Supporting Information

Charge state enhanced propene binding to yttrium-doped gold clusters

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Supporting information contains:

- Method test – Table S1, Table S2
- Optimized structures of neutral clusters and complexes – Figure S1
- Optimized structures of the isomers of cationic clusters and complexes with \( E_{\text{rel}} < 0.1 \) eV – Figure S2
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- XYZ coordinates and total energies of the optimized clusters and cluster-propene complexes
Table S1: Adsorption energies of propene on \( \text{Au}_{4}^{+} \),\( \text{Au}_{5}^{+} \), \( \text{Au}_{6}^{+} \), \( \text{Au}_{3}Y^{+} \), \( \text{Au}_{4}Y^{+} \), \( \text{Au}_{5}Y^{+} \) (\( E \), eV) calculated using the CCSD(T)/def2-TZVP, TPSSh/def2-TZVP+XDM, CAM-B3LYP/def2-TZVP+XDM, LRC-\( \omega \)PBE/def2-TZVP+XDM, PBE0/CRENBL, PBE0/CRENBL+XDM and PBE0/CRENBL(SO) methods and the deviation of the adsorption energies from the \( \text{Au}_{5}^{+} \) adsorption energy (\( \Delta E_{1} \), kJ/mol, to show the accuracy for the size dependence and doping trends) and from the CCSD(T)/def2-TZVP benchmarks (\( \Delta E_{2} \), kJ/mol), respectively. The values are given in eV. Relative to the CCSD(T) benchmark, the LRC-\( \omega \)PBE method gives the most accurate energies. Using this method, the largest deviation from the benchmarks is 0.12 eV. This value is used to estimate error bars for the calculated relative adsorption energies. For the neutral case, 0.09 eV was used to estimate error bars, based on the same calculation method.

|          | CCSD(T)/def2-TZVP | TPSSh+XDM/def2-TZVP | CAM-B3LYP+XDM/def2-TZVP | LRC-\( \omega \)PBE+XDM/def2-TZVP | PBE0/CRENBL | PBE0+XDM/CRENBL | PBE0/CRENBL(SO) |
|----------|-------------------|---------------------|-------------------------|---------------------------------|-------------|-----------------|-----------------|
| \( \text{E} \) | \( \Delta E_{1} \) | \( \Delta E_{1} \) | \( \Delta E_{2} \) | \( \Delta E_{1} \) | \( \Delta E_{1} \) | \( \Delta E_{2} \) | \( \Delta E_{1} \) |
| \( \text{Au}_{4}^{+} \) | 2.01 | 0.15 | 1.85 | -0.16 | 1.69 | -0.32 | 0.22 | 1.87 | -0.14 | 0.19 | 1.62 | -0.39 | -0.08 | 1.78 | -0.23 | -0.05 | 1.60 | -0.41 | -0.05 |
| \( \text{Au}_{5}^{+} \) | 1.86 | 0.00 | 1.81 | -0.05 | 1.48 | -0.38 | 0.00 | 1.68 | -0.18 | 0.00 | 1.55 | -0.31 | 0.00 | 1.73 | -0.13 | 0.00 | 1.55 | -0.31 | 0.00 |
| \( \text{Au}_{6}^{+} \) | 1.83 | -0.03 | 1.68 | -0.15 | -0.13 | 1.55 | -0.28 | 0.07 | 1.68 | -0.15 | 0.00 | 1.51 | -0.32 | 0.04 | 1.65 | -0.18 | 0.08 | 1.50 | -0.33 | 0.05 |
| \( \text{Au}_{3}Y^{+} \) | 1.28 | -0.58 | 1.15 | -0.13 | -0.66 | 1.15 | -0.13 | -0.32 | 1.15 | -0.13 | -0.53 | 1.06 | -0.22 | 0.49 | 1.20 | -0.08 | 0.54 | 1.10 | -0.18 | 0.45 |
| \( \text{Au}_{4}Y^{+} \) | 1.60 | -0.26 | 1.23 | -0.37 | -0.58 | 1.27 | -0.33 | 0.21 | 1.31 | -0.29 | -0.38 | 1.04 | -0.56 | 0.51 | 1.20 | -0.40 | 0.54 | 0.92 | -0.68 | 0.63 |
| \( \text{Au}_{5}Y^{+} \) | 1.29 | -0.57 | 1.22 | -0.07 | -0.59 | 1.01 | -0.28 | -0.47 | 1.18 | -0.11 | -0.50 | 0.98 | -0.31 | 0.57 | 1.14 | -0.15 | 0.59 | 1.01 | -0.28 | 0.54 |

(a) The PBE0(SO) computations were carried out using the NWChem program.\(^{1}\)
Table S2: Propene adsorption energies on cationic gold and yttrium-doped gold clusters using the LRC-ωPBE/def2-TZVP+XDM method.

| \( n \) | \( \text{LRC-ωPBE/def2-TZVP+XDM} \) | \( \text{Au}_{n}^{+} \) | \( \text{Au}_{n-1}Y^{+} \) |
| --- | --- | --- | --- |
| 4 | | 1.90 | 1.18 |
| 5 | | 1.73 | 1.33 |
| 6 | | 1.72 | 1.2 |
| 7 | | 1.99 | 1.34 |
| 8 | | 1.55 | 1.42 |
| 9 | | 1.35 | 1.35 |
| 10 | | 1.53 | 1.45 |
| 11 | | 1.39 | 1.27 |
| 12 | | 1.35 | 1.28 |
| 13 | | 1.30 | 1.30 |
| 14 | | 1.42 | 1.23 |
| 15 | | 1.49 | 1.54 |
Figure S1: Optimized structures of the lowest energy neutral $\text{Au}_n$ and $\text{Au}_{n-1}Y$ ($n = 5-15$) clusters and the corresponding $\text{Au}_n\text{-C}_3\text{H}_6$ and $\text{Au}_{n-1}Y\text{-C}_3\text{H}_6$ complexes, calculated using the BP86/LANL2DZ method. Au, yellow; Y, blue; C, grey; H, white
Figure S2: Optimized structures of the lowest energy cationic $\text{Au}_n^+$ and $\text{Au}_{n-1}^+\text{Y}^+$ ($n = 5-15$) clusters and the corresponding $\text{Au}_n^+-\text{C}_3\text{H}_6$ and $\text{Au}_{n-1}^+\text{Y}^+-\text{C}_3\text{H}_6$ complexes. The relative energies are given in eV. (Method: LRC-$\omega$PBE/def2-TZVP+XDM)
Figure S3: Optimized structures and proposed growth paths of the lowest energy $\text{Au}_{n+1}^+$ clusters. The most stable $\text{Au}_9^+$ cluster was found by using the CALYPSO program. (Method: LRC-$\omega$PBE/def2-TZVP+XDM)
Figure S4: LUMOs of $\text{Au}_{n+}^+$ clusters.

Figure S5: LUMOs of $\text{Au}_{n-1}Y^+$. The energies of the orbitals are given in eV. For $n=11$, LUMO and LUMO+1 are quasi-degenerate.
Dissociation of propene on gold and yttrium-doped gold clusters

To test whether the gold and yttrium-doped gold clusters are able to dissociate propene after the adsorption we remove the different hydrogens from the propene and put on the cluster in the case of Au$_6$, Au$_5$Y and Au$_6$Y clusters. We found that after the geometry optimization the energies of these geometries are larger in every case than that of the undissociated cases.

![Graph showing energy levels for intact and dissociated propene adduct of Au$_5$Y$^+$, Au$_6$Y$^+$ and Au$_6^+$ clusters. Method: LRC-$\omega$PBE/def2-TZVP+XDM)](image)

*Figure S6: Intact and dissociated propene adduct of Au$_5$Y$^+$, Au$_6$Y$^+$ and Au$_6^+$ clusters (Method: LRC-$\omega$PBE/def2-TZVP+XDM)*
Table S3: Natural charges of the atoms in the neutral and cationic Au$_n$ clusters. The atoms where the propene is bound are marked with bold.

| $n$ | $Au_n^+$ | $Au_n$ |
|-----|---------|-------|
| 4   |         |       |
| Au  | 0.31    | -     |
| Au  | 0.19    | -     |
| Au  | 0.31    | -     |
| Au  | 0.19    | -     |
| 5   |         |       |
| Au  | 0.24    | 0.11  |
| Au  | 0.25    | **0.02** |
| Au  | **0.02** | 0.02  |
| Au  | 0.25    | -0.08 |
| Au  | 0.24    | -0.08 |
| 6   |         |       |
| Au  | **0.09** | 0.09  |
| Au  | 0.25    | 0.09  |
| Au  | 0.21    | 0.09  |
| Au  | 0.20    | -0.09 |
| Au  | 0.17    | -0.09 |
| Au  | 0.09    | **-0.09** |
| 7   |         |       |
| Au  | 0.15    | 0.01  |
| Au  | 0.15    | 0.09  |
| Au  | 0.15    | 0.08  |
| Au  | 0.15    | **0.03** |
| Au  | 0.15    | -0.05 |
| Au  | **0.09** | -0.08 |
| Au  | 0.15    | -0.06 |
| 8   |         |       |
| Au  | 0.12    | 0.06  |
| Au  | 0.11    | 0.06  |
| Au  | **0.17** | 0.06  |
| Au  | 0.14    | 0.06  |
| Au  | 0.11    | **-0.06** |
| Au  | 0.10    | -0.06 |
| Au  | 0.11    | -0.06 |
| Au  | 0.14    | -0.06 |
| 8_2 |         |       |
| Au  | 0.18    | -     |
| Au  | 0.06    | -     |
| Au | 0.17  | -   |
|----|-------|-----|
| Au | 0.09  | -   |
| Au | 0.18  | -   |
| Au | 0.06  | -   |
| Au | 0.09  | -   |
| Au | 0.17  | -   |
| Au | 0.10  | 0.08|
| Au | 0.14  | 0.05|
| Au | 0.10  | -0.06|
| Au | 0.14  | 0.00|
| Au | 0.10  | -0.06|
| Au | 0.14  | 0.05|
| Au | 0.09  | 0.09|
| Au | 0.09  | -0.07|
| Au | 0.09  | -0.07|

| Au | 0.09  | -0.05|
|Au  | 0.12  | -0.03|
| Au | 0.09  | 0.12|
| Au | 0.08  | -0.05|
| Au | 0.12  | 0.01|
| Au | 0.15  | 0.01|
| Au | 0.08  | 0.12|
| Au | 0.09  | -0.05|
| Au | 0.07  | -0.05|
| Au | 0.04  | -0.03|

| Au | 0.06  |
|----|-------|
| Au | 0.13  |
| Au | 0.07  |
| Au | 0.12  |
| Au | 0.06  |

| Au | 0.13  |
|----|-------|
| Au | 0.12  |
| Au | 0.13  |
| Au | 0.12  |
| Au | 0.06  |

| Au | 0.10  | 0.09|
|----|-------|
| Au | 0.10  | 0.09|
|   |   |   |
|---|---|---|
| Au | 0.10 | 0.09 |
| Au | 0.10 | 0.09 |
| Au | 0.10 | 0.09 |
| Au | **0.10** | 0.09 |
| Au | 0.09 | -0.11 |
| Au | 0.09 | -0.11 |
| Au | 0.08 | -0.11 |
| Au | 0.08 | -0.11 |
| Au | 0.08 | **-0.11** |
| **12** |   |   |
| Au | -0.02 | 0.05 |
| Au | -0.02 | 0.08 |
| Au | 0.1 | 0.08 |
| Au | 0.12 | 0.08 |
| Au | 0.12 | 0.08 |
| Au | 0.10 | 0.03 |
| Au | 0.12 | **0.04** |
| Au | 0.12 | -0.13 |
| Au | 0.01 | -0.13 |
| Au | 0.10 | 0.08 |
| Au | **0.10** | -0.11 |
| Au | 0.14 | -0.16 |
| **13** |   |   |
| Au | -0.05 | 0.04 |
| Au | 0.17 | 0.07 |
| Au | -0.05 | 0.07 |
| Au | 0.17 | 0.02 |
| Au | **0.14** | **-0.06** |
| Au | -0.01 | 0.03 |
| Au | 0.14 | -0.05 |
| Au | 0.14 | 0.07 |
| Au | -0.01 | 0.07 |
| Au | 0.14 | -0.08 |
| Au | 0.03 | **-0.08** |
| Au | **0.18** | **-0.05** |
| Au | 0.03 | -0.06 |
| **14** |   |   |
| Au | 0.04 | 0.12 |
| Au | 0.00 | 0.12 |
| Au | **0.18** | 0.04 |
| Au | 0.11 | 0.11 |
Table S4: Natural charges of the atoms in the neutral and cationic yttrium-doped clusters. The atoms where the propene is bound are marked with bold.

|   | $Au_{n-1}Y^+$ | $Au_{n-1}Y$ |
|---|--------------|--------------|
| 4 |              |              |
|   | $Y$ | 1.46 | - |
| Au | -0.08 | - |
| Au | -0.08 | - |
| Au | -0.31 | - |
| 5 |              |              |
|   | $Y$ | 1.37 | 1.27 |
| Au | 0.02 | -0.34 |
| Au | **0.02** | -0.13 |
| Au | -0.21 | -0.34 |
| Au | -0.21 | -0.46 |
|   | \( Y \) |   | \( Au \) |   | \( Au \) |   | \( Au \) |   | \( Au \) |   | \( Au \) |   | \( Au \) |   | \( Au \) |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 |   | 1.13 | 1.16 |   | 0.10 | -0.30 |   | 0.10 | -0.06 |   | -0.12 | -0.06 |   | -0.12 | -0.30 |   | -0.09 | -0.44 |
| 7 |   | 1.03 | 0.51 |   | 0.14 | -0.14 |   | 0.14 | 0.02 |   | -0.15 | -0.14 |   | -0.15 | -0.14 |   | 0.14 | 0.18 |   | 0.15 | -0.14 |
| 8 |   | 0.65 | 0.51 |   | 0.06 | -0.12 |   | 0.02 | -0.12 |   | 0.05 | -0.03 |   | 0.02 | -0.03 |   | 0.06 | -0.08 |   | 0.09 | -0.08 |   | 0.05 | -0.05 |
| 9 |   | 0.65 | 0.04 |   | 0.09 | -0.05 |   | 0.02 | -0.05 |   | 0.02 | -0.03 |   | 0.09 | -0.04 |   | 0.06 | 0.03 |   | 0.01 | 0.03 |   | 0.01 | 0.03 |   | 0.06 | 0.03 |
| 10|   | 0.03 | -0.10 |   | 0.07 | -0.05 |   | 0.15 | 0.00 |   | 0.05 | -0.05 |   | 0.12 | 0.02 |   | 0.16 | 0.02 |   | 0.11 | 0.04 |   | 0.07 | 0.04 |
|   | 10 | 11 | 12 | 13 |
|---|----|----|----|----|
|   | Au | Au | Au | Au |
|   | 0.07 | 0.04 | 0.16 | 0.04 |
|   | 10.2 |   |   |   |
|   | 0.19 |   |   |   |
|   |   |   |   |   |
|   |   | 0.09 |   |   |
|   |   | 0.22 |   |   |
|   |   | 0.19 |   |   |
|   |   | 0.09 |   |   |
|   |   | 0.05 |   |   |
|   |   | 0.18 |   |   |
|   |   | 0.05 |   |   |
|   |   | 0.22 |   |   |
|   |   | 0.22 |   |   |
|   |   |   | 0.24 | 0.02 |
|   |   |   | 0.24 | 0.02 |
|   |   |   | 0.06 | 0.11 |
|   |   |   | 0.17 | 0.00 |
|   |   |   | 0.24 | 0.01 |
|   |   |   | 0.16 | 0.14 |
|   |   |   | 0.06 | 0.00 |
|   |   |   | 0.16 | 0.00 |
|   |   |   | 0.04 | -0.06 |
|   |   |   | 0.21 | 0.03 |
| Y | -0.23 | -0.38 | -1.06 | -1.50 |
| Au | 0.19 | 0.04 | 0.14 | 0.19 |
| Au |   | 0.24 | 0.26 | 0.24 |
| Au |   | 0.15 | 0.15 | 0.24 |
| Au |   |   | 0.24 | 0.24 |
| Au |   |   |   | 0.24 |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Y |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
| Au |   |   |   |   |
|    | Au  | Y   |
|----|-----|-----|
| 14 | 0.18| -2.08|
|    | 0.13| -2.48|
|    | 0.21| 0.27|
|    | 0.15| 0.18|
|    | 0.27| 0.15|
|    | 0.16| 0.15|
|    | 0.16| 0.20|
|    | 0.29| 0.15|
|    | 0.27| 0.20|
|    | 0.19| 0.15|
| 15 | 0.25| -2.66|
|    | 0.29| -3.67|
|    | 0.24| 0.23|
|    | 0.23| 0.23|
|    | 0.30| 0.16|
|    | 0.25| 0.16|
|    | 0.21| 0.13|
|    | 0.27| 0.13|
|    | 0.25| 0.23|
|    | 0.33| 0.28|
|    | 0.34| 0.28|
|    | 0.28| 0.28|
|    | 0.31| 0.28|
|    | 0.27| 0.28|
|    | 0.20| 0.26|
|    | 0.21| 0.28|
|    | 0.27| 0.26|
|    | 0.20| 0.28|
|    | 0.19| 0.23|
|    | 0.24| 0.23|
Figure S7: Natural charges of the atoms in the small neutral and cationic yttrium-doped clusters where the propene prefers to bind also to the yttrium atom. The atom where the propene is preferentially bound is marked with red star. The charge of the yttrium atom is colored with blue. For the cationic Au₅Y⁺ in the case of the most stable isomer structural reorganization takes place. The original geometry of the most stable cluster is marked with a) and the reorganized cluster is marked with b).
Figure S8: Electrostatic potential of the selected cationic \(\text{Au}_8\), \(\text{Au}_5\text{Y}\) and \(\text{Au}_{11}\text{Y}\) clusters.

Table S5: Natural charges of the atoms in the cationic cluster-propene complexes. The atoms where the propene is bound are marked with bold.

| \(n\) | \(\text{Au}_n^+\text{C}_3\text{H}_6\) | \(\text{Au}_{n-1}\text{Y}^+\text{C}_3\text{H}_6\) |
|---|---|---|
| \(4\) | \(\text{Au}/\text{Y}\) | \(0.20\) | \(1.43\) |
| | \(\text{Au}\) | \(0.17\) | \(-0.10\) |
| | \(\text{Au}\) | \(0.36\) | \(-0.08\) |
| | \(\text{Au}\) | \(0.16\) | \(-0.35\) |
| | \(\text{C}\) | \(-0.51\) | \(-0.67\) |
| | \(\text{C}\) | \(-0.16\) | \(-0.02\) |
| | \(\text{C}\) | \(-0.64\) | \(-0.65\) |
| | \(\text{H}\) | \(0.24\) | \(0.23\) |
| | \(\text{H}\) | \(0.24\) | \(0.25\) |
| | \(\text{H}\) | \(0.23\) | \(0.22\) |
| | \(\text{H}\) | \(0.22\) | \(0.27\) |
| | \(\text{H}\) | \(0.23\) | \(0.25\) |
| | \(\text{H}\) | \(0.25\) | \(0.22\) |
| \(5\) | \(\text{Au}/\text{Y}\) | \(0.16\) | \(1.47\) | \(1.24\) |
| | \(\text{Au}\) | \(0.19\) | \(0.40\) | \(0.01\) |
| | \(\text{Au}\) | \(0.36\) | \(-0.27\) | \(0.02\) |
| | \(\text{Au}\) | \(0.03\) | \(-0.29\) | \(-0.21\) |
| | \(\text{Au}\) | \(0.14\) | \(-0.36\) | \(-0.19\) |
| | \(\text{C}\) | \(-0.52\) | \(-0.51\) | \(-0.67\) |
| | \(\text{C}\) | \(-0.15\) | \(-0.19\) | \(0.00\) |
|   |  6   |  7   |  8   |
|---|------|------|------|
| C | -0.64 | -0.63 | -0.65 |
| H |  0.24 |  0.23 |  0.24 |
| H |  0.23 |  0.24 |  0.25 |
| H |  0.23 |  0.23 |  0.23 |
| H |  0.24 |  0.23 |  0.25 |
| H |  0.25 |  0.22 |  0.22 |
| H |  0.22 |  0.24 |  0.26 |
| Au/Y |  0.23 | 1.23 | **0.97** | 1.22 |
| Au |  0.09 | -0.21 |  0.09 | -0.08 |
| Au |  0.09 | -0.08 |  0.10 | -0.07 |
| Au | **0.28** | **0.27** | -0.11 | -0.21 |
| Au |  0.06 | -0.07 | -0.11 | -0.22 |
| Au |  0.06 | -0.22 | -0.06 | **0.26** |
| C | -0.48 | -0.51 | -0.65 | -0.50 |
| C | -0.12 | -0.16 | -0.02 | -0.16 |
| C | -0.64 | -0.64 | -0.65 | -0.64 |
| H |  0.24 |  0.23 |  0.25 |  0.23 |
| H |  0.24 |  0.24 |  0.24 |  0.24 |
| H |  0.23 |  0.22 |  0.22 |  0.23 |
| H |  0.22 |  0.23 |  0.26 |  0.24 |
| H |  0.25 |  0.24 |  0.22 |  0.23 |
| H |  0.24 |  0.22 |  0.25 |  0.22 |
| Au/Y |  0.09 | 1.13 |      |      |
| Au |  0.09 |  0.09 |      |      |
| Au |  0.10 |  0.10 |      |      |
| Au |  0.04 | -0.33 |      |      |
| Au |  0.11 | -0.19 |      |      |
| Au |  0.05 | **0.32** |      |      |
| Au | **0.40** | -0.18 |      |      |
| C | -0.50 | -0.52 |      |      |
| C | -0.16 | -0.16 |      |      |
| C | -0.64 | -0.64 |      |      |
| H |  0.24 |  0.23 |      |      |
| H |  0.24 |  0.24 |      |      |
| H |  0.23 |  0.23 |      |      |
| H |  0.25 |  0.25 |      |      |
| H |  0.23 |  0.22 |      |      |
| H |  0.22 |  0.23 |      |      |
| Au/Y |  0.13 | **0.30** | 0.73 |      |
| Au |  0.07 |  0.00 | **0.25** |      |
| Au | **0.41** |  0.09 |  0.01 |      |
| Au | -0.01 |  0.10 | -0.07 |      |
|   | Au       | C      | H      |
|---|---------|--------|--------|
| 9 | Au/¥    | 0.11   | 0.59   |
|   | Au      | 0.03   | -0.01  |
|   | Au      | 0.12   | 0.01   |
|   | Au      | 0.20   | 0.26   |
|   | Au      | 0.06   | 0.06   |
|   | Au      | 0.12   | 0.03   |
|   | Au      | 0.10   | -0.06  |
|   | Au      | 0.03   | -0.02  |
|   | Au      | 0.15   | 0.02   |
|   | C       | -0.51  | -0.49  |
|   | C       | -0.14  | -0.15  |
|   | C       | -0.64  | -0.64  |
|   | H       | 0.24   | 0.24   |
|   | H       | 0.23   | 0.23   |
|   | H       | 0.22   | 0.23   |
|   | H       | 0.22   | 0.23   |
|   | H       | 0.23   | 0.22   |
|   | H       | 0.25   | 0.25   |
| 10| Au/¥    | 0.04   | -0.04  | 0.30   | -0.18 |
|   | Au      | 0.09   | 0.32   | 0.03   | -0.03 |
|   | Au      | 0.04   | -0.01  | 0.08   | 0.37  |
|   | Au      | 0.14   | 0.16   | 0.12   | 0.02  |
|   | Au      | 0.03   | 0.06   | 0.04   | 0.08  |
|   | Au      | 0.09   | -0.01  | 0.18   | 0.15  |
|   | Au      | 0.04   | 0.10   | 0.00   | 0.03  |
|   | Au      | 0.30   | 0.14   | -0.01  | 0.18  |
|   | Au      | 0.13   | 0.13   | 0.02   | 0.18  |
|   | Au      | 0.04   | 0.08   | 0.12   | 0.13  |
|   | C       | -0.52  | -0.52  | -0.48  | -0.50 |
|   | C       | -0.17  | -0.17  | -0.15  | -0.18 |
|    | C  |     |     |     |     |
|----|----|-----|-----|-----|-----|
|    | -0.64 | -0.64 | -0.64 | -0.63 |     |
| H  | 0.24  | 0.24  | 0.23  | 0.23  |     |
| H  | 0.23  | 0.23  | 0.23  | 0.23  |     |
| H  | 0.23  | 0.23  | 0.22  | 0.22  |     |
| H  | 0.23  | 0.23  | 0.23  | 0.24  |     |
| H  | 0.25  | 0.25  | 0.25  | 0.23  |     |
| H  | 0.22  | 0.22  | 0.22  | 0.22  |     |

11

| Au/Y | 0.11 | -0.41 |
|------|------|-------|
| Au   | 0.10 | 0.06  |
| Au   | 0.10 | 0.19  |
| Au   | 0.09 | 0.01  |
| Au   | 0.09 | 0.07  |
| Au   | 0.08 | 0.20  |
| Au   | **0.21** | 0.13 |
| Au   | 0.09 | 0.12  |
| Au   | 0.01 | **0.34** |
| Au   | 0.01 | 0.01  |
| Au   | 0.01 | 0.20  |
| C    | -0.51 | -0.49 |
| C    | -0.15 | -0.17 |
| C    | -0.64 | -0.64 |
| H    | 0.24  | 0.23  |
| H    | 0.23  | 0.23  |
| H    | 0.22  | 0.22  |
| H    | 0.25  | 0.23  |
| H    | 0.22  | 0.24  |
| H    | 0.23  | 0.22  |

12

| Au/Y | -0.04 | -0.89 |
|------|-------|-------|
| Au   | -0.05 | 0.19  |
| Au   | 0.10  | 0.15  |
| Au   | 0.11  | 0.15  |
| Au   | 0.10  | 0.14  |
| Au   | 0.10  | 0.21  |
| Au   | 0.10  | 0.12  |
| Au   | 0.11  | 0.14  |
| Au   | -0.01 | 0.12  |
| Au   | **0.24** | 0.06 |
| Au   | 0.07  | **0.37** |
| Au   | 0.07  | 0.17  |
| C    | -0.51 | -0.50 |
| C    | -0.15 | -0.17 |
| C    | -0.64 | -0.64 |
| H    | 0.23  | 0.23  |
|     | 0.24 | 0.24 |
|-----|------|------|
|     | 0.22 | 0.23 |
|     | 0.23 | 0.23 |
|     | 0.22 | 0.24 |
|     | 0.25 | 0.22 |
| **13** |  
| Au/Y | -0.10 | -1.49 |
| Au   | 0.17  | 0.19  |
| Au   | 0.17  | 0.05  |
| Au   | 0.12  | 0.14  |
| Au   | -0.05 | 0.17  |
| Au   | 0.15  | 0.14  |
| Au   | 0.13  | 0.26  |
| Au   | -0.05 | 0.37  |
| Au   | 0.15  | 0.15  |
| Au   | 0.18  | 0.26  |
| Au   | 0.15  | 0.26  |
| Au   | -0.04 | 0.16  |
| C    | -0.50 | -0.49 |
| C    | -0.15 | -0.17 |
| C    | -0.64 | -0.64 |
|     | 0.24  | 0.23  |
|     | 0.23  | 0.23  |
|     | 0.22  | 0.22  |
|     | 0.24  | 0.23  |
|     | 0.23  | 0.22  |
|     | 0.22  | 0.24  |
| **14** |  
| Au/Y | 0.27  | -2.30 |
| Au   | 0.11  | 0.27  |
| Au   | 0.11  | 0.21  |
| Au   | 0.12  | 0.43  |
| Au   | 0.08  | 0.21  |
| Au   | 0.12  | 0.32  |
| Au   | -0.01 | 0.29  |
| Au   | 0.12  | 0.31  |
| Au   | 0.12  | 0.20  |
| Au   | -0.02 | 0.15  |
| Au   | 0.03  | 0.25  |
| Au   | -0.01 | 0.24  |
| Au   | -0.04 | 0.15  |
| Au   | -0.05 | 0.17  |
| C    | -0.50 | -0.49 |
| C    | -0.18 | -0.16 |
Localized orbital locators (LOL) and bond critical points of the electron density

We used the localized orbital locator (LOL) and the Bader analysis to analyze the chemical bonds between the cluster and propene. LOL is a bonding descriptor, based on the kinetic energy density. It characterizes the atomic shells and the different elements of chemical bonding (e.g. bonds, lone pairs, etc.) correctly, thus it is considered a valuable tool in the analysis of chemical bonding. The Bader analysis defines the chemical bonds by bond critical points (BCP) and the corresponding bond paths, starting from the bond critical point and leading to the nuclei. In this approach, a
covalent bond is characterized by a \( \sim 0.1 \) a.u. electron density at the BCP and a negative Laplacian, while electrostatic interactions and ionic bonds are characterized by a lower, \( \sim 0.01 \) a.u. electron density and a positive Laplacian.

The LOL profiles of the neutral and the cationic clusters indicate the formation of two-electron three-center bonds between the metal atoms in both cases (Figure S9). In the case of the yttrium doped gold clusters, increased localization in the vicinity of the yttrium atom can be observed. The LOL profile of the propene-cluster complex is approximately the union of that of the reactants. Slightly increased localization can be observed near to the propene adsorption site. The absence of the basin between the propene and cluster shows that there is no covalent bond between the two fragments, neither in the neutral, nor in the cationic case.

*Figure S9: Localized Orbital Locator isosurfaces (green lobes) of propene, selected clusters (\( \text{Au}_8^+ \), \( \text{Au}_8\text{Y}^+ \), \( \text{Au}_5\text{Y}^+ \)) and complexes (\( \text{Au}_8^+\text{-C}_3\text{H}_6 \), \( \text{Au}_8\text{Y}^+\text{-C}_3\text{H}_6 \), \( \text{Au}_5\text{Y}^+\text{-C}_3\text{H}_6 \)). LOL =0.3.*
The topological analysis of the electron density (Bader analysis) fully supports this conclusion. The electron density at the BCP is small (~0.07 a.u.) and the Laplacian of the electron density is positive in the BCP of the carbon-gold chemical bond. If propene binds to the yttrium atom, the electron density at the BCP is even smaller (~0.03 a.u.) while the Laplacian is also positive. These values indicate electrostatic interactions between the cluster and propene, similarly to what we observed in the neutral case.

**Natural charges and bond indices**

The natural charges clearly show that the positive charge resides mainly in the metal atoms of the cluster-propene complex cations, while the propene is approximately neutral with an overall charge of ~0.1 in all cases (Figure S10).

![Figure S10: Total natural charge of clusters with respect to the cluster size](image)

The Wiberg bond indices between the carbon atom and the adjacent metal atom (~0.3 for Au-C and ~0.15 for Y-C) are small, clearly showing that there is no covalent bond between the propene and the cluster (Table S5).
Upon propene adsorption the C1-C2 (single C-C bond in propene) bond indices are decreasing, while the C2-C3 (double C-C bond in propene) bond indices are increasing slightly. The C1-C2 decrease is smaller if propene binds to the yttrium atom. The natural charges change also with the adsorption: the charge of C1 becomes more negative, that of C2 becomes slightly less negative, and that of C3 changes only a slightly. For M=Y these values change more significantly. These changes imply donation-back donation mechanism for the adsorption – for the yttrium connected propene complexes in somewhat less extent, similarly to the neutral case.

Table S6: Natural charges of carbon atoms in propene and Wiberg bond indices between the carbon atoms in propene and between the carbon atoms and the adjacent metal atom of the cluster (M=Au or Y). See Figure S9 for labelling of the carbon atoms.

|                 | C3H6 | Au8+-C3H6 | Au8Y+-C3H6 | Au5Y+-C3H6 |
|-----------------|------|-----------|------------|------------|
| **Natural charge** |      |           |            |            |
| C1              | -0.39| -0.48     | -0.49      | -0.65      |
| C2              | -0.17| -0.15     | -0.15      | -0.02      |
| C3              | -0.61| -0.64     | -0.64      | -0.65      |
| **Wiberg bond index** |      |           |            |            |
| C1-C2           | 1.98 | 1.64      | 1.67       | 1.82       |
| C2-C3           | 1.06 | 1.08      | 1.08       | 1.09       |
| M-C1            | -    | 0.28      | 0.26       | 0.16       |
| M-C2            | -    | 0.22      | 0.21       | 0.07       |

Table S7: Total electron density transfer (dQ) due to the donation/back-donation

|      | Au_n |            | Au_{n+1}Y |            |
|------|------|------------|-----------|------------|
| n    | donation [e^-] | back-donation [e^-] | donation [e^-] | back-donation [e^-] |
| 4    | 0.049 | 0.019 | 0.017 | 0.008 |
| 5    | 0.050 | 0.024 | 0.047 | 0.031 |
| 6    | 0.031 | 0.013 | 0.040 | 0.016 |
| 7    | 0.048 | 0.019 | 0.042 | 0.020 |
| 8    | 0.050 | 0.023 | 0.040 | 0.015 |
| 9    | 0.036 | 0.013 | 0.040 | 0.016 |
| 10   | 0.045 | 0.020 | 0.037 | 0.008 |
| 11   | 0.038 | 0.015 | 0.038 | 0.016 |
| 12   | 0.037 | 0.010 | 0.041 | 0.015 |
| 13   | 0.035 | 0.010 | 0.039 | 0.017 |
| 14   | 0.042 | 0.011 | 0.041 | 0.017 |
| 15   | 0.039 | 0.011 | 0.042 | 0.018 |
XYZ coordinates of the optimized clusters and cluster-propene complexes on BP86/LANL2DZ level and total energies (in Hartree) on TPSSh/DEF2-TZVP level. The imaginary frequencies are also collected.

| Au₄   | E = -542.5743802783 |
|-------|---------------------|
|       | Imaginary frequencies: no |
|       | Au 0.0000000000 -1.3803040121 -0.0007572594 |
|       | Au -2.3393335920 0.0000000000 0.0007572819 |
|       | Au 0.0000000000 1.3803040121 -0.0007572594 |
|       | Au 2.3393335920 0.0000000000 0.0007572819 |

| Au₅   | E = -678.3407782094 |
|-------|---------------------|
|       | Imaginary frequencies: no |
|       | Au 2.3895648628 -0.2122536028 -1.3066017067 |
|       | Au 2.3758360989 -0.1006243499 1.3145272555 |
|       | Au 0.0000000000 0.0000000000 -0.0158509752 |
|       | Au -2.3758360989 0.1006243499 1.3145272555 |
|       | Au -2.3895648628 0.2122536028 -1.3066017067 |

| Au₆   | E = -814.0738594346 |
|-------|---------------------|
|       | Imaginary frequencies: 7.69i |
|       | Au 3.0712936987 0.5507920995 -0.0011969724 |
|       | Au 0.5588870226 1.4579207060 -0.0043913798 |
|       | Au 1.0897603175 -1.2295960643 0.0058922629 |
|       | Au -1.0299810566 -2.8557853623 0.0006903003 |
|       | Au -1.9547718750 2.3635730766 0.0060239140 |
|       | Au -1.7351881074 -0.2869044556 -0.0070181250 |

| Au₇   | E = -949.8430618484 |
|-------|---------------------|
|       | Imaginary frequencies: 15.68i |
|       | Au 0.0000043728 -2.7633400310 -0.0019236486 |
|       | Au -2.3903138740 -1.3808124924 0.0009751180 |
|       | Au 2.3903173091 -1.3808049435 0.0009762656 |
|       | Au -2.3903173091 1.3808049435 0.0009762656 |
|       | Au -0.0000043728 2.7633400310 -0.0019236486 |
|       | Au 2.3903138740 1.3808124924 0.0009751180 |
|       | Au 0.0000000000 0.0000000000 -0.000554339 |

| Au₈   | E = -1085.57469121 |
|-------|---------------------|
|       | Imaginary frequencies: no |
|       | Au 1.1006707262 -1.4565183166 -0.3746391609 |
|       | Au 1.2572762841 1.2995896245 0.2929809925 |
|        |        |        |        |
|--------|--------|--------|--------|
| Au     | -1.1174583150 | 0.3142991095 | -1.1066985955 |
| Au     | -1.3537382201  | -1.5491602035 | 1.0898381950 |
| Au     | -0.8289563470  | 2.9427446016  | -0.4422446878 |
| Au     | 3.3712748464   | -0.3245249559 | 0.4631711771 |
| Au     | -1.1898894154  | -2.3687301544 | -1.5937890532 |
| Au     | -1.2391795592  | 1.1423002948  | 1.6713811328 |

**Au$_8$**

$E = -1085.5772889538$

Imaginary frequencies: no

| Au     | 2.2560829760  | -2.7946706324 | 0.0000000000 |
|--------|--------------|--------------|---------------|
| Au     | 1.4514516312  | -0.2454413555 | 0.0000000000 |
| Au     | 3.0438221840  | 1.9011571129  | 0.0000000000 |
| Au     | 0.3946151437  | 2.3487843741  | 0.0000000000 |
| Au     | -2.2557145182 | 2.7943797303  | 0.0000000000 |
| Au     | -1.4517762135 | 0.2449200541  | 0.0000000000 |
| Au     | -0.3941948172 | -2.3484931196 | 0.0000000000 |
| Au     | -3.0442863860 | -1.9006361639 | 0.0000000000 |

**Au$_9$**

$E = -1221.3450007571$

Imaginary frequencies: no

| Au     | -1.4435679158 | -1.4253483185 | -0.3044344582 |
|--------|--------------|--------------|---------------|
| Au     | -3.0310180985 | 0.0000000000 | -1.9094087071 |
| Au     | -1.4435679158 | 1.4253483185 | -0.3044344582 |
| Au     | -0.0000000000 | -2.7434437009 | 1.6267357212 |
| Au     | 0.0000000000  | 2.7434437009 | 1.6267357212 |
| Au     | 1.4435679158  | 1.4253483185 | -0.3044344582 |
| Au     | 1.4435679158  | -1.4253483185 | -0.3044344582 |
| Au     | 3.0310180985  | -0.0000000000 | -1.9094087071 |
| Au     | 0.0000000000  | -0.0000000000 | 1.7830825309 |

**Au$_{10}$**

$E = -1357.0743424524$

Imaginary frequencies: no

| Au     | 1.4723020649  | -2.7937434748 | 1.1856879886 |
|--------|--------------|--------------|---------------|
| Au     | -0.8447522962 | -1.4461003856 | 1.1884080831 |
| Au     | -3.1911941706 | -0.0004392188 | 1.1419107511 |
| Au     | 0.9882220622  | -1.4004237831 | -1.2119723024 |
| Au     | -0.1583335436 | 0.0002066204  | -3.3669848424 |
| Au     | -1.6916889563 | -0.0000761359 | -1.1692589273 |
| Au     | 1.8094643899  | 0.0000169920  | 1.0704248418 |
| Au     | -0.8449913801 | 1.4465765277  | 1.1885435328 |
| Au     | 0.9882788243  | 1.4004857976  | -1.2120886686 |
| Au     | 1.4726930056  | 2.7934970604  | 1.1853295433 |
Au_{10, 2}
E = -1357.0779997346

Imaginary frequencies: no

|    |    |    |    |
|----|----|----|----|
| Au | -0.1059420176 | -3.2429463268 | -1.7215855269 |
| Au | -1.6338403814 | -1.4676510742 | -0.4497245567 |
| Au | -1.057264103  | 3.2431287249  | -1.723156338  |
| Au | 1.1740989409  | -1.4338172805 | -0.2300140244 |
| Au | 3.5475599423  | -0.0001865396 | -0.1336925807 |
| Au | -1.6336440922 | 1.4677699438  | -0.4495679711 |
| Au | 1.8705060017  | 0.0000973144  | 2.1101162716  |
| Au | -0.8226002083 | 0.0000781573  | 1.8652707430  |
| Au | 1.1743258559  | 1.4337809459  | -0.2300299119 |

Au_{11}
E = -1492.85438007

Imaginary frequencies: no

|    |    |    |    |
|----|----|----|----|
| Au | -1.4358424706 | -0.8266298692 | -1.4096452454 |
| Au | 1.4357642393  | -0.8267661147 | -1.4096448933 |
| Au | 0.0000791966  | 1.6593430361  | -1.4103971578 |
| Au | 1.4357642393  | -0.8267661147 | 1.4096448933  |
| Au | -1.4358424706 | -0.8266298692 | 1.4096452454  |
| Au | 0.0000791966  | 1.6593430361  | 1.4103971578  |
| Au | -0.0000002774 | 0.0014043241  | 3.5904155375  |
| Au | -0.0000002774 | 0.0014043241  | -3.5904155375 |
| Au | -3.3879797627 | -1.9663448369 | 0.0000000000  |
| Au | 0.0001865696  | 3.9183117669  | 0.0000000000  |
| Au | 3.3877918174  | -1.9666696823 | 0.0000000000  |

Au_{12}
E = -1628.582367701

Imaginary frequencies: no

|    |    |    |    |
|----|----|----|----|
| Au | -3.6379985979 | 0.0000000000 | -0.4119190203 |
| Au | 3.6379985979  | 0.0000000000 | -0.4119190203 |
| Au | -1.3966754453 | 0.0000000000 | -2.0284178046 |
| Au | -1.3983923214 | -1.4244599880 | 0.4225767235 |
| Au | -1.3983923214 | 1.4244599880  | 0.4225767235  |
| Au | 1.3966754453  | 0.0000000000  | -2.0284178046 |
| Au | 1.3983923214  | 1.4244599880  | 0.4225767235  |
| Au | 1.3983923214  | -1.4244599880 | 0.4225767235  |
| Au | 0.0000000000  | 0.0000000000  | -4.3145044807 |
| Au | 0.0000000000  | -2.7117405798 | 2.4419596052  |
| Au | 0.0000000000  | 2.7117405798  | 2.4419596052  |
| Au | 0.0000000000  | 0.0000000000  | 2.6209520260  |

Au_{13}
E = -1764.3412932263
Imaginary frequencies: no
Au       -2.4443402821    0.0000000000   -2.0902142638
Au        0.0000000000   -1.3898978257   -1.9832211282
Au        2.4443402821    0.0000000000   -2.0902142638
Au        0.0000000000    1.3898978257   -1.9832211282
Au       -1.5764748052   -1.4128110124    0.3448918302
Au        0.0000000000   -3.5999229622   -0.2546448751
Au        1.5764748052   -1.4128110124    0.3448918302
Au       -1.5764748052    1.4128110124    0.3448918302
Au        0.0000000000    3.5999229622   -0.2546448751
Au        1.5764748052    1.4128110124    0.3448918302
Au       -2.7148161391    0.0000000000    2.4542639267
Au        0.0000000000    0.0000000000    2.3680506348
Au        2.7148161391    0.0000000000    2.4542639267

Au_{14}
E = -1900.0795148249
Imaginary frequencies: no
Au       1.5274999491   -1.9594068076   -0.5676136476
Au      -1.3933653360   -0.3521212564    1.2074845085
Au        0.2634624187   1.9267490237   1.5920075150
Au       2.0975824720    0.7719943676   -0.2908772430
Au       1.3008138540   -0.7528289077   2.0030792151
Au       -1.2147317404   -2.1680295764   -0.9520516611
Au       -3.6770601977   -1.4872954525    0.0365060970
Au       -2.3101346917    0.4334484470   -1.3515773401
Au       -0.1502782018   2.1753092874   -1.2129862853
Au       -2.1185534929   2.5003932608   -3.0183514741
Au       -0.4757241324   0.4026228663    3.7500969278
Au       1.9183329547    3.5145850599    0.0790212787
Au       0.4645123353   -3.8727404911   -2.125600290
Au       3.7676434684   -1.1326798211    0.8508656431

Au_{15}
E = -2035.8493584813
Imaginary frequencies: 12.78i; 2.01i
Au        2.5531996531   -2.0434859199    0.2578637122
Au        3.6848153730    0.4419246214    0.2453348085
Au        1.2935548031   0.9601525846    1.6738958874
Au        2.4627224821   3.0757640058    0.1347620335
Au       -0.3019728230    2.8863786541    0.1761552467
Au       -1.4596039635    0.5795233537    1.6666031366
Au       -1.5529294427    0.5420618914   -1.1962044769
Au       -0.0315840861   -0.0127860363   -3.4209799499
Au        0.2097235208   -1.6941739901   -1.2619361830
Au  0.3637100929  -3.9412367791  0.3139578801  0.3139578801
Au  -3.7903185225  -0.2842190011  0.2799128119  0.2799128119
Au  -2.0239235084  -2.3575430181  0.3461130874  0.3461130874
Au  1.355565962  0.8872270834  -1.2227335331  -1.2227335331
Au  -3.0227358970  2.4989232133  0.1921468015  0.1921468015

Au-C$_3$H$_6$
E = -660.5986783356
Imaginary frequencies: 6.83i

Au  -2.3564336420  1.0602483273  0.7837987913
Au  1.7663462450  0.1054283177  -1.2115459320  -1.2115459320
Au  -0.3013113758  -0.8119534148  0.4286785731  0.4286785731
Au  -0.2023248536  1.7774238690  -0.6101611756  -0.6101611756
C  -0.9523131055  -2.6216505878  1.6175834936  1.6175834936
C  0.2787548506  -3.0443011634  1.0757554990  1.0757554990
C  1.5814303092  -3.0578847538  1.8252832582  1.8252832582
H  -1.894297116  -2.9134276930  1.1380310709  1.1380310709
H  -1.0101465384  -2.2902520757  2.6620705733  2.6620705733
H  0.2590859158  -3.5721240173  0.1101424364  0.1101424364
H  1.5543549234  -2.4396863591  2.7367622245  2.7367622245
H  2.4285518528  -2.7403278957  1.1920616314  1.1920616314
H  1.7993764259  -4.1038672805  2.1268604381  2.1268604381

Au$_5$-C$_3$H$_6$
E = -796.3611800924
Imaginary frequencies: 3.52i

Au  2.4642437464  -0.5715435256  2.6310072150  2.6310072150
Au  2.296571266  0.1859450070  0.1069465118  0.1069465118
Au  -0.2757123225  0.0025893833  -1.1957600006  -1.1957600006
Au  -2.3299372958  -0.8933635047  0.3204308599  0.3204308599
Au  0.0153836133  -0.7002872986  1.4869104496  1.4869104496
C  0.8937008588  0.8513202001  -2.9435947587  -2.9435947587
C  -0.4204630249  0.6751904883  -2.4385974414  -3.4385974414
C  1.4278813268  1.7774646551  -3.5948330267  -3.5948330267
H  1.6638544100  0.1046334294  -3.1707292410  -3.1707292410
H  1.2385497534  1.8529658459  -2.6580278755  -2.6580278755
H  -0.6498239580  -0.2763532442  -3.9424300244  -3.9424300244
H  -2.4510866362  1.4353669413  -3.3619342527  -3.3619342527
H  -1.4412571290  2.0853705032  -4.6616052634  -4.6616052634
H  -1.1896475565  2.6648554769  -2.9871218594  -2.9871218594

Au$_5$-C$_3$H$_6$$_2$
E = -796.3606700129
Imaginary frequencies: 21.79i; 10.15i

Au  2.6515095544  -2.3356910003  -0.6207402125  -0.6207402125
Au  3.2420470962 -0.5523037574  1.2057611261
Au  0.6171173846 -0.9843451895  0.5974078863
Au -1.2162746270  0.7098187071 -0.7210248693
Au -1.8489937314 -0.6772204364  1.4673353819
C  -0.7956788300  2.0772396795 -2.4540452249
C  -2.0187348632  2.075144165 -2.3899260817
C  -3.0440504753  3.1609860545 -1.7652139267
H  -0.2220198002  2.9188880016 -2.0459678877
H  -0.2761752018  1.4268677912 -3.1678207339
H  -2.7425946455  1.3369121262 -3.0007092222
H  -3.9131295072  2.7542471887 -1.2364054737
H  -2.4569387000  3.7980134439 -1.0758742561
H  -3.4301014447  3.8057097822 -2.5766062452

Au₆-C₃H₆
E = -932.0906520675
Imaginary frequencies: 14.18i
Au  2.0961903078  0.0976945570  0.2699359294
Au -0.4133695825  1.3556735734  0.2155947815
Au -0.1372576183 -1.3562406278 -0.6109526408
Au -2.5451513065 -0.1133484148 -0.5842078158
Au  1.8043383253  2.6578237041  0.9900425159
Au  2.3046365771 -2.4652567257 -0.4649749055
C  -4.6329327251  0.0312293462 -1.4812496210
C  -4.9284787853 -0.5074264505 -0.2172576251
C  -5.4091262818  0.2824523606  0.9632167610
H  -4.5458385417 -0.6213364684 -2.3590111843
H  -4.7757017729  1.1020412042 -1.6775119596
H  -4.9530412692 -1.6031615123 -0.1184550913
H  -5.2770756551  1.3684001934  0.8335257683
H  -6.4921565795  0.0801650216  1.0987844277
H  -4.9210998284 -0.0401673557  1.8997737128

Au₇-C₃H₆
E = -1067.8630511446
Imaginary frequencies: 4.94i
Au  1.7849037577 -2.0166291273 -0.3234018417
Au  1.3691802588  0.5734204255 -1.0823412945
Au -0.8280078966 -1.2728774549 -0.6708131149
Au  0.7803295595  2.9891721169 -2.0110385971
Au -1.3176390625  1.3624461616 -1.6518544977
Au -3.2698629800 -0.4332340311 -1.2820818758
Au  0.7336419883 -0.3423114477  1.5648202052
C  0.4901940103  0.1308419129  3.7768376295
C  0.0989119370  1.1379414152  3.3041433425
C  0.9657405023  2.3666111753  3.3320488940
H  1.4849345819  -0.2758069496  4.2170882411
H  -0.2648077472  -0.8918332317  4.0094092488
H  -0.9671912902  1.2962304346  3.0819718049
H   0.6244768922  3.0136686130  4.1661084948
H   0.8612824250  2.9649710371  2.4109278636
H   2.0302031143  2.1338270641  3.4964575819

Au₈-C₃H₆
E = -1203.583245148
Imaginary frequencies: no
Au  2.2543992765  0.5990349980  -0.0752119415
Au  -0.4796946924  1.1363020938  0.0546064847
Au  -1.6532374677  -1.2739272023  -1.0991787434
Au   0.6106557529  -1.5824102548  0.7887430362
Au   -3.1858582523  0.9513099737  -0.1458095769
Au   1.2866141895  3.0340743917  -0.5649014213
Au   3.2360112225  -1.8576821957  0.3592536901
Au  -1.8496848697  -0.8096751851  1.6240453826
C  -2.2116632854  -1.9862552308  -3.1474050227
C  -1.0847347640  -2.7738637785  -2.826226020
C   0.3069340254  -2.5196729537  -3.3399541978
H  -2.1118791431  -1.1248195094  -3.8197079219
H  -3.2238857749  -2.3851287019  -3.009745200
H  -1.2608680742  -3.7508577172  -2.3513996930
H   0.4359163702  -1.9457010683  -3.7267489007
H   0.5096064881  -3.2284267200  -4.1689305568
H   1.0697458271  -2.7114035930  -2.5658905939

Au₈-C₃H₆₂
E = -1203.5872494836
Imaginary frequencies: no
Au  -1.5323589504  0.5123424531  1.6198883329
Au   0.7259814075  0.4726824650  0.1436485211
Au   2.7115653400  2.2419385639  0.4000234871
Au   3.0710416145  0.3567986987  -1.4641943579
Au   3.3682135117  -1.5455421216  -3.318090513
Au   1.1249941245  -1.6046872443  -1.8779204423
Au  -1.1440700533  -1.4664632242  -0.2474998062
Au  -0.8432276475  -3.4020652834  -2.1083315008
C  -3.3746769442  2.1215901508  2.7872987826
C  -2.3648020174  1.2926543613  3.7569718153
C  -2.1125022613  0.2637367818  4.8219469909
H  -4.0675909278  0.3659437155  2.7734878245
H  -3.6744991162  2.1062927617  2.2206382234
H  -1.8151675643  2.2420960546  3.8517128331
H  -2.4888659540  0.6582379454  5.7879759269
Au-C₃H₆
E = -1339.3552724777
Imaginary frequencies: no
Au 0.3759054702 -1.6406084396 0.3715047785
Au -1.5427879270 -3.352255592 1.1606256058
Au -2.2983223886 -0.7853130548 1.0043744499
Au 2.4292494341 0.1899526761 -0.0948998247
Au -2.6744869883 1.9148591092 1.2527173483
Au -2.3176265125 0.9783278441 -1.2914872156
Au 0.2987329989 -0.0255986603 -1.9143714423
Au -1.5935957975 0.3419874094 -3.7752934571
Au -0.1007989412 1.1265142475 0.6434254392
C 4.6839407026 0.3240365439 0.4707916384
C 4.6584754865 1.1765187337 -0.6315947223
C 4.5726836097 2.6756110457 -0.5708614868
H 4.9834403560 -0.7251417418 0.3570096078
H 4.6769825747 0.7262080212 1.4922005100
H 4.8429106253 0.7399365576 -1.6248486020
H 4.3275246483 3.0488631568 0.4366857148
H 3.8404353407 3.0729440992 -1.2959952821
H 5.555212942 3.0974585460 -0.8633261809

Au-C₃H₆₂
E = -1339.3547337395
Imaginary frequencies: 19.65i
Au -1.0088439502 0.9676875048 1.0379550800
Au 0.6696679962 1.8492603120 2.9285187940
Au 1.4974167080 -0.2926232936 1.5770931954
Au -2.9899233105 -0.2038266456 -0.5413023157
Au 1.9619784623 -2.6557872628 0.3009719571
Au 1.9348939024 -0.4216874468 -1.2847525393
Au -0.6574289856 0.7362995940 -1.7381963561
Au 1.5248116420 1.4586646658 -3.1193747490
Au -0.5478916157 -1.5661536352 -0.1387973586
C -5.2772222157 -0.0860826287 -0.9576282436
C -5.2654814263 -1.1228155714 -0.0261643725
C -5.5293138185 -0.9676895833 1.4451433469
H -5.5317012400 0.9375489233 -0.6529494407
H -5.3072542204 -0.3015324164 -2.0326281086
H -5.1778867777 -2.1532302626 -0.4026197120
H -4.8132162581 -1.5481921108 2.0535998817
H -6.5330807462 -1.3809478611 1.6719485829
H -5.5101420258 0.0854428634 1.7685323434
Au$_9$-C$_3$H$_6$$_3$

E = -1339.3537893227

Imaginary frequencies: 5.54i

Au       -0.7337439190   -1.2552235141    0.9031868038
Au       -3.1400559784   -0.1201435695    0.3204882495
Au       -0.8907702586    1.3950160827    0.3014259529
Au       1.6950840973   -2.3942810161    1.6109989592
Au       1.4547141473    2.9108537431    0.3624954193
Au       1.2600437471   1.0881546005   -1.6514294827
Au       1.4172605675   -1.6802541631   -1.0096775407
Au       1.4451365765   -0.7974148311   -3.5283829010
Au       1.7473841449    0.2973330915    1.1014172094
C        -5.2535056870   -0.5215304502   -0.5565722822
C        -5.5157641760   -0.5168227830    0.8133368808
C        -6.0818473757    0.6451860738    1.5830745864
H        -5.4676346845    0.3615931027   -1.1719105365
H        -5.0785630156   -1.4627911934   -1.0908773153
H        -5.4523235678   -1.4734052536    1.3538272415
H        -7.1336833919    0.4168969207    1.8478045910
H        -6.0711667754    1.5816749795    1.0023227540
H        -5.5499754535    0.8049226531    2.5376625954

Au$_{10}$-C$_3$H$_6$

E = -1475.0768603224

Imaginary frequencies: no

Au       1.0569687541    0.7756889500    3.0387495520
Au       1.9654531827    1.4030434677    0.3825890973
Au       0.6853094258   -0.4415773230   -3.8112356820
Au       -0.7920229911   1.3609321908    1.0794412516
Au       -2.9208322392    1.3367201508    0.6134491921
Au       -0.1571855078    0.8451470167   -1.5713612616
Au       0.6954993929   -1.0620513555    1.0235755891
Au       0.3054618263   -1.9683656415   -1.6685206407
Au       -2.0067985426   -1.1309466769   -0.1205214891
Au       -0.6095532247   -3.419673273    0.4631161369
C        3.5904062368    2.5246822595   -0.7297800924
C        4.2866815938    2.0952258703    0.4133371652
C        5.1976773225    0.8978119262    0.4576191553
H        3.1771032341    3.5399276130   -0.7754707336
H        3.7154532372    2.0024769604   -1.6861737597
H        4.3128303375    2.7644076174    1.2856945986
H        5.0676096800    0.3135781398    1.3853914238
H        6.2485811316    1.2529057751    0.4560331521
H        5.0618484941    0.2332265240   -0.4109672207
Au$_{10}$-2-C$_3$H$_6$

$E = -1475.0876247066$

Imaginary frequencies: 9.52i

|        |          |          |          |          |
|--------|----------|----------|----------|----------|
| Au     | -0.4725488300 | -3.0333933995 | 2.3437983639 |
| Au     | -1.1297839044 | -0.8699538705 | 0.9091454453 |
| Au     | 0.8622982968  | -0.8017114068 | -3.7710175719 |
| Au     | 1.5557093609  | -1.6631266946 | 1.3138013583 |
| Au     | 3.7445681057  | -0.2002385890 | 0.6882221589 |
| Au     | -0.5788573714 | 0.0668369455  | -1.6866576904 |
| Au     | 1.1707666944  | 1.0721519685  | 0.5985871886 |
| Au     | -1.4760782381 | 1.9178285574  | 0.3273933346 |
| Au     | 2.1475341562  | -0.6505677113 | -1.4538341303 |
| Au     | -3.1651395426 | -0.025946020  | -0.7544875122 |
| C      | -1.2627657833 | 4.0288995193  | 1.1491648623 |
| C      | -2.5890671332 | 4.0251300585  | 0.6807123706 |
| C      | -3.044262256  | 4.6147698156  | -0.6294289522 |
| H      | -1.0500506769 | 3.8550480124  | 2.2103900955 |
| H      | -0.4686650084 | 4.5047652698  | 0.5604725174 |
| H      | -3.3839913772 | 3.7389884790  | 1.3851757967 |
| H      | -3.7838052834 | 3.9799781497  | -1.1332573845 |
| H      | -3.5315076183 | 5.860849360   | -0.4298912230 |
| H      | -2.1937746889 | 4.7993893274  | -1.3180511912 |

Au$_{11}$-C$_3$H$_6$

$E = -1610.8596794$

Imaginary frequencies: no

|        |          |          |          |          |
|--------|----------|----------|----------|----------|
| Au     | 1.6158650072 | -1.4937475596 | -0.8961989333 |
| Au     | 1.8381073870 | 1.3652251445  | -0.6459440714 |
| Au     | 1.4373530777 | -0.2612212511 | 1.6956816939 |
| Au     | -0.9767512655 | 1.5824296092  | -0.9206465275 |
| Au     | -1.1828003129 | -1.1931369854 | -1.1739400254 |
| Au     | -1.362348187 | 0.0109063023  | 1.3569438979 |
| Au     | -3.4242184731 | 0.3274272185  | -0.4957328104 |
| Au     | 3.7869105252  | -0.3182961285 | 0.2896824815 |
| Au     | 0.1502280796  | -3.1900707385 | -2.3440355294 |
| Au     | -0.2440172823 | -0.3034211593 | 3.7647671285 |
| Au     | 0.6861420058  | 3.5076649297  | -1.7381375648 |
| C      | -5.5987533716 | 0.9403079834  | -0.9844711319 |
| C      | -5.8067614574 | -0.3320127974 | -0.4509178185 |
| C      | -6.2247514507 | -0.6177328009 | 0.9647869221 |
| H      | -5.5312005287 | 1.0865313910  | -2.0694133912 |
| H      | -5.7701342018 | 1.8376445115  | -0.3762600751 |
| H      | -5.7975097749  | -1.1888801438 | -1.1413690804 |
| H      | -7.2811297316  | -0.9542149601 | 0.9632104353 |
| H      | -6.1483258748  | 0.2690569416  | 1.6145108807 |
| H      | -5.6384142104  | -1.4431940518 | 1.4060937850 |
### Au$_{12}$-C$_3$H$_6$

E = -1746.5849473961

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | 0.3548275735 | 3.4308483974 | 1.3947595198 |
| Au      | 0.4225247718  | -3.6703228094 | 0.0528711315 |
| Au      | 1.6116993984  | 1.0750749191  | 2.0503333977 |
| Au      | 0.6693871085  | 1.5453963504  | -0.6163998168 |
| Au      | -1.1709679461 | 1.1082531845  | 1.5593356702 |
| Au      | 1.6091858669  | -1.6736238457 | 1.5328892773 |
| Au      | -1.1740397266 | -1.6093047609 | 1.0323330093 |
| Au      | 0.6809438232  | -1.1737850382 | -1.1262383623 |
| Au      | 3.4885942375  | -0.5423534599 | 3.0605238557 |
| Au      | 0.2093127043  | 0.6276838876  | -3.2238633553 |
| Au      | -3.5036600870 | -0.1532799482 | 0.7582429310 |
| Au      | -1.7835876227 | 0.2644779839  | -1.3068879422 |
| C       | 0.0463784963  | 1.0620343757  | -5.4925610114 |
| C       | 1.4107134708  | 0.7864582891  | -5.3910176348 |
| C       | 2.4974323789  | 1.8204286673  | -5.2913970403 |
| H       | -0.3139966289 | 2.0976254933  | -5.5405171659 |
| H       | -0.6592537746 | 0.2807320350  | -5.8002627286 |
| H       | 1.7372892269  | -0.2556176313 | -5.5271746586 |
| H       | 3.2433383482  | 1.5572090261  | -4.5205486610 |
| H       | 2.1032688145  | 2.8286656683  | -5.0852154554 |
| H       | 3.0457284893  | 1.8546934218  | -6.2543589913 |

### Au$_{13}$-C$_3$H$_6$

E = -1882.3408445957

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | -1.1485328152 | -0.3808597121 | -2.6581516597 |
| Au      | -1.5337493890 | -2.2273836915 | -0.5888193842 |
| Au      | 0.5135622457  | -4.0229399364 | 0.1122769698 |
| Au      | 0.9661566319  | -2.0084396640 | -1.7874890668 |
| Au      | -1.3899821273 | 0.4886020467  | 0.1901297816 |
| Au      | -3.0199926115 | -1.2584139917 | 1.5731307456 |
| Au      | -0.3453326867 | -1.8854186399 | 1.9461387426 |
| Au      | 1.0966475644  | 0.7068815231  | -1.0080531818 |
| Au      | 3.4136300578  | -0.6804700737 | -1.5737845856 |
| Au      | 2.1931383398  | -1.6538903551 | 0.7222206367 |
| Au      | 0.0009153787  | 2.9332972186  | 0.3305358631 |
| Au      | 0.9157422675  | 0.7829963892  | 1.8083021592 |
| Au      | 1.8999374963  | -1.1648902467 | 3.4375125258 |
| C       | -0.1710747875 | 5.1654552244  | -0.3528690210 |
| C       | -0.5665350044 | 5.2629702203  | 0.9790496069 |
| C       | -1.9923260755 | 5.3025874877  | 1.4567796665 |
| H       | 0.8653029919  | 5.3715610406  | -0.6459943670 |


\[ Au_{13}-C_3H_6 \_2 \]

\[ E = -1882.3377232783 \]

Imaginary frequencies: no

\[ Au -0.3608708990 -1.7426906331 -2.5906479504 \]
\[ Au -1.2613166183 -1.5746975339 -0.0349994274 \]
\[ Au 0.3163329637 -3.5234169732 1.5256833336 \]
\[ Au 0.1534974250 -0.9362464454 2.3506900668 \]
\[ Au 0.9149469409 0.5396384014 -1.509410982 \]
\[ Au 3.5860771669 -0.2152195118 -1.106212201 \]
\[ Au 2.2544581763 0.6583456569 1.0884540167 \]
\[ Au -0.2940209789 3.0007784293 -1.3015728165 \]
\[ Au -0.6804031477 1.3716538489 0.8612335899 \]
\[ Au 0.9445243066 1.5149525924 3.2686024962 \]
\[ C -3.9826604493 0.3085336065 -2.6056450002 \]
\[ C -3.9863296781 1.6617604761 -2.2320402599 \]
\[ C -4.5825233407 2.196069032 -0.9548317712 \]
\[ H -4.4274921296 -0.4512543914 -1.9519383295 \]
\[ H -3.8036401166 0.0179589648 -3.6472015132 \]
\[ H -3.7279571142 2.4048607544 -3.0007307773 \]
\[ H -5.5799826165 2.6264662964 -1.1765723675 \]
\[ H -3.9713050653 3.0083658911 -0.5260919935 \]
\[ H -4.7106523532 1.4091995558 -0.1920834512 \]

\[ Au_{14}-C_3H_6 \]

\[ E = -2018.0847339652 \]

Imaginary frequencies: no

\[ Au 2.3848007591 2.4615901510 0.2218278973 \]
\[ Au -1.9516872213 -0.9885546837 1.3044835570 \]
\[ Au -1.8484752349 -0.8571359383 -1.4777220503 \]
\[ Au 0.4293797965 1.0362597980 -1.3110067390 \]
\[ Au -2.2746175286 1.6204415698 0.0169887442 \]
\[ Au 0.3409117561 0.8930447814 1.4615014532 \]
\[ Au -0.3809398246 -0.7485003661 3.5678614961 \]
\[ Au 0.6138282676 -2.0474462971 1.3145584682 \]
\[ Au 0.7144688856 -1.9143019871 -1.4757065265 \]
\[ Au 2.7735448858 -3.0521596640 -0.0599116462 \]
\[ Au -4.2132871766 -0.2817730802 -0.1407689394 \]
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Au      | -0.1640509327 | -0.3732708528 | -3.6189073522 |
| Au      | 2.6254397244  | -0.2561629333  | 0.0747380945  |
| Au      | -0.3658198382 | 3.4535283799   | 0.1914192654  |
| C       | 3.1573346000  | 4.6494171649   | 0.3978311174  |
| C       | 4.3141959869  | 3.8629670510   | 0.2928240397  |
| C       | 5.1164604298  | 3.6832328688   | -0.9689166342 |
| H       | 2.7719732153  | 5.1907244066   | -0.4745780900 |
| H       | 2.7857145428  | 4.963886712    | 1.3796912240  |
| H       | 4.7860523404  | 3.5150008057   | 1.2237770954  |
| H       | 6.0282460470  | 4.3105700387   | -0.9018805285 |
| H       | 5.4602705121  | 2.6413408875   | -1.0909350088 |
| H       | 4.5584440694  | 3.9867380180   | -1.8697856655 |

**Au$_{15}$-C$_3$H$_6**

$E = -2153.856271005$

Imaginary frequencies: 14.96i; 12.31i

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Au      | 0.7075524072  | 0.4209341100  | -1.4733057208 |
| Au      | -1.2517596030 | -1.7221302867 | -1.4261843114 |
| Au      | -1.9199295644 | 2.5999985807  | 0.8320860709  |
| Au      | -2.1136126791 | 1.1012151246  | -1.5172285395 |
| Au      | -0.2671864243 | -2.7315136103 | 0.9892147300  |
| Au      | -3.8647032799 | 0.6305063283  | 0.5752175412  |
| Au      | -2.9820292906 | -2.2168239738 | 0.6788248593  |
| Au      | 0.9672288001  | 2.0534137450  | 0.8045276633  |
| Au      | 1.8195237146  | -0.6690452858 | 0.8637243409  |
| Au      | -0.8793313989 | -0.1387770899 | -3.6592111872 |
| Au      | -1.1046500578 | -0.0666731448 | 0.9999787685  |
| Au      | -0.0631334297 | 4.2349332194  | 1.9309671678  |
| Au      | 2.1841630614  | -2.9921284234 | 2.1064172578  |
| Au      | -5.5477626935 | -1.4396469387 | 0.9086814300  |
| Au      | 3.2496666671  | 1.2234480169  | -0.5918762196 |
| C       | 5.4234949114  | 1.3719265187  | -1.2899864319 |
| C       | 5.0187130981  | 2.7106235200  | -1.3407815076 |
| C       | 5.3022618004  | 3.7388109719  | -0.2808562043 |
| H       | 5.4111230234  | 0.7515309268  | -2.1941994509 |
| H       | 6.0164664276  | 0.9986245346  | -0.4452971970 |
| H       | 4.5976499708  | 3.0871035847  | -2.2848981727 |
| H       | 4.4220513690  | 4.3748628937  | -0.0823465207 |
| H       | 6.1021682762  | 4.4132478530  | -0.6472789169 |
| H       | 5.6448203039  | 3.2879469925  | 0.6642973955  |

**Au$_3$Y**

$E = -445.281022319$

Imaginary frequencies: no

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Y       | 0.5542823043 | 0.9348077511 | 0.0000000000 |
| Au      | -1.5192264553 | -0.2308946657 | -1.3903137889 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | -1.5192264553 | -0.2308946657 | 1.3903137889 |
| Au      | 2.7393634478  | -0.4440412103 | 0.0000000000 |

**Au\_Y**

\( E = -581.0487429007 \)

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.0012802707 | -1.1266405950 | 0.0564069460 |
| Au      | -1.3247791224 | 1.3484526282 | -0.0026388099 |
| Au      | 1.3224278679  | 1.3498623788 | 0.0032654151 |
| Au      | -2.7567953211 | -1.0721617794 | -0.0127848433 |
| Au      | 2.7585296545  | -1.0700156793 | -0.0156184686 |

**Au\_5Y**

\( E = -716.7900775479 \)

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | -0.6373357992 | 0.2908661779 | -0.3552022448 |
| Au      | 1.9312315829  | 1.5236078289 | -0.1189476177 |
| Au      | -0.6765671472 | -2.3865286560 | 0.6408851663 |
| Au      | -2.9704744844 | -1.2919012419 | -0.3607424823 |
| Au      | -0.1201012656 | 2.8965810924 | -1.2915185634 |
| Au      | 1.6792848370  | -1.0296590640 | 0.7954545520 |

**Au\_5Y\_2**

\( E = -716.7829136443 \)

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.2475540305  | 0.1870421423 | 1.3526635523 |
| Au      | 1.0677376230  | 0.3154002962 | -1.4338746935 |
| Au      | 1.73213114008 | 2.3098291435 | 0.3290036222 |
| Au      | -2.5383705260 | 0.2078847763 | 1.3947959697 |
| Au      | 1.0656993701  | -2.1688515160 | 0.0504533471 |
| Au      | -1.3511461306 | -0.8394709953 | -0.8447720369 |

**Au\_5Y\_3**

\( E = -716.7870133368 \)

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.6434609236  | 0.9211594511 | -0.7074684630 |
| Au      | -0.6654357760 | 3.0665849111 | 0.4685684117 |
| Au      | -1.9000938756 | 0.6138227937 | 0.3393070955 |
| Au      | 3.1746663433  | -0.1767339753 | -0.3937468725 |
| Au      | 0.9591225251  | -1.7978139367 | -0.2982835687 |
| Au      | -1.6986341633 | -2.0044865857 | -0.1467253091 |

**Au\_6Y**

\( E = -852.5531487049 \)

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.3276573742  | -0.0013777457 | 1.1880223800 |
Au 0.6330235302 1.3800798381 -1.4124627037
Au -1.7227779260 -0.0105025996 -0.9441529020
Au 1.6931051356 -2.4397325453 0.8712119227
Au 1.6418944083 2.4667193269 0.8764593324
Au 0.6354233185 -1.3931515212 -1.4160223826
Au -2.4426129081 -0.0007214168 1.6862629894

Au\_Y\_2
E = -852.5527778571
Imaginary frequencies: no
Y -0.6970096919 0.9531576641 0.0360721003
Au 2.1550329026 0.3285251905 0.2347116310
Au -2.4722849496 -1.2195048423 -0.0699255495
Au -3.3698737264 1.5158198265 -0.0893132523
Au 1.3961631184 2.8698402391 0.235552167
Au 0.0721590953 -1.8452177729 0.0543776907
Au 2.7365323372 -2.2459868090 0.2013457273

Au\_Y\_3
E = -852.5497493906
Imaginary frequencies: no
Y 0.0113395126 -1.3063309119 0.0936071213
Au -2.6943809920 -2.0288910681 -0.0167066096
Au -2.1583263928 0.6881597972 -0.088569047
Au 2.3749561493 -0.5419742514 -1.3274743501
Au 2.2263766488 -0.4249118414 1.6699490375
Au 0.0519127497 1.2118240182 1.4954751713
Au 0.2010086907 1.0937731946 -1.4838285132

Au\_Y\_4
E = -852.5486169239
Imaginary frequencies: no
Y -0.1472471019 -0.6695064221 -1.2728888763
Au -0.9491766715 -3.1441901587 -1.2925576000
Au -1.0399506840 1.2000896193 0.8214734770
Au 2.7354456832 -0.6407605942 -1.4179804460
Au 1.7087204186 0.2820012055 0.8162832715
Au 0.4618340289 1.1125196770 3.0182812641
Au -2.4344566693 1.0920981506 -1.4008448467

Au\_Y
E = -988.2992975214
Imaginary frequencies: no
Y 0.4179799244 -0.2582517716 -0.0076451993
Au -2.3709253275 -0.7546291566 -0.2561209333
Au 1.8409193337 2.1739244826 0.6691225012
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | 3.2772180482 | -0.2659772329 | 0.3268546429 |
| Au      | -0.7456662858 | -2.8490325155 | -0.5684990079 |
| Au      | -0.8213004198 | 2.2512658287  | 0.4901086467  |
| Au      | -3.3963882329 | 1.6652457827  | 0.1510993972  |
| Au      | 2.0813790310 | -2.5939892902 | -0.2761471521 |

**Au₈Y**

$E = -1124.0629679158$

Imaginary frequencies: 7.56i

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | -0.1738106943 | -0.4520732352 | 0.1224969822 |
| Au      | 2.3738015142 | -1.7850164831 | 0.4570388248 |
| Au      | -0.4332660898 | 2.3783335336  | 0.0449825355  |
| Au      | -2.8836048458 | 0.4389820120  | -0.3933045203 |
| Au      | 0.2397199117 | -3.3052155795 | 0.0778552300  |
| Au      | 1.9743633743 | 1.3753484944  | 0.4277528626  |
| Au      | 4.2802469249 | 0.0097272201  | 0.8122556411  |
| Au      | -2.4362040772 | -2.1687259438 | -0.3691765254 |
| Au      | -3.0191180682 | 3.0794037519  | -0.3491576235 |

**Au₈Y₂**

$E = -1124.057551584$

Imaginary frequencies: 8.50i

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.4639896780 | 0.0804908471 | 0.0652212170 |
| Au      | -1.7380892985 | -1.9162510985 | -0.1713884684 |
| Au      | -0.5320160460 | 2.7931300558  | -0.0250233122 |
| Au      | 3.2425883877  | 0.7945354949  | 0.1341729236  |
| Au      | 0.6987421247  | -2.8297569660 | 0.1609330240  |
| Au      | -2.3481443984 | 0.9457815246  | -0.3989558702 |
| Au      | -4.1905185996 | -0.9756927345 | -0.6509292863 |
| Au      | 2.7335967976  | -1.4425506165 | -1.1978089191 |
| Au      | 1.7310828710  | 2.4345551779  | 1.5815492164  |

**Au₉Y**

$E = -1259.7987370179$

Imaginary frequencies: no

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | 0.2243130744 | -0.5291672149 | -0.4990128275 |
| Au      | 2.7820239677  | -1.5031286669 | 0.5860408414 |
| Au      | -0.9728955866 | 1.4110158744  | 1.3925082919 |
| Au      | -2.6247882577 | 0.0328524801  | -0.6219903749 |
| Au      | 0.6215422946  | -3.1240375439 | 0.8448631892 |
| Au      | 0.5412400517  | -0.5300872250 | 2.3476218244 |
| Au      | 2.7324028981  | 0.8934805043  | -0.9453115199 |
| Au      | -1.8870430480 | -2.5379588328 | -0.3764042565 |
| Au      | -2.2364902490 | 2.7380256023  | -0.7665250410 |
| Au      | 0.4578307537  | 2.3231315762  | -1.0189291632 |
\( \text{Au}_9 \text{Y}_2 \)

\begin{align*}
\text{E} &= -1259.7983957749 \\
\text{Imaginary frequencies: no} \\
\text{Y} &\quad 0.2377691374 \quad -0.1385571039 \quad 0.7828038868 \\
\text{Au} &\quad 2.7824449548 \quad 1.1507589773 \quad 0.6778046629 \\
\text{Au} &\quad -0.7536591894 \quad -0.9151117797 \quad -1.8313537569 \\
\text{Au} &\quad -3.3452346693 \quad 0.2160043482 \quad -1.8506270993 \\
\text{Au} &\quad 0.5943982934 \quad 2.7676816640 \quad 0.8535822297 \\
\text{Au} &\quad 1.8037527681 \quad -1.2709432264 \quad -1.2822092844 \\
\text{Au} &\quad 4.1329400279 \quad -1.0653252192 \quad 0.0851688533 \\
\text{Au} &\quad -1.6256781043 \quad 1.8092431118 \quad -0.3592005427 \\
\text{Au} &\quad -2.6465015577 \quad -0.8119230182 \quad 0.5278089932 \\
\text{Au} &\quad -1.3850454905 \quad -1.5957267122 \quad 2.7044369105 \\
\end{align*}

\( \text{Au}_9 \text{Y}_3 \)

\begin{align*}
\text{E} &= -1259.7960531339 \\
\text{Imaginary frequencies: no} \\
\text{Y} &\quad -0.6067652677 \quad -0.1629053067 \quad 0.7392155250 \\
\text{Au} &\quad 2.1396064878 \quad 0.5328777486 \quad -0.2831490442 \\
\text{Au} &\quad -0.9051125465 \quad -3.0658016109 \quad 0.4807057360 \\
\text{Au} &\quad -2.7423754560 \quad 1.1957456524 \quad -0.8518070828 \\
\text{Au} &\quad 0.4129885392 \quad 2.5639193434 \quad 0.2740717370 \\
\text{Au} &\quad 1.555658316 \quad -2.1187719093 \quad 0.9277333800 \\
\text{Au} &\quad 3.9281670759 \quad -0.8702945918 \quad 1.1243944003 \\
\text{Au} &\quad -2.0255806664 \quad 2.4108070087 \quad 1.5246961170 \\
\text{Au} &\quad -2.1123618007 \quad -1.4057839343 \quad -1.4043536601 \\
\text{Au} &\quad -0.1188858420 \quad 0.8025114208 \quad -1.9370238224 \\
\end{align*}

\( \text{Au}_{10} \text{Y} \)

\begin{align*}
\text{E} &= -1395.5781359152 \\
\text{Imaginary frequencies: 6.25i} \\
\text{Y} &\quad -0.0784158867 \quad 0.4064953002 \quad 0.9207820118 \\
\text{Au} &\quad 2.5224853487 \quad -0.9904508698 \quad 0.9510249671 \\
\text{Au} &\quad -1.5229178498 \quad 0.0996604431 \quad -1.6565239850 \\
\text{Au} &\quad -2.1878417481 \quad 2.3673765838 \quad -0.0264459093 \\
\text{Au} &\quad 2.6754582433 \quad 1.653425175 \quad 0.4991637016 \\
\text{Au} &\quad 1.1095320580 \quad 0.9075861377 \quad -1.7564196721 \\
\text{Au} &\quad 1.1287487252 \quad -3.3559079882 \quad 1.0429475735 \\
\text{Au} &\quad 0.4282414834 \quad 3.1879684766 \quad -0.1344416387 \\
\text{Au} &\quad -3.0597488880 \quad -0.1750914792 \quad 0.7325057697 \\
\text{Au} &\quad -1.3807321551 \quad -2.2334734357 \quad 1.1367340469 \\
\text{Au} &\quad 0.5016791952 \quad -1.7261480358 \quad -1.1066252353 \\
\end{align*}

\( \text{Au}_{10} \text{Y}_2 \)

\begin{align*}
\text{E} &= -1395.5776027734 \\
\end{align*}
Imaginary frequencies: 14.96i

Y        -0.1289769415   -0.2349178442    0.9483767847
Au        2.8672257819   -1.9303987531    0.2611960402
Au       -1.4718729594   -0.1673657351   -1.6805927771
Au       -1.4911143306    2.3963407487    1.1006389400
Au        2.6336109679    0.7289208800    0.7340533697
Au        1.2301953051   -0.7575239720   -1.6449469395
Au       -3.1324789706    0.3031224959    0.6177541059
Au    0.3505287439    1.8386091018   -1.1288797092

Au_{11}Y

E = -1531.3192627014

Imaginary frequencies: no

Y        -0.0868813772   -0.1813726645    0.8392844116
Au    1.9865697806    1.6842681721    1.9936696027
Au        -1.5809039993   -1.3320600240   -1.4626531972
Au       -3.0201548245   -1.2835053735   -1.0090690112
Au     -0.2652583706   -2.9177961276    0.7969346000
Au       -0.8820521473    1.3803105904   -1.6059607229
Au        2.9682238964   -0.3914698122    0.3391484070
Au     -2.6251386960    1.5331501567    0.6677864669
Au     -1.0965510757   -3.1033474364    0.7375897438
Au     -1.5028247216   -2.6911564165    0.0805902143
Au    1.1025799430    -0.6434671519   -1.8904732428
Au    1.8076849274    1.9059479000   -0.8511623072

Au_{12}Y

E = -1667.0851452714

Imaginary frequencies: no

Y        -0.0689837175   -0.2250646866    0.4670346233
Au    2.1899728175    1.1285532827    2.1750575002
Au     -2.1496606346   -0.3997261205   -1.7497425665
Au     -2.9699554262   -0.8019908571   -1.0251316410
Au     0.2988542680    2.8803106913    1.0678467166
Au     0.3922898844    0.5312371635   -2.4641872839
Au    2.3936854244   -1.5121051873    1.6653722629
Au     -1.4207322508    2.1362071269   -1.0397081807
Au     -1.7549437024   -2.8329941539   -0.4191412746
Au     0.8972331986   -3.1564534016    0.0236361597
Au     2.3194441206   -1.0722543977   -1.2194502498
Au    2.1987857888   1.5897002157   -0.5930350262
Au    -2.1940406221    1.7026403887    1.6390070735
Au$_{13}$Y
E = -1802.839659287
Imaginary frequencies: no

Y 0.0387511245 0.0010188891 0.5453532720
Au 2.9159059493 0.1535891947 1.4619507914
Au -2.4208988761 0.9226576553 -1.0512944191
Au -2.2111536311 1.6167649220 1.7948952866
Au 2.4020198534 2.4297751793 -0.0385368645
Au -0.1333836418 0.0335658806 -2.5040165593
Au 1.7569159318 -2.3054830790 1.5262632389
Au -0.1736184735 2.5172440274 -1.1845295159
Au -2.8645045914 -0.9699224967 1.130977818
Au -0.8647519141 -2.9433941876 0.9985979041
Au 0.8714076774 -2.3351412760 -1.2719899668
Au 2.4351429080 -0.0646329267 -1.3588829691
Au 0.2250289151 2.8141559817 1.6397256169
Au -1.9503272475 -1.8802137894 -1.3816032180

Au$_{13}$Y$_2$
E = -1802.8353747458
Imaginary frequencies: no

Y -0.0826523218 0.0396210567 0.5683087821
Au 2.2227370453 1.4488374775 2.0150913549
Au -2.0533357828 -0.0713877025 -1.6725334421
Au -2.2855277997 -2.0151751889 0.5821107658
Au 0.5097956530 3.1148773279 0.6159016777
Au 0.7778427344 -0.2328571058 -2.6095070463
Au 2.1383580725 -1.2688774254 2.2239337668
Au -0.3863017054 2.2190704074 -1.8873502947
Au -0.5347184556 -2.4685984221 -1.5282451837
Au 0.3150854244 -3.0192091061 1.0916352167
Au 2.1635687907 -1.5757008225 -0.5981108061
Au 2.2560230414 1.3102004329 -0.8189629468
Au -2.1512466066 2.2038153181 0.2625337484
Au -2.7405741367 0.2355026032 2.0583665380

Au$_{14}$Y
E = -1938.6082485850
Imaginary frequencies: 8.11i

Au 0.574219 0.041331 2.630682
Y 0.146944 -0.027446 -0.476025
Au -0.504725 -2.346699 1.498588
Au 2.201616 -1.717274 1.097380
Au 2.621784 1.177067 1.136371
Au -2.684744 -1.309422 -0.020608
Au -2.443877 1.596931 0.366562
Au  0.086726  2.461016  1.270899
Au  3.178616 -0.310614 -1.193434
Au  1.974496  2.252098 -1.411075
Au -0.740219  2.640929 -1.649169
Au -2.402916  0.403546 -2.226535
Au -1.152507 -2.174129 -2.186741
Au  1.482685 -2.533901 -1.550549
Au -2.263696 -0.167332  2.472628

Au₃Y-C₃H₆
E = -563.2784397983
Imaginary frequencies: no
Y     0.4113196605  0.8397840658  -1.0215625178
Au   -1.9454181965  0.8459993326   0.4649511761
Au   -1.5764700807 -1.0588351754  -1.4960807205
Au    2.6003162358  0.1180741663   0.2042980306
C     0.8063141397  3.2978064888  -1.8876590832
C    -0.3728075315  3.8868366576  -1.5036480716
C    -1.5761251168  4.0784554715  -2.3712108856
H     0.9759362487  3.0348807168  -2.9465521928
H     1.7047915276  3.3727117735  -1.2519478879
H    -0.4476254427  4.2849335093  -0.4790987589
H    -1.7573668731  5.1659782970  -2.4931465264
H    -2.4912067716  3.6793374847  -1.8932449858
H    -1.4621866510  3.6379434679  -3.3749060019

Au₄Y-C₃H₆
E = -699.0480296263
Imaginary frequencies: no
Y     1.0240996616 -1.4147147721   1.1206791162
Au   -0.7204504677  0.6917051978  -1.0636707861
Au    0.3539086529  1.2296276685   1.3811203123
Au    0.0528396431 -1.9566337947  -1.3565828465
Au    3.4175626027 -2.1938971526   1.7758339945
C    -1.8080617146  1.2938675907  -2.9214824749
C    -1.8925718368  2.4440707700  -2.0990602148
C    -3.1247743769  2.8469868395  -1.3326046193
H    -2.6720537350  0.6263741554  -3.0277832591
H    -1.0437138835  1.2312935261  -3.7051779023
H    -1.1145012660  3.2127771416  -2.2156387785
H    -2.8774313639  3.3299727059  -0.3724842139
H    -3.8047513262  1.9990467666  -1.1484184625
H    -3.6774602971  3.6006808547  -1.9306835813

Au₄Y-C₃H₆₂
E = -699.0471736197
Imaginary frequencies: 18.36i; 10.85i

| Element | X             | Y             | Z             |
|---------|---------------|---------------|---------------|
| Y       | 0.1048623003  | -0.2939471924 | 0.8564819601  |
| Au      | 1.2867252505  | 0.2887961134  | -1.6522835179 |
| Au      | -1.1892304542 | 1.1103649638  | -1.2510703837 |
| Au      | 2.5017069945  | -1.5105974920 | 0.1275218670  |
| Au      | -2.6636557501 | 0.0640381725  | 0.8829838727  |
| C       | 0.7349697176  | 1.5030152634  | 2.6486374711  |
| C       | 1.5197171397  | 2.3238638801  | 1.8755156589  |
| C       | 3.0087017733  | 2.2660506374  | 1.7789611070  |
| H       | 1.2014183983  | 0.8145638697  | 3.3737364852  |
| H       | -0.3328125957 | 1.7382731229  | 2.7961577723  |
| H       | 1.0222605285  | 3.1032441059  | 1.2770206656  |
| H       | 3.3322064760  | 2.1234514120  | 0.7292225634  |
| H       | 3.4522165111  | 1.4762265959  | 2.4056972317  |
| H       | 3.4319378946  | 3.2427234143  | 2.0891442019  |

$\text{Au}_5\text{Y-C}_3\text{H}_6$

$E = -834.7891816867$

Imaginary frequencies: no

| Element | X             | Y             | Z             |
|---------|---------------|---------------|---------------|
| Y       | 0.8230661417  | -2.1779539276 | 0.4470177652  |
| Au      | 2.6221299635  | -1.5517079989 | -1.5036309125 |
| Au      | 1.0975926179  | 0.4905080160  | -0.3134909539 |
| Au      | -0.7343866186 | 1.9328143085  | 1.1250098463  |
| Au      | -1.4862543966 | -0.6273550551 | 0.7161818660  |
| Au      | -1.6189650698 | -3.3703367766 | 0.1822662403  |
| C       | -1.5379167383 | 3.7677384802  | 2.2307225201  |
| C       | -0.5432444610 | 4.3428697099  | 1.4294668325  |
| C       | -0.7938238172 | 5.0469807825  | 0.1237945053  |
| H       | -2.5935526777 | 3.8297374085  | 1.9376033055  |
| H       | -1.3316536265 | 3.5140926419  | 3.2771719785  |
| H       | 0.4688894076  | 4.4356300198  | 1.8516623873  |
| H       | -0.0308282584 | 4.7945895508  | -0.6330520837 |
| H       | -0.7181658338 | 6.1408556560  | 0.2901388759  |
| H       | -1.7945671051 | 4.8341371206  | -0.2858471657 |

$\text{Au}_5\text{Y-C}_3\text{H}_6 \_2$

$E = -834.7886222835$

Imaginary frequencies: 8.98i

| Element | X             | Y             | Z             |
|---------|---------------|---------------|---------------|
| Y       | 0.1664609533  | 1.6021506360  | 2.4566983657  |
| Au      | 1.3982198695  | 0.8313879896  | 0.0684119206  |
| Au      | -1.4697490130 | 0.2115495783  | 0.6749703320  |
| Au      | -2.5409632047 | 2.0279477265  | 2.4942957997  |
| Au      | 2.2556693193  | 3.0860163117  | 1.5125839443  |
| Au      | 0.0638208178  | -1.3149965639 | -0.9460107825 |
| C       | -0.1763957601 | -3.3810678696 | -1.9467891307 |
| C       | 0.5893481219  | -2.6885102206 | -2.8906660020 |
| Atoms | X        | Y        | Z        |
|-------|----------|----------|----------|
| C     | 0.0419321842 | -2.0306862628 | -4.1281913304 |
| H     | -1.2586375001 | -3.4985877675 | -2.0838225641 |
| H     | 0.3032753041 | -4.0435591182 | -1.2170958779 |
| H     | 1.6851054955 | -2.7581680834 | -2.8167630182 |
| H     | 0.3231834187 | -2.6409577424 | -5.0099264924 |
| H     | 0.4819875929 | -1.0306414561 | -4.2890394403 |
| H     | -1.0566749517 | -1.9433400321 | -4.1074726447 |

\[ \text{Au}_5\text{Y-C}_3\text{H}_6 \]

\[ \text{E} = -834.7861309501 \]

Imaginary frequencies: no

| Atoms | X        | Y        | Z        |
|-------|----------|----------|----------|
| Y     | -0.0240284794 | 0.0560655430 | 0.6866119072 |
| Au    | 2.1277710968 | -0.7844504891 | -0.9848727264 |
| Au    | -2.4375785800 | -0.7212088336 | -0.6477494289 |
| Au    | -2.4325014258 | 1.5503162201 | 0.8468642161 |
| Au    | 2.5618870347 | 1.2467168735 | 0.7637685244 |
| Au    | -0.2138982074 | -2.0688901842 | -1.4068933477 |
| C     | -0.0137576194 | -1.1286180331 | 3.0334285718 |
| C     | 0.1864200386 | -2.4210729255 | 2.6184311351 |
| C     | 1.5133211496 | -3.0993186803 | 2.4929322303 |
| H     | -1.0287790489 | -0.7688084761 | 3.2667762404 |
| H     | 0.8294601945 | -0.5327016161 | 3.4220665842 |
| H     | -0.6970513821 | -3.0310362728 | 2.3729428973 |
| H     | 1.5688912773 | -3.9158062775 | 3.2422188975 |
| H     | 2.3639957273 | -2.4194165757 | 2.6621670902 |
| H     | 1.6235197356 | -3.5913299460 | 1.5086238932 |

\[ \text{Au}_6\text{Y-C}_3\text{H}_6 \]

\[ \text{E} = -970.5538712545 \]

Imaginary frequencies: 13.38i

| Atoms | X        | Y        | Z        |
|-------|----------|----------|----------|
| Y     | -0.6736049745 | 1.2604106715 | 1.9301380150 |
| Au    | 1.4218443265 | 0.8124206146 | 0.0111603965 |
| Au    | -1.1657774578 | 0.4635117444 | -0.8018700893 |
| Au    | -0.45777111480 | -1.3733105992 | 2.4453284827 |
| Au    | 1.7662631608 | 2.6970910005 | 1.9286041193 |
| Au    | 0.4368636242 | -1.7344935273 | -0.3612725190 |
| Au    | -2.9725545414 | 2.029996529 | 0.4710679570 |
| C     | 0.6677431605 | -4.0052215248 | -0.4956855670 |
| C     | 1.1802051992 | -3.5594775016 | -1.7253640519 |
| C     | 2.6459585758 | -3.4224176540 | -2.0401603276 |
| H     | 1.3460508562 | -4.2939709053 | 0.3165038793 |
| H     | -0.3695840470 | -4.3524508708 | -0.4184163077 |
| H     | 0.4885139879 | -3.4855893647 | -2.5774454210 |
| H     | 2.9510367881 | -4.2729050059 | -2.6828186789 |
| H     | 3.2731573162 | -3.4380710412 | -1.1339332637 |
| H     | 2.8598714878 | -2.5047126455 | -2.6149487742 |
### Au\(_7\)Y-C\(_3\)H\(_6\)

**E** = \(-1106.30385621\)

Imaginary frequencies: no

|                | \(x\)            | \(y\)            | \(z\)            |
|----------------|------------------|------------------|------------------|
| Y              | \(-1.3965404107\) | \(-0.2097040541\)| \(0.2682568801\) |
| Au             | \(3.2457739078\) | \(0.9012314534\) | \(0.2717635234\) |
| Au             | \(1.3531325433\) | \(-1.0526050598\)| \(0.2356381267\) |
| Au             | \(-0.5895835158\)| \(-2.949427963\) | \(0.2690635385\) |
| Au             | \(0.7015026398\) | \(1.6864216805\) | \(-0.2681740167\)|
| Au             | \(-1.8667864621\)| \(2.4178886251\) | \(-0.7337168149\) |
| Au             | \(-3.3088301101\)| \(-2.2056390086\)| \(-0.4175129925\) |
| Au             | \(-3.9220890767\)| \(0.3728353028\) | \(-0.9073404008\) |
| C              | \(5.4725753643\) | \(1.3966669816\) | \(-0.0393461879\) |
| C              | \(5.3745362804\) | \(1.4455296393\) | \(1.3534649757\) |
| C              | \(5.7685258262\) | \(0.3305306116\) | \(2.2830789636\) |
| H              | \(5.4055863121\) | \(2.3136473469\) | \(-0.6370116270\) |
| H              | \(5.8823166160\) | \(0.5115247524\) | \(-0.5419623920\) |
| H              | \(5.1330849154\) | \(2.4127490332\) | \(1.8199658865\) |
| H              | \(5.0295305155\) | \(0.1869716622\) | \(3.0909596897\) |
| H              | \(5.9187013044\) | \(-0.6252645707\)| \(1.7547396122\) |
| H              | \(6.7216164977\) | \(0.6015452697\) | \(2.7805085007\) |

### Au\(_8\)Y-C\(_3\)H\(_6\)

**E** = \(-1242.0673841134\)

Imaginary frequencies: 2.20i

|                | \(x\)            | \(y\)            | \(z\)            |
|----------------|------------------|------------------|------------------|
| Y              | \(0.9943981743\) | \(0.5728881532\) | \(-0.0515722736\) |
| Au             | \(1.5630287053\) | \(-2.1190508936\)| \(0.6337199306\) |
| Au             | \(-0.9593356663\)| \(-1.3273573022\)| \(0.8142959175\) |
| Au             | \(-3.5734696400\)| \(-0.4579006736\)| \(1.0014612590\) |
| Au             | \(4.2376118470\) | \(-2.2966743987\)| \(0.2672973303\) |
| Au             | \(3.8219725461\) | \(0.2399309004\) | \(-0.3644701762\) |
| Au             | \(-0.0172087044\)| \(3.1827330415\) | \(-0.7208457369\) |
| Au             | \(-1.8051851120\)| \(1.3621183532\) | \(0.1412874565\) |
| Au             | \(2.8061398027\) | \(2.6350919314\) | \(-0.8732327023\) |
| C              | \(-5.4503312957\)| \(-1.1525299436\)| \(2.1315937054\) |
| C              | \(-5.6486088438\)| \(-1.7305681472\)| \(0.8739223408\) |
| C              | \(-6.5232787063\)| \(-1.1619656998\)| \(-0.2093459764\)|
| H              | \(-5.0091707719\)| \(-1.7323822298\)| \(2.9510770574\) |
| H              | \(-5.9646782988\)| \(-0.2228254165\)| \(2.4078717163\) |
| H              | \(-5.2632662139\)| \(-2.7477067017\)| \(0.7075055512\) |
| H              | \(-6.0396396860\)| \(-1.2245184120\)| \(-1.2000124355\)|
| H              | \(-6.8135403572\)| \(-0.1169344750\)| \(-0.0134670331\) |
| H              | \(-7.4479977648\)| \(-1.7696553289\)| \(-0.2753876670\) |

### Au\(_9\)Y-C\(_3\)H\(_6\)

**E** = \(-1377.7989311046\)
Imaginary frequencies: no

Y     0.3917336847  -0.3954936617   0.3283126608
Au    2.1102361829  -2.5551670010  -0.6868508798
Au    -1.6896781194   1.5217956891  -0.2311264578
Au    -1.2714940141   0.6443414195   2.6065563161
Au    3.1656205197  -0.9022060984  1.1606620269
Au    0.4666621711   1.9354417925  -1.6395250180
Au    -0.6657325693  -2.9734138632  -0.4105785248
Au    1.3357161925   0.2785913495   2.9654257569
Au   -3.7790318015   0.8839556472   1.5543633225
Au   -2.4585264860  -1.2925572845   0.5857310064
C    2.5768704642   2.6493639828  -2.3906199632
C    1.9910882589   2.2156120696  -3.5764266270
C    1.2909344291   3.1042262728  -4.5673160604
H    3.2566366329   1.9980073429  -1.8300000153
H    2.5803354187   3.7129018958  -2.1201342346
H    2.1594892505   1.1739603567  -3.8865313083
H    0.3408372633   2.6618408816  -4.9174947290
H    1.9309108422   3.2117787264  -5.4661683845
H    1.0953483349   4.1124206624  -4.1663777988

AuY-C₃H₆₂
E = -1377.7981761747

Imaginary frequencies: 2.60i

Y    -0.1076413408   0.6927824335   1.9946407409
Au   2.4266414444   -0.4294880134   2.9643373250
Au   0.1390652897  -0.7650160837  -1.6878402116
Au  -0.1370795200   1.7677495104  -0.7365862933
Au   2.5255659032   2.148616161   2.0536606367
Au   2.0834238191   0.1322937216   0.1287317947
Au   0.1170778305  -1.3238066843   4.1026365622
Au   0.3062476923   3.6076070933  1.2594644606
Au  -2.1281188347  -0.1691137533   0.0528354126
Au  -2.1762816862  -1.2575343512   2.5033800004
C    0.8384475969  -2.5383480132  -2.9770269244
C   -0.5496346267  -2.5431448477  -3.1752523500
C   -1.2516598414  -1.9406937906  -4.3633100933
H    1.5095473470  -2.0924129096  -3.7214085796
H    1.2964421777  -3.2083662527  -2.2400728393
H   -1.1604571509  -3.1763377216  -2.5144253363
H   -2.1745302151  -1.4112086207  -4.0686285731
H   -1.5633082260  -2.7585186569  -5.0438684356
H   -0.6064294614  -1.2525225400  -4.9332564722

Au₉Y-C₃H₆₃
E = -1377.7968437111
Imaginary frequencies: 20.04i; 16.65i; 7.85i
Y    0.3530148721  -0.3560859103   0.3975884316
Au   3.2985043515  -0.4098193640   0.041115022
Au  -1.0784665003   1.4228427555  -1.4567891919
Au  -3.0212181336   1.3312365315   0.4484856039
Au   2.1327640784   2.0030811592   0.8605469746
Au   1.6601109981   1.0786819059  -1.8288808705
Au   2.0645991911  -2.7291437623   0.6298747198
Au  -0.5118728989   2.3035056857   1.3392531627
Au  -2.2240480113  -1.1084467011  -0.7849165349
Au  -0.6421236153  -3.0791751643   0.0884154830
Y    0.4058676855   0.7026335038   0.8777426990
Au   3.0797012972   1.8105128911   0.2439527107
Au  -1.0710676585  -0.6807541732  -1.2755808430
Au  -2.5708005615   0.5459455576   0.8098036346
Au   1.0728974966   3.5778925552   0.5296187932
Au  -0.4891616635   2.1055429584  -1.5504955805
Au   3.0151897080  -0.9491109126   0.2197587154
Au  -1.6312213671   3.0859489688   0.8485045122
Au  -2.1721073696  -2.2328025952   0.7240618997
Au   0.6244490623  -2.2108526848   0.4708650788
Au   1.5260068136   0.2964250131  -1.8293371486
C    -2.8901076104  -4.1069847201   1.8968402302
C    -4.0583082839  -3.3435176597   1.8039529521
C    -5.1418387808  -3.5631472315   0.7809349310
H    -2.7154947339  -4.9439034947   1.2093660033
H    -2.2666375546  -4.0698108285   2.7970973996
H    -4.2874745523  -2.6436489719   2.6210008150
H    -5.5149653950  -2.6114750516   0.3634956442
H    -6.0069176296  -4.0519213375   1.2726666818
H    -4.8097319974  -4.2137006215  -0.0447062330

Au_{10}Y-C_3H_6
E  =  -1513.5771640883

Imaginary frequencies: no
Y    0.4058676855   0.7026335038   0.8777426990
Au   3.0797012972   1.8105128911   0.2439527107
Au  -1.0710676585  -0.6807541732  -1.2755808430
Au  -2.5708005615   0.5459455576   0.8098036346
Au   1.0728974966   3.5778925552   0.5296187932
Au  -0.4891616635   2.1055429584  -1.5504955805
Au   3.0151897080  -0.9491109126   0.2197587154
Au  -1.6312213671   3.0859489688   0.8485045122
Au  -2.1721073696  -2.2328025952   0.7240618997
Au   0.6244490623  -2.2108526848   0.4708650788
Au   1.5260068136   0.2964250131  -1.8293371486
C    -2.8901076104  -4.1069847201   1.8968402302
C    -4.0583082839  -3.3435176597   1.8039529521
C    -5.1418387808  -3.5631472315   0.7809349310
H    -2.7154947339  -4.9439034947   1.2093660033
H    -2.2666375546  -4.0698108285   2.7970973996
H    -4.2874745523  -2.6436489719   2.6210008150
H    -5.5149653950  -2.6114750516   0.3634956442
H    -6.0069176296  -4.0519213375   1.2726666818
H    -4.8097319974  -4.2137006215  -0.0447062330

Au_{10}Y-C_3H_6_2
E = -1513.5747342932
Imaginary frequencies: no
Y  -0.5378778938  -0.1485986898  1.4601270062
Au  2.1043565494  0.8889699880  2.2524846947
Au  0.1306365145  -1.4788063554  -1.0014379482
Au  -3.0007415764  0.6794118776  0.0479290598
Au  0.3104051996  -1.4788063554  -1.0014379482
Au  2.2664273154  0.2546727414  -0.6461249923
Au  1.9018049666  -1.7741594558  1.6709638964
Au  -1.9504889970  3.2180283855  -0.0659725603
Au  -2.5519865532  -0.5423643026  -3.1027062405
Au  -0.2801286939  -3.3404688932  1.0501707183
Au  -0.3567186446  1.1963882420  -1.146313940
C  4.4841447363  0.8189701198  -0.9267316158
C  4.0264363953  0.6757662104  -2.2448563610
C  4.2436507457  0.6757662104  -2.2448563610
H  5.0568988976  0.0168785837  -0.445820318
H  4.5381560109  1.8103254791  -0.4624159642
H  3.6438232498  1.5703221858  -2.758306192
H  4.5682264895  -1.4178095254  -2.5168061136
H  5.0310978535  -0.3145788260  -3.8492941290
H  3.3370249004  -0.8059636608  -3.6749689205

\text{Au}_{11}\text{Y-C}_3\text{H}_6
E = -1649.3160582259
Imaginary frequencies: 7.65i
Y  0.0142590044  0.1698645790  1.3150233709
Au  3.1487293021  -0.5862734124  1.2889798494
Au  -2.3254658477  0.9461049290  -0.2886486967
Au  -2.0738353899  2.3716596422  2.2574267397
Au  2.4662572937  1.9222747419  0.4871479341
Au  0.1538491530  1.8243161698  -1.1787903434
Au  1.2509107810  -2.5703230653  0.9972927232
Au  0.2004058253  3.2839386612  1.2538504498
Au  -2.9417957130  -0.3696297451  2.1581587085
Au  -1.1650700850  -2.3911123785  2.142247849
Au  -0.9135854141  -0.4204633139  -2.3356370557
Au  1.6396953852  -0.5965663304  -1.0661059744
C  -1.1157800543  -2.1589512884  -3.8297171095
C  -2.4516816316  -1.8984221025  -3.4940145855
C  -3.4080406391  -1.0978258262  -4.3365289343
H  -0.6910713986  -1.7776799267  -4.7669447447
H  -0.5624936404  -2.9630298266  -3.3312968314
H  -2.8895697423  -2.4584841922  -2.6543988533
H  -4.0732874225  -0.4667851574  -3.7219726765
H  -4.0656907987  1.800758287  -4.8877737745
H        -2.8913565486   -0.4650161603   -5.0765151821
Au        3.0678671901    0.0482915902   -1.883747802
Au       -1.7346943561    0.0918032171   -1.4041120061
Au       -2.0461860969    2.2416281571    0.4865700094
Au        2.7695146719    2.3413698874    0.2528747848
Au        0.7027732559    1.2943737548   -2.2406691068
Au        1.6193798263   -2.1493032951    0.9780603949
Au        0.3129351072    3.4088564889   -0.3298820473
Au       -3.1655856153    -0.3268099076    0.8842028207
Au       -1.0825285506    -2.1559891082    0.4165408998
Au        0.6646040745   -1.4859879569   -1.7315883527
Au        2.9438250735   -0.1941979995   -0.9564297411
C        -4.5804147976   -1.3273105495    2.4202930213
C        -4.9783692322    0.0192122715   -2.4529707897
C        -6.1624539449    0.5813089618    1.7106251057
H        -3.8864207664   -1.7198445822    3.1702476509
H        -5.1452491935   -2.0583877427    1.833113724
H        -4.5129121925    0.6785194485    3.2001452972
H        -6.5355070285   -0.1071279378    0.9348971021
H        -5.9302860223    1.5567237831    1.2478950342
H        -6.9834773016    0.7626035311    2.4328897645

Au_{11}Y-C_3H_6_2
E = -1649.3143012406
Imaginary frequencies: 17.06i

Y        0.3887035239    0.5417319834    0.6024513067
Au       -3.0678671901   -0.0482915902   -1.883747802
Au       -2.7346943561   -0.0918032171   -1.4041120061
Au       -2.2461860969   -2.2416281571    0.4865700094
Au        2.7695146719   -2.3413698874    0.2528747848
Au        0.7027732559    1.2943737548   -2.2406691068
Au        1.6193798263   -2.1493032951    0.9780603949
Au        0.3129351072    3.4088564889   -0.3298820473
Au       -3.1655856153   -0.3268099076    0.8842028207
Au       -1.0825285506   -2.1559891082    0.4165408998
Au        0.6646040745   -1.4859879569   -1.7315883527
Au        2.9438250735  -0.1941979995   -0.9564297411
C        -4.5804147976   -1.3273105495    2.4202930213
C        -4.9783692322    0.0192122715   -2.4529707897
C        -6.1624539449    0.5813089618    1.7106251057
H        -3.8864207664   -1.7198445822    3.1702476509
H        -5.1452491935   -2.0583877427    1.833113724
H        -4.5129121925    0.6785194485    3.2001452972
H        -6.5355070285  -0.1071279378    0.9348971021
H        -5.9302860223    1.5567237831    1.2478950342
H        -6.9834773016    0.7626035311    2.4328897645

Au_{11}Y-C_3H_6_3
E = -1649.3136373615
Imaginary frequencies: 18.50i

Y        0.3887035239    0.5417319834    0.6024513067
Au       -3.0678671901   -0.0482915902   -1.883747802
Au       -2.7346943561   -0.0918032171   -1.4041120061
Au       -2.2461860969   -2.2416281571    0.4865700094
Au        2.7695146719   -2.3413698874    0.2528747848
Au        0.7027732559    1.2943737548   -2.2406691068
Au        1.6193798263   -2.1493032951    0.9780603949
Au        0.3129351072    3.4088564889  -0.3298820473
Au       -3.1655856153   -0.3268099076    0.8842028207
Au       -1.0825285506   -2.1559891082    0.4165408998
Au        0.6646040745   -1.4859879569   -1.7315883527
Au        2.9438250735   -0.1941979995   -0.9564297411
C         3.1093305402    3.1670189262   -1.4142317163
C         2.4079202762    3.1669056445   -2.6234257504
C         1.3638363092    4.1717671077   -3.0146337636
H        -4.0275410590    2.5797829286   -1.2984248001
Au_{11} Y-C_{3}H_{6}.4
E = -1649.313434636
Imaginary frequencies: 13.88i

Y       -0.6051377943  0.1621928665  0.9807631533
Au      2.1128022596  0.3435727815  2.2693241770
Au     -2.2913384976  0.1794278483  1.4310099157
Au     -3.4327481506  1.2345124437  2.0696394766
Au     -0.0149525051  1.8271434891  1.4713701991
Au      1.6912544045  0.8567749980  0.6024319402
Au     -1.4944368295  3.0838143773  0.6546962175
Au     -3.1607592793  1.4833450208  0.7973787410
Au     -0.8684910922 -2.7880880651  0.1950112026
Au      0.2967877499  0.9189467206  1.6781305181
Au      2.5355635886  0.6355539542  0.6531866772
C       4.3409594262  0.5383287282  2.1164246568
C       4.8058706947  0.4480503811  1.59552059
C       5.7533859389  1.0437048493  0.0424098188
H       4.6670335180  0.5084257186  2.0955189971
H       3.8815291426  0.8918576392  3.0463725351
H       4.6061544721  2.5171252218  1.3242031533
H       5.4670841771  1.5924944169  0.9056771288
H       6.7625031041  1.4861737075  0.2982945526
H       5.8305453112  0.0170404596  0.1210829040

Au_{11} Y-C_{3}H_{6}.5
E = -1649.3122838016
Imaginary frequencies: no

Y       -0.6193010160 -0.2809302437  0.9724151172
Au      1.0349598422  2.1940472575  2.3433711451
Au     -1.8699127807  1.3655319845  1.1973492083
Au     -1.6730952752  2.4709282587  1.4928809935
Au      3.2907276581  1.2391755054  0.3880305750
Au      0.8203056249  0.6904077869  1.5327564480
Au     -0.1989112920 -3.0647561972  0.1006190682
Au      0.9448391265  2.2436791821  0.8834448672
Au     -3.5230176128  0.3802846534  1.0417143921
Au     -2.8142274288 -2.1545515545  0.3089049507
Au     -1.1759517245 -1.2195560950  1.9349328677
Au      2.0613091326 -1.2125380829  0.0711640545
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 5.5825351962 | 1.6023082801 | -0.4573131506 |
| C       | 5.1125767850  | 2.8453409733  | -0.0257790638 |
| C       | 5.1070047501  | 3.3124718698  | 1.4048777371  |
| H       | 6.0010131235  | 0.8834134448  | 0.2581814856  |
| H       | 5.7942524510  | 1.4215426125  | -1.5180330849 |
| H       | 4.8773547879  | 3.6012098367  | 1.6650572072  |
| H       | 5.9194014951  | 4.0546101023  | 1.5410616655  |
| H       | 5.2746779705  | 2.4882587547  | 2.1174119294  |

$\text{Au}_{12}\text{Y-C}_3\text{H}_6$

$E = -1785.0846655903$

Imaginary frequencies: no

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Y       | 0.5178624961 | 0.3641909575 | 0.3716730726 |
| Au      | 2.8332627023  | -0.5940817652 | 1.9998507148 |
| Au      | -1.7568721474 | 0.3569907734  | -1.5634536617 |
| Au      | -1.7690103341 | 2.2490564284  | 0.6590542434  |
| Au      | 3.0475474090  | 1.9395211468  | 0.7880394168  |
| Au      | 0.9162275113  | -0.0764927607 | -2.5926384027 |
| Au      | 0.7569207053  | -2.3168314771 | 1.8059229324  |
| Au      | 0.0825029201  | 2.4142031652  | -1.8878459993 |
| Au      | -3.3314426543 | -0.0950071490 | 0.6258498938  |
| Au      | -1.3472550247 | -1.9886055965 | -0.0543285037 |
| Au      | 1.2726530940  | -2.3463889175 | -1.0229526342 |
| Au      | 3.1728256479  | -0.3958081864 | -0.8432477644 |
| Au      | 0.7302529304  | 3.3913011914  | 0.6982225124  |

$E = -1785.0824904491$

Imaginary frequencies: no

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Y       | 0.6749600785 | -0.2355863891 | -0.8318534189 |
| Au      | 0.9703686678  | -3.0812410205 | -1.9032099047 |
| Au      | -0.9135731516 | 1.8866288847  | 0.5626561188  |
| Au      | -1.0143070616 | 3.0959132162  | -1.9860296386 |
| Au      | -1.6211062140 | -2.0743209984 | -1.3559258484 |
| Au      | -0.0554410205 | -0.2151501211 | 2.0475740552  |
| Au      | 3.2463383313  | -1.7222742917 | -1.3373364649 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Au      | -2.6276008853 | -0.3058076271 | 0.7816204649 |
| Au      | 1.4852110796  | 2.5941168329  | -0.9758639928 |
| Au      | 3.3884334255  | 0.8661987275  | -0.2147988955 |
| Au      | 2.4435000783  | -1.3381863885 | 1.3889585474  |
| Au      | 0.1781875328  | -2.7617998398 | 0.7941921301  |
| Au      | -2.0026325090 | 0.5538451199  | -1.9344934680 |
| C       | -4.5968014267 | -1.3475105769 | 1.3270609495  |
| C       | -4.3689084144 | -0.4731576506 | 2.4041243984  |
| C       | -5.0402659803 | 0.8652707270  | 2.5723470836  |
| H       | -5.8304605345 | 0.7731852420  | 3.3447723187  |
| H       | -5.5136804158 | 1.2169468823  | 1.6409442794  |
| H       | -4.3373406148 | 1.6363816516  | 2.9328960174  |

**Au$_{13}$Y-C$_3$H$_6$**

E = -1920.8367526031

Imaginary frequencies: 4.48i

Au  0.2718913948 -0.1900214893  2.4756023021
Y  0.4125797525  0.1241703318 -0.4967567725
Au -1.5244829263 -1.7183191704  0.8993631263
Au -3.3489708841  0.4535812753  0.2095195640
Au -1.1439960829  1.9756990087  1.3065248107
Au  1.1312937559 -2.4738754716  1.0122017824
Au  2.9784504857 -0.3547585716  1.3931975401
Au  1.6133872482  2.1301402772  1.5215655981
Au -1.7115309269  1.9269308575 -1.5301071086
Au  0.8534098374  2.9720887654 -1.2079892493
Au  3.1035424536  1.3537566189 -0.8848692085
Au  2.8037774603 -1.5200326322 -1.2007371961
Au  0.2801965463 -2.5336535064 -1.8135877755
Au -2.0165682073 -0.9417194927 -1.8466079215
C   -5.0357634361  0.8969697050  1.7215348762
C   -5.5229223327 -0.2437779395  1.0695590618
C   -6.5257615473 -0.2282596420 -0.0514859710
H   -5.3986516454  1.8949365760  1.4461817343
H   -4.5171540523  0.8095094988  2.6827878222
H   -5.2874074313 -1.2259367296  1.5047481320
H   -6.2638417692 -0.9467958936 -0.8478432227
H   -6.6471671202  0.7737949432 -0.4941517880
H   -7.5100558082 -0.5494374701  0.3462372368

**Au$_{13}$Y-C$_3$H$_6$_2**

E = -1920.8339221636

Imaginary frequencies: no
Au$_{13}$Y-C$_3$H$_6$-3
E = -1920.8338644617

Imaginary frequencies: 20.46i

| Element | Coordinates (Å) |
|---------|-----------------|
| Y       | 0.4991012265  -0.3367501409  -0.6324727102 |
| Au      | 1.1273245324  -3.3702125020  -0.8064935761 |
| Au      | -1.4891949612  1.8605585605  -0.1070854507 |
| Au      | -1.4476425724  2.0744893828  -2.9440435382 |
| Au      | -1.5182348896  -2.577771958  -0.5194853026 |
| Au      | -0.6038282957  0.3655805261  2.0890647418 |
| Au      | 3.1916401405  -1.6197136227  -0.5097599295 |
| Au      | -2.9905354476  0.4284299900  0.8067191441 |
| Au      | 1.0501037539  2.3162893219  -1.9109380502 |
| Au      | 3.1628941882  1.1391983653  -0.6164903539 |
| Au      | 1.0948702939  2.3443182253  0.9553044372 |
| C       | -5.0412580214  -1.2694119956  1.4750437975 |
| C       | -5.3641545449  1.032446752  2.4244113787 |
| H       | -6.1688712137  1.1542300161  3.1853826888 |
| H       | -5.8018645324  1.3641222357  1.4467642535 |
### Au_{13}Y-C_{3}H_{6} \_4

**E = -1920.8336726618**

Imaginary frequencies: 22.15i

| Atoms | x      | y      | z      |
|-------|--------|--------|--------|
| H     | 4.8532165054 | -1.0748928987 | 2.5164118690 |
| H     | 3.4272617603  | 1.0287766538  | 4.3543483649 |
| H     | 4.6460891327  | -0.1408330484 | 4.9413178510 |
| H     | 3.0922630335  | -0.7386066191 | 4.3370408475 |

### Au_{14}Y-C_{3}H_{6}

**E = -2056.6151237891**

Imaginary frequencies: 11.21i

| Atoms | x      | y      | z      |
|-------|--------|--------|--------|
| Au    | 0.1013394426 | -2.0887116441 | -1.4971967591 |
| Y     | -0.4160179728  | 0.4520574051  | 0.2094598981 |
| Au    | 0.2792048470  | -2.2230101497 | 1.4384515065 |
| Au    | -2.1819506691  | -2.2234417855 | 0.1145332437 |
| Au    | -2.0896453768  | -0.5587022590 | -2.2632805953 |
| Au    | 2.0763076571   | -0.1237587168 | 1.8242629800 |
| Au    | 2.4727431545   | 0.9343295566  | -0.7628522027 |
| Au    | 0.5119506230   | 0.4425503367  | -2.6832904709 |
| Au    | -3.4738900053  | 0.2993597005  | 0.0587952511 |
| Au    | -2.1061618812  | 2.1747734273  | -1.5998098075 |
| Au    | 0.4909347426   | 2.9789655717  | -1.2084698937 |
### Au$_{14}$Y-C$_6$H$_6$$_2$

E = -2056.6148499307

Imaginary frequencies: no

|          | x     | y     | z     |
|----------|-------|-------|-------|
| Au       | -0.7653288097  | 2.0214934420  | 1.9337506554  |
| Y        | 0.2435703583   | -0.5434156370  | -0.7386564649  |
| Au       | -0.5648904450  | -1.853953237   | 1.8619288928   |
| Au       | 1.3818370262   | 0.120783286    | 2.0810507587   |
| Au       | 1.2675095660   | 2.1548181815   | 0.0935038173   |
| Au       | -2.0588265830  | -2.582231591   | -0.4093943092  |
| Au       | -2.7143859388  | -0.1747187219  | -2.0124212341  |
| Au       | -1.3220610760  | 2.0236542558   | -0.9344952763  |
| Au       | 3.2157902845   | 0.0698617364   | -0.2135194058  |
| Au       | 2.0519070694   | 1.2074719116   | -2.4533732749  |
| Au       | -0.4011296481  | 0.5875441153   | -3.4570155209  |
| Au       | -1.0305542554  | -2.1869904205  | -3.0171759084  |
| Au       | 0.5121787905   | -3.5281665014  | -1.0323495454  |
| Au       | 2.1566213382   | -2.3221165158  | 0.7967987231   |
| Au       | -2.4619780214  | -0.0843619579  | 0.7514541323   |
| C        | -1.7614772556  | 2.2681459337   | 4.0042012863   |
| C        | -2.6135378331  | 2.9954652362   | 3.1622083190   |
| C        | -2.5738716156  | 4.4897272188   | 2.9808064783   |
| H        | -1.0015147765  | 2.7793014612   | 4.6083450071   |
| H        | -2.0017196493  | 1.2377249459   | 4.2881364060   |
| H        | -3.4864648652  | 2.4762568800   | 2.7400586412   |
| H        | -3.4212448052  | 4.9388822620   | 3.5370980379   |
| H        | -2.705593406   | 4.7785774782   | 1.9233611629   |
| H        | -1.6407673619  | 4.9362951021   | 3.3615816086   |

### Au$_{14}$Y-C$_6$H$_6$$_3$

E = -2056.6146695937

Imaginary frequencies: no
Au  0.8619873507  -2.6787578337  -1.8249367798
Y  -0.2146641539  -0.6218475261   0.1293673834
Au  0.9892880828   0.2198297535  -2.5055506091
Au  2.7783182116  -0.8891997831  -0.6910952976
Au  1.5636637011  -3.0144031485   0.8829392806
Au  0.2192162347   2.3515568775  -0.8244283008
Au -3.2771700170  -0.5119365890  -0.1885148930
Au -1.7511815141  -1.9306994773  -2.1137643190
Au  2.1004904488  -0.4298979914   2.0373548759
Au -0.1044603985  -1.9949932980   2.8598057718
Au -2.1244070979  -0.2200324547   2.4196130718
Au -2.1281239319   1.9404773121   0.6026896102
Au  0.2805788948   1.6805210831   2.0195157434
Au  2.7854699423   1.7168179524   0.4666096930
Au -1.7294604084   0.8724140757  -2.1262538637
C   4.0714869717   3.1949938512  -0.7650969444
C   3.7032926196   3.9652599093   0.3451617513
C   4.5720854122  4.1907162797   1.5539664737
H   5.0572995319   2.7161355459  -0.8107439982
H   3.5218748061   3.2736383122  -1.7095805655
H   2.8018866450   4.5904852924   0.2682621037
H   5.4191003381   3.4871435345   1.5990617846
H   3.9954732783   4.1252186228   2.4932152798
H   4.9818133287   5.2201533008   1.5095647849

$\text{Au}_{14}\text{Y-C}_3\text{H}_6\_4$

E = -2056.6124983503

Imaginary frequencies: 20.99i; 16.88i

Au  0.5048467908  -0.4091961421  -3.2758597078
Y  -0.0103808582   0.1606916705  -0.2800464902
Au  1.1755429179  -2.5577851796   0.0119819807
Au -0.7112916607  -2.5110481976  -2.0513303556
Au -1.1150255824  1.8541659803  -2.4621867375
Au  2.4002582827  -0.5657301700   1.5423512505
Au  2.5960716652   1.9743298245   0.2344596558
Au  1.7367984400   1.9255644802  -2.3777718105
Au -2.5949131630  -0.4260918486  -1.6182928583
Au -2.6821439007   2.0778713226  -0.2631693106
Au -0.0160329383   3.1288839222  -0.0839131281
Au  0.6825542233   1.6588169144   2.2876117243
Au -0.2263774598  -0.9792933978   2.5208017591
Au -1.7702197704  -2.1127943633   0.5699449395
Au  2.7221363259  -0.5266234352  -1.2435143018
C  -3.7817885021   2.9101051133   1.5710610708
C  -4.6656977007  1.9407904408   1.0696202194
C   5.8573447353   2.2384016207   0.1972142735
XYZ coordinates of the optimized cluster-propene complexes with one hydrogen dissociated from the propene to the cluster for Au$_6$, Au$_5$Y and Au$_6$Y on BP86/LANL2DZ level and total energies (in Hartree) on TPSSH/DEF2-TZVP level. The imaginary frequencies are also collected.

Au$_6$-C$_3$H$_6$-1
E = -932.038041454
Imaginary frequencies: no

Au
-3.9316431946  3.9739365657  1.3481501543
-3.1118168944  2.6760671555  2.4054222476
-4.6045025894  0.9253421393  1.4861098857
-5.8004300141  3.2340315260 -0.2729733713
-6.7719973608  2.2096236895  0.8232557939
-5.9906403804  1.4737410802 -0.5872410608

Au$_6$-C$_3$H$_6$-2
E = -932.0680784138
Imaginary frequencies: no

Au
1.7735547903  0.6954551700  0.0593961193
-0.9946588131  0.9240531312 -0.0848282185
0.1887806277 -1.7104021797 -0.056975119
-2.6996729030 -1.2177911083 -0.179395185
0.5396010905  3.0893985708 -0.0320925895
2.8579636239 -1.7333478597  0.1315166035

C
-4.6311357212 -0.6118243638 -0.2263060926
-5.3456025429 -0.3096655886  0.9018129303
-6.5915479165  0.5287316733  0.9054806543
-5.0503436710 -0.5230346248 -1.2403321713
-4.9969511765 -0.6616759628  1.8846729510
-6.8939297020  0.8536620134 -0.1013819326
-7.4158295050 -0.0584469222  1.3629137006
-6.4624770057  1.4185105893  1.5514189401
-1.3506567455 -2.4143584644 -0.216387325

Au$_6$-C$_3$H$_6$-2
E = -932.0680784138
Imaginary frequencies: no

Au
1.1395146896 -0.6127978630 -0.0299369560
0.8715487320  0.7444409178  0.0249112220
0.7896431459 -0.5772264529  0.0412424290
1.8328941409  2.2668141115 -0.1583283284
3.2235279001  0.5322297433  0.0818804437
-0.6847981706 -3.0885456710 -0.0930471596
-3.8396724091  1.2499435300 -0.7768536024
-3.3746606747  0.4817022658  0.2933095367
-4.0121036689  0.3855040360  1.6454804151
-3.5518725983  1.0401639298 -1.8151108909
-4.7236593163  1.8921745228 -0.6402749278
-4.7671735627  1.1832263461  1.7876250262
H  -4.5360066832  -0.5879964252  1.7205845673
H  -3.2827302761  0.4252799488  2.4711711013
H  -0.2968735214  3.1149930557  0.0334393262

\( \text{Au}_5 \text{Y-C}_3 \text{H}_6 \_1 \)
E = -834.7481763940
Imaginary frequencies: 10.47i

Y   -0.0100753465  -0.5615205866  -0.1075080385
Au   -2.5033481294   0.7385368406   0.4695820530
Au   2.2693862276   1.2392977300  -0.4357936416
Au   2.7488142901  -1.4301817182  -0.0119926529
Au   -2.3471961601  -1.8094804361  -0.8409297949
Au   -0.3715704178   2.3020980850   0.2113975774
C   1.2823330513  -2.5761144702   1.0096876921
C   0.8981982763  -2.2725253231   2.2890153577
C   0.0534792610  -3.1551399393   3.1698627014
H   1.0190332368  -3.5452791080   0.5544712847
H   1.2534071729  -1.3364017396   2.7579224069
H   0.6519622632  -3.4695434123   4.0481277362
H   -0.2968755966  -4.0595713825   2.6471301225
H   -0.8194576194  -2.6066282494   3.5705360418
H   1.2900265026   2.7606908132  -0.185583408

\( \text{Au}_5 \text{Y-C}_3 \text{H}_6 \_2 \)
E = -834.7390237583
Imaginary frequencies: 17.68i

Y   0.1664094621  -0.8732671924   0.4913525973
Au   -2.6354514313   0.605849798   0.3703773396
Au   2.1349401886   1.2465765764  -0.2777329622
Au   3.0272644852  -1.2119322294  -0.2307598411
Au   -2.1970705334  -1.6802433245  -0.9985709002
Au   -0.4593083909   2.0823204116   0.0463212440
C   0.2672418821  -3.0631411815  1.9276879736
C   0.0935425080  -1.8441909394   2.5187118766
C   -0.0220559013  -1.6250021488   4.0024620259
H   0.3408002376  -3.2141176982   0.8159445821
H   0.3549131212  -4.0310781749   2.4416107743
H   0.7855775497  -0.9577413335   4.3580738740
H   0.0204191112  -2.5628550849   4.5870334344
H   -0.9712052211  -1.1122671908   4.2471572847
H   1.1875559229   2.7699006978  -0.1668980354

\( \text{Au}_5 \text{Y-C}_3 \text{H}_6 \_3 \)
E = -834.7747595710
Imaginary frequencies: 9.12i

Y   0.0120726769  -0.6659371952   0.2925744522
Au  -2.5839662406  0.6205876541  0.4126748318
Au   1.9545209020  1.1821960034 -0.9268240218
Au   2.7804061680  1.1821960034 -0.9268240218
Au  -2.3439487677 -1.7689304727 -0.8293505656
Au  -0.1794420882  2.2088861019  0.4704423867
C   2.4897700455  2.8371613645  1.5229287066
C   1.4740683144  2.2616496637  2.4029320763
C   0.0918616750  2.3571908991  2.2336309060
H   3.4911043616  2.9468757323  1.965888688
H   2.1886987213  3.7025596150  0.9133744702
H   1.8482920743  1.6424890919  3.2332371715
H  -0.3342747318  3.1240975977  1.5651265397
H  -0.5812026624 -1.9966449091  3.026522952
H  -1.9936802684  2.1264744305  1.0319946100

\( \text{Au}_6\text{Y-C}_3\text{H}_6\text{.1} \)
E = -970.4854220650
Imaginary frequencies: no
Y  -1.0838297179  -0.4339842207  -1.0261558913
Au  0.3083200159  -1.2806378394  1.3548204305
Au  -0.8197394703  1.1620347203  1.3647709763
Au  1.2513702726  0.5522469963  -2.0517011617
Au  -0.7071363656  -3.1523465820  -0.3829514428
Au  1.9392247477  0.9434968983  0.5963218553
Au  -2.8351329615  1.6966143249  -0.4104322064
C   3.6688144415   1.9000733434  -0.0234538455
C   4.8634046294   1.2884484606  -0.1358106521
C   5.2430014751  -0.1127103564  0.2533700001
H   3.4705381773   2.9562890270  -0.2403841522
H   5.6704170459   1.1897750222  -0.5796145575
H   5.5918186246  -0.6853739470  -0.6265897878
H   4.3971743343  -0.6532857594   0.7127240843
H   6.0815917247  -0.0992550737   0.9745883257
H   2.5908129258   1.2631166948  2.0193013856

\( \text{Au}_6\text{Y-C}_3\text{H}_6\text{.2} \)
E = -970.5288599421
Imaginary frequencies: 17.42i
Y   0.0898643033  0.4771893386  -0.1732320867
Au  2.0604876452   1.1177072474  1.6762554625
Au  -1.1058859468  -2.3403761728  -0.0347590840
Au  -1.6196996121   2.6253407149  -0.8036631602
Au  2.9497749198   0.4769205925   0.8209562692
Au  -2.7918452253   0.4184696457   0.1935865106
Au  1.4319837222  -1.9871373431  -0.5050703712
C  -3.4209914336  -2.5306060640  -0.0277176362
Au₆Y-C₃H₆₃₃
E = -970.5536714556
Imaginary frequencies: 9.74i

Y 1.3383374955 0.1203139409 -0.9484732442
Au -0.2709448113 1.3527252387 1.1010268382
Au 0.0757686574 -1.3584064752 1.1816851251
Au -0.9173644608 -0.2365029819 -2.3732979261
Au 1.7502426493 2.7723320841 -0.0397886807
Au -2.2985756399 -0.3154028071 0.2105683148
Au 2.4329905833 -2.2483343347 0.1540325072
C -4.4594907877 -0.6385627864 -0.4301338494
C -4.5618667103 0.5048904286 0.9657562816
C -4.9995124608 0.7477362897 1.6761873662
H -4.7131973181 0.2011909578 -1.0889375837
H -4.4286876531 -1.6324948844 -0.8921275284
H -4.5127172388 -1.4200124152 1.5742484684
H -6.0524059889 0.6197941665 2.0000565435
H -4.4115737050 0.9281845532 2.5925761398
H -4.9486019299 1.6389482893 1.0299136013
XYZ coordinates of the optimized clusters and cluster-propene complexes and total energies (in Hartree) on LRC-ωPBE/def2-TZVP+XDM level.

Au₄
E = -542.876207478283
Au 0.0000000000 -1.3319672315 0.0000500623
Au -2.3103296544 0.0000000000 -0.0000500623
Au 0.0000000000 1.3319672315 0.0000500623
Au 2.3103296544 0.0000000000 -0.0000500623

Au₅
E = -678.721463100737
Au 2.3473859286 0.0541456636 1.2801965724
Au 2.3286944660 -0.0546678997 -1.2870463118
Au 0.0000000000 0.0000000000 0.0136994789
Au -2.3286944660 0.0546678997 -1.2870463118
Au -2.3473859286 -0.0541456636 1.2801965724

Au₆
E = -814.521701019185
Au 3.0090369630 0.5717176954 0.0002161333
Au 0.5379977447 1.4358532960 0.0011092181
Au 1.0250958034 -1.1369178220 -0.0014543346
Au -0.9633014463 -2.8423698188 -0.0003812031
Au -1.9372493812 2.2903678862 -0.0014366718
Au -1.6715793866 -0.3186512368 0.0019468580

Au₇
E = -950.370953199763
Au 2.6917207532 -0.0001917551 0.0018159984
Au 1.3456004375 2.3290192669 -0.0009160986
Au 1.3452706249 -2.3292095017 -0.0009170368
Au -1.3452706249 2.3292095017 -0.0009170368
Au -2.6917207532 0.0001917551 0.0018159984
Au -1.3456004375 -2.3290192669 -0.0009160986
Au 0.0000000000 0.0000000000 0.0000342741

Au₈
E = -1086.18306961367
Au 1.4787232259 1.0393341837 -0.1818874140
Au -1.2730516833 1.2555595423 -0.1619137797
Au -0.0914706580 -1.1994123342 -0.9656308943
Au 1.2370224742 -1.2183602814 1.5055989693
Au -2.7438783542 -0.8697048289 -0.9333740105
Au 0.2776142764 3.3374788348 0.1394184925
Au 2.5785458083 -1.3151673667 -0.8898017861
Au -1.4635050893 -1.0297277495 1.4875904229
Au$_8$ 2
E = -1086.1781595999
Au  2.3866804899 -2.5586680240 0.0000000000
Au  0.0443025060  -1.4059327586 0.0000000000
Au  -2.1911122881 -2.7053609757 0.0000000000
Au  -2.3268472442  0.0738887542 0.0000000000
Au  -2.3867488903  2.5586699887 0.0000000000
Au  -0.0443284038  1.4059902153 0.0000000000
Au  -2.3269256973  0.0738719354 0.0000000000
Au  -2.2191242610  2.7053183731 0.0000000000

Au$_9$
E = -1222.0309375423
Au  3.0332718976  0.4957181757  0.7722388805
Au  0.5746240362  1.5198428574  0.8267479315
Au  -1.9458673520  2.3797375474  0.7680954925
Au  1.0285528425 -1.2578311156  0.8263314846
Au  -1.0878370903 -2.8759999472  0.7642421113
Au  -1.6032951249 -0.2621007773  0.8253296979
Au  1.5492793321  0.2527292472  -1.5927600174
Au  -0.9931929190  1.2152830337  -1.5947804079
Au  -0.5555356222 -1.4673790212  -1.5954451729

Au$_{10}$
E = -1357.83861841529
Au  1.0325638322  -2.8453035146  1.3406215362
Au  -1.1212901581 -1.4641374886  0.7855088452
Au  -3.2944859999  0.0062477628  0.1869574337
Au  1.2464090960 -1.3141337291 -0.9498429418
Au  0.7830942535  0.2098444511 -3.2082372939
Au  -1.2526318271  0.1103651949 -1.5623946349
Au  1.8208291370  0.1103651949 -1.5623946349
Au  1.3890148297 -0.1075402350  1.4987530072
Au  -1.1064459910  1.3600536693  0.9734487777
Au  1.2599745984  1.4140124602 -0.7687897824
Au  1.0637973663  2.6305914290  1.7039750530

Au$_{10}$ 2
E = -1357.84295424075
Au  -0.1126455899  -3.2439011826  -1.6145197744
Au  -1.5845773802  -1.4359301060  -0.4554235704
Au  -0.1124586787  3.2439424276  -1.6144880787
Au  1.1563753245 -1.4018476331  -0.2625925467
Au  3.4761344136 -0.0001338126  -0.0977828528
Au  -1.5844322775  1.4360020742  -0.4553956519
Au  1.8208291370  -0.000248425  2.0548480465
|  | Au     | 11   | E = -1493.70513722813 |
|---|--------|------|----------------------|
|  | -0.8215633104 | -0.0000231906 | 1.8036565919  |
|  | 1.1565227410  | 1.4018040254  | -0.2626458400  |
|  | -3.3941843792  | 0.0001122402 | 0.9043436765  |
|  | 1.1565227410  | 1.4018040254  | -0.2626458400  |
|  | -3.3941843792  | 0.0001122402 | 0.9043436765  |
|  | 0.0000522204  | 1.6265869499 | -1.3728827135  |
|  | 1.4063034868  | -0.8114175691 | 1.3723926634  |
|  | -1.4063552794  | -0.8113274057 | 1.3723926563  |
|  | 0.0000522204  | 1.6265869499 | -1.3728827135  |
|  | -1.4063034868  | -0.8114175691 | 1.3723926634  |
|  | 0.0000000000  | 0.0024415917 | 3.5058271100  |
|  | 0.0000000000  | 0.0024415917 | -3.5058271100  |
|  | 0.0000000000  | 1.6265869499 | -1.3728827135  |
|  | 1.6265869499  | 0.0000000000 | 1.3723926634  |
|  | 0.0000000000  | 1.6265869499 | -1.3728827135  |
|  | -1.4063034868  | -0.8114175691 | 1.3723926634  |
|  | -1.4063552794  | -0.8113274057 | 1.3723926563  |
|  | 0.0000522204  | 1.6265869499 | -1.3728827135  |
|  | 1.4063034868  | -0.8114175691 | 1.3723926634  |
|  | -1.4063552794  | -0.8113274057 | 1.3723926563  |
|  | 0.0000522204  | 1.6265869499 | -1.3728827135  |
|  | -1.4063034868  | -0.8114175691 | 1.3723926634  |
|  | 0.0000522204  | 1.6265869499 | -1.3728827135  |

|  | Au     | 12   | E = -1629.50396897513 |
|---|--------|------|----------------------|
|  | -3.5527771546  | 0.0000000000 | -0.4161795928 |
|  | 3.5527771546  | 0.0000000000 | -0.4161795928 |
|  | -1.3528779790  | 0.0000000000 | -1.9812786808 |
|  | -1.3713355292  | -1.3879813927 | 0.4251714314 |
|  | -1.3713355292  | 1.3879813927 | 0.4251714314 |
|  | 1.3528779790  | 0.0000000000 | -1.9812786808 |
|  | 1.3713355292  | 1.3879813927 | 0.4251714314 |
|  | 1.3713355292  | -1.3879813927 | 0.4251714314 |
|  | 0.0000000000  | 0.0000000000 | -4.2256940357 |
|  | 0.0000000000  | -2.6634966857 | 2.3864548339 |
|  | 0.0000000000  | 2.6634966857 | 2.3864548339 |
|  | 0.0000000000  | 0.0000000000 | 2.5470151895 |

|  | Au     | 13   | E = -1765.34510914659 |
|---|--------|------|----------------------|
|  | 0.0000000000  | 2.3980328318 | 2.0543429160 |
|  | 1.3486181164  | 0.0000000000 | 1.9274349750 |
|  | 0.0000000000  | -2.3980328318 | 2.0543429160 |
|  | -1.3486181164 | 0.0000000000 | 1.9274349750 |
|  | 1.3818140118  | 1.5290364429 | -0.3469897570 |
|  | 3.5310080953  | 0.0000000000 | 0.2743414264 |
|  | 1.3818140118  | -1.5290364429 | -0.3469897570 |
|  | -1.3818140118 | 1.5290364429 | -0.3469897570 |
|  | -3.5310080953 | 0.0000000000 | 0.2743414264 |
|  | -1.3818140118 | -1.5290364429 | -0.3469897570 |
|  | 0.0000000000  | 2.6641815513 | -2.3990645075 |
| Au       | 0.0000000000 | 0.0000000000 | -2.3261505919 |
| Au       | 0.0000000000 | -2.6641815513 | -2.3990645075 |

\( \text{Au}_{14} \)

\[ E = -1901.1603196283 \]

| Au       | -0.2596528712 | 2.1810937533 | -1.0262815925 |
| Au       | 0.5915231175  | 0.0199130863 | 1.6001590594  |
| Au       | -1.6532051012 | -1.5352052323| 1.0942124493  |
| Au       | -1.7439443343 | -0.1004723885| -1.2975124879 |
| Au       | -1.8295702110 | 1.2935679156 | 1.1177140617  |
| Au       | 2.1845839776  | 1.5408404619 | -0.0697422475 |
| Au       | 3.3220362689  | 0.1904894782 | 1.9351483162  |
| Au       | 2.3600514880  | -1.2447092680| -0.1043176694 |
| Au       | 0.0152678079  | -2.1822505050| -1.0637982889 |
| Au       | 2.3136734660  | -3.2913589473| -1.7096976103 |
| Au       | -1.5272815298 | -0.1258813963| 3.3657189752  |
| Au       | -2.6670025914 | -2.6484361310| -1.1235160291 |
| Au       | 1.8739012434  | 3.5953944999 | 1.6364933387  |
| Au       | -2.9803807304 | 2.3068697231 | -1.0815935975 |

\( \text{Au}_{15} \)

\[ E = -2037.00166314082 \]

| Au       | 2.4747049492  | -1.8709086442 | 0.0999636165 |
| Au       | 3.6812251771  | 0.4954076721  | 0.3693993781 |
| Au       | 1.2640905700  | 0.9236462294  | 1.7204927594 |
| Au       | 2.3888830097  | 3.0091445471  | 0.2101229513 |
| Au       | -0.2911264678 | 2.7404089524  | 0.1330575050 |
| Au       | -1.4321138890 | 0.5911326587  | 1.6922373261 |
| Au       | -1.5303426458 | 0.4595579857  | -1.0892777720|
| Au       | -0.0079421700 | 0.1649515866  | -3.2933907327|
| Au       | 0.1477449301  | -1.7148020825 | -1.3787196588|
| Au       | 0.4104572457  | -3.8530007334 | 0.2003046400 |
| Au       | -3.7166494012 | -0.2836636581 | 0.3436969333 |
| Au       | -2.0164872642 | -2.330954043  | 0.1995519742 |
| Au       | 0.2020274244  | -1.508674658  | 1.6256163987 |
| Au       | 1.3927567228  | 0.7379952059  | -1.0606490295|
| Au       | -2.9672281908 | 2.4418931503  | 0.2275937105 |

\( \text{Au}_{4}-\text{C}_{3}\text{H}_{6} \)

\[ E = -660.791671589258 \]

| Au       | 2.3184603369  | -0.2296047049 | -0.1246222151 |
| Au       | -2.2065452550 | 0.6510273863  | 0.2377019738  |
| Au       | -0.2290428548 | -1.2301889441 | 0.0807216270  |
| Au       | 0.2663755827  | 1.4037544213  | -0.1498021013 |
| C        | 0.0941220253  | -3.3833946138 | 0.2028820972  |
| C        | -1.2779902266 | -3.2040457477 | 0.1991738031  |
C   -2.1492921721  -3.4285615695  -0.9962320187  
H    0.6274164643  -3.5289781158   1.1407845681  
H    0.6072138754  -3.6894258770  -0.7082745029  
H   -1.7841813884  -3.1531237928   1.1655933373  
H   -1.5841543888  -3.3947359029  -1.9315819977  
H   -2.9715213666  -2.7086878637  -1.0448407387  
H   -2.6035100496  -4.4239542963  -0.9073568175  

Au₅-C₃H₆
E = -796.630577707172
Au  2.8651560836  -0.3876384505   0.0994894043  
Au  1.1905120274   1.5791902778  -0.0106264193  
Au  -1.6219873063   0.9257641534  -0.1022026260  
Au  -2.2026021527  -1.6596343769  -0.0671591636  
Au  0.2835126735  -0.9879870454   0.0124621020  
C  -1.7007578668   3.1008284971  -0.1428561218  
C  -3.9441640596   2.6241072413   0.971214330  
H  -1.2095701104   3.4238398989  -1.0595045537  
H  -1.3094894879   2.6356234777  -0.194989437  
H  -1.3461640596  -2.6241072413   0.971214330  
H  -4.5844503858   1.7368424527   0.9649275052  
H  -4.6076270220   3.4949080586   0.8883793476  
H  -3.4169950019   2.6838450049   1.9270495976  

Au₆-C₃H₆
E = -932.43016107037
Au  1.6731470593   0.1252470394   0.0874070349  
Au  -0.7616932188   1.3023854608   0.0859753340  
Au  -0.5095132290  -1.4439083758  -0.1749617325  
Au  -2.9047129798  -0.2725635871  -0.1226347186  
Au  1.4498034411   2.7223826945   0.3124929204  
Au  1.9223281919  -2.4686252257  -0.1391454630  
C  -4.9891549645  -0.4187956964  -0.7797348701  
C  -5.040362790  -0.4532873252   0.5983086643  
C  -5.3951184678   0.7196551333   1.4635608982  
H  -5.008336814   -1.3417400020  -1.3578179185  
H  -5.208685639   0.5028424232  -1.3186762003  
H  -5.0376812521  -1.4317933625  1.0838472476  
H  -5.3377647438   1.6612092489   0.9242251741  
H  -6.4266423945   0.5769565318  1.8133907039  
H  -4.7635942238   0.7597570036   2.3560340958  

Au₇-C₃H₆
E = -1068.28880327553
Au  2.3308074318  -0.7570058802  -1.3652036763
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Au      | 0.740982323 | 1.2852046843 | -0.6146437939 |
| Au      | 0.0358225143 | -1.4062813755 | -0.1205940362 |
| Au      | -1.0691368612 | 3.1112635995 | -0.2279858201 |
| Au      | -1.7747108361 | 0.6379324988 | 0.3256228583 |
| Au      | -2.3604780022 | -1.8880034977 | 0.7682222668 |
| Au      | 2.1938744760 | -0.2461684548 | 1.2499863657 |
| C       | 3.3282391310 | -0.0600229477 | 3.1002325764 |
| C       | 2.0023331771 | 0.1277348936 | 3.4402903251 |
| C       | 1.3673336183 | 1.4610114586 | 3.6818233873 |
| H       | 3.9929504047 | 0.7953012467 | 2.9814083151 |
| H       | 3.7985621004 | -1.0334164414 | 3.2301414843 |
| H       | 1.4382236786 | -0.7427598652 | 3.7824262195 |
| H       | 1.2733537163 | 1.6081402116 | 4.7652128895 |
| H       | 0.3579322883 | 1.5060357483 | 3.2621514380 |
| H       | 1.9641489499 | 2.2810247715 | 3.2735197739 |

**Au₈-C₃H₆**

\[ E = -1204.08463024198 \]

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Au      | 2.1054779499 | 0.6817116531 | -0.2402088314 |
| Au      | -0.5740670830 | 1.0698659959 | 0.0736006817 |
| Au      | -1.5807746206 | -1.2513385504 | -1.1837465867 |
| Au      | 0.7368245684 | -1.5813325342 | 0.5168399545 |
| Au      | -3.2370059693 | 0.6560925250 | -0.0028055727 |
| Au      | 1.0234891133 | 3.0496296101 | -0.5040660109 |
| Au      | 3.3062553665 | -1.6433593185 | 0.0280451444 |
| Au      | -1.6935142604 | -1.0312261770 | 1.5097373199 |
| C       | -2.1205669068 | -1.8084503513 | -3.2088032612 |
| C       | -0.9173143836 | -2.4397776791 | -2.9346994764 |
| C       | 0.4107155294 | -1.9634078538 | -3.4377175222 |
| H       | -2.1385109014 | -0.8974735648 | -3.8058747106 |
| H       | -3.0614596793 | -2.3469573773 | -3.1096294891 |
| H       | -0.9555378794 | -3.4688437733 | -2.5718802681 |
| H       | 0.3863187894 | -0.9075125012 | -3.7214154538 |
| H       | 0.6769463310 | -2.5525018302 | -4.3244428784 |
| H       | 1.2008529163 | -2.1148432186 | -2.6966888032 |

**Au₈-C₃H₆₂**

\[ E = -1204.0805227080 \]

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Au      | 3.4565072446 | 0.3251035275 | 0.1213396746 |
| Au      | 0.9151843494 | 0.9883124068 | 0.4132881936 |
| Au      | 0.1128157802 | 3.2725090747 | 1.4034395262 |
| Au      | -1.7595226175 | 1.6032135014 | 0.6316154907 |
| Au      | -3.5987789417 | -0.0995250851 | -0.1484066795 |
| Au      | -1.1078935381 | -0.8238383561 | -0.4098547000 |
| Au      | 1.5232276582 | -1.3975509037 | -0.6084074022 |
| Au      | -0.3201192582 | -3.1393778776 | -1.3687864679 |
C         5.5674501931    0.3162793679    0.7244334535
C         5.5717263434    0.5897573352   -0.6254759689
C         5.8720365403   -0.4120518257   -1.6942027833
H         5.7834852097   -0.6879793581    1.0875015141
H         5.624401376    1.1238110531   -1.4530767211
H         5.5760218010    1.6376094537   -0.9336486493
H         5.8720365403   -0.4120518257   -1.6942027833
H         5.2043612155   -0.2961251199   -2.5535541837
H         5.8119698132   -1.4389042180   -1.3236033045

Au         0.7136102540   -1.6303029414   -0.7608857490
Au       -1.4908796131   -2.8354074312   -1.535507251
Au       -1.7850632053   -0.9897969057    0.2839980077
Au        3.0302840345   -0.7453015245    0.3993786936
Au       -1.8556803073    0.5944474689    2.4523614866
Au       -1.0825266430    1.7736976406    0.1691258080
Au       -1.396078575    1.0241501367   -0.9027324653
Au       0.0200053831    3.0950220066   -1.7945639321
Au        0.6108210276   -0.0732772079    1.5290166698
C         4.9471096536   -1.7034562090    1.0494511356
C         5.2424124092   -0.3704829880    0.938401931
C         5.3015359299    0.5880869807    2.0840252150
H         5.1592585719   -2.3891158339    0.2304379040
H         4.7323026666   -2.1460053915    2.0218650560
H         5.6424233561   -0.0133268277   -0.0133124267
H         4.8501361246    0.1734893281    2.9894724091
H         4.8156664643   -1.5383655714    1.8398977864
H         6.3536157570    0.8158891193    2.2965381335

Au9-C3H6
E = -1339.93714896661
Au       -1.4908796131   -2.8354074312   -1.535507251
Au       -1.7850632053   -0.9897969057    0.2839980077
Au        3.0302840345   -0.7453015245    0.3993786936
Au       -1.8556803073    0.5944474689    2.4523614866
Au       -1.0825266430    1.7736976406    0.1691258080
Au       -1.396078575    1.0241501367   -0.9027324653
Au       0.0200053831    3.0950220066   -1.7945639321
Au        0.6108210276   -0.0732772079    1.5290166698
C         4.9471096536   -1.7034562090    1.0494511356
C         5.2424124092   -0.3704829880    0.938401931
C         5.3015359299    0.5880869807    2.0840252150
H         5.1592585719   -2.3891158339    0.2304379040
H         4.7323026666   -2.1460053915    2.0218650560
H         5.6424233561   -0.0133268277   -0.0133124267
H         4.8501361246    0.1734893281    2.9894724091
H         4.8156664643   -1.5383655714    1.8398977864
H         6.3536157570    0.8158891193    2.2965381335

Au10-C3H6
E = -1475.73259927424
Au        3.3406577288   -0.5894002822   -0.7477627850
Au        1.9367481057    1.7544811427   -0.2163437490
Au       -2.5979847206    2.5846210219    0.1022867766
Au        1.5331415721   -0.5289988757    1.2827469556
Au       -0.4796320695    -1.0413872893    2.9648403131
Au       -0.5709295326    1.1789768936    1.0880793072
Au        0.7305798490   -0.4952324064   -1.3839680944
Au       -1.9053860157    0.4452137309   -1.2076588513
Au       -1.0338650179   -1.6891996646    0.4775727379
Au       -1.3676070438   -1.9876530003   -2.1942531487
C         2.0105727030    3.9292648040   -0.2374227618
C         3.0886855452    3.5137224041   -0.9983319969
C         3.1056469619    3.5119543338   -2.4960363577
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 2.1470272426 | 4.2117377983 | 0.8049219417 |
| H    | 1.0959900605 | 4.2711351157 | -0.7201768940 |
| H    | 4.0572428411 | 3.4244831057 | -0.5034166909 |
| H    | 3.6407763887 | 2.6451928160 | -2.8943793761 |
| H    | 3.6383441294 | 4.4064791207 | -2.8428879798 |
| H    | 2.0959406072 | 3.5334231112 | -2.9155828018 |

**Au\textsubscript{10} \cdot 2C\textsubscript{6}H\textsubscript{6}**

\[ E = -1475.72420023605 \]

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Au   | 0.7249846755 | -3.2770954206 | -1.4180312068 |
| Au   | -0.8836626264 | -1.4654172845 | -0.4017919509 |
| Au   | 0.2276354088 | 3.2315268857 | -1.6642940699 |
| Au   | 1.8451534370 | -1.3197783902 | -0.1203085905 |
| Au   | 3.1623180506 | 0.2990070005 | 1.5419602381 |
| Au   | -1.0985995997 | 1.2744515224 | -0.5210734495 |
| Au   | 0.4072450277 | 0.0920628153 | 1.8045582925 |
| Au   | -2.3147962830 | -0.1185750943 | 1.5855197326 |
| Au   | 1.6168001335 | 1.567058143 | -0.2258966862 |
| Au   | -3.2723837086 | -0.2922437763 | -0.9452242520 |
| C    | -2.7411243586 | -0.0832396690 | 3.7232717665 |
| C    | -3.9756854120 | -0.0786779082 | 3.0959100929 |
| C    | -4.8256367584 | 1.1423169196 | 2.9293983572 |
| H    | -2.3229321731 | -1.0114402590 | 4.1079708499 |
| H    | -2.3300387733 | 0.8413572918 | 4.1261720077 |
| H    | -4.4713524184 | -1.0387719000 | 2.9411263877 |
| H    | -5.3540210350 | 1.1416425373 | 1.9717398113 |
| H    | -5.5896569075 | 1.1467926441 | 3.7175327948 |
| H    | -4.2424199774 | 2.0631839304 | 3.0172252572 |

**Au\textsubscript{11} \cdot C\textsubscript{3}H\textsubscript{6}**

\[ E = -1611.60128828568 \]

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Au   | 1.4507569611 | -0.0871385939 | 1.6376985617 |
| Au   | 1.5778771625 | -1.1432327052 | -0.9749325396 |
| Au   | 1.2984117286 | 1.6328316843 | -0.5885436150 |
| Au   | -1.1729839951 | -1.3757860891 | -0.9765434771 |
| Au   | -1.2927824206 | -0.3565657343 | 1.5547091963 |
| Au   | -1.4399523150 | 1.3263053984 | -0.6124600215 |
| Au   | -3.5242518363 | -0.3436839629 | -0.0325137699 |
| Au   | 3.5642472055 | 0.3439934704 | 0.0452835529 |
| Au   | 0.0456602872 | -0.5235281556 | 3.7915465212 |
| Au   | -0.2891401046 | 3.5219121266 | -1.4353621856 |
| Au   | 0.3552838979 | -3.0010061772 | -2.3358161349 |
| C    | -5.6393072296 | -0.8786253662 | -0.4604918989 |
| C    | -5.7070440349 | 0.0889186918 | 0.5092937023 |
| H    | -5.9985682765 | 1.5332996037 | 0.2542064635 |
| H    | -5.6825763725 | -1.9338003019 | -0.1951628710 |
H  -5.8000778932  -0.6255814419  -1.5082148524
H  -5.7469247092  -0.2346023777  1.5516822617
H  -7.0281822895  1.7439714236  0.5697269362
H  -5.9034680444  1.7905418272  -0.8042405930
H  -5.3465393188  2.1853016257  0.8442930034

Au_{12}-C_3H_6
E = -1747.39864506264
Au  -0.4150304932  -3.5053319775  -0.1205496634
Au  -0.4322245942  3.5644190628  0.0402550281
Au  -1.9563166789  -1.3183963195  -0.4563591084
Au  0.7559516777  1.3451334561  1.5798898887
Au  0.7451886440  1.4219906765  -1.1186788778
Au  -4.0524608019  0.0461097812  -1.2382731923
Au  2.9062130767  0.0870510690  -2.1487392294
Au  1.7216169162  -0.0347329645  3.1385862926
Au  2.4344276121  0.0265025140  0.5720185811
C  4.7773138148  0.0997287582  -3.3535748668
C  3.7692847669  0.0201303631  -4.2801309213
C  3.3223353722  -1.2404233157  -4.9482079621
H  5.3235622851  -0.7934231374  -3.0506754051
H  5.2222619797  1.0606658916  -3.0994033114
H  3.3899603221  0.9525037023  -4.7039539042
H  2.2303641410  -1.3020845033  -5.0003491621
H  3.7108189295  -2.1309193859  -4.4465263998
H  3.6891273303  -1.2391088243  -5.9824091052

Au_{13}-C_3H_6
E = -1883.23813788974
Au  -0.2899625575  0.8241613619  -3.0698376964
Au  1.2332591438  -1.0887440346  -1.8058937745
Au  3.2109748000  -0.3671800552  -0.0231628589
Au  1.4998387693  1.5055739781  -1.0992592480
Au  -1.4186862277  -0.9964715513  -1.0871961940
Au  -0.1189526641  -3.3765925353  -1.1593117405
Au  0.8364578694  -1.7783902384  0.8203319109
Au  -1.1482610473  1.6051336518  -0.3700678429
Au  0.6064850193  3.3932387509  0.6678137272
Au  1.1040866769  0.8730817607  1.5461697812
Au  -3.5862727482  0.3666146129  -0.0602975542
Au  -1.5214668054  -0.3185627344  1.5939464594
Au  0.3650886523  -0.9937139093  3.3824441516
C  -5.6387591973  0.7169418994  -0.8749166419
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -5.8050678952 | 0.5434817118 | 0.4743921767 |
| C    | -6.2498529372 | -0.7296349000 | 1.1212195787 |
| H    | -5.5671668202 | 1.7157137047 | -1.3019337817 |
| H    | -5.8232475913 | -0.1046240974 | -1.5664681219 |
| H    | -5.8091206273 | 1.4344001437 | 1.1064423081 |
| H    | -7.2985983678 | -0.6225792372 | 1.4256276433 |
| H    | -5.6762430152 | -0.9412109899 | 2.0293921917 |
| H    | -6.1751798565 | -1.5825851451 | 0.4411146497 |

$Au_{14}$-$C_3H_6$

$E = -2019.05700433738$

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Au   | 2.3858356312 | 2.4488796457 | 0.2115318831 |
| Au   | -1.8474985698 | -0.9093782722 | 1.2681495860 |
| Au   | -1.7467079860 | -0.7833997852 | -1.4531351320 |
| Au   | 0.4833152540 | 1.0682612964 | -1.2927065044 |
| Au   | -2.1494951348 | 1.6155130240 | 0.0065131742 |
| Au   | 0.3905963165 | 0.9280829927 | 1.4267597048 |
| Au   | -0.3187954020 | -0.6821147588 | 3.4813723990 |
| Au   | 0.6622876217 | -1.9446354901 | 1.2776738093 |
| Au   | 0.7649261448 | -1.8090811086 | -1.4451721887 |
| Au   | 2.7640946558 | -2.9573125366 | -0.0629025620 |
| Au   | -4.0638198932 | -0.2382630235 | -0.1460030335 |
| Au   | -0.1006011732 | -0.3135355941 | -3.5448733178 |
| Au   | 2.6175204814 | -0.2214951834 | 0.0689620460 |
| Au   | -0.2949048369 | 3.4316752491 | 0.1703585161 |
| C    | 3.1031732915 | 4.5369528774 | 0.3524733717 |
| C    | 4.2149296934 | 3.7165391820 | 0.3127468934 |
| C    | 5.0618126480 | 3.5030500228 | -0.9033122689 |
| H    | 2.7821508406 | 5.0652648618 | -0.5444271550 |
| H    | 2.7300198226 | 4.9102386567 | 1.3042083274 |
| H    | 4.6582316191 | 3.4149200337 | 1.2638092886 |
| H    | 5.9543696285 | 4.1368271564 | -0.8247857683 |
| H    | 5.4063662350 | 2.4671783751 | -0.9743408807 |
| H    | 4.5332280494 | 3.7695784638 | -1.8227286264 |

$Au_{15}$-$C_3H_6$

$E = -2154.90156606888$

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Au   | -1.9284680910 | -2.3617233382 | -0.2412920317 |
| Au   | -3.7359204237 | -0.4032420874 | -0.2728969940 |
| Au   | -1.4670768146 | 0.4309676068 | -1.6756579998 |
| Au   | -3.0330141291 | 2.3176827744 | -0.2591852333 |
| Au   | -0.3791148518 | 2.7295972648 | -0.1534431675 |
| Au   | 1.1835941952 | 0.9919183508 | -1.7859175029 |
| Au   | 1.2951385477 | 0.7331403319 | 1.016604571 |
| Au   | -0.0288873094 | 0.2711985592 | 3.3872869755 |
| Au   | 0.1318991369 | -1.6802523183 | 1.4553312638 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | 0.4715771822 | -3.8540223423 | -0.1002909991 |
| Au      | 3.5906072274  | 0.5214738307  | -0.3798985025  |
| Au      | 2.5346206171  | -1.8893229460 | 0.0950445046  |
| Au      | 0.3657123321  | -1.5173492984 | -1.5583546608 |
| Au      | -1.5264851212 | 0.4328948440  | 1.1117414693  |
| Au      | 2.3107929443  | 3.0237428658  | -0.2160297151 |
| C       | 0.0586107131  | 0.2136529094  | 5.5993674962  |
| C       | 0.2829595899  | 1.5232229842  | 5.2482738738  |
| C       | 1.6322500559  | 2.1657256658  | 5.1722945142  |
| H       | -0.9368143627 | -0.1204710765 | 5.8875531006  |
| H       | 0.8904152024  | -0.4450235313 | 5.8475972624  |
| H       | -0.5754434587 | 2.1979221704  | 5.2191476253  |
| H       | 1.7611500944  | 2.8230050989  | 6.0412142339  |
| H       | 1.7252264905  | 2.7936756782  | 4.2800012789  |
| H       | 2.4380569637  | 1.4265773916  | 5.1763850570  |

\( \text{Au}_3\text{Y} \)
\[ E = -445.515149007483 \]
\[ \begin{align*}
Y & \quad 0.5462894587 \quad -1.0330002416 \quad 0.0000000000 \\
\text{Au} & \quad -1.5269615948 \quad 0.1280323367 \quad 1.3417287169 \\
\text{Au} & \quad -1.5269615948 \quad 0.1280323367 \quad -1.3417287169 \\
\text{Au} & \quad 2.7797439585 \quad 0.2329271810 \quad 0.0000000000
\end{align*} \]

\( \text{Au}_4\text{Y} \)
\[ E = -581.355107907814 \]
\[ \begin{align*}
Y & \quad 0.0005403741 \quad -1.1374626624 \quad 0.0572855741 \\
\text{Au} & \quad -1.2891362486 \quad 1.2897585257 \quad -0.0002766846 \\
\text{Au} & \quad 1.2883081767 \quad 1.2908949357 \quad -0.0001249425 \\
\text{Au} & \quad -2.7607217544 \quad -1.0078249595 \quad -0.0140708525 \\
\text{Au} & \quad 2.7615599800 \quad -1.0058115808 \quad -0.0142695648
\end{align*} \]

\( \text{Au}_5\text{Y} \)
\[ E = -717.1734969000705 \]
\[ \begin{align*}
Y & \quad 0.0007530712 \quad -0.6932704341 \quad 0.0144401714 \\
\text{Au} & \quad -2.3340313127 \quad 0.8622322037 \quad 0.0144558110 \\
\text{Au} & \quad 2.3319532952 \quad 0.8672008613 \quad -0.0244251837 \\
\text{Au} & \quad 2.6122683407 \quad -1.7663832498 \quad 0.0181399909 \\
\text{Au} & \quad -2.6083480138 \quad -1.7720319268 \quad -0.0200093994 \\
\text{Au} & \quad -0.0023684473 \quad 2.1538778251 \quad 0.0045900194
\end{align*} \]

\( \text{Au}_6\text{Y} \)
\[ E = -853.014796933774 \]
\[ \begin{align*}
Y & \quad 0.0156755856 \quad 0.0154977239 \quad 1.1733764321 \\
\text{Au} & \quad 1.1101804136 \quad -1.0974766514 \quad -1.2582674842 \\
\text{Au} & \quad 0.3458245972 \quad 1.4948576883 \quad -1.2876550944 \\
\text{Au} & \quad -2.6932549805 \quad -0.7820723016 \quad 1.1184031813
\end{align*} \]
| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Au      | 2.0706572997 | -1.9232941907 | 1.0655748343 |
| Au      | -1.5161430171 | -0.4623724444 | -1.232320739 |
| Au      | 0.6723041016  | 2.7592949555  | 1.0150343147 |

**Au,Y**

E = -988.837958146004

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Y       | 0.5829510092 | 0.0011386801 | 0.6408944751 |
| Au      | -1.7272342817 | 1.4514185762 | -0.1024536625 |
| Au      | 0.5271871085  | -2.7418608416 | -0.0714546540 |
| Au      | 2.9686800641  | -1.3070893637 | -0.1302012728 |
| Au      | 0.5266950690  | 2.7386944688  | -0.0832852764 |
| Au      | -1.7274063227 | -1.4552763222 | -0.0914663559 |
| Au      | -3.8997386985 | -0.0020858455 | -0.0292419984 |
| Au      | 2.9778756434  | 1.3155122910  | -0.0966730922 |

**Au,Y**

E = -1124.67894772093

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Y       | -0.0069893829 | -0.4993787413 | -0.5270363057 |
| Au      | -2.7777354479 | -0.5931486639 | 0.1043386953 |
| Au      | 1.3003342926  | 1.8912721380  | 0.0571564759 |
| Au      | 2.7692391275  | -0.6285121271 | 0.0781288290 |
| Au      | -1.5085647750 | -2.8411517026 | 0.1196797210 |
| Au      | -1.2855811505 | 1.9124065765  | 0.0459422879 |
| Au      | -3.9368535147 | 1.7204774082  | 0.0019116819 |
| Au      | 1.4902042779  | -2.8707939655 | 0.0348473243 |
| Au      | 3.9500381811  | 1.6764947463  | 0.0508346963 |

**Au,Y**

E = -1260.48673823265

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Y       | 0.3864161418  | -0.0046358185 | 0.8166979632 |
| Au      | 2.8743708752  | -1.3376062581 | 0.1248829105 |
| Au      | -1.317868728  | 0.0116753905  | -1.5709591815 |
| Au      | -1.7555802342 | 1.8638537298  | 0.5635347720 |
| Au      | 2.8843871894  | 1.3139721506  | 0.1358399906 |
| Au      | 1.2335042594  | 0.0008897716  | -1.8772371364 |
| Au      | 0.6198020864  | -2.8736442613 | 0.8116129910 |
| Au      | 0.6425521643  | 2.8625148495  | 0.8330896952 |
| Au      | -3.6087631927 | 0.0143013110  | -0.0112815943 |
| Au      | -1.7701126931 | -1.8540637771 | 0.5487123234 |

**Au,Y_2**

E = -1260.49021333860

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Au      | -1.9716472185 | -2.2012027028 | -0.7227172268 |
| Au      | -2.8781379262 | 0.3222504791  | -0.6601109009 |
| Au      | -1.2963055211 | 2.5236439382  | -0.4640700687 |
| Au      | 1.5032649906  | 2.3898314653  | -0.5046958674 |
Au  2.8827066271  0.0616698795 -0.7665352365
Au  1.7353976531 -2.3641420512 -0.7666415070
Au -0.0776870410 -1.8057392386  1.2934477268
Au -1.2812155294  0.6276773804  1.5774472267
Au  1.3978481938  0.4747234477  1.5233614791
Y  -0.0190789013 -0.0661585789 -1.0275295972

Au10Y
E = -1396.34428893178
Y  -0.1085274750  0.0029979900 -0.9753408038
Au  1.8004538363 -2.1380389064 -0.4421580433
Au -0.8338625897  1.3354977428  1.4903529079
Au -2.7733310040  1.3173111934 -0.5795952192
Au -0.6648722524 -3.0414835281 -0.707269602
Au -0.7988698622 -1.3612828031  1.4838949170
Au  3.3993770349  0.0173575318 -0.5051160118
Au -2.7532497864 -1.3396776832 -0.5764225726
Au -0.6966775757  3.0307145880 -0.6932098347
Au  1.7835001546  2.1629063192 -0.4497775777
Au  1.5331840913  0.0182295191  1.4598748489

Au11Y
E = -1532.16232228304
Y  -0.1324582996  0.0012914553  0.8283918772
Au  2.6975732491 -0.0093135252  1.8257841113
Au -2.0561178089  0.0033800030 -1.3675864944
Au -2.8694835728  1.3675989481  0.9257682894
Au  1.8326460563  2.2745662905  0.4563141317
Au  0.2700419235  1.3779632914 -1.7483706848
Au  1.8140166553 -2.2877714297  0.4600274077
Au -0.7677047677  2.8967021898  0.3860284351
Au -2.8827634353 -1.3437205612  0.9305179075
Au -0.7918276879 -2.8872780425  0.3884133277
Au  0.2625515834 -1.3824579149 -1.7483309581
Au  2.5469929597 -0.0102222791 -0.9168962600

Au12Y
E = -1668.00820269477
Y  -0.0258506216 -0.1693815418  0.4904945044
Au  2.4938742572  1.4099848903  1.6579661069
Au -2.2368260280 -0.8085982585 -1.4993352371
Au -2.8788078346 -0.1916163363  1.2321860697
Au  0.5127871895  2.7656193024  0.2907931585
Au  0.0526610793  0.3915030540 -2.4378962976
Au  2.6408962173 -1.2093306140  1.1981910641
Au -1.7803942977  1.7607925828 -0.9702809300
|      | x      | y      | z      |
|------|--------|--------|--------|
| Au   | -1.8302745715 | -2.5986233353 | 0.5574652221 |
| Au   | 0.7900220220  | -3.0823696532 | 0.5541419608 |
| Au   | 1.7735373600  | -1.5510634990 | -1.5190682221 |
| Au   | 2.2773289976  | 1.0134162536  | -1.0086173446 |
| Au   | -1.7983500400 | 2.1978487216  | 1.6985314249  |

\[ \text{E} = -1803.83865000443 \]

|      | x      | y      | z      |
|------|--------|--------|--------|
| Au   | 13     | Y      |        |
| E    |        |        |        |
| Y    | 0.0905338779 | 0.0005355636 | 0.5268434228 |
| Au   | 2.2388547582  | -1.9840055400 | 1.3668740556 |
| Au   | -1.1198182087 | 2.2612973952  | -1.1012035152 |
| Au   | -0.2960769742 | 2.7992141888  | 1.5777285275  |
| Au   | 3.2242155703  | 0.0036650688  | -0.1834751656 |
| Au   | -0.1908671771 | -0.0021250825 | -2.4156280579 |
| Au   | -0.2896128327 | -2.7977669319 | 1.5821172376  |
| Au   | 1.5273283009  | 1.8480484570  | -1.3323849844 |
| Au   | -2.5407570869 | 1.3720414928  | 1.2301651376  |
| Au   | -2.5373690777 | -1.3760408223 | 1.2322390541  |
| Au   | -1.1444456865 | -2.2656392662 | -1.0977132301 |
| Au   | 1.5317345791  | -1.8465179926 | -1.3295349011 |
| Au   | 2.2344664908  | 1.9915617628  | 1.3637851187  |
| Au   | -2.7259564387 | -0.0040830964 | -1.1460455420 |

\[ \text{E} = -1939.69622908470 \]

|      | x      | y      | z      |
|------|--------|--------|--------|
| Au   | 14     | Y      |        |
| E    |        |        |        |
| Y    | -0.0037090994 | 0.0059053469 | -0.3805204973 |
| Au   | 1.4140540798  | 0.0731007790 | 2.5364061780 |
| Au   | 0.1423026146  | -2.2704153799 | 1.5158914394 |
| Au   | 2.5835367666  | -1.3504713262 | 0.5837584611 |
| Au   | 2.3870238815  | 1.5837298903  | 0.5335024206 |
| Au   | -2.3821010484 | -1.5972056042 | 0.5391378408 |
| Au   | -2.5584197713 | 1.3479460907  | 0.6568260103 |
| Au   | -0.1099188308 | 2.2351671515  | 1.5915619084 |
| Au   | 2.7474737705  | 0.0789493796  | -1.7403170437 |
| Au   | 1.2351972152  | 2.3806346842  | -1.8033169497 |
| Au   | -1.4058200398 | 2.3636672515  | -1.6000608727 |
| Au   | -2.7817379710 | -0.0389214973 | -1.6888334835 |
| Au   | -1.2742170760 | -2.3391987427 | -1.8359776407 |
| Au   | 1.3694267304  | -2.3281232478 | -1.6570437528 |
| Au   | -1.3666549887 | -0.1377996478 | 2.5531207530 |

\[ \text{E} = -563.401969138099 \]

|      | x      | y      | z      |
|------|--------|--------|--------|
| Au   | 3      | Y-C_3H_6|        |
| E    |        |        |        |
| Y    | 0.5122550675 | 0.6330121186 | -0.4299826166 |
| Au   | -1.5382311943 | 0.5380379916 | 1.4168198900  |
| Au   | -1.8490081855 | -0.7162096396 | -0.9254914035 |
\[
\text{Au\textsubscript{4}Y-C\textsubscript{3}H\textsubscript{6}}
\]
\[
E = -699.249267729939
\]
\[
\begin{array}{cccc}
\text{Y} & -1.0200962166 & 0.0389210806 & -0.6302674012 \\
\text{Au} & 2.1314537191 & -0.1941523457 & 0.1704597114 \\
\text{Au} & 0.7862024501 & 2.0651468914 & -0.3027823857 \\
\text{Au} & 0.4427554041 & -2.2333663257 & -0.2821762172 \\
\text{Au} & -3.3373943622 & 0.8279000101 & 0.5044029540 \\
\text{C} & 4.0284024498 & -1.0374112127 & 0.7774979474 \\
\text{C} & 4.1966924196 & 0.3439085029 & 0.7353818128 \\
\text{C} & 4.9297732169 & 1.0583570006 & -0.3607568123 \\
\text{H} & 4.4083782691 & -1.6577729881 & -0.0333241936 \\
\text{H} & 3.8419216858 & -1.5398368072 & 1.7247375812 \\
\text{H} & 4.0833693297 & 0.8296704000 & 1.6719172661 \\
\text{H} & 4.5065462709 & 2.0474301378 & -0.5569985997 \\
\text{H} & 4.9386416685 & 0.4857760788 & -1.2911535273 \\
\text{H} & 5.9698173323 & 1.2093557718 & -0.0454380927 \\
\end{array}
\]
\[
\text{Au\textsubscript{5}Y-C\textsubscript{3}H\textsubscript{6} \_2}
\]
\[
E = -699.248258403245
\]
\[
\begin{array}{cccc}
\text{Y} & 0.0605802693 & -1.0869487390 & -0.0886846325 \\
\text{Au} & -1.6696634834 & 1.0716462918 & 0.1334191865 \\
\text{Au} & 0.7846273240 & 1.5671314910 & -0.4721866729 \\
\text{Au} & -2.5361302220 & -1.3823943614 & 0.9024913578 \\
\text{Au} & 2.7345898784 & -0.3234637050 & -0.303341913 \\
\text{C} & -0.1474506925 & -2.3882450258 & -2.3535040871 \\
\text{C} & -0.4098753989 & -1.2467532661 & -3.015634367 \\
\text{C} & -1.7623637182 & -0.7462228471 & -3.3633946395 \\
\text{H} & -0.9550259390 & -3.0693567101 & -2.0687588998 \\
\text{H} & 0.8843531289 & -2.7427349014 & -2.2551863309 \\
\text{H} & 0.4365672954 & -0.6403734739 & -3.3508594143 \\
\text{H} & -1.8845422943 & 0.2957103961 & -3.0453202287 \\
\text{H} & -2.5602047106 & -1.3604945549 & -2.9382616285 \\
\text{H} & -1.8614569583 & -0.7449913577 & -4.4568140411 \\
\end{array}
\]
\[
\text{Au\textsubscript{3}Y-C\textsubscript{3}H\textsubscript{6}}
\]
\[
E = -835.063234245562
\]

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Y       | 1.5883736583 | 0.1414017149 | 0.8352314228 |
| Au      | 1.7045405738 | 2.7013517923 | -0.0905280014 |
| Au      | -0.6488030625 | 1.3662357046 | -0.1489251759 |
| Au      | -2.7406554463 | -0.2903665550 | 0.1264993835 |
| Au      | -0.3865897695 | -1.4823044244 | -0.1453246340 |
| Au      | 2.1750298619 | -2.3417468787 | -0.1404249100 |
| C       | -4.8215413052 | -0.9186882819 | 0.5078405701 |
| C       | -4.9000781668 | 0.4074880172 | 0.1510147548 |
| C       | -5.2968023991 | 0.8970668904 | -1.2056903164 |
| H       | -5.048326809  | -1.699032157 | -0.2192191891 |
| H       | -4.8106665916 | -1.2112800613 | 1.5563506296 |
| H       | -4.8924620711 | 1.1519424067 | 0.9500696471 |
| H       | -4.6907094922 | 1.7519018665 | -1.5212714248 |
| H       | -6.3372470086 | 1.2433701982 | -1.1622893825 |
| H       | -5.2290175812 | 0.1098719719 | -1.9614002221 |

\[
\text{Au}_5\text{Y-C}_3\text{H}_6\_2
\]

\[
E = -835.06233900462
\]

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Y       | -0.0383109777 | -0.6268998807 | 0.4793384373 |
| Au      | -2.1549110376 | 1.0230724974 | -0.3405254028 |
| Au      | 2.3463542032 | 0.7386259943 | -0.1040456489 |
| Au      | 2.4425488904 | -1.8998235242 | -0.1083976142 |
| Au      | -2.6579656144 | -1.5624809206 | -0.1466456042 |
| Au      | 0.1642705180 | 2.2521642308 | 0.0419437174 |
| C       | 0.0388689034 | -0.9816750807 | 3.0865756120 |
| C       | -0.3340304568 | 0.2890244219 | 3.3187965915 |
| C       | -1.7268011286 | 0.7459710355 | 3.5551239685 |
| H       | 1.0965978083 | -2.555270858 | 3.058084608 |
| H       | -0.6960375184 | -1.7927754984 | 3.1114331337 |
| H       | 0.4449731832 | 1.0543220642 | 3.3694471772 |
| H       | -1.8021449071 | 1.1194641942 | 4.5845690068 |
| H       | -2.4595983957 | -0.0538058453 | 3.4182449422 |
| H       | -1.9755594891 | 1.5914327762 | 2.9033946674 |

\[
\text{Au}_6\text{Y-C}_3\text{H}_6
\]

\[
E = -970.908460946390
\]

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Y       | 1.1704532867 | 0.0627547578 | -0.9302544524 |
| Au      | -0.3493827365 | 1.3557451699 | 1.0430164349 |
| Au      | -0.0390065495 | -1.2915228875 | 1.2083725684 |
| Au      | -1.0791931443 | -0.2863188718 | -2.3262337514 |
| Au      | 1.6100154822 | 2.7428263142 | -0.0371475655 |
| Au      | -2.3632998940 | -0.2767802835 | 0.2738612908 |
| Au      | 2.2114470420 | -2.3028083915 | 0.2889440566 |
| C       | -4.4139380088 | -0.5694636784 | -0.4353884014 |
| C       | -4.4980383203 | -0.4043761564 | 0.9343890565 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -4.926722312 | 0.8635957600 | 1.6050682253 |
| H       | -4.6530259970 | 0.2580680499 | -1.1024709102 |
| H       | -4.4180746033 | -1.5672605611 | -0.8706727087 |
| H       | -4.5078209784 | -1.3018705939 | 1.5555617860 |
| H       | -5.9790600288 | 0.7640522524 | 1.9000505506 |
| H       | -4.8395682464 | 1.7281169654 | 0.9409650685 |
| H       | -4.3542125640 | 1.0507933680 | 2.5182586177 |

**Au-Y-C\textsubscript{3}H\textsubscript{6}**

\[E = -1106.73390290117\]

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | -0.7614315572 | 0.0398879940 | -0.7101262741 |
| Au      | 3.8467957012  | -0.1467200832 | 0.1260340010 |
| Au      | 1.6160940180  | 1.3094801230 | 0.1055925817 |
| Au      | -0.5682790058 | 2.7693770274 | 0.0172870543 |
| Au      | 1.5222355940  | -1.4405699622 | 0.0200034504 |
| Au      | -0.7624134854 | -2.7347173292 | -0.1527257541 |
| Au      | -3.0604933875 | 1.4093349749 | 0.1536853681 |
| Au      | -3.1510360508 | -1.210321558 | 0.0822539722 |
| C       | 5.9565344007  | -0.2445092875 | 0.8044276079 |
| C       | 6.0190779948  | -0.878780755  | -0.557609614 |
| C       | 6.2887383047  | 1.2093363897  | -1.2525057856 |
| H       | 6.0238268159  | -1.2337161600 | 1.2544317367 |
| H       | 6.967277316  | 0.6077559268 | 1.4687678151 |
| H       | 6.0857248793  | -0.9874919058 | -1.1733020793 |
| H       | 5.6442089827  | 1.3398804806  | -2.372741589 |
| H       | 6.1678276529  | 2.0662303153  | -0.5841258435 |
| H       | 7.3232350061  | 1.2017869864  | -1.6179151671 |

**Au\textsubscript{8}Y-C\textsubscript{3}H\textsubscript{6}**

\[E = -1242.57213385282\]

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Y       | -0.3029036254 | -0.5279212501 | -0.0238231890 |
| Au      | -0.9703565964 | 2.1666971110 | 0.0655722717 |
| Au      | 1.5569304847  | 1.5171441449 | 0.0665194360 |
| Au      | 4.1773739629  | 0.8295710334 | 0.0936367444 |
| Au      | -3.6219460731 | 2.4294626062 | 0.0462886054 |
| Au      | -3.0794711708 | -0.0982351512 | -0.0100474054 |
| Au      | 0.7300146044  | -3.1471002645 | -0.1325194515 |
| Au      | 2.4550215685  | -1.1486428076 | -0.0370556174 |
| Au      | -2.2719552545 | -2.5602088699 | -0.0738807022 |
| C       | 6.0524573759  | 1.7959599017 | 0.7828522886 |
| C       | 6.0564600581  | 1.9294404249 | -0.5828836591 |
| C       | 6.8316371876  | 1.0585762803 | -1.5203936733 |
| H       | 5.6950415935  | 2.6019804362 | 1.4212285034 |
| H       | 6.6310196524  | 1.0077116752 | 1.2641869591 |
| H       | 5.6411904836  | 2.8453464785 | -1.0085893393 |
| H       | 6.2425432676  | 0.7930830902 | -2.4038753433 |
Au_3Y-C_3H_6
E = -1378.38460273518

Y  -0.7014925511  -0.1513304324   0.0120312916
Au  -3.1893197257   0.6263656305  -1.2584888221
Au   1.7234312586  -1.6405272139  -0.0357284353
Au   1.6227297789   0.8533011258  1.4907266801
Au  -3.1762524724   0.5265168548  1.3724741601
Au  -0.3465105215  -3.1498525686  -0.0214033885
Au  -0.7505608760   1.2693505505  -2.4570914750
Au   1.7160516282  -1.552322803  2.5413123348
Au   3.7520655278   0.2192170490  -0.0108956811
Au   1.6020521295   0.9200645952  -1.4495359649
C  -2.1460489443  -4.3335226029   0.6031342154
C  -1.9784125109  -4.6104373660  -0.7271233733
C  -1.2894015318  -5.8248141319  -1.2631556053
H  -2.8600299879  -3.5793730749   0.9292838516
H  -1.7719420544  -5.0164600446  1.3656805885
H  -2.5375608883  -4.0142773473  -1.4509467799
H  -0.6198908562  -5.7533700556  -2.0931315648
H  -2.0463310236  -6.5108524216  -1.6632560838
H  -0.7245095199  -6.3527450498  -0.4897268586

Au_3Y-C_3H_6_2
E = -1378.38304275921

Au  -1.5437174099  -2.4046803524  -0.3026786156
Au  -3.1914656339  -0.1832578295  -0.3670682410
Au  -1.6761497916   2.0908976188   0.0976228391
Au   0.9591992152   2.7194663773  -0.4889679423
Au   2.7230641784   0.7367953415  -0.9099653475
Au   2.2551848039  -1.8828597548  -1.2450323970
Au   0.8782077289  -1.8304364236  1.1317899269
Au  -1.2890657248  -0.2229422849  1.5647514089
Au   1.2357854381   0.8282181828  1.5498864114
Y  -0.0269509628  -0.3784931589  -0.9889624525
C  -4.9771435441  -0.7407459867  -1.5290905978
C  -5.1016262330   0.6072999225  -1.2525858070
C  -5.9780040536   1.1633568276  -0.1711879716
H  -5.5133776616  -1.4771274633  -0.9317691700
H  -4.6048107758  -1.0781493407  -2.4939901637
H  -4.7689817538   1.3168334517  -2.0118373138
H  -6.9204299166   1.5004863927  -0.6209780852
H  -5.5225333732   2.0314131287   0.3139859817
H  -6.2155686291   0.4134995411   0.5888374149
|        |        |        |        |
|--------|--------|--------|--------|
| Au     | 0.0930685256 | 0.0534323621 | 0.9205970814 |
| Y      | 2.8299471436 | -1.0457270325 | 0.8906470333 |
| Au     | -1.4425416096 | -0.2252938489 | -1.5133927539 |
| Au     | -1.9453750584 | 1.9942122264 | 0.0606282641 |
| Au     | 2.6082051712 | 1.5697459410 | 0.7391337752 |
| Au     | 0.8354474082 | 1.3207509022 | -1.5721177945 |
| Au     | 0.9388752269 | -2.9595516671 | 0.8257631363 |
| Au     | 0.4300557625 | 3.1304441414 | 0.4816255165 |
| Au     | -3.4773379343 | -0.2780996632 | 0.2836436253 |
| Au     | -1.5927816659 | -2.2848506389 | 0.3269302706 |
| Au     | 1.0727682600 | -1.3408156048 | -1.4115147005 |
| C      | -5.3217244141 | -1.0184569987 | 1.2689211230 |
| C      | -5.4886635188 | 0.3414741569 | 1.1364712090 |
| C      | -6.3104701111 | 0.9907949636 | 0.0658999635 |
| H      | -5.7849270562 | -1.7039022500 | 0.5600412946 |
| H      | -4.9746360382 | -1.4467250615 | 2.2070408712 |
| H      | -5.2141098409 | 0.9737117349 | 1.9828022933 |
| H      | -5.8424232503 | 1.9081026739 | -0.3036688415 |
| H      | -7.2819355941 | 1.2740557212 | 0.4903190585 |
| H      | -6.4910140534 | 0.3170488048 | -0.7763635366 |

|        |        |        |        |
|--------|--------|--------|--------|
| Au     | 0.150572736 | -0.1957326401 | 0.4606350449 |
| Y      | 3.1016860177 | 0.0530042225 | 1.2643824433 |
| Au     | -2.0896039587 | 0.5727765131 | -1.4155108648 |
| Au     | -2.9032886497 | 0.9712943048 | 1.1375261965 |
| Au     | 1.7473023468 | 2.2645046964 | 0.5412102713 |
| Au     | 0.3458628549 | 1.7061823836 | -1.8315446769 |
| Au     | 2.0866367137 | -2.3135473933 | 0.3786735287 |
| Au     | -0.9119710356 | 2.6642406116 | 0.5013285721 |
| Au     | -2.5915144568 | -1.5998289564 | 0.2968014615 |
| Au     | -0.4266294633 | 3.0730171958 | 0.5643105490 |
| Au     | -0.0201835792 | 0.7991184636 | -2.7174178309 |
| Au     | 2.3284548047 | 0.0912828301 | -1.3282407420 |
| C      | 0.3430149722 | -2.7728035588 | -3.6295554309 |
| C      | -1.0257560250 | -2.6058519480 | -3.6258325783 |
| C      | -1.8331086676 | -2.2085002704 | -4.8221822911 |
| H      | 0.9184724918 | -2.5928848816 | -4.5371189288 |
| H      | 0.8330065094 | -3.3371429267 | -2.8388464444 |
| H      | -1.5824173280 | -3.0108231357 | -2.7783321693 |
| H      | -2.6446560251 | -1.5259825277 | -4.5528632283 |
| H      | -2.2967024208 | -3.1080793934 | -5.2466493730 |
| H      | -1.2174839296 | -1.7449988612 | -5.5982067377 |
\[
\text{Au}_{12}\text{Y-C}_3\text{H}_6
\]
\[E = -1785.90065080658\]
\[
\begin{array}{cccc}
\text{Y} & 0.0795881801 & 0.0872109237 & -0.4590646981 \\
\text{Au} & -2.2032387368 & -1.0855678304 & -1.8691352421 \\
\text{Au} & 2.1197203159 & 0.2394907919 & 1.5984433542 \\
\text{Au} & 2.4088572521 & 1.9036702372 & -0.6652939516 \\
\text{Au} & -2.2802922191 & 1.6137349032 & -1.4476145654 \\
\text{Au} & -0.5255553990 & -0.0246379133 & 2.4369100709 \\
\text{Au} & -0.1961278463 & -2.7928109826 & -1.4876098086 \\
\text{Au} & 0.4073810902 & 2.3308407543 & 1.5440922241 \\
\text{Au} & 3.4365675352 & -0.6546824013 & -0.5707663214 \\
\text{Au} & 1.5362803596 & -2.2829988794 & 0.6434319311 \\
\text{Au} & -1.2271879703 & -2.2253188278 & 0.9968778926 \\
\text{Au} & -2.7193740245 & -0.0369931024 & 0.7149046695 \\
\text{Au} & -0.0239135471 & 3.0121169392 & -1.1280591014 \\
\text{C} & 4.6347011590 & -2.0147060743 & -1.8447243098 \\
\text{C} & 4.9820945811 & -0.7357547621 & -2.2207216450 \\
\text{C} & 6.2269684850 & -0.0330311713 & -1.7752043953 \\
\text{H} & 3.9016713936 & -2.5808412248 & -2.4155213760 \\
\text{H} & 5.2682741801 & -2.5816691214 & -1.1635317676 \\
\text{H} & 4.4609544974 & -0.2953637045 & -3.0726208009 \\
\text{H} & 6.0420970265 & 1.0265482657 & -1.5745795593 \\
\text{H} & 6.6628953277 & -0.4952631980 & -0.8850505605 \\
\text{H} & 6.9674476400 & -0.0834227501 & -2.5834565870 \\
\end{array}
\]

\[
\text{Au}_{13}\text{Y-C}_3\text{H}_6
\]
\[E = -1921.72867424674\]
\[
\begin{array}{cccc}
\text{Y} & 0.1183617533 & 0.0401991952 & -0.5142495598 \\
\text{Au} & -1.6981793165 & -1.8787985875 & 0.8067356495 \\
\text{Au} & -3.4608537463 & 0.3041148577 & 0.2656011359 \\
\text{Au} & -1.3343091674 & 1.9657215541 & 1.1946436749 \\
\text{Au} & 0.9177758911 & -2.4642086891 & 1.0107026900 \\
\text{Au} & 2.6887241226 & -0.3798208570 & 1.2387912329 \\
\text{Au} & 1.3405187729 & 2.0006452909 & 1.4562643954 \\
\text{Au} & -2.000958496 & 1.7696487111 & -1.5386788339 \\
\text{Au} & 0.4782994315 & 2.8693700079 & -1.1603518010 \\
\text{Au} & 2.7025202068 & 1.2923205585 & -0.9871731302 \\
\text{Au} & 2.4331091383 & -1.5500465168 & -1.2721687531 \\
\text{Au} & -0.0416002225 & -2.6254887334 & -1.7085256423 \\
\text{Au} & -2.2685260262 & -1.0329802677 & -1.8172852795 \\
\text{C} & -5.0790991590 & 0.9384400862 & 1.6329997956 \\
\text{C} & -5.2450860678 & -0.4189621978 & 1.4583681539 \\
\text{C} & -6.2512943704 & -1.0368214474 & 0.5383540093 \\
\text{H} & -5.6880695338 & 1.6457825823 & 1.0713283274 \\
\end{array}
\]
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