse
Peak 2:	2780 ± 156.7	5.8	3.59e+8 ± 2.08e+7	2.0	35.2	Monodisperse
Peak 3:	0.000 ± 0.000	0	0.0 ± 0.0	0.0	0.0	

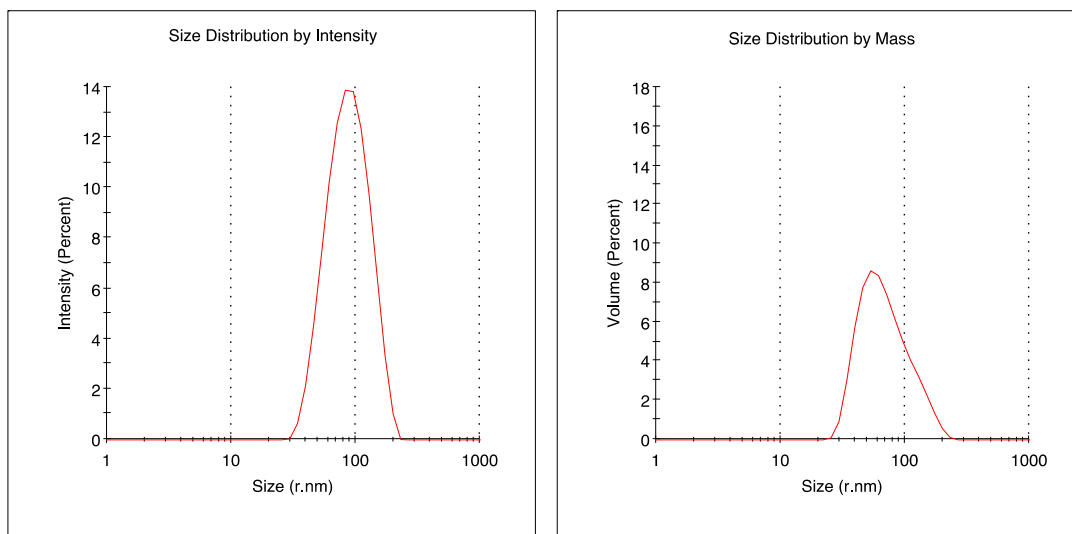


Figure S6. DLS of Au nanoparticles.

## Cartesian Coordinates of Complexes 1 to 16

### 1. Benzene@Ag<sub>26</sub>

Ag	-8.2577035	2.7791402	4.9619427
Ag	-5.8450899	3.5630459	3.4900353
Ag	-6.7666262	0.7268483	3.4900353
Ag	-3.4936040	4.3270898	2.0257809
Ag	-5.3133281	-1.2734449	2.0257809
Ag	-4.3478903	1.5087648	2.1233220
Ag	-1.1007463	5.1045765	0.5683060
Ag	-3.8344607	-3.3089313	0.5683060
Ag	-2.8947447	-0.5115848	0.6248074
Ag	-1.9847392	2.2891243	0.6248074
Ag	1.3204794	5.8912804	-0.8272902
Ag	-2.3380609	-5.3685489	-0.8272902
Ag	-1.4058719	-2.5688605	-0.8138478
Ag	-0.4979226	0.2578344	-0.8374952
Ag	0.4290207	3.0783580	-0.8138478
Ag	3.7193835	6.6707316	-2.2724729
Ag	-0.8554567	-7.4091787	-2.2724729
Ag	0.1014382	-4.6065212	-2.1450832
Ag	0.9953692	-1.7805537	-2.1899282
Ag	1.9083103	1.0291903	-2.1899282
Ag	2.8461670	3.8408855	-2.1450832
Ag	1.3282218	-6.4838182	-3.8920761
Ag	2.2438372	-3.7219348	-3.8920761
Ag	3.1717438	-0.9345124	-3.8920761
Ag	4.0594573	1.8659693	-3.8920761
Ag	4.9421033	4.6385653	-3.8920761
C	0.8101121	-1.5871438	1.9131578
C	1.7700609	-2.1686804	1.0819971
C	2.7838619	-1.3823478	0.5270771
C	2.8338033	-0.0135571	0.8014617

C	1.8723206	0.5687529	1.6318012
C	0.8623468	-0.2185941	2.1888115
H	0.0184809	-2.2035592	2.3471048
H	1.7303104	-3.2390845	0.8663585
H	3.5376557	-1.8371439	-0.1204005
H	3.6291785	0.6009322	0.3712507
H	1.9100536	1.6401706	1.8447178
H	0.1116273	0.2374497	2.8383355

## 2. Toluene@Ag26

Ag	-8.2159718	2.7361579	4.6969403
Ag	-5.8033596	3.5200632	3.2250337
Ag	-6.7248954	0.6838672	3.2250337
Ag	-3.4518750	4.2841068	1.7607801
Ag	-5.2715981	-1.3164248	1.7607801
Ag	-4.3061608	1.4657833	1.8583212
Ag	-1.0590186	5.0615930	0.3033059
Ag	-3.7927315	-3.3519101	0.3033059
Ag	-2.8530160	-0.5545652	0.3598074
Ag	-1.9430111	2.2461424	0.3598074
Ag	1.3622057	5.8482964	-1.0922894
Ag	-2.2963326	-5.4115267	-1.0922894
Ag	-1.3641441	-2.6118398	-1.0788470
Ag	-0.4561953	0.2148536	-1.1024945
Ag	0.4707475	3.0353756	-1.0788470
Ag	3.7611084	6.6277472	-2.5374714
Ag	-0.8137292	-7.4521552	-2.5374714
Ag	0.1431651	-4.6494993	-2.4100816
Ag	1.0370957	-1.8235334	-2.4549266
Ag	1.9500363	0.9862089	-2.4549266
Ag	2.8878924	3.7979026	-2.4100816
Ag	1.3699481	-6.5267953	-4.1570737
Ag	2.2855630	-3.7649134	-4.1570737
Ag	3.2134691	-0.9774925	-4.1570737

Ag	4.1011820	1.8229876	-4.1570737
Ag	4.9838276	4.5955820	-4.1570737
C	0.8435434	-1.6341507	1.6670652
C	1.7702261	-2.1999079	0.7892404
C	2.7764392	-1.4124211	0.2262287
C	2.8337565	-0.0519359	0.5366521
C	1.9034710	0.5088585	1.4136306
C	0.9030119	-0.2751695	2.0060871
H	0.0681593	-2.2647976	2.1119152
H	1.7106781	-3.2646301	0.5504203
H	3.5161396	-1.8556609	-0.4445938
H	3.6178284	0.5762773	0.1056307
H	1.9665265	1.5738201	1.6557427
C	-0.0816950	0.3290796	2.9612990
H	0.3844365	1.1034328	3.5877263
H	-0.9112922	0.8119128	2.4125122
H	-0.5303424	-0.4288762	3.6189855

### 3. *o*-Xylene@Ag26

Ag	-8.3496468	2.5836660	4.5583090
Ag	-5.9370364	3.3675707	3.0864037
Ag	-6.8585717	0.5313771	3.0864037
Ag	-3.5855540	4.1316137	1.6221514
Ag	-5.4052756	-1.4689134	1.6221514
Ag	-4.4398390	1.3132926	1.7196923
Ag	-1.1926997	4.9090991	0.1646785
Ag	-3.9264102	-3.5043969	0.1646785
Ag	-2.9866956	-0.7070543	0.2211798
Ag	-2.0766911	2.0936508	0.2211798
Ag	1.2285227	5.6958019	-1.2309157
Ag	-2.4300124	-5.5640117	-1.2309157
Ag	-1.4978249	-2.7643272	-1.2174734
Ag	-0.5898766	0.0623638	-1.2411208
Ag	0.3370652	2.8828835	-1.2174734



Ag	3.6274235	6.4752520	-2.6760965
Ag	-0.9474102	-7.6046384	-2.6760965
Ag	0.0094832	-4.8019849	-2.5487070
Ag	0.9034130	-1.9760214	-2.5935519
Ag	1.8163529	0.8337185	-2.5935519
Ag	2.7542080	3.6454098	-2.5487070
Ag	1.2362651	-6.6792794	-4.2956975
Ag	2.1518793	-3.9173998	-4.2956975
Ag	3.0797844	-1.1299813	-4.2956975
Ag	3.9674969	1.6704966	-4.2956975
Ag	4.8501414	4.4430886	-4.2956975
C	0.6819460	-1.8237143	1.4904132
C	1.6169220	-2.3850190	0.6192215
C	2.6314899	-1.5870861	0.0919879
C	2.6936176	-0.2363978	0.4394649
C	1.7689803	0.3361206	1.3222240
C	0.7455068	-0.4747152	1.8609567
H	-0.1124970	-2.4504772	1.9063271
H	1.5522703	-3.4436111	0.3571959
H	3.3782170	-2.0123703	-0.5826973
H	3.4920587	0.3896282	0.0302110
C	-0.2464409	0.0983716	2.8272223
H	0.2504173	0.5157387	3.7179556
H	-0.8206214	0.9249150	2.3720189
H	-0.9701787	-0.6579695	3.1606987
C	1.8808698	1.7800304	1.7112808
H	0.9309394	2.3190395	1.5547917
H	2.1274542	1.8887628	2.7807415
H	2.6566401	2.2951497	1.1279501
<b>4. m-Xylene@Ag26</b>			
Ag	-8.5048983	2.6510200	4.6704976
Ag	-6.0922833	3.4349262	3.1985894
Ag	-7.0138202	0.5987270	3.1985894

Ag	-3.7407962	4.1989706	1.7343342
Ag	-5.5605213	-1.4015673	1.7343342
Ag	-4.5950829	1.3806440	1.8318753
Ag	-1.3479371	4.9764577	0.2768584
Ag	-4.0816531	-3.4370549	0.2768584
Ag	-3.1419365	-0.6397068	0.3333599
Ag	-2.2319305	2.1610039	0.3333599
Ag	1.0732900	5.7631620	-1.1187385
Ag	-2.5852524	-5.4966737	-1.1187385
Ag	-1.6530629	-2.6969837	-1.1052961
Ag	-0.7451130	0.1297128	-1.1289436
Ag	0.1818307	2.9502380	-1.1052961
Ag	3.4721954	6.5426136	-2.5639221
Ag	-1.1026473	-7.5373045	-2.5639221
Ag	-0.1457520	-4.7346455	-2.4365323
Ag	0.7481796	-1.9086764	-2.4813773
Ag	1.6611212	0.9010691	-2.4813773
Ag	2.5989784	3.7127659	-2.4365323
Ag	1.0810324	-6.6119436	-4.1835262
Ag	1.9966483	-3.8500586	-4.1835262
Ag	2.9245554	-1.0626346	-4.1835262
Ag	3.8122694	1.7378487	-4.1835262
Ag	4.6949159	4.5104462	-4.1835262
C	0.4400445	-1.6635009	1.6365725
C	1.3876164	-2.2184380	0.7749808
C	2.4420272	-1.4433825	0.2905428
C	2.5584310	-0.0957900	0.6581621
C	1.5868392	0.4465885	1.5112788
C	0.5344889	-0.3209346	2.0274875
H	-0.3724530	-2.2851397	2.0240526
H	1.3084597	-3.2693146	0.4855895
H	3.1915792	-1.8916625	-0.3678167
H	1.6703064	1.4982376	1.8045385

C	-0.4675677	0.2836487	2.9649582
H	-0.0104355	1.0441071	3.6144565
H	-1.2798464	0.7823940	2.4042166
H	-0.9417337	-0.4782412	3.5998057
C	3.7279046	0.7302242	0.2075652
H	3.4478654	1.7862158	0.0736753
H	4.5392605	0.6931942	0.9537402
H	4.1400617	0.3645565	-0.7450365

### 5. *p*-Xylene@Ag26

Ag	-8.5184745	2.8961445	4.7557510
Ag	-6.1058615	3.6800500	3.2838440
Ag	-7.0273976	0.8438532	3.2838440
Ag	-3.7543763	4.4440938	1.8195900
Ag	-5.5740999	-1.1564393	1.8195900
Ag	-4.6086624	1.6257696	1.9171311
Ag	-1.3615193	5.2215803	0.3621154
Ag	-4.0952329	-3.1919253	0.3621154
Ag	-3.1555172	-0.3945795	0.4186169
Ag	-2.2455119	2.4061289	0.4186169
Ag	1.0597057	6.0082840	-1.0334803
Ag	-2.5988335	-5.2515424	-1.0334803
Ag	-1.6666448	-2.4518547	-1.0200379
Ag	-0.7586957	0.3748394	-1.0436854
Ag	0.1682473	3.1953622	-1.0200379
Ag	3.4586092	6.7877348	-2.4786627
Ag	-1.1162297	-7.2921714	-2.4786627
Ag	-0.1593351	-4.4895148	-2.3512729
Ag	0.7345956	-1.6635481	-2.3961179
Ag	1.6475365	1.1461951	-2.3961179
Ag	2.5853929	3.9578895	-2.3512729
Ag	1.0674481	-6.3668113	-4.0982653
Ag	1.9830634	-3.6049285	-4.0982653
Ag	2.9109696	-0.8175069	-4.0982653

Ag	3.7986829	1.9829740	-4.0982653
Ag	4.6813286	4.7555691	-4.0982653
C	0.5520787	-1.4695377	1.7071810
C	1.5120451	-2.0491111	0.8767659
C	2.5555765	-1.2890291	0.3309249
C	2.5657352	0.0850328	0.6063661
C	1.6036233	0.6651594	1.4343914
C	0.5933723	-0.1058206	2.0249589
H	-0.2359997	-2.0973735	2.1337418
H	1.4600353	-3.1204882	0.6635094
H	3.3567903	0.7123986	0.1844553
H	1.6542446	1.7383582	1.6420372
C	-0.4056874	0.5076455	2.9592400
H	0.0543238	1.2839922	3.5878913
H	-1.2292233	0.9898738	2.4006799
H	-0.8632759	-0.2465861	3.6153513
C	3.6497883	-1.9330007	-0.4708210
H	4.4531148	-2.3005142	0.1895684
H	3.2758719	-2.7946552	-1.0457315
H	4.0979535	-1.2235105	-1.1817158

**6. 1,2,3-Trimethylbenzene@Ag26**

Ag	-8.6226506	2.5160551	4.5550624
Ag	-6.2100356	3.2999613	3.0831542
Ag	-7.1315725	0.4637621	3.0831542
Ag	-3.8585485	4.0640057	1.6188990
Ag	-5.6782736	-1.5365322	1.6188990
Ag	-4.7128352	1.2456791	1.7164401
Ag	-1.4656894	4.8414928	0.1614232
Ag	-4.1994054	-3.5720198	0.1614232
Ag	-3.2596888	-0.7746717	0.2179247
Ag	-2.3496828	2.0260390	0.2179247
Ag	0.9555377	5.6281971	-1.2341737
Ag	-2.7030047	-5.6316386	-1.2341737

Ag	-1.7708152	-2.8319486	-1.2207313
Ag	-0.8628653	-0.0052521	-1.2443788
Ag	0.0640784	2.8152731	-1.2207313
Ag	3.3544431	6.4076487	-2.6793573
Ag	-1.2203996	-7.6722694	-2.6793573
Ag	-0.2635043	-4.8696104	-2.5519675
Ag	0.6304273	-2.0436413	-2.5968125
Ag	1.5433689	0.7661042	-2.5968125
Ag	2.4812261	3.5778010	-2.5519675
Ag	0.9632801	-6.7469085	-4.2989614
Ag	1.8788960	-3.9850235	-4.2989614
Ag	2.8068031	-1.1975995	-4.2989614
Ag	3.6945171	1.6028838	-4.2989614
Ag	4.5771636	4.3754813	-4.2989614
C	0.3404680	-1.8358435	1.4311430
C	1.3051293	-2.4007315	0.5988542
C	2.3730109	-1.6229359	0.1577096
C	2.4912689	-0.2777368	0.5332898
C	1.5001856	0.2988167	1.3588155
C	0.4286224	-0.4951780	1.8252632
H	-0.4886169	-2.4481747	1.7978328
H	1.2315635	-3.4506072	0.3056596
H	3.1450558	-2.0683217	-0.4755676
C	-0.5917294	0.0752933	2.7655084
H	-0.1276349	0.4256051	3.7017668
H	-1.1112252	0.9466106	2.3292670
H	-1.3605980	-0.6671796	3.0213744
C	1.5983659	1.7324511	1.7964536
H	0.6174497	2.2314761	1.7710953
H	1.9654025	1.8089080	2.8348607
H	2.2761753	2.3184913	1.1634225
C	3.6945806	0.5068232	0.0922809
H	3.4138354	1.4127911	-0.4726083

H	4.2948291	0.8402014	0.9540906
H	4.3412351	-0.0967162	-0.5589659

**7. 1,3,5-Trifluorobenzene@Ag26**

Ag	-8.1970272	2.7611173	4.9132608
Ag	-5.7844163	3.5450222	3.4413551
Ag	-6.7059516	0.7088278	3.4413551
Ag	-3.4329332	4.3090654	1.9771024
Ag	-5.2526551	-1.2914630	1.9771024
Ag	-4.2872184	1.4907436	2.0746433
Ag	-1.0400780	5.0865512	0.5196290
Ag	-3.7737896	-3.3269471	0.5196290
Ag	-2.8340744	-0.5296038	0.5761304
Ag	-1.9240701	2.2711022	0.5761304
Ag	1.3811449	5.8732542	-0.8759655
Ag	-2.2773914	-5.3865627	-0.8759655
Ag	-1.3452033	-2.5868773	-0.8625232
Ag	-0.4372550	0.2398145	-0.8861706
Ag	0.4896870	3.0603350	-0.8625232
Ag	3.7800462	6.6527044	-2.3211467
Ag	-0.7947887	-7.4271899	-2.3211467
Ag	0.1621049	-4.6245357	-2.1937571
Ag	1.0560351	-1.7985714	-2.2386020
Ag	1.9689751	1.0111693	-2.2386020
Ag	2.9068308	3.8228615	-2.1937571
Ag	1.3888873	-6.5018306	-3.9407481
Ag	2.3045016	-3.7399502	-3.9407481
Ag	3.2324073	-0.9525309	-3.9407481
Ag	4.1201197	1.8479477	-3.9407481
Ag	5.0027648	4.6205404	-3.9407481
C	0.6399146	-1.5467492	1.9827920
C	1.6590614	-2.1089307	1.2209490
C	2.7051687	-1.3577741	0.6942959
C	2.7159894	0.0042818	0.9751156

C	1.7268830	0.6250899	1.7311907
C	0.7037300	-0.1782617	2.2238025
H	-0.1753400	-2.1549589	2.3752395
H	3.4880466	-1.8172622	0.0912523
H	1.7528023	1.6972310	1.9249455
F	-0.2695093	0.3902387	2.9272696
F	3.6976026	0.7479030	0.4774308
F	1.6202725	-3.4119476	0.9692254

#### 8. Hexafluorobenzene@Ag26

Ag	-8.0506230	2.5568396	4.7662591
Ag	-5.6380080	3.3407458	3.2943509
Ag	-6.5595449	0.5045466	3.2943509
Ag	-3.2865209	4.1047902	1.8300957
Ag	-5.1062460	-1.4957477	1.8300957
Ag	-4.1408076	1.2864636	1.9276368
Ag	-0.8936618	4.8822773	0.3726199
Ag	-3.6273778	-3.5312353	0.3726199
Ag	-2.6876612	-0.7338872	0.4291214
Ag	-1.7776552	2.0668235	0.4291214
Ag	1.5275653	5.6689816	-1.0229770
Ag	-2.1309771	-5.5908541	-1.0229770
Ag	-1.1987876	-2.7911641	-1.0095346
Ag	-0.2908377	0.0355324	-1.0331821
Ag	0.6361060	2.8560576	-1.0095346
Ag	3.9264707	6.4484332	-2.4681606
Ag	-0.6483720	-7.6314849	-2.4681606
Ag	0.3085233	-4.8288259	-2.3407708
Ag	1.2024549	-2.0028568	-2.3856158
Ag	2.1153965	0.8068887	-2.3856158
Ag	3.0532537	3.6185855	-2.3407708
Ag	1.5353077	-6.7061240	-4.0877647
Ag	2.4509236	-3.9442390	-4.0877647
Ag	3.3788307	-1.1568150	-4.0877647

Ag	4.2665447	1.6436683	-4.0877647
Ag	5.1491912	4.4162658	-4.0877647
C	0.4156077	-1.2115423	2.2583135
C	1.4585849	-1.6722735	1.4561909
C	2.4251154	-0.7811780	0.9915998
C	2.3522545	0.5686582	1.3336755
C	1.3072527	1.0285118	2.1344886
C	0.3382711	0.1384206	2.5951586
F	-0.6726162	0.5796609	3.3196139
F	1.2197906	2.3115301	2.4302359
F	3.2552311	1.4146548	0.8778823
F	3.3916019	-1.2095799	0.2016527
F	1.5137781	-2.9443162	1.1132394
F	-0.5195427	-2.0475337	2.6680565

### 9. Benzene@Au26

Au	-8.2119654	2.7398584	4.9583477
Au	-5.7993549	3.5237631	3.4864423
Au	-6.7208901	0.6875694	3.4864423
Au	-3.4478724	4.2878059	2.0221900
Au	-5.2675940	-1.3127209	2.0221900
Au	-4.3021577	1.4694849	2.1197310
Au	-1.0550182	5.0652915	0.5647171
Au	-3.7887286	-3.3482044	0.5647171
Au	-2.8490141	-0.5508619	0.6212185
Au	-1.9390097	2.2498433	0.6212185
Au	1.3662041	5.8519944	-0.8308771
Au	-2.2923309	-5.4078192	-0.8308771
Au	-1.3601433	-2.6081347	-0.8174347
Au	-0.4521951	0.2185562	-0.8410821
Au	0.4747468	3.0390759	-0.8174347
Au	3.7651050	6.6314444	-2.2760578
Au	-0.8097287	-7.4484461	-2.2760578
Au	0.1471647	-4.6457926	-2.1486682



Au	1.0410943	-1.8198290	-2.1935132
Au	1.9540343	0.9899110	-2.1935132
Au	2.8918896	3.8016023	-2.1486682
Au	1.3739465	-6.5230869	-3.8956586
Au	2.2895607	-3.7612073	-3.8956586
Au	3.2174659	-0.9737889	-3.8956586
Au	4.1051783	1.8266889	-3.8956586
Au	4.9878229	4.5992809	-3.8956586
C	0.6864266	-1.5001409	1.8783110
C	1.6762438	-2.0816177	1.0811475
C	2.7137709	-1.2959547	0.5696219
C	2.7582443	0.0717872	0.8535069
C	1.7674835	0.6530192	1.6511036
C	0.7331862	-0.1332275	2.1633949
H	-0.1277255	-2.1130692	2.2730164
H	1.6369131	-3.1498991	0.8546230
H	3.4906062	-1.7507417	-0.0501718
H	3.5706561	0.6875006	0.4591637
H	1.8014475	1.7228789	1.8713391
H	-0.0460126	0.3228600	2.7782977

#### 10. Toluene@Au26

Au	-7.8901982	2.5648460	4.4967150
Au	-5.4775860	3.3487513	3.0248084
Au	-6.3991218	0.5125553	3.0248084
Au	-3.1261014	4.1127949	1.5605548
Au	-4.9458245	-1.4877367	1.5605548
Au	-3.9803872	1.2944714	1.6580959
Au	-0.7332450	4.8902811	0.1030806
Au	-3.4669579	-3.5232220	0.1030806
Au	-2.5272424	-0.7258771	0.1595821
Au	-1.6172375	2.0748305	0.1595821
Au	1.6879793	5.6769845	-1.2925147
Au	-1.9705590	-5.5828386	-1.2925147

Au	-1.0383705	-2.7831517	-1.2790723
Au	-0.1304217	0.0435417	-1.3027198
Au	0.7965211	2.8640637	-1.2790723
Au	4.0868820	6.4564353	-2.7376967
Au	-0.4879556	-7.6234671	-2.7376967
Au	0.4689387	-4.8208112	-2.6103069
Au	1.3628693	-1.9948453	-2.6551519
Au	2.2758099	0.8148970	-2.6551519
Au	3.2136660	3.6265907	-2.6103069
Au	1.6957217	-6.6981072	-4.3572990
Au	2.6113366	-3.9362253	-4.3572990
Au	3.5392427	-1.1488044	-4.3572990
Au	4.4269556	1.6516757	-4.3572990
Au	5.3096012	4.4242701	-4.3572990
C	0.4554605	-1.4162575	1.8503913
C	1.5185413	-1.7174259	0.9948065
C	2.4031165	-0.7134122	0.5925830
C	2.2067113	0.5941480	1.0450421
C	1.1425301	0.8886923	1.9012981
C	0.2565257	-0.1121420	2.3276679
H	-0.2329107	-2.2104106	2.1528709
H	1.6530300	-2.7406750	0.6353543
H	3.2366351	-0.9473848	-0.0743249
H	2.8837331	1.3903496	0.7252700
H	0.9988053	1.9169427	2.2454575
C	-0.8532166	0.1978561	3.2891884
H	-0.5072151	0.0895449	4.3305804
H	-1.2162944	1.2302917	3.1698054
H	-1.7098539	-0.4795369	3.1531729
<b>11. o-Xylene@Au26</b>			
Au	-8.2654385	2.5981965	4.5446282
Au	-5.8528370	3.3820984	3.0727284
Au	-6.7743688	0.5459152	3.0727284

Au	-3.5013631	4.1461385	1.6084814
Au	-5.3210782	-1.4543680	1.6084814
Au	-4.3556450	1.3278277	1.7060218
Au	-1.1085175	4.9236212	0.1510138
Au	-3.8422181	-3.4898440	0.1510138
Au	-2.9025069	-0.6925117	0.2075150
Au	-1.9925058	2.1081832	0.2075150
Au	1.3126960	5.7103211	-1.2445753
Au	-2.3458258	-5.5494514	-1.2445753
Au	-1.4136418	-2.7497772	-1.2311330
Au	-0.5056967	0.0769037	-1.2547804
Au	0.4212418	2.8974131	-1.2311330
Au	3.7115880	6.4897685	-2.6897509
Au	-0.8632290	-7.5900707	-2.6897509
Au	0.0936609	-4.7874275	-2.5623619
Au	0.9875875	-1.9614742	-2.6072065
Au	1.9005240	0.8482554	-2.6072065
Au	2.8383758	3.6599365	-2.5623619
Au	1.3204384	-6.6647151	-4.3093462
Au	2.2360492	-3.9028455	-4.3093462
Au	3.1639510	-1.1154372	-4.3093462
Au	4.0516602	1.6850304	-4.3093462
Au	4.9343015	4.4576124	-4.3093462
C	0.6198553	-1.8665920	1.4304753
C	1.6012899	-2.3596952	0.5671135
C	2.5980163	-1.5037501	0.0982455
C	2.5963416	-0.1646464	0.4961656
C	1.6263450	0.3387379	1.3742131
C	0.6208437	-0.5307951	1.8535632
H	-0.1609316	-2.5389269	1.7977931
H	1.5840349	-3.4089041	0.2624952
H	3.3800703	-1.8737807	-0.5692413
H	3.3796397	0.5074165	0.1329696

C	-0.4160577	-0.0367587	2.8155704
H	0.0418691	0.3181528	3.7530827
H	-0.9787511	0.8171213	2.3991285
H	-1.1457534	-0.8199320	3.0628421
C	1.6746813	1.7687111	1.8229466
H	0.7048275	2.2735168	1.6817029
H	1.9118014	1.8417800	2.8975776
H	2.4315655	2.3388437	1.2666782

## 12. *m*-Xylene@Au26

Au	-8.2695838	2.4726990	4.5260075
Au	-5.8569688	3.2566052	3.0540993
Au	-6.7785057	0.4204060	3.0540993
Au	-3.5054817	4.0206496	1.5898441
Au	-5.3252068	-1.5798883	1.5898441
Au	-4.3597684	1.2023230	1.6873852
Au	-1.1126226	4.7981367	0.1323683
Au	-3.8463386	-3.6153759	0.1323683
Au	-2.9066220	-0.8180278	0.1888698
Au	-1.9966160	1.9826829	0.1888698
Au	1.3086045	5.5848410	-1.2632286
Au	-2.3499379	-5.6749947	-1.2632286
Au	-1.4177484	-2.8753047	-1.2497862
Au	-0.5097985	-0.0486082	-1.2734337
Au	0.4171452	2.7719170	-1.2497862
Au	3.7075099	6.3642926	-2.7084122
Au	-0.8673328	-7.7156255	-2.7084122
Au	0.0895625	-4.9129665	-2.5810224
Au	0.9834941	-2.0869974	-2.6258674
Au	1.8964357	0.7227481	-2.6258674
Au	2.8342929	3.5344449	-2.5810224
Au	1.3163469	-6.7902646	-4.3280163
Au	2.2319628	-4.0283796	-4.3280163
Au	3.1598699	-1.2409556	-4.3280163

Au	4.0475839	1.5595277	-4.3280163
Au	4.9302304	4.3321252	-4.3280163
C	0.3142364	-1.5600431	1.6544978
C	1.3879083	-1.8746938	0.8181592
C	2.3245659	-0.8985431	0.4725439
C	2.1962544	0.4125432	0.9560971
C	1.0987739	0.7114691	1.7784432
C	0.1607913	-0.2593137	2.1556250
H	-0.4111182	-2.3336997	1.9216123
H	1.4936444	-2.8911470	0.4305715
H	3.1675121	-1.1584672	-0.1737052
H	0.9827703	1.7342875	2.1508174
C	-0.9527849	0.0762241	3.1044833
H	-0.6133144	-0.0224341	4.1490077
H	-1.3060408	1.1105313	2.9716891
H	-1.8160147	-0.5937110	2.9739913
C	3.2371001	1.4515948	0.6579448
H	2.8026403	2.4613778	0.6057797
H	4.0068678	1.4614537	1.4479349
H	3.7460514	1.2565760	-0.2980282

### 13. *p*-Xylene@Au26

Au	-8.2603263	2.6441027	4.5666563
Au	-5.8477133	3.4280081	3.0947493
Au	-6.7692494	0.5918114	3.0947493
Au	-3.4962281	4.1920519	1.6304953
Au	-5.3159517	-1.4084812	1.6304953
Au	-4.3505142	1.3737278	1.7280364
Au	-1.1033711	4.9695385	0.1730207
Au	-3.8370847	-3.4439672	0.1730207
Au	-2.8973690	-0.6466214	0.2295222
Au	-1.9873637	2.1540871	0.2295222
Au	1.3178539	5.7562421	-1.2225750
Au	-2.3406853	-5.5035843	-1.2225750

Au	-1.4084966	-2.7038966	-1.2091326
Au	-0.5005475	0.1227975	-1.2327801
Au	0.4263955	2.9433203	-1.2091326
Au	3.7167574	6.5356930	-2.6677574
Au	-0.8580815	-7.5442133	-2.6677574
Au	0.0988131	-4.7415566	-2.5403676
Au	0.9927438	-1.9155900	-2.5852126
Au	1.9056847	0.8941532	-2.5852126
Au	2.8435411	3.7058476	-2.5403676
Au	1.3255963	-6.6188531	-4.2873600
Au	2.2412116	-3.8569703	-4.2873600
Au	3.1691178	-1.0695488	-4.2873600
Au	4.0568311	1.7309322	-4.2873600
Au	4.9394768	4.5035273	-4.2873600
C	0.2641928	-1.2834828	1.8270430
C	1.3462604	-1.6440663	1.0207965
C	2.3010652	-0.6988674	0.6178974
C	2.0939156	0.6325464	1.0060668
C	1.0106368	0.9930491	1.8112915
C	0.0891455	0.0377554	2.2619313
H	-0.4544025	-2.0504149	2.1307483
H	1.4554777	-2.6859702	0.7060750
H	2.7983358	1.4035861	0.6805692
H	0.8867117	2.0401295	2.1024697
C	-1.0181765	0.4067676	3.2053629
H	-0.6950181	0.2792045	4.2521412
H	-1.3262608	1.4568379	3.0841845
H	-1.9077264	-0.2248990	3.0584037
C	3.5243410	-1.1061429	-0.1507663
H	4.3353353	-1.3932472	0.5389919
H	3.3280968	-1.9698391	-0.8042398
H	3.9038376	-0.2866276	-0.7795718

**14. 1,2,3-Trimethylbenzene@Au26**

Au	-8.5932249	2.5066497	4.5673202
Au	-6.1806127	3.2905551	3.0954136
Au	-7.1021486	0.4543591	3.0954136
Au	-3.8291283	4.0545987	1.6311601
Au	-5.6488513	-1.5459330	1.6311601
Au	-4.6834139	1.2362752	1.7287011
Au	-1.4362718	4.8320848	0.1736859
Au	-4.1699848	-3.5814184	0.1736859
Au	-3.2302692	-0.7840734	0.2301873
Au	-2.3202643	2.0166342	0.2301873
Au	0.9849526	5.6187883	-1.2219094
Au	-2.6735858	-5.6410348	-1.2219094
Au	-1.7413973	-2.8413480	-1.2084671
Au	-0.8334484	-0.0146547	-1.2321145
Au	0.0934942	2.8058673	-1.2084671
Au	3.3838552	6.3982389	-2.6670914
Au	-1.1909823	-7.6816632	-2.6670914
Au	-0.2340881	-4.8790074	-2.5397017
Au	0.6598426	-2.0530415	-2.5845467
Au	1.5727831	0.7567008	-2.5845467
Au	2.5106392	3.5683944	-2.5397017
Au	0.9926950	-6.7563035	-4.2866936
Au	1.9083098	-3.9944215	-4.2866936
Au	2.8362159	-1.2070007	-4.2866936
Au	3.7239289	1.5934795	-4.2866936
Au	4.6065744	4.3660739	-4.2866936
C	0.3139640	-1.8309900	1.3959287
C	1.2835824	-2.3824486	0.5585268
C	2.3432412	-1.5914052	0.1196682
C	2.4504418	-0.2468853	0.5056490
C	1.4542612	0.3152341	1.3380026
C	0.3901155	-0.4921781	1.7998501
H	-0.5082206	-2.4531408	1.7600010

H	1.2194843	-3.4314684	0.2602229
H	3.1187442	-2.0259315	-0.5170500
C	-0.6314318	0.0569435	2.7499179
H	-0.1653312	0.4060654	3.6851112
H	-1.1655552	0.9237989	2.3222105
H	-1.3889088	-0.6973852	3.0030096
C	1.5495413	1.7429873	1.7933022
H	0.5641349	2.2319828	1.8027804
H	1.9465255	1.8041620	2.8216241
H	2.2045032	2.3446503	1.1506468
C	3.6573569	0.5434943	0.0853821
H	3.3864563	1.4844623	-0.4225992
H	4.2755127	0.8169636	0.9563124
H	4.2843735	-0.0333949	-0.6083603

**15. 1,3,5-Trifluorobenzene@Au26**

Au	-8.1105694	2.6793594	4.8596043
Au	-5.6979655	3.4632618	3.3877034
Au	-6.6194983	0.6270761	3.3877034
Au	-3.3464900	4.2273024	1.9234552
Au	-5.1662063	-1.3732085	1.9234552
Au	-4.2007726	1.4089893	2.0209956
Au	-0.9536423	5.0047859	0.4659862
Au	-3.6873453	-3.4086861	0.4659862
Au	-2.7476331	-0.6113515	0.5224876
Au	-1.8376313	2.1893457	0.5224876
Au	1.4675734	5.7914867	-0.9296039
Au	-2.1909515	-5.4682955	-0.9296039
Au	-1.2587666	-2.6686186	-0.9161616
Au	-0.3508207	0.1580645	-0.9398090
Au	0.5761181	2.9785762	-0.9161616
Au	3.8664674	6.5709346	-2.3747807
Au	-0.7083533	-7.5089167	-2.3747807
Au	0.2485371	-4.7062709	-2.2473917



Au	1.1424644	-1.8803153	-2.2922361
Au	2.0554018	0.9294168	-2.2922361
Au	2.9932544	3.7411004	-2.2473917
Au	1.4753158	-6.5835599	-3.9943774
Au	2.3909272	-3.8216880	-3.9943774
Au	3.3188298	-1.0342775	-3.9943774
Au	4.2065398	1.7661923	-3.9943774
Au	5.0891819	4.5387766	-3.9943774
C	0.4922182	-1.4520572	2.0414402
C	1.5509926	-1.9178809	1.2671510
C	2.5606861	-1.0845287	0.7953494
C	2.4874420	0.2623329	1.1374778
C	1.4542479	0.7879772	1.9080345
C	0.4744683	-0.0956318	2.3491521
H	-0.2914818	-2.1236977	2.3921384
H	3.3777233	-1.4712803	0.1862509
H	1.4151556	1.8489833	2.1542001
F	-0.5338138	0.3796117	3.0712979
F	3.4326745	1.0829276	0.6968436
F	1.5901390	-3.2064275	0.9533149

**16. Hexafluorobenzene@Au26**

Au	-8.0505919	2.5568744	4.7662524
Au	-5.6379769	3.3407806	3.2943442
Au	-6.5595138	0.5045814	3.2943442
Au	-3.2864898	4.1048250	1.8300890
Au	-5.1062149	-1.4957129	1.8300890
Au	-4.1407765	1.2864984	1.9276301
Au	-0.8936307	4.8823121	0.3726132
Au	-3.6273467	-3.5312005	0.3726132
Au	-2.6876301	-0.7338524	0.4291147
Au	-1.7776241	2.0668583	0.4291147
Au	1.5275964	5.6690164	-1.0229837
Au	-2.1309460	-5.5908193	-1.0229837

Au	-1.1987565	-2.7911293	-1.0095413
Au	-0.2908066	0.0355672	-1.0331888
Au	0.6361371	2.8560924	-1.0095413
Au	3.9265018	6.4484680	-2.4681673
Au	-0.6483409	-7.6314501	-2.4681673
Au	0.3085544	-4.8287911	-2.3407775
Au	1.2024860	-2.0028220	-2.3856225
Au	2.1154276	0.8069235	-2.3856225
Au	3.0532848	3.6186203	-2.3407775
Au	1.5353388	-6.7060892	-4.0877714
Au	2.4509547	-3.9442042	-4.0877714
Au	3.3788618	-1.1567802	-4.0877714
Au	4.2665758	1.6437031	-4.0877714
Au	5.1492223	4.4163006	-4.0877714
C	0.3860262	-1.2190504	2.2024372
C	1.4304731	-1.6726946	1.3972865
C	2.3935149	-0.7757710	0.9354111
C	2.3108844	0.5739303	1.2764233
C	1.2623495	1.0273249	2.0766787
C	0.3009070	0.1303319	2.5404828
F	-0.7065488	0.5627102	3.2740792
F	1.1678602	2.3088453	2.3741759
F	3.2098056	1.4245411	0.8220114
F	3.3689423	-1.1993468	0.1548439
F	1.4949490	-2.9445403	1.0562700
F	-0.5364333	-2.0631498	2.6219239