

Electronic Supplementary Information

Aerobic oxidation of methanol to formic acid on Au_{20}^- : a theoretical study on the reaction mechanism

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Additional optimized structures and energies considered in DFT calculation with M06 functional

Here we report some information on the results for optimized structures, selected geometrical parameters, the Cartesian coordinates and the corresponding calculated energies of the coadsorption of oxygen molecule and the methoxy species, aerobic oxidation of methanol to formic acid along pathway I and II on Au_{20}^-

Figure S1. Optimized Structures of the Coadsorption of Oxygen Molecule and Methoxy Species on Au_{20}^- .

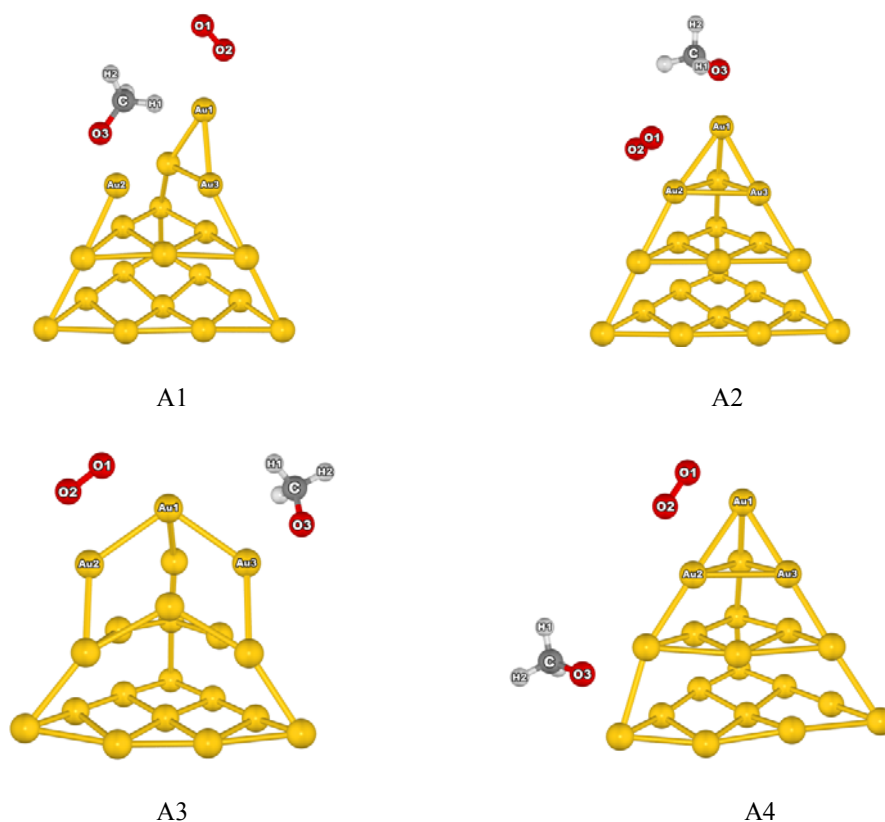
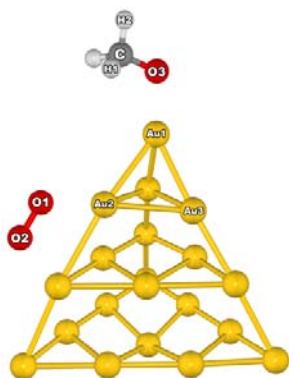
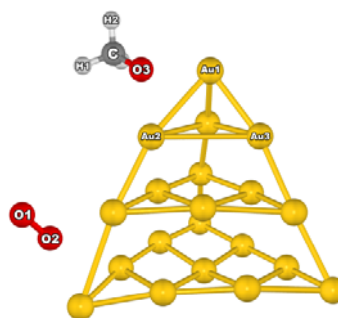


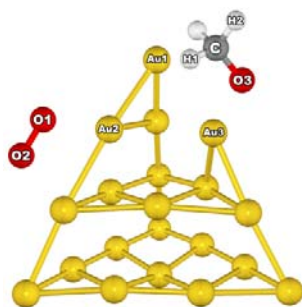
figure continued



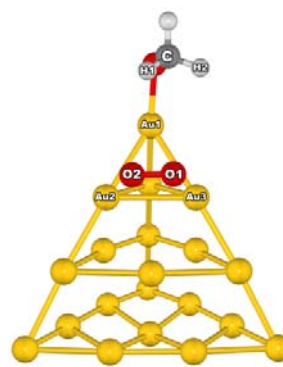
A5



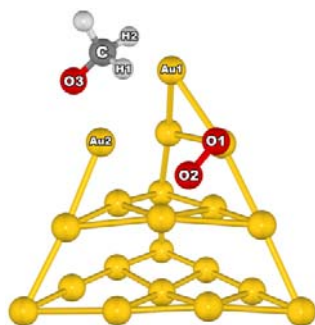
A6



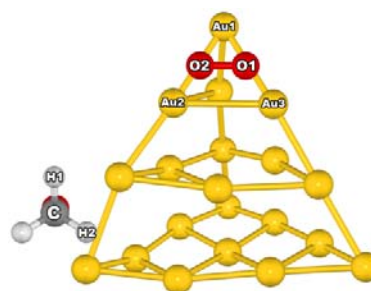
A7



A8



A9



A10

Table S1. Calculated adsorption energies (E_{O_2}), BSSE energies (E_{BSSE}) and corrected adsorption energies (E_{O_2+BSSE}) for the stable O_2 adsorption structures. Four gold atoms, which are located close to O_2 , were selected for the BSSE calculations.

Structure	E_{O_2} (kcal/mol)	E_{BSSE} (kcal/mol)	E_{O_2+BSSE} (kcal/mol)
BR1	-18.1	1.1	-17.0
BR2	-5.8	1.2	-4.6
BR3	-7.1	1.1	-6.0
T1	-13.7	1.0	-12.7
T3	-2.4	1.1	-1.3
FCC	-2.3	1.0	-1.3
HCP	-0.9	0.5	-0.4

Table S2. Calculated Energies (E_{co-ads} , kcal/mol) of Coadsorption of Oxygen Molecule and Methoxy Species on Au_{20}^- .

Structure	E_{co-ads}
A1	-26.4
A2	-28.8
A3	-26.6
A4	-34.1
A5	-37.6
A6	-25.6
A7	-23.8
A8	-29.1
A9	-18.4
A10	-26.5

Table S3. Selected interatomic distances (Å) and Mulliken charges of intermediates and TS and vibrational frequency (ν , in cm^{-1}) of O–O bond for the coadsorption of oxygen molecule and methoxy species on Au_{20}^- (A1–A5).

	A1	A2	A3	A4	A5
$R_{\text{O1-O2}}$	1.351	1.351	1.351	1.342	1.346
$R_{\text{O1-H1}}$	3.462	2.552	5.440	6.857	4.712
$R_{\text{C-H1}}$	1.111	1.103	1.103	1.104	1.103
$R_{\text{C-O3}}$	1.383	1.434	1.422	1.433	1.420
$R_{\text{O1-Au}}$	2.212	2.282	2.314	2.382	2.366
$R_{\text{O2-Au}}$	2.084	2.081	2.110	2.466	2.391
$R_{\text{O3-Au}}$	2.081	2.083	2.111	2.340	2.100
q_{O1}	-0.187	-0.212	-0.215	-0.204	-0.203
q_{O2}	-0.253	-0.273	-0.248	-0.209	-0.205
q_{C}	-0.086	-0.281	-0.270	-0.294	-0.268
q_{O3}	-0.593	-0.649	-0.629	-0.591	-0.647
q_{Au1}	-0.258	-0.214	-0.211	-0.287	-0.257
q_{Au2}	-0.103	0.015	-0.145	0.053	0.026
$\nu_{\text{O1-O2}}$	1201	1152	1217	1235	1215

Table S4. Selected interatomic distances (Å) and Mulliken charges of intermediates and TS and vibrational frequency (ν , in cm^{-1}) of O–O bond for the coadsorption of oxygen molecule and methoxy species on Au_{20}^- (A6–A10).

	A6	A7	A8	A9	A10
$R_{\text{O1-O2}}$	1.338	1.343	1.347	1.338	1.342
$R_{\text{O1-H1}}$	5.730	4.957	3.288	2.842	6.532
$R_{\text{C-H1}}$	1.102	1.102	1.101	1.102	1.104
$R_{\text{C-O3}}$	1.428	1.403	1.422	1.440	1.432
$R_{\text{O1-Au}}$	3.823	2.420	2.490	2.452	2.454
$R_{\text{O2-Au}}$	2.572	2.412	2.472	2.501	2.510
$R_{\text{O3-Au}}$	2.353	2.131	2.093	2.304	2.331
q_{O1}	-0.200	-0.200	-0.209	-0.200	-0.201
q_{O2}	-0.203	-0.208	-0.209	-0.207	-0.207
q_{C}	-0.295	-0.253	-0.276	-0.317	-0.296
q_{O3}	-0.591	-0.617	-0.647	-0.601	-0.592
q_{Au1}	-0.275	-0.396	-0.184	-0.296	-0.357
q_{Au2}	0.109	0.097	0.130	0.055	0.088
Freq	1214	1219	1217	1238	1218

Table S5. Selected interatomic distances (Å) involved in the mechanism of aerobic oxidation of methanol to formaldehyde on Au_{20}^- .

	coadsorption			transition state			formaldehyde		
	A1	A2	A3	TS A1	TS A2	TS A3	B1	B2	B3
$R_{\text{O1-O2}}$	1.351	1.351	1.351	1.446	1.312	1.451	1.438	1.512	1.510
$R_{\text{O1-H1}}$	3.462	2.552	5.440	1.260	1.064	1.273	0.964	0.979	0.980
$R_{\text{C-H1}}$	1.111	1.103	1.103	1.317	1.693	1.317	2.804	2.768	3.149
$R_{\text{C-O3}}$	1.383	1.434	1.422	1.359	1.314	1.355	1.201	1.242	1.229
$R_{\text{O2-Au}}$	2.212	2.282	2.314	2.115	3.100	2.228	2.157	2.317	2.291
$R_{\text{O3-Au}}$	2.084	2.081	2.110	2.195	2.209	2.236	2.857	2.474	4.736
q_{O1}	-0.187	-0.212	-0.215	-0.382	-0.275	-0.305	-0.203	-0.475	-0.442
q_{O2}	-0.253	-0.273	-0.248	-0.406	-0.058	-0.377	-0.523	-0.313	-0.354
q_{C}	-0.086	-0.281	-0.270	-0.312	-0.205	-0.305	-0.132	0.129	0.068
q_{H1}	0.114	0.193	0.157	0.389	0.298	0.373	0.267	0.418	0.404
q_{O3}	-0.593	-0.649	-0.629	-0.507	-0.461	-0.536	-0.221	-0.415	-0.432
q_{Au1}	-0.258	-0.214	-0.211	-0.223	0.146	0.131	-0.183	-0.200	-0.335
q_{Au2}	-0.103	0.015	-0.145	0.062	0.108	-0.072	0.256	-0.117	-0.066

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

	Au₂₀⁻		
	X	Y	Z
Au	0.000000	4.170579	3.068010
Au	0.000000	-4.170579	3.068010
Au	4.170579	0.000000	-3.068010
Au	-4.170579	0.000000	-3.068010
Au	-1.612350	0.000000	1.155936
Au	1.612350	0.000000	1.155936
Au	0.000000	-1.612350	-1.155936
Au	0.000000	1.612350	-1.155936
Au	0.000000	1.385857	3.138860
Au	1.385857	0.000000	-3.138860
Au	-1.385857	0.000000	-3.138860
Au	0.000000	-1.385857	3.138860
Au	-1.474887	2.947159	0.936280
Au	2.947159	-1.474887	-0.936280
Au	1.474887	-2.947159	0.936280
Au	-2.947159	1.474887	-0.936280
Au	1.474887	2.947159	0.936280
Au	2.947159	1.474887	-0.936280
Au	-1.474887	-2.947159	0.936280
Au	-2.947159	-1.474887	-0.936280

A1

	X	Y	Z
Au	-2.47484100	-1.37782900	1.02352300
Au	-0.04246500	-0.07014000	0.67959800
Au	2.78975600	0.18326200	0.70558200
Au	1.26543900	1.93818600	-0.99971800
Au	-1.64931300	2.12680500	-1.18753300
Au	-0.00994800	3.62370000	-2.92960900
Au	1.49530400	-1.13752900	-1.57779200
Au	-1.43464800	-1.14232800	-1.54726600
Au	-0.21235600	0.79949900	-3.36471200
Au	-0.08647400	-2.03517800	-3.88604100
Au	2.97676600	3.64791700	-2.86746700
Au	1.51861000	5.25059700	-4.68324100
Au	4.39809700	-1.02503500	-1.68282500
Au	3.15494000	0.83557900	-3.56923300
Au	1.47003200	2.48786300	-5.27034200
Au	3.04303300	-2.07270900	-3.85606000
Au	1.43393400	-0.22250200	-5.67455200
Au	1.61237000	-3.00742500	-6.05526800
Au	5.70418800	0.15394700	0.47772500
Au	4.28080100	1.97541200	-1.13098700
O	-4.95423085	-1.52618729	2.75002926
O	-3.91481115	-2.31861571	2.40971874
C	-4.01558200	1.57473500	0.58085700
H	-4.21051000	0.59047300	0.11183700
H	-4.98707800	1.93407000	0.96125400
H	-3.39124000	1.36356500	1.47005200
O	-3.48086100	2.50935600	-0.27446100

A2

	X	Y	Z
Au	-2.915558	0.974840	0.637704
Au	-0.153835	0.535447	0.655500
Au	2.674700	0.205687	0.731476
Au	1.568696	2.222149	-1.049603
Au	-1.357477	2.357835	-1.223215
Au	0.207899	3.866010	-3.037642
Au	1.150605	-0.896811	-1.494217
Au	-1.811378	-0.665788	-1.641581
Au	-0.137642	0.991710	-3.451122
Au	-0.340478	-1.857183	-3.766190
Au	3.296128	3.586074	-2.985460
Au	2.035618	5.233278	-4.851864
Au	4.105481	-1.167492	-1.535967
Au	3.157984	0.725224	-3.547476
Au	1.633650	2.487949	-5.306383
Au	2.694294	-2.148018	-3.691367
Au	1.403396	-0.233295	-5.669000
Au	1.176494	-3.024939	-5.891130
Au	5.591332	-0.015692	0.554723
Au	4.468763	1.844082	-1.190987
O	-3.726103	-1.844959	-1.243975
O	-3.709471	-2.421501	-0.027551
C	-5.654143	-0.054047	1.285925
H	-6.564239	0.061776	1.896437
H	-5.956256	-0.037969	0.227555
H	-5.237343	-1.051526	1.477805
O	-4.751262	1.000603	1.618891

A3

	X	Y	Z
Au	-2.295986	-1.508781	0.080250
Au	0.129129	-0.421783	1.342623
Au	2.807890	-0.868861	0.215541
Au	1.322286	1.403719	-0.713153
Au	-1.532771	0.946043	-0.892747
Au	-0.440669	3.136790	-2.281229
Au	0.475768	-1.421581	-1.256447
Au	-1.824370	-1.930949	-2.841068
Au	-0.246714	0.479989	-3.479866
Au	0.683832	-2.176880	-4.057542
Au	2.620572	3.529975	-2.245681
Au	0.936870	5.249661	-3.689283
Au	4.669909	-1.043975	-2.091598
Au	2.988937	0.883413	-3.418154
Au	1.179099	2.694228	-4.821084
Au	3.541825	-1.744721	-4.455342
Au	1.538914	0.160566	-5.838459
Au	1.937388	-2.486268	-6.652777
Au	5.612671	-0.295299	0.451917
Au	4.224422	1.715589	-0.911861
O	-3.818683	-2.936884	-2.240410
O	-3.984855	-2.957757	-0.896910
C	-1.500558	0.502208	3.707449
H	-1.736348	1.441196	3.177622
H	-1.534075	0.723923	4.787173
H	-2.325595	-0.200250	3.495023
O	-0.221596	-0.018061	3.383014

A4

	X	Y	Z
Au	-2.786205	0.449623	0.692926
Au	0.006061	0.294728	0.704504
Au	2.755964	0.111056	0.642448
Au	1.490898	2.122274	-1.013619
Au	-1.437027	2.096706	-1.072216
Au	-0.069430	3.602670	-2.962687
Au	1.314461	-1.160623	-1.709154
Au	-1.608289	-1.080080	-1.509643
Au	-0.197655	0.676283	-3.404721
Au	-0.492871	-2.192866	-3.798978
Au	3.035094	3.662291	-2.948162
Au	1.517726	5.163710	-4.753523
Au	4.281554	-1.051018	-1.610279
Au	3.114034	0.797885	-3.498711
Au	1.402096	2.360581	-5.251630
Au	3.185653	-2.095536	-3.943075
Au	1.535708	-0.378546	-5.643177
Au	1.477107	-3.162353	-5.798883
Au	5.605477	0.226139	0.586406
Au	4.398771	2.017416	-1.179914
O	-3.689168	-2.061454	-0.624225
O	-4.254212	-1.397181	0.409586
C	-1.737763	-3.367119	-6.435209
H	-1.757667	-4.134505	-7.222746
H	-2.744563	-3.312396	-5.997784
H	-1.526530	-2.397725	-6.914672
O	-0.771145	-3.710108	-5.440365

A5

	X	Y	Z
Au	-2.915826	0.288888	0.673027
Au	-0.096205	0.085479	0.595363
Au	2.709576	0.059681	0.661558
Au	1.417047	2.052608	-0.984366
Au	-1.506663	1.852734	-1.207971
Au	-0.102203	3.568604	-2.922739
Au	1.334627	-1.118283	-1.659157
Au	-1.688087	-1.069991	-1.584395
Au	-0.120063	0.683317	-3.494129
Au	-0.068436	-2.170618	-3.966525
Au	2.997202	3.648108	-2.868962
Au	1.506726	5.228926	-4.632057
Au	4.329622	-1.016170	-1.686024
Au	3.368269	0.853035	-3.694973
Au	1.530802	2.476660	-5.254361
Au	3.010354	-2.047862	-3.865258
Au	1.544974	-0.233375	-5.711957
Au	1.696507	-2.991171	-6.142371
Au	5.585217	0.138207	0.561210
Au	4.342350	1.967804	-1.153279
O	-2.019198	-3.491854	-3.591663
O	-2.705782	-2.976680	-2.549986
C	-5.650986	-0.809366	1.319067
H	-6.493599	-0.837715	2.029483
H	-6.068855	-0.541262	0.334426
H	-5.263961	-1.838106	1.235796
O	-4.683889	0.118112	1.788280

A6

	X	Y	Z
Au	-2.692398	0.193012	0.666367
Au	0.029868	0.333204	0.906461
Au	2.763156	-0.041051	0.598380
Au	1.502932	2.034339	-0.963560
Au	-1.409544	2.043955	-0.979863
Au	-0.069804	3.658289	-2.792251
Au	1.055102	-1.081825	-1.640406
Au	-1.855240	-1.071235	-1.900171
Au	-0.261829	0.771286	-3.466390
Au	-0.356382	-2.123526	-3.996436
Au	3.047109	3.635784	-2.858629
Au	1.520410	5.313698	-4.492113
Au	4.072015	-1.199715	-1.770841
Au	2.979119	0.802877	-3.556663
Au	1.326770	2.559963	-5.191899
Au	2.753770	-2.063268	-4.028025
Au	1.377513	-0.139039	-5.810273
Au	1.659334	-2.814922	-6.464208
Au	5.624516	-0.099422	0.349435
Au	4.405770	1.844339	-1.238175
O	-0.620184	-3.681747	-5.644518
O	-1.678931	-4.508320	-5.698487
C	-4.944227	-0.645127	-1.584112
H	-5.857958	-0.690073	-0.973832
H	-4.786526	0.405159	-1.877626
H	-5.124991	-1.225938	-2.499262
O	-3.840343	-1.182632	-0.853232

A7

	X	Y	Z
Au	-2.870717	1.294504	0.397013
Au	0.249195	0.868655	1.026768
Au	3.014978	0.635140	0.623570
Au	1.591915	2.377293	-1.136175
Au	-1.265800	2.487491	-1.447773
Au	0.275445	3.829572	-3.321762
Au	1.256068	-0.608734	-1.335877
Au	-1.672693	-0.463315	-1.444446
Au	-0.024900	0.889732	-3.547648
Au	-0.215779	-2.004907	-3.502833
Au	3.260632	3.690607	-3.279984
Au	1.933419	5.086553	-5.324342
Au	4.337196	-0.913274	-1.531863
Au	3.246525	0.784923	-3.618499
Au	1.694379	2.293344	-5.561265
Au	2.758899	-2.089118	-3.437794
Au	1.512723	-0.456204	-5.634756
Au	1.381962	-3.242950	-5.594979
Au	5.843307	0.475546	0.437880
Au	4.592084	2.173744	-1.425353
O	-2.197948	-3.225521	-2.894112
O	-2.826958	-2.531379	-1.921236
C	-1.835929	-0.093396	3.086193
H	-2.137494	-0.123282	4.146480
H	-2.707030	0.362564	2.541496
H	-1.767418	-1.132553	2.721954
O	-0.650324	0.640021	2.947405

A8

	X	Y	Z
Au	-2.832206	0.063599	0.678437
Au	-0.072606	0.107969	0.608315
Au	2.774387	0.107176	0.676852
Au	1.335109	2.045723	-0.985876
Au	-1.593473	1.906024	-1.212950
Au	-0.102247	3.635305	-2.906953
Au	1.359210	-1.195248	-1.529328
Au	-1.566253	-1.036752	-1.724653
Au	-0.083903	0.792007	-3.496825
Au	-0.048981	-2.095324	-3.870762
Au	2.970770	3.647092	-2.877047
Au	1.506834	5.234226	-4.677281
Au	4.313835	-1.043267	-1.637867
Au	3.183321	0.824984	-3.565435
Au	1.506236	2.500092	-5.277126
Au	3.021500	-2.070097	-3.837374
Au	1.528091	-0.222074	-5.731233
Au	1.569000	-3.007281	-6.055620
Au	5.739058	0.174045	0.432037
Au	4.290927	1.978874	-1.132821
O	-3.695171	-0.094701	-2.559615
O	-3.696619	1.239460	-2.360497
C	-5.761702	-0.458565	0.675238
H	-5.641639	-1.397689	0.110320
H	-5.884381	0.345807	-0.065916
H	-6.704966	-0.534313	1.241170
O	-4.696058	-0.219601	1.588597

A9

	X	Y	Z
Au	-1.958297	0.763331	1.355309
Au	0.604826	-0.128636	1.238351
Au	3.340239	0.163787	0.598211
Au	1.499946	1.896463	-0.771751
Au	-1.305521	2.819879	-0.719152
Au	0.460870	3.872060	-2.519952
Au	1.520562	-1.111917	-1.334501
Au	-1.330232	-0.924252	-0.821378
Au	-0.459064	1.068392	-2.980178
Au	-0.385436	-1.960090	-3.267247
Au	3.349495	3.576312	-3.073136
Au	1.715696	5.265407	-4.641850
Au	4.415604	-1.183173	-1.965933
Au	2.810290	0.758541	-3.461531
Au	1.181817	2.521094	-5.076519
Au	2.669780	-2.130229	-3.875784
Au	0.819466	-0.189279	-5.357021
Au	0.731421	-2.969781	-5.723333
Au	6.161814	-0.099258	-0.054915
Au	4.675110	1.807342	-1.490600
O	-3.313662	-0.173466	-2.135859
O	-2.888276	0.739674	-3.031411
C	-4.329615	2.395457	-0.038189
H	-4.605575	3.262254	-0.653378
H	-5.112987	2.253386	0.719197
H	-4.301510	1.509967	-0.685725
O	-3.070946	2.635207	0.618865

A10

	X	Y	Z
Au	-2.115090	-1.472198	1.131729
Au	0.545504	-0.918991	0.879650
Au	3.232368	-0.629294	0.483404
Au	1.356894	1.597994	-0.528468
Au	-1.507152	0.994709	-0.266254
Au	-0.751312	3.405793	-1.399605
Au	1.539259	-1.510498	-1.755372
Au	-1.374740	-1.632765	-1.703120
Au	-0.256078	0.918799	-2.923018
Au	-0.041165	-1.849083	-4.119209
Au	2.834104	3.726989	-2.148802
Au	0.807867	5.414789	-2.932884
Au	4.484181	-1.137304	-2.175401
Au	2.899630	1.031302	-3.300698
Au	1.122746	3.093444	-4.411153
Au	2.951343	-1.676742	-4.392215
Au	1.064586	0.543072	-5.516035
Au	1.278335	-2.080842	-6.615443
Au	6.044102	-0.339317	0.004792
Au	4.310703	1.751861	-0.881053
O	-3.710266	-0.911292	-1.622071
O	-3.798428	0.276767	-0.981553
C	-2.424919	5.712235	-2.705201
H	-2.348818	5.150120	-3.649334
H	-2.565434	6.773873	-2.955305
H	-3.328303	5.367938	-2.183124
O	-1.269799	5.551841	-1.876969

TS_A1

	X	Y	Z
Au	-2.791174	-0.088046	0.257587
Au	0.085008	-0.110111	0.730639
Au	2.916577	0.066360	0.600612
Au	1.336160	1.858424	-0.991974
Au	-1.529308	1.948039	-0.948642
Au	-0.225704	3.469078	-2.939111
Au	1.504078	-1.154191	-1.624443
Au	-1.342197	-1.810911	-1.773673
Au	-0.288706	0.592200	-3.308537
Au	0.206869	-2.152783	-4.024908
Au	2.762627	3.681301	-2.856686
Au	1.357491	5.200999	-4.746943
Au	4.482297	-0.923072	-1.768455
Au	3.117834	0.891815	-3.608398
Au	1.279118	2.445162	-5.244201
Au	3.207407	-2.006800	-3.944400
Au	1.556497	-0.206145	-5.801243
Au	1.828617	-2.992015	-6.198404
Au	5.759133	0.315758	0.407592
Au	4.304353	2.086855	-1.227954
O	-3.017246	-2.335709	-0.401573
O	-2.702027	-3.397575	0.536428
C	-1.552128	-2.163235	2.489479
H	-1.599537	-2.917677	3.291035
H	-2.357830	-1.408581	2.589373
H	-2.040676	-2.839885	1.470404
O	-0.303988	-1.681892	2.273003

TS_A2

	X	Y	Z
Au	-2.884847	0.179990	0.374111
Au	-0.057805	0.121610	0.542968
Au	2.742600	0.154049	0.680511
Au	1.455548	2.009155	-1.123687
Au	-1.484793	1.968887	-1.353586
Au	0.027894	3.655916	-3.013505
Au	1.469058	-1.231573	-1.546916
Au	-1.458244	-0.962050	-1.767461
Au	-0.110128	0.824773	-3.664671
Au	-0.016048	-2.067074	-3.898508
Au	3.033507	3.642384	-2.976418
Au	1.431786	5.274416	-4.873204
Au	4.405521	-0.996941	-1.626458
Au	3.185859	0.791320	-3.538466
Au	1.676141	2.496503	-5.316481
Au	3.074557	-2.123022	-3.790430
Au	1.582367	-0.247492	-5.764258
Au	1.631840	-3.054446	-6.008809
Au	5.575590	-0.054677	0.751086
Au	4.380095	1.910251	-1.125895
O	-4.415334	3.443724	0.805617
O	-4.279986	2.878386	-0.370157
C	-4.710316	1.298750	2.506694
H	-4.583749	2.654567	1.500036
H	-3.815229	1.523277	3.115860
H	-5.673554	1.466740	3.021122
O	-4.672501	0.287492	1.667890

TS_A3

	X	Y	Z
Au	-2.791174	-0.088046	0.257587
Au	0.085008	-0.110111	0.730639
Au	2.916577	0.066360	0.600612
Au	1.336160	1.858424	-0.991974
Au	-1.529308	1.948039	-0.948642
Au	-0.225704	3.469078	-2.939111
Au	1.504078	-1.154191	-1.624443
Au	-1.342197	-1.810911	-1.773673
Au	-0.288706	0.592200	-3.308537
Au	0.206869	-2.152783	-4.024908
Au	2.762627	3.681301	-2.856686
Au	1.357491	5.200999	-4.746943
Au	4.482297	-0.923072	-1.768455
Au	3.117834	0.891815	-3.608398
Au	1.279118	2.445162	-5.244201
Au	3.207407	-2.006800	-3.944400
Au	1.556497	-0.206145	-5.801243
Au	1.828617	-2.992015	-6.198404
Au	5.759133	0.315758	0.407592
Au	4.304353	2.086855	-1.227954
O	-3.017246	-2.335709	-0.401573
O	-2.702027	-3.397575	0.536428
C	-1.552128	-2.163235	2.489479
H	-1.599537	-2.917677	3.291035
H	-2.357830	-1.408581	2.589373
H	-2.040676	-2.839885	1.470404
O	-0.303988	-1.681892	2.273003

B1

	X	Y	Z
Au	-4.282057	-0.422446	2.833839
Au	-1.450958	-0.461590	2.929645
Au	1.352312	-0.540682	3.027873
Au	4.187973	-0.391444	3.119752
Au	3.003284	1.291733	1.199074
Au	0.069629	1.518953	1.408331
Au	-2.864464	1.312219	1.131089
Au	-1.424870	3.058422	-0.535605
Au	1.657936	3.064011	-0.462502
Au	0.213560	4.668881	-2.252345
Au	2.973057	-1.617288	0.722908
Au	0.052108	-1.695783	0.723553
Au	-2.888487	-1.599134	0.546500
Au	1.775046	0.228801	-1.186496
Au	-1.534561	0.240029	-1.249477
Au	0.137000	1.937640	-2.914278
Au	-1.387751	-2.648066	-1.591864
Au	1.602738	-2.656605	-1.571928
Au	0.220855	-0.798292	-3.393627
Au	-0.021196	-3.569157	-3.900801
O	-6.444156	-2.405495	3.334720
O	-6.054890	-1.119418	3.846155
C	-4.487690	-3.801422	2.687452
H	-4.002185	-3.017530	3.303040
H	-5.009500	-4.597002	3.256463
H	-6.769907	-2.189559	2.453742
O	-4.406626	-3.828564	1.489184

B2

	X	Y	Z
Au	-2.887981	-0.068556	0.396638
Au	-0.093242	-0.057683	0.613592
Au	2.680340	0.106349	0.725075
Au	1.294853	1.934896	-1.047079
Au	-1.659038	2.057546	-1.298300
Au	-0.059805	3.631319	-2.964204
Au	1.442742	-1.299957	-1.534288
Au	-1.519277	-1.172736	-1.698235
Au	-0.234118	0.780018	-3.453565
Au	-0.018207	-2.121129	-3.871249
Au	2.899446	3.662069	-2.848846
Au	1.306933	5.280529	-4.798457
Au	4.380552	-0.966454	-1.589163
Au	3.102017	0.811712	-3.466478
Au	1.539639	2.493306	-5.213875
Au	3.090334	-2.108771	-3.774953
Au	1.462902	-0.230737	-5.649189
Au	1.677535	-3.014179	-6.020083
Au	5.497584	-0.035328	0.833551
Au	4.254096	1.922284	-1.036420
O	-2.510887	3.112142	1.559163
O	-3.220990	2.631190	0.314008
C	-3.040113	1.531447	3.091648
H	-1.564309	3.057212	1.314685
H	-1.961013	1.335400	3.128443
H	-3.406917	2.372638	3.687982
O	-3.825362	0.743941	2.537466

B3

	X	Y	Z
Au	-1.998482	-0.338407	0.649540
Au	0.785937	-0.048343	0.551287
Au	3.543672	0.151274	0.207384
Au	1.830397	2.091556	-1.136245
Au	-1.075118	1.812126	-0.759293
Au	-0.119243	3.508176	-2.733986
Au	2.010199	-1.089927	-1.916188
Au	-0.843171	-1.783657	-1.738955
Au	-0.093332	0.611558	-3.291854
Au	0.459631	-2.110150	-4.146286
Au	2.924314	3.896024	-3.115777
Au	1.015782	5.325435	-4.607137
Au	4.901128	-0.639506	-2.335179
Au	3.215828	1.099098	-3.957524
Au	1.068283	2.582636	-5.266316
Au	3.381651	-1.769235	-4.467526
Au	1.485160	-0.037099	-5.957581
Au	1.564345	-2.780276	-6.639344
Au	6.304482	0.649085	-0.053090
Au	4.703106	2.232424	-1.759619
O	-2.213899	-2.664579	-0.128229
O	-1.451044	-3.605244	0.773240
C	-3.324851	-3.100208	2.561173
H	-3.724789	-3.422782	1.592477
H	-2.732813	-2.165464	2.523253
H	-0.620400	-3.114837	0.948401
O	-3.539683	-3.692877	3.616227

TS_B1

	X	Y	Z
Au	-4.054158	-0.333421	3.106955
Au	-1.266449	-0.416572	3.057279
Au	1.551715	-0.374573	3.023672
Au	4.435746	-0.345694	2.720985
Au	3.058917	1.477507	1.098919
Au	0.178949	1.604345	1.439054
Au	-2.741015	1.370809	1.370770
Au	-1.465843	3.038201	-0.474957
Au	1.641324	3.107452	-0.631039
Au	0.017501	4.699507	-2.270716
Au	3.014708	-1.561761	0.631878
Au	0.073730	-1.665363	0.821690
Au	-2.816445	-1.841960	0.776474
Au	1.758615	0.275156	-1.240097
Au	-1.514609	0.147310	-0.958215
Au	-0.007477	1.913118	-2.852288
Au	-1.342339	-2.677575	-1.543355
Au	1.639188	-2.619490	-1.515883
Au	0.011860	-0.816069	-3.331227
Au	0.300919	-3.638015	-3.776935
O	-6.324231	-2.457581	2.646505
O	-5.955129	-1.138262	3.724506
C	-5.075908	-3.444395	2.379977
H	-4.454017	-3.185001	3.247763
H	-5.592027	-4.405318	2.518059
H	-6.393114	-1.937678	1.818228
O	-4.594094	-3.229572	1.164473

C1

	X	Y	Z
Au	-3.817296	-0.964147	3.695561
Au	-1.061004	-0.757968	3.255159
Au	1.740924	-0.355303	3.025372
Au	4.596354	0.115972	2.469807
Au	2.849730	1.651029	0.938564
Au	-0.020824	1.298129	1.429296
Au	-2.916879	0.714337	1.615571
Au	-1.969284	2.566928	-0.306865
Au	1.080304	3.047563	-0.656983
Au	-0.795212	4.333023	-2.287339
Au	3.144065	-1.369016	0.577198
Au	0.234306	-1.858699	0.960849
Au	-2.681946	-2.272236	1.147970
Au	1.570610	0.239291	-1.275571
Au	-1.657891	-0.282505	-0.809740
Au	-0.525532	1.589704	-2.795747
Au	-1.204228	-3.115338	-1.169423
Au	1.795591	-2.657580	-1.446408
Au	-0.140005	-1.104449	-3.215695
Au	0.287413	-3.862802	-3.494646
O	-5.456477	-1.587250	-0.427177
O	-5.231221	-1.307197	5.091220
C	-5.625648	-2.363746	0.769467
H	-5.758002	-1.602860	1.565906
H	-6.582258	-2.921402	0.678288
H	-4.940152	-2.158192	-1.004300
O	-4.625221	-3.232694	0.976493

TS_C1

	X	Y	Z
Au	-4.160535	-0.739330	2.964580
Au	-1.386514	-0.579270	3.028704
Au	1.460576	-0.483974	3.004921
Au	4.370270	-0.186280	2.763778
Au	2.907942	1.528628	1.124111
Au	-0.005855	1.385541	1.330234
Au	-2.916262	1.085567	1.282711
Au	-1.687133	2.842282	-0.557041
Au	1.404423	3.110770	-0.571765
Au	-0.169076	4.582065	-2.344191
Au	3.024235	-1.486953	0.674116
Au	0.052513	-1.755221	0.783426
Au	-2.856416	-2.155274	0.570160
Au	1.731454	0.291605	-1.242958
Au	-1.594003	-0.048678	-1.038984
Au	-0.136152	1.822856	-2.876754
Au	-1.197082	-2.848774	-1.592141
Au	1.802193	-2.604755	-1.514432
Au	0.133493	-0.856248	-3.390094
Au	0.447997	-3.635267	-3.764180
O	-6.209727	-2.185895	0.292416
O	-5.961744	-1.673801	3.322678
C	-5.724753	-3.155182	1.240749
H	-5.891525	-2.606406	2.338532
H	-6.434433	-3.991990	1.208771
H	-5.852881	-1.308314	0.521083
O	-4.445367	-3.558508	1.086432

D1

	X	Y	Z
Au	-4.058154	-0.812235	2.807519
Au	-1.232649	-0.697681	2.896572
Au	1.579924	-0.534092	2.992113
Au	4.430130	-0.538371	2.986929
Au	3.105926	1.443089	1.246853
Au	0.191365	1.376846	1.336478
Au	-2.739908	1.104465	1.160530
Au	-1.423013	3.011347	-0.425021
Au	1.595582	3.203378	-0.457006
Au	-0.166916	4.847410	-2.192556
Au	3.249524	-1.418461	0.588385
Au	0.325322	-1.807462	0.694631
Au	-2.616593	-1.779250	0.534579
Au	1.912670	0.407335	-1.202945
Au	-1.391496	0.216805	-1.261402
Au	0.239354	2.120685	-2.819888
Au	-1.126125	-2.636501	-1.677436
Au	1.947618	-2.495518	-1.616014
Au	0.321749	-0.585635	-3.460798
Au	0.522776	-3.364566	-3.876206
O	-7.520171	-3.629082	1.023919
O	-5.926863	-1.252518	3.702680
C	-6.304589	-3.108830	1.304109
H	-6.321713	-0.406424	3.917213
H	-6.341961	-2.435358	2.186814
H	-7.391392	-4.182956	0.241232
O	-5.340317	-3.372441	0.645828

E1

	X	Y	Z
Au	-4.232461	-0.657222	2.740451
Au	-1.403180	-0.656931	2.891624
Au	1.414598	-0.648778	3.004374
Au	4.275147	-0.587056	2.888966
Au	3.028625	1.332715	1.276270
Au	0.104554	1.360969	1.380814
Au	-2.813557	1.232540	1.150637
Au	-1.400053	3.084216	-0.411193
Au	1.680629	3.116022	-0.354439
Au	0.196842	4.801063	-2.032817
Au	3.062082	-1.628796	0.589647
Au	0.139774	-1.764729	0.648487
Au	-2.781075	-1.620884	0.490912
Au	1.852776	0.332518	-1.193164
Au	-1.422950	0.303458	-1.259233
Au	0.239314	2.117619	-2.838289
Au	-1.331767	-2.559498	-1.728199
Au	1.751599	-2.538930	-1.671000
Au	0.275221	-0.577446	-3.467802
Au	0.308587	-3.338633	-3.934077
O	-6.011617	-0.921683	3.741252
H	-6.369783	-0.046437	3.900300

F1

	X	Y	Z
Au	-3.753343	-0.363025	3.304441
Au	-0.986910	-0.458662	3.110972
Au	1.793998	-0.507324	2.910844
Au	4.627541	-0.461759	2.503684
Au	3.251510	1.365279	0.894301
Au	0.362467	1.462855	1.337363
Au	-2.581514	1.291778	1.412203
Au	-1.363452	2.999874	-0.422969
Au	1.737631	3.048745	-0.699197
Au	0.060623	4.617460	-2.298206
Au	3.111025	-1.659327	0.464647
Au	0.155191	-1.709769	0.773992
Au	-2.778204	-1.798954	0.837511
Au	1.779791	0.202050	-1.339989
Au	-1.461312	0.121425	-0.982259
Au	-0.033247	1.874967	-2.896070
Au	-1.377542	-2.726917	-1.444096
Au	1.639417	-2.694292	-1.616450
Au	-0.014608	-0.834243	-3.391489
Au	0.023376	-3.628175	-3.725515
O	-6.193294	-1.749084	2.086732
O	-5.588790	-0.628252	4.869237
C	-5.457593	-3.082917	1.925083
H	-5.009802	-3.206645	2.924141
H	-6.262869	-3.815050	1.775288
H	-6.155600	-1.288049	1.233863
O	-4.616631	-3.029120	0.876048
O	-6.815250	-0.819437	4.311104
H	-6.641977	-1.203444	3.344522

TS_F1

	X	Y	Z
Au	-3.985416	-0.704222	3.093145
Au	-1.225551	-0.514467	3.091914
Au	1.570405	-0.400787	2.992841
Au	4.409782	-0.150048	2.704846
Au	2.990774	1.553518	1.001205
Au	0.090004	1.443728	1.319912
Au	-2.829434	1.095857	1.323089
Au	-1.668208	2.851549	-0.510285
Au	1.428423	3.103760	-0.682054
Au	-0.286313	4.525099	-2.378284
Au	3.081821	-1.469897	0.617055
Au	0.129186	-1.739488	0.824770
Au	-2.776170	-2.057022	0.723257
Au	1.686848	0.259166	-1.265127
Au	-1.575582	-0.040022	-1.034138
Au	-0.181827	1.775689	-2.907696
Au	-1.233226	-2.883284	-1.464591
Au	1.766650	-2.646233	-1.495065
Au	0.052236	-0.928170	-3.366113
Au	0.318842	-3.714458	-3.665438
O	-6.159875	-1.941272	0.333557
O	-5.927472	-1.863059	3.523416
C	-5.796151	-3.004374	1.198151
H	-6.002246	-2.466469	2.465283
H	-6.569951	-3.774557	1.106521
H	-5.470956	-1.248799	0.314979
O	-4.539138	-3.424392	1.215892
O	-7.039082	-0.878133	3.539590
H	-7.602573	-1.244792	4.248438

G1

	X	Y	Z
Au	-3.513136	-1.417298	3.555536
Au	-0.816361	-0.931316	3.299623
Au	1.889740	-0.378654	2.932591
Au	4.617373	0.209445	2.520894
Au	2.825911	1.692340	0.888900
Au	-0.031239	1.219708	1.475990
Au	-2.894230	0.524550	1.552756
Au	-1.991510	2.519219	-0.183799
Au	0.892358	3.075137	-0.562176
Au	-1.056848	4.290554	-2.234155
Au	3.343742	-1.200279	0.392163
Au	0.514169	-1.924070	0.908069
Au	-2.418055	-2.335581	1.041919
Au	1.461717	0.276027	-1.242658
Au	-1.722782	-0.360677	-0.918584
Au	-0.635719	1.586778	-2.776706
Au	-0.955551	-3.223070	-1.189280
Au	1.913888	-2.608621	-1.543707
Au	-0.146782	-1.097601	-3.245214
Au	0.420936	-3.795570	-3.653556
O	-5.732126	-1.446760	0.839586
O	-6.232254	-1.329125	3.889557
C	-6.189597	-2.728740	0.898134
H	-7.223296	-2.726370	1.249856
H	-4.767177	-1.360327	0.615022
O	-5.545568	-3.717928	0.608689
O	-6.842112	-0.268681	3.034131
H	-6.390639	-0.463763	2.172375
H	-6.037981	-0.818994	4.701849