

Supplementary Information:

Promoting Ethylene Epoxidation on Gold Nanocluster: Self and CO Induced O₂ Activation

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Content:

Figure 1S. Energy diagrams for the CO-promoted trimolecular ethylene oxidation (black line) and CO-promoted trimolecular CO oxidation (blue line) on the gold nanocluster. The energy and bond length are in the unit of eV and Å, respectively.

Cartesian coordinates of intermediates and transition states mentioned in the potential energy surfaces in the paper (Figures 1~3) and C₂H₄ adsorbed on Au(111) surface.

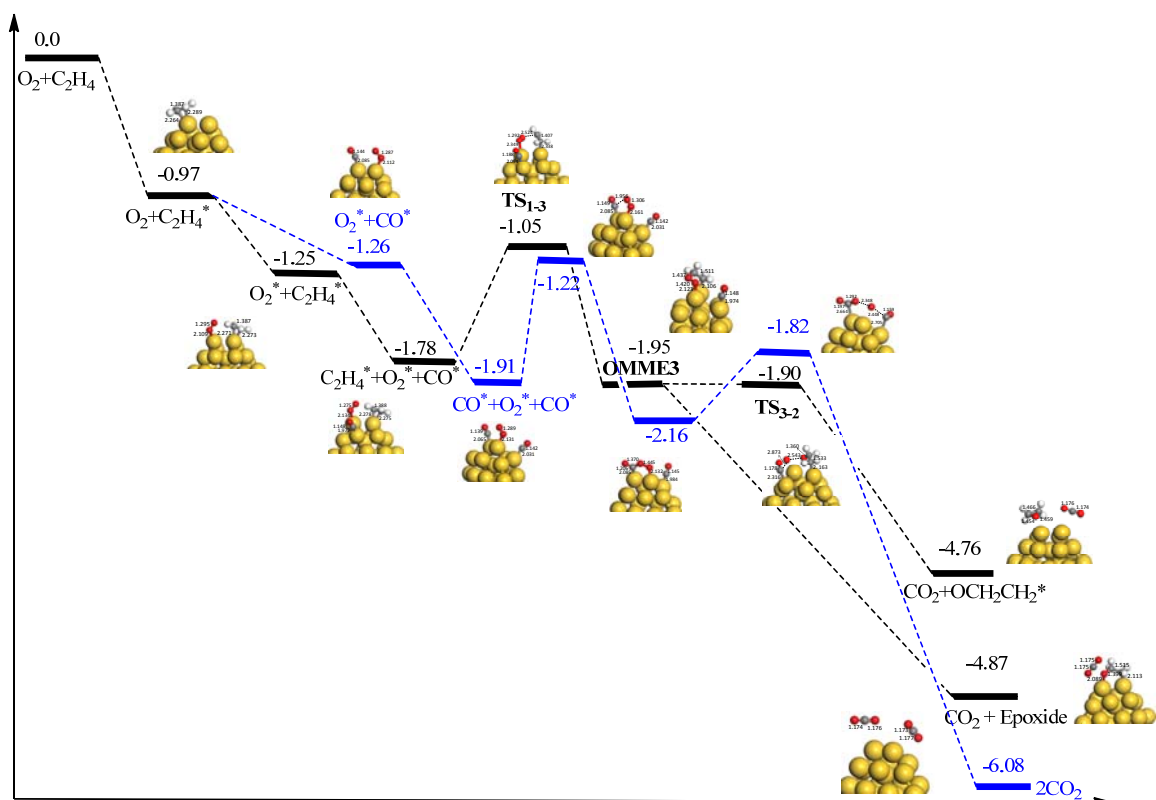


Figure 1S. Energy diagrams for the CO-promoted trimolecular ethylene oxidation (black line) and CO-promoted trimolecular CO oxidation (blue line) on the gold nanocluster. The energy and bond length are in the unit of eV and Å, respectively.

Cartesian coordinates of intermediates and transition states mentioned in the potential energy surfaces in the paper (Figures 1~3).

(a) Au₂₉-C₂H₄*

Au	5.87680000	6.51640000	5.89400000
Au	10.74000000	7.21540000	7.94200000
Au	6.96460000	11.25160000	6.59380000
Au	8.06580000	6.50920000	4.15520000
Au	13.47860000	8.25400000	5.03840000
Au	11.73640000	10.00820000	6.75240000
Au	10.65080000	7.72700000	5.19120000
Au	8.26000000	5.29220000	6.77540000
Au	10.78140000	4.38280000	7.74920000
Au	9.33360000	10.70640000	8.15600000
Au	13.51480000	8.08200000	7.86820000
Au	9.30200000	8.93260000	2.97720000
Au	5.30820000	9.02060000	6.93060000
Au	6.88260000	9.18020000	4.48340000
Au	8.35620000	8.27840000	6.77940000
Au	11.50540000	9.51020000	9.57120000
Au	13.12520000	5.45440000	9.08300000
Au	10.40880000	4.83240000	4.96680000
Au	8.71580000	5.47060000	9.56340000
Au	12.95580000	5.64980000	6.28860000
Au	10.17600000	6.13100000	2.37260000
Au	11.79700000	10.47700000	3.94340000
Au	8.87140000	8.39060000	9.96420000
Au	9.34800000	10.72240000	5.25480000
Au	11.17320000	6.79000000	10.67540000
Au	12.13380000	8.17560000	2.47400000
Au	6.55780000	7.08520000	8.70500000
Au	12.76680000	5.65840000	3.54660000
Au	6.73620000	9.99540000	9.18500000
C	10.99020000	6.83920000	12.93100000
C	11.94760000	5.88200000	12.62840000
H	13.01280000	6.11960000	12.66680000
H	11.68600000	4.82220000	12.58840000
H	11.27920000	7.85320000	13.21460000
H	9.95660000	6.55280000	13.13820000

(b) Au₂₉-O₂*+C₂H₄*

Au	5.91940000	6.44180000	5.88680000
Au	10.75340000	7.26140000	7.97380000
Au	6.87580000	11.20000000	6.50960000
Au	8.12740000	6.44660000	4.16720000
Au	13.47700000	8.35760000	5.04100000
Au	11.67020000	10.10860000	6.72340000
Au	10.66620000	7.76620000	5.20320000
Au	8.34260000	5.29320000	6.80660000
Au	10.88720000	4.43480000	7.83340000
Au	9.25660000	10.74080000	8.10600000
Au	13.50020000	8.26640000	7.86660000
Au	9.30440000	8.87580000	2.93800000
Au	5.29340000	8.91780000	6.91880000
Au	6.89020000	9.07580000	4.46120000
Au	8.36520000	8.26940000	6.79100000
Au	11.43340000	9.58700000	9.55640000
Au	13.12780000	5.61520000	9.13880000
Au	10.50020000	4.86460000	5.01280000
Au	8.76600000	5.50180000	9.58760000
Au	12.96440000	5.78380000	6.33080000
Au	10.24820000	6.11540000	2.39120000
Au	11.75160000	10.52100000	3.90220000
Au	8.80360000	8.45880000	9.94800000
Au	9.28220000	10.70580000	5.18580000
Au	11.08520000	6.93660000	10.76680000
Au	12.15040000	8.20200000	2.48620000
Au	6.57280000	7.05380000	8.71120000
Au	12.86040000	5.71220000	3.57600000
Au	6.66240000	10.02420000	9.14020000
O	14.72868026	5.19195171	11.62482042
O	14.83993954	5.40842357	10.35279632
C	11.28720000	6.93360000	13.03120000
C	11.72620000	5.70420000	12.56420000
H	12.79160000	5.50580000	12.40140000
H	11.05700000	4.83920000	12.57380000
H	11.99980000	7.73540000	13.24300000
H	10.27580000	7.06440000	13.42380000

(c) TS₁

Au	5.52440000	9.29620000	6.68180000
Au	10.45060000	8.98180000	8.59280000
Au	6.85820000	13.44020000	8.89280000
Au	7.66060000	9.74980000	4.92760000
Au	13.16760000	10.91700000	6.01860000
Au	11.54760000	12.08820000	8.38180000
Au	10.33320000	10.49100000	6.19820000
Au	7.88640000	7.75860000	7.01300000
Au	10.37500000	6.39800000	7.44440000
Au	9.23620000	12.29420000	10.05400000
Au	13.29920000	9.90700000	8.65200000
Au	8.96740000	12.37560000	4.53640000
Au	5.13540000	11.24740000	8.58100000
Au	6.63560000	12.17540000	6.21000000
Au	8.13160000	10.52300000	8.01260000
Au	11.36320000	10.57980000	10.82260000
Au	12.73540000	7.08200000	8.99860000
Au	9.92700000	7.85920000	5.01500000
Au	8.45360000	6.92760000	9.65800000
Au	12.50000000	8.08740000	6.42700000
Au	9.68780000	9.94380000	3.01540000
Au	11.54380000	13.40780000	5.86260000
Au	8.69340000	9.53720000	11.05280000
Au	9.15600000	13.30080000	7.30340000
Au	10.83480000	7.70000000	11.14220000
Au	11.73360000	11.76240000	3.65500000
Au	6.34800000	8.80560000	9.50600000
Au	12.30260000	9.00560000	3.83980000
Au	6.65020000	11.42280000	10.96920000
O	13.87080000	5.18140000	10.75560000
O	14.31940000	6.28080000	10.21140000
C	11.79980000	6.85940000	12.86620000
C	12.16440000	5.55920000	12.54900000
H	13.18900000	5.21100000	12.60840000
H	11.41100000	4.85100000	12.18340000
H	12.61360000	7.53780000	13.13140000
H	10.97960000	6.84860000	13.58960000

(d) OMME

Au	5.28240000	11.71420000	7.65800000
Au	10.20300000	10.53280000	9.15560000
Au	6.96840000	14.88880000	10.93980000
Au	7.38740000	12.53280000	6.02480000
Au	12.98580000	13.01860000	7.11060000
Au	11.53660000	13.51940000	9.82180000
Au	10.13440000	12.71200000	7.33080000
Au	7.54260000	10.01260000	7.45060000
Au	9.88200000	8.40160000	7.23440000
Au	9.29460000	13.31720000	11.61040000
Au	13.13840000	11.25340000	9.30700000
Au	8.86680000	15.09240000	6.36640000
Au	5.05720000	12.99920000	10.07820000
Au	6.56420000	14.50140000	8.01180000
Au	8.01620000	12.33380000	9.18720000
Au	11.33260000	11.34560000	11.67280000
Au	12.22920000	8.49300000	8.98100000
Au	9.51480000	10.58040000	5.43480000
Au	8.21040000	8.39880000	9.71600000
Au	12.10260000	10.21340000	6.75600000
Au	9.36460000	13.17840000	4.17360000
Au	11.52600000	15.49540000	7.78960000
Au	8.58760000	10.45620000	11.78080000
Au	9.19180000	15.12420000	9.27200000
Au	10.59660000	8.48280000	11.41780000
Au	11.54240000	14.66340000	5.15740000
Au	6.17540000	10.33760000	10.17100000
Au	11.93720000	11.91940000	4.57520000
Au	6.64740000	12.38020000	12.33220000
O	12.44140000	5.86180000	10.07700000
O	13.38080000	6.83980000	9.65600000
C	12.09440000	7.22180000	12.18340000
C	12.28820000	5.88620000	11.50520000
H	13.19220000	5.41480000	11.94440000
H	11.43460000	5.21040000	11.66480000
H	13.00320000	7.83780000	12.13440000
H	11.82540000	7.04880000	13.23800000

(e) TS₂

Au	5.06580000	11.92220000	7.46940000
Au	9.92500000	10.65560000	9.08700000
Au	6.74040000	15.15360000	10.66380000
Au	7.22180000	12.68520000	5.85580000
Au	12.80140000	13.06160000	7.09320000
Au	11.33880000	13.62780000	9.76000000
Au	9.93200000	12.81780000	7.27340000
Au	7.28880000	10.18820000	7.30700000
Au	9.64080000	8.53940000	7.22300000
Au	9.09160000	13.56260000	11.44340000
Au	12.82300000	11.28700000	9.29800000
Au	8.74720000	15.20060000	6.16380000
Au	4.81440000	13.29100000	9.84460000
Au	6.41660000	14.70160000	7.78140000
Au	7.78060000	12.52660000	9.08420000
Au	11.04340000	11.33000000	11.61700000
Au	11.93520000	8.55640000	8.91640000
Au	9.32900000	10.68080000	5.36160000
Au	7.93780000	8.60320000	9.62160000
Au	11.88540000	10.29880000	6.71200000
Au	9.25100000	13.23200000	4.02920000
Au	11.44620000	15.62220000	7.69880000
Au	8.33920000	10.55300000	11.69020000
Au	9.03300000	15.31400000	9.05340000
Au	10.25540000	8.45760000	11.72960000
Au	11.41060000	14.64420000	5.11860000
Au	5.90500000	10.59580000	10.04140000
Au	11.80160000	11.92700000	4.46620000
Au	6.48360000	12.60660000	12.07800000
O	10.45620000	6.30260000	11.44700000
O	12.76120000	7.22500000	10.00520000
C	11.43720000	7.38660000	13.14840000
C	11.44120000	6.02400000	12.47140000
H	12.44580000	5.76580000	12.06260000
H	11.11200000	5.16820000	13.11720000
H	12.34260000	7.98900000	13.21480000
H	10.75620000	7.47840000	14.01360000

(f) TS₃

Au	5.16700000	11.80020000	7.64800000
Au	10.11040000	10.64980000	9.06540000
Au	6.92060000	14.99340000	10.89780000
Au	7.26700000	12.63680000	6.00360000
Au	12.89220000	13.11260000	6.97800000
Au	11.51040000	13.61600000	9.70500000
Au	10.04160000	12.83240000	7.24440000
Au	7.42020000	10.10680000	7.37820000
Au	9.78460000	8.51900000	7.14860000
Au	9.27920000	13.42240000	11.51780000
Au	13.02400000	11.30600000	9.16540000
Au	8.72340000	15.21240000	6.30320000
Au	5.00820000	13.11960000	10.06480000
Au	6.46760000	14.61960000	7.98440000
Au	7.92300000	12.44660000	9.14320000
Au	11.29640000	11.40600000	11.54760000
Au	12.09780000	8.54560000	8.81940000
Au	9.37120000	10.69880000	5.35140000
Au	8.16260000	8.52200000	9.62640000
Au	11.98160000	10.32120000	6.62380000
Au	9.19860000	13.28720000	4.10460000
Au	11.47200000	15.62400000	7.70820000
Au	8.57960000	10.50880000	11.72440000
Au	9.14060000	15.21800000	9.19640000
Au	10.47400000	8.47480000	11.37740000
Au	11.36700000	14.75680000	5.09380000
Au	6.11480000	10.43280000	10.12960000
Au	11.79700000	12.03340000	4.42940000
Au	6.67580000	12.44740000	12.27200000
O	12.62680000	5.30700000	10.73480000
O	13.21280000	7.25900000	9.73720000
C	12.09700000	6.87420000	12.51120000
C	12.48440000	5.57940000	11.97020000
H	13.03780000	4.94880000	12.69240000
H	11.28420000	5.53380000	12.25040000
H	12.36920000	7.76120000	11.94240000
H	11.87200000	6.89200000	13.58640000

(g) Au₂₉- C₂H₄*+O₂*+C₂H₄*

Au	5.85680000	6.63620000	5.85020000
Au	10.85760000	7.29040000	7.83580000
Au	6.89780000	11.28640000	6.48500000
Au	7.95520000	6.49140000	4.00680000
Au	13.34780000	8.28200000	4.91940000
Au	11.66380000	10.00920000	6.59240000
Au	10.53540000	7.71400000	5.08020000
Au	8.28000000	5.44520000	6.67880000
Au	10.76660000	4.41140000	7.61940000
Au	9.34900000	10.87140000	8.01680000
Au	13.55980000	8.19800000	7.81420000
Au	9.22900000	8.92120000	2.85940000
Au	5.27260000	9.07500000	7.01480000
Au	6.85800000	9.14960000	4.46220000
Au	8.38560000	8.38240000	6.79040000
Au	11.50500000	9.66340000	9.45660000
Au	13.07880000	5.28140000	8.93500000
Au	10.34560000	4.83760000	4.82800000
Au	8.88420000	5.65140000	9.44840000
Au	12.87920000	5.73000000	6.17140000
Au	10.08160000	6.14640000	2.25040000
Au	11.69680000	10.49220000	3.77840000
Au	8.92360000	8.53920000	9.90240000
Au	9.26440000	10.75100000	5.10560000
Au	11.29660000	6.98160000	10.58100000
Au	12.04080000	8.20000000	2.30320000
Au	6.61720000	7.18720000	8.69420000
Au	12.70100000	5.70940000	3.41440000
Au	6.80720000	10.15880000	9.13380000
O	14.95400000	5.91660000	11.28020000
O	14.78040000	5.08740000	10.29400000
C	11.52460000	7.10240000	12.84140000
C	11.95400000	5.84560000	12.44500000
H	13.01900000	5.65260000	12.28180000
H	11.28460000	4.98400000	12.50920000
H	12.24280000	7.91020000	13.00260000
H	10.51460000	7.26320000	13.22680000
C	15.80920000	8.31800000	8.15540000
C	15.21780000	8.60580000	9.37460000
H	15.10160000	7.83020000	10.13800000
H	15.06440000	9.64340000	9.68220000
H	16.16980000	7.30960000	7.93920000
H	16.14860000	9.11380000	7.48780000

(h) TS₁₋₁

Au	5.01380000	10.26860000	6.93440000
Au	10.30720000	9.66280000	8.73840000
Au	6.71180000	14.38120000	9.73580000
Au	7.15160000	10.90440000	4.93240000
Au	13.20940000	11.81640000	6.25280000
Au	11.59240000	12.79160000	8.85420000
Au	10.09880000	11.33540000	6.26040000
Au	7.50640000	8.59180000	7.02240000
Au	9.93220000	6.77480000	7.04720000
Au	9.33820000	13.08180000	10.88340000
Au	13.16440000	10.29320000	8.90220000
Au	8.73980000	13.76200000	4.91120000
Au	4.70720000	12.12380000	9.25980000
Au	6.29760000	13.30100000	6.75120000
Au	7.95740000	11.41560000	8.56280000
Au	11.59740000	11.07600000	11.47360000
Au	12.29120000	7.40520000	8.74240000
Au	9.53000000	8.66600000	4.68820000
Au	8.34980000	7.31600000	9.68060000
Au	12.45120000	8.77420000	6.19340000
Au	9.33340000	11.25260000	2.93000000
Au	11.64500000	14.54600000	6.40380000
Au	8.58480000	9.98040000	11.58120000
Au	9.10460000	14.41380000	7.95980000
Au	10.80020000	8.06080000	11.24340000
Au	11.62300000	13.11000000	3.79000000
Au	6.03860000	9.31420000	9.82800000
Au	12.14120000	10.11900000	3.65080000
Au	6.50140000	12.02240000	11.75100000
O	12.82826451	5.06861941	9.98400885
O	13.76906451	5.96401941	9.87480885
C	12.20808938	7.04824430	12.78609786
C	12.27648938	5.66004430	12.49249786

H	13.24408938	5.13404430	12.43149786
H	11.38028938	5.04924430	12.37969786
H	13.10228938	7.64184430	12.61989786
H	11.53448938	7.45464430	13.56769786
C	15.47220000	10.83480000	9.59480000
C	15.40760000	9.43100000	9.72880000
H	15.65460000	8.74880000	8.91580000
H	15.11580000	8.98580000	10.69840000
H	15.84000000	11.28640000	8.65320000
H	15.27300000	11.51720000	10.42980000

(i) OMME1

Au	5.21080000	11.76920000	7.63360000
Au	10.24740000	10.58080000	9.07100000
Au	6.94120000	14.91760000	10.76800000
Au	7.18920000	12.55500000	5.82520000
Au	12.79360000	12.88740000	6.98760000
Au	11.38980000	13.36840000	9.56720000
Au	9.94580000	12.60420000	7.07120000
Au	7.49560000	10.12940000	7.39260000
Au	9.69180000	8.38760000	7.09820000
Au	9.28420000	13.46840000	11.54720000
Au	13.05840000	11.06140000	9.27800000
Au	8.78640000	15.05500000	6.21420000
Au	4.98160000	13.02940000	10.07840000
Au	6.51020000	14.46960000	7.90220000
Au	8.03340000	12.38120000	9.15980000
Au	11.26600000	11.47380000	11.72280000
Au	11.95740000	8.29420000	8.83400000
Au	9.33140000	10.47400000	5.20720000
Au	8.27960000	8.54760000	9.67900000
Au	11.96380000	10.10180000	6.64460000
Au	9.21040000	13.09720000	4.00060000
Au	11.46540000	15.41340000	7.57640000
Au	8.56460000	10.55860000	11.75120000
Au	9.15760000	15.18540000	9.10220000
Au	10.64880000	8.63300000	11.44720000
Au	11.41040000	14.58180000	4.93820000
Au	6.16840000	10.42720000	10.13920000
Au	11.76820000	11.81180000	4.46640000
Au	6.65080000	12.49540000	12.30200000
O	12.16620000	5.79000000	10.22780000
O	13.09180000	6.65380000	9.57300000
C	12.15600000	7.37560000	12.20420000
C	12.22440000	5.96920000	11.65000000
H	13.17040000	5.50920000	12.00540000
H	11.38660000	5.34760000	12.00140000
H	13.08360000	7.93180000	12.01060000
H	11.98860000	7.32060000	13.29180000
C	15.13060000	11.36580000	10.14320000
C	15.08700000	10.06380000	9.66960000
H	15.47320000	9.81520000	8.67900000
H	14.87840000	9.22140000	10.33220000
H	15.57000000	12.16220000	9.53820000
H	14.97300000	11.58440000	11.20140000

(j) TS_{1,2}

Au	5.19540000	11.99740000	7.62600000
Au	10.07760000	10.43420000	9.10180000
Au	7.13460000	14.96740000	10.86860000
Au	7.31700000	12.67960000	5.94420000
Au	12.90180000	12.53640000	7.12160000
Au	11.47900000	13.14260000	9.72640000
Au	10.04900000	12.52980000	7.18580000
Au	7.32280000	10.14720000	7.38320000
Au	9.46720000	8.32540000	7.11180000
Au	9.33580000	13.29040000	11.61640000
Au	12.88920000	10.69900000	9.39460000
Au	9.05040000	15.06580000	6.34300000
Au	5.06400000	13.27180000	10.06480000
Au	6.69920000	14.67120000	7.97800000
Au	7.99640000	12.39560000	9.16360000
Au	11.18100000	11.15820000	11.79100000
Au	11.68580000	7.95900000	8.80620000
Au	9.23820000	10.48180000	5.28640000
Au	7.99460000	8.49020000	9.64240000
Au	11.87320000	9.82500000	6.70080000
Au	9.37520000	13.12460000	4.10880000
Au	11.76020000	15.17720000	7.77740000
Au	8.41100000	10.45600000	11.73500000

Au	9.38900000	15.07460000	9.23800000
Au	10.36940000	8.37120000	11.36800000
Au	11.67260000	14.36120000	5.14200000
Au	6.01840000	10.53860000	10.09060000
Au	11.79040000	11.58540000	4.55640000
Au	6.62900000	12.51000000	12.29840000
O	12.91480000	6.48540000	10.34660000
O	14.11300000	7.14140000	10.67120000
C	11.69420000	7.13080000	12.41560000
C	12.31140000	6.03160000	11.60140000
H	13.12920000	5.52220000	12.14780000
H	11.58840000	5.25960000	11.31280000
H	12.49580000	7.80800000	12.74540000
H	11.14080000	6.71660000	13.27140000
C	15.01740000	10.38120000	10.05920000
C	15.21480000	9.01220000	9.84220000
H	15.14480000	8.62800000	8.81620000
H	15.60800000	8.36340000	10.61900000
H	15.37180000	11.08380000	9.26560000
H	15.06700000	10.74900000	11.09220000

(k) OMME2

Au	5.21000000	12.10260000	7.63080000
Au	10.01360000	10.37500000	9.12240000
Au	7.24960000	14.99220000	10.91560000
Au	7.39860000	12.72740000	6.00760000
Au	12.97320000	12.35080000	7.20220000
Au	11.54680000	13.02280000	9.83660000
Au	10.12480000	12.48880000	7.26800000
Au	7.25500000	10.15020000	7.36520000
Au	9.36560000	8.28440000	7.11500000
Au	9.36180000	13.18680000	11.65740000
Au	12.87140000	10.48760000	9.46200000
Au	9.21540000	15.06000000	6.41760000
Au	5.12660000	13.38000000	10.06560000
Au	6.82920000	14.74860000	8.02600000
Au	7.99240000	12.39140000	9.16640000
Au	11.13460000	10.98140000	11.80760000
Au	11.54400000	7.84460000	8.80520000
Au	9.22760000	10.47840000	5.33240000
Au	7.88680000	8.47200000	9.62680000
Au	11.84820000	9.68540000	6.70880000
Au	9.47680000	13.12160000	4.17000000
Au	11.92820000	15.03040000	7.88440000
Au	8.33900000	10.39320000	11.72880000
Au	9.51900000	14.99020000	9.30580000
Au	10.22320000	8.23200000	11.35460000
Au	11.81080000	14.23180000	5.24580000
Au	5.96960000	10.58360000	10.06660000
Au	11.81800000	11.47200000	4.60740000
Au	6.63200000	12.50960000	12.29360000
O	14.57930000	8.01170000	7.08060000
O	14.84970000	7.91750000	8.54850000
C	12.59620000	6.51210000	7.58640000
C	14.09070000	6.71060000	6.69710000
H	14.90980000	5.99480000	6.90500000
H	13.99290000	6.82260000	5.60650000
H	12.74960000	6.27090000	8.64770000
H	12.24150000	5.60800000	7.06590000
C	14.79860000	9.86680000	10.02600000
C	15.52690000	9.12980000	8.92410000
H	15.65830000	9.75800000	8.03130000
H	16.53740000	8.82920000	9.27060000
H	15.36150000	10.76840000	10.31050000
H	14.65010000	9.23320000	10.91230000

(l) TS₂₋₁

Au	5.17640000	11.94700000	7.62200000
Au	10.18080000	10.41480000	9.22220000
Au	7.13280000	15.00960000	10.83560000
Au	7.32920000	12.57940000	5.97300000
Au	12.98360000	12.31800000	7.42800000
Au	11.55780000	13.00400000	9.74160000
Au	10.06820000	12.49540000	7.22680000
Au	7.30780000	10.07340000	7.44320000
Au	9.50600000	8.26180000	7.36560000
Au	9.34100000	13.30440000	11.57320000
Au	13.35500000	10.62620000	9.80120000
Au	9.05440000	15.00700000	6.29900000
Au	5.06080000	13.31060000	10.01860000

Au	6.73060000	14.62160000	7.95220000
Au	8.02620000	12.32640000	9.16980000
Au	11.16260000	11.14560000	11.82360000
Au	11.76340000	7.99780000	9.00100000
Au	9.27600000	10.37960000	5.43580000
Au	7.87980000	8.50060000	9.73260000
Au	11.87240000	9.79460000	6.88620000
Au	9.40080000	13.02560000	4.16080000
Au	11.78500000	15.11320000	7.82800000
Au	8.32860000	10.54500000	11.76420000
Au	9.39860000	15.02880000	9.21040000
Au	10.17180000	8.39480000	11.53200000
Au	11.73180000	14.18520000	5.25360000
Au	5.95380000	10.57220000	10.12580000
Au	11.83060000	11.45100000	4.68720000
Au	6.56780000	12.60320000	12.30340000
O	12.70900000	6.54780000	10.21600000
O	14.05600000	9.12760000	11.11640000
C	11.42960000	6.93820000	12.35520000
C	12.04820000	6.01420000	11.30920000
H	12.82840000	5.43800000	11.85860000
H	11.28140000	5.28400000	10.99720000
H	12.17080000	7.54860000	12.89580000
H	10.82120000	6.36520000	13.08440000
C	15.46500000	9.83540000	9.60540000
C	15.14540000	8.56020000	10.34720000
H	14.82600000	7.72920000	9.68660000
H	15.94080000	8.14900000	11.00900000
H	15.59180000	9.86620000	8.52020000
H	16.04100000	10.55260000	10.18960000

(m) TS₃₋₁

Au	5.20320000	12.04560000	7.70040000
Au	10.10920000	10.32580000	9.18540000
Au	7.31760000	15.02460000	10.90860000
Au	7.37140000	12.62760000	6.04060000
Au	12.97920000	12.29540000	7.18680000
Au	11.62740000	12.98320000	9.76300000
Au	10.12020000	12.43960000	7.25840000
Au	7.27120000	10.10460000	7.48360000
Au	9.41280000	8.20540000	7.29500000
Au	9.44820000	13.23380000	11.62720000
Au	13.16380000	10.55820000	9.45260000
Au	9.18280000	14.99200000	6.33940000
Au	5.18680000	13.38100000	10.10080000
Au	6.85700000	14.69300000	8.01700000
Au	8.05640000	12.35880000	9.20900000
Au	11.21960000	11.03020000	11.78080000
Au	11.71460000	7.83140000	8.96320000
Au	9.21200000	10.38820000	5.41720000
Au	7.85760000	8.48600000	9.75540000
Au	11.79500000	9.66820000	6.82440000
Au	9.42600000	13.00820000	4.18520000
Au	11.92120000	15.02640000	7.79740000
Au	8.39800000	10.47880000	11.80580000
Au	9.55160000	14.98940000	9.23940000
Au	10.21820000	8.31660000	11.49320000
Au	11.79340000	14.14740000	5.19400000
Au	5.99520000	10.60040000	10.19900000
Au	11.79960000	11.37360000	4.60240000
Au	6.70240000	12.60660000	12.36180000
O	12.71520000	6.45540000	10.23200000
O	14.62000000	8.56200000	10.70960000
C	11.36560000	6.76320000	12.31800000
C	11.98060000	5.86000000	11.25340000
H	12.71480000	5.20140000	11.78380000
H	11.19740000	5.18680000	10.84300000
H	12.12880000	7.30200000	12.90860000
H	10.70900000	6.17860000	12.98600000
C	15.84160000	10.47420000	10.04080000
C	15.69300000	9.05260000	10.20900000
H	15.42600000	9.27140000	9.04480000
H	16.65320000	8.48640000	10.18720000
H	16.56020000	10.86740000	9.30920000
H	15.32160000	11.16580000	10.70800000

(n) Au₂₉-C₂H₄*+O₂*+CO₂*

Au	5.84400000	6.54460000	5.83840000
Au	10.86660000	7.21460000	7.92360000
Au	6.91020000	11.19740000	6.57380000

Au	7.98620000	6.46940000	4.04600000
Au	13.37380000	8.22900000	5.03240000
Au	11.67720000	9.93840000	6.74500000
Au	10.57920000	7.63820000	5.15320000
Au	8.25580000	5.36160000	6.70640000
Au	10.74160000	4.35300000	7.62180000
Au	9.31280000	10.78340000	8.15680000
Au	13.55180000	8.12700000	7.92800000
Au	9.27420000	8.92360000	2.96660000
Au	5.24820000	8.99240000	6.98980000
Au	6.88420000	9.10940000	4.52440000
Au	8.41600000	8.30480000	6.84400000
Au	11.47480000	9.56340000	9.59900000
Au	12.98520000	5.27880000	9.05140000
Au	10.33000000	4.77340000	4.85000000
Au	8.84800000	5.57760000	9.47220000
Au	12.94080000	5.61280000	6.23860000
Au	10.11640000	6.14820000	2.28960000
Au	11.74700000	10.45540000	3.93800000
Au	8.86300000	8.47200000	9.99460000
Au	9.30660000	10.71120000	5.24400000
Au	11.18340000	6.90160000	10.70600000
Au	12.07020000	8.20900000	2.38960000
Au	6.58600000	7.09100000	8.67620000
Au	12.69420000	5.71980000	3.50380000
Au	6.71280000	10.01140000	9.18320000
O	14.67395632	5.30645277	11.53847617
O	14.73936153	5.24064631	10.26668601
C	11.42320000	6.99740000	12.96640000
C	11.69020000	5.69460000	12.57020000
H	12.72120000	5.36160000	12.42180000
H	10.91580000	4.92640000	12.63080000
H	12.24000000	7.70480000	13.12980000
H	10.44020000	7.28740000	13.34320000
C	15.39600000	8.30200000	8.61840000
O	16.51380000	8.46100000	8.82720000

(o)TS₁₋₃

Au	5.00000000	10.81140000	7.09560000
Au	10.34820000	10.07020000	8.99520000
Au	6.66666667	14.67460000	10.32120000
Au	7.24740000	11.63240000	5.27280000
Au	13.27360000	12.48440000	6.69900000
Au	11.59460000	13.23940000	9.40540000
Au	10.17220000	11.98060000	6.68560000
Au	7.47940000	9.08360000	7.13120000
Au	9.93920000	7.30300000	7.03180000
Au	9.25920000	13.23660000	11.39060000
Au	13.31760000	10.90600000	9.27020000
Au	8.81820000	14.50440000	5.49040000
Au	4.69980000	12.45120000	9.58120000
Au	6.31120000	13.88980000	7.22200000
Au	7.93000000	11.78920000	8.87240000
Au	11.54940000	11.21060000	11.80740000
Au	12.38907168	7.69282304	8.90498301
Au	9.59440000	9.43820000	4.87180000
Au	8.34340000	7.58980000	9.70720000
Au	12.47280000	9.43240000	6.47520000
Au	9.45760000	12.19480000	3.33333333
Au	11.66920000	15.19920000	7.08420000
Au	8.53980000	10.09160000	11.79800000
Au	9.07880000	14.86600000	8.58960000
Au	10.74260000	8.20980000	11.37540000
Au	11.75500000	13.96600000	4.35940000
Au	6.00420000	9.59220000	9.95320000
Au	12.22740000	10.96540000	4.00840000
Au	6.41540000	12.13160000	12.10740000
O	12.90660000	5.20840000	10.00220000
O	13.82300000	6.11200000	9.88680000
C	12.30640000	7.05320000	12.67260000
C	12.36360000	5.66960000	12.42320000
H	13.31460000	5.12260000	12.40860000
H	11.46900000	5.04680000	12.21880000
H	13.20340000	7.64300000	12.49700000
H	11.73100000	7.38200000	13.56460000
C	15.06080000	9.80640000	9.93200000
O	16.12660000	9.33440000	10.16140000

(p)OMME3

Au	5.27220000	11.69660000	7.56660000
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Au	10.29500000	10.58000000	9.16520000
Au	6.89520000	14.83620000	10.83860000
Au	7.36240000	12.55900000	5.92700000
Au	12.93420000	13.05060000	7.22860000
Au	11.48640000	13.47780000	9.75020000
Au	10.08300000	12.68420000	7.25520000
Au	7.57280000	10.06520000	7.38480000
Au	9.84060000	8.42980000	7.14000000
Au	9.26300000	13.37920000	11.59200000
Au	13.27640000	11.39120000	9.51020000
Au	8.86120000	15.10120000	6.35100000
Au	5.02660000	12.91620000	10.02340000
Au	6.53400000	14.47360000	7.93760000
Au	8.01920000	12.33500000	9.17500000
Au	11.29800000	11.43900000	11.76800000
Au	12.04400000	8.30500000	8.87640000
Au	9.53020000	10.58940000	5.33920000
Au	8.32640000	8.44500000	9.65600000
Au	12.10160000	10.23720000	6.82560000
Au	9.41400000	13.23000000	4.17020000
Au	11.46860000	15.58100000	7.78300000
Au	8.59520000	10.47700000	11.73640000
Au	9.15740000	15.12760000	9.24080000
Au	10.70520000	8.59200000	11.45920000
Au	11.58540000	14.73360000	5.16040000
Au	6.20940000	10.30640000	10.09060000
Au	11.97900000	11.97680000	4.66920000
Au	6.62880000	12.35600000	12.28660000
O	12.35300000	5.78820000	10.22740000
O	13.24080000	6.71880000	9.62520000
C	12.21420000	7.34080000	12.22940000
C	12.33100000	5.94820000	11.65540000
H	13.26740000	5.50160000	12.04960000
H	11.49000000	5.30420000	11.95360000
H	13.13320000	7.92120000	12.07080000
H	12.01680000	7.26140000	13.31040000
C	14.75980000	10.18440000	10.00000000
O	15.71140000	9.61480000	10.29820000

(q)TS₃₋₂

Au	4.92220000	11.67740000	7.46800000
Au	10.30440000	10.52160000	9.22400000
Au	6.76680000	15.17640000	11.01660000
Au	7.17100000	12.60300000	5.76900000
Au	13.20080000	13.07600000	7.17760000
Au	11.63760000	13.61900000	9.90760000
Au	10.11060000	12.72260000	7.19620000
Au	7.33520000	9.90200000	7.32580000
Au	9.76020000	8.10000000	7.08860000
Au	9.29220000	13.53280000	11.85620000
Au	13.49260000	11.04980000	9.57560000
Au	8.79720000	15.38040000	6.21740000
Au	4.70440000	13.10580000	10.08180000
Au	6.32600000	14.70780000	7.87640000
Au	7.90980000	12.37880000	9.25420000
Au	11.50900000	11.40680000	11.99020000
Au	12.28340000	8.08080000	8.93180000
Au	9.42620000	10.42460000	5.13800000
Au	8.15380000	8.17240000	9.72520000
Au	12.25080000	10.10760000	6.77380000
Au	9.32140000	13.26840000	3.86080000
Au	11.68460000	15.81340000	7.81440000
Au	8.45460000	10.43840000	11.97160000
Au	9.14700000	15.39560000	9.29440000
Au	10.55980000	8.50460000	11.47120000
Au	11.69020000	14.88400000	4.98140000
Au	5.90180000	10.18880000	10.17840000
Au	12.09200000	11.88940000	4.39420000
Au	6.44740000	12.44440000	12.54520000
O	12.15040000	5.87760000	10.22200000
O	14.15700000	6.94980000	9.08660000
C	12.15120000	7.27900000	12.27440000
C	12.24320000	5.91580000	11.57840000
H	13.20220000	5.42620000	11.94180000
H	11.38260000	5.26860000	11.98960000
H	13.05380000	7.92420000	12.20360000
H	11.84600000	7.15040000	13.34320000
C	15.20260000	9.51300000	9.85400000
O	16.03860000	8.93560000	10.44980000

(r)C₂H₄-Au(111)

Au	4.28283231	7.47712274	21.56604067
Au	-4.27119618	7.47839644	7.17470648
Au	1.46537413	0.78324841	4.61199611
Au	-0.01129008	1.63250426	2.09341334
Au	-1.48440721	7.47764721	21.58170597
Au	-1.38136904	7.47345150	7.20074177
Au	4.34793410	0.78534626	4.62015972
Au	2.87291365	1.63430242	2.10444524
Au	1.39836904	7.47697290	21.55986281
Au	1.50456497	7.47539951	7.20714027
Au	7.22781213	0.78729427	4.59964039
Au	5.75296472	1.63235441	2.08194017
Au	7.16660347	2.48213473	21.56449621
Au	-1.38733850	2.48505674	7.19963858
Au	0.02145547	3.27999318	4.62258674
Au	-1.45083978	4.12917411	2.09098633
Au	1.39867184	2.48370812	21.58280916
Au	1.50067184	2.48610566	7.20714027
Au	2.90315030	3.28358950	4.62126291
Au	1.43219601	4.13089735	2.10951992
Au	4.28248626	2.48228457	21.56648195
Au	4.38972036	2.48205980	7.17911924
Au	5.78748380	3.28486320	4.59324188
Au	4.31250662	4.13134689	2.08370527
Au	5.72506395	4.97910427	21.56912960
Au	-2.82675844	4.97790550	7.20294815
Au	-1.42185759	5.77643826	4.61883589
Au	-2.89588312	6.62606873	2.09341334
Au	-0.04256489	4.98090243	21.58236788
Au	0.06047329	4.97895443	7.22236429
Au	1.46221637	5.78220736	4.61398186
Au	-0.01176590	6.62816658	2.10621035
Au	2.83995182	4.98007828	21.56736450
Au	2.94666684	4.98389937	7.20669899
Au	4.34386794	5.77913550	4.60493570
Au	2.87027498	6.62936536	2.07973379
C	2.56890346	0.69491381	9.29525830
C	1.80701792	1.79800988	9.28885980
H	3.65949894	0.75185553	9.28246130
H	-2.19918588	7.18859303	9.31290934
H	2.24819606	2.79711237	9.27451833
H	0.71646569	1.73964461	9.30651084
Tv	8.65140000	0.00000000	0.00000000
Tv	-4.32570000	7.49233218	0.00000000
Tv	0.00000000	0.00000000	22.06380000