Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

On the influence of Ag/Au nanoparticle and π-system sizes in the stability of noncovalent adducts: A theoretical study

Sergi Burguera,[a] María de las Nieves Piña,[a] and Antonio Bauzá*,[a]

[a]Department of Chemistry, Universitat de les Illes Balears, Ctra. de Valldemossa km 7.5, Palma de Mallorca (Baleares), 07122, Spain; E-mail: antonio.bauza@uib.es

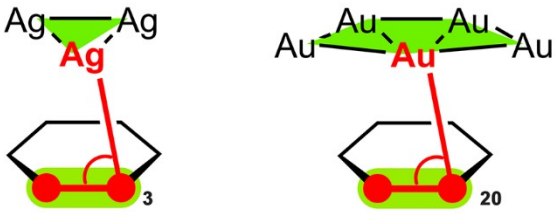

Fig. S1 Schematic representation of the Rg···C–C angles frozen during the optimization procedure of complexes **3** and **20**.

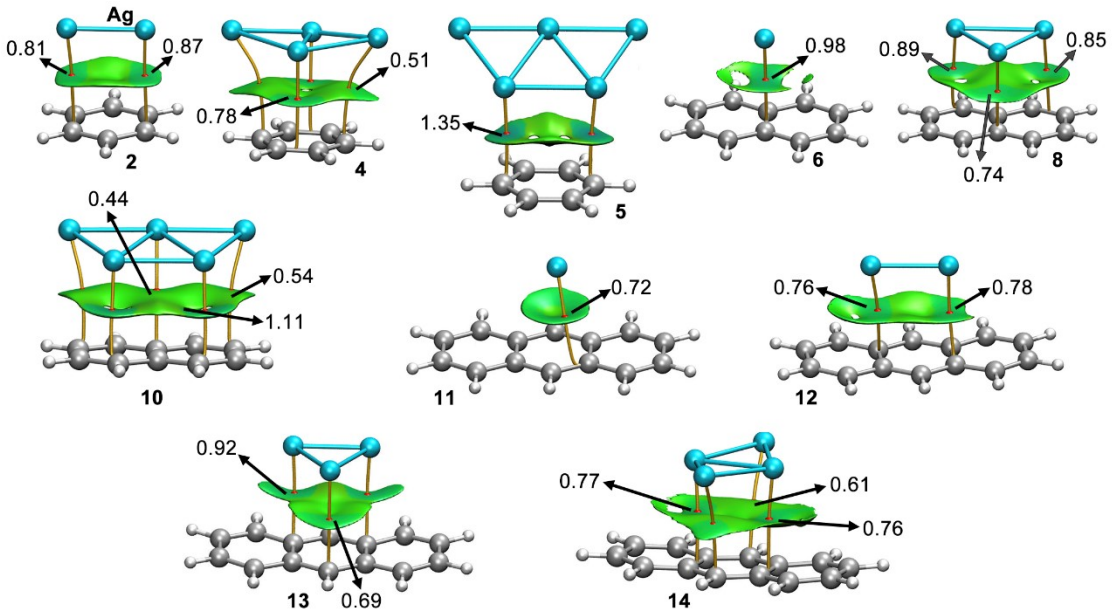

Fig. S2 Distribution of intermolecular bcps (red dots) and bond paths in Ag complexes **2**, **4**, **5**, **6**, **10**, **11**, **12**, **13** and **14**. The values of the density ($\rho \cdot 10^2$) related to the Rg-π interactions are also included in a.u. NCIplot color range−0.03 au≤(signλ_2)ρ≤+0.03 au.

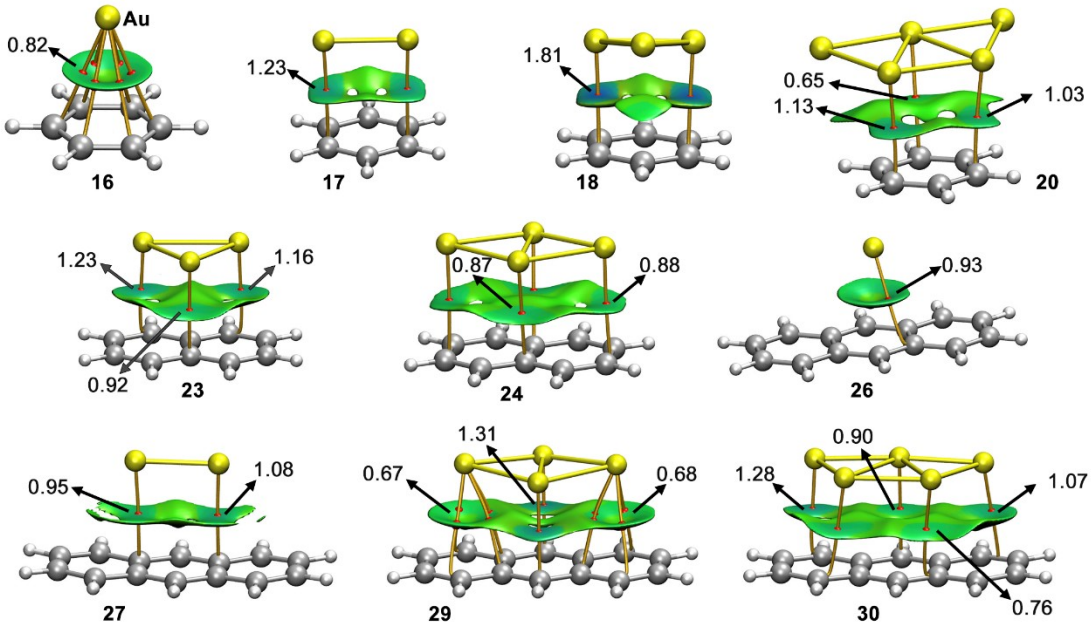

Fig. S3 Distribution of intermolecular bcps (red dots) and bond paths in Au complexes **16**, **17**, **18**, **20**, **23**, **24**, **26**, **27**, **29** and **30**. The values of the density ($\rho \cdot 10^2$) related to the Rg-π interactions are also included in a.u. NCIplot color range−0.03 au≤(signλ_2)ρ≤+0.03 au.

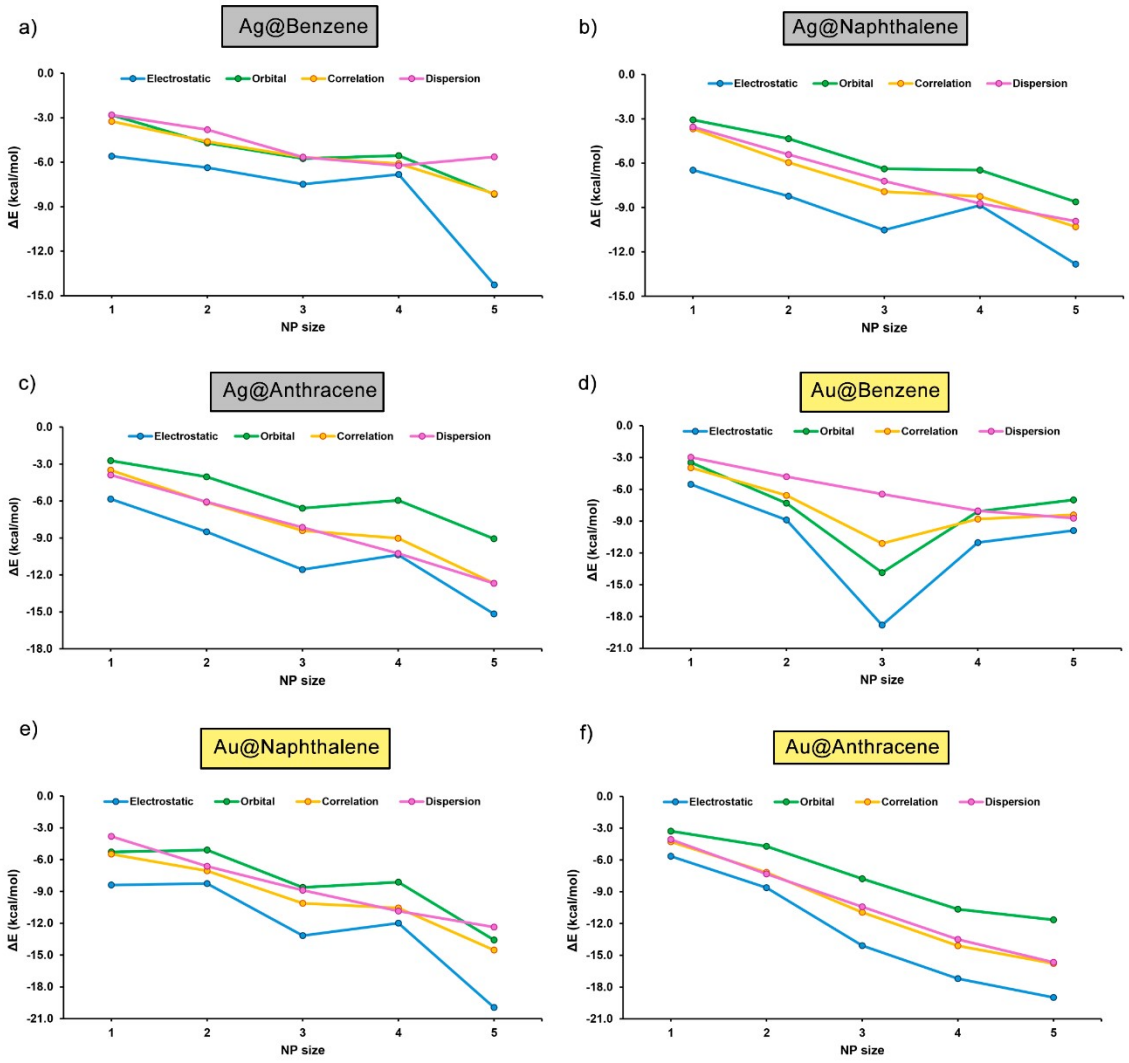

Fig. S4 Attractive interaction energy terms (ΔE in kcal/mol) *vs* NP size for (a) **Ag@Benzene**, (b) **Ag@Naphthalene**, (c) **Ag@Anthracene**, (d) **Au@Benzene**, (e) **Au@Naphthalene** and (f) **Au@Anthracene**.

Table S1. Average values of the laplacian of ρ ($\nabla^2\rho$x100), the potential (Vx100) and kinetic (Gx100) energy densities as well as the total energy density (Hx100) in a.u. for complexes **1** to **30**.

Complex	∇^2Px100	Vx100	Gx100	Hx100
1	1.87	-0.33	0.40	0.07
2	2.04	-0.40	0.45	0.06
3	1.93	-0.38	0.43	0.05
4	1.63	-0.29	0.35	0.06
5	3.47	-0.83	0.85	0.02
6	2.65	-0.55	0.61	0.06
7	1.69	-0.29	0.36	0.06
8	2.11	-0.41	0.47	0.06
9	1.77	-0.31	0.38	0.07
10	1.87	-0.37	0.42	0.05
11	1.99	-0.37	0.43	0.06
12	2.09	-0.38	0.45	0.07
13	2.29	-0.43	0.50	0.07
14	1.81	-0.33	0.39	0.06
15	1.99	-0.38	0.44	0.06
16	2.49	-0.48	0.55	0.07
17	3.05	-0.69	0.73	0.03
18	4.40	-1.14	1.12	-0.02
19	2.34	-0.47	0.53	0.06
20	2.51	-0.51	0.57	0.06
21	4.06	-1.00	1.01	0.01
22	2.22	-0.40	0.48	0.08
23	2.87	-0.62	0.67	0.05
24	2.43	-0.47	0.54	0.07
25	0.27	-0.59	0.63	0.04
26	2.69	-0.55	0.61	0.06
27	2.81	-0.58	0.64	0.06
28	2.97	-0.63	0.69	0.05
29	2.25	-0.43	0.50	0.07
30	2.63	-0.54	0.60	0.06

Table S2. Donor and acceptor NBOs with indication of the second-order interaction energy $E^{(2)}$ in complexes **2**, **4**, **5**, **6**, **8**, **10** to **14**, **16** to **18**, **20**, **23**, **24**, **26**, **27**, **29** and **30**. LP, BD, BD* and s* and p* stand for lone pair, bonding orbital, antibonding orbital and unfilled s and p orbitals, respectively. Energy values are in kcal/mol.

Complex	Donor	Acceptor	$E^{(2)}$
2	BD C–C	5p* Ag	1.33
	BD C–C	BD*Ag–Ag	2.06
4	BD C–C	5p* Ag	3.51
	BD C–C	BD*Ag–Ag	0.45
5	BD C–C	5p* Ag	0.83
	BD C–C	BD*Ag–Ag	1.88
6	BD C–C	5p* Ag	0.53
8	BD C–C	5p* Ag	1.11
10	BD C–C	5p* Ag	1.13
	BD C–C	BD*Ag–Ag	2.14
11	BD C–C	5p* Ag	0.37
	5s Ag	BD* C–C	0.28
12	BD C–C	5p* Ag	1.26
	BD C–C	BD*Ag–Ag	1.64
	5s Ag	BD* C–C	0.41
13	BD C–C	5p* Ag	0.48
	BD C–C	BD*Ag–Ag	1.32
	5s Ag	BD* C–C	0.60
14	BD C–C	5p* Ag	8.24
	BD C–C	BD*Ag–Ag	0.64
	5s Ag	BD* C–C	0.38
16	BD C–C	6s* Au	0.14
	BD C–C	6p* Au	0.64
	5d Au	BD* C–C	0.21
17	BD C–C	6p* Au	1.85
	BD C–C	BD* Au–Au	3.71

	5d Au	BD* C–C	1.38
18	BD C–C	6p* Au	2.47
	BD C–C	BD* Au–Au	3.83
	5d Au	BD* C–C	1.83
20	BD C–C	6s* Au	1.08
	BD C–C	6p* Au	1.07
	BD C–C	BD* Au–Au	1.86
	5d Au	BD* C–C	0.57
23	BD C–C	6s* Au	1.61
	BD C–C	6p* Au	1.28
	5d Au	BD* C–C	0.75
24	BD C–C	6s* Au	11.21
	BD C–C	6p* Au	1.22
	BD C–C	BD* Au–Au	1.40
	5d Au	BD* C–C	1.00
26	BD C–C	6s* Au	0.64
27	BD C–C	6s* Au	0.48
	BD C–C	BD* Au–Au	1.11
	5d Au	BD* C–C	1.14
29	BD C–C	6s* Au	12.74
	BD C–C	6p* Au	4.07
	BD C–C	BD* Au–Au	1.78
	5d Au	BD* C–C	1.30
30	BD C–C	6s* Au	0.68
	BD C–C	6p* Au	1.67
	6s Au	BD* C–C	0.66
	5d Au	BD* C–C	1.32

Table S3. Energy Decomposition Analysis into exchange-repulsion ($E_{ex\text{-}rep}$), electrostatics (E_{el}), orbital (E_{orb}), electron correlation + dispersion terms ($E_{cor+disp}$) in kcal/mol for complexes **1** to **30**.

Complex	$E_{ex\text{-}rep}$	E_{el}	E_{orb}	$E_{cor} + E_{disp}$
1 (Ag_1@B)	10.5	–5.6	–2.8	–6.0
2 (Ag_2@B)	15.4	–6.4	–4.7	–8.4
3 (Ag_3@B)	18.4	–7.5	–5.7	–11.4
4 (Ag_4@B)	18.1	–6.8	–5.6	–12.3
5 (Ag_5@B)	28.9	–14.3	–8.2	–13.7
6 (Ag_1@N)	12.5	–6.5	–3.1	–7.2
7 (Ag_2@N)	17.7	–8.2	–4.3	–11.4
8 (Ag_3@N)	24.2	–10.5	–6.4	–15.1
9 (Ag_4@N)	23.8	–8.9	–6.5	–17.0
10 (Ag_5@N)	31.2	–12.8	–8.6	–20.2
11 (Ag_1@A)	11.3	–5.8	–2.7	–7.4
12 (Ag_2@A)	17.9	–8.5	–4.0	–12.2
13 (Ag_3@A)	24.9	–11.6	–6.6	–16.5
14 (Ag_4@A)	24.5	–10.4	–5.9	–19.3
15 (Ag_5@A)	36.0	–15.2	–9.1	–25.4
16 (Au_1@B)	11.7	–5.5	–3.5	–7.0
17 (Au_2@B)	22.0	–8.9	–7.3	–11.4
18 (Au_3@B)	41.1	–18.8	–13.9	–17.6
19 (Au_4@B)	26.9	–11.0	–8.1	–16.8
20 (Au_5@B)	25.2	–9.9	–7.0	–15.7
21 (Au_1@N)	18.1	–8.4	–5.3	–9.3
22 (Au_2@N)	19.7	–8.3	–5.1	–13.7
23 (Au_3@N)	30.9	–13.2	–8.6	–19.0
24 (Au_4@N)	30.5	–12.0	–8.1	–20.5
25 (Au_5@N)	46.6	–19.9	–13.6	–27.4
26 (Au_1@A)	12.4	–5.7	–3.3	–8.4
27 (Au_2@A)	20.0	–8.6	–4.7	–14.5
28 (Au_3@A)	31.2	–14.1	–7.8	–21.3
29 (Au_4@A)	41.1	–17.2	–10.7	–27.6
30 (Au_5@A)	45.1	–19.0	–11.7	–31.5

Cartesian coordinates of complexes 1 to 30

1

C	0.0000001	1.3885463	-1.4400049
C	-1.2026530	0.6943198	-1.4400053
C	-1.2026466	-0.6943212	-1.4400053
C	-0.0000004	-1.3885384	-1.4400049
C	1.2026479	-0.6943219	-1.4400053
C	1.2026524	0.6943201	-1.4400053
H	-0.0000001	2.4724690	-1.4345783
H	-2.1412638	1.2363593	-1.4345718
H	-2.1412658	-1.2363600	-1.4345718
H	0.0000001	-2.4724726	-1.4345783
H	2.1412653	-1.2363598	-1.4345718
H	2.1412639	1.2363593	-1.4345718
Ag	0.0000000	-0.0000000	1.8350095

2

C	0.0090712	-0.4843625	-1.3894168
C	1.2102165	-0.4760741	-0.6951683
C	1.2102165	-0.4760741	0.6951683
C	0.0090712	-0.4843625	1.3894168
C	-1.1917098	-0.4871956	0.6950007
C	-1.1917098	-0.4871956	-0.6950007
H	0.0090510	-0.4802897	-2.4731072
H	2.1493577	-0.4765871	-1.2369888
H	2.1493577	-0.4765871	1.2369888
H	0.0090510	-0.4802897	2.4731072
H	-2.1308690	-0.4943437	1.2367443
H	-2.1308690	-0.4943437	-1.2367443
Ag	-1.3466222	2.9191823	0.0000000
Ag	1.2363871	2.8785230	0.0000000

3

C	-2.0442388	1.1433681	-1.6177763
C	-1.7028939	-0.0516418	-2.2273836
C	-2.0346088	-1.2412627	-1.6077917

C	-2.7179693	-1.2337080	-0.3962142
C	-3.0668174	-0.0327058	0.2094450
C	-2.7271569	1.1634067	-0.4070262
H	-1.8007385	2.0821838	-2.1057697
H	-1.1702127	-0.0522108	-3.1705349
H	-1.7717842	-2.1862561	-2.0700111
H	-2.9810746	-2.1725274	0.0777036
H	-3.5933576	-0.0317312	1.1561858
H	-2.9889264	2.1091428	0.0527433
Ag	0.9178570	1.2879164	-0.4604166
Ag	0.2363333	0.0390966	1.9219099
Ag	1.2250423	-1.2924875	-0.3263991

4

C	1.3841186	0.0993841	2.9184605
C	0.7757703	-1.1509835	2.9184261
C	-0.6078322	-1.2491361	2.9194226
C	-1.3845141	-0.0997873	2.9186782
C	-0.7761980	1.1506032	2.9184138
C	0.6074475	1.2487229	2.9191874
H	2.4655022	0.1772949	2.9200227
H	1.3817980	-2.0498611	2.9190705
H	-1.0817664	-2.2230481	2.9023552
H	-2.4659146	-0.1777053	2.9203683
H	-1.3822029	2.0494777	2.9190306
H	1.0813835	2.2226540	2.9019360
Ag	1.0346431	2.1890223	-0.7082909
Ag	1.1862437	-0.5628400	-0.4545954
Ag	-1.1863751	0.5641286	-0.4556698
Ag	-1.0346911	-2.1878335	-0.7082170

5

C	-2.7410832	-0.0477471	-0.6933276
C	-2.7410719	-0.0477466	0.6933108
C	-2.6628251	1.1555282	1.3870888
C	-2.5954962	2.3582943	0.6936550
C	-2.5955012	2.3583027	-0.6936630

C	-2.6628418	1.1555352	-1.3870990
H	-2.7893649	-0.9838369	-1.2365848
H	-2.7893294	-0.9838425	1.2365671
H	-2.6720310	1.1550681	2.4713784
H	-2.5397745	3.2945716	1.2367746
H	-2.5397990	3.2945773	-1.2367782
H	-2.6720895	1.1550808	-2.4713874
Ag	1.3189305	-1.5691015	-2.7014375
Ag	0.3881550	0.6529901	-1.3978790
Ag	1.3434417	-1.5491823	0.0000165
Ag	0.3881649	0.6530017	1.3978957
Ag	1.3189147	-1.5690931	2.7014698

6

Ag	1.9260892	-0.2239201	0.0000001
C	-0.9333825	2.5414963	-0.7043352
C	-1.0995700	1.3726996	-1.3947419
C	-1.2757705	0.1477445	-0.7119801
C	-1.2757719	0.1477354	0.7119798
C	-1.0995689	1.3727053	1.3947406
C	-0.9333829	2.5414910	0.7043356
H	-1.4362735	-1.0762919	-2.4792346
H	-0.7970055	3.4737045	-1.2400564
H	-1.0940130	1.3693817	-2.4795832
C	-1.4393149	-1.0789542	-1.3944837
C	-1.4393167	-1.0789674	1.3944742
H	-1.0940124	1.3693857	2.4795846
H	-0.7970056	3.4737044	1.2400586
C	-1.5941765	-2.2493563	0.7043832
C	-1.5941784	-2.2493742	-0.7043782
H	-1.4362726	-1.0762866	2.4792375
H	-1.7153552	-3.1836649	1.2402656
H	-1.7153545	-3.1836587	-1.2402664

7

Ag	-1.9917814	-0.0529321	-0.0000031
Ag	-0.2470816	-1.9547052	0.0000014

C	-0.2329583	3.0951497	-0.7048086
C	0.5480985	2.2081951	-1.3942993
C	1.3619214	1.2777783	-0.7108386
C	1.3619261	1.2777723	0.7108350
C	0.5480902	2.2082045	1.3942949
C	-0.2329596	3.0951522	0.7048081
H	2.1451922	0.3269255	-2.4792342
H	-0.8556890	3.8018777	-1.2410704
H	0.5448623	2.1999821	-2.4789152
C	2.1524751	0.3280258	-1.3945617
C	2.1524877	0.3280112	1.3945412
H	0.5448613	2.1999822	2.4789141
H	-0.8556923	3.8018824	1.2410813
C	2.9030161	-0.5854601	0.7051005
C	2.9030421	-0.5854921	-0.7050976
H	2.1451912	0.3269241	2.4792509
H	3.5015876	-1.3126166	1.2417794
H	3.5015830	-1.3126136	-1.2417785

8

C	-0.8451867	2.5225856	-0.7349994
C	-0.9864709	1.3483322	-1.4219169
C	-1.1788431	0.1266452	-0.7373686
C	-1.2266298	0.1353199	0.6829670
C	-1.0807373	1.3643432	1.3637576
C	-0.8933022	2.5313535	0.6721469
C	-1.3377412	-1.1012278	-1.4189912
C	-1.4374190	-1.0824452	1.3666342
C	-1.5901987	-2.2560394	0.6776973
C	-1.5375125	-2.2652895	-0.7295326
H	-0.7021373	3.4529566	-1.2717397
H	-0.9485891	1.3382724	-2.5064030
H	-1.1206178	1.3684963	2.4479106
H	-0.7862022	3.4680124	1.2064972
H	-1.2976971	-1.1055847	-2.5033302
H	-1.4771860	-1.0727221	2.4507564
H	-1.7548822	-3.1833117	1.2138649

H	-1.6644564	-3.1992862	-1.2639738
Ag	-4.5154295	0.6260367	-1.4591644
Ag	-4.3276350	2.1179396	0.7592492
Ag	-4.7941199	-1.0086414	0.6024531

9

C	-2.4183812	-0.7039659	2.2914803
C	-1.2371541	-1.3938057	2.2884448
C	-0.0000241	-0.7115295	2.2875244
C	0.0000218	0.7115055	2.2875238
C	-1.2371648	1.3938256	2.2884391
C	-2.4183943	0.7039627	2.2914812
H	1.2351938	-2.4789258	2.2886816
H	-3.3602745	-1.2398720	2.2886573
H	-1.2352082	-2.4789234	2.2886839
C	1.2371843	-1.3937734	2.2884414
C	1.2371625	1.3938148	2.2884411
H	-1.2352037	2.4789258	2.2886789
H	-3.3602684	1.2398639	2.2886570
C	2.4183974	0.7039845	2.2914778
C	2.4183903	-0.7040066	2.2914794
H	1.2352005	2.4789104	2.2886871
H	3.3602636	1.2398938	2.2886522
H	3.3602587	-1.2398803	2.2886502
Ag	2.4309551	-0.0000101	-1.2041975
Ag	0.0000002	1.3109838	-1.1501145
Ag	-0.0000004	-1.3109750	-1.1501242
Ag	-2.4309547	-0.0000030	-1.2041965

10

C	1.8340805	1.7181231	2.4176995
C	2.3847062	1.3056641	1.2359941
C	1.8470490	1.7268784	0.0000106
C	0.7221707	2.5967618	-0.0000088
C	0.1731845	3.0038820	1.2365695
C	0.7157186	2.5739822	2.4190994
H	3.2398525	0.6382386	-1.2324541

H	2.2506886	1.3800756	3.3589331
H	3.2398482	0.6382434	1.2324569
C	2.3846999	1.3056730	-1.2360075
C	0.1731752	3.0038929	-1.2365549
H	-0.6858745	3.6664319	1.2344536
H	0.2843939	2.8917130	3.3611772
C	0.7157278	2.5739733	-2.4190998
C	1.8340822	1.7181161	-2.4176984
H	-0.6858696	3.6664266	-1.2344552
H	0.2843912	2.8917130	-3.3611815
H	2.2506861	1.3800786	-3.3589301
Ag	0.0440911	-1.5316969	2.7035657
Ag	-1.5330328	0.2762740	1.3926803
Ag	0.0316625	-1.5489615	-0.0000001
Ag	-1.5330297	0.2762742	-1.3926838
Ag	0.0440933	-1.5316999	-2.7035655

11

C	-2.7825198	-2.4562721	-0.1292727
C	-1.4218952	-2.4567193	-0.1294486
C	-0.6921088	-1.2368378	-0.1359856
C	-1.4188760	-0.0001978	-0.1419155
C	-2.8397286	-0.0444267	-0.1406940
C	-3.5011925	-1.2334105	-0.1349187
C	0.7002650	-1.2051354	-0.1283743
C	-0.7141663	1.2008950	-0.1408022
C	0.6782874	1.2329611	-0.1420622
C	1.4054660	-0.0038176	-0.1352817
C	2.8262212	0.0406431	-0.1227294
H	3.3736235	-0.8957700	-0.1139944
C	3.4873985	1.2298218	-0.1164903
C	2.7686137	2.4525868	-0.1240282
C	1.4080854	2.4529532	-0.1370022
H	1.2502693	-2.1412201	-0.1184784
H	-3.3265393	-3.3937511	-0.1235692
H	-0.8699580	-3.3907252	-0.1223344
H	-3.3870152	0.8921498	-0.1420980

H	-4.5848881	-1.2526661	-0.1333137
H	-1.2642142	2.1369630	-0.1399331
H	4.5709594	1.2492351	-0.1039768
H	3.3125005	3.3901162	-0.1174646
H	0.8561111	3.3869422	-0.1394729
Ag	0.1653008	0.0456825	3.1136410

12

C	-2.7502525	-2.4510303	-0.1881202
C	-1.3893443	-2.4507570	-0.2170761
C	-0.6600276	-1.2317167	-0.2822760
C	-1.3876231	0.0033659	-0.3237883
C	-2.8088992	-0.0412645	-0.2981050
C	-3.4701605	-1.2291558	-0.2292468
C	0.7303900	-1.2005445	-0.2715768
C	-0.6865014	1.2042698	-0.3534364
C	0.7038979	1.2366646	-0.3234133
C	1.4321499	0.0010165	-0.2805026
C	2.8526513	0.0489620	-0.2232871
H	3.4006325	-0.8865372	-0.1879832
C	3.5121755	1.2394790	-0.2059478
C	2.7920850	2.4610065	-0.2488154
C	1.4323881	2.4580310	-0.3074056
H	1.2804594	-2.1353600	-0.2281591
H	-3.2931497	-3.3874757	-0.1316734
H	-0.8364763	-3.3833901	-0.1802698
H	-3.3562060	0.8947420	-0.3256917
H	-4.5536190	-1.2479709	-0.2047250
H	-1.2376592	2.1392174	-0.3727883
H	4.5948314	1.2608357	-0.1585798
H	3.3338671	3.3996984	-0.2326368
H	0.8789396	3.3906352	-0.3362007
Ag	-1.4188693	-0.6121800	3.0617928
Ag	0.9043206	0.5194586	3.0499125

13

C	2.3155681	-0.2324978	-3.6339260

C	2.6488973	-0.8397589	-2.4621403
C	2.4151427	-0.1998892	-1.2154031
C	1.8425068	1.1147346	-1.2138694
C	1.5036138	1.7139448	-2.4598317
C	1.7303152	1.0591418	-3.6331058
C	2.6942244	-0.8191033	-0.0000072
C	1.5903916	1.7455801	-0.0000029
C	1.8425195	1.1147341	1.2138622
C	2.4150754	-0.1999242	1.2153906
C	2.6487170	-0.8398417	2.4621247
H	3.0843262	-1.8331584	2.4602939
C	2.3154883	-0.2325340	3.6339149
C	1.7304282	1.0591934	3.6331051
C	1.5037072	1.7139833	2.4598280
H	3.1192546	-1.8178104	-0.0000098
H	2.4916388	-0.7364211	-4.5770893
H	3.0846720	-1.8330032	-2.4603162
H	1.0658860	2.7067095	-2.4553491
H	1.4667258	1.5256889	-4.5753443
H	1.1390876	2.7325017	0.0000006
H	2.4914574	-0.7365023	4.5770731
H	1.4669156	1.5257761	4.5753474
H	1.0661043	2.7068038	2.4553461
Ag	-0.6833010	-1.8457780	0.0000790
Ag	-1.4165925	0.4940246	1.2723417
Ag	-1.4166410	0.4939238	-1.2723123

14

C	-0.5411203	3.6170800	-0.7095066
C	-0.5787218	2.4441319	-1.3995768
C	-0.6080837	1.1967057	-0.7175360
C	-0.6080837	1.1967057	0.7175360
C	-0.5787218	2.4441319	1.3995768
C	-0.5411203	3.6170800	0.7095066
C	-0.5810254	-0.0170008	-1.3962425
C	-0.5810254	-0.0170008	1.3962425
C	-0.5196184	-1.2293056	0.7174708

C	-0.5196184	-1.2293056	-0.7174708
C	-0.3970725	-2.4710252	-1.3995032
H	-0.3877592	-2.4668622	-2.4840113
C	-0.2707293	-3.6377899	-0.7095239
C	-0.2707293	-3.6377899	0.7095239
C	-0.3970725	-2.4710252	1.3995032
H	-0.5533299	-0.0159127	-2.4809716
H	-0.5074034	4.5603992	-1.2423179
H	-0.5695114	2.4407093	-2.4841389
H	-0.5695114	2.4407093	2.4841389
H	-0.5074034	4.5603992	1.2423179
H	-0.5533299	-0.0159127	2.4809716
H	-0.1657146	-4.5757874	-1.2423566
H	-0.1657146	-4.5757874	1.2423566
H	-0.3877592	-2.4668622	2.4840113
Ag	2.8072560	-1.2409733	0.0000000
Ag	2.9220418	0.0790732	-2.4235644
Ag	2.9220418	0.0790732	2.4235644
Ag	2.7088402	1.3921421	0.0000000

15

C	1.8981053	1.7214744	2.4894527
C	2.4579492	1.3184889	1.2806754
C	1.9116699	1.7048963	0.0597046
C	0.7536756	2.5489621	0.0473788
C	0.1968016	2.9551232	1.2563735
C	0.7332506	2.5558126	2.4764584
H	3.3203035	0.6211974	-1.1701645
H	3.3314103	0.6736368	1.2900082
C	2.4474696	1.2652814	-1.1809809
C	0.1904830	2.9178619	-1.2044241
H	-0.6896927	3.5815793	1.2473739
C	0.7301653	2.4740526	-2.3725289
C	1.8733165	1.6338615	-2.3609459
H	-0.6871335	3.5555061	-1.2096646
H	0.2855645	2.7561640	-3.3197476
H	2.2906197	1.2879326	-3.2995655

C	0.1439645	2.9250017	3.7170156
C	2.4251239	1.3066123	3.7429436
C	1.8317213	1.6829744	4.9111531
H	2.2436956	1.3575836	5.8594413
C	0.6734512	2.5006951	4.8974160
H	0.2097515	2.7841499	5.8349947
H	3.3093047	0.6781235	3.7512295
H	-0.7412019	3.5520832	3.7032061
Ag	0.2275004	-1.1747722	3.9759436
Ag	-1.8578822	0.2168007	2.9052522
Ag	-0.0621292	-1.1674311	1.2830153
Ag	-2.0946076	0.3444342	0.1402691
Ag	-0.2201955	-0.8892248	-1.4074301

16

C	-0.0000002	-1.3887966	-1.4341266
C	1.2027685	-0.6944477	-1.4340933
C	1.2027684	0.6944476	-1.4340933
C	-0.0000001	1.3887967	-1.4341266
C	-1.2027682	0.6944473	-1.4340933
C	-1.2027681	-0.6944473	-1.4340933
H	0.0000000	-2.4726882	-1.4296144
H	2.1414545	-1.2364313	-1.4296863
H	2.1414545	1.2364313	-1.4296863
H	-0.0000000	2.4726882	-1.4296144
H	-2.1414547	1.2364314	-1.4296863
H	-2.1414547	-1.2364313	-1.4296863
Au	0.0000000	0.0000000	1.7701304

17

C	-0.0000000	-1.3906371	0.4656009
C	1.2006660	-0.6959073	0.4596149
C	1.2006660	0.6959073	0.4596149
C	-0.0000000	1.3906371	0.4656009
C	-1.2006660	0.6959073	0.4596149
C	-1.2006660	-0.6959073	0.4596149
H	-0.0000000	-2.4741534	0.4633498

H	2.1400827	-1.2368232	0.4632815
H	2.1400827	1.2368232	0.4632815
H	-0.0000000	2.4741534	0.4633498
H	-2.1400827	1.2368232	0.4632815
H	-2.1400827	-1.2368232	0.4632815
Au	1.2697973	0.0000000	-2.7747435
Au	-1.2697973	0.0000000	-2.7747435

18

C	-3.1099500	1.2008503	-0.6615261
C	-3.2312850	0.0000599	-1.3474654
C	-3.1108387	-1.2005227	-0.6613286
C	-2.9019375	-1.1999362	0.7182462
C	-2.8110200	0.0001347	1.4085971
C	-2.9012888	1.2002933	0.7181628
H	-3.2039029	2.1411589	-1.1925177
H	-3.3960112	0.0000200	-2.4181385
H	-3.2043466	-2.1408523	-1.1923122
H	-2.8266517	-2.1391791	1.2539741
H	-2.6403991	0.0001472	2.4778916
H	-2.8263356	2.1395458	1.2539690
Au	-0.0296007	1.2992585	-0.3763343
Au	-0.0235579	-1.3028072	-0.3813546
Au	0.8997061	0.0018290	1.8724735

19

C	1.3840906	0.1000569	2.8843243
C	0.7747531	-1.1517235	2.8847712
C	-0.6087134	-1.2502798	2.8904861
C	-1.3844793	-0.1004052	2.8845415
C	-0.7751491	1.1513648	2.8847794
C	0.6083042	1.2499324	2.8902798
H	2.4653929	0.1766409	2.8840061
H	1.3814215	-2.0499679	2.8841149
H	-1.0829246	-2.2240613	2.8753660
H	-2.4657812	-0.1769303	2.8843334
H	-1.3818260	2.0495975	2.8841171

H	1.0824551	2.2237417	2.8750341
Au	-1.1895208	0.5632132	-0.3756138
Au	-1.0061467	-2.1299374	-0.5935419
Au	1.1894057	-0.5622050	-0.3749302
Au	1.0061307	2.1310556	-0.5934694

20

Au	0.5234914	1.2803828	-1.2681470
Au	0.5666845	1.1788998	1.4333524
Au	0.5517361	-1.2284723	2.6212051
Au	0.4508235	-1.2033206	-0.0072854
Au	0.3496980	-1.0265586	-2.6299381
C	-2.6973515	1.7196244	1.1581527
C	-2.6096865	2.3587051	-0.0728767
C	-2.7270918	1.6246153	-1.2456688
C	-2.9377446	0.2535612	-1.1861371
C	-3.0263540	-0.3841134	0.0430986
C	-2.9037602	0.3486995	1.2161204
H	-2.5961142	2.2986864	2.0689514
H	-2.4406658	3.4287075	-0.1085308
H	-2.6310141	2.1174613	-2.2065224
H	-3.0143811	-0.3219592	-2.1010017
H	-3.1955228	-1.4535942	0.0878810
H	-2.9562127	-0.1521658	2.1755457

21

C	-0.9312582	2.5425428	-0.7043590
C	-1.0858858	1.3728586	-1.3953406
C	-1.2508914	0.1452930	-0.7129412
C	-1.2508904	0.1452966	0.7129431
C	-1.0858852	1.3728568	1.3953377
C	-0.9312574	2.5425483	0.7043625
H	-1.4194067	-1.0781454	-2.4801387
H	-0.8036803	3.4760796	-1.2399033
H	-1.0826377	1.3690283	-2.4800705
C	-1.4233506	-1.0810996	-1.3953991
C	-1.4233510	-1.0811029	1.3954043

H	-1.0826373	1.3690315	2.4800765
H	-0.8036803	3.4760797	1.2398985
C	-1.5898546	-2.2490874	0.7044237
C	-1.5898551	-2.2490907	-0.7044293
H	-1.4194076	-1.0781476	2.4801333
H	-1.7200835	-3.1823426	1.2398633
H	-1.7200835	-3.1823418	-1.2398614
Au	1.7704602	-0.2206828	0.0000002

22

C	-0.2369464	3.0931684	-0.7048737
C	0.5457544	2.2078060	-1.3946665
C	1.3609439	1.2786970	-0.7110816
C	1.3609481	1.2786888	0.7111015
C	0.5457579	2.2078025	1.3946460
C	-0.2369595	3.0931796	0.7048874
H	2.1415085	0.3243932	-2.4793488
H	-0.8617565	3.7980539	-1.2412336
H	0.5405716	2.1991146	-2.4793669
C	2.1481018	0.3262629	-1.3947443
C	2.1480980	0.3262684	1.3947069
H	0.5405706	2.1991143	2.4793721
H	-0.8617494	3.7980444	1.2412271
C	2.8937043	-0.5913596	0.7051239
C	2.8937072	-0.5913618	-0.7051118
H	2.1415088	0.3243931	2.4793637
H	3.4891400	-1.3211859	1.2413291
H	3.4891394	-1.3211865	-1.2413320
Au	-1.9443370	-0.0229632	-0.0000006
Au	-0.2361270	-1.8919227	0.0000018

23

C	-0.9220599	2.5387727	-0.7525261
C	-1.0310148	1.3609531	-1.4390488
C	-1.2267276	0.1383901	-0.7557485
C	-1.3069731	0.1494021	0.6626538
C	-1.1945878	1.3821231	1.3435817

C	-1.0053722	2.5506660	0.6529680
C	-1.3630008	-1.0920223	-1.4387095
C	-1.5257381	-1.0683576	1.3440489
C	-1.6547883	-2.2449050	0.6539655
C	-1.5719240	-2.2559485	-0.7517135
H	-0.7782128	3.4695712	-1.2882400
H	-0.9663042	1.3482976	-2.5221457
H	-1.2605234	1.3888133	2.4262764
H	-0.9216874	3.4895012	1.1876224
H	-1.2991130	-1.0972713	-2.5218436
H	-1.5927206	-1.0564214	2.4266349
H	-1.8251320	-3.1719145	1.1885737
H	-1.6829208	-3.1914935	-1.2871119
Au	-4.5154295	0.6260367	-1.4591644
Au	-4.3322283	2.0814487	0.7049884
Au	-4.7641317	-0.9248138	0.6371661

24

C	-2.4186597	-0.7042010	2.2758212
C	-1.2374023	-1.3940284	2.2757479
C	-0.0000011	-0.7114212	2.2770318
C	0.0000127	0.7114229	2.2770285
C	-1.2374079	1.3940170	2.2757267
C	-2.4186871	0.7042106	2.2758158
H	1.2351801	-2.4789840	2.2743282
H	-3.3605624	-1.2399119	2.2704573
H	-1.2351763	-2.4789692	2.2743263
C	1.2373821	-1.3940314	2.2757225
C	1.2373838	1.3940285	2.2757272
H	-1.2351839	2.4789770	2.2743337
H	-3.3605580	1.2399088	2.2704586
C	2.4186628	0.7041852	2.2758239
C	2.4186799	-0.7041888	2.2758251
H	1.2351881	2.4789860	2.2743282
H	3.3605767	1.2399222	2.2704565
H	3.3605697	-1.2399200	2.2704577
Au	0.0000246	1.3130626	-1.0881333

Au	0.0000245	-1.3130715	-1.0881413
Au	2.3648241	0.0000010	-1.1338554
Au	-2.3648705	0.0000057	-1.1338385

25

C	1.8220311	1.7030249	2.4181800
C	2.3744827	1.2943975	1.2357364
C	1.8392927	1.7196041	0.0000070
C	0.7137732	2.5881657	-0.0000028
C	0.1576814	2.9869353	1.2370493
C	0.7011866	2.5550627	2.4208438
H	3.2270798	0.6239204	-1.2310959
H	2.2366289	1.3609053	3.3586742
H	3.2270713	0.6239271	1.2310875
C	2.3744742	1.2944041	-1.2357391
C	0.1576665	2.9869382	-1.2370449
H	-0.7024954	3.6478552	1.2356471
H	0.2665138	2.8686900	3.3626700
C	0.7011903	2.5550600	-2.4208288
C	1.8220431	1.7030188	-2.4181921
H	-0.7024877	3.6478550	-1.2356548
H	0.2665088	2.8686882	-3.3626709
H	2.2366239	1.3609061	-3.3586616
Au	0.0461355	-1.4924806	2.6272610
Au	-1.4434652	0.3657727	1.3604532
Au	-1.4434618	0.3657732	-1.3604582
Au	0.0461385	-1.4924829	-2.6272604
Au	0.0918834	-1.5158834	0.0000003

26

Au	1.4319554	1.0892426	4.0395233
C	-1.5251549	-1.4167430	0.8623180
C	-0.1645122	-1.4171505	0.8653394
C	0.5652350	-0.1972884	0.8627898
C	-0.1615873	1.0396058	0.8560193
C	-1.5823937	0.9951622	0.8547307
C	-2.2438581	-0.1939341	0.8576668

C	1.9576826	-0.1657409	0.8732764
C	0.5430720	2.2407555	0.8581369
C	1.9356325	2.2730204	0.8601764
C	2.6631407	1.0358302	0.8680860
C	4.0839212	1.0803357	0.8764672
H	4.6312574	0.1438826	0.8847391
C	4.7450768	2.2695136	0.8765501
C	4.0263526	3.4922709	0.8692863
C	2.6657559	3.4928717	0.8618651
H	2.5077485	-1.1017201	0.8846919
H	-2.0691781	-2.3542928	0.8644969
H	0.3874787	-2.3511676	0.8717201
H	-2.1298292	1.9316594	0.8532724
H	-3.3275747	-0.2132938	0.8571689
H	-0.0069826	3.1768609	0.8594247
H	5.8287345	2.2889161	0.8833065
H	4.5703573	4.4297535	0.8707441
H	2.1138807	4.4268604	0.8587609

27

Au	-0.0870753	-0.0504750	-1.0552309
Au	-2.2274371	-1.4038586	-0.9946236
C	-3.7133712	-3.3998182	-4.2315807
C	-2.3530409	-3.4003123	-4.2716981
C	-1.6227474	-2.1808780	-4.3211532
C	-2.3497670	-0.9440427	-4.3382277
C	-3.7710828	-0.9882036	-4.2988241
C	-4.4323569	-2.1768112	-4.2438299
C	-0.2321213	-2.1509553	-4.3229908
C	-1.6476337	0.2563116	-4.3558751
C	-0.2568810	0.2865123	-4.3313573
C	0.4707559	-0.9504407	-4.3175345
C	1.8911857	-0.9051531	-4.2676494
H	2.4381541	-1.8417957	-4.2558080
C	2.5522947	0.2836828	-4.2231926
C	1.8334716	1.5065820	-4.2303111
C	0.4731726	1.5070677	-4.2857795

H	0.3175698	-3.0867563	-4.3009518
H	-4.2566248	-4.3367136	-4.1868861
H	-1.8007216	-4.3339942	-4.2566754
H	-4.3178630	-0.0515108	-4.3050005
H	-5.5155016	-2.1952056	-4.2084165
H	-2.1975509	1.1921797	-4.3502480
H	3.6350214	0.3025577	-4.1784010
H	2.3761915	2.4440972	-4.1914637
H	-0.0793432	2.4406888	-4.2897153

28

Au	-2.3750554	1.5691370	1.2923776
Au	-2.3734323	1.5671709	-1.2917506
Au	-3.4191229	-0.6437386	-0.0008286
C	0.0125053	-0.7376709	-3.6315249
C	-0.1876411	-1.3994644	-2.4592520
C	0.1338533	-0.7938783	-1.2144376
C	0.6896447	0.5293750	-1.2140653
C	0.8889800	1.1843399	-2.4626817
C	0.5563721	0.5725566	-3.6333098
C	-0.1173755	-1.4254050	0.0000492
C	0.9735743	1.1478367	0.0000045
C	0.6898324	0.5293779	1.2140494
C	0.1338437	-0.7938303	1.2144600
C	-0.1876813	-1.3993348	2.4593293
H	-0.6167429	-2.3952810	2.4536127
C	0.0127244	-0.7375776	3.6315683
C	0.5568909	0.5725405	3.6332923
C	0.8894479	1.1842695	2.4626302
H	-0.5509606	-2.4199368	0.0000586
H	-0.2491188	-1.2069074	-4.5726875
H	-0.6165751	-2.3954722	-2.4534880
H	1.3064924	2.1855087	-2.4609918
H	0.7058026	1.0865439	-4.5758387
H	1.3790992	2.1546797	-0.0000292
H	-0.2488811	-1.2067458	4.5727618
H	0.7064729	1.0865086	4.5757932

H	1.3070508	2.1853981	2.4608985

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Au	2.7267092	0.0856678	-1.3143403
Au	2.7267092	0.0856678	1.3143403
Au	2.7975502	2.4549880	0.0000000
Au	2.9813085	-2.2707442	0.0000000
C	-0.5937120	3.6201280	-0.7091118
C	-0.5655089	2.4472543	-1.3987627
C	-0.5302255	1.2025385	-0.7157862
C	-0.5302255	1.2025385	0.7157862
C	-0.5655089	2.4472543	1.3987627
C	-0.5937120	3.6201280	0.7091118
C	-0.4710889	-0.0148422	-1.3942270
C	-0.4710889	-0.0148422	1.3942270
C	-0.4396966	-1.2332527	0.7157436
C	-0.4396966	-1.2332527	-0.7157436
C	-0.3853344	-2.4773877	-1.3985283
H	-0.3759290	-2.4741081	-2.4830921
C	-0.3301885	-3.6494148	-0.7090751
C	-0.3301885	-3.6494148	0.7090751
C	-0.3853344	-2.4773877	1.3985283
H	-0.4774216	-0.0152006	-2.4803057
H	-0.6113774	4.5637101	-1.2418220
H	-0.5554403	2.4446640	-2.4833718
H	-0.5554403	2.4446640	2.4833718
H	-0.6113774	4.5637101	1.2418220
H	-0.4774216	-0.0152006	2.4803057
H	-0.2802155	-4.5918783	-1.2417744
H	-0.2802155	-4.5918783	1.2417744
H	-0.3759290	-2.4741081	2.4830921

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C	1.8939870	1.7159348	2.4894250
C	2.4531734	1.3121119	1.2803863
C	1.9085941	1.7013931	0.0591490
C	0.7499891	2.5442332	0.0471901

C	0.1931203	2.9499745	1.2565494
C	0.7293315	2.5502184	2.4765380
H	3.3139317	0.6131719	-1.1701669
H	3.3244423	0.6644255	1.2896175
C	2.4420999	1.2584983	-1.1811422
C	0.1834079	2.9090712	-1.2045608
H	-0.6967597	3.5714432	1.2475837
C	0.7217013	2.4634175	-2.3725632
C	1.8652639	1.6239211	-2.3612681
H	-0.6958985	3.5441524	-1.2094548
H	0.2749999	2.7424384	-3.3196785
H	2.2816516	1.2763206	-3.2996064
Au	0.2308332	-1.1171761	3.9077348
Au	-1.8308604	0.2558121	2.8660586
Au	-2.0571553	0.3778348	0.1736597
Au	-0.2082950	-0.8562155	-1.3311859
Au	0.0289534	-1.0963579	1.2815150
C	0.1374856	2.9155492	3.7175616
C	2.4163668	1.2940119	3.7423345
C	1.8217350	1.6687433	4.9115261
H	2.2325009	1.3401169	5.8591145
C	0.6655678	2.4888361	4.8979687
H	0.2011713	2.7713125	5.8353902
H	3.2984611	0.6628248	3.7503039
H	-0.7473451	3.5428434	3.7038737