Supplementary Material

Catalytic oxidation of benzyl alcohol to benzaldehyde on Au_8 and Au_6Pd_2 clusters: A DFT study on the reaction mechanism

Jitlada Kodchasee[1], Chanon Chanloi[1], Pongtanawat Khemthong[2], Boontida Uapipatanakul[1], Masahiro Ehara[3,4*] Karan Bobuatong[1*]

[1] Department of Chemistry, Faculty of Science and Technology, Rajamangala University of Technology Thanyaburi, Pathum Thani 12110, Thailand
[2] National Nanotechnology Center (NANOTEC), National Science and Technology, Development Agency, 111 Thailand Science Park, Paholyothin Rd., Pathum thani 12120, Thailand
[3] Institute for Molecular Science and Research Center for Computational Science, 38 Nishigo-Naka, Myodaiji, Okazaki 444-8585, Japan
[4] Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto Daigaku-Katsura, Kyoto 615-8510, Japan

Structures of Au_8 and Au_6Pd_2

To validate the reliability of the present computational method, we first performed geometry optimization for various two-dimensional (2D) and three-dimensional (3D) Au_8 isomers. The optimized structures of Au_8 isomers are shown in Figure S1, and the relative energies are compiled in Table S1. Comparing the relative stability among Au_8 isomers, the 2D structure with D_{4h} symmetry is the lowest energy structure, which is separated by 3.8 kcal/mol from the next lowest 3D C_s isomer. This planar structure agrees with the guideline for the study on the dimensionality of the gold clusters; neutral gold clusters (Au_n) have a planar structure for $n \leq 8$, whereas the crossover from planar to nonplanar structures occurs at clusters larger than Au_8.[75-78] The calculated average nearest-neighbor bond length of gold atoms is 2.80 Å, which also agree well with previous experimental (2.79 Å)[79] and theoretical studies (2.69-2.77 Å).[80-82]

The Mulliken charges presented in Figure 1a indicates that the charge distribution is not uniform over all the atoms of Au_8. The high electron densities appear at the apex sites where the gold atoms are less coordinated; meanwhile, the highly coordinated gold atoms have a lower electron density. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the planar D_{4h} cluster, which are depicted in Figure 1b reveals that HOMO is localized at low-coordinated gold atoms. This also agrees well with the report of Metiu and co-workers[83] where the valence electrons of gold cluster are not delocalized over the entire cluster but localized at the apex, corner and step. Although it was reported that the complete basis set limit (CBS) beyond the MP2 and CCSD(T) level of theory is required for predicting the dimensionality of Au8 cluster,[75] the practical choice of DFT calculations with moderate basis sets which reproduce the results of wavefunction theories is useful for simulating the catalytic reactions of gold clusters. Accordingly, the hybrid meta-GGA functional, M06 functional employed in this study provides a similar trend of energetics and electronic properties compared to previous theoretical studies. Based on the present results together with the previous studies,[58-65] it is reasonable to adopt the present computational method for further calculations of the aerobic oxidation of benzyl alcohol.

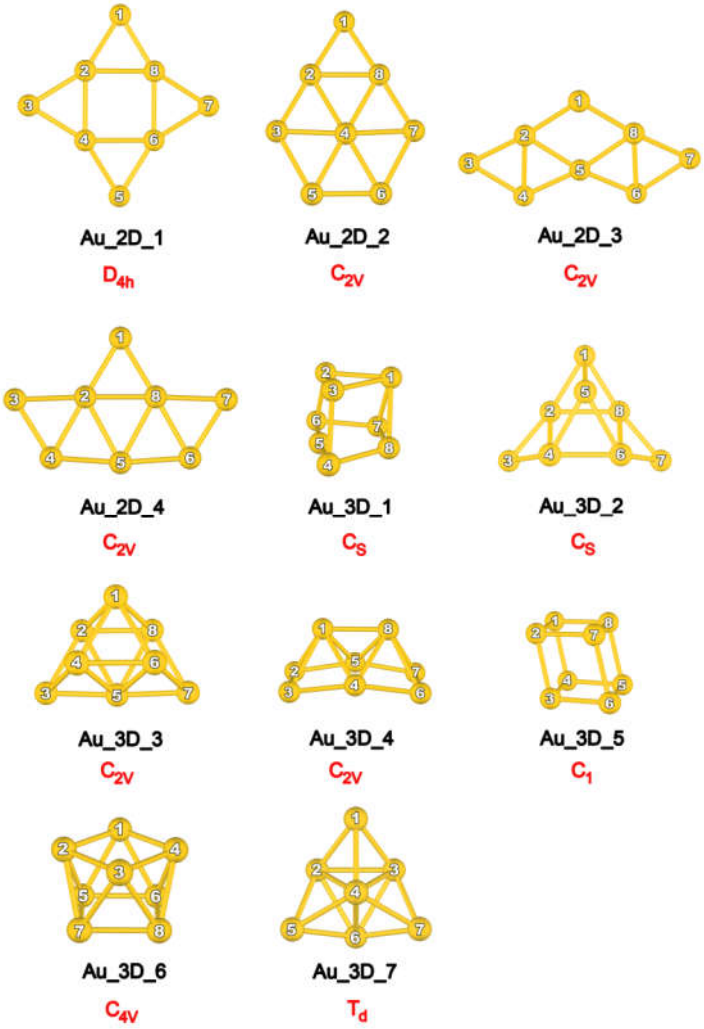


Figure S1. Optimized structures of two-dimensional (2D) and three-dimensional (3D) Au_8 isomers.

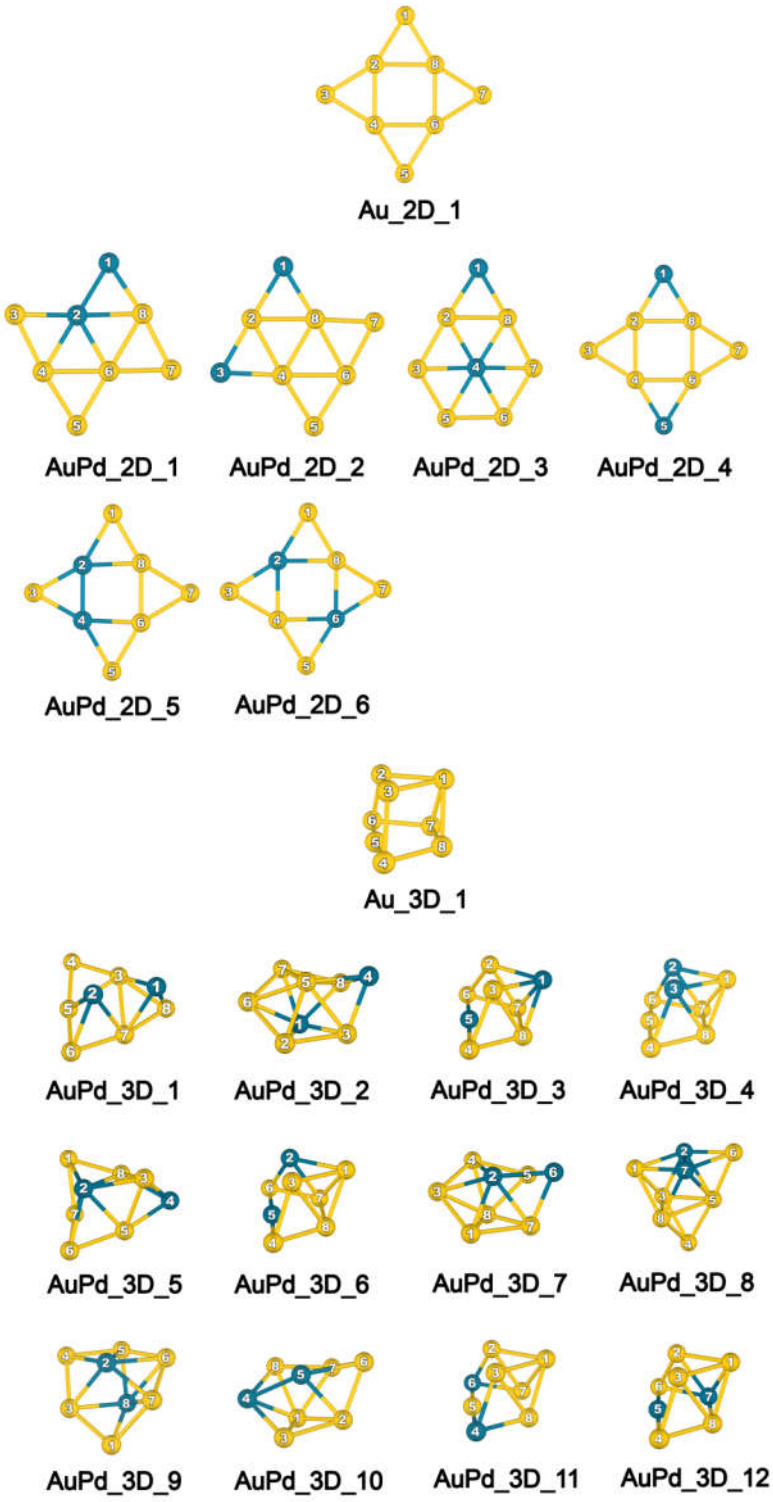


Figure S2. Planar (Au_2D_1) and 3-dimensional (Au_3D_1) of the lowest-energy isomers of Au_8 and their possible Au_6Pd_2 isomers.

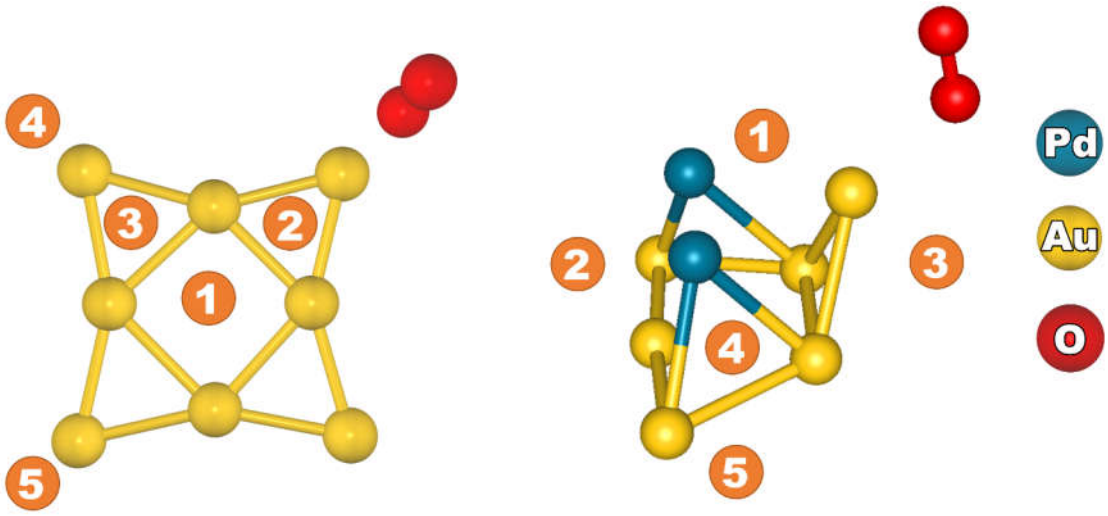


Figure S3. Initial positions of benzyl alcohol, intermeadtes and products on Au_8 and Au_6Pd_2 for the structural optimization.

Figure S4. Optimized structures for the complexes between benzyl alcohol and O_2 on Au_8 and Au_6Pd_2 clusters . The values in parenthesises denote the relative adsorption energy of the different complex geometries in kcal/mol.

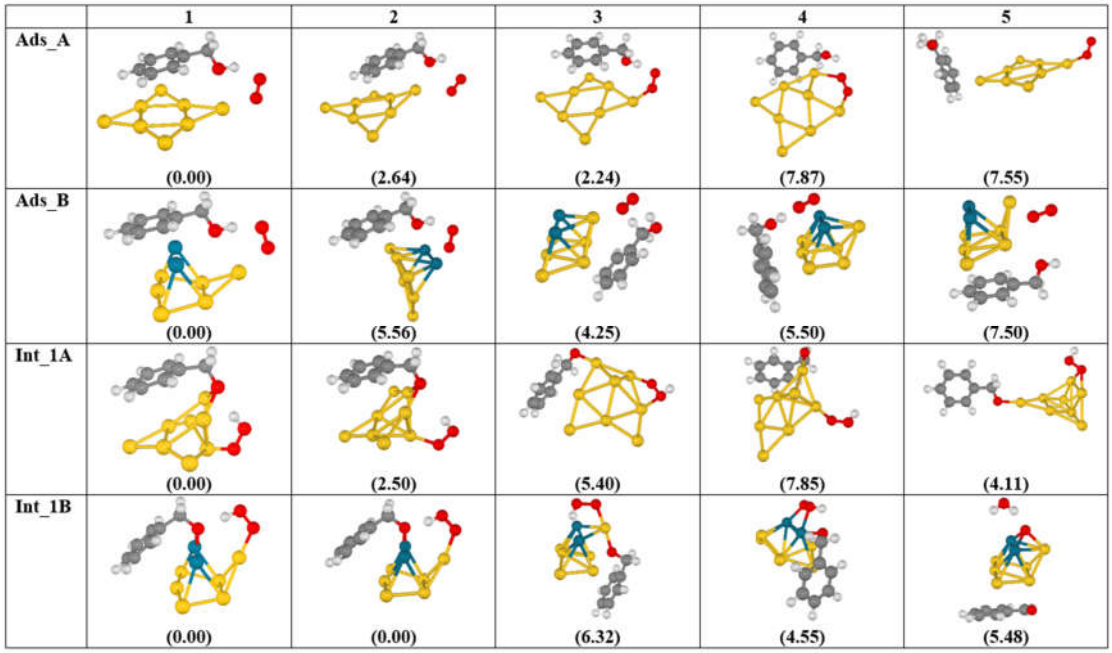


Figure S5. Optimized structures for the complexes between benzyl alcohol and O_2 on Au_8 and Au_6Pd_2 clusters . The values in parenthesises denote the relative adsorption energy of the different complex geometries in kcal/mol (Cond't).

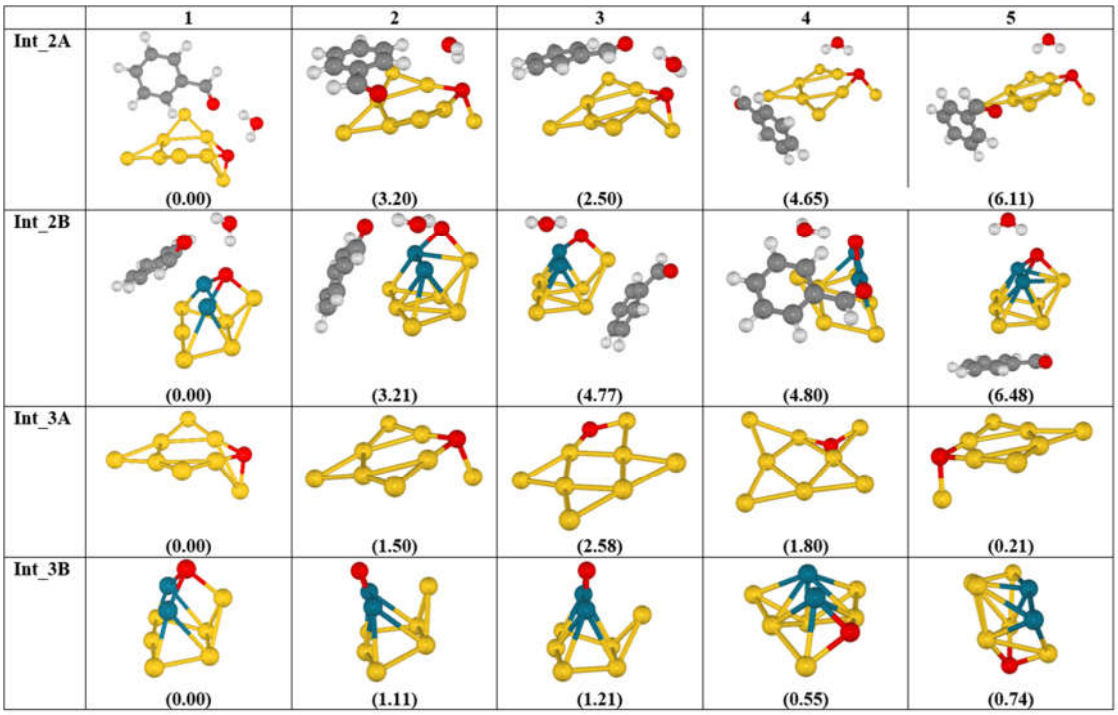


Figure S6. Optimized structures for the complexes between benzyl alcohol and O_2 on Au_8 and Au_6Pd_2 clusters . The values in parenthesises denote the relative adsorption energy of the different complex geometries in kcal/mol (Cond't).

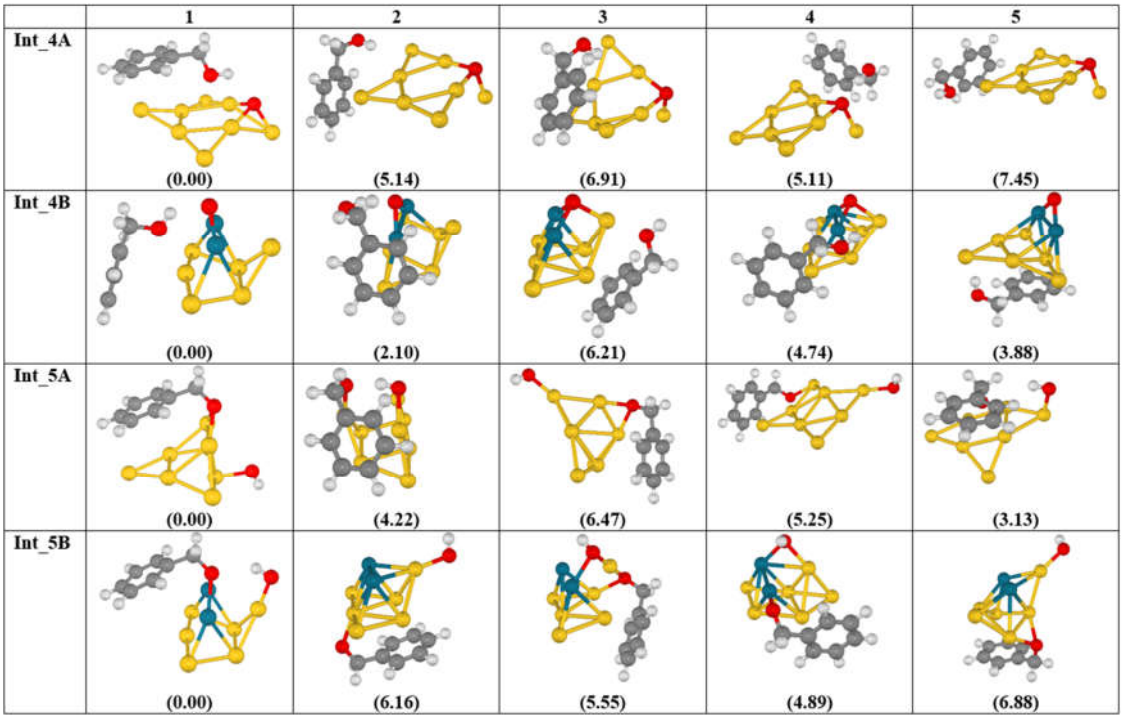


Figure S7. Optimized structures for the complexes between benzyl alcohol and O_2 on Au_8 and Au_6Pd_2 clusters . The values in parenthesises denote the relative adsorption energy of the different complex geometries in kcal/mol (Cond't).

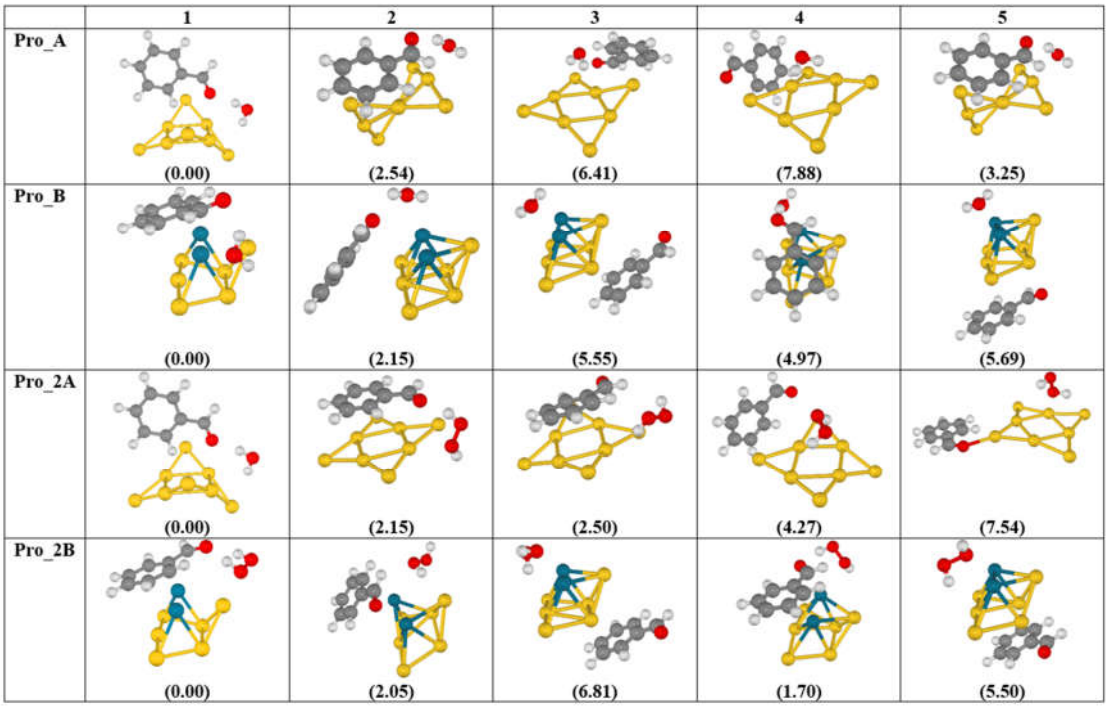


Table S1. The relative energy of the 2D and 3D Au_8 isomers. All values are shown in kcal/mol.

Structure	Energy
Au_2D_1	0.0
Au_2D_2	12.3
Au_2D_3	31.0
Au_2D_4	18.9
Au_3D_1	3.8
Au_3D_2	14.4
Au_3D_3	20.1
Au_3D_4	12.8
Au_3D_5	26.3
Au_3D_6	15.3
Au_3D_7	7.4

Table S2. The relative energy of 2-dimensional (2D) and 3-dimensional (3D) Au_6Pd_2 isomers. All values are shown in kcal/mol.

Structure	Energy
AuPd_2D_1	2.85
AuPd_2D_2	27.04
AuPd_2D_3	33.10
AuPd_2D_4	40.91
AuPd_2D_5	55.92
AuPd_2D_6	8.00
AuPd_3D_1	7.84
AuPd_3D_2	3.62
AuPd_3D_3	15.39
AuPd_3D_4	0.00
AuPd_3D_5	4.05
AuPd_3D_6	5.55
AuPd_3D_7	7.48
AuPd_3D_8	9.76
AuPd_3D_9	12.99
AuPd_3D_10	5.36
AuPd_3D_11	24.26
AuPd_3D_12	6.36

Table S3. Selected interatomic distances (Å) and partial charges (Mulliken charge on atom) of adsorption complex for the molecular O_2 over Au_8 and Au_6Pd_2.

	O_2	Au_8	Au_6Pd_2	Au_8O_2	$Au_6Pd_2O_2$
$R_{O1\text{-}Au}$	–	–	–	2.38	2.39
$R_{O1\text{-}O2}$	1.20	–	–	1.29	1.30
∠OOAu	–	–	–	114.7	121.4
Mulliken charge					
q_{Au}	–	-0.094	-0.145	-0.081	-0.068
q_{O1}	0.00	–	–	-0.181	-0.213
q_{O2}	0.00	–	–	-0.205	-0.239
NBO					
q_{Au}	–	0.155	0.081	0.131	0.135
q_{O1}	0.00	–	–	-0.263	-0.254
q_{O2}	0.00	–	–	-0.160	-0.158

Table S4. Selected interatomic distances (Å) and partial charges (Mulliken charge on atom) of adsorption complex, intermediates, transition states, and products for the aerobic oxidation of benzyl alcohol over Au_8 and Au_6Pd_2 generating benzaldehyde and H_2O.

	Adsorption		1st TS		Int_1		2nd TS	
	Ads_A	Ads_B	TS_1A	TS_1B	Int_1A	Int_1B	TS_2A	TS_2B
$R_{O1\text{-}H1}$	0.98	0.99	1.08	1.32	2.36	1.80	3.48	4.12
$R_{O2\text{-}H1}$	1.85	1.72	1.38	1.10	0.98	0.99	0.98	0.94
$R_{O2\text{-}O3}$	1.29	1.30	1.31	1.34	1.44	1.37	1.43	1.47
$R_{O3\text{-}Au}$	2.23	2.23	2.15	2.12	2.08	2.10	2.16	2.09
$R_{O2\text{-}H2}$	4.12	3.74	3.10	2.83	5.11	3.75	1.28	1.35
$R_{O3\text{-}H2}$	4.93	4.73	4.22	4.05	6.07	4.79	2.14	2.41
$R_{C\text{-}O1}$	1.40	1.40	1.41	1.40	1.42	1.41	1.31	1.37
Mulliken charge								
q_{Au}	-0.079	-0.065	0.081	0.008	0.103	-0.049	0.039	-0.035
q_{O1}	-0.529	-0.524	-0.581	-0.592	-0.578	-0.580	-0.494	-0.593
q_{O2}	-0.239	-0.266	-0.338	-0.295	-0.349	-0.283	-0.280	-0.414
q_{O3}	-0.219	-0.234	-0.256	-0.274	-0.384	-0.311	-0.353	-0.321
q_{H1}	0.357	0.380	0.473	0.490	0.390	0.407	0.405	0.412
q_{H2}	0.077	0.094	0.146	0.125	0.136	0.143	0.347	0.145
q_{Pd1}	–	0.101	–	0.174	–	0.202	–	0.207
q_{Pd2}	–	0.101	–	0.039	–	0.202	–	0.207
NBO								
q_{Au}	0.082	0.014	-0.098	-0.005	-0.101	0.034	-0.038	0.041
q_{O1}	-0.352	-0.359	-0.379	-0.604	-0.548	-0.577	-0.456	-0.593
q_{O2}	-0.150	-0.145	-0.361	-0.318	-0.269	-0.351	-0.278	-0.414
q_{O3}	-0.258	-0.221	-0.244	-0.298	-0.374	-0.308	-0.326	-0.321
q_{H1}	0.536	0.640	0.439	0.548	0.352	0.406	0.498	0.413
q_{H2}	0.079	0.077	0.151	0.158	0.199	0.144	0.344	0.141
q_{Pd1}	–	-0.015	–	-0.168	–	-0.054	–	-0.098
q_{Pd2}	–	-0.015	–	-0.024	–	-0.054	–	-0.098

Table S5. Selected interatomic distances (Å) and partial charges (Mulliken charge on atom) of adsorption complex, intermediates, transition states, and products for the aerobic oxidation of benzyl alcohol over Au_8 and Au_6Pd_2 generating benzaldehyde and H_2O (cond't).

	Int_2		Int_3		Int_4		3rd TS	
	Int_2A	Int_2B	Int_3A	Int_3A	Int_4A	Int_4B	TS_3A	TS_3B
$R_{O1\text{-}H1}$	3.17	2.19	–	–	0.97	0.99	1.18	1.10
$R_{O2\text{-}H1}$	0.97	0.96	–	–	–	–	–	–
$R_{O2\text{-}O3}$	2.76	2.78	–	–	–	–	–	–
$R_{O3\text{-}Au}$	2.04	2.10	–	–	2.05	3.19	2.04	1.94
$R_{O2\text{-}H2}$	0.97	0.97	–	–	–	–	–	–
$R_{O3\text{-}H2}$	1.87	1.86	–	–	4.59	3.33	3.70	3.78
$R_{C\text{-}O1}$	1.22	1.23	–	–	1.41	1.38	1.40	1.42
Mulliken charge								
q_{Au}	0.247	0.112	0.226	0.070	0.196	0.195	0.197	0.112
q_{O1}	-0.398	-0.408	–	–	-0.506	-0.580	-0.502	-0.570
q_{O2}	-0.651	-0.682	–	–	–	–	–	–
q_{O3}	-0.654	-0.586	-0.502	-0.545	-0.612	-0.663	-0.610	-0.652
q_{H1}	0.372	0.347	–	–	0.372	0.396	0.320	0.490
q_{H2}	0.343	0.378	–	–	0.112	0.126	0.111	0.224
q_{Pd1}	–	0.138	–	0.277	–	0.279	–	0.266
q_{Pd2}	–	0.175	–	0.277	–	0.279	–	0.093
NBO								
q_{Au}	-0.273	-0.110	-0.378	-0.072	-0.273	-0.110	-0.181	-0.112
q_{O1}	-0.366	-0.411	–	–	-0.366	-0.411	-0.503	-0.554
q_{O2}	-0.687	-0.669	–	–	–	–	–	–
q_{O3}	-0.645	-0.524	-0.506	-0.577	-0.645	-0.524	-0.680	-0.694
q_{H1}	0.371	0.356	–	–	0.371	0.356	0.310	0.488
q_{H2}	0.342	0.387	–	–	0.342	0.387	0.111	0.225
q_{Pd1}	–	-0.088	–	-0.114	–	-0.011	–	-0.087
q_{Pd2}	–	-0.011	–	-0.114	–	-0.011	–	-0.010

Table S6. Selected interatomic distances (Å) and partial charges (Mulliken charge on atom) of adsorption complex, intermediates, transition states, and products for the aerobic oxidation of benzyl alcohol over Au_8 and Au_6Pd_2 generating benzaldehyde and H_2O (Cond't).

	Int_5		4rd TS		Product	
	Int_5A	Int_5B	TS_4A	TS_4B	Pro_A	Pro_B
$R_{O1\text{-}H1}$	5.20	2.36	4.08	4.43	3.17	2.06
$R_{O3\text{-}Au}$	2.07	2.03	2.13	2.07	3.65	3.67
$R_{O3\text{-}H2}$	6.16	4.54	1.39	2.15	0.97	0.96
$R_{C\text{-}O1}$	1.41	1.41	1.34	1.35	1.22	1.23
Mulliken charge						
q_{Au}	0.007	0.077	0.094	0.082	-0.088	-0.139
q_{O1}	-0.524	-0.573	-0.537	-0.560	-0.405	-0.461
q_{O3}	-0.609	-0.646	-0.612	-0.634	-0.641	-0.576
q_{H1}	0.320	0.340	0.346	0.328	0.356	0.364
q_{H2}	0.124	0.149	0.235	0.304	0.362	0.365
q_{Pd1}	–	0.281	–	0.257	–	0.097
q_{Pd2}	–	0.281	–	0.081	–	-0.023
NBO						
q_{Au}	-0.013	-0.077	-0.094	-0.082	0.088	0.139
q_{O1}	-0.514	-0.524	-0.547	-0.560	-0.405	-0.454
q_{O3}	-0.705	-0.682	-0.684	-0.634	-0.641	-0.558
q_{H1}	0.365	0.319	0.328	0.328	0.356	0.374
q_{H2}	0.115	0.137	0.239	0.304	0.362	0.334
q_{Pd1}	–	-0.072	–	-0.266	–	-0.091
q_{Pd2}	–	-0.072	–	-0.074	–	0.021

Table S7. Selected interatomic distances (Å) and partial charges (Mulliken charge on atom) of adsorption complex, intermediates, transition states, and products for the aerobic oxidation of benzyl alcohol over Au_8 and Au_6Pd_2 generating benzaldehyde and H_2O_2.

	Int_1		5th TS		Product	
	Int_1A	Int_1B	TS_5A	TS_5B	Pro_2A	Pro_2B
$R_{O1\text{-}H1}$	2.36	1.80	4.39	3.89	3.90	2.02
$R_{O2\text{-}H1}$	0.98	0.99	0.97	0.97	0.97	0.98
$R_{O2\text{-}O3}$	1.44	1.37	1.42	1.41	1.44	1.44
$R_{O3\text{-}Au}$	2.08	2.10	2.17	2.21	4.82	2.41
$R_{O2\text{-}H2}$	5.11	3.75	2.17	2.26	1.84	1.90
$R_{O3\text{-}H2}$	6.07	4.79	1.37	1.76	0.98	0.98
$R_{C\text{-}O1}$	1.42	1.41	1.33	1.34	1.22	1.23
Mulliken charge						
q_{Au}	0.103	-0.049	0.087	-0.005	-0.104	-0.048
q_{O1}	-0.578	-0.580	-0.538	-0.499	0.423	-0.513
q_{O2}	-0.283	-0.349	-0.300	-0.293	-0.296	-0.318
q_{O3}	-0.384	-0.311	-0.401	-0.352	-0.366	-0.310
q_{H1}	0.390	0.407	0.368	0.366	0.384	0.377
q_{H2}	0.136	0.143	0.311	0.243	0.393	0.388
q_{Pd1}	–	0.202	–	0.193	–	-0.007
q_{Pd2}	–	0.202	–	0.099	–	0.060
NBO						
q_{Au}	-0.101	0.034	-0.039	0.004	0.089	0.055
q_{O1}	-0.548	-0.577	-0.522	-0.432	0.454	-0.632
q_{O2}	-0.269	-0.351	-0.311	-0.301	-0.288	-0.211
q_{O3}	-0.374	-0.308	-0.402	-0.354	-0.364	-0.315
q_{H1}	0.352	0.406	0.377	0.397	0.393	0.324
q_{H2}	0.199	0.144	0.313	0.244	0.402	0.373
q_{Pd1}	–	-0.054	–	-0.161	–	0.002
q_{Pd2}	–	-0.054	–	-0.017	–	-0.030

Optimized Structures in Cartesian Coordinates of Reactants, Intermediates, Transition States and Products.

	Ads_A				TS_1A		
	X	Y	Z		X	Y	Z
Au	-0.5273	1.1507	1.3886	Au	-0.6410	-1.5359	1.3501
Au	-0.6198	3.5214	0.0000	Au	0.0737	-3.7201	-0.5160
Au	-0.5273	1.1507	-1.3886	Au	-0.0392	-1.1190	-1.5584
Au	-0.0923	-1.6693	1.4336	Au	0.3268	1.1541	1.3184
Au	-0.0290	-4.0089	0.0000	Au	-0.1771	3.4829	-0.0198
Au	-0.0923	-1.6693	-1.4336	Au	1.1403	1.5194	-1.3981
C	3.0678	-0.4328	-1.2055	C	-2.2010	-0.6758	-2.9979
C	3.2344	0.9485	-1.2012	C	-2.5892	-1.2575	-1.7768
C	3.3339	1.6507	0.0000	C	-3.1365	-0.4497	-0.7569
C	3.2344	0.9485	1.2012	C	-3.2706	0.9139	-0.9807
C	3.0678	-0.4328	1.2055	C	-2.8872	1.4882	-2.1949
C	2.9939	-1.1291	0.0000	C	-2.3455	0.7019	-3.2009
H	2.9839	-0.9681	-2.1502	H	-1.8522	-1.3148	-3.8071
H	3.2695	1.4976	-2.1427	H	-2.5951	-2.3469	-1.6596
H	3.2695	1.4976	2.1427	H	-3.6794	1.5442	-0.1911
H	2.9839	-0.9681	2.1502	H	-3.0002	2.5595	-2.3429
H	2.8619	-2.2100	0.0000	H	-2.0460	1.1448	-4.1470
C	3.4209	3.1511	0.0000	C	-3.6576	-1.0720	0.5104
H	3.9876	3.4849	0.8895	H	-3.8447	-0.2890	1.2568
H	3.9876	3.4849	-0.8895	H	-4.6271	-1.5520	0.2921
O	2.1121	3.6385	0.0000	O	-2.8144	-2.0415	1.0876
H	2.0332	4.6143	0.0000	H	-2.9019	-2.9580	0.5371
Au	-0.2040	-0.2657	3.7719	Au	1.7760	-0.9219	2.3554
Au	-0.2040	-0.2657	-3.7719	Au	2.5618	-0.6328	-2.2516

O	-0.3056	5.7332	0.0000	O	-1.7820	-4.6527	0.0368
O	0.9336	6.1015	0.0000	O	-2.8812	-4.0417	-0.3316

	Int_1A				**TS_2A**		
	X	Y	Z		X	Y	Z
Au	1.7418	1.2991	1.6148	Au	-0.5049	-1.5525	-1.0656
Au	-0.8313	1.5818	0.0000	Au	1.7041	-1.2912	1.7070
Au	1.7418	1.2991	-1.6148	Au	2.0468	0.2914	-0.7770
Au	-0.1707	-0.8736	1.4454	Au	-2.7164	0.0301	-0.2613
Au	-1.0069	-3.0395	0.0000	Au	-2.9074	2.6263	-1.2021
Au	-0.1707	-0.8736	-1.4454	Au	-0.4062	1.5209	-1.2199
C	3.2288	-2.2024	-1.2077	C	5.4065	-1.7790	-1.1362
C	3.7654	-0.9179	-1.2020	C	4.3009	-2.5964	-1.2104
C	4.0094	-0.2495	0.0000	C	3.1312	-2.1691	-1.8760
C	3.7654	-0.9179	1.2020	C	3.1025	-0.8568	-2.4530
C	3.2288	-2.2024	1.2077	C	4.2765	-0.0515	-2.3904
C	2.9428	-2.8402	0.0000	C	5.3985	-0.4978	-1.7205
H	3.0364	-2.7063	-2.1527	H	6.2977	-2.1253	-0.6187
H	3.9969	-0.4209	-2.1455	H	4.3087	-3.5779	-0.7371
H	3.9969	-0.4209	2.1455	H	2.3258	-0.6611	-3.1947
H	3.0364	-2.7063	2.1527	H	4.2777	0.9155	-2.8883
H	2.5215	-3.8429	0.0000	H	6.2827	0.1310	-1.6612
C	4.2980	1.2277	0.0000	C	1.9593	-3.0214	-1.9416
H	4.8791	1.5122	0.8925	H	2.1744	-4.0994	-2.1022
H	4.8791	1.5122	-0.8925	H	1.8153	-3.3837	-0.6327
O	3.0922	1.9804	0.0000	O	0.8422	-2.5748	-2.4679
Au	0.0900	0.7394	3.6627	Au	-1.1879	-1.2326	1.6545
Au	0.0900	0.7394	-3.6627	Au	0.6182	1.1987	1.4826

O	0.6129	4.1783	0.0000	O	1.6554	-3.9615	0.5002
O	-0.7287	3.6611	0.0000	O	2.4100	-3.3257	1.5391
H	1.2138	3.4104	0.0000	H	0.7193	-3.8581	0.7653

Int_2A

	X	Y	Z
Au	0.5808	-1.1898	1.4313
Au	0.5808	0.4847	3.6024
Au	-1.0357	1.1477	1.5673
Au	0.5808	-1.1898	-1.4313
Au	0.5808	0.4847	-3.6024
Au	-1.0357	1.1477	-1.5673
Au	1.4002	-3.3606	0.0000
Au	-3.7091	0.2523	0.0000
O	-2.3671	1.7824	0.0000
O	-1.7363	4.4683	0.0000
H	-2.2512	3.6474	0.0000
H	-0.8222	4.1541	0.0000
C	3.1855	2.5540	0.0000
C	2.9620	1.1732	0.0000
C	4.0366	0.2978	0.0000
C	5.3381	0.8023	0.0000
C	5.5673	2.1764	0.0000
C	4.4900	3.0533	0.0000
H	1.9335	0.8103	0.0000
H	3.8576	-0.7763	0.0000
H	6.1824	0.1166	0.0000
H	6.5845	2.5597	0.0000

Int_3A

	X	Y	Z
Au	-0.6309	1.1667	1.4257
Au	-0.6309	-0.2632	3.7617
Au	0.2701	-1.5278	1.5752
Au	-0.6309	1.1667	-1.4257
Au	-0.6309	-0.2632	-3.7617
Au	0.2701	-1.5278	-1.5752
Au	-1.0043	3.4547	0.0000
Au	2.8846	-1.9238	0.0000
O	1.0192	-2.7884	0.0000

H	4.6499	4.1313	0.0000
C	2.0529	3.4827	0.0000
H	2.3304	4.5612	0.0000
O	0.8823	3.1463	0.0000

Int_4A

	X	Y	Z
Au	0.3554	0.4671	1.4115
Au	0.9424	-0.8579	3.7537
Au	0.4759	-2.3850	1.6028
Au	0.3554	0.4671	-1.4115
Au	0.9424	-0.8579	-3.7537
Au	0.4759	-2.3850	-1.6028
C	-3.4513	2.2882	-1.2109
C	-3.4736	0.8962	-1.2041
C	-3.4895	0.1911	0.0000
C	-3.4736	0.8962	1.2041
C	-3.4513	2.2882	1.2109
C	-3.4337	2.9916	0.0000
H	-3.4444	2.8305	-2.1535
H	-3.4622	0.3437	-2.1433
H	-3.4622	0.3437	2.1433
H	-3.4444	2.8305	2.1535
H	-3.4531	4.0799	0.0000
C	-3.4338	-1.3089	0.0000
H	-3.9557	-1.6969	0.8898
H	-3.9557	-1.6969	-0.8898
O	-2.0717	-1.6836	0.0000

TS_3A

	X	Y	Z
Au	0.8539	0.8639	1.4088
Au	1.3563	-0.8076	3.5498
Au	-0.2816	-1.7470	1.6287
Au	0.8539	0.8639	-1.4088
Au	1.3563	-0.8076	-3.5498
Au	-0.2816	-1.7470	-1.6287
C	-2.9943	2.8117	-1.2141
C	-3.2028	1.4352	-1.2045
C	-3.3099	0.7371	0.0000
C	-3.2028	1.4352	1.2045
C	-2.9943	2.8117	1.2141
C	-2.8775	3.5124	0.0000
H	-2.9238	3.3497	-2.1565
H	-3.2700	0.8866	-2.1436
H	-3.2700	0.8866	2.1436
H	-2.9238	3.3497	2.1565
H	-2.7870	4.5971	0.0000
C	-3.4244	-0.7620	0.0000
H	-3.9917	-1.0881	0.8890
H	-3.9917	-1.0881	-0.8890
O	-2.1377	-1.3108	0.0000

H	-1.9782	-2.6472	0.0000	H	-1.9299	-2.4713	0.0000
Au	-0.7147	2.5414	0.0000	Au	-0.4255	2.8205	0.0000
Au	1.9421	-4.5518	0.0000	Au	0.6296	-3.9651	0.0000
O	0.0341	-3.7890	0.0000	O	-1.3578	-3.5275	0.0000

	Pro_A				**TS_5A**		
	X	Y	Z		X	Y	Z
Au	1.1837	0.7437	1.4419	Au	1.5039	0.1146	1.8761
Au	-0.7895	0.6248	3.3293	Au	-0.2926	-2.1635	0.9476
Au	-0.7895	-1.3336	1.4349	Au	-1.4656	0.6199	0.9103
Au	1.1837	0.7437	-1.4419	Au	1.2791	1.6022	-0.4658
Au	-0.7895	0.6248	-3.3293	Au	0.8014	3.2287	-2.6090
Au	-0.7895	-1.3336	-1.4349	Au	-1.3634	1.8116	-1.6515
Au	3.3543	1.5478	0.0000	C	-4.0571	-0.0380	3.8083
Au	-0.3598	-3.6216	0.0000	C	-2.7919	-0.4822	4.1239
O	-3.7779	-2.3404	0.0000	C	-1.6547	0.2804	3.7872
H	-2.9005	-2.7413	0.0000	C	-1.8356	1.4795	3.0324
H	-3.6092	-1.3857	0.0000	C	-3.1580	1.9321	2.7536
C	-2.8312	2.8029	0.0000	C	-4.2493	1.1775	3.1258
C	-1.4319	2.8256	0.0000	H	-4.9221	-0.6296	4.0987
C	-0.7595	4.0383	0.0000	H	-2.6524	-1.4173	4.6654
C	-1.4848	5.2305	0.0000	H	-0.9903	2.1687	2.9904
C	-2.8781	5.2148	0.0000	H	-3.2890	2.8843	2.2451
C	-3.5518	4.0003	0.0000	H	-5.2550	1.5204	2.8995
H	-0.8895	1.8800	0.0000	C	-0.3150	-0.1771	4.1641
H	0.3286	4.0550	0.0000	H	-0.2582	-0.5959	5.1899
H	-0.9576	6.1819	0.0000	H	-0.3083	-1.3419	3.6397
H	-3.4341	6.1487	0.0000	O	0.7308	0.5728	3.8272

H	-4.6411	3.9691	0.0000	Au	1.8940	-1.1386	-0.5973
C	-3.5521	1.5299	0.0000	Au	-0.9883	-0.9642	-1.4113
H	-4.6617	1.6211	0.0000	O	0.9876	-3.0738	3.4504
O	-3.0241	0.4311	0.0000	O	-0.2987	-2.5958	3.0760
				H	0.7503	-3.8113	4.0319

	Pro_2A				**Ads_B**		
	X	Y	Z		X	Y	Z
Au	1.1988	0.6544	1.4407	Au	0.6634	-1.4216	1.4076
Au	-0.8434	0.7139	3.2676	Au	-1.6024	-0.3471	2.7712
Au	-0.8434	-1.3213	1.4503	Au	-1.7133	-0.0938	0.0000
Au	1.1988	0.6544	-1.4407	Au	-1.6024	-0.3471	-2.7712
Au	-0.8434	0.7139	-3.2676	Pd	0.2261	1.3713	1.5060
Au	-0.8434	-1.3213	-1.4503	Au	0.6634	-1.4216	-1.4076
Au	3.4055	1.3639	0.0000	Au	3.0437	-1.2700	0.0000
Au	-0.0157	-3.5055	0.0000	Pd	0.2261	1.3713	-1.5060
O	-4.4593	-1.6323	0.0000	C	-0.7650	3.8951	1.2091
H	-4.2541	-0.6726	0.0000	C	0.6056	3.5584	1.2195
C	-2.6464	3.1365	0.0000	C	1.3018	3.3874	0.0000
C	-1.2681	2.8932	0.0000	C	0.6056	3.5584	-1.2195
C	-0.3796	3.9578	0.0000	C	-0.7650	3.8951	-1.2091
C	-0.8674	5.2651	0.0000	C	-1.4415	4.0513	0.0000
C	-2.2389	5.5135	0.0000	H	-1.2796	4.0588	2.1528
C	-3.1294	4.4482	0.0000	H	1.1803	3.6080	2.1499
H	-0.9192	1.8607	0.0000	H	1.1803	3.6080	-2.1499
H	0.6922	3.7662	0.0000	H	-1.2796	4.0588	-2.1528
H	-0.1701	6.0998	0.0000	H	-2.5020	4.2921	0.0000
H	-2.6077	6.5358	0.0000	C	2.7687	3.0633	0.0000

H	-4.2051	4.6234	0.0000	H	3.2340	3.5271	-0.8900
C	-3.5889	2.0207	0.0000	H	3.2340	3.5271	0.8900
H	-4.6629	2.3165	0.0000	O	2.9155	1.6733	0.0000
O	-3.2692	0.8432	0.0000	H	3.8719	1.4033	0.0000
O	-3.0973	-2.0999	0.0000	O	5.3950	0.6074	0.0000
H	-3.2239	-3.0613	0.0000	O	5.1948	-0.6787	0.0000

	Int_1B				**TS_2B**		
	X	Y	Z		X	Y	Z
Au	1.2853	-0.4108	1.3986	Au	-0.8830	-1.0680	1.72067
Au	-1.1930	-0.8579	2.7452	Au	-1.2390	-3.0044	-0.36576
Au	-1.5069	-0.9505	0.0000	Au	0.9063	-1.3385	-0.90688
Au	-1.1930	-0.8579	-2.7452	Au	3.2898	0.1169	-0.72472
Pd	-0.8773	1.5456	1.3923	Au	1.4755	0.4821	1.40916
Au	1.2853	-0.4108	-1.3986	Au	-1.0884	1.6921	1.45799
Au	1.8587	1.9205	0.0000	C	-4.4797	1.9334	-1.69406
Pd	-0.8773	1.5456	-1.3923	C	-3.4562	2.8732	-1.78097
C	-4.5711	0.9538	1.2054	C	-2.1841	2.5075	-2.23532
C	-3.8072	2.1212	1.2049	C	-1.9650	1.1696	-2.65647
C	-3.4180	2.7104	0.0000	C	-3.0210	0.2309	-2.61634
C	-3.8072	2.1212	-1.2049	C	-4.2714	0.6160	-2.09461
C	-4.5711	0.9538	-1.2054	H	-5.4520	2.2314	-1.30568
C	-4.9473	0.3667	0.0000	H	-3.6230	3.8998	-1.45277
H	-4.8667	0.4998	2.1487	H	-1.0317	0.9375	-3.16926
H	-3.5125	2.5841	2.1485	H	-2.9056	-0.7395	-3.09783
H	-3.5125	2.5841	-2.1485	H	-5.0787	-0.1110	-2.04106
H	-4.8667	0.4998	-2.1487	C	-1.0897	3.4868	-2.28040
H	-5.5392	-0.5452	0.0000	H	-1.3900	4.4745	-2.69042

C	-2.3806	3.7906	0.0000	H	-0.9664	3.9474	-0.94736
H	-2.4736	4.4383	-0.8887	O	0.1463	3.1124	-2.49692
H	-2.4736	4.4383	0.8887	O	-0.4964	4.2716	0.11535
O	-1.1007	3.1944	0.0000	O	-1.3866	3.8695	1.18524
H	0.3358	4.2859	0.0000	Pd	0.8855	1.5229	-1.12596
O	1.1427	4.8586	0.0000	Pd	-1.7015	-0.1913	-0.79501
O	2.2119	3.9945	0.0000	H	0.2573	3.6315	0.14316

Int_2B

	X	Y	Z
Au	-2.2566	-0.8682	-0.0990
Au	-2.4757	1.7184	-1.2824
Au	0.1016	0.5744	-1.3912
Au	2.3420	-1.0804	-1.4357
Au	0.1257	-2.3793	-0.2291
Au	-0.6521	-1.2004	2.1743
C	4.6552	1.5644	-0.7183
C	3.7650	2.6356	-0.7580
C	2.9307	2.9076	0.3238
C	2.9873	2.1051	1.4910
C	3.8840	1.0190	1.5230
C	4.6961	0.7485	0.4074
H	5.2904	1.3457	-1.5734
H	3.6977	3.2622	-1.6476
H	2.4428	2.4171	2.3852
H	4.0074	0.4489	2.4416
H	5.3714	-0.1046	0.4352
C	1.9616	3.9962	0.2088

Int_3B

	X	Y	Z
Au	-0.5632	1.3106	1.4697
Au	1.4921	-0.1282	2.8049
Au	1.6023	-0.4961	0.0000
Au	1.4921	-0.1282	-2.8049
Au	-0.5632	1.3106	-1.4697
Au	-2.6085	0.1216	0.0000
O	-1.9319	-2.0719	0.0000
Pd	-0.5632	-1.5289	-1.4748
Pd	-0.5632	-1.5289	1.4748

H	1.9996	4.5291	-0.7723
O	1.1534	4.3324	1.0545
O	0.3014	0.7441	2.5873
O	0.8755	3.1435	3.7723
H	0.8127	3.6226	2.9338
H	0.6040	2.2359	3.5196
Pd	1.6298	0.2580	1.0300
Pd	-0.9721	1.5298	1.0764

	Int_4B				**TS_3B**		
	X	Y	Z		X	Y	Z
Au	-1.0537	-1.3847	1.4619	Au	1.1021	0.8336	2.7686
Au	-0.4825	0.9707	2.7769	Au	0.7538	-1.7112	1.4575
Au	-0.3106	1.2566	0.0000	Au	1.1021	0.8336	-2.7686
Au	-0.4825	0.9707	-2.7769	Au	0.7538	-1.7112	-1.4575
Au	-1.0537	-1.3847	-1.4619	C	-0.6435	5.1691	-1.2045
Au	0.6144	-3.0434	0.0000	C	-1.6931	4.2562	-1.2010
C	-0.6678	5.0975	1.2053	C	-2.2385	3.8040	0.0000
C	0.6215	4.5734	1.2026	C	-1.6931	4.2562	1.2010
C	1.2789	4.3118	0.0000	C	-0.6435	5.1691	1.2045
C	0.6215	4.5734	-1.2026	C	-0.1198	5.6307	0.0000
C	-0.6678	5.0975	-1.2053	H	-0.2282	5.5159	-2.1487
C	-1.3146	5.3581	0.0000	H	-2.0950	3.8768	-2.1410
H	-1.1687	5.3036	2.1488	H	-2.0950	3.8768	2.1410
H	1.1307	4.3566	2.1423	H	-0.2282	5.5159	2.1487
H	1.1307	4.3566	-2.1423	H	0.7022	6.3440	0.0000
H	-1.1687	5.3036	-2.1488	C	-3.3189	2.7603	0.0000
H	-2.3211	5.7699	0.0000	H	-3.9602	2.8893	0.8912

C	2.6026	3.6036	0.0000	H	-3.9602	2.8893	-0.8912
H	3.1887	3.8847	-0.8904	O	-2.6985	1.5127	0.0000
H	3.1887	3.8847	0.8904	H	-3.1761	0.5417	0.0000
O	2.2823	2.2340	0.0000	Au	0.9352	1.0765	0.0000
H	3.0179	1.5842	0.0000	Au	-1.5531	-2.3599	0.0000
O	3.1347	-0.3032	0.0000	O	-3.0272	-0.8148	0.0000
Pd	1.6691	-0.4240	-1.3302	Pd	-1.3203	0.1819	1.4920
Pd	1.6691	-0.4240	1.3302	Pd	-1.3203	0.1819	-1.4920

Pro_B

	X	Y	Z
Au	1.4385	1.1038	-1.6834
Au	3.1538	0.2009	0.3661
Au	0.8521	-1.2941	0.0412
Au	-1.4263	-2.7522	-0.6155
Au	-0.9950	-0.4843	-2.2247
Au	-1.1381	2.1765	-1.2837
C	-0.4407	-0.7470	3.7079
C	0.0094	0.5575	3.4928
C	-0.7905	1.4862	2.7968
C	-2.0779	1.0831	2.3051
C	-2.5319	-0.2303	2.5690
C	-1.6930	-1.1353	3.2562
H	0.1901	-1.4550	4.2385
H	0.9602	0.8920	3.9072
H	-2.7531	1.8686	1.9674
H	-3.5678	-0.5006	2.3706
H	-2.0514	-2.1445	3.4463

TS_5B

	X	Y	Z
Au	-1.3587	-0.9448	-1.3432
Au	-2.4387	1.6574	-1.8040
Au	0.1223	1.7581	-0.7013
Au	2.8668	1.3926	-0.3718
Au	1.4066	-1.0083	-0.7719
Au	-0.5246	-2.0316	1.0660
C	-3.9929	-0.0537	3.7452
C	-2.7275	-0.4408	4.1890
C	-1.5907	0.2780	3.8229
C	-1.7364	1.4344	3.0230
C	-3.0189	1.8348	2.5838
C	-4.1442	1.0648	2.9343
H	-4.8662	-0.6408	4.0246
H	-2.6105	-1.3331	4.8051
H	-0.8677	2.0744	2.8699
H	-3.1479	2.7942	2.0851
H	-5.1307	1.3662	2.5884

C	-0.4005	2.9031	2.7779	C	-0.2342	-0.2051	4.2362
H	0.5565	3.1159	3.3083	H	-0.1946	-0.4082	5.3298
O	-1.0482	3.8055	2.2588	H	-0.2424	-1.3584	3.8002
O	1.3868	3.9179	0.7399	O	0.8333	0.4196	3.7671
H	0.5420	4.2878	1.0469	H	0.9256	-3.7329	4.1052
H	1.3609	3.9724	-0.2216	O	-0.3423	-2.6817	3.2252
Pd	-1.7558	-0.1038	0.4225	O	1.0051	-3.1395	3.3470
Pd	0.6557	1.4714	0.9762	Pd	1.1116	0.4155	1.6164
				Pd	-1.9851	0.6935	0.8494

Pro_2B

	X	Y	Z
Au	0.8791	-0.6079	1.4287
Au	-1.4386	-2.0884	2.0974
Au	-1.2453	-1.4164	-0.5744
Au	-0.7448	-0.6795	-3.1875
Pd	-1.5976	0.6916	1.4345
Au	1.2187	0.1829	-1.3286
Au	0.9880	2.0927	0.6769
Pd	-1.2890	1.4234	-1.3389
C	-3.8030	1.4033	1.4574
C	-2.9387	2.4256	1.0156
C	-2.8632	2.7147	-0.3948
C	-3.6448	1.9626	-1.3073
C	-4.4870	0.9366	-0.8355
C	-4.5545	0.6572	0.5138
H	-4.0125	1.2895	2.5191
H	-2.5391	3.1638	1.7117

H	-3.6944	2.2749	-2.3501
H	-5.0813	0.3661	-1.5438
H	-5.2085	-0.1339	0.8727
C	-2.1048	3.8580	-0.8915
H	-2.2261	4.0575	-1.9773
H	-0.3510	4.4503	1.3254
O	-1.4049	4.6054	-0.2057
H	0.5445	5.1331	-0.2265
O	1.1766	5.2266	0.5129
O	0.6118	4.3349	1.4852

	Au_8O_2				$Au_6Pd_2O_2$		
	X	Y	Z		X	Y	Z
Au	0.0188	1.2869	1.3696	Au	1.5835	0.2765	1.4485
Au	0.0192	-0.0429	3.7471	Au	0.0352	-1.7328	2.7571
Au	0.0188	-1.5814	1.4989	Au	-0.0407	-1.8435	0.0000
Au	0.0188	1.2869	-1.3696	Au	0.0352	-1.7328	-2.7571
Au	0.0192	-0.0429	-3.7471	Pd	-1.1978	0.4650	1.4134
Au	0.0188	-1.5814	-1.4989	Au	1.5835	0.2765	-1.4485
Au	0.0186	3.5351	0.0000	Au	0.5669	2.4403	0.0000
Au	0.0186	-3.9590	0.0000	Pd	-1.1978	0.4650	-1.4134
O	-0.2113	5.2076	0.0000	O	-0.2818	5.5914	0.0000
O	-1.2821	5.6439	0.0000	O	0.6919	4.8286	0.0000

	Ads_A_2				Ads_A_3		
	X	Y	Z		X	Y	Z
Au	-0.7018	1.2873	1.4076	Au	-2.0542	-0.2898	-0.30383
Au	-1.3011	3.5429	0.0000	Au	-2.5788	2.4176	0.02028
Au	-0.7018	1.2873	-1.4076	Au	0.0358	1.6062	-0.27518
Au	1.1110	-0.9567	1.4426	Au	0.6076	-1.4945	-0.28506
Au	2.9656	-2.3378	0.0000	Au	3.2518	-2.1342	0.24280
Au	1.1110	-0.9567	-1.4426	Au	2.6635	0.4977	0.10214
C	2.3798	2.8637	-1.2073	C	-0.2178	-1.4332	2.79833
C	1.8524	4.1513	-1.2051	C	-1.4647	-0.8145	2.71006
C	1.5794	4.8021	0.0000	C	-2.6154	-1.5689	2.46747
C	1.8524	4.1513	1.2051	C	-2.5040	-2.9549	2.33484
C	2.3798	2.8637	1.2073	C	-1.2638	-3.5768	2.42855
C	2.6438	2.2199	0.0000	C	-0.1177	-2.8153	2.65434
H	2.5790	2.3560	-2.1491	H	0.6748	-0.8355	2.97657
H	1.6298	4.6543	-2.1461	H	-1.5452	0.2675	2.81898
H	1.6298	4.6543	2.1461	H	-3.4019	-3.5418	2.14288
H	2.5790	2.3560	2.1491	H	-1.1875	-4.6566	2.32352
H	3.0464	1.2070	0.0000	H	0.8555	-3.2975	2.72192
C	0.9028	6.1368	0.0000	C	-3.9391	-0.9009	2.25092
H	1.1913	6.7129	0.8920	H	-4.7382	-1.4567	2.76520
H	1.1913	6.7129	-0.8920	H	-3.9198	0.1221	2.65761
O	-0.5093	5.9117	0.0000	O	-4.2141	-0.8681	0.84913
H	-1.0059	6.7386	0.0000	H	-4.8569	-0.1399	0.69877
Au	-0.2125	-0.1711	3.6815	Au	-1.5861	-2.8315	-1.21912
Au	-0.2125	-0.1711	-3.6815	Au	2.2581	3.1872	-0.00789
O	-3.4852	5.3788	0.0000	O	-4.7320	2.0472	-0.21772

O	-3.3031	6.5685	0.0000	O	-5.3495	1.5943	0.78977

Ads_A_4

	X	Y	Z
Au	-0.2034	-1.0740	-0.9051
Au	0.7619	-3.5025	0.0974
Au	2.4219	-1.3063	0.1155
Au	-1.4983	1.2993	-0.1845
Au	-0.1551	3.6952	-0.0398
Au	1.3920	1.4249	0.0241
C	-5.2378	2.0223	-0.7900
C	-5.6997	0.8470	-0.2100
C	-5.1965	0.4160	1.0212
C	-4.2333	1.1880	1.6730
C	-3.7768	2.3798	1.1011
C	-4.2764	2.7918	-0.1366
H	-5.6291	2.3439	-1.7516
H	-6.4440	0.2374	-0.7205
H	-3.8298	0.8554	2.6290
H	-3.0579	2.9992	1.6350
H	-3.9138	3.7155	-0.5830
C	-5.6229	-0.9094	1.5758
H	-5.2454	-1.0274	2.6016
H	-6.7201	-0.9886	1.6009
O	-5.0928	-1.9222	0.7174
H	-5.0076	-2.7576	1.1930
Au	-2.7921	-1.1929	-0.0244
Au	4.0528	0.8799	0.3505
O	-1.3610	-3.9880	0.7729

Ads_A_5

	X	Y	Z
Au	-1.9876	-1.3943	0.0616
Au	-4.1672	0.2551	0.2659
Au	-1.6987	1.4122	0.0428
Au	0.8816	-1.3146	-0.2547
Au	3.3409	-0.1494	-0.5810
Au	1.1684	1.4696	-0.3077
C	5.9110	0.4293	-0.7176
C	6.2983	0.6896	0.5992
C	6.4230	-0.3522	1.5129
C	6.1363	-1.6619	1.1088
C	5.7475	-1.9356	-0.1938
C	5.6323	-0.8891	-1.1263
H	5.8640	1.2396	-1.4422
H	6.5074	1.7029	0.9257
H	6.2185	-2.4738	1.8298
H	5.5336	-2.9553	-0.5021
H	5.4309	-1.1079	-2.1734
C	6.8902	-0.0899	2.9176
H	6.3272	-0.7412	3.6083
H	7.9479	-0.3986	2.9934
O	6.7232	1.2660	3.2314
H	7.3371	1.5230	3.9235
Au	-0.5094	-3.6735	-0.0884
Au	-0.3343	3.7620	-0.1278
O	-6.1580	-0.7595	0.5859

O	-2.3320	-3.5214	0.1009	O	-6.5908	-0.8732	1.7326

Int_1A_2

	X	Y	Z
Au	-1.6653	0.3255	1.5598
Au	-0.6232	-2.0191	0.0000
Au	-1.6653	0.3255	-1.5598
Au	1.1367	-0.1800	1.4108
Au	3.5141	0.0685	0.0000
Au	1.1367	-0.1800	-1.4108
C	0.1796	3.6967	-1.2045
C	-1.1661	3.3412	-1.2012
C	-1.8471	3.1288	0.0000
C	-1.1661	3.3412	1.2012
C	0.1796	3.6967	1.2045
C	0.8586	3.8590	0.0000
H	0.7025	3.8194	-2.1511
H	-1.6902	3.1910	-2.1469
H	-1.6902	3.1910	2.1469
H	0.7025	3.8194	2.1511
H	1.9168	4.1112	0.0000
C	-3.2062	2.4790	0.0000
H	-3.7721	2.8045	0.8917
H	-3.7721	2.8045	-0.8917
O	-3.1230	1.0702	0.0000
Au	-0.1829	0.0840	3.8395
Au	-0.1829	0.0840	-3.8395
O	-3.3749	-3.1101	0.0000
O	-2.0087	-3.5866	0.0000

Int_1A_3

	X	Y	Z
Au	-0.2953	-1.0137	1.4525
Au	-0.7073	-2.8225	-0.6047
Au	-2.6610	-0.5692	-0.4412
Au	1.9230	0.5674	0.2205
Au	1.3874	3.1829	-0.3137
Au	-0.7518	1.4775	-0.0372
C	4.6500	1.5892	0.6698
C	4.4352	0.2177	0.4386
C	4.5011	-0.3022	-0.8695
C	4.7442	0.5808	-1.9274
C	4.9520	1.9345	-1.6937
C	4.9097	2.4454	-0.3940
H	4.6208	1.9697	1.6887
H	4.3491	-0.4847	1.2672
H	4.7895	0.1885	-2.9431
H	5.1510	2.6011	-2.5298
H	5.0875	3.5034	-0.2142
C	4.3972	-1.7900	-1.1192
H	3.8450	-1.9338	-2.0698
H	5.4308	-2.1304	-1.3361
O	3.9140	-2.5461	-0.0744
Au	1.9006	-2.2854	0.3352
Au	-3.4462	1.9666	0.1676
O	-3.4735	-2.5726	-1.3373
O	-2.3760	-3.4349	-1.7564

H	-3.2923	-2.1468	0.0000	H	-3.9224	-3.1228	-0.6733

Int_1A_4

	X	Y	Z
Au	-0.5546	-2.1516	-1.5309
Au	-0.8267	-1.9566	1.2612
Au	1.7119	-1.2945	0.1739
Au	-0.5544	0.5385	-0.4799
Au	-0.2729	3.2000	0.1276
Au	1.9668	1.6406	0.0156
C	-2.9146	3.7763	-0.8052
C	-3.6198	2.5950	-0.6059
C	-3.8139	2.0884	0.6842
C	-3.2728	2.7759	1.7744
C	-2.5599	3.9560	1.5914
C	-2.3636	4.4692	0.2920
H	-2.7888	4.1769	-1.8086
H	-4.0414	2.0430	-1.4434
H	-3.4112	2.3775	2.7788
H	-2.1596	4.4943	2.4476
H	-1.9225	5.4560	0.1532
C	-4.6277	0.8314	0.8981
H	-4.2710	0.3504	1.8308
H	-5.6649	1.1575	1.1168
O	-4.6835	-0.0275	-0.1840
Au	-2.9004	-0.9906	-0.5576
Au	4.1259	-0.1452	-0.0808
O	-0.7343	-3.6643	3.5055
O	-0.5833	-2.2715	3.2668

Int_1A_5

	X	Y	Z
Au	-1.8373	-1.5313	1.4580
Au	-1.8785	0.0001	-1.0209
Au	-1.8373	1.5312	1.4580
Au	0.5862	-1.4091	-0.3628
Au	2.9379	-0.0002	-0.3841
Au	0.5864	1.4090	-0.3626
C	9.1047	0.0007	-0.7744
C	7.7179	0.0004	-0.6420
C	7.1339	-0.0002	0.6215
C	7.9573	-0.0007	1.7493
C	9.3399	-0.0004	1.6190
C	9.9198	0.0003	0.3519
H	9.5510	0.0013	-1.7673
H	7.0656	0.0008	-1.5112
H	7.5021	-0.0013	2.7412
H	9.9692	-0.0008	2.5071
H	11.0027	0.0005	0.2458
C	5.6336	-0.0005	0.8018
H	5.3717	-0.8825	1.4212
H	5.3715	0.8811	1.4215
O	4.9716	-0.0003	-0.4202
Au	-1.8947	-2.8343	-0.9182
Au	-1.8942	2.8346	-0.9179
O	-0.7482	-0.0003	3.7402
O	-2.0149	-0.0000	3.0471

H	-1.6377	-3.7035	3.8516	H	-1.0577	0.0008	4.6580

	Int_2A_2				**Int_2A_3**		
	X	Y	Z		X	Y	Z
Au	0.3227	1.9576	-0.2776	Au	1.9277	0.4537	-0.4104
Au	2.8054	2.5717	0.6946	Au	3.4664	-1.6890	0.3199
Au	2.1870	-0.0373	0.5651	Au	0.8017	-2.0374	0.3976
Au	-1.6326	-0.0604	-0.7907	Au	-0.7161	1.5309	-0.5077
Au	-2.7652	-2.3107	0.3093	Au	-3.3852	1.6757	0.1565
Au	-0.0964	-2.2263	0.1533	Au	-2.1447	-0.6780	0.5234
Au	-1.9671	2.5052	-1.6530	Au	1.4440	2.9427	-1.4082
Au	2.8090	-2.6813	-1.1007	Au	-1.5874	-3.0125	-1.3925
O	2.0271	-2.1854	0.7046	O	-1.1978	-2.7311	0.5893
O	0.8076	-1.8129	3.2386	O	-2.8060	-1.9695	2.7459
H	1.4398	-2.0386	2.5360	H	-2.4070	-2.6799	2.2180
H	0.1844	-2.5457	3.2294	H	-2.0404	-1.5772	3.2020
C	-3.3048	0.8388	2.2247	C	0.4357	1.6172	2.8172
C	-2.0994	0.1982	2.5434	C	1.7669	1.1894	2.7484
C	-0.9535	0.9435	2.7841	C	2.7660	2.0992	2.4305
C	-1.0112	2.3370	2.7039	C	2.4391	3.4334	2.1837
C	-2.2111	2.9853	2.4099	C	1.1148	3.8619	2.2464
C	-3.3571	2.2370	2.1784	C	0.1121	2.9522	2.5593
H	-2.0674	-0.8878	2.6020	H	1.9914	0.1433	2.9493
H	-0.0276	0.4225	3.0272	H	3.8011	1.7694	2.3703
H	-0.1106	2.9216	2.8858	H	3.2247	4.1442	1.9365
H	-2.2466	4.0706	2.3586	H	0.8674	4.9016	2.0475
H	-4.3006	2.7283	1.9409	H	-0.9305	3.2673	2.6046
C	-4.5158	0.0883	1.8923	C	-0.6299	0.6660	3.1555
H	-5.4334	0.7140	1.8090	H	-1.6596	1.0939	3.1520

O	-4.5937	-1.1152	1.6902	O	-0.4441	-0.5092	3.4219

Int_2A_4

	X	Y	Z
Au	0.6621	2.2001	-0.1069
Au	3.3915	2.3896	-0.0676
Au	2.4047	-0.0626	0.3848
Au	-1.3465	0.2263	-0.0628
Au	-2.6796	-2.2008	-0.0112
Au	-0.0515	-2.2009	0.4502
Au	-1.9665	2.8808	-0.2082
Au	2.7943	-3.0042	-0.7746
O	2.0844	-2.1303	0.9094
O	1.0364	-1.2421	3.3951
H	1.5796	-1.7060	2.7388
H	0.7017	-0.4746	2.9196
C	-5.0737	0.6740	0.1589
C	-4.7275	0.4901	-1.1877
C	-4.7691	-0.7780	-1.7422
C	-5.1257	-1.8790	-0.9455
C	-5.4699	-1.6960	0.4015
C	-5.4550	-0.4132	0.9456
H	-4.4333	1.3554	-1.7778
H	-4.5088	-0.9308	-2.7860
H	-5.1972	-2.8695	-1.3919
H	-5.7661	-2.5486	1.0073
H	-5.7227	-0.2551	1.9893
C	-4.9991	2.0060	0.7716
H	-5.4372	2.0802	1.7912

Int_2A_5

	X	Y	Z
Au	0.3291	2.1775	0.0122
Au	2.9813	2.8135	0.2365
Au	2.4032	0.1991	0.3947
Au	-1.3652	-0.0818	-0.0093
Au	-2.3322	-2.6488	0.2413
Au	0.3101	-2.2919	0.3548
Au	-2.3464	2.4465	-0.3880
Au	3.1360	-2.4597	-1.1445
O	2.4280	-1.9523	0.6864
O	1.6450	-1.0753	3.3010
H	2.0898	-1.5700	2.5957
H	0.8734	-0.6949	2.8683
C	-5.1514	-0.1611	0.1320
C	-4.7085	-0.2110	-1.1974
C	-4.5996	0.9593	-1.9301
C	-4.8989	2.1909	-1.3281
C	-5.3432	2.2421	-0.0012
C	-5.4817	1.0611	0.7210
H	-4.4618	-1.1754	-1.6366
H	-4.2624	0.9312	-2.9627
H	-4.8401	3.1069	-1.9140
H	-5.5909	3.1982	0.4525
H	-5.8321	1.0832	1.7519
C	-5.2514	-1.3841	0.9346
H	-5.7876	-1.2704	1.9018

O	-4.4917	2.9844	0.2474	O	-4.7916	-2.4711	0.6176

Int_3A_2

	X	Y	Z
Au	1.5748	-1.398	-0.5247
Au	3.7980	0.094	-0.3896
Au	1.4257	1.385	0.0477
Au	-1.5753	-1.397	-0.5237
Au	-3.7977	0.097	-0.3900
Au	-1.4248	1.387	0.0468
Au	-0.0017	-3.509	1.1646
Au	0.0010	3.626	0.6464
O	-0.0006	-2.839	-0.7665

Int_3A_3

	X	Y	Z
Au	-1.4190	-1.9496	-0.0015
Au	-3.7222	-0.5614	0.1306
Au	-1.3984	0.9366	0.0087
Au	1.1837	-0.8234	-0.0338
Au	3.8228	0.0623	0.1573
Au	1.3184	2.0728	-0.0326
Au	0.8091	-3.5288	-0.1276
Au	-0.9352	3.5919	-0.0979
O	3.3641	1.9707	-0.0313

Int_3A_4

	X	Y	Z
Au	-1.3515	1.9035	0.0000
Au	0.8508	3.5592	-0.4119
Au	1.2362	0.8323	0.0313
Au	-1.5095	-0.9773	0.0290
Au	-0.7779	-3.5152	-0.6828
Au	1.1701	-1.9754	0.4780
Au	-3.7477	0.5516	0.3588
Au	3.8531	-0.2508	0.0629
O	2.7299	-1.2624	1.3282

Int_3A_5

	X	Y	Z
Au	1.4249	1.3869	0.0471
Au	3.7980	0.0963	-0.3874
Au	1.5753	-1.3973	-0.5248
Au	-1.4255	1.3861	0.0472
Au	-3.7980	0.0945	-0.3873
Au	-1.5748	-1.3982	-0.5248
Au	-0.0010	3.6273	0.6443
Au	0.0010	-3.5081	1.1635
O	0.0006	-2.8399	-0.7680

	Int_4A_2				Int_4A_3		
	X	Y	Z		X	Y	Z
Au	1.3176	0.5072	-0.0775	Au	1.1525	-1.5369	0.4407
Au	1.5677	3.2322	-0.3672	Au	2.9673	-1.5348	-1.6024
Au	-0.9106	2.2030	-0.4902	Au	1.9853	0.8633	-0.8760
Au	0.0770	-1.9999	-0.0636	Au	-1.4034	-0.3298	0.9423
Au	-2.3472	-3.2726	-0.3092	Au	-3.2112	0.9678	-0.6871
Au	-2.4357	-0.6026	-0.4575	Au	-0.8022	2.0931	-0.3457
C	5.2741	-2.1630	1.3824	C	-3.9178	-0.4629	-2.9293
C	5.2565	-1.5777	0.1038	C	-2.6830	-1.0852	-3.1188
C	5.1812	-0.1776	-0.0372	C	-2.2430	-2.0656	-2.2317
C	5.1139	0.6110	1.1092	C	-3.0643	-2.4384	-1.1609
C	5.1341	0.0273	2.3746	C	-4.2991	-1.8305	-0.9657
C	5.2084	-1.3545	2.5179	C	-4.7310	-0.8224	-1.8408
H	5.3591	-3.2432	1.4777	H	-4.2603	0.2933	-3.6323
H	5.3902	-2.2002	-0.7823	H	-2.0363	-0.7949	-3.9429
H	5.0298	1.6896	0.9942	H	-2.7174	-3.1983	-0.4604
H	5.0836	0.6596	3.2577	H	-4.9225	-2.1192	-0.1229
H	5.2166	-1.8051	3.5066	H	-5.7143	-0.3723	-1.7190
C	5.1711	0.4507	-1.4082	C	-0.8908	-2.7097	-2.4089
H	6.1947	0.7430	-1.6814	H	-0.4838	-2.9676	-1.4115
H	4.8517	-0.3028	-2.1483	H	-1.0014	-3.6576	-2.9540
O	4.4023	1.6218	-1.4837	O	0.0092	-1.9305	-3.1525
H	3.4670	1.3809	-1.3820	H	0.2931	-1.1858	-2.6008
Au	2.7704	-1.7937	0.2232	Au	-0.4986	-2.4732	2.3903
Au	-3.4631	1.7680	1.2622	Au	1.6045	2.8998	1.4411
O	-2.9194	1.4887	-0.6886	O	1.2505	2.8660	-0.5681

	Int_4A_4				Int_4A_5		
	X	Y	Z		X	Y	Z
Au	-0.2055	2.1871	0.1379	Au	-1.4401	-0.5816	-0.0633
Au	-2.8846	1.9458	-0.2279	Au	-1.4182	-3.3089	-0.3982
Au	-1.3750	-0.3226	-0.2608	Au	0.9679	-2.0890	-0.5220
Au	2.1656	0.5214	-0.0428	Au	-0.0637	1.8539	0.0020
Au	3.7285	-1.6947	-0.5469	Au	2.2451	3.3333	-0.2654
Au	1.0927	-2.0955	-0.5001	Au	2.5173	0.6829	-0.4800
C	-4.9558	0.8383	-1.8378	C	-5.3970	-1.2949	1.5315
C	-4.6582	-0.5170	-1.7486	C	-5.7872	0.0304	1.3844
C	-4.7253	-1.1788	-0.5197	C	-5.6453	0.6751	0.1531
C	-5.1061	-0.4664	0.6206	C	-5.1106	-0.0247	-0.9301
C	-5.4043	0.8899	0.5467	C	-4.7229	-1.3544	-0.7864
C	-5.3160	1.5637	-0.6863	C	-4.8655	-1.9872	0.4454
H	-4.9072	1.3467	-2.7980	H	-5.5070	-1.7906	2.4926
H	-4.3511	-1.0820	-2.6253	H	-6.1956	0.5822	2.2303
H	-5.1501	-0.9784	1.5818	H	-4.9816	0.4814	-1.8865
H	-5.7024	1.4362	1.4385	H	-4.3003	-1.8920	-1.6328
H	-5.6333	2.6023	-0.7676	H	-4.5582	-3.0253	0.5610
C	-4.4148	-2.6553	-0.4306	C	-5.9661	2.1305	0.0346
H	-3.9962	-2.8633	0.5755	H	-6.0216	2.4250	-1.0232
H	-5.3644	-3.2113	-0.4805	H	-6.9276	2.3645	0.5148
O	-3.5996	-3.1360	-1.4493	O	-4.9231	2.8597	0.7018
H	-2.6682	-2.9201	-1.2379	H	-4.9809	3.7950	0.4736
Au	2.3277	3.1619	0.5539	Au	-2.7556	1.7713	0.3687
Au	-1.2743	-2.9466	1.4495	Au	3.5409	-1.7083	1.2015
O	-1.0463	-2.4832	-0.5250	O	2.9911	-1.4015	-0.7440

	Int_5A_2				Int_5A_3		
	X	Y	Z		X	Y	Z
Au	1.4036	0.8390	1.5542	Au	1.4156	1.4132	0.3134
Au	0.9231	-1.6450	0.1512	Au	3.3040	-0.6215	-0.2408
Au	-1.4064	-0.3193	1.3701	Au	1.1949	-1.1278	1.5512
Au	1.5644	0.8863	-1.5338	Au	-1.4000	1.0374	-0.3601
Au	-0.6271	2.2784	-0.5568	Au	-2.0608	-1.0712	-2.1248
Au	-0.9774	-0.2415	-1.7156	Au	-1.5069	-1.8447	0.4391
C	-4.2041	-0.1677	1.3710	C	-4.5349	-0.3985	1.9379
C	-3.6988	1.1079	1.6615	C	-3.5808	-1.2036	2.5562
C	-3.6019	2.0850	0.6586	C	-2.3421	-0.6787	2.9522
C	-4.0331	1.7616	-0.6260	C	-2.0861	0.6780	2.7310
C	-4.5496	0.4972	-0.9207	C	-3.0387	1.4858	2.1059
C	-4.6326	-0.4701	0.0721	C	-4.2632	0.9465	1.7068
H	-4.3110	-0.9022	2.1680	H	-5.4935	-0.8201	1.6451
H	-3.4097	1.3629	2.6822	H	-3.7900	-2.2571	2.7454
H	-3.9584	2.5152	-1.4108	H	-1.1309	1.1036	3.0423
H	-4.8931	0.2743	-1.9287	H	-2.8330	2.5444	1.9562
H	-5.0428	-1.4537	-0.1480	H	-5.0061	1.5814	1.2303
C	-2.9402	3.4118	0.9510	C	-1.2798	-1.6001	3.4881
H	-3.2589	4.1361	0.1764	H	-0.6058	-1.0401	4.1572
H	-3.3271	3.7921	1.9157	H	-1.7588	-2.3890	4.0925
O	-1.5551	3.3163	1.0428	O	-0.5457	-2.2207	2.4504
Au	3.4521	-0.4383	0.2503	Au	-0.3118	3.5266	-0.0306
Au	-1.6670	-2.5977	-0.2051	Au	0.6849	-0.9099	-1.2738
O	-0.3964	1.2664	2.6395	O	5.2318	-0.9916	-0.7359
H	-0.7781	2.0780	2.2247	H	5.6122	-0.1685	-1.0641

	Int_5A_4				Int_5A_5		
	X	Y	Z		X	Y	Z
Au	-0.7710	-1.2881	0.4551	Au	-0.1900	2.0375	0.3781
Au	-3.3927	-1.8703	0.0826	Au	2.4570	2.7227	-0.1985
Au	-2.6494	0.7991	-0.0335	Au	1.8146	-0.1153	-0.2263
Au	1.9282	-0.5605	-0.5426	Au	-2.2303	0.1076	0.2438
Au	2.8383	1.9456	0.1589	Au	-2.8871	-2.5436	0.3700
Au	0.1504	1.5459	-0.1435	Au	-0.3037	-1.9663	-0.2652
C	4.8918	0.7011	1.7798	C	4.0527	-1.7718	2.1716
C	4.5721	-0.6447	1.6233	C	3.1313	-0.7360	2.3000
C	4.6755	-1.2613	0.3735	C	1.8407	-0.9630	2.8062
C	5.1653	-0.5225	-0.7138	C	1.4829	-2.2633	3.1902
C	5.4888	0.8198	-0.5712	C	2.3937	-3.3088	3.0789
C	5.3238	1.4543	0.6743	C	3.6864	-3.0683	2.5750
H	4.8002	1.1769	2.7532	H	5.0422	-1.5686	1.7664
H	4.1986	-1.2172	2.4711	H	3.3698	0.2583	1.9186
H	5.2533	-1.0103	-1.6833	H	0.4799	-2.4486	3.5779
H	5.8622	1.3881	-1.4197	H	2.1007	-4.3111	3.3880
H	5.6420	2.4872	0.8082	H	4.3995	-3.8858	2.4943
C	4.1592	-2.6591	0.1425	C	0.8275	0.1598	2.8705
H	4.9622	-3.2836	-0.2885	H	0.1850	-0.0276	3.7622
H	3.8958	-3.1075	1.1151	H	1.3710	1.1063	3.1133
O	3.0832	-2.6443	-0.7668	O	0.0745	0.2739	1.7297
Au	1.0522	-3.2296	-0.1162	Au	-2.6181	2.7597	-0.5884
Au	-1.8985	3.4024	-0.0712	Au	2.0331	-2.3206	-1.7663
O	-5.3148	-2.3999	-0.1856	O	3.3909	3.0214	1.5404
H	-5.7647	-2.2173	0.6490	H	2.8719	2.3692	2.0431

	Pro_A_2				Pro_A_3		
	X	Y	Z		X	Y	Z
Au	1.9004	0.2239	-0.0123	Au	-0.3939	-2.2922	-0.1708
Au	2.1787	2.4057	-1.6731	Au	-3.0874	-2.5756	-0.5023
Au	-0.0148	2.3175	-0.0662	Au	-2.2278	-0.0388	0.0286
Au	0.6517	-2.3925	0.0494	Au	1.2356	0.0239	-0.3099
Au	-1.8804	-2.4891	-0.8989	Au	2.1798	2.5859	-0.6020
Au	-1.1694	-0.2741	0.6048	Au	-0.4667	2.2783	-0.1208
Au	3.2325	-2.0181	0.8488	Au	2.2572	-2.4354	0.3874
Au	-1.7139	1.9259	2.1214	Au	-3.0665	2.4737	0.6809
O	-1.4562	4.2258	-0.7693	O	1.1340	0.5490	2.8500
H	-1.8913	4.4363	0.0639	H	0.9516	1.2858	2.2524
H	-2.1031	3.6918	-1.2714	H	0.5471	-0.1480	2.5338
C	-4.1453	0.2302	-1.1121	C	5.0334	0.2511	-0.0204
C	-3.8089	-0.5022	-2.2525	C	4.3034	0.4325	1.1626
C	-4.1379	-1.8555	-2.3229	C	4.0803	-0.6403	2.0115
C	-4.8182	-2.4642	-1.2571	C	4.5780	-1.9084	1.6719
C	-5.1647	-1.7258	-0.1249	C	5.3196	-2.0907	0.4967
C	-4.8230	-0.3824	-0.0523	C	5.5505	-1.0071	-0.3428
H	-3.2689	-0.0063	-3.0560	H	3.9122	1.4186	1.4056
H	-3.8981	-2.4302	-3.2151	H	3.4782	-0.4986	2.9056
H	-5.0807	-3.5179	-1.3201	H	4.4372	-2.7438	2.3565
H	-5.6870	-2.2050	0.6981	H	5.7161	-3.0726	0.2512
H	-5.0599	0.2011	0.8370	H	6.1220	-1.1331	-1.2615
C	-3.7345	1.6344	-0.9892	C	5.2283	1.3517	-0.9672
H	-3.9896	2.1080	-0.0126	H	5.9546	1.1439	-1.7831
O	-3.1470	2.2577	-1.8556	O	4.6579	2.4325	-0.9300

	Pro_2A_2				Pro_2A_3		
	X	Y	Z		X	Y	Z
Au	2.3087	-0.4473	-0.1269	Au	-1.9911	0.9793	-0.0903
Au	2.2213	-3.1540	-0.2300	Au	-1.3065	3.5301	0.5352
Au	-0.1995	-1.8611	-0.3497	Au	0.7314	1.9404	-0.3149
Au	0.5638	1.8398	-0.2442	Au	-1.1818	-1.7916	-0.2230
Au	-1.8216	3.1670	-0.4354	Au	0.9858	-3.4537	-0.1454
Au	-1.9331	0.4490	-0.3683	Au	1.4975	-0.8067	-0.5531
Au	3.2864	2.0906	-0.1058	Au	-3.7792	-1.0465	-0.4934
Au	-2.9007	-2.1147	-0.3153	Au	3.2630	1.2369	-0.9867
O	-5.1521	-0.6366	0.5808	O	5.3579	-0.0080	0.5297
H	-4.6651	-0.4617	1.4200	H	5.2296	0.7517	1.1276
C	-1.0517	-0.2340	2.9777	C	1.3474	-0.2950	2.8641
C	-0.7833	1.1387	3.0441	C	-0.0439	-0.1675	2.7814
C	0.5265	1.5749	3.1718	C	-0.8490	-1.2874	2.9543
C	1.5676	0.6459	3.2345	C	-0.2667	-2.5294	3.2193
C	1.3050	-0.7209	3.1701	C	1.1184	-2.6590	3.3017
C	-0.0066	-1.1607	3.0382	C	1.9266	-1.5411	3.1253
H	-1.6136	1.8386	2.9784	H	-0.4725	0.8162	2.5852
H	0.7459	2.6400	3.2089	H	-1.9319	-1.1930	2.8932
H	2.5950	0.9935	3.3226	H	-0.9010	-3.4037	3.3515
H	2.1221	-1.4376	3.2053	H	1.5646	-3.6283	3.5132
H	-0.2281	-2.2261	2.9625	H	3.0134	-1.6179	3.1825
C	-2.4169	-0.7156	2.7682	C	2.2189	0.8807	2.7006
H	-2.5134	-1.8253	2.7181	H	3.3101	0.6440	2.7626
O	-3.3953	0.0034	2.6313	O	1.8308	2.0146	2.5057
O	-4.8264	0.5715	-0.1269	O	4.6014	-1.0194	1.1907

H	-4.7764	0.2294	-1.0314	H	3.8512	-1.1390	0.5734

Pro_2A_4

	X	Y	Z
Au	1.2715	-0.2159	-0.2125
Au	1.8878	-2.8453	0.2751
Au	-0.7184	-2.2432	-0.1738
Au	-0.1222	2.2651	-0.1616
Au	-2.6925	2.8962	0.4903
Au	-2.2190	0.2387	0.0488
Au	2.5599	2.1852	-0.5470
Au	-3.4199	-2.1487	-0.5085
O	-0.7574	0.3688	2.8132
H	-0.4922	1.1212	2.2524
C	4.9322	-0.5877	0.6285
C	4.7064	-0.6542	-0.7530
C	4.8417	0.4875	-1.5278
C	5.1782	1.7087	-0.9209
C	5.4126	1.7727	0.4588
C	5.2967	0.6205	1.2279
H	4.4304	-1.6079	-1.1983
H	4.6730	0.4465	-2.6007
H	5.3228	2.5958	-1.5359
H	5.6885	2.7177	0.9191
H	5.4726	0.6544	2.3020
C	4.7579	-1.7750	1.4713
H	5.0950	-1.6601	2.5242
O	4.2738	-2.8322	1.0957
O	0.4358	-0.4123	2.8365

Pro_2A_5

	X	Y	Z
Au	1.3012	-0.6077	0.1622
Au	1.1596	-3.3314	-0.1409
Au	-1.2003	-1.9651	-0.0801
Au	0.1348	1.9176	0.0192
Au	-2.1683	3.3520	-0.3769
Au	-2.4353	0.6515	-0.2591
Au	2.8312	1.6485	0.3031
Au	-3.9092	-1.6465	-0.0816
O	-1.1594	-0.0455	3.8295
H	-0.4694	0.6132	3.6670
C	6.4048	0.5925	-0.2617
C	5.4215	-0.4072	-0.3123
C	5.7830	-1.7201	-0.5786
C	7.1251	-2.0445	-0.7923
C	8.1100	-1.0590	-0.7389
C	7.7490	0.2562	-0.4748
H	4.3708	-0.1547	-0.1415
H	5.0157	-2.4910	-0.6188
H	7.4035	-3.0766	-1.0028
H	9.1538	-1.3182	-0.9038
H	8.5079	1.0387	-0.4328
C	6.1077	1.9988	0.0037
H	7.0039	2.6544	0.0022
O	5.0114	2.5270	0.1621
O	-1.3827	-0.4986	2.4910

H	0.2100	-1.1352	2.2222	H	-2.3299	-0.3147	2.3818
	Ads_B_2				**Ads_B_3**		
	X	Y	Z		X	Y	Z
Au	0.2365	1.4741	1.4300	Au	-0.2244	-1.6321	0.7708
Au	0.4419	-0.8808	2.8478	Au	2.5572	-2.2426	0.3378
Au	0.4670	-1.1936	0.0000	Au	1.9004	0.4329	0.2281
Au	0.4419	-0.8808	-2.8478	Au	1.2015	3.1118	0.2742
Pd	-1.9150	-0.4775	1.4121	Pd	0.8234	-1.3949	-1.7213
Au	0.2365	1.4741	-1.4300	Au	-0.9503	1.2940	0.7107
Au	0.4237	3.8003	0.0000	Au	-1.8340	-0.4566	-1.4426
Pd	-1.9150	-0.4775	-1.4121	Pd	0.1572	1.4781	-1.7880
C	2.5955	-4.0364	1.2055	C	-1.4810	0.2635	3.0727
C	1.2180	-4.2399	1.2035	C	-2.6651	0.7492	2.5018
C	0.5155	-4.3491	0.0000	C	-3.5967	-0.1328	1.9062
C	1.2180	-4.2399	-1.2035	C	-3.3372	-1.4915	1.9081
C	2.5955	-4.0364	-1.2055	C	-2.1561	-1.9951	2.4783
C	3.2854	-3.9349	0.0000	C	-1.2106	-1.1265	3.0496
H	3.1312	-3.9595	2.1492	H	-0.8086	0.9362	3.6014
H	0.6706	-4.3195	2.1434	H	-2.9264	1.8041	2.6135
H	0.6706	-4.3195	-2.1434	H	-4.0741	-2.1557	1.4648
H	3.1312	-3.9595	-2.1492	H	-2.0034	-3.0712	2.5438
H	4.3619	-3.7821	0.0000	H	-0.3501	-1.5183	3.5883
C	-0.9816	-4.4785	0.0000	C	-4.8571	0.4159	1.2821
H	-1.3083	-5.0415	-0.8900	H	-5.3904	1.0065	2.0457
H	-1.3083	-5.0415	0.8900	H	-4.5554	1.1368	0.4974
O	-1.4953	-3.1690	0.0000	O	-5.7057	-0.5628	0.7915
H	-2.4714	-3.0971	0.0000	H	-5.4738	-0.6944	-0.1524
O	-3.9389	-1.9094	0.0000	O	-3.7288	-1.4710	-1.7002

O	-3.4335	-0.7133	0.0000	O	-4.7023	-0.6483	-1.7692

Ads_B_4

	X	Y	Z
Au	-0.1138	-1.8824	-1.1283
Au	-2.6378	-1.0459	-0.4566
Au	-0.6661	1.0669	-0.3570
Au	1.5117	2.8192	-0.4188
Pd	-0.5692	-1.1750	1.5099
Au	2.0771	0.1609	-1.0995
Au	2.0586	-2.0477	0.6824
Pd	1.5510	0.7558	1.5408
C	-4.9148	0.0798	0.0420
C	-4.3626	0.7590	1.1412
C	-3.6465	1.9376	0.9568
C	-3.4964	2.4451	-0.3429
C	-4.0602	1.7965	-1.4368
C	-4.7694	0.6081	-1.2510
H	-5.5155	-0.8139	0.2008
H	-4.4720	0.3460	2.1432
H	-2.9364	3.3702	-0.4828
H	-3.9454	2.2104	-2.4353
H	-5.2226	0.0983	-2.0978
C	-2.9610	2.6330	2.1040
H	-3.2279	3.6987	2.1006
H	-3.3131	2.2092	3.0579
O	-1.5578	2.5587	1.9982
H	-1.2959	1.6988	2.3900
O	-1.2492	0.0035	3.1134

Ads_B_5

	X	Y	Z
Au	0.7686	-1.4377	0.8162
Au	3.0122	-0.5376	-0.7175
Au	0.8949	1.2180	-0.6267
Au	-1.3503	2.8061	-0.5180
Pd	0.6057	-1.3865	-1.9676
Au	-1.5556	0.3420	0.9191
Au	-1.7141	-2.2073	-0.2396
Pd	-1.6174	0.3182	-1.8682
C	1.0718	3.1904	1.9806
C	0.4285	2.3093	2.9962
C	1.1204	1.0885	3.4811
C	2.4550	0.8504	2.8810
C	3.0127	1.7923	1.8669
C	2.3180	2.9144	1.4253
H	0.5619	4.1108	1.6626
H	-0.4790	2.6541	3.5373
H	3.1067	0.0717	3.3332
H	4.0195	1.6193	1.4605
H	2.7502	3.5777	0.6591
C	0.5683	0.2204	4.6428
H	1.3928	-0.2066	5.2448
H	-0.0504	0.8256	5.3324
O	-0.1632	-0.7593	4.1149
H	-0.5291	-1.3314	4.8132
O	-2.3798	-3.2192	2.2605

O	0.0432	-0.2750	3.2581	O	-1.7669	-2.3811	1.5897

Int_1B_2

	X	Y	Z
Au	-1.2075	-1.2518	1.4056
Au	-0.8203	1.2146	2.7461
Au	-0.7933	1.5269	0.0000
Au	-0.8203	1.2146	-2.7461
Pd	1.3446	0.0111	1.3469
Au	-1.2075	-1.2518	-1.4056
Au	0.7040	-2.7105	0.0000
Pd	1.3446	0.0111	-1.3469
C	1.8399	3.9588	1.2060
C	2.7112	2.8723	1.2044
C	3.1475	2.3165	0.0000
C	2.7112	2.8723	-1.2044
C	1.8399	3.9588	-1.2060
C	1.3988	4.4983	0.0000
H	1.5025	4.3831	2.1491
H	3.0547	2.4436	2.1472
H	3.0547	2.4436	-2.1472
H	1.5025	4.3831	-2.1491
H	0.7185	5.3466	0.0000
C	3.9140	1.0302	0.0000
H	4.5627	0.9518	-0.8882
H	4.5627	0.9518	0.8882
O	3.0244	-0.0697	0.0000
H	3.3971	-1.7146	0.0000
O	3.7565	-2.6396	0.0000

Int_1B_3

	X	Y	Z
Au	1.0464	0.5573	1.6043
Au	0.2006	-1.8124	2.7588
Au	-0.3745	-1.4700	0.0000
Au	0.2006	-1.8124	-2.7588
Pd	-1.6776	0.0771	1.9560
Au	1.0464	0.5573	-1.6043
Au	-1.5722	2.2208	0.0000
Pd	-1.6776	0.0771	-1.9560
C	4.3233	1.1571	-1.2060
C	3.3123	2.1219	-1.2085
C	2.7912	2.6055	0.0000
C	3.3123	2.1219	1.2085
C	4.3233	1.1571	1.2060
C	4.8147	0.6639	0.0000
H	4.7240	0.7936	-2.1494
H	2.9509	2.5404	-2.1507
H	2.9509	2.5404	2.1507
H	4.7240	0.7936	2.1494
H	5.5940	-0.0932	0.0000
C	1.4947	3.3631	0.0000
H	1.4032	4.0014	0.8938
H	1.4032	4.0014	-0.8938
O	0.5296	2.3367	0.0000
H	-3.1030	0.0154	0.0000
O	-3.9425	0.5114	0.0000

O	2.7201	-3.5235	0.0000	O	-3.5591	1.9223	0.0000

Int_1B_4

	X	Y	Z
Au	2.0523	1.0546	-0.7134
Au	1.3450	-1.9192	-0.1816
Au	-1.3420	-1.9753	0.5479
Au	-3.2852	-0.3493	-0.8567
Pd	0.6373	0.1403	1.6104
Au	-0.5540	0.1016	-1.2396
Au	-0.2083	2.6450	-0.1754
Pd	-1.9562	0.8062	1.2707
C	4.6726	0.4742	-1.1494
C	4.3080	0.5284	0.2077
C	4.0161	-0.6529	0.9177
C	4.1257	-1.8731	0.2498
C	4.5004	-1.9272	-1.1019
C	4.7527	-0.7598	-1.8074
H	4.9387	1.3911	-1.6722
H	4.3181	1.4741	0.7515
H	3.9454	-2.7972	0.8018
H	4.5796	-2.8920	-1.5981
H	5.0283	-0.7989	-2.8575
C	3.4792	-0.5526	2.3266
H	3.1663	-1.5652	2.6550
H	4.3232	-0.2721	2.9908
O	2.5015	0.4026	2.4667
H	0.4811	1.7494	3.5394
O	-0.1280	0.9921	3.4452

Int_1B_5

	X	Y	Z
Au	1.1794	0.0798	1.4901
Au	-0.9421	-1.1674	2.8048
Au	-1.1182	-1.1596	0.0000
Au	-0.9421	-1.1674	-2.8048
Pd	-1.4253	1.2314	1.5236
Au	1.1794	0.0798	-1.4901
Au	0.4233	2.6397	0.0000
Pd	-1.4253	1.2314	-1.5236
C	1.5975	-3.8638	-1.2061
C	2.4769	-2.7846	-1.2036
C	2.9124	-2.2224	0.0000
C	2.4769	-2.7846	1.2036
C	1.5975	-3.8638	1.2061
C	1.1480	-4.3978	0.0000
H	1.2678	-4.2944	-2.1495
H	2.8372	-2.3686	-2.1466
H	2.8372	-2.3686	2.1466
H	1.2678	-4.2944	2.1495
H	0.4677	-5.2464	0.0000
C	3.7060	-0.9463	0.0000
H	4.3571	-0.9123	0.8901
H	4.3571	-0.9123	-0.8901
O	2.8767	0.1971	0.0000
H	-0.5131	5.1758	0.0000
O	0.3632	5.5796	0.0000

O	-1.3556	1.5701	3.0761	O	1.2779	4.4744	0.0000

	Int_2B_2				**Int_2B_3**		
	X	Y	Z		X	Y	Z
Au	-2.1360	0.4128	-0.9591	Au	-1.0651	1.2181	-0.9380
Au	-1.0437	2.9971	-0.3375	Au	0.9604	3.2042	-0.4315
Au	0.8573	1.0121	-0.6115	Au	1.7460	0.5172	-0.3474
Au	2.5258	-1.1850	-0.8387	Au	2.6908	-2.1129	-0.2473
Au	-0.2157	-1.6850	-1.3649	Au	-0.1057	-1.7896	-0.7892
Au	-2.1592	-1.8497	0.7620	Au	-2.1320	-0.7090	1.1138
C	4.3162	2.1447	-0.2110	C	-2.1449	-2.0808	-2.3431
C	3.3940	2.2760	0.8227	C	-3.0187	-2.1286	-1.2406
C	3.2695	1.2679	1.7838	C	-3.7246	-0.9868	-0.8365
C	4.0673	0.1225	1.7102	C	-3.5590	0.2237	-1.5554
C	4.9791	-0.0140	0.6690	C	-2.6961	0.2744	-2.6537
C	5.1031	0.9990	-0.2881	C	-2.0031	-0.8849	-3.0535
H	4.4146	2.9274	-0.9583	H	-1.6826	-2.9951	-2.7124
H	2.7594	3.1602	0.8901	H	-3.1943	-3.0682	-0.7186
H	3.9425	-0.6527	2.4636	H	-4.1653	1.0806	-1.2686
H	5.6068	-0.9003	0.6068	H	-2.6369	1.1759	-3.2606
H	5.8207	0.8889	-1.0978	H	-1.3572	-0.8518	-3.9272
C	2.2233	1.3823	2.8092	C	-4.8444	-1.1254	0.1439
H	1.6073	2.3093	2.7479	H	-4.9157	-2.1355	0.6080
O	1.9979	0.5348	3.6557	O	-5.6305	-0.2374	0.3869
O	-0.7941	-2.0713	2.4485	O	-0.8681	-0.4886	2.6617
O	-0.8153	0.2986	3.6831	O	0.2681	1.6176	3.8466
H	0.1112	0.4138	3.9619	H	1.1841	1.3450	3.9645
H	-0.8944	-0.6702	3.4586	H	-0.2376	0.7760	3.7485
Pd	0.6227	-1.3780	1.2954	Pd	0.8262	-1.2973	1.6657

Pd	-1.0367	0.8754	1.5415	Pd	-0.1014	1.5555	1.5338

Int_2B_4

	X	Y	Z
Au	1.0380	0.5760	-1.4358
Au	1.5816	-1.8666	-0.3202
Au	-1.0150	-1.3929	-1.0904
Au	-3.5235	-0.7056	0.0005
Au	-1.6115	1.3383	0.0438
Au	0.5818	3.0000	-0.1183
C	5.6237	-0.9939	-0.8034
C	5.2372	0.1803	-0.1668
C	4.2970	0.1394	0.8652
C	3.7815	-1.0890	1.3034
C	4.1997	-2.2684	0.6889
C	5.1066	-2.2126	-0.3757
H	6.3356	-0.9607	-1.6235
H	5.6465	1.1396	-0.4816
H	3.0954	-1.1134	2.1491
H	3.8311	-3.2217	1.0607
H	5.4213	-3.1337	-0.8602
C	3.8537	1.3955	1.4650
H	4.5532	2.2507	1.3548
O	2.7946	1.5769	2.0517
O	0.3719	-0.8550	2.7992
O	1.3899	-3.1345	1.8236
H	0.6205	-3.6999	1.6976
H	1.0332	-2.3160	2.2850
Pd	-1.3584	-0.9476	1.7773

Int_2B_5

	X	Y	Z
Au	0.3530	1.3678	1.3487
Au	-0.7805	2.9046	-0.8068
Au	-1.0408	0.1455	-1.0161
Au	-1.2648	-2.6445	-0.9945
Au	0.2004	-1.6963	1.2308
Au	2.6542	-0.3458	1.1040
C	-4.8830	-1.0652	0.8257
C	-3.8944	-0.8991	1.7862
C	-3.2317	0.3278	1.9059
C	-3.5632	1.3926	1.0543
C	-4.5507	1.2222	0.0930
C	-5.2057	-0.0050	-0.0201
H	-5.4001	-2.0163	0.7288
H	-3.6228	-1.7193	2.4507
H	-3.0387	2.3397	1.1720
H	-4.8112	2.0433	-0.5705
H	-5.9791	-0.1340	-0.7737
C	-2.1575	0.4664	2.8840
H	-1.9751	-0.4325	3.5159
O	-1.4563	1.4628	3.0333
O	2.9266	-0.2676	-1.0719
O	3.6625	0.4035	-3.7021
H	2.7556	0.2247	-3.9684
H	3.6513	0.2034	-2.7527
Pd	1.2872	-1.4485	-1.2394

Pd	0.7791	0.6097	1.5679	Pd	1.5972	1.4330	-1.0534

Int_3B_2

	X	Y	Z
Au	1.4484	0.7805	-1.2040
Au	2.7800	-1.4050	-0.1302
Au	0.0021	-1.6776	0.0227
Au	-2.7762	-1.4112	-0.1265
Au	-1.4511	0.7751	-1.2067
Au	-0.0053	2.5826	0.3232
O	0.0007	0.7593	3.0634
Pd	-1.3242	0.2397	1.7259
Pd	1.3276	0.2388	1.7281

Int_3B_3

	X	Y	Z
Au	1.4486	0.7784	-1.2034
Au	2.7788	-1.4077	-0.1293
Au	0.0008	-1.6781	0.0225
Au	-2.7772	-1.4100	-0.1281
Au	-1.4500	0.7768	-1.2041
Au	-0.0017	2.5849	0.3212
O	0.0003	0.7593	3.0634
Pd	-1.3253	0.2391	1.7269
Pd	1.3264	0.2396	1.7269

Int_3B_4

	X	Y	Z
Au	-0.1731	-1.9858	-0.0897
Au	-3.1792	-0.2452	-0.7879
Au	-1.0918	1.4774	-0.0633
Au	1.3280	2.7559	0.2419
Au	1.4232	0.3383	-1.2089
Au	2.5407	-1.9004	0.0214
O	-2.2914	-1.9739	0.3442
Pd	0.9347	0.1406	1.4812
Pd	-1.9923	-0.5534	1.6990

Int_3B_5

	X	Y	Z
Au	1.1997	-1.6130	0.5883
Au	3.0476	0.0028	-0.7951
Au	1.3301	1.4255	0.7709
Au	-1.3795	2.3875	-0.3544
Au	-1.2612	-0.0198	1.2930
Au	-1.4413	-2.3590	-0.1425
O	-0.5732	2.0923	1.6009
Pd	-2.6306	-0.0160	-1.2104
Pd	0.1622	-0.0456	-1.4040

	Int_4B_2				Int_4B_3		
	X	Y	Z		X	Y	Z
Au	0.5824	0.9024	-1.6427	Au	-1.6365	-1.6365	0.6768
Au	2.2254	-1.2995	-1.2819	Au	-2.6560	-2.6560	0.2912
Au	-0.3584	-1.6369	-0.3464	Au	0.1569	0.1569	0.2593
Au	-3.0234	-1.5234	0.4660	Au	2.9741	2.9741	0.2837
Au	-2.1952	0.8430	-0.7232	Au	1.5154	1.5154	0.6811
Au	-0.3279	2.6092	0.3349	Au	-0.1806	-0.1806	-1.4660
C	4.8399	-0.8613	0.0644	C	1.2428	1.2428	3.0679
C	4.3110	-1.1235	1.3179	C	0.8067	0.8067	2.1792
C	3.7025	-0.0953	2.0744	C	-0.5683	-0.5683	1.9413
C	3.5855	1.1875	1.4898	C	-1.4897	-1.4897	2.6033
C	4.1149	1.4409	0.2072	C	-1.0455	-1.0455	3.4904
C	4.7538	0.4310	-0.4898	C	0.3123	0.3123	3.7103
H	5.3512	-1.6507	-0.4838	H	2.3027	2.3027	3.2962
H	4.3881	-2.1136	1.7639	H	1.5226	1.5226	1.7153
H	3.2044	2.0114	2.0951	H	-2.5589	-2.5589	2.4899
H	4.0284	2.4378	-0.2188	H	-1.7755	-1.7755	3.9945
H	5.1823	0.6296	-1.4693	H	0.6580	0.6580	4.3826
C	3.3917	-0.3343	3.5398	C	-1.0433	-1.0433	0.9992
H	4.3270	-0.6499	4.0258	H	-2.1025	-2.1025	0.7530
H	3.0925	0.6229	3.9973	H	-0.9358	-0.9358	1.4585
O	2.4476	-1.3370	3.7532	O	-0.2389	-0.2389	-0.1865
H	1.5798	-0.9131	3.5704	H	-0.4882	-0.4882	-0.7641
O	0.6125	0.4461	2.8450	O	-0.0755	-0.0755	-2.7671
Pd	-1.1042	0.0965	1.8510	Pd	1.5153	1.5153	-1.7293
Pd	1.4705	0.1468	1.1268	Pd	-1.4520	-1.4520	-1.7275

	Int_4B_4				Int_4B_5		
	X	Y	Z		X	Y	Z
Au	0.0654	0.6039	-1.3436	Au	-1.1723	1.2241	-0.5863
Au	2.5285	-0.6647	-0.7212	Au	-2.9644	-0.8260	-0.3639
Au	0.1763	-1.9686	-0.1224	Au	-0.1394	-1.4344	0.6023
Au	-2.4512	-2.1825	0.7094	Au	2.8277	-1.3682	0.9618
Au	-2.7665	0.3304	-0.6930	Au	1.6356	0.9009	-0.0649
Au	-1.3372	2.6226	0.0860	Au	0.4926	3.3760	-0.2271
C	5.3062	-0.9114	-0.9386	C	-1.3400	-2.1699	2.9416
C	4.9488	0.3731	-0.5016	C	-0.6336	-0.9620	3.0869
C	4.8956	0.6544	0.8712	C	-1.3088	0.2721	3.0466
C	5.1924	-0.3514	1.7867	C	-2.6881	0.2751	2.8725
C	5.5508	-1.6239	1.3500	C	-3.3925	-0.9251	2.7368
C	5.6043	-1.9094	-0.0097	C	-2.7263	-2.1475	2.7648
H	5.3676	-1.1155	-2.0053	H	-0.8083	-3.1164	3.0193
H	4.7628	1.1678	-1.2225	H	0.4311	-0.9839	3.3257
H	5.1331	-0.1384	2.8529	H	-3.2038	1.2320	2.8394
H	5.7781	-2.4000	2.0764	H	-4.4749	-0.9020	2.6232
H	5.8787	-2.9047	-0.3490	H	-3.2779	-3.0780	2.6583
C	4.5417	2.0248	1.3405	C	-0.5381	1.5556	3.2390
H	4.2551	1.9932	2.4022	H	-0.3544	1.6987	4.3142
H	5.4155	2.6894	1.2409	H	0.4560	1.4517	2.7650
O	3.4746	2.5423	0.5468	O	-1.2165	2.6954	2.7865
H	3.2264	3.4199	0.8624	H	-1.0436	2.7973	1.8424
O	-0.3115	1.9084	2.0180	O	0.6479	-1.8250	-3.1479
Pd	-1.0392	0.1168	1.5128	Pd	1.7176	-1.5786	-1.5584
Pd	1.4223	1.4395	0.9860	Pd	-0.8723	-1.2339	-2.1385

	Int_5B_2				Int_5B_3		
	X	Y	Z		X	Y	Z
Au	-0.5781	1.0095	1.5487	Au	-1.7951	0.7734	0.5811
Au	1.3809	-0.6447	2.7981	Au	-2.6715	-1.9501	0.1344
Au	1.5196	-0.5195	0.0000	Au	0.0450	-1.4938	0.4150
Au	1.3809	-0.6447	-2.7981	Au	2.8366	-1.7153	0.5097
Au	-0.5781	1.0095	-1.5487	Au	1.8794	0.8363	0.6782
Au	-2.7373	-0.1967	0.0000	Au	0.1347	2.1474	-1.5034
C	0.0720	3.4415	1.2122	C	-0.4609	1.5379	3.9414
C	1.3914	2.9486	1.1976	C	0.3190	2.3329	3.0939
C	2.0477	2.6485	0.0000	C	-0.2406	2.9898	2.0042
C	1.3914	2.9486	-1.1976	C	-1.6304	2.8645	1.7770
C	0.0720	3.4415	-1.2122	C	-2.4205	2.0647	2.6328
C	-0.5966	3.6740	0.0000	C	-1.8191	1.3925	3.7105
H	-0.3907	3.7429	2.1517	H	0.0022	1.0364	4.7872
H	1.9137	2.7800	2.1398	H	1.3866	2.4484	3.2868
H	1.9137	2.7800	-2.1398	H	-2.1031	3.4890	1.0169
H	-0.3907	3.7429	-2.1517	H	-3.5016	2.0468	2.5111
H	-1.6126	4.0608	0.0000	H	-2.4290	0.7801	4.3688
C	3.3989	1.9626	0.0000	C	0.6331	3.7604	1.0511
H	3.9474	2.3433	-0.8881	H	0.0343	4.5356	0.5445
H	3.9474	2.3433	0.8881	H	1.4155	4.2774	1.6320
O	3.3736	0.5812	0.0000	O	1.2741	2.9470	0.0978
H	-5.2100	-0.3145	0.0000	H	-0.2545	1.0278	-3.7212
O	-4.6531	0.4741	0.0000	O	-0.9188	1.3221	-3.0840
Pd	-0.7737	-1.7104	-1.4084	Pd	1.5217	-0.5459	-1.7506
Pd	-0.7737	-1.7104	1.4084	Pd	-1.4694	-0.4256	-1.8188

	Int_5B_4				Int_5B_5		
	X	Y	Z		X	Y	Z
Au	-1.7682	-2.3353	-0.5109	Au	1.8094	-0.2104	1.4389
Au	-1.4356	0.5031	-0.8256	Au	2.9542	-1.6045	-0.5896
Au	1.3574	1.5607	-0.9475	Au	1.0062	0.2989	-1.4007
Au	3.4574	-0.2610	-0.5709	Au	-0.8965	2.3401	-1.0140
Au	0.8782	-1.3253	-0.5579	Au	-1.1125	0.3784	1.1110
Au	-0.8916	-0.9236	1.6999	Au	-2.6231	-1.8872	0.3527
C	-4.9952	0.9842	0.1883	C	-0.8170	4.3325	0.5345
C	-4.1398	2.0389	0.4867	C	-0.6696	3.6039	1.7267
C	-3.2604	2.5403	-0.4770	C	0.5539	3.0290	2.0645
C	-3.2278	1.9235	-1.7470	C	1.6571	3.2328	1.2220
C	-4.0947	0.8507	-2.0418	C	1.5324	3.9417	0.0368
C	-4.9775	0.3877	-1.0737	C	0.2874	4.4850	-0.3292
H	-5.6860	0.6204	0.9456	H	-1.7580	4.8291	0.3070
H	-4.1380	2.4941	1.4754	H	-1.5263	3.4664	2.3862
H	-2.6167	2.3665	-2.5366	H	2.6193	2.7999	1.4989
H	-4.0773	0.4051	-3.0340	H	2.3923	4.0829	-0.6130
H	-5.6507	-0.4354	-1.2994	H	0.1974	5.0977	-1.2237
C	-2.3358	3.6867	-0.1411	C	0.6470	2.0812	3.2309
H	-1.7225	3.9223	-1.0335	H	1.6408	2.1780	3.7030
H	-2.9765	4.5772	0.0277	H	-0.1037	2.3695	3.9875
O	-1.5900	3.4999	0.9995	O	0.4154	0.7511	2.8515
H	-0.0091	0.5831	3.6525	H	-4.7704	-3.0544	0.1288
O	0.3790	-0.2355	3.3178	O	-4.0890	-3.1908	0.7995
Pd	1.8030	0.2293	1.6838	Pd	-1.8129	-0.1318	-1.6178
Pd	-0.2259	2.0449	1.1731	Pd	0.1100	-1.9637	-0.1706

	Pro_B_2				Pro_B_3		
	X	Y	Z		X	Y	Z
Au	0.7399	-0.0635	-1.8682	Au	0.0534	-1.7742	-0.5469
Au	2.1187	-2.0687	-0.4464	Au	-2.7971	-1.5309	-0.8234
Au	-0.4504	-1.5465	0.4275	Au	-1.4751	0.8798	-0.6097
Au	-3.1106	-1.0646	1.0106	Au	-0.0195	3.2329	-0.5665
Au	-2.0630	0.4314	-1.1692	Au	1.5607	0.8387	-0.4312
Au	-0.0183	2.4473	-0.8425	Au	1.4633	-0.9370	1.8534
C	0.8817	-4.6329	3.5516	C	1.5427	-2.1374	-2.6812
C	1.1424	-3.2688	3.7065	C	2.5667	-2.6555	-1.8731
C	0.0678	-2.3517	3.7740	C	3.5991	-1.8309	-1.4319
C	-1.2578	-2.8215	3.6415	C	3.6304	-0.4817	-1.8045
C	-1.4987	-4.1776	3.5063	C	2.6148	0.0481	-2.6150
C	-0.4303	-5.0821	3.4699	C	1.5716	-0.7888	-3.0510
H	1.7073	-5.3385	3.5107	H	0.7679	-2.7920	-3.0785
H	2.1617	-2.9114	3.8525	H	2.5568	-3.7068	-1.5852
H	-2.0642	-2.0931	3.6789	H	4.4634	0.1312	-1.4664
H	-2.5199	-4.5415	3.4268	H	2.6749	1.0713	-2.9786
H	-0.6296	-6.1466	3.3697	H	0.7791	-0.3809	-3.6752
C	0.3327	-0.9218	3.9725	C	4.6327	-2.3603	-0.5193
H	1.4006	-0.6604	4.1465	H	4.5239	-3.4459	-0.2807
H	-0.4447	1.7558	4.1090	H	-2.7819	0.8264	2.9580
O	-0.5467	-0.0604	4.0033	O	5.5229	-1.6932	-0.0456
H	-0.5497	2.6782	2.8614	H	-1.6660	0.3520	3.9013
O	-1.0810	2.1944	3.5007	O	-2.4342	0.0430	3.4039
Pd	-1.2550	1.0743	1.3505	Pd	0.0605	1.5579	1.7189
Pd	1.6023	0.5190	0.7181	Pd	-1.3878	-0.9851	1.5859

	Pro_B_4				Pro_B_5		
	X	Y	Z		X	Y	Z
Au	0.7404	-0.0640	-1.8665	Au	0.4206	-1.3835	1.2358
Au	2.1168	-2.0710	-0.4445	Au	2.4263	-1.4828	-0.8122
Au	-0.4529	-1.5461	0.4273	Au	0.8351	0.7740	-0.8765
Au	-3.1128	-1.0620	1.0096	Au	-0.7838	2.9989	-0.5468
Au	-2.0629	0.4332	-1.1699	Au	-1.3789	0.9343	1.3133
Au	-0.0168	2.4467	-0.8410	Au	-2.4201	-1.6115	0.6212
C	4.9008	0.9909	0.0419	C	4.0913	2.6976	0.2915
C	3.8559	1.7124	0.6250	C	3.0792	2.4134	1.2019
C	3.3657	1.3348	1.8968	C	3.0376	1.1681	1.8359
C	3.9107	0.2042	2.5455	C	4.0115	0.2013	1.5557
C	4.9569	-0.4884	1.9613	C	5.0282	0.4929	0.6586
C	5.4562	-0.0899	0.7154	C	5.0630	1.7365	0.0249
H	5.2845	1.2880	-0.9304	H	4.1182	3.6609	-0.2107
H	3.4645	2.6093	0.1449	H	2.3070	3.1512	1.4191
H	3.5035	-0.0751	3.5142	H	3.9542	-0.7621	2.0589
H	5.3912	-1.3449	2.4706	H	5.7948	-0.2482	0.4447
H	6.2827	-0.6364	0.2669	H	5.8596	1.9574	-0.6816
C	2.2927	2.1097	2.5314	C	1.9234	0.8649	2.7331
H	1.9846	3.0265	1.9804	H	1.2764	1.7372	2.9918
H	0.0493	1.9035	3.6199	H	-1.2783	-1.4282	-3.8175
O	1.7903	1.8209	3.6182	O	1.6581	-0.2494	3.1645
H	-1.1928	2.8208	3.4330	H	-2.3658	-2.1073	-2.9746
O	-0.9123	1.9009	3.4140	O	-1.4685	-2.2331	-3.3160
Pd	-1.2540	1.0742	1.3505	Pd	-1.9916	0.5087	-1.3239
Pd	1.6026	0.5166	0.7202	Pd	-0.3436	-1.8494	-1.3213

	Pro_2B_2				Pro_2B_3		
	X	Y	Z		X	Y	Z
Au	-0.3895	1.4482	-1.1825	Au	0.1546	-1.8731	-0.3597
Au	-2.4112	-0.3917	-1.8027	Au	2.9392	-1.2776	-0.8481
Au	-0.0778	-1.4926	-0.7436	Au	1.2551	0.9101	-0.8445
Au	2.4125	-2.2567	0.1672	Au	-0.4880	3.0475	-0.9564
Pd	-1.7614	0.1735	0.8959	Pd	1.6057	-0.6555	1.5676
Au	2.3498	0.4244	-0.6717	Au	-1.7420	0.5094	-0.3955
Au	1.1353	2.5624	0.8325	Au	-1.2032	-0.9713	2.0354
Pd	1.0236	-0.1793	1.6286	Pd	-0.2244	1.6702	1.5050
C	-3.3287	-3.1453	1.8209	C	-2.0913	-0.9961	-2.7071
C	-2.2789	-2.4222	2.3566	C	-3.2583	-0.9961	-1.9443
C	-2.4567	-1.0585	2.6835	C	-3.5657	-2.1041	-1.1290
C	-3.6989	-0.4332	2.4134	C	-2.7154	-3.1979	-1.0850
C	-4.7426	-1.1783	1.8560	C	-1.5356	-3.2059	-1.8454
C	-4.5607	-2.5258	1.5734	C	-1.2213	-2.1041	-2.6539
H	-3.1941	-4.1980	1.5856	H	-1.8613	-0.1586	-3.3622
H	-1.3075	-2.8743	2.5479	H	-3.9820	-0.1833	-2.0078
H	-3.8508	0.6055	2.7067	H	-2.9602	-4.0463	-0.4474
H	-5.6974	-0.7001	1.6551	H	-0.8999	-4.0894	-1.8623
H	-5.3798	-3.1027	1.1507	H	-0.3317	-2.1226	-3.2801
C	-1.3499	-0.2654	3.2246	C	-4.7753	-2.0704	-0.2804
H	-1.6084	0.7573	3.5705	H	-4.9378	-2.9909	0.3286
H	-1.4929	2.7434	1.2863	H	1.7546	3.2462	2.9983
O	-0.1987	-0.7140	3.4068	O	-5.5337	-1.1309	-0.2259
H	-3.1180	4.4322	0.7953	H	2.5731	1.5728	1.6055
O	-2.9015	3.5991	0.3497	O	2.7356	1.6859	2.5674

O	-2.4536	2.8096	1.4521	O	1.5172	2.3060	2.9974

Pro_2B_4

	X	Y	Z
Au	1.5654	-1.6042	-0.1124
Au	2.4273	0.2272	-2.0712
Au	-0.3036	0.3076	-1.5368
Au	-2.9954	-0.1929	-1.1008
Pd	1.5715	1.0683	0.5156
Au	-1.3145	-1.8529	0.4401
Au	0.5095	-0.8982	2.4179
Pd	-1.3988	0.8135	1.0724
C	-2.4070	3.8939	-0.5098
C	-1.0584	3.6962	-0.2677
C	-0.6309	3.1829	0.9733
C	-1.5853	2.8638	1.9721
C	-2.9550	3.0310	1.6883
C	-3.3556	3.5481	0.4581
H	-2.7311	4.3063	-1.4618
H	-0.2991	3.9503	-1.0045
H	-1.2490	2.6365	2.9870
H	-3.6915	2.7956	2.4521
H	-4.4137	3.6905	0.2549
C	0.8049	3.1257	1.3030
H	1.0453	2.9084	2.3641
H	3.9163	1.0918	2.0964
O	1.6969	3.4829	0.5075
H	3.3298	3.2930	1.3285
O	3.9899	2.9616	1.9781

Pro_2B_5

	X	Y	Z
Au	1.6076	0.9485	-0.1758
Au	2.4839	-1.8188	-0.3689
Au	-0.0642	-1.4235	0.6037
Au	-2.6111	-1.0295	1.6113
Pd	0.5702	-0.6372	-2.1054
Au	-1.2863	1.4057	0.8548
Au	-0.4846	2.0055	-1.8381
Pd	-2.0951	-0.2727	-1.0820
C	2.8934	-0.1190	3.2876
C	1.8857	0.8181	3.1341
C	2.0780	1.9078	2.2700
C	3.2853	2.0364	1.5529
C	4.2873	1.0766	1.7062
C	4.0890	0.0090	2.5741
H	2.7526	-0.9631	3.9576
H	0.9396	0.7373	3.6654
H	3.4491	2.9176	0.9316
H	5.2165	1.1703	1.1509
H	4.8705	-0.7368	2.6966
C	1.0357	2.9417	2.1277
H	1.3282	3.8243	1.5148
H	-2.9517	-2.0504	-3.1334
O	-0.0767	2.8629	2.6234
H	-1.7921	-2.9481	-1.1396
O	-1.9685	-3.2540	-2.0499

O	3.3202	1.7777	2.4298	O	-2.0757	-1.9915	-2.7250