

Endohedrally Doped Gold Cages: Efficient Catalysts of O₂ Activation and CO Oxidation

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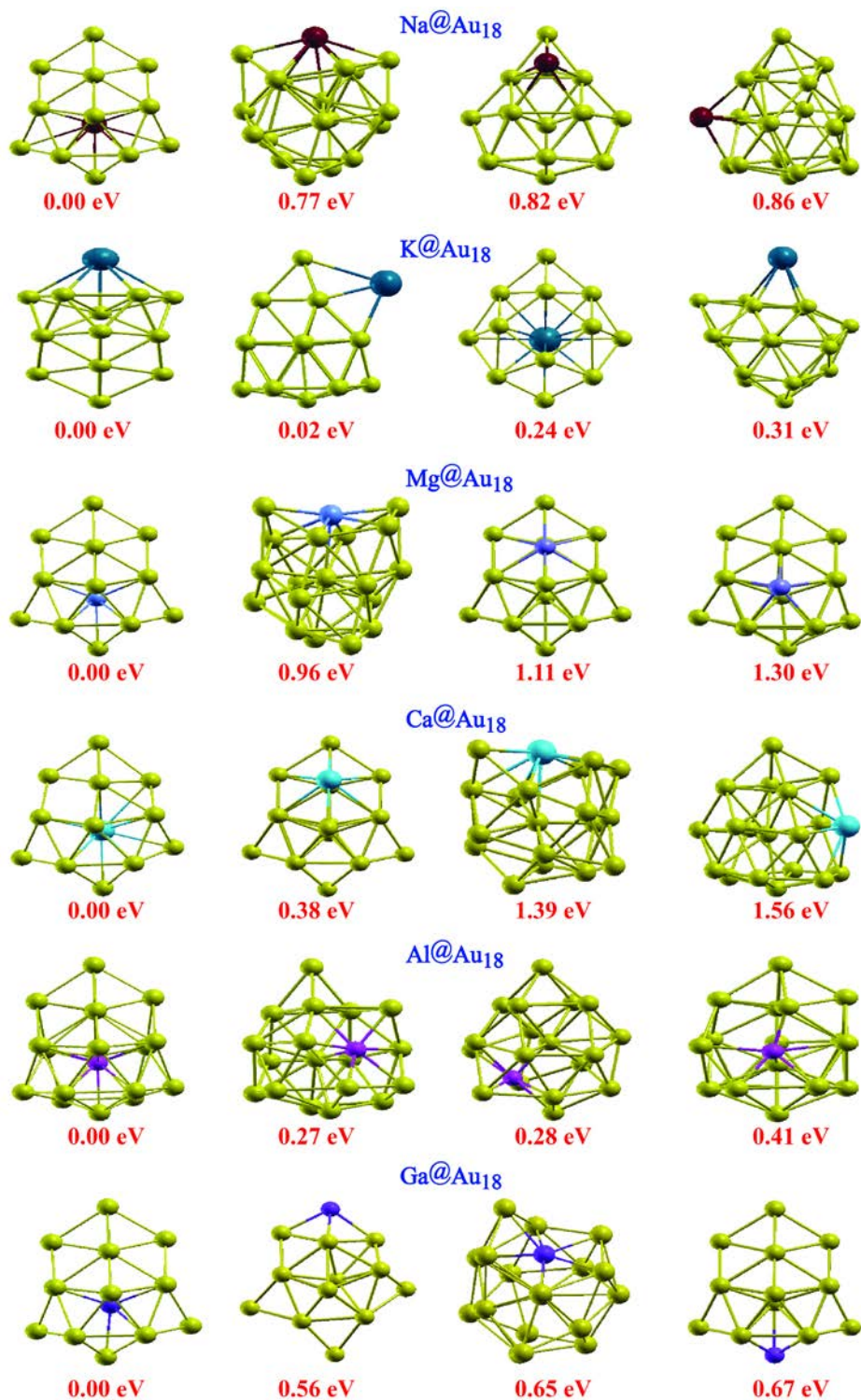


Fig. S1: Relative energies of the four lowest energy isomers of the $M@Au_{18}$ nanocages ($M = Na, K, Mg, Ca, Al$ and Ga).

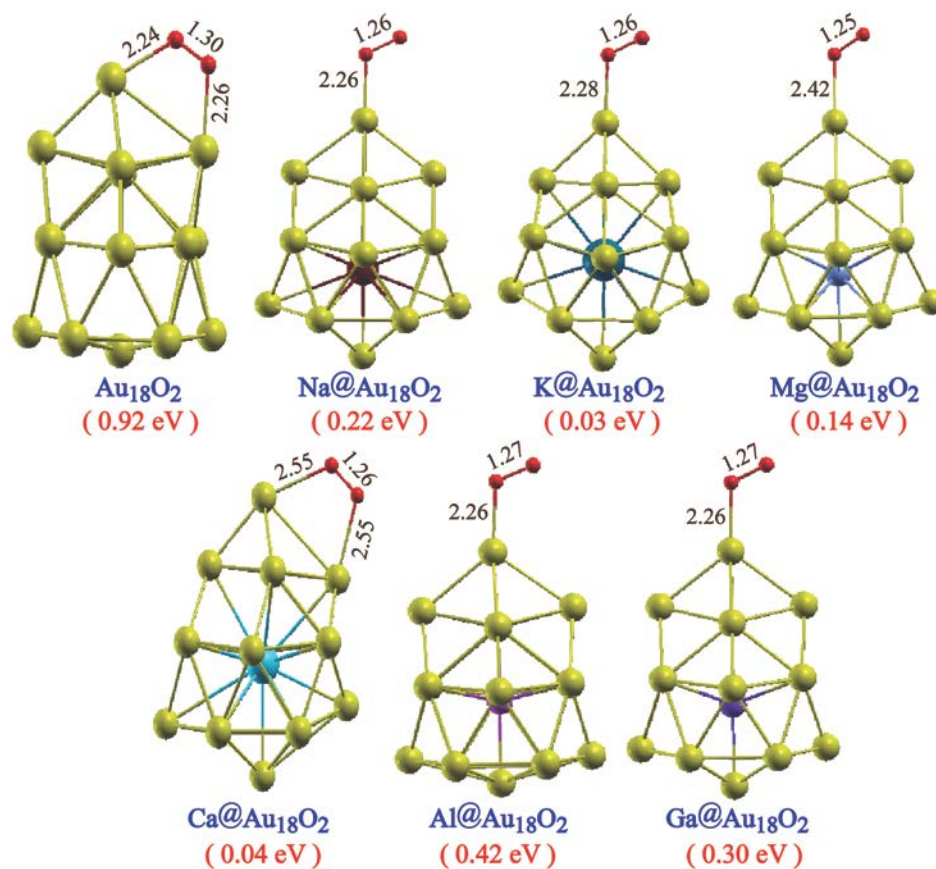


Fig. S2: Optimized geometries of the atop isomers (bridged for the pristine and Ca doped) of the doped gold cages with their relative energies with respect to lowest energy isomers.

Cartesian coordinates of the reactant, the transition state and the product for CO oxidation on the Au_{18} and M@Au_{18} ($\text{M} = \text{Na}, \text{K}, \text{Mg}, \text{Ca}, \text{Al}$ and Ga) clusters.

$\text{Au}_{18}/\text{PBE}$:

Reactant

Au	-2.236537	-1.713118	-0.001512
Au	-0.298376	-1.442450	2.097290
Au	2.248050	2.449521	-1.429317
Au	-0.299016	1.442221	-2.097242
Au	-0.298082	-1.437716	-2.099140

Au	-2.674584	0.001700	-2.250411
Au	-0.035272	-3.332311	-0.003189
Au	2.249015	-2.448796	1.429450
Au	2.249270	-2.445691	-1.434028
Au	2.043258	0.003224	-2.785706
Au	-2.674622	-0.002582	2.250396
Au	-2.237556	1.712743	0.001515
Au	-0.036555	3.332242	0.003058
Au	-0.298817	1.437682	2.099292
Au	2.248135	2.446427	1.433915
Au	2.043181	-0.002559	2.785718
Au	2.444876	0.000413	0.000046
Au	-4.436367	-0.000949	-0.000134

I(1)

O	-6.690078	-0.049648	-0.784376
O	-7.355152	0.090486	0.258405
Au	-4.316854	-0.046189	-0.698338
Au	-2.029458	1.451147	-0.346908
Au	-0.430932	1.540318	1.926553
Au	2.629469	0.021290	0.287692
Au	1.855716	0.200382	2.978428
Au	2.165881	2.565604	1.499348
Au	0.038409	3.261001	-0.280804
Au	0.103722	1.285421	-2.333319
Au	2.555762	-0.168971	-2.518053

Au	2.506933	-2.506608	-0.997497
Au	2.167941	-2.340301	1.827605
Au	0.040749	-3.270964	0.155408
Au	0.104358	-1.585772	-2.138582
Au	-2.230574	-0.181398	-2.693597
Au	-2.041645	-1.504567	-0.155284
Au	-2.917242	0.138007	2.082182
Au	-0.426313	-1.257093	2.094319
Au	2.503536	2.351668	-1.324219
C	-4.386870	0.214850	3.409682
O	-5.174238	0.262398	4.239982

TS(1)

O	-6.161411	-0.540481	0.385952
O	-6.254504	-1.733307	-0.228111
Au	-4.394096	0.782746	0.039414
Au	-2.010747	0.454494	1.395409
Au	0.253209	0.356430	2.928431
Au	0.112488	2.304357	0.840568
Au	2.378213	2.414068	-0.864258
Au	2.141803	0.787409	-3.119292
Au	1.757540	-2.014061	-2.792065
Au	-0.408114	-0.341251	-3.609827
Au	-0.175104	2.002193	-1.996128
Au	-2.392583	2.663184	-0.371675
Au	-2.361006	0.165944	-1.754927

Au	-0.745520	-2.094370	-1.437660
Au	1.582300	-3.071578	-0.185994
Au	2.191880	-1.504932	2.044796
Au	2.618132	1.296126	1.689628
Au	2.446240	-0.401503	-0.569619
Au	-3.126202	-1.953328	0.179840
Au	-0.539698	-1.903330	1.353350
C	-4.999453	-2.669143	-0.376731
O	-5.270825	-3.704027	-0.881330

I(2)

O	5.919367	-0.289491	0.664454
O	5.930699	0.737311	1.592147
Au	4.282614	-0.302742	-0.750139
Au	1.928475	-1.631219	-0.158251
Au	0.452621	-1.354145	2.179570
Au	-2.618201	0.131709	0.305229
Au	-1.785294	0.266732	3.008956
Au	-2.233088	-2.232217	1.847937
Au	-0.212226	-3.308169	0.175929
Au	-0.160784	-1.590302	-2.101629
Au	-2.517028	-0.067896	-2.520660
Au	-2.407028	2.438506	-1.313598
Au	-2.076968	2.642029	1.499417
Au	0.089602	3.282338	-0.290250
Au	-0.022957	1.258538	-2.318447

Au	2.293698	-0.337907	-2.679716
Au	2.141397	1.469083	-0.462119
Au	2.957195	0.021363	2.003289
Au	0.466766	1.419206	1.776911
Au	-2.644769	-2.388819	-0.960862
C	4.796577	0.908318	2.474093
O	4.954001	1.674576	3.377339

TS(2)

O	-5.246286	0.845142	1.044084
O	-5.702451	-0.492544	1.963809
Au	-4.330858	0.348626	-0.823243
Au	-1.922904	1.722529	-0.434582
Au	-0.446972	1.771492	1.915340
Au	2.519293	-0.017906	0.366428
Au	1.713186	0.289009	3.037789
Au	2.256829	2.585305	1.532061
Au	0.253722	3.383526	-0.313048
Au	0.159003	1.381422	-2.360201
Au	2.473276	-0.274244	-2.444671
Au	2.249922	-2.567285	-0.877238
Au	1.852467	-2.297450	1.960592
Au	-0.247920	-3.187898	0.268225
Au	-0.059548	-1.479549	-2.044501
Au	-2.327011	0.058413	-2.727190
Au	-2.226546	-1.374242	-0.225108

Au	-2.971238	0.451162	1.977859
Au	-0.644760	-1.045123	2.110977
Au	2.641762	2.260116	-1.293446
C	-4.670902	-0.751547	2.690824
O	-4.525941	-1.549580	3.585636

Product

O	-4.730725	-0.276049	-1.846083
Au	-4.429354	-0.019602	0.166239
Au	-2.148296	-1.639681	0.101280
Au	-0.304785	-1.444682	-2.057987
Au	2.462850	0.005345	-0.023504
Au	2.040089	-0.046853	-2.790200
Au	2.278529	-2.477063	-1.408063
Au	-0.002273	-3.339810	0.024556
Au	-0.217093	-1.404639	2.092548
Au	2.098763	0.062477	2.778630
Au	2.254039	2.484443	1.362085
Au	2.262579	2.432394	-1.496786
Au	-0.040591	3.336180	-0.104171
Au	-0.249960	1.510461	2.082464
Au	-2.646646	0.041896	2.408287
Au	-2.154745	1.598611	0.036698
Au	-2.718323	-0.030178	-2.309483
Au	-0.320130	1.368768	-2.123656
Au	2.314408	-2.410112	1.448008

Na@Au₁₈/PBE:

Reactant

Au	2.221547	0.000105	1.664412
Au	2.729775	-2.248939	0.000140
Au	0.434530	-2.309037	-1.581459
Au	0.434542	-2.308646	1.581815
Au	-1.749611	-3.115368	0.000268
Au	-3.473765	-0.006653	-0.000078
Au	-2.251730	-1.419167	-2.146517
Au	-2.253040	1.417417	-2.140181
Au	0.433826	2.308849	-1.575420
Au	0.433884	2.308916	1.575162
Au	2.734060	2.247753	-0.000233
Au	2.221451	-0.000163	-1.664434
Au	-0.051712	0.002598	-3.180516
Au	-0.051607	0.003048	3.180640
Au	-2.251699	-1.418740	2.146659
Au	-2.253039	1.417609	2.140004
Au	-1.752477	3.122454	-0.000121
Au	4.514545	-0.001671	-0.000112
Na	-0.498994	-0.002616	-0.000198

I(I)

O	6.253704	-1.878085	-0.360552
O	6.832766	-0.865169	0.144379
Au	4.030835	-1.710663	-0.580677

Au	1.399384	-2.146922	-1.354094
Au	-1.246621	-2.353772	-2.006839
Au	0.202309	-0.024331	-3.062702
Au	-1.068589	2.398256	-2.030067
Au	-1.263521	3.039896	0.783547
Au	-2.142068	0.777635	2.212122
Au	0.751638	1.516433	2.107217
Au	1.230475	2.741165	-0.447595
Au	2.431007	0.467946	-1.434685
Au	3.395156	1.609814	1.005834
Au	-0.043022	-0.990100	2.982231
Au	-2.587589	-2.014566	2.554359
Au	-3.041054	-1.304263	-0.073513
Au	-2.576653	0.051498	-2.560594
Au	-3.301460	1.476427	-0.284791
Na	-0.443034	0.144412	-0.201342
Au	2.012240	-0.969607	1.188420
Au	-0.478295	-2.678901	0.712453
C	5.224566	1.966390	1.694632
O	6.275571	2.196186	2.079598

TS(1)

O	-5.934961	-0.191998	-0.290574
O	-6.225116	0.986768	0.284355
Au	-3.955835	-1.078762	0.003030
Au	-1.605219	-2.464739	0.125514

Au	1.341903	-2.966586	0.205777
Au	-0.142016	-2.199257	2.498227
Au	0.337323	0.539199	3.181567
Au	1.326416	3.675473	-0.170818
Au	2.325935	1.481393	-1.557212
Au	-0.673275	2.151474	-1.513852
Au	-0.690577	2.316034	1.293205
Au	-2.010240	-0.131801	1.802926
Au	-3.147158	1.791333	-0.160724
Au	0.440211	0.182752	-3.183505
Au	2.469347	-1.358875	-1.894149
Au	3.965433	-0.196230	0.085269
Au	2.405209	-1.129655	2.148372
Au	2.285978	1.650695	1.489552
Na	0.429287	-0.183613	0.033878
Au	-1.941520	-0.345044	-1.820714
Au	-0.061623	-2.471920	-2.214979
C	-5.136450	2.159680	0.359356
O	-5.604406	3.149276	0.802354

I(2)

O	-5.818974	-0.081201	-0.418990
O	-6.016994	1.040029	0.458623
Au	-3.984240	-1.125270	-0.119915
Au	-1.639129	-2.500474	0.087599
Au	1.343362	-2.957309	0.245850

Au	-0.224236	-2.174804	2.478661
Au	0.206766	0.565725	3.161649
Au	1.270679	3.687944	-0.233397
Au	2.317978	1.480298	-1.570660
Au	-0.663451	2.141144	-1.611913
Au	-0.741527	2.339479	1.230534
Au	-2.087334	-0.133511	1.727075
Au	-3.140539	1.760331	-0.267632
Au	0.470802	0.130793	-3.204109
Au	2.494835	-1.365174	-1.843316
Au	3.914200	-0.121151	0.161849
Au	2.327101	-1.085193	2.192648
Au	2.173836	1.688406	1.494332
Na	0.388973	-0.189509	0.011939
Au	-1.937647	-0.373700	-1.887018
Au	-0.029005	-2.494630	-2.196240
C	-5.098975	2.045818	0.502730
O	-5.340114	3.071206	1.087676

TS(2)

O	-5.265424	0.453548	-0.713616
O	-5.838813	1.308675	0.636894
Au	-3.945062	-1.173253	-0.220343
Au	-1.642868	-2.559184	0.065589
Au	1.317842	-2.968191	0.319964
Au	-0.295082	-2.146506	2.495121

Au	0.109173	0.620896	3.146094
Au	1.242217	3.708166	-0.276032
Au	2.344919	1.475026	-1.506825
Au	-0.641214	2.110833	-1.681967
Au	-0.821124	2.344347	1.142854
Au	-2.149021	-0.148260	1.697867
Au	-3.123039	1.739784	-0.345562
Au	0.580654	0.099627	-3.200442
Au	2.538374	-1.362645	-1.726913
Au	3.934545	-0.106664	0.283066
Au	2.247594	-1.048096	2.240564
Au	2.085395	1.719297	1.492074
Na	0.344966	-0.201921	0.013507
Au	-1.883889	-0.409372	-1.981119
Au	0.044133	-2.524487	-2.172518
C	-4.930303	2.168909	0.882467
O	-4.864919	3.096968	1.653029

Product

O	-4.734983	1.563560	-0.327836
Au	-4.177946	-0.405081	0.031796
Au	-2.136179	-2.228237	0.091935
Au	0.768579	-3.096357	0.103071
Au	-0.586453	-2.160642	2.408256
Au	0.324095	0.437713	3.175898
Au	1.789379	3.476465	-0.121068

Au	2.346588	1.187716	-1.589306
Au	-0.429761	2.328873	-1.478681
Au	-0.387580	2.445646	1.362458
Au	-2.104299	0.177285	1.845117
Au	-2.815231	2.354670	-0.011564
Au	0.268464	0.236061	-3.212373
Au	2.080152	-1.636003	-2.001685
Au	3.736593	-0.721730	-0.022282
Au	2.109248	-1.513884	2.063143
Au	2.404226	1.287711	1.493576
Na	0.241762	-0.211070	0.009273
Au	-2.134471	0.032428	-1.854605
Au	-0.609574	-2.331580	-2.251779

K@Au₁₈/PBE:

Reactant

Au	-2.280307	2.001091	0.000135
Au	-2.379610	0.000098	-2.103343
Au	-0.497457	-2.029349	-2.388452
Au	-0.497554	2.029718	-2.388112
Au	1.331948	0.000349	-3.094542
Au	3.531758	0.000187	0.000291
Au	2.261415	-2.095877	-1.442426
Au	2.261134	-2.096025	1.442474
Au	-0.497762	-2.030145	2.388087
Au	-0.498383	2.029417	2.388323

Au	-2.379894	-0.000786	2.102865
Au	-2.280128	-2.001330	-0.000613
Au	0.159490	-3.352237	-0.000333
Au	0.159047	3.352211	0.000277
Au	2.261245	2.096472	-1.442006
Au	2.260825	2.096146	1.442922
Au	1.330925	-0.000093	3.094812
Au	-4.304439	0.000156	-0.000376
K	0.240118	-0.000006	0.000084

I(1)

O	-6.247504	1.666981	0.002874
O	-6.911241	0.584301	-0.082980
Au	-3.985894	1.530821	0.005084
Au	-1.388693	2.521314	-0.001714
Au	1.264528	3.284331	-0.003344
Au	0.298911	2.016661	-2.354294
Au	0.165622	-0.702661	-3.156144
Au	1.605324	-2.584106	-1.491669
Au	1.609041	-2.579667	1.496111
Au	-1.229823	-2.385935	1.415387
Au	-1.232845	-2.387364	-1.409034
Au	-2.071933	0.385487	-1.782529
Au	-3.503043	-1.421130	0.003833
Au	0.169037	-0.695814	3.157370
Au	2.642498	0.226231	2.315750

Au	3.483675	1.597884	-0.004393
Au	2.640480	0.218860	-2.319333
Au	3.564590	-1.222040	-0.001260
K	0.519350	-0.031864	-0.000143
Au	-2.069762	0.388324	1.785470
Au	0.300137	2.021864	2.350263
C	-5.371182	-2.141753	0.011064
O	-6.382088	-2.673268	0.017307

TS(1)

O	5.951025	0.692089	-0.422533
O	6.354751	-0.570602	-0.672240
Au	3.833997	1.235121	-0.706261
Au	1.361299	2.315384	-0.978771
Au	-1.266026	3.155760	-1.141989
Au	-0.225047	2.739079	1.468017
Au	-0.143187	0.422720	3.167466
Au	-1.584686	-1.909208	2.297679
Au	-1.750865	-2.895139	-0.471030
Au	1.101578	-2.755645	-0.593742
Au	1.269293	-1.756960	2.044938
Au	2.064919	0.972612	1.498299
Au	3.477166	-1.450382	0.330020
Au	-0.406171	-1.771625	-2.755427
Au	-2.815101	-0.529632	-2.196111
Au	-3.531287	1.590784	-0.487497

Au	-2.595018	1.162897	2.113402
Au	-3.574517	-1.013093	0.530638
K	-0.551480	-0.009158	-0.016756
Au	1.889217	-0.324678	-2.041276
Au	-0.490448	1.089494	-2.936989
C	5.429981	-1.777492	-0.335484
O	5.948814	-2.817239	-0.564787

I(2)

O	5.787066	0.404102	-0.125912
O	5.936698	-0.788418	-0.939639
Au	3.899483	1.369113	-0.393800
Au	1.466764	2.487152	-0.754630
Au	-1.159040	3.277768	-1.005706
Au	-0.163018	2.812825	1.599311
Au	-0.385242	0.462660	3.184652
Au	-1.518015	-2.020934	2.313747
Au	-1.661863	-2.999032	-0.403010
Au	1.089478	-3.032152	-0.127138
Au	1.316406	-1.648010	2.352785
Au	2.069141	1.060551	1.766912
Au	3.251324	-1.328218	0.308110
Au	0.103831	-1.868944	-2.520483
Au	-2.556029	-1.077572	-2.280690
Au	-3.117801	1.338091	-1.069320
Au	-2.631864	1.460809	1.728127

Au	-3.425957	-0.955212	0.524068
K	-0.325428	-0.076470	0.065969
Au	2.016110	0.096716	-2.175521
Au	-0.604974	1.043706	-2.758302
C	5.020286	-1.771753	-0.802314
O	5.145169	-2.838518	-1.344361

TS(2)

O	-5.414879	0.101931	0.880539
O	-6.199076	-0.570872	-0.463803
Au	-3.858580	1.554154	0.361488
Au	-1.409326	2.626492	0.060558
Au	1.252461	3.304061	-0.258833
Au	0.052559	1.879927	-2.398841
Au	-0.130414	-0.952328	-2.963965
Au	1.299729	-2.763586	-1.266349
Au	1.585901	-2.503149	1.648976
Au	-1.276802	-2.211689	1.830587
Au	-1.491520	-2.457163	-0.999936
Au	-2.248461	0.375742	-1.665862
Au	-3.568401	-1.373760	0.428871
Au	0.376361	-0.488572	3.313535
Au	2.768029	0.307081	2.191541
Au	3.451604	1.532108	-0.220175
Au	2.364372	0.148203	-2.410541

Au	3.377616	-1.259743	-0.131626
K	0.384607	-0.019776	0.081348
Au	-1.912062	0.634700	2.179557
Au	0.537194	2.199362	2.263472
C	-5.418836	-1.516840	-0.819163
O	-5.494322	-2.374788	-1.662146

Product

O	-4.451033	0.364869	0.021629
Au	-3.056940	1.816905	0.717082
Au	-0.794964	3.173212	-0.123180
Au	1.517192	2.702780	-1.576427
Au	-0.765417	1.592586	-2.655926
Au	-0.994458	-1.202617	-2.765614
Au	1.094436	-2.733294	-1.796251
Au	1.141155	-2.624463	1.295675
Au	-1.441852	-2.187461	2.290436
Au	-1.282201	-2.996609	-0.419749
Au	-3.077931	0.359851	-1.843819
Au	-3.368412	-1.424739	0.476617
Au	0.152580	-0.228588	3.443709
Au	2.517200	-0.243031	2.025812
Au	3.373366	1.121034	-0.282287
Au	1.786612	-0.029920	-2.445262
Au	3.156821	-1.624160	-0.345962

K -0.216552 0.013521 0.122071

Au -1.015528 2.133928 2.528208

Au 1.561162 2.354384 1.445390

Mg@Au₁₈/PBE:

Reactant

Au -2.183663 0.000009 -1.522375

Au -2.840278 -2.262553 -0.000003

Au -0.411419 -2.225491 1.459092

Au -0.411418 -2.225488 -1.459097

Au 1.785370 -3.250818 -0.000003

Au 3.575513 -0.000129 0.000001

Au 2.241253 -1.416122 2.078376

Au 2.241289 1.416089 2.078196

Au -0.411398 2.225469 1.459017

Au -0.411397 2.225472 -1.459013

Au -2.840351 2.262516 0.000001

Au -2.183664 0.000006 1.522373

Au 0.054781 0.000037 3.171146

Au 0.054783 0.000044 -3.171146

Au 2.241255 -1.416117 -2.078378

Au 2.241291 1.416094 -2.078191

Au 1.785207 3.251106 0.000004

Au -4.637352 -0.000107 -0.000002

Mg 0.725483 -0.000114 0.000000

I(1)

O	6.836854	-0.823753	0.549903
O	7.491523	0.237473	0.642509
Au	4.463853	-0.703881	-0.083447
Au	2.032751	-0.248362	1.380575
Au	-0.122752	-0.051063	3.141729
Au	-0.018327	-2.331561	1.464607
Au	-2.394416	-3.025603	0.036476
Au	-2.558582	-1.146312	-2.019969
Au	-2.190414	1.654495	-2.142360
Au	-0.181945	-0.082148	-3.132726
Au	-0.048404	-2.338388	-1.442601
Au	2.342045	-2.679177	-0.019337
Au	2.058944	-0.272073	-1.492475
Au	0.552806	2.087051	-1.443861
Au	-1.527054	3.352257	-0.004913
Au	-2.143590	1.676448	2.165277
Au	-2.513967	-1.127110	2.076250
Au	-3.627361	0.509651	0.036605
Mg	-0.840129	0.052503	0.009630
Au	3.131620	1.943216	-0.047237
Au	0.578750	2.122954	1.420484
C	4.365109	3.486847	-0.078497
O	5.047659	4.406017	-0.092113
TS(1)			
O	-6.161411	-0.540481	0.385952

O	-6.254504	-1.733307	-0.228111
Au	-4.394096	0.782746	0.039414
Au	-1.967582	0.388964	1.479774
Au	0.228074	0.218366	3.134586
Au	0.080153	2.452451	1.328557
Au	2.471204	2.710789	-0.186117
Au	2.556682	1.061440	-2.430721
Au	2.164345	-1.718353	-1.897288
Au	0.139804	-0.125156	-3.125101
Au	0.043675	2.288442	-1.578462
Au	-2.394414	2.672007	-0.113336
Au	-2.022586	0.229980	-1.457495
Au	-0.605079	-2.172746	-1.303262
Au	1.413643	-3.466978	0.171313
Au	2.203852	-1.507491	2.013472
Au	2.612110	1.315598	2.214019
Au	3.569715	-0.121475	-0.041260
Mg	0.763011	0.028812	-0.010439
Au	-3.126202	-1.953328	0.179840
Au	-0.586823	-2.024919	1.554307
C	-4.999453	-2.669143	-0.376731
O	-5.270825	-3.704027	-0.881330
I(2)			
O	-5.900047	-0.672311	0.593371
O	-6.016775	-1.760273	-0.327540

Au	-4.424074	0.796470	0.085053
Au	-2.007293	0.385633	1.495851
Au	0.198443	0.293577	3.139820
Au	0.025863	2.432932	1.280237
Au	2.381072	2.970688	-0.226508
Au	2.526497	0.984005	-2.166960
Au	2.106032	-1.816302	-2.233575
Au	0.077729	-0.109564	-3.134760
Au	-0.011402	2.253217	-1.579764
Au	-2.474389	2.698535	-0.136658
Au	-2.058908	0.204729	-1.425272
Au	-0.595225	-2.213819	-1.303066
Au	1.621264	-3.112808	0.187439
Au	2.206735	-1.519130	2.399089
Au	2.582449	1.253270	1.937796
Au	3.434917	-0.640913	-0.015275
Mg	0.725969	-0.032337	-0.013800
Au	-3.053387	-2.025533	0.210243
Au	-0.548258	-2.016285	1.609745
C	-4.957048	-2.617711	-0.481952
O	-5.086477	-3.640322	-1.102576
TS(2)			
O	-5.346469	0.616374	-0.261871
O	-5.880861	1.500335	1.111937
Au	-4.301316	-1.250489	0.061110

Au	-1.950603	-0.516863	-1.416996
Au	0.200636	-0.116248	-3.083697
Au	0.265351	-2.437248	-1.409546
Au	2.698432	-2.524789	0.040931
Au	2.666120	-0.917632	2.314055
Au	2.016340	1.826824	1.848978
Au	0.184914	0.048677	3.126957
Au	0.265802	-2.338978	1.497764
Au	-2.148334	-2.933188	0.056622
Au	-1.972364	-0.503674	1.531345
Au	-0.780062	2.084228	1.385696
Au	1.100916	3.599952	-0.108739
Au	2.058816	1.738993	-1.970574
Au	2.709123	-1.044756	-2.303255
Au	3.584900	0.381642	-0.015416
Mg	0.764733	0.014122	-0.025989
Au	-3.208706	1.702614	0.048667
Au	-0.776883	2.020939	-1.493460
C	-4.894538	2.271972	1.367897
O	-4.739597	3.155355	2.177131

Product

O	4.989440	1.486310	-0.214772
Au	4.411982	-0.480899	-0.000023
Au	2.082798	-0.071151	1.543532
Au	-0.164391	0.303074	3.132335

Au	0.368699	-2.274809	1.929006
Au	-1.588206	-2.921919	0.022147
Au	-2.281812	-1.370182	-2.225730
Au	-2.248646	1.386358	-1.555881
Au	-0.163936	0.243448	-3.137698
Au	0.370681	-2.312651	-1.888572
Au	2.443777	-2.524976	0.032280
Au	2.077676	-0.102257	-1.538787
Au	0.527360	2.301794	-1.393938
Au	-1.624334	3.627992	-0.025566
Au	-2.248729	1.416818	1.534733
Au	-2.278024	-1.328022	2.237818
Au	-3.688997	-0.535282	0.002352
Mg	-0.456210	-0.243018	0.002288
Au	3.017644	2.185985	-0.013249
Au	0.550494	2.343081	1.366643

Ca@Au₁₈/PBE:

Reactant

Au	2.326173	0.046457	1.838686
Au	2.482863	-2.083780	-0.000002
Au	0.567819	-2.315866	-2.010860
Au	0.567842	-2.315835	2.010888
Au	-1.237948	-3.182903	0.000034
Au	-3.587590	-0.322911	0.000021
Au	-2.164985	-1.553220	-2.150423

Au	-2.367596	1.282970	-2.045960
Au	0.326275	2.434079	-1.515813
Au	0.326279	2.434114	1.515769
Au	2.630835	2.169484	-0.000018
Au	2.326142	0.046446	-1.838701
Au	-0.076380	0.186661	-3.203898
Au	-0.076339	0.186717	3.203886
Au	-2.164959	-1.553182	2.150472
Au	-2.367572	1.283008	2.045960
Au	-1.966912	3.132624	-0.000023
Au	4.546039	0.158617	-0.000019
Ca	-0.355448	-0.132239	0.000002

I(1)

O	-6.610281	-1.559284	0.503018
O	-7.615118	-0.822155	0.386140
Au	-4.415743	-0.741249	-0.092067
Au	-2.109837	-0.249230	-1.570471
Au	0.165149	0.153063	-3.141577
Au	0.063029	-2.415041	-1.996031
Au	2.068944	-2.909666	-0.015032
Au	2.565104	-1.179476	2.174714
Au	2.222553	1.635433	2.141587
Au	0.106640	0.092090	3.146228
Au	0.025382	-2.454484	1.938821
Au	-1.902683	-2.651029	-0.048759

Au	-2.125318	-0.285642	1.504899
Au	-0.721104	2.226478	1.459280
Au	1.479137	3.327206	0.051125
Au	2.266860	1.680650	-2.062489
Au	2.610999	-1.133763	-2.152601
Au	3.739748	0.342614	0.046672
Ca	0.647627	-0.097049	0.001055
Au	-3.223609	1.868022	-0.038037
Au	-0.679440	2.262105	-1.443008
C	-4.450678	3.417113	0.015568
O	-5.146787	4.326450	0.051885

TS(1)

O	6.215506	-0.045539	-0.389128
O	6.422453	1.129586	0.233396
Au	4.300000	-1.185977	-0.053312
Au	2.157546	-0.370266	1.587311
Au	-0.100500	-0.009887	3.092320
Au	-0.323666	-2.520271	1.679516
Au	-2.698359	-2.528909	0.128029
Au	-2.779704	-0.923880	-2.122289
Au	-1.993091	1.805418	-2.222191
Au	-0.235251	-0.235199	-3.117461
Au	-0.357046	-2.618163	-1.498430
Au	1.976367	-2.719584	0.080625
Au	2.065020	-0.511182	-1.639980

Au	0.909922	2.050767	-1.637495
Au	-1.072662	3.370862	-0.107259
Au	-1.936495	1.943660	2.131583
Au	-2.688637	-0.786956	2.290404
Au	-3.592670	0.800102	0.026572
Ca	-0.635448	0.007398	0.004506
Au	3.334987	1.675434	-0.182905
Au	0.945148	2.169714	1.448557
C	5.268608	2.159525	0.427177
O	5.628996	3.146675	0.973564

I(2)

O	-5.891099	0.596207	0.259319
O	-5.803561	1.672972	-0.686854
Au	-4.358574	-0.902652	0.073695
Au	-2.137578	-0.231200	-1.574892
Au	0.104070	0.184808	-3.120627
Au	0.028214	-2.332980	-1.789805
Au	2.503826	-2.654428	-0.461101
Au	2.808237	-1.214665	1.886101
Au	2.134075	1.513211	2.354107
Au	0.343038	-0.641801	3.090267
Au	0.181371	-2.730541	1.163749
Au	-2.315845	-2.701996	-0.193614
Au	-2.036668	-0.610923	1.662125
Au	-0.759228	1.851568	2.142319

Au	0.995158	3.235797	0.432359
Au	1.953994	2.097153	-1.967892
Au	2.664911	-0.632296	-2.355852
Au	3.614013	0.794264	-0.021902
Ca	0.609078	0.073272	0.007449
Au	-2.987476	1.839599	0.388483
Au	-0.870613	2.341866	-1.486728
C	-4.720129	2.500722	-0.650833
O	-4.704088	3.524872	-1.283280

TS(2)

O	-5.184745	0.957342	0.110124
O	-5.649121	1.881727	1.442790
Au	-4.174869	-0.968772	0.281719
Au	-2.109404	-0.199504	-1.477514
Au	0.101711	0.134144	-3.106679
Au	0.010848	-2.468654	-1.975289
Au	2.169117	-2.925642	-0.177939
Au	2.809537	-1.284133	2.021909
Au	2.409337	1.553166	2.061939
Au	0.475288	-0.093407	3.225744
Au	0.211558	-2.587249	1.844629
Au	-1.940675	-2.608152	0.028270
Au	-1.885902	-0.412531	1.846188
Au	-0.488177	2.144883	1.686222
Au	1.539648	3.281107	0.060617

Au	2.212306	1.688281	-2.117697
Au	2.591305	-1.138787	-2.290240
Au	3.779333	0.304205	-0.125931
Ca	0.688301	-0.147032	0.005694
Au	-2.960687	1.929252	0.428254
Au	-0.688457	2.244088	-1.317992
C	-4.596743	2.570061	1.730816
O	-4.431214	3.421299	2.571418

Product

O	5.162958	0.792330	0.144694
Au	4.124803	-1.001461	-0.036173
Au	2.197194	-0.206632	1.827070
Au	-0.189266	0.499867	3.096063
Au	0.269307	-2.220878	2.267313
Au	-1.232192	-2.966474	-0.012922
Au	-2.423609	-1.304224	-2.066821
Au	-2.577351	1.529581	-1.800130
Au	-0.259454	0.570606	-3.074428
Au	0.199218	-2.169631	-2.328320
Au	1.815029	-2.522521	-0.060689
Au	2.158843	-0.184337	-1.863602
Au	1.063972	2.462391	-1.430291
Au	-1.270853	3.188949	0.005706
Au	-2.499688	1.519813	1.863345

Au	-2.357915	-1.326010	2.106925
Au	-3.848754	-0.235952	0.047471
Ca	-0.413714	0.036352	-0.001019
Au	3.369279	1.841867	-0.000411
Au	1.043345	2.435605	1.445498

Al@Au₁₈/PBE:

Reactant

Au	2.277718	1.617123	-0.318542
Au	2.773098	0.456119	2.285079
Au	0.382478	-1.058894	2.567635
Au	0.316528	1.707052	1.712709
Au	-1.925968	0.602138	2.948108
Au	-3.130034	0.025351	-0.007672
Au	-2.202325	-1.962552	1.841183
Au	-2.201136	-2.519478	-0.957802
Au	0.384628	-1.958688	-1.974049
Au	0.318784	0.927713	-2.233257
Au	2.774808	-0.446226	-2.285778
Au	2.106625	-1.386191	0.273748
Au	0.049227	-3.209899	0.634429
Au	0.025491	3.240166	-0.638927
Au	-2.254278	2.556847	0.940993
Au	-2.251507	2.008011	-1.843638

Au -1.924708 -0.564210 -2.952521

Au 4.571765 0.031008 -0.003997

Al -0.554182 -0.397382 0.074741

I(1)

O -6.124362 1.648085 -0.290739

O -6.706007 0.513473 -0.201595

Au -3.883483 1.643573 -0.204146

Au -1.332639 2.693524 -0.468972

Au 1.197873 3.728503 -0.883428

Au 0.561260 1.312922 -2.211589

Au 0.009036 -1.321754 -3.033601

Au 1.165511 -2.542265 -0.716737

Au 1.707774 -2.181791 2.078692

Au -0.973561 -1.880459 1.273991

Au -1.652077 -2.824113 -1.307285

Au -1.698740 -0.024738 -1.158806

Au -3.604528 -1.386589 0.484693

Au 0.160290 -0.099111 3.222263

Au 2.772780 0.469617 2.263030

Au 2.826477 1.455490 -0.426935

Au 2.651781 -0.662409 -2.390107

Au 3.612894 -1.250067 0.161573

Al 0.791561 -0.104873 0.259596

Au -1.908248 0.829556 1.639628

Au 0.637706 2.221542 1.527165

C -5.519553 -1.897524 0.752160

O -6.536053 -2.359612 0.993251

TS(1)

O -5.860085 1.289887 -0.624562

O -6.522790 0.390397 0.111520

Au -3.722403 1.672433 -0.359648

Au -1.204927 2.735806 -0.551018

Au 1.362532 3.664806 -0.951541

Au 0.638126 1.256984 -2.297205

Au -0.028625 -1.424942 -3.014550

Au 1.029072 -2.574825 -0.656445

Au 1.560912 -2.215137 2.126901

Au -1.159324 -1.793313 1.361508

Au -1.788089 -2.811612 -1.205601

Au -1.534230 -0.028800 -1.079473

Au -3.741078 -1.188154 0.404253

Au 0.157586 -0.019558 3.225127

Au 2.810505 0.404555 2.293446

Au 2.829528 1.308454 -0.445644

Au 2.630693 -0.811949 -2.392843

Au 3.505009 -1.363220 0.187520

Al 0.787727 -0.158402 0.425657

Au -1.861076 1.013607 1.657700

Au 0.744079 2.270474 1.500904

C -5.784404 -0.966870 0.681631

O -6.563221 -1.641877 1.251639

I(2)

O -5.633189 1.049646 -0.677268

O -6.239383 0.445551 0.482315

Au -3.648039 1.770899 -0.381088

Au -1.118460 2.816170 -0.516413

Au 1.497474 3.651705 -0.868591

Au 0.657434 1.320960 -2.302029

Au -0.098995 -1.333954 -3.060201

Au 0.939478 -2.583184 -0.712657

Au 1.484978 -2.301779 2.121826

Au -1.217816 -1.789243 1.367831

Au -1.827459 -2.764133 -1.252952

Au -1.486129 0.029785 -1.029510

Au -3.765280 -1.217971 0.270407

Au 0.146462 -0.051446 3.223505

Au 2.816134 0.288713 2.300449

Au 2.828610 1.223509 -0.425289

Au 2.565059 -0.824337 -2.414110

Au 3.394120 -1.490841 0.158157

Al 0.768886 -0.201342 0.506254

Au -1.825759 1.083348 1.660722

Au 0.803556 2.249400 1.547530

C -5.705721 -0.734560 0.927751

O -6.283081 -1.383414 1.761548

TS(2)

O	-5.300672	0.485626	-0.541223
O	-6.077757	0.173065	0.941535
Au	-3.647777	1.841932	-0.379312
Au	-1.151408	2.875623	-0.385323
Au	1.465839	3.732792	-0.504515
Au	0.769067	1.526872	-2.215404
Au	0.104792	-1.106813	-3.185688
Au	1.003268	-2.476270	-0.876539
Au	1.400098	-2.447109	1.959708
Au	-1.271376	-2.030840	1.147154
Au	-1.769635	-2.603941	-1.606815
Au	-1.458824	0.153898	-1.221194
Au	-3.689590	-1.232445	0.098843
Au	-0.036382	-0.357985	3.223566
Au	2.652813	0.126240	2.456504
Au	2.741323	1.263796	-0.175400
Au	2.713933	-0.609998	-2.346349
Au	3.444046	-1.430125	0.210916
Al	0.629988	-0.228201	0.515043
Au	-1.890160	0.841498	1.582123
Au	0.655530	2.127700	1.750019
C	-5.465286	-0.856675	1.384729
O	-5.647456	-1.569254	2.342799

Product

O	-5.147947	0.337580	-0.095286
Au	-3.700660	1.806657	-0.199892
Au	-1.186110	2.835927	-0.648621
Au	1.440502	3.568133	-1.193311
Au	0.493211	1.176287	-2.425768
Au	-0.277612	-1.530732	-2.940341
Au	0.821647	-2.682794	-0.595042
Au	1.327454	-2.209178	2.200945
Au	-1.437245	-1.622440	1.587261
Au	-1.929889	-2.863541	-0.973864
Au	-1.523097	-0.000807	-0.905467
Au	-3.876595	-1.283769	0.189354
Au	0.123594	0.122570	3.275972
Au	2.754639	0.370701	2.256572
Au	2.688370	1.153976	-0.558789
Au	2.419955	-0.969702	-2.424937
Au	3.249212	-1.511510	0.176609
Al	0.664454	-0.226934	0.550390
Au	-1.799982	1.325490	1.743133
Au	0.824578	2.317890	1.355266

Ga@Au₁₈/PBE:

Reactant

Au	-2.223764	-0.092931	1.617023
Au	-2.884124	2.160275	0.000011
Au	-0.503411	2.217215	-1.485072

Au	-0.503411	2.217194	1.485094
Au	1.656149	3.281818	0.000014
Au	3.336422	-0.080999	0.000003
Au	2.161850	1.472750	-2.090776
Au	2.282400	-1.357518	-2.337392
Au	-0.288854	-2.211553	-1.486052
Au	-0.288857	-2.211558	1.486022
Au	-2.662672	-2.398583	-0.000017
Au	-2.223751	-0.092913	-1.617020
Au	-0.007408	0.028226	-3.253257
Au	-0.007416	0.028187	3.253257
Au	2.161846	1.472724	2.090800
Au	2.282396	-1.357546	2.337382
Au	2.018225	-2.898951	-0.000014
Au	-4.544459	-0.195553	-0.000007
Ga	0.608654	0.050240	-0.000005

I(1)

O	-6.619420	-1.182247	-0.000713
O	-7.454702	-0.225067	0.005524
Au	-4.425529	-0.712240	-0.000512
Au	-2.066975	-0.241233	-1.456390
Au	0.068614	-0.057756	-3.202021
Au	0.079486	-2.342212	-1.481985
Au	2.502570	-2.744159	0.000528
Au	2.525260	-1.142378	2.277454

Au	2.155294	1.668041	2.347672
Au	0.067865	-0.057106	3.201981
Au	0.079155	-2.341915	1.482403
Au	-2.271922	-2.688370	-0.000024
Au	-2.067345	-0.240993	1.455952
Au	-0.543861	2.133595	1.445691
Au	1.676442	3.113097	-0.000156
Au	2.155856	1.667560	-2.347572
Au	2.525794	-1.142845	-2.276703
Au	3.220589	0.429229	0.000301
Ga	0.594999	-0.030392	0.000033
Au	-3.092449	2.010912	-0.000667
Au	-0.543512	2.133355	-1.446369
C	-4.416644	3.488796	-0.000557
O	-5.116686	4.393227	-0.000382

TS(1)

O	-5.722362	0.021424	0.759573
O	-6.197982	0.690391	-0.261108
Au	-4.207190	-1.568171	0.300356
Au	-2.285250	-0.517714	-1.433141
Au	0.003930	-0.590952	-2.948841
Au	0.673142	-2.752799	-1.155937
Au	3.026133	-2.142928	0.302023
Au	2.683345	-0.499210	2.505354
Au	1.865336	2.223183	2.155513

Au	0.072708	0.281017	3.193641
Au	0.475294	-2.146220	1.684509
Au	-1.786357	-2.866245	0.128366
Au	-2.009679	-0.358518	1.530474
Au	-0.798125	2.163814	1.171148
Au	1.301835	3.191789	-0.431672
Au	1.798780	1.590442	-2.677865
Au	2.713640	-1.092058	-2.304618
Au	2.766669	0.713621	-0.097390
Ga	0.244689	-0.155967	-0.165915
Au	-3.294753	1.958982	-0.047970
Au	-0.885217	1.914213	-1.712027
C	-5.275835	2.289413	-0.540676
O	-5.949070	3.090801	-1.049018

I(2)

O	-5.893764	0.222919	0.611028
O	-6.014920	1.485453	-0.056069
Au	-4.298096	-1.008229	-0.118524
Au	-2.102484	0.103430	-1.485397
Au	-0.040466	0.982249	-3.061648
Au	0.151364	-1.755056	-2.173127
Au	2.622781	-2.325516	-0.895642
Au	2.690375	-1.748124	1.832633
Au	2.152005	0.912497	2.777976
Au	0.217081	-1.124172	3.032376

Au	0.257071	-2.716107	0.623549
Au	-2.191985	-2.668973	-0.824001
Au	-1.973461	-0.880873	1.405194
Au	-0.603771	1.504511	2.108985
Au	1.540621	2.980399	0.990937
Au	1.949838	2.478478	-1.736414
Au	2.514794	-0.163353	-2.673698
Au	2.917915	0.474979	0.063176
Ga	0.326868	-0.030886	-0.027570
Au	-3.115551	1.779696	0.768065
Au	-0.704097	2.470647	-0.661913
C	-5.017774	2.411461	0.100101
O	-5.185944	3.549928	-0.251906

TS(2)

O	-5.280850	0.936581	-0.204137
O	-6.020748	-0.071823	-1.360855
Au	-3.493306	2.008340	-0.949440
Au	-1.895339	1.225606	1.287470
Au	0.330316	2.816757	1.663016
Au	1.884722	2.931862	-0.659263
Au	3.647335	0.753098	-0.741897
Au	2.749851	-1.538860	-1.981922
Au	1.173315	-3.286011	-0.424258
Au	0.055780	-1.837860	-2.663895
Au	1.086650	0.816695	-2.359548

Au	-0.856874	2.645289	-1.063664
Au	-1.753407	0.111701	-2.033163
Au	-1.384039	-2.211556	-0.171926
Au	0.461083	-2.613439	2.223639
Au	0.447484	0.163794	2.802170
Au	2.777379	1.473918	1.838537
Au	2.485018	-1.161239	0.954534
Ga	0.213268	0.018779	0.038930
Au	-3.699085	-0.789098	0.198589
Au	-1.989393	-1.285494	2.491424
C	-5.389198	-1.170749	-1.228033
O	-5.504361	-2.266561	-1.717584

Product

O	-5.076851	0.256102	-0.703923
Au	-3.677556	1.703694	-1.264227
Au	-2.188152	0.970791	1.156611
Au	-0.167205	2.693258	1.817833
Au	1.561351	3.134354	-0.340421
Au	3.458055	1.107801	-0.493924
Au	2.969895	-1.205864	-1.892927
Au	1.453507	-3.141056	-0.518051
Au	0.345115	-1.706676	-2.768337
Au	1.082927	1.004812	-2.208247
Au	-1.076751	2.596595	-1.005874
Au	-1.653561	0.071690	-2.222421

Au	-1.245857	-2.358052	-0.435121
Au	0.458127	-2.709194	2.085891
Au	0.139823	0.016964	2.814385
Au	2.403179	1.600407	2.097211
Au	2.418013	-0.996923	1.060586
Ga	0.074512	-0.056216	0.049471
Au	-3.690748	-1.141581	-0.059995
Au	-2.105290	-1.644893	2.228900