

## **Supporting information**

This supporting information file contains two sections:

Section A reports the total energies obtained after optimization (0K, Fixed Nuclei). Gibbs free energies computed at 298.15K (1 atm.) from quadratic vibration frequencies complete these data. Reaction free energies are given in the two last columns for the cohesion and mixing processes as described in the text.

Section B reports for all the clusters described in the main text, the Cartesian coordinates obtained after full optimisation at B3LYP level with the LANL2DZ pseudopotential.

## A) Energies

| Clusters | E<br>(Hartree) | G<br>(Hartree) | $\Delta G_c$<br>(kcal/mol) | $\Delta G_{mix}$<br>(kcal/mol) |           |             |             |        |
|----------|----------------|----------------|----------------------------|--------------------------------|-----------|-------------|-------------|--------|
| Pd       | -126.70676     | -126.72336     | -                          | -                              | Au9_D     | -1219.45073 | -1219.51556 | -27.50 |
| Au       | -135.43979     | -135.45791     | -                          | -                              | Au9_E     | -1219.44963 | -1219.51324 | -27.34 |
| Pd2_A    | -253.4488      | -253.4746      | -8.75                      | -                              | Au10_A    | -1354.97778 | -1355.04453 | -29.21 |
| Pd3_A    | -380.21428     | -380.2464      | -15.96                     | -                              | Au10_B    | -1354.97769 | -1355.04367 | -29.15 |
| Pd4_A    | -507.01061     | -507.04531     | -23.83                     | -                              | Au10_C    | -1354.97661 | -1355.04161 | -29.02 |
| Pd5_A    | -633.77692     | -633.81582     | -24.98                     | -                              | Au10_D    | -1354.97324 | -1355.03904 | -28.86 |
| Pd5_B    | -633.77281     | -633.80889     | -24.11                     | -                              | Au11_A    | -1490.47757 | -1490.54817 | -29.16 |
| Pd6_A    | -760.55155     | -760.59181     | -26.32                     | -                              | Au11_B    | -1490.47083 | -1490.54279 | -28.85 |
| Pd7_A    | -887.31755     | -887.36296     | -26.84                     | -                              | Au11_C    | -1490.46864 | -1490.54073 | -28.74 |
| Pd7_B    | -887.31386     | -887.35869     | -26.46                     | -                              | Au11_D    | -1490.4683  | -1490.54001 | -28.69 |
| Pd7_C    | -887.31109     | -887.35572     | -26.19                     | -                              | Au12_A    | -1625.99229 | -1626.06821 | -29.98 |
| Pd8_A    | -1014.0855     | -1014.13461    | -27.28                     | -                              | Au12_B    | -1625.99138 | -1626.06511 | -29.82 |
| Pd8_B    | -1014.08501    | -1014.13341    | -27.18                     | -                              | Au12_C    | -1625.99038 | -1626.0665  | -29.89 |
| Pd8_C    | -1014.08377    | -1014.13182    | -27.06                     | -                              | Au12_D    | -1625.98343 | -1626.05924 | -29.51 |
| Pd8_D    | -1014.08116    | -1014.12991    | -26.91                     | -                              | Au13_A    | -1761.4875  | -1761.56838 | -29.71 |
| Pd9_A    | -1140.8665     | -1140.91693    | -28.36                     | -                              | Au13_B    | -1761.48542 | -1761.56585 | -29.59 |
| Pd9_B    | -1140.85878    | -1140.90955    | -27.84                     | -                              | Au13_C    | -1761.48378 | -1761.56472 | -29.54 |
| Pd9_C    | -1140.85863    | -1140.91066    | -27.92                     | -                              | Au13_D    | -1761.48286 | -1761.56322 | -29.46 |
| Pd9_D    | -1140.85722    | -1140.90827    | -27.75                     | -                              | Au14_A    | -1897.00305 | -1897.08626 | -30.28 |
| Pd10_A   | -1267.6393     | -1267.69385    | -28.88                     | -                              | Au14_B    | -1897.00108 | -1897.08401 | -30.18 |
| Pd10_B   | -1267.63674    | -1267.6909     | -28.70                     | -                              | Au14_C    | -1897.00033 | -1897.08389 | -30.17 |
| Pd10_C   | -1267.63509    | -1267.6884     | -28.54                     | -                              | Au14_D    | -1896.99799 | -1897.08303 | -30.13 |
| Pd10_D   | -1267.63428    | -1267.6883     | -28.53                     | -                              | Au14_E    | -1896.99766 | -1897.08209 | -30.09 |
| Pd11_A   | -1394.41583    | -1394.47157    | -29.36                     | -                              | Au1Pd1_A  | -262.20398  | -262.23097  | -15.59 |
| Pd11_B   | -1394.41246    | -1394.46865    | -29.19                     | -                              | Au1Pd2_A  | -388.97637  | -389.00881  | -21.79 |
| Pd11_C   | -1394.41143    | -1394.4682     | -29.16                     | -                              | Au1Pd3_A  | -515.75152  | -515.78771  | -25.06 |
| Pd11_D   | -1394.4114     | -1394.46597    | -29.04                     | -                              | Au1Pd4_A  | -642.51496  | -642.55391  | -25.42 |
| Pd11_E   | -1394.41012    | -1394.46707    | -29.10                     | -                              | Au1Pd4_B  | -642.51327  | -642.55215  | -25.20 |
| Pd12_A   | -1521.19575    | -1521.25578    | -30.09                     | -                              | Au1Pd4_C  | -642.51186  | -642.55163  | -25.14 |
| Pd12_B   | -1521.19145    | -1521.24971    | -29.78                     | -                              | Au1Pd5_A  | -769.28317  | -769.32604  | -26.29 |
| Pd12_C   | -1521.18912    | -1521.24775    | -29.67                     | -                              | Au1Pd5_B  | -769.27891  | -769.32238  | -25.90 |
| Pd12_D   | -1521.18891    | -1521.24767    | -29.67                     | -                              | Au1Pd5_C  | -769.27869  | -769.32151  | -25.81 |
| Pd13_A   | -1647.97846    | -1648.03864    | -30.65                     | -                              | Au1Pd5_D  | -769.27742  | -769.32127  | -25.79 |
| Pd13_B   | -1647.97164    | -1648.03328    | -30.39                     | -                              | Au1Pd6_A  | -896.06024  | -896.10633  | -27.63 |
| Pd14_A   | -1774.75258    | -1774.81504    | -30.84                     | -                              | Au1Pd6_B  | -896.05836  | -896.10541  | -27.55 |
| Pd14_B   | -1774.74851    | -1774.81218    | -30.71                     | -                              | Au1Pd6_C  | -896.0553   | -896.10232  | -27.27 |
| Au2_A    | -270.94842     | -270.97491     | -18.54                     | -                              | Au1Pd7_A  | -1022.83222 | -1022.88263 | -28.33 |
| Au3_A    | -406.42051     | -406.45642     | -17.30                     | -                              | Au1Pd7_B  | -1022.83136 | -1022.8809  | -28.20 |
| Au4_A    | -541.93317     | -541.97364     | -22.28                     | -                              | Au1Pd7_C  | -1022.831   | -1022.88045 | -28.16 |
| Au4_B    | -541.93047     | -541.9687      | -21.50                     | -                              | Au1Pd7_D  | -1022.8302  | -1022.87991 | -28.12 |
| Au5_A    | -677.43435     | -677.47889     | -23.76                     | -                              | Au1Pd7_E  | -1022.82956 | -1022.88014 | -28.14 |
| Au6_A    | -812.97032     | -813.01665     | -28.15                     | -                              | Au1Pd8_A  | -1149.60882 | -1149.66107 | -29.02 |
| Au7_A    | -948.44924     | -948.50408     | -26.78                     | -                              | Au1Pd8_B  | -1149.60647 | -1149.66037 | -28.98 |
| Au7_B    | -948.44038     | -948.49531     | -25.99                     | -                              | Au1Pd8_C  | -1149.60302 | -1149.6548  | -28.59 |
| Au8_A    | -1083.97819    | -1084.03547    | -29.19                     | -                              | Au1Pd8_D  | -1149.60142 | -1149.65308 | -28.47 |
| Au9_A    | -1219.45768    | -1219.52072    | -27.86                     | -                              | Au1Pd9_A  | -1276.38146 | -1276.43601 | -29.36 |
| Au9_B    | -1219.45449    | -1219.51784    | -27.66                     | -                              | Au1Pd9_B  | -1276.37922 | -1276.43411 | -29.24 |
| Au9_C    | -1219.45255    | -1219.51537    | -27.48                     | -                              | Au1Pd9_C  | -1276.37818 | -1276.43344 | -29.20 |
|          |                |                |                            |                                | Au1Pd9_D  | -1276.37496 | -1276.42973 | -28.97 |
|          |                |                |                            |                                | Au1Pd10_A | -1403.16189 | -1403.21893 | -30.09 |
|          |                |                |                            |                                | Au1Pd10_B | -1403.15906 | -1403.21776 | -30.02 |
|          |                |                |                            |                                | Au1Pd10_C | -1403.15837 | -1403.21547 | -29.89 |
|          |                |                |                            |                                | Au1Pd11_A | -1529.93959 | -1529.99948 | -30.57 |
|          |                |                |                            |                                | Au1Pd11_B | -1529.93591 | -1529.99505 | -30.34 |

|           |             |             |        |       |         |             |             |        |       |
|-----------|-------------|-------------|--------|-------|---------|-------------|-------------|--------|-------|
| Au1Pd12_A | -1656.71778 | -1656.77987 | -30.97 | -0.40 | Pd4Au3  | -913.5379   | -913.58714  | -28.68 | -1.87 |
| Au1Pd12_B | -1656.71566 | -1656.77651 | -30.81 | -0.23 | Pd4Au4  | -1049.05129 | -1049.10356 | -29.69 | -1.45 |
| Au1Pd13_A | -1783.49602 | -1783.56146 | -31.37 | -0.57 | Pd4Au5  | -1184.56353 | -1184.62009 | -30.48 | -2.40 |
| Au1Pd13_B | -1783.49495 | -1783.55735 | -31.19 | -0.39 | Pd4Au6  | -1320.09081 | -1320.1496  | -31.92 | -2.85 |
| Pd1Au1_A  | -262.20398  | -262.23097  | -15.59 | -1.95 | Pd4Au7  | -1455.58759 | -1455.65081 | -31.49 | -2.26 |
| Pd1Au2_A  | -397.71089  | -397.74374  | -21.87 | -5.02 | Pd4Au8  | -1591.10166 | -1591.16728 | -31.93 | -1.91 |
| Pd1Au3_A  | -533.20701  | -533.2461   | -23.38 | -0.71 | Pd4Au9  | -1726.61163 | -1726.68189 | -32.21 | -2.21 |
| Pd1Au3_B  | -533.20209  | -533.24222  | -22.77 | -0.10 | Pd4Au10 | -1862.12597 | -1862.19743 | -32.49 | -2.05 |
| Pd1Au4_A  | -668.71415  | -668.75757  | -25.42 | -1.42 | Pd5Au2  | -904.8007   | -904.84838  | -28.31 | -1.48 |
| Pd1Au5_A  | -804.23268  | -804.28041  | -27.98 | -0.13 | Pd5Au3  | -1040.31757 | -1040.36988 | -29.76 | -1.76 |
| Pd1Au6_A  | -939.74061  | -939.79157  | -28.75 | -1.97 | Pd5Au4  | -1175.82829 | -1175.88239 | -30.26 | -2.12 |
| Pd1Au6_B  | -939.73598  | -939.78814  | -28.45 | -1.66 | Pd5Au5  | -1311.35541 | -1311.41405 | -31.86 | -2.82 |
| Pd1Au6_C  | -939.73492  | -939.78635  | -28.29 | -1.50 | Pd5Au6  | -1446.86058 | -1446.92229 | -31.83 | -2.58 |
| Pd1Au7_A  | -1075.2349  | -1075.29138 | -28.45 | 0.51  | Pd5Au7  | -1582.37468 | -1582.43963 | -32.29 | -2.26 |
| Pd1Au7_B  | -1075.23469 | -1075.29315 | -28.59 | 0.37  | Pd5Au8  | -1717.88433 | -1717.95433 | -32.55 | -2.47 |
| Pd1Au7_C  | -1075.23449 | -1075.293   | -28.57 | 0.38  | Pd5Au9  | -1853.3986  | -1853.47152 | -32.88 | -2.40 |
| Pd1Au8_A  | -1210.75845 | -1210.81785 | -30.07 | -2.15 | Pd6Au2  | -1031.57307 | -1031.62295 | -28.79 | -1.03 |
| Pd1Au8_B  | -1210.74705 | -1210.80623 | -29.26 | -1.34 | Pd6Au3  | -1167.09374 | -1167.14775 | -30.25 | -2.06 |
| Pd1Au9_A  | -1346.24655 | -1346.31367 | -29.44 | -0.26 | Pd6Au4  | -1302.61922 | -1302.6769  | -31.70 | -2.68 |
| Pd1Au9_B  | -1346.24469 | -1346.31058 | -29.24 | -0.07 | Pd6Au5  | -1438.12996 | -1438.19231 | -32.09 | -2.83 |
| Pd1Au9_C  | -1346.24383 | -1346.30893 | -29.14 | 0.03  | Pd6Au6  | -1573.64167 | -1573.70599 | -32.34 | -2.30 |
| Pd1Au9_D  | -1346.24058 | -1346.30752 | -29.05 | 0.12  | Pd6Au7  | -1709.15356 | -1709.22181 | -32.64 | -2.50 |
| Pd1Au10_A | -1481.76649 | -1481.83579 | -30.43 | -1.25 | Pd6Au8  | -1844.66943 | -1844.74226 | -33.12 | -2.60 |
| Pd1Au10_B | -1481.764   | -1481.83272 | -30.25 | -1.07 | Pd7Au2  | -1158.348   | -1158.40057 | -29.37 | -1.13 |
| Pd1Au10_C | -1481.76366 | -1481.83165 | -30.19 | -1.01 | Pd7Au3  | -1293.87846 | -1293.9335  | -31.14 | -2.16 |
| Pd1Au11_A | -1617.26683 | -1617.34191 | -30.41 | -0.42 | Pd7Au4  | -1429.39388 | -1429.4557  | -31.98 | -2.69 |
| Pd1Au11_B | -1617.26009 | -1617.33239 | -29.91 | 0.08  | Pd7Au5  | -1564.90856 | -1564.97181 | -32.36 | -2.31 |
| Pd1Au11_C | -1617.25416 | -1617.32574 | -29.57 | 0.42  | Pd7Au6  | -1700.41791 | -1700.4851  | -32.54 | -2.32 |
| Pd1Au12_A | -1752.78386 | -1752.85907 | -30.93 | -1.15 | Pd7Au7  | -1835.93916 | -1836.01045 | -33.24 | -2.68 |
| Pd1Au12_B | -1752.7818  | -1752.85997 | -30.97 | -1.19 | Pd8Au2  | -1285.12726 | -1285.18111 | -30.02 | -1.08 |
| Pd1Au13_A | -1888.28877 | -1888.36892 | -31.05 | -0.73 | Pd8Au3  | -1420.64839 | -1420.70876 | -31.27 | -1.97 |
| Pd1Au13_B | -1888.27461 | -1888.35517 | -30.43 | -0.12 | Pd8Au4  | -1556.17369 | -1556.23656 | -32.32 | -2.26 |
| Pd2Au2    | -524.4773   | -524.51358  | -23.70 | -0.64 | Pd8Au5  | -1691.68297 | -1691.74895 | -32.46 | -2.17 |
| Pd2Au3    | -659.98105  | -660.02353  | -25.49 | -1.24 | Pd8Au6  | -1827.20527 | -1827.27562 | -33.23 | -2.63 |
| Pd2Au4    | -795.49106  | -795.53817  | -27.17 | 0.37  | Pd9Au2  | -1411.90323 | -1411.96168 | -30.56 | -1.23 |
| Pd2Au5    | -931.0116   | -931.06238  | -29.23 | -2.44 | Pd9Au3  | -1547.42508 | -1547.48592 | -31.48 | -1.41 |
| Pd2Au6    | -1066.51543 | -1066.57056 | -29.52 | -0.81 | Pd9Au4  | -1682.94972 | -1683.0141  | -32.45 | -2.09 |
| Pd2Au7    | -1202.0278  | -1202.08688 | -30.32 | -2.35 | Pd9Au5  | -1818.47334 | -1818.5426  | -33.29 | -2.66 |
| Pd2Au8    | -1337.54481 | -1337.60505 | -31.07 | -1.92 | Pd10Au2 | -1538.68149 | -1538.74244 | -31.01 | -0.94 |
| Pd2Au9    | -1473.03724 | -1473.10521 | -30.65 | -1.46 | Pd10Au3 | -1674.20861 | -1674.27178 | -32.07 | -1.64 |
| Pd2Au10   | -1608.55572 | -1608.6265  | -31.41 | -1.41 | Pd10Au4 | -1809.73097 | -1809.79891 | -32.89 | -2.21 |
| Pd2Au11   | -1744.05909 | -1744.13372 | -31.38 | -1.52 | Pd11Au2 | -1665.46411 | -1665.52636 | -31.55 | -1.04 |
| Pd2Au12   | -1879.56753 | -1879.64568 | -31.56 | -1.20 | Pd11Au3 | -1800.9882  | -1801.05356 | -32.40 | -1.68 |
| Pd3Au2    | -651.25235  | -651.29426  | -26.15 | -1.66 | Pd12Au2 | -1792.24672 | -1792.31007 | -32.00 | -1.24 |
| Pd3Au3    | -786.75879  | -786.80468  | -27.28 | -0.05 |         |             |             |        |       |
| Pd3Au4    | -922.27533  | -922.3253   | -29.01 | -2.20 |         |             |             |        |       |
| Pd3Au5    | -1057.78509 | -1057.83828 | -29.70 | -1.23 |         |             |             |        |       |
| Pd3Au6    | -1193.29395 | -1193.35102 | -30.22 | -2.20 |         |             |             |        |       |
| Pd3Au7    | -1328.8162  | -1328.87623 | -31.42 | -2.32 |         |             |             |        |       |
| Pd3Au8    | -1464.31432 | -1464.37796 | -31.07 | -1.85 |         |             |             |        |       |
| Pd3Au9    | -1599.82772 | -1599.89759 | -31.71 | -1.70 |         |             |             |        |       |
| Pd3Au10   | -1735.34068 | -1735.41109 | -31.95 | -2.02 |         |             |             |        |       |
| Pd3Au11   | -1870.83815 | -1870.9148  | -31.72 | -1.32 |         |             |             |        |       |
| Pd4Au2    | -778.02502  | -778.07011  | -27.28 | -0.35 |         |             |             |        |       |

## B) cartesian coordinates

### Pd<sub>n</sub> clusters

#### Pd2\_A

| Atom | X       | Y       | Z        | Charges |
|------|---------|---------|----------|---------|
| Pd   | 0.00000 | 0.00000 | 1.26325  | 0.00000 |
| Pd   | 0.00000 | 0.00000 | -1.26325 | 0.00000 |

#### Pd3\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Pd   | 0.00000 | 1.37841  | -0.71467 | 0.03224  |
| Pd   | 0.00000 | 0.00000  | 1.42934  | -0.06449 |
| Pd   | 0.00000 | -1.37841 | -0.71467 | 0.03224  |

#### Pd4\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 1.56648  | -0.52024 | 0.00749  |
| Pd   | 1.35661  | -0.78324 | -0.52024 | 0.00749  |
| Pd   | -1.35661 | -0.78324 | -0.52024 | 0.00749  |
| Pd   | 0.00000  | 0.00000  | 1.56072  | -0.02248 |

#### Pd5\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 1.75657  | 0.00000  | 0.02952  |
| Pd   | 1.52124  | -0.87829 | 0.00000  | 0.02952  |
| Pd   | -1.52124 | -0.87829 | 0.00000  | 0.02952  |
| Pd   | 0.00000  | 0.00000  | 1.93427  | -0.04429 |
| Pd   | 0.00000  | 0.00000  | -1.93427 | -0.04429 |

#### Pd5\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | 1.58848  | -0.03431 |
| Pd   | 0.00000  | 1.85020  | -0.39712 | 0.00858  |
| Pd   | 1.85020  | 0.00000  | -0.39712 | 0.00858  |
| Pd   | 0.00000  | -1.85020 | -0.39712 | 0.00858  |
| Pd   | -1.85020 | 0.00000  | -0.39712 | 0.00858  |

#### Pd6\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 1.86829  | 0.00000  | 0.00400  |
| Pd   | 1.86829  | 0.00000  | 0.00000  | 0.00400  |
| Pd   | -1.86829 | 0.00000  | 0.00000  | 0.00400  |
| Pd   | 0.00000  | 0.00000  | 2.02283  | -0.00799 |
| Pd   | 0.00000  | 0.00000  | -2.02283 | -0.00799 |
| Pd   | 0.00000  | -1.86829 | 0.00000  | 0.00400  |

#### Pd7\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | 2.35843  | -0.00189 |
| Pd   | 0.00000  | 2.17285  | 0.68768  | 0.06661  |
| Pd   | 0.00000  | -2.17285 | 0.68768  | 0.06661  |
| Pd   | -0.02579 | 1.38406  | -1.87060 | 0.03677  |
| Pd   | 0.02579  | -1.38406 | -1.87060 | 0.03677  |
| Pd   | 1.50741  | -0.12247 | 0.00371  | -0.10244 |
| Pd   | -1.50741 | 0.12247  | 0.00371  | -0.10244 |

#### Pd7\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.80989 | 2.11363  | 0.00000  | 0.06718  |
| Pd   | 0.30209  | 1.08446  | 1.31472  | -0.03833 |
| Pd   | 2.29483  | -0.28112 | 0.00000  | -0.02307 |
| Pd   | 0.30209  | -1.69501 | -1.34740 | 0.02910  |
| Pd   | -1.69331 | -0.61142 | 0.00000  | -0.02565 |
| Pd   | 0.30209  | -1.69501 | 1.34740  | 0.02910  |
| Pd   | 0.30209  | 1.08446  | -1.31472 | -0.03833 |

#### Pd7\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.00162  | -0.84131 | 1.30401  | -0.02848 |
| Pd   | -0.06834 | -0.10578 | -1.34563 | -0.07881 |
| Pd   | -0.94396 | 1.13596  | 1.16509  | -0.04207 |
| Pd   | -1.49036 | -1.57913 | 0.42548  | 0.03264  |
| Pd   | 1.55888  | 1.58467  | 0.10680  | 0.04187  |
| Pd   | 2.53115  | -0.66783 | -0.80416 | 0.06308  |
| Pd   | -2.58899 | 0.47341  | -0.85160 | 0.01178  |

#### Pd8\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Pd   | 2.68422 | -1.11380 | -0.02742 | -0.01503 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 2.22208  | 1.43050  | -0.08388 | -0.00716 |
| Pd | 0.64883  | -0.31286 | 1.44733  | -0.00515 |
| Pd | 0.49256  | -0.41339 | -1.40014 | -0.01192 |
| Pd | -1.16724 | -1.86576 | 0.10823  | 0.03962  |
| Pd | -0.53750 | 1.81984  | -0.04219 | 0.05943  |
| Pd | -2.13144 | 0.31601  | 1.37337  | -0.02119 |
| Pd | -2.21151 | 0.13947  | -1.37530 | -0.03861 |

Pd8\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.23963 | 3.27518  | 0.26453  | 0.01362  |
| Pd   | 0.23963  | -3.27518 | 0.26453  | 0.01362  |
| Pd   | -1.60114 | 1.59233  | -1.19101 | -0.00732 |
| Pd   | 1.60114  | -1.59233 | -1.19101 | -0.00732 |
| Pd   | -0.98747 | 1.07099  | 1.44357  | 0.01449  |
| Pd   | 0.98747  | -1.07099 | 1.44357  | 0.01449  |
| Pd   | -0.98747 | -1.03196 | -0.51709 | -0.02080 |
| Pd   | 0.98747  | 1.03196  | -0.51709 | -0.02080 |

Pd8\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.31414  | 2.58804  | 0.00000  | -0.04366 |
| Pd   | 0.26138  | 1.04260  | 2.23534  | 0.05644  |
| Pd   | 0.26138  | -1.64064 | 1.38452  | 0.02316  |
| Pd   | 0.26138  | -1.64064 | -1.38452 | 0.02316  |
| Pd   | 0.26138  | 1.04260  | -2.23534 | 0.05644  |
| Pd   | -1.22944 | 0.39660  | 0.00000  | -0.04071 |
| Pd   | 1.73559  | 0.40670  | 0.00000  | -0.04699 |
| Pd   | -1.86578 | -2.19525 | 0.00000  | -0.02785 |

Pd8\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.01736 | -0.60232 | -0.93325 | -0.07636 |
| Pd   | -2.28586 | 0.89943  | -0.91521 | -0.02770 |
| Pd   | 0.09503  | 2.00889  | 0.06377  | 0.01432  |
| Pd   | 2.40623  | 0.83632  | -0.87670 | -0.00524 |
| Pd   | -1.43858 | 0.15055  | 1.49624  | -0.02774 |
| Pd   | 1.36520  | -0.00860 | 1.56353  | 0.01734  |
| Pd   | 2.31708  | -1.67034 | -0.20164 | 0.03712  |
| Pd   | -2.44175 | -1.61395 | -0.19674 | 0.06825  |

Pd9\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.32055 | 1.60322  | -0.24727 | -0.00356 |
| Pd   | 2.29521  | 1.56948  | -0.16552 | -0.01766 |
| Pd   | -2.20387 | -0.97878 | -1.22533 | -0.05312 |
| Pd   | 2.42350  | -0.95368 | -1.11715 | -0.00934 |
| Pd   | -2.34001 | -0.65707 | 1.35022  | -0.00541 |
| Pd   | 2.22961  | -0.49841 | 1.44569  | -0.05498 |
| Pd   | 0.05173  | 0.57575  | -1.40833 | 0.04291  |
| Pd   | -0.15565 | 0.97123  | 1.16857  | 0.04212  |
| Pd   | 0.02003  | -1.63173 | 0.19911  | 0.05902  |

Pd9\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.34454  | 2.15447  | -0.49881 | 0.01205  |
| Pd   | -1.41996 | 0.26138  | -1.46276 | -0.02291 |
| Pd   | 1.41982  | -0.26151 | -1.46283 | -0.02285 |
| Pd   | 0.00011  | 0.00002  | 1.19449  | -0.08122 |
| Pd   | -0.34450 | -2.15450 | -0.49865 | 0.01204  |
| Pd   | 2.62366  | 1.08996  | 0.65365  | 0.03902  |
| Pd   | -2.16613 | 1.49141  | 0.71062  | 0.01243  |
| Pd   | 2.16610  | -1.49139 | 0.71060  | 0.01243  |
| Pd   | -2.62366 | -1.08983 | 0.65369  | 0.03900  |

Pd9\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.98655 | 0.38731  | -0.68996 | -0.03981 |
| Pd   | -2.03691 | -0.69802 | 1.61172  | -0.03358 |
| Pd   | -1.00679 | 1.70690  | 0.72927  | 0.04523  |
| Pd   | -1.09668 | -1.80862 | -0.53134 | 0.08099  |
| Pd   | -0.48601 | 0.60701  | -1.56944 | 0.00390  |
| Pd   | 0.70944  | -0.45984 | 1.21186  | -0.05448 |
| Pd   | 1.80341  | 1.59996  | -0.24765 | -0.00704 |
| Pd   | 1.76655  | -1.05619 | -1.22074 | -0.01020 |
| Pd   | 3.33353  | -0.27850 | 0.70629  | 0.01499  |

Pd9\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.92316 | 0.90042  | 1.24777  | -0.06328 |
| Pd   | -0.19337 | 2.35598  | -0.11558 | 0.13853  |
| Pd   | 1.96653  | 0.89826  | -1.19453 | -0.03130 |
| Pd   | 1.43057  | -1.73264 | -0.53082 | 0.04430  |
| Pd   | -1.29250 | -1.77865 | 0.59107  | 0.02362  |
| Pd   | 0.69086  | 0.16802  | 1.28677  | -0.05379 |
| Pd   | -0.70419 | -0.04767 | -1.34634 | -0.10258 |

|    |          |          |          |         |
|----|----------|----------|----------|---------|
| Pd | 3.25674  | -0.31088 | 0.71081  | 0.01616 |
| Pd | -3.23149 | -0.45283 | -0.64916 | 0.02833 |

Pd10\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.90698 | 0.25735  | -1.24150 | -0.00790 |
| Pd   | -1.27715 | 1.93050  | 0.20541  | 0.04344  |
| Pd   | 1.60402  | 1.84143  | 0.22340  | 0.01692  |
| Pd   | 1.27715  | -1.93050 | -0.20541 | 0.04344  |
| Pd   | -1.60402 | -1.84143 | -0.22340 | 0.01692  |
| Pd   | 0.10312  | -0.24366 | 1.40249  | -0.02584 |
| Pd   | -0.10312 | 0.24366  | -1.40249 | -0.02584 |
| Pd   | 2.90698  | -0.25735 | 1.24150  | -0.00790 |
| Pd   | -2.71672 | -0.10577 | 1.41917  | -0.02663 |
| Pd   | 2.71672  | 0.10577  | -1.41917 | -0.02663 |

Pd10\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.79193 | -2.07694 | -0.00843 | 0.03686  |
| Pd   | 2.13315  | -1.39628 | -1.24484 | 0.02098  |
| Pd   | 2.96391  | -0.06448 | 1.03043  | -0.05427 |
| Pd   | 0.63490  | 1.44744  | 1.07812  | 0.06896  |
| Pd   | -1.87972 | 0.05387  | 1.53358  | -0.05843 |
| Pd   | -0.20691 | -0.06782 | -1.15822 | -0.09307 |
| Pd   | 0.63322  | -1.31638 | 1.12158  | 0.05785  |
| Pd   | 2.16011  | 1.29082  | -1.15936 | -0.00208 |
| Pd   | -1.58263 | 2.15138  | -0.21339 | 0.01109  |
| Pd   | -3.06411 | -0.02160 | -0.97947 | 0.01212  |

Pd10\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 2.30345  | 0.00912  | -1.43271 | -0.05373 |
| Pd   | 1.19152  | 2.32601  | -0.64714 | 0.09280  |
| Pd   | -1.23715 | 1.94179  | 0.91002  | -0.00216 |
| Pd   | -1.53788 | -0.75942 | 1.47732  | 0.00344  |
| Pd   | 0.72443  | -1.83781 | 0.02041  | 0.06329  |
| Pd   | -0.49314 | 0.34236  | -1.19962 | -0.07769 |
| Pd   | 1.04618  | 0.53643  | 1.33395  | -0.04209 |
| Pd   | -3.17083 | 0.37766  | -0.43280 | -0.00047 |
| Pd   | -1.96599 | -1.91878 | -0.82014 | -0.00209 |
| Pd   | 3.13941  | -1.01736 | 0.79072  | 0.01869  |

Pd10\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.89109  | -1.30388 | -1.05003 | -0.01318 |
| Pd   | 2.05886  | 1.40888  | -0.88260 | 0.00684  |
| Pd   | -0.33248 | 2.13465  | 0.54719  | 0.09158  |
| Pd   | -1.67098 | -0.16696 | 1.55010  | -0.09102 |
| Pd   | -0.51754 | -2.19651 | 0.25071  | 0.09632  |
| Pd   | -0.53503 | 0.18543  | -1.22468 | -0.11500 |
| Pd   | 1.11669  | -0.14577 | 1.28869  | -0.05442 |
| Pd   | -2.75150 | 1.49097  | -0.45177 | 0.01942  |
| Pd   | -2.91762 | -1.27282 | -0.52742 | 0.01698  |
| Pd   | 3.65852  | -0.13399 | 0.49981  | 0.04248  |

Pd11\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | 2.35758  | -0.00321 |
| Pd   | -2.40515 | 0.82622  | 0.96238  | -0.00859 |
| Pd   | -2.45969 | -0.83693 | -1.07103 | -0.00779 |
| Pd   | 1.03711  | -0.77778 | -2.57260 | -0.01128 |
| Pd   | 2.40515  | -0.82622 | 0.96238  | -0.00859 |
| Pd   | 0.00000  | 1.28695  | -0.17241 | 0.06563  |
| Pd   | 0.00000  | -1.28695 | -0.17241 | 0.06563  |
| Pd   | -1.03711 | 0.77778  | -2.57260 | -0.01128 |
| Pd   | 1.96790  | 1.67638  | 1.67488  | -0.03637 |
| Pd   | -1.96790 | -1.67638 | 1.67488  | -0.03637 |
| Pd   | 2.45969  | 0.83693  | -1.07103 | -0.00779 |

Pd11\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.18075  | 1.89768  | 0.62819  | 0.02500  |
| Pd   | 1.76582  | -2.01671 | -0.52798 | -0.00221 |
| Pd   | -1.12684 | -2.32521 | -0.78623 | 0.02345  |
| Pd   | -2.59926 | 0.12989  | -1.01661 | -0.02446 |
| Pd   | -0.89776 | 2.60017  | -0.93197 | 0.00277  |
| Pd   | 0.18246  | -0.69963 | 1.22140  | 0.00221  |
| Pd   | 0.07206  | 0.15799  | -1.26212 | -0.00839 |
| Pd   | -2.46974 | -1.34824 | 1.20041  | -0.00629 |
| Pd   | -1.69304 | 1.40754  | 1.22593  | -0.00744 |
| Pd   | 2.80780  | -0.13837 | 1.40780  | -0.00324 |
| Pd   | 2.77775  | 0.33490  | -1.15884 | -0.00140 |

Pd11\_C

| Atom | X        | Y        | Z       | Charges |
|------|----------|----------|---------|---------|
| Pd   | -1.93773 | -0.67104 | 1.44918 | 0.02719 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -1.28399 | 2.09162  | 0.99299  | -0.05598 |
| Pd | 0.68183  | 2.52909  | -0.66906 | 0.02301  |
| Pd | 2.01069  | -0.84160 | -1.52040 | 0.01982  |
| Pd | 0.13874  | -2.20911 | 0.19604  | -0.00590 |
| Pd | 0.74301  | 0.29497  | 1.34300  | 0.00107  |
| Pd | -0.43894 | 0.17011  | -1.13695 | -0.06426 |
| Pd | 2.89646  | 1.21429  | -0.10095 | 0.00716  |
| Pd | 2.61280  | -1.52911 | 0.92811  | 0.01006  |
| Pd | -2.37892 | -1.80522 | -0.85916 | -0.00874 |
| Pd | -3.04393 | 0.75601  | -0.62280 | 0.04657  |

Pd11\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | 2.90762  | -0.05997 |
| Pd   | -1.44065 | -1.69465 | 1.46243  | 0.05647  |
| Pd   | -1.06818 | -1.01622 | -1.33208 | -0.03335 |
| Pd   | 1.06818  | 1.01622  | -1.33208 | -0.03335 |
| Pd   | 1.44065  | 1.69465  | 1.46243  | 0.05647  |
| Pd   | -1.13695 | 0.98274  | 0.64387  | -0.02718 |
| Pd   | 1.13695  | -0.98274 | 0.64387  | -0.02718 |
| Pd   | -1.37979 | 1.74146  | -1.91460 | 0.02729  |
| Pd   | 0.00000  | 3.32389  | -0.31344 | 0.00675  |
| Pd   | 1.37979  | -1.74146 | -1.91460 | 0.02729  |
| Pd   | 0.00000  | -3.32389 | -0.31344 | 0.00675  |

Pd11\_E

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.32829 | 0.47702  | -0.66859 | -0.04536 |
| Pd   | -1.28584 | 1.90266  | 1.35719  | 0.02713  |
| Pd   | 1.25361  | 1.63137  | 0.60521  | -0.00791 |
| Pd   | 1.63793  | -1.98856 | -0.46872 | -0.03327 |
| Pd   | -1.19550 | -2.12801 | -1.12871 | 0.00035  |
| Pd   | -0.39280 | -0.71022 | 1.16387  | -0.04707 |
| Pd   | 0.36979  | 0.21806  | -1.43246 | 0.05184  |
| Pd   | 2.35228  | -0.60896 | 1.65070  | 0.00862  |
| Pd   | -2.84595 | -1.64282 | 0.81971  | 0.05719  |
| Pd   | 3.14279  | 0.16621  | -0.79438 | 0.01985  |
| Pd   | -0.70801 | 2.68324  | -1.10382 | -0.03137 |

Pd12\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.50868 | 1.90466  | 0.93351  | -0.03071 |
| Pd   | -2.74928 | 0.73522  | -1.07285 | 0.00749  |
| Pd   | -1.49445 | -1.91677 | -0.93329 | -0.03064 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 2.52999  | -1.00625 | 0.85420  | -0.00176 |
| Pd | 1.45407  | 1.85990  | 1.38311  | -0.01743 |
| Pd | -0.06368 | 0.47020  | -1.19927 | 0.03745  |
| Pd | -0.05706 | -0.47050 | 1.19826  | 0.03691  |
| Pd | 1.46844  | -1.84783 | -1.38325 | -0.01769 |
| Pd | 0.30895  | 3.04080  | -0.69595 | 0.00540  |
| Pd | 0.33248  | -3.03850 | 0.69510  | 0.00553  |
| Pd | -2.74033 | -0.75687 | 1.07539  | 0.00737  |
| Pd | 2.51957  | 1.02594  | -0.85497 | -0.00194 |

Pd12\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.33150 | -2.94465 | 0.05888  | 0.05757  |
| Pd   | -2.33236 | -0.98589 | -1.41048 | 0.02160  |
| Pd   | -2.95963 | 1.32038  | 0.07808  | 0.02249  |
| Pd   | -0.87774 | 2.22141  | 1.47161  | 0.01179  |
| Pd   | 1.23802  | 2.95288  | -0.11602 | 0.03300  |
| Pd   | 2.10780  | 0.86160  | -1.55947 | -0.00458 |
| Pd   | 3.05168  | -1.19551 | -0.08704 | 0.04305  |
| Pd   | 1.06304  | -2.09312 | 1.52840  | -0.00323 |
| Pd   | 0.46728  | -1.37918 | -1.08983 | -0.06255 |
| Pd   | -0.58501 | 1.20228  | -1.14323 | -0.02735 |
| Pd   | -1.20937 | -0.51696 | 1.11759  | -0.05284 |
| Pd   | 1.36781  | 0.55676  | 1.15150  | -0.03897 |

Pd12\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.88705 | -1.14430 | 1.01933  | -0.00191 |
| Pd   | -1.72721 | -1.90048 | -1.22771 | 0.03072  |
| Pd   | 1.21006  | -2.08725 | -1.28809 | 0.01905  |
| Pd   | 1.50324  | 0.80163  | 1.52316  | -0.01814 |
| Pd   | -1.28141 | 1.18746  | 1.49253  | 0.05415  |
| Pd   | 0.04425  | 0.34694  | -0.95335 | -0.11315 |
| Pd   | -0.22736 | -1.44506 | 1.12379  | 0.00879  |
| Pd   | 2.80852  | 0.00747  | -0.89290 | 0.00750  |
| Pd   | -2.71007 | 0.62496  | -0.91524 | -0.01340 |
| Pd   | 2.44772  | -1.79254 | 1.02877  | 0.00355  |
| Pd   | 1.71873  | 2.60889  | -0.38500 | 0.01860  |
| Pd   | -0.89943 | 2.79228  | -0.52532 | 0.00424  |

Pd12\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.27656 | -2.50910 | 0.18064  | -0.03617 |
| Pd   | 1.25340  | -1.97051 | -1.37325 | 0.06547  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 1.73953  | 0.85323  | -1.16148 | -0.04204 |
| Pd | 0.07740  | 1.69717  | 1.06433  | 0.01081  |
| Pd | -1.69363 | -0.43999 | 1.76539  | 0.03118  |
| Pd | -0.82923 | -0.17328 | -1.04054 | -0.11903 |
| Pd | 1.00358  | -0.98228 | 1.08836  | -0.07267 |
| Pd | -0.48891 | 2.46545  | -1.51440 | 0.02446  |
| Pd | -2.47948 | 1.74199  | 0.07852  | -0.02823 |
| Pd | -3.37506 | -0.95954 | -0.33441 | 0.08864  |
| Pd | 2.67909  | 1.27217  | 1.37352  | 0.05600  |
| Pd | 3.38988  | -0.99531 | -0.12669 | 0.02158  |

#### Pd13\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 2.88873  | -1.27029 | 1.08782  | -0.02289 |
| Pd   | 2.87208  | 0.32396  | -1.01263 | 0.02704  |
| Pd   | 1.10665  | 2.61244  | -0.92640 | 0.01637  |
| Pd   | -1.55113 | 0.53298  | 1.25655  | -0.02359 |
| Pd   | 0.20618  | -1.73269 | 1.22959  | 0.04730  |
| Pd   | 0.02962  | 0.07491  | -0.99659 | -0.12750 |
| Pd   | 1.30757  | 0.90837  | 1.30810  | 0.02973  |
| Pd   | -1.66854 | 2.29150  | -0.97457 | 0.02247  |
| Pd   | 1.72514  | -2.14054 | -1.12205 | 0.00651  |
| Pd   | -0.39779 | 3.01201  | 1.20489  | -0.01980 |
| Pd   | -2.83916 | -0.28230 | -1.06947 | 0.05799  |
| Pd   | -1.23516 | -2.34020 | -1.16268 | -0.01023 |
| Pd   | -2.44418 | -1.99016 | 1.17743  | -0.00339 |

#### Pd13\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.01816 | 1.17992  | -1.54654 | 0.01605  |
| Pd   | -1.68855 | -1.67819 | -1.40485 | -0.02562 |
| Pd   | -1.58641 | -2.67580 | 1.01299  | 0.01407  |
| Pd   | 2.19604  | -0.78134 | 1.45034  | -0.00524 |
| Pd   | 0.99780  | 2.02303  | 1.53915  | 0.00186  |
| Pd   | 0.47563  | 0.03458  | -1.08923 | 0.01462  |
| Pd   | -0.53926 | -0.22220 | 1.25628  | 0.03903  |
| Pd   | 0.85323  | -2.47163 | -0.10849 | -0.05280 |
| Pd   | 0.35824  | 2.72244  | -0.97977 | -0.01705 |
| Pd   | -3.09165 | -0.26770 | 0.48859  | 0.01147  |
| Pd   | 2.73614  | 1.21899  | -0.24015 | -0.00545 |
| Pd   | -1.73077 | 2.29717  | 0.76568  | -0.01327 |
| Pd   | 3.03770  | -1.37928 | -1.14399 | 0.02233  |

#### Pd14\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.76615 | -1.83776 | -0.14842 | 0.03066  |
| Pd   | -2.07384 | 0.15052  | -1.78221 | -0.01036 |
| Pd   | -1.33270 | 2.56663  | -0.07436 | 0.00970  |
| Pd   | 0.71044  | 1.98867  | 1.73034  | 0.02822  |
| Pd   | 3.02262  | 1.18511  | 0.16037  | 0.03190  |
| Pd   | 2.61720  | -0.89111 | -1.41891 | 0.06593  |
| Pd   | 1.86685  | -3.11351 | -0.04373 | 0.03555  |
| Pd   | -0.46911 | -2.65155 | 1.47968  | 0.06200  |
| Pd   | -0.15284 | -1.79503 | -1.12435 | -0.07807 |
| Pd   | 0.52459  | 0.84943  | -0.98871 | -0.11701 |
| Pd   | -1.18123 | -0.00991 | 1.09244  | -0.11693 |
| Pd   | 1.43225  | -0.77271 | 1.24533  | -0.06111 |
| Pd   | 1.29659  | 3.35325  | -0.42206 | 0.06080  |
| Pd   | -3.49467 | 0.97798  | 0.29459  | 0.05872  |

#### Pd14\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.45310 | 1.61644  | 0.53969  | 0.07206  |
| Pd   | -2.42595 | -1.21679 | 1.16755  | 0.05763  |
| Pd   | 0.29381  | -1.96395 | 1.83057  | 0.08198  |
| Pd   | 1.96611  | 0.37329  | 1.53747  | -0.03835 |
| Pd   | 0.28198  | 2.58157  | 0.85268  | 0.08956  |
| Pd   | -0.27473 | -0.01269 | -0.05710 | -0.49862 |
| Pd   | -0.76923 | 0.36265  | 2.56731  | -0.01741 |
| Pd   | 1.91402  | -1.61883 | -0.55167 | -0.00592 |
| Pd   | 1.83411  | 1.27142  | -1.20847 | -0.01176 |
| Pd   | -0.87655 | 2.21659  | -1.52371 | -0.00745 |
| Pd   | -2.53155 | -0.30974 | -1.62324 | 0.07000  |
| Pd   | -0.79872 | -2.61683 | -0.80601 | 0.01824  |
| Pd   | -0.08264 | -0.72879 | -2.54351 | 0.09834  |
| Pd   | 3.92244  | 0.04566  | -0.18155 | 0.09170  |

### Au<sub>m</sub> clusters

#### Au2\_A

| Atom | X       | Y       | Z        | Charges |
|------|---------|---------|----------|---------|
| Au   | 0.00000 | 0.00000 | 1.28670  | 0.00000 |
| Au   | 0.00000 | 0.00000 | -1.28670 | 0.00000 |

#### Au3\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 0.59160  | -0.07187 |
| Au   | 0.00000 | 2.48681  | -0.29580 | 0.03594  |
| Au   | 0.00000 | -2.48681 | -0.29580 | 0.03594  |

|    |         |         |         |          |
|----|---------|---------|---------|----------|
| Au | 2.04345 | 3.06985 | 0.00000 | -0.06132 |
|----|---------|---------|---------|----------|

Au4\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 0.59193  | -0.05887 |
| Au   | 0.00000 | 0.00000  | 3.17763  | -0.15798 |
| Au   | 0.00000 | 1.31616  | -1.88478 | 0.10843  |
| Au   | 0.00000 | -1.31616 | -1.88478 | 0.10843  |

Au4\_B

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 2.42370  | -0.27744 |
| Au   | 0.00000 | 1.33970  | 0.00000  | 0.27744  |
| Au   | 0.00000 | -1.33970 | 0.00000  | 0.27744  |
| Au   | 0.00000 | 0.00000  | -2.42370 | -0.27744 |

Au5\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 1.04388  | 0.12311  |
| Au   | 0.00000 | 1.38897  | -1.47105 | 0.02997  |
| Au   | 0.00000 | -1.38897 | -1.47105 | 0.02997  |
| Au   | 0.00000 | 2.69634  | 0.94911  | -0.09153 |
| Au   | 0.00000 | -2.69634 | 0.94911  | -0.09153 |

Au6\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 1.67487  | 0.00000 | 0.10163  |
| Au   | -1.45048 | -0.83744 | 0.00000 | 0.10163  |
| Au   | 1.45048  | -0.83744 | 0.00000 | 0.10163  |
| Au   | 0.00000  | -3.11886 | 0.00000 | -0.10163 |
| Au   | -2.70101 | 1.55943  | 0.00000 | -0.10163 |
| Au   | 2.70101  | 1.55943  | 0.00000 | -0.10163 |

Au7\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.92412  | -1.73672 | 0.00000 | 0.01368  |
| Au   | -1.83379 | -0.95560 | 0.00000 | 0.09929  |
| Au   | 0.00000  | 1.22190  | 0.00000 | 0.09663  |
| Au   | 2.64515  | 0.36660  | 0.00000 | 0.01038  |
| Au   | -2.68575 | 1.60046  | 0.00000 | -0.06445 |
| Au   | -1.09318 | -3.56649 | 0.00000 | -0.09421 |

Au7\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.00000  | 1.45870  | -2.40912 | -0.09341 |
| Au   | 0.00000  | -1.45870 | -2.40912 | -0.09341 |
| Au   | 2.70155  | -0.12554 | 1.90121  | -0.08918 |
| Au   | -2.70155 | 0.12554  | 1.90121  | -0.08918 |
| Au   | 1.47673  | 0.13956  | -0.49175 | 0.12787  |
| Au   | 0.00000  | 0.00000  | 1.99932  | 0.10943  |
| Au   | -1.47673 | -0.13956 | -0.49175 | 0.12787  |

Au8\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 2.03094  | 0.00000 | 0.07321  |
| Au   | 2.03094  | 0.00000  | 0.00000 | 0.07321  |
| Au   | 0.00000  | -2.03094 | 0.00000 | 0.07321  |
| Au   | -2.03094 | 0.00000  | 0.00000 | 0.07321  |
| Au   | 2.62926  | -2.62926 | 0.00000 | -0.07321 |
| Au   | 2.62926  | 2.62926  | 0.00000 | -0.07321 |
| Au   | -2.62926 | -2.62926 | 0.00000 | -0.07321 |
| Au   | -2.62926 | 2.62926  | 0.00000 | -0.07321 |

Au9\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 1.00171  | 0.08927  |
| Au   | 0.00000 | 2.35905  | -0.46175 | 0.05239  |
| Au   | 0.00000 | 2.44792  | 2.30017  | -0.06947 |
| Au   | 0.00000 | 0.00000  | 3.79015  | 0.01463  |
| Au   | 0.00000 | -2.44792 | 2.30017  | -0.06947 |
| Au   | 0.00000 | -2.35905 | -0.46175 | 0.05239  |
| Au   | 0.00000 | 0.00000  | -2.15193 | 0.10724  |
| Au   | 0.00000 | -2.52626 | -3.15838 | -0.08850 |
| Au   | 0.00000 | 2.52626  | -3.15838 | -0.08850 |

Au9\_B

| Atom | X        | Y        | Z        | Charges |
|------|----------|----------|----------|---------|
| Au   | 0.00000  | 0.00000  | 1.90268  | 0.06726 |
| Au   | -1.46397 | 1.45661  | -0.15053 | 0.08629 |
| Au   | 1.46397  | 1.45661  | -0.15053 | 0.08629 |
| Au   | 1.46397  | -1.45661 | -0.15053 | 0.08629 |
| Au   | -1.46397 | -1.45661 | -0.15053 | 0.08629 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 0.00000  | 3.73325  | 0.02854  | -0.10164 |
| Au | 0.00000  | -3.73325 | 0.02854  | -0.10164 |
| Au | 3.68578  | 0.00000  | -0.67882 | -0.10456 |
| Au | -3.68578 | 0.00000  | -0.67882 | -0.10456 |

Au9\_C

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 0.50633  | 0.05601  |
| Au   | 0.00000 | 1.35329  | -1.90015 | 0.03848  |
| Au   | 0.00000 | 2.95523  | 0.57773  | 0.06675  |
| Au   | 0.00000 | 1.44637  | 2.87869  | -0.00918 |
| Au   | 0.00000 | -1.44637 | 2.87869  | -0.00918 |
| Au   | 0.00000 | -2.95523 | 0.57773  | 0.06675  |
| Au   | 0.00000 | -1.35329 | -1.90015 | 0.03848  |
| Au   | 0.00000 | -4.15309 | -1.80943 | -0.12406 |
| Au   | 0.00000 | 4.15309  | -1.80943 | -0.12406 |

Au9\_D

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 0.01908  | 0.10990  |
| Au   | 0.00000 | 0.00000  | 2.81391  | -0.00939 |
| Au   | 0.00000 | 2.43668  | 1.54815  | -0.04695 |
| Au   | 0.00000 | 2.39979  | -1.49945 | 0.02365  |
| Au   | 0.00000 | 0.00000  | -2.83159 | -0.04709 |
| Au   | 0.00000 | -2.39979 | -1.49945 | 0.02365  |
| Au   | 0.00000 | -2.43668 | 1.54815  | -0.04695 |
| Au   | 0.00000 | -4.65122 | -0.04940 | -0.00341 |
| Au   | 0.00000 | 4.65122  | -0.04940 | -0.00341 |

Au9\_E

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.05982  | 0.62865  | 1.47790  | 0.11849  |
| Au   | -1.21586 | 1.82521  | 0.00000  | -0.04649 |
| Au   | 1.05982  | 0.62865  | -1.47790 | 0.11849  |
| Au   | -2.87845 | -0.32961 | 0.00000  | -0.00667 |
| Au   | -0.79088 | -1.55960 | 1.38740  | 0.05537  |
| Au   | -0.79088 | -1.55960 | -1.38740 | 0.05537  |
| Au   | 1.05982  | -1.27775 | 3.38574  | -0.12077 |
| Au   | 1.05982  | -1.27775 | -3.38574 | -0.12077 |
| Au   | 1.43680  | 2.92181  | 0.00000  | -0.05303 |

Au10\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.99635 | 0.99530  | 1.02586  | 0.06849  |
| Au   | 0.99635  | 0.99530  | -1.02586 | 0.06849  |
| Au   | 0.99635  | -0.99530 | 1.02586  | 0.06849  |
| Au   | -0.99635 | -0.99530 | -1.02586 | 0.06849  |
| Au   | 0.00000  | 0.00000  | -3.60689 | 0.10366  |
| Au   | 0.00000  | 0.00000  | 3.60689  | 0.10366  |
| Au   | 1.90138  | 1.90972  | -3.42591 | -0.12032 |
| Au   | -1.90138 | -1.90972 | -3.42591 | -0.12032 |
| Au   | -1.90138 | 1.90972  | 3.42591  | -0.12032 |
| Au   | 1.90138  | -1.90972 | 3.42591  | -0.12032 |

Au10\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.67546  | 1.90232  | 0.00000  | 0.11542  |
| Au   | -1.32795 | 0.31414  | 1.47554  | 0.11574  |
| Au   | -1.32795 | 0.31414  | -1.47554 | 0.11574  |
| Au   | 0.47589  | -1.89405 | -1.37867 | 0.05236  |
| Au   | 0.47589  | -1.89405 | 1.37867  | 0.05236  |
| Au   | -2.01503 | 2.55611  | 0.00000  | 0.00547  |
| Au   | 2.34509  | -0.40665 | 0.00000  | 0.05147  |
| Au   | -1.32795 | -1.52753 | -3.43752 | -0.16993 |
| Au   | -1.32795 | -1.52753 | 3.43752  | -0.16993 |
| Au   | 3.35450  | 2.16309  | 0.00000  | -0.16868 |

Au10\_C

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 1.42442  | 0.12138  |
| Au   | 0.00000 | 2.43877  | 0.00000  | 0.00977  |
| Au   | 0.00000 | 2.42788  | 2.79075  | -0.05495 |
| Au   | 0.00000 | 0.00000  | 4.20952  | -0.02125 |
| Au   | 0.00000 | -2.42788 | 2.79075  | -0.05495 |
| Au   | 0.00000 | -2.43877 | 0.00000  | 0.00977  |
| Au   | 0.00000 | 0.00000  | -1.42442 | 0.12138  |
| Au   | 0.00000 | -2.42788 | -2.79075 | -0.05495 |
| Au   | 0.00000 | 2.42788  | -2.79075 | -0.05495 |
| Au   | 0.00000 | 0.00000  | -4.20952 | -0.02125 |

Au10\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.46299  | 1.43040  | -0.38675 | 0.13312  |
| Au   | 0.00000  | 1.32469  | 2.11169  | -0.03585 |
| Au   | -1.46299 | 1.43040  | -0.38675 | 0.13312  |
| Au   | 0.00000  | -1.32469 | 2.11169  | -0.03585 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.46299  | -1.43040 | -0.38675 | 0.13312  |
| Au | -1.46299 | -1.43040 | -0.38675 | 0.13312  |
| Au | 0.00000  | -3.66544 | 0.32797  | -0.17983 |
| Au | 0.00000  | 3.66544  | 0.32797  | -0.17983 |
| Au | 3.36292  | 0.00000  | -1.66617 | -0.05057 |
| Au | -3.36292 | 0.00000  | -1.66617 | -0.05057 |

Au11\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.43457  | 0.83088  | 1.40067  | 0.10524  |
| Au   | -0.00070 | -1.65781 | 1.40067  | 0.10523  |
| Au   | -1.43745 | 0.82900  | 1.40081  | 0.10492  |
| Au   | -0.00070 | -1.65781 | -1.40067 | 0.10523  |
| Au   | 1.43457  | 0.83088  | -1.40067 | 0.10524  |
| Au   | -1.43745 | 0.82900  | -1.40081 | 0.10492  |
| Au   | -0.00070 | 0.00041  | -3.66972 | -0.13129 |
| Au   | -0.00070 | 0.00041  | 3.66972  | -0.13129 |
| Au   | 3.45828  | 1.99129  | 0.00000  | -0.12251 |
| Au   | -3.45812 | 1.99436  | 0.00000  | -0.12316 |
| Au   | 0.00842  | -3.99059 | 0.00000  | -0.12253 |

Au11\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 1.34338  | 0.00000 | 0.06589  |
| Au   | 1.91325  | -0.82170 | 0.00000 | 0.03278  |
| Au   | 2.74893  | 1.97606  | 0.00000 | 0.03975  |
| Au   | 0.89387  | 3.99444  | 0.00000 | -0.06646 |
| Au   | -1.91498 | 3.37776  | 0.00000 | 0.00006  |
| Au   | -2.79673 | 0.74750  | 0.00000 | 0.00296  |
| Au   | -0.86828 | -1.30639 | 0.00000 | 0.06885  |
| Au   | -3.65566 | -1.89185 | 0.00000 | -0.06843 |
| Au   | 0.93673  | -3.42711 | 0.00000 | 0.00201  |
| Au   | -1.80563 | -3.95791 | 0.00000 | -0.00655 |
| Au   | 4.54849  | -0.03418 | 0.00000 | -0.07087 |

Au11\_C

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 0.00000  | -0.01657 |
| Au   | 0.00000 | 2.40444  | 1.38403  | 0.02080  |
| Au   | 0.00000 | 2.40444  | -1.38403 | 0.02080  |
| Au   | 0.00000 | 0.00000  | -3.02731 | 0.10234  |
| Au   | 0.00000 | -2.40444 | -1.38403 | 0.02080  |
| Au   | 0.00000 | -2.40444 | 1.38403  | 0.02080  |
| Au   | 0.00000 | 0.00000  | 3.02731  | 0.10234  |

|    |         |          |          |          |
|----|---------|----------|----------|----------|
| Au | 0.00000 | -2.47781 | 4.12367  | -0.06783 |
| Au | 0.00000 | 2.47781  | 4.12367  | -0.06783 |
| Au | 0.00000 | 2.47781  | -4.12367 | -0.06783 |
| Au | 0.00000 | -2.47781 | -4.12367 | -0.06783 |

Au11\_D

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 0.95173  | 0.00000 | 0.08013  |
| Au   | 2.69873  | 0.11963  | 0.00000 | -0.01574 |
| Au   | 2.02686  | 2.88194  | 0.00000 | -0.07908 |
| Au   | -0.59275 | 3.71651  | 0.00000 | 0.07607  |
| Au   | -2.70333 | 1.67032  | 0.00000 | 0.03671  |
| Au   | -2.05172 | -0.99616 | 0.00000 | -0.00053 |
| Au   | 0.63099  | -1.84087 | 0.00000 | 0.12154  |
| Au   | -1.39813 | -3.74598 | 0.00000 | -0.08880 |
| Au   | 3.31108  | -2.57763 | 0.00000 | -0.00562 |
| Au   | 1.30794  | -4.55284 | 0.00000 | -0.01387 |
| Au   | -3.22969 | 4.37334  | 0.00000 | -0.11082 |

Au12\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.32297 | 0.91414  | 0.00000  | 0.08062  |
| Au   | 0.34778  | -1.63676 | 1.40107  | 0.07429  |
| Au   | 0.34778  | -1.63676 | -1.40107 | 0.07429  |
| Au   | 2.33622  | 0.45723  | -1.46120 | 0.10458  |
| Au   | 2.33622  | 0.45723  | 1.46120  | 0.10458  |
| Au   | -2.04511 | -1.54379 | 0.00000  | 0.01866  |
| Au   | 1.97479  | 2.73690  | 0.00000  | -0.01556 |
| Au   | 2.33622  | -1.52332 | -3.28114 | -0.13259 |
| Au   | 2.33622  | -1.52332 | 3.28114  | -0.13259 |
| Au   | -3.22738 | 1.10734  | 0.00000  | 0.09456  |
| Au   | -1.66965 | 3.30719  | 0.00000  | -0.10659 |
| Au   | -4.75014 | -1.11607 | 0.00000  | -0.16423 |

Au12\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 1.59751  | 0.00000 | 0.05485  |
| Au   | 1.38348  | -0.79875 | 0.00000 | 0.05485  |
| Au   | 2.85038  | 1.64645  | 0.00000 | -0.01083 |
| Au   | 1.39206  | 4.03363  | 0.00000 | -0.02164 |
| Au   | -1.39569 | 4.03443  | 0.00000 | -0.02239 |
| Au   | -2.85106 | 1.64528  | 0.00000 | -0.01083 |
| Au   | -1.38348 | -0.79875 | 0.00000 | 0.05485  |
| Au   | -4.18925 | -0.81126 | 0.00000 | -0.02164 |

|    |          |          |         |          |
|----|----------|----------|---------|----------|
| Au | 0.00068  | -3.29173 | 0.00000 | -0.01083 |
| Au | -2.79607 | -3.22592 | 0.00000 | -0.02239 |
| Au | 4.19176  | -0.80851 | 0.00000 | -0.02239 |
| Au | 2.79720  | -3.22237 | 0.00000 | -0.02164 |

Au12\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.24120  | -1.91250 | 1.38343  | 0.04034  |
| Au   | 0.24120  | -1.91250 | -1.38343 | 0.04034  |
| Au   | -2.71285 | 1.02927  | 0.00000  | 0.08286  |
| Au   | 2.05386  | 0.27960  | -1.46546 | 0.09471  |
| Au   | 2.05386  | 0.27960  | 1.46546  | 0.09471  |
| Au   | 0.03063  | 1.79808  | 0.00000  | 0.05105  |
| Au   | 2.76856  | 2.49697  | 0.00000  | 0.02839  |
| Au   | -2.11589 | -1.73399 | 0.00000  | -0.01407 |
| Au   | 2.05386  | -1.55922 | 3.41777  | -0.12652 |
| Au   | -1.98000 | 3.61520  | 0.00000  | -0.00969 |
| Au   | 2.05386  | -1.55922 | -3.41777 | -0.12652 |
| Au   | -4.68829 | -0.82131 | 0.00000  | -0.15560 |

Au12\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -1.51919 | -0.53868 | 0.00000  | 0.06868  |
| Au   | 1.66421  | 0.64485  | 1.43260  | 0.11599  |
| Au   | 1.66421  | 0.64485  | -1.43260 | 0.11599  |
| Au   | -0.97172 | 0.15154  | -2.80490 | 0.04819  |
| Au   | -3.26676 | 0.88545  | -1.65053 | -0.08529 |
| Au   | -3.26676 | 0.88545  | 1.65053  | -0.08529 |
| Au   | -0.97172 | 0.15154  | 2.80490  | 0.04819  |
| Au   | 1.41217  | -0.74625 | 3.82821  | -0.14546 |
| Au   | 0.53210  | -1.98609 | 1.35381  | 0.03700  |
| Au   | 0.53210  | -1.98609 | -1.35381 | 0.03700  |
| Au   | 2.77918  | 2.63969  | 0.00000  | -0.00957 |
| Au   | 1.41217  | -0.74625 | -3.82821 | -0.14546 |

Au13\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 2.29457  | 1.56408  | 0.00000 | 0.05727  |
| Au   | -1.87983 | 0.41339  | 1.42888 | 0.08839  |
| Au   | -0.29489 | -1.89181 | 1.42820 | 0.08823  |
| Au   | 2.09083  | -1.21501 | 0.00000 | 0.04191  |
| Au   | 4.51226  | -0.02138 | 0.00000 | -0.07352 |
| Au   | -0.36976 | 2.37889  | 0.00000 | 0.04173  |
| Au   | -3.16898 | 2.45638  | 0.00000 | -0.07195 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -1.87983 | 0.41339  | -1.42888 | 0.08839  |
| Au | -0.29489 | -1.89181 | -1.42820 | 0.08823  |
| Au | -1.87983 | -1.28355 | -3.54955 | -0.10187 |
| Au | -1.87983 | -1.28355 | 3.54955  | -0.10187 |
| Au | 1.13119  | -3.84384 | 0.00000  | -0.07181 |
| Au | 1.61901  | 4.20480  | 0.00000  | -0.07312 |

Au13\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Au   | 0.00000  | 1.32169  | 0.00000 | 0.01185  |
| Au   | -0.80859 | -1.33060 | 0.00000 | 0.04809  |
| Au   | -2.82506 | 0.64834  | 0.00000 | 0.04244  |
| Au   | -1.86907 | 3.43399  | 0.00000 | 0.07543  |
| Au   | 0.79259  | 4.06717  | 0.00000 | -0.09381 |
| Au   | 2.75339  | 2.03064  | 0.00000 | 0.02685  |
| Au   | 1.89209  | -0.71261 | 0.00000 | 0.06525  |
| Au   | 4.60923  | 0.01319  | 0.00000 | -0.01955 |
| Au   | 1.15289  | -3.46051 | 0.00000 | -0.02559 |
| Au   | 3.85149  | -2.71275 | 0.00000 | -0.02295 |
| Au   | -3.50456 | -2.07631 | 0.00000 | -0.03121 |
| Au   | -1.54850 | -4.05993 | 0.00000 | -0.03227 |
| Au   | -4.49591 | 2.83770  | 0.00000 | -0.04453 |

Au13\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.21316 | 1.10068  | 0.00000  | -0.01051 |
| Au   | 0.46609  | -1.52821 | 1.42206  | 0.10450  |
| Au   | 2.28312  | 0.71352  | 1.44525  | 0.10849  |
| Au   | 1.91147  | 3.05783  | 0.00000  | -0.05079 |
| Au   | -1.25608 | 3.66430  | 0.00000  | -0.13025 |
| Au   | -2.97432 | 1.53026  | 0.00000  | 0.10368  |
| Au   | -2.06747 | -1.20770 | 0.00000  | 0.07238  |
| Au   | -4.70883 | -0.56148 | 0.00000  | -0.13334 |
| Au   | -0.75629 | -3.65296 | 0.00000  | -0.04800 |
| Au   | 0.46609  | -1.52821 | -1.42206 | 0.10450  |
| Au   | 2.28312  | 0.71352  | -1.44525 | 0.10849  |
| Au   | 2.28312  | -1.15078 | -3.41165 | -0.11457 |
| Au   | 2.28312  | -1.15078 | 3.41165  | -0.11457 |

Au13\_D

| Atom | X        | Y        | Z       | Charges |
|------|----------|----------|---------|---------|
| Au   | -0.35014 | 0.31329  | 0.00000 | 0.05963 |
| Au   | 0.26362  | -2.21980 | 1.40547 | 0.07327 |
| Au   | 2.24257  | -0.01612 | 1.40572 | 0.07301 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.62293  | 2.33070  | 0.00000  | 0.06220  |
| Au | -1.29582 | 3.02168  | 0.00000  | 0.02980  |
| Au | -3.14640 | 0.94764  | 0.00000  | 0.03083  |
| Au | -2.13863 | -1.87134 | 0.00000  | 0.06332  |
| Au | -4.81908 | -1.17270 | 0.00000  | -0.11953 |
| Au | 0.26362  | -2.21980 | -1.40547 | 0.07327  |
| Au | 2.24257  | -0.01612 | -1.40572 | 0.07301  |
| Au | 2.24257  | -2.00629 | -3.25710 | -0.15017 |
| Au | 2.24257  | -2.00629 | 3.25710  | -0.15017 |
| Au | 0.62962  | 4.91514  | 0.00000  | -0.11847 |

Au14\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.28926 | 0.65861  | 0.00000  | -0.04235 |
| Au   | 0.56615  | -1.94998 | 1.44347  | 0.10120  |
| Au   | 2.22926  | 0.43648  | 1.40899  | 0.09111  |
| Au   | 1.67125  | 2.79051  | 0.00000  | 0.00447  |
| Au   | -1.43856 | 3.17876  | 0.00000  | 0.01338  |
| Au   | -3.04614 | 0.94498  | 0.00000  | 0.06218  |
| Au   | -2.06043 | -1.74243 | 0.00000  | 0.08455  |
| Au   | -4.70948 | -1.26759 | 0.00000  | -0.17529 |
| Au   | -0.58846 | -4.04883 | 0.00000  | 0.08165  |
| Au   | 0.56615  | -1.94998 | -1.44347 | 0.10120  |
| Au   | 2.22926  | 0.43648  | -1.40899 | 0.09111  |
| Au   | 2.22926  | -1.34011 | -3.48111 | -0.13401 |
| Au   | 2.22926  | -1.34011 | 3.48111  | -0.13401 |
| Au   | 0.41174  | 5.19322  | 0.00000  | -0.14521 |

Au14\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.05135 | 1.62103  | 1.65027  | 0.09235  |
| Au   | -1.37180 | -0.77795 | 1.49632  | 0.10122  |
| Au   | 1.41945  | -0.69640 | 1.49593  | 0.10202  |
| Au   | -0.05647 | 1.62705  | -1.65242 | 0.09336  |
| Au   | 1.41563  | -0.68727 | -1.49070 | 0.10122  |
| Au   | -1.37542 | -0.77376 | -1.49803 | 0.10177  |
| Au   | -2.35567 | 2.18620  | 0.00369  | -0.03061 |
| Au   | 2.23323  | 2.26360  | -0.00646 | -0.02679 |
| Au   | -3.76431 | -0.16647 | 0.00092  | -0.07327 |
| Au   | 3.79006  | 0.00630  | -0.00135 | -0.07562 |
| Au   | 2.84444  | -2.74331 | -0.00122 | -0.12768 |
| Au   | -2.71259 | -2.88024 | -0.00240 | -0.13023 |
| Au   | 0.07229  | -2.94738 | -0.00151 | 0.01513  |
| Au   | -0.08749 | 3.96860  | 0.00697  | -0.14286 |

Au14\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.30253  | 0.30482  | 0.00000  | 0.06492  |
| Au   | 1.43659  | -1.81652 | 1.55940  | 0.06398  |
| Au   | -1.37499 | -1.87208 | 1.43358  | 0.09326  |
| Au   | -1.37499 | -1.87208 | -1.43358 | 0.09326  |
| Au   | 1.43659  | -1.81652 | -1.55940 | 0.06398  |
| Au   | -0.12182 | 0.13933  | 2.86127  | 0.02075  |
| Au   | -0.12182 | 0.13933  | -2.86127 | 0.02075  |
| Au   | -3.22025 | -3.25329 | 0.00000  | -0.13145 |
| Au   | 3.24747  | -3.12306 | 0.00000  | -0.20079 |
| Au   | -0.08435 | 2.79743  | 1.50585  | 0.08325  |
| Au   | 2.18407  | 2.60177  | 0.00000  | 0.07245  |
| Au   | -0.08435 | 2.79743  | -1.50585 | 0.08325  |
| Au   | -1.11235 | 2.48672  | 3.95659  | -0.16379 |
| Au   | -1.11235 | 2.48672  | -3.95659 | -0.16379 |

Au14\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.25390  | 0.94930  | 0.00000  | 0.06432  |
| Au   | -1.83992 | -0.43977 | 1.41374  | 0.07205  |
| Au   | -1.83992 | -0.43977 | -1.41374 | 0.07205  |
| Au   | 0.02001  | -2.63351 | -1.39234 | 0.04635  |
| Au   | 0.02001  | -2.63351 | 1.39234  | 0.04635  |
| Au   | -2.48047 | 1.88627  | 0.00000  | 0.03225  |
| Au   | 2.99500  | 0.34981  | 0.00000  | 0.09473  |
| Au   | -1.83992 | -2.30407 | -3.36696 | -0.14833 |
| Au   | -1.83992 | -2.30407 | 3.36696  | -0.14833 |
| Au   | -0.29351 | 3.78522  | 0.00000  | 0.11785  |
| Au   | 2.32324  | 2.98346  | 0.00000  | -0.03771 |
| Au   | -2.81872 | 4.64710  | 0.00000  | -0.08809 |
| Au   | 2.36395  | -2.39910 | 0.00000  | -0.02245 |
| Au   | 4.97627  | -1.44736 | 0.00000  | -0.10105 |

Au14\_E

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.78409 | 0.28523  | 0.00000  | -0.03066 |
| Au   | 0.94630  | -1.89245 | 1.44716  | 0.11524  |
| Au   | 1.93582  | 0.84585  | 1.44762  | 0.11560  |
| Au   | 0.22933  | 2.85498  | 0.00000  | -0.01561 |
| Au   | -2.47029 | 2.54761  | 0.00000  | 0.01789  |
| Au   | -1.65425 | -2.33614 | 0.00000  | -0.01598 |
| Au   | 0.54806  | -4.21240 | 0.00000  | -0.12675 |
| Au   | 0.94630  | -1.89245 | -1.44716 | 0.11524  |
| Au   | 1.93582  | 0.84585  | -1.44762 | 0.11560  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.93582  | -0.70330 | -3.65641 | -0.01739 |
| Au | 1.93582  | -0.70330 | 3.65641  | -0.01739 |
| Au | 3.12420  | 2.87843  | 0.00000  | -0.12753 |
| Au | -3.52870 | -0.36951 | 0.00000  | 0.01796  |
| Au | -5.10014 | 1.85160  | 0.00000  | -0.14621 |

## Pd<sub>n</sub>Au<sub>1</sub> clusters

Au1Pd1\_A

| Atom | X       | Y       | Z        | Charges  |
|------|---------|---------|----------|----------|
| Au   | 0.00000 | 0.00000 | 0.94226  | -0.26184 |
| Pd   | 0.00000 | 0.00000 | -1.61822 | 0.26184  |

Au1Pd2\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Au   | 0.00000 | 0.00000  | 1.26081  | -0.24324 |
| Pd   | 0.00000 | 1.28572  | -1.08265 | 0.12162  |
| Pd   | 0.00000 | -1.28572 | -1.08265 | 0.12162  |

Au1Pd3\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.46301 | 1.38201  | 0.00000  | -0.12441 |
| Pd   | 1.72119  | -0.30392 | 0.00000  | 0.04151  |
| Pd   | -0.46301 | -1.03476 | 1.33126  | 0.04145  |
| Pd   | -0.46301 | -1.03476 | -1.33126 | 0.04145  |

Au1Pd4\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.00000  | 0.00000  | 1.45478  | -0.09272 |
| Pd   | 0.00000  | 2.20214  | -0.15461 | 0.03340  |
| Pd   | 0.00000  | -2.20214 | -0.15461 | 0.03340  |
| Pd   | -1.31079 | 0.00000  | -1.09460 | 0.01296  |
| Pd   | 1.31079  | 0.00000  | -1.09460 | 0.01296  |

Au1Pd4\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.00000  | 0.00000  | 1.45313  | -0.10812 |
| Pd   | 0.00000  | 1.86890  | -0.62390 | 0.02703  |
| Pd   | 0.00000  | -1.86890 | -0.62390 | 0.02703  |
| Pd   | 1.86890  | 0.00000  | -0.62390 | 0.02703  |
| Pd   | -1.86890 | 0.00000  | -0.62390 | 0.02703  |

Au1Pd4\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.89080  | -0.03553 | 0.00010  | -0.12756 |
| Pd   | -0.18554 | 1.69672  | -0.02314 | 0.02268  |
| Pd   | -2.34668 | 0.07771  | -0.00304 | 0.00391  |
| Pd   | -0.35839 | -0.83471 | 1.41749  | 0.05038  |
| Pd   | -0.35664 | -0.87870 | -1.39149 | 0.05059  |

Au1Pd5\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.70544  | -0.27249 | -0.00106 | -0.02389 |
| Pd   | 0.04853  | 1.41572  | 1.40617  | -0.02953 |
| Pd   | -0.48674 | -1.33732 | -1.37222 | 0.02005  |
| Pd   | 0.04721  | 1.41831  | -1.40343 | -0.02954 |
| Pd   | -2.05269 | 0.31109  | 0.00089  | 0.04315  |
| Pd   | -0.48522 | -1.33982 | 1.37042  | 0.01975  |

Au1Pd5\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.64766  | -0.44957 | -0.00060 | -0.20551 |
| Pd   | -1.40076 | 0.73539  | 1.40157  | 0.00469  |
| Pd   | 0.02394  | -1.17486 | -0.00151 | 0.01117  |
| Pd   | -2.64246 | -1.06020 | -0.00113 | 0.04975  |
| Pd   | 0.87459  | 1.53131  | 0.00117  | 0.13499  |
| Pd   | -1.40238 | 0.74044  | -1.39907 | 0.00490  |

Au1Pd5\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.10102  | -0.56401 | -0.04378 | -0.10460 |
| Pd   | -0.10603 | -0.38663 | 1.54250  | 0.02228  |
| Pd   | -0.25330 | -0.34937 | -1.51162 | 0.02138  |
| Pd   | 0.75313  | 1.82876  | 0.00961  | 0.03151  |
| Pd   | -1.89426 | 1.24877  | 0.02133  | -0.00330 |
| Pd   | -2.10781 | -1.37291 | 0.01337  | 0.03273  |

Au1Pd5\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -0.00401 | -0.78053 | -1.20474 | -0.07931 |
| Pd   | 0.00392  | 0.33846  | 1.64095  | -0.03192 |

|    |          |          |          |         |
|----|----------|----------|----------|---------|
| Pd | 1.38965  | 1.50528  | -0.34541 | 0.00905 |
| Pd | -1.38765 | 1.50878  | -0.34685 | 0.00683 |
| Pd | -2.07559 | -1.00508 | 0.56415  | 0.04636 |
| Pd | 2.07655  | -1.00696 | 0.55617  | 0.04900 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -0.84098 | -0.83121 | 1.30043  | 0.07615  |
| Pd | 1.47211  | 0.76482  | 1.34301  | -0.03704 |
| Pd | 3.62845  | 0.06426  | -0.08564 | 0.07235  |

Au1Pd6\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.87064  | -0.09094 | 0.00005  | -0.28471 |
| Pd   | 0.64884  | 1.43105  | -0.00197 | 0.08828  |
| Pd   | -0.84367 | 0.06699  | 1.87566  | 0.11656  |
| Pd   | -2.21549 | -1.43846 | 0.00107  | -0.02622 |
| Pd   | 0.45311  | -1.35531 | -0.00215 | 0.04793  |
| Pd   | -2.12365 | 1.38372  | 0.00268  | -0.05794 |
| Pd   | -0.84916 | 0.06820  | -1.87537 | 0.11609  |

Au1Pd7\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -3.35594 | 0.00000  | 0.00794  | -0.26443 |
| Pd   | -1.04557 | 1.38331  | 0.06320  | 0.10132  |
| Pd   | -1.04558 | -1.38332 | 0.06321  | 0.10133  |
| Pd   | 1.48949  | 2.22055  | -0.07865 | 0.03138  |
| Pd   | 1.48949  | -2.22055 | -0.07860 | 0.03138  |
| Pd   | 3.11637  | -0.00002 | 0.01272  | 0.05859  |
| Pd   | 1.00218  | 0.00005  | 1.50600  | -0.00361 |
| Pd   | 0.75710  | -0.00004 | -1.50151 | -0.05597 |

Au1Pd6\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -2.77187 | -0.06091 | -0.08469 | -0.36869 |
| Pd   | -0.37360 | -1.42367 | 0.64930  | 0.14895  |
| Pd   | 2.10156  | -1.25481 | -0.85028 | 0.01844  |
| Pd   | 1.98953  | 1.41341  | -0.60292 | -0.01637 |
| Pd   | 1.86422  | -0.14647 | 1.50051  | -0.04736 |
| Pd   | -0.32422 | 0.17324  | -1.41981 | 0.10167  |
| Pd   | -0.49710 | 1.34291  | 0.86864  | 0.16336  |

Au1Pd7\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.14505  | -0.51957 | 0.06064  | -0.19866 |
| Pd   | -3.54351 | 0.33296  | 0.46688  | 0.06637  |
| Pd   | 1.43369  | 1.54635  | -0.87543 | 0.12316  |
| Pd   | -2.19819 | -0.91478 | -1.39856 | 0.00997  |
| Pd   | 0.98309  | 0.48885  | 1.49718  | 0.07853  |
| Pd   | -1.42705 | -0.99559 | 1.24116  | -0.01718 |
| Pd   | -1.19341 | 1.36943  | -0.21315 | -0.05821 |
| Pd   | 0.54410  | -0.93490 | -0.82223 | -0.00398 |

Au1Pd6\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -2.61633 | -0.63832 | -0.20759 | -0.27416 |
| Pd   | -0.63459 | 0.33386  | 1.57570  | 0.09473  |
| Pd   | 1.85336  | -1.06284 | 1.22299  | 0.03682  |
| Pd   | 2.68173  | -0.45834 | -1.15807 | 0.03272  |
| Pd   | 1.60574  | 1.47350  | 0.19173  | -0.05790 |
| Pd   | 0.05810  | -0.84636 | -0.87003 | 0.00261  |
| Pd   | -1.07110 | 1.65643  | -0.60579 | 0.16518  |

Au1Pd7\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -2.72981 | -0.86432 | -0.00020 | -0.23984 |
| Pd   | -1.87745 | 1.73658  | 0.00013  | 0.13378  |
| Pd   | -0.30070 | -0.31690 | -1.29899 | 0.01369  |
| Pd   | -0.30023 | -0.31582 | 1.29991  | 0.01386  |
| Pd   | 1.66372  | -1.97529 | 0.00087  | 0.11769  |
| Pd   | 0.72275  | 1.99484  | -0.00085 | 0.07183  |
| Pd   | 2.39006  | 0.17977  | -1.33341 | -0.05542 |
| Pd   | 2.39000  | 0.18120  | 1.33268  | -0.05560 |

Au1Pd7\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -3.17869 | -0.02244 | -0.02049 | -0.22001 |
| Pd   | 1.60730  | -1.60000 | 0.00875  | -0.01373 |
| Pd   | -0.83450 | -0.84497 | -1.30120 | 0.08876  |
| Pd   | -0.91817 | 1.61593  | 0.05748  | 0.05665  |
| Pd   | 1.34484  | 0.86972  | -1.28763 | -0.02312 |

Au1Pd8\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.45407  | 1.15400  | -0.01748 | -0.13379 |
| Pd   | -2.25285 | 1.69031  | -0.03456 | -0.01384 |
| Pd   | 1.92413  | -1.14452 | 1.41902  | 0.03323  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -2.63483 | -0.49859 | 1.35990  | -0.00438 |
| Pd | 1.93290  | -1.18997 | -1.37788 | 0.03332  |
| Pd | -2.63594 | -0.55503 | -1.33688 | -0.00539 |
| Pd | -0.04690 | 0.68961  | 1.35316  | 0.04135  |
| Pd | -0.04622 | 0.63463  | -1.37999 | 0.04318  |
| Pd | -0.45488 | -1.60832 | 0.02725  | 0.00631  |

Au1Pd8\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.32421  | -0.16479 | 0.45095  | -0.19095 |
| Pd   | -3.34957 | 0.22087  | -0.51719 | 0.03771  |
| Pd   | 0.61478  | -0.40890 | 1.09643  | -0.01963 |
| Pd   | -0.97226 | 0.59337  | -1.57091 | -0.01105 |
| Pd   | -1.32908 | -1.78628 | -0.52617 | 0.04227  |
| Pd   | 1.36379  | -0.95011 | -1.38827 | 0.06125  |
| Pd   | -2.07203 | -0.69550 | 1.78486  | -0.01554 |
| Pd   | 1.36508  | 1.62912  | -0.42854 | 0.06220  |
| Pd   | -1.32968 | 1.68044  | 0.77534  | 0.03373  |

Au1Pd8\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.67650  | -0.70708 | -0.40568 | -0.20477 |
| Pd   | -0.84795 | 2.12472  | 0.47742  | 0.04439  |
| Pd   | 0.96232  | 0.52300  | 1.56295  | 0.06902  |
| Pd   | -1.81181 | -0.31849 | 1.42951  | -0.05106 |
| Pd   | -0.11085 | 0.01371  | -1.15571 | -0.04499 |
| Pd   | 0.37446  | -2.00568 | 0.62999  | 0.03878  |
| Pd   | -2.84609 | 0.76704  | -0.90855 | 0.00941  |
| Pd   | 1.76773  | 1.85261  | -0.61916 | 0.08590  |
| Pd   | -2.08440 | -1.74257 | -0.71973 | 0.05331  |

Au1Pd8\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.86962  | -0.47247 | -0.58863 | -0.25436 |
| Pd   | -1.98064 | -2.30440 | 0.85821  | 0.04638  |
| Pd   | 0.44244  | 0.76429  | -1.14656 | -0.00757 |
| Pd   | -1.34264 | 0.22868  | 1.21827  | -0.07618 |
| Pd   | 0.51293  | -1.70123 | 0.17639  | 0.09038  |
| Pd   | -1.76279 | -1.02149 | -1.38154 | 0.03478  |
| Pd   | 1.45083  | 0.54798  | 1.57409  | 0.04024  |
| Pd   | -2.07921 | 1.70829  | -0.98710 | 0.03771  |
| Pd   | -0.16919 | 2.58930  | 0.69915  | 0.08862  |

Au1Pd9\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.94233  | -0.17875 | -0.90075 | -0.12337 |
| Pd   | -2.62790 | -0.33799 | -1.61937 | 0.01892  |
| Pd   | -3.24759 | 0.23722  | 1.03032  | 0.03443  |
| Pd   | 0.14207  | -0.19911 | -1.33930 | -0.05430 |
| Pd   | -0.60355 | 0.28386  | 1.44138  | -0.06574 |
| Pd   | -1.66005 | -1.92449 | 0.19190  | 0.03909  |
| Pd   | -1.62483 | 1.88762  | -0.38340 | 0.00220  |
| Pd   | 2.17862  | 0.27942  | 1.79327  | 0.05102  |
| Pd   | 1.15437  | -1.83372 | 0.52811  | 0.04366  |
| Pd   | 1.23573  | 1.91418  | -0.09598 | 0.05408  |

Au1Pd9\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -3.21339 | -0.62772 | -0.55183 | -0.20959 |
| Pd   | -1.88747 | 0.65461  | 1.52861  | 0.10269  |
| Pd   | -0.27348 | 2.58115  | 0.64040  | 0.09939  |
| Pd   | 1.77721  | 1.76808  | -1.06773 | -0.02775 |
| Pd   | 1.35483  | -1.00958 | -1.43512 | 0.02872  |
| Pd   | -0.78797 | -1.69033 | 0.24682  | 0.05409  |
| Pd   | 0.92201  | 0.26819  | 1.22475  | -0.10492 |
| Pd   | -0.84020 | 0.76923  | -1.14823 | 0.01121  |
| Pd   | 3.42518  | -0.05731 | 0.12858  | 0.01654  |
| Pd   | 1.82854  | -2.20600 | 0.82964  | 0.02964  |

Au1Pd9\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.57978  | -0.11205 | 0.39248  | -0.14830 |
| Pd   | 1.49317  | -1.20267 | -1.20435 | 0.08530  |
| Pd   | 1.73444  | 1.41364  | -1.00051 | 0.08955  |
| Pd   | -0.53008 | 2.11646  | 0.54988  | 0.05243  |
| Pd   | -1.87941 | -0.15394 | 1.58658  | -0.05691 |
| Pd   | -0.76477 | -2.22759 | 0.20017  | 0.05424  |
| Pd   | -0.91680 | 0.17948  | -1.25300 | -0.13654 |
| Pd   | 0.93139  | -0.17638 | 1.18397  | -0.06074 |
| Pd   | -3.01929 | 1.51628  | -0.33570 | 0.04436  |
| Pd   | -3.19655 | -1.27285 | -0.40108 | 0.07660  |

Au1Pd9\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.30554  | -0.37710 | -0.40932 | -0.22444 |
| Pd   | -3.13813 | -0.23792 | 0.50551  | 0.00407  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -0.88976 | -1.77882 | 1.17398  | 0.04840  |
| Pd | 1.51200  | -0.43813 | 1.71540  | 0.03111  |
| Pd | 1.27996  | 1.49452  | -0.37439 | 0.07513  |
| Pd | -1.39956 | 0.72787  | -1.37282 | -0.01427 |
| Pd | 0.64679  | -1.16139 | -0.85905 | 0.01126  |
| Pd | -0.88127 | 0.92638  | 1.41400  | -0.03652 |
| Pd | -1.95130 | -1.91782 | -1.31184 | 0.02420  |
| Pd | -0.85562 | 3.03293  | -0.18782 | 0.08108  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -0.80252 | -1.98024 | -0.74710 | 0.11508  |
| Pd | -0.72715 | -0.28039 | 1.32288  | 0.03620  |
| Pd | 0.98830  | 0.15262  | -1.16138 | -0.07449 |
| Pd | 1.74528  | -1.28293 | 1.55207  | -0.00093 |
| Pd | 3.46585  | -0.02139 | -0.16654 | 0.05410  |
| Pd | 0.20846  | 2.73347  | -1.29037 | 0.00318  |

Au1Pd11\_A

Au1Pd10\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 1.23473  | 2.72653  | -0.45957 | -0.19853 |
| Pd   | -2.93905 | 0.07176  | 1.28739  | -0.02053 |
| Pd   | -2.18739 | -1.68728 | -0.86195 | 0.03163  |
| Pd   | 0.44721  | -2.57603 | -1.01180 | 0.04968  |
| Pd   | 1.82381  | 0.62598  | 1.20960  | 0.06964  |
| Pd   | -0.90425 | 1.76082  | 0.96477  | 0.08745  |
| Pd   | 0.09542  | 0.18194  | -1.10317 | -0.06603 |
| Pd   | -0.51265 | -1.06149 | 1.27461  | -0.01696 |
| Pd   | 2.63771  | -0.65907 | -0.89734 | 0.07974  |
| Pd   | -2.51342 | 0.87608  | -1.18275 | 0.03891  |
| Pd   | 1.93209  | -2.21524 | 1.10991  | -0.05499 |

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.14085  | -0.56884 | 0.31859  | -0.13328 |
| Pd   | -2.04677 | -1.23496 | 1.47377  | 0.00118  |
| Pd   | -1.77917 | 1.62189  | 0.99519  | -0.00045 |
| Pd   | -0.52725 | 3.03026  | -1.06564 | -0.02286 |
| Pd   | 1.71789  | 1.45731  | -0.95220 | 0.02903  |
| Pd   | 1.25049  | -1.64636 | -1.34017 | 0.05923  |
| Pd   | 0.47461  | -0.07811 | 1.08314  | -0.02716 |
| Pd   | -0.77964 | 0.29390  | -1.22422 | -0.01932 |
| Pd   | 0.75996  | 2.66505  | 1.18875  | 0.02275  |
| Pd   | 0.32909  | -2.73825 | 0.82743  | 0.06466  |
| Pd   | -3.28823 | -0.06643 | -0.48596 | 0.09517  |
| Pd   | -1.50506 | -2.32738 | -1.04725 | -0.06894 |

Au1Pd10\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.90302  | -1.59156 | 0.13175  | -0.20766 |
| Pd   | 1.80058  | 0.62378  | -1.12705 | 0.04986  |
| Pd   | 1.47429  | 2.49647  | 0.88051  | 0.01437  |
| Pd   | -1.13987 | 1.67366  | 1.05105  | 0.04194  |
| Pd   | -1.69628 | -1.25008 | 1.44286  | -0.01062 |
| Pd   | 0.28310  | -2.07309 | -0.52689 | 0.10119  |
| Pd   | -0.99710 | 0.25930  | -1.14317 | -0.07495 |
| Pd   | 0.88463  | -0.09037 | 1.35379  | 0.05441  |
| Pd   | -3.38663 | 0.42302  | 0.12831  | 0.04273  |
| Pd   | -2.36718 | -2.04670 | -0.92208 | -0.00125 |
| Pd   | 0.15883  | 2.71735  | -1.36361 | -0.01002 |

Au1Pd11\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 2.15439  | -1.44116 | -1.19546 | -0.09287 |
| Pd   | 0.55119  | -2.01992 | 1.01442  | -0.02972 |
| Pd   | 1.89389  | 1.29239  | -0.60855 | -0.00798 |
| Pd   | -1.86652 | 1.68708  | 0.44835  | -0.04578 |
| Pd   | -2.05633 | -0.96405 | 1.60440  | -0.00764 |
| Pd   | -0.49052 | -0.33983 | -1.08330 | -0.04677 |
| Pd   | 0.41687  | 0.60896  | 1.42663  | 0.07306  |
| Pd   | -0.39781 | 2.39914  | -1.60136 | 0.03114  |
| Pd   | -1.79746 | -2.57757 | -0.41289 | 0.04710  |
| Pd   | 0.37098  | 3.26168  | 0.77299  | -0.01850 |
| Pd   | 2.89588  | -0.48324 | 1.29922  | 0.05040  |
| Pd   | -3.22011 | -0.38962 | -0.80683 | 0.04757  |

Au1Pd10\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -3.21048 | -1.05382 | 0.21323  | -0.20318 |
| Pd   | -1.70558 | 0.86774  | -1.06063 | 0.03374  |
| Pd   | -1.03011 | 2.45405  | 0.99384  | 0.03645  |
| Pd   | 1.53037  | 1.51251  | 1.01061  | 0.02252  |
| Pd   | 1.84075  | -2.34561 | -0.81956 | -0.02266 |

Au1Pd12\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | -3.29174 | -0.25395 | 0.77330  | -0.08812 |
| Pd   | -1.82714 | -1.42434 | -1.40646 | 0.07740  |
| Pd   | 0.66740  | -2.76973 | -1.10691 | -0.00921 |
| Pd   | 1.57221  | 0.07313  | 1.41456  | 0.07161  |
| Pd   | -0.98513 | 1.30900  | 1.07642  | -0.05476 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 0.41824  | 0.04673  | -1.07662 | -0.09859 |
| Pd | -0.80821 | -1.50342 | 1.05826  | -0.03575 |
| Pd | 2.88305  | -1.26246 | -0.74026 | 0.03150  |
| Pd | -2.12777 | 1.21965  | -1.36063 | 0.07622  |
| Pd | 1.76593  | -2.59155 | 1.27348  | -0.00363 |
| Pd | 2.54821  | 1.67229  | -0.76601 | 0.03464  |
| Pd | 0.18705  | 2.90273  | -1.03102 | 0.00256  |
| Pd | 1.35936  | 2.76412  | 1.33712  | -0.00386 |

Au1Pd12\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 0.12380  | 3.03124  | -0.48880 | -0.18388 |
| Pd   | 0.34097  | 0.39218  | -1.42769 | 0.01324  |
| Pd   | 0.40763  | -1.68374 | 0.29431  | 0.00412  |
| Pd   | 0.17616  | 1.05914  | 1.44439  | 0.03189  |
| Pd   | 0.57498  | -2.06499 | -2.36884 | -0.01229 |
| Pd   | 0.40855  | -1.08921 | 2.92646  | -0.03859 |
| Pd   | 2.49511  | 1.36827  | -0.14232 | 0.09460  |
| Pd   | 2.61323  | -0.70990 | 1.52882  | 0.02457  |
| Pd   | 2.78437  | -1.20160 | -1.28856 | 0.04811  |
| Pd   | -2.10838 | 1.31522  | -0.30274 | 0.01744  |
| Pd   | -1.96340 | -0.81431 | 1.50496  | -0.03302 |
| Pd   | -1.89320 | -1.33574 | -1.26887 | -0.04378 |
| Pd   | -4.04862 | -0.44115 | -0.06047 | 0.07760  |

Au1Pd13\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Au   | 3.56760  | -0.28249 | -0.03510 | -0.09863 |
| Pd   | -0.21751 | -3.34915 | -0.17310 | 0.01954  |
| Pd   | -1.58753 | -1.65369 | -1.73459 | 0.01600  |
| Pd   | -2.97349 | 0.20326  | 0.03081  | 0.02751  |
| Pd   | -1.38880 | 1.79431  | 1.69909  | 0.02574  |
| Pd   | 0.31937  | 3.36901  | 0.10137  | 0.00024  |
| Pd   | 1.99606  | 1.75789  | -1.23474 | 0.13138  |
| Pd   | 1.72975  | -1.92172 | 1.37304  | 0.07356  |
| Pd   | 1.13296  | -1.06665 | -1.19361 | -0.07977 |
| Pd   | -0.61181 | 0.95784  | -1.06618 | -0.10830 |
| Pd   | -0.68701 | -0.88533 | 1.08582  | -0.11136 |
| Pd   | 1.31601  | 0.94936  | 1.17331  | -0.01588 |
| Pd   | -2.39238 | 2.86673  | -0.45517 | 0.06747  |
| Pd   | -2.76260 | -2.53671 | 0.45423  | 0.05248  |

Au1Pd13\_B

| Atom | X | Y | Z | Charges |
|------|---|---|---|---------|
|------|---|---|---|---------|

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 0.00005  | 3.09773  | -0.00031 | -0.17638 |
| Pd | 0.00002  | 0.60919  | -1.33827 | 0.03005  |
| Pd | 0.00002  | 0.60919  | 1.33783  | 0.02999  |
| Pd | -0.00006 | -2.00663 | 0.00027  | 0.03747  |
| Pd | 0.00000  | -1.68276 | 2.65721  | -0.05780 |
| Pd | -0.00007 | -1.68332 | -2.65672 | -0.05783 |
| Pd | -2.29559 | -0.98716 | -1.38646 | -0.01404 |
| Pd | -2.29561 | -0.98675 | 1.38686  | -0.01403 |
| Pd | -2.32643 | 1.51047  | -0.00026 | 0.04395  |
| Pd | 2.29546  | -0.98720 | -1.38647 | -0.01406 |
| Pd | 2.29560  | -0.98680 | 1.38680  | -0.01403 |
| Pd | 2.32654  | 1.51049  | -0.00031 | 0.04398  |
| Pd | 4.37275  | -0.11943 | -0.00004 | 0.08137  |
| Pd | -4.37272 | -0.11929 | 0.00010  | 0.08137  |

**Pd<sub>1</sub>Au<sub>m</sub> clusters**

Pd1Au1\_A

| Atom | X       | Y       | Z        | Charges  |
|------|---------|---------|----------|----------|
| Pd   | 0.00000 | 0.00000 | -1.61822 | 0.26184  |
| Au   | 0.00000 | 0.00000 | 0.94226  | -0.26184 |

Pd1Au2\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Pd   | 0.00000 | 0.00000  | 1.78449  | 0.07904  |
| Au   | 0.00000 | 1.36479  | -0.51953 | -0.03952 |
| Au   | 0.00000 | -1.36479 | -0.51953 | -0.03952 |

Pd1Au3\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Pd   | 0.00000 | 0.00000  | -1.58698 | 0.24653  |
| Au   | 0.00000 | 0.00000  | 1.20582  | 0.12182  |
| Au   | 0.00000 | 2.33873  | -0.14088 | -0.18418 |
| Au   | 0.00000 | -2.33873 | -0.14088 | -0.18418 |

Pd1Au3\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | -0.11871 | -2.12429 | 0.00000 | 0.33241  |
| Au   | 0.00000  | 0.57150  | 0.00000 | -0.03395 |
| Au   | 2.45466  | 1.44485  | 0.00000 | -0.12428 |
| Au   | -2.38554 | -0.77942 | 0.00000 | -0.17417 |

Pd1Au4\_A

| Atom | X       | Y        | Z        | Charges  |
|------|---------|----------|----------|----------|
| Pd   | 0.00000 | 0.00000  | 1.09079  | 0.09076  |
| Au   | 0.00000 | 1.38517  | -1.33406 | 0.02000  |
| Au   | 0.00000 | -1.38517 | -1.33406 | 0.02000  |
| Au   | 0.00000 | 2.72119  | 1.01649  | -0.06538 |
| Au   | 0.00000 | -2.72119 | 1.01649  | -0.06538 |

Pd1Au5\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | 1.59718  | -0.76274 | 0.00000 | 0.25982  |
| Au   | 0.00000  | 1.61527  | 0.00000 | 0.07650  |
| Au   | -1.25950 | -1.01610 | 0.00000 | 0.07698  |
| Au   | -2.68236 | 1.28267  | 0.00000 | -0.08740 |
| Au   | 2.66975  | 1.71730  | 0.00000 | -0.16286 |
| Au   | 0.34210  | -3.15502 | 0.00000 | -0.16304 |

Pd1Au6\_A

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | 0.00000  | 0.00000  | 0.00000 | -0.12190 |
| Au   | 0.00000  | 2.76730  | 0.00000 | 0.02032  |
| Au   | 2.39655  | 1.38365  | 0.00000 | 0.02032  |
| Au   | 2.39655  | -1.38365 | 0.00000 | 0.02032  |
| Au   | 0.00000  | -2.76730 | 0.00000 | 0.02032  |
| Au   | -2.39655 | -1.38365 | 0.00000 | 0.02032  |
| Au   | -2.39655 | 1.38365  | 0.00000 | 0.02032  |

Pd1Au6\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.49545  | 2.47138  | 0.00000  | 0.04368  |
| Au   | -1.17240 | 2.71864  | 0.00000  | -0.02172 |
| Au   | 0.05955  | 0.64180  | 1.49241  | 0.06352  |
| Au   | 0.05955  | -1.79143 | 2.70204  | -0.12562 |
| Au   | 0.05955  | 0.64180  | -1.49241 | 0.06352  |
| Au   | 0.06343  | -1.85841 | 0.00000  | 0.10225  |
| Au   | 0.05955  | -1.79143 | -2.70204 | -0.12562 |

Pd1Au6\_C

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | -1.43852 | -1.13187 | 0.00000 | 0.04688  |
| Au   | -0.11097 | 3.26196  | 0.00000 | -0.11230 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.22228  | -1.46155 | 0.00000  | 0.16112  |
| Au | -0.06842 | 0.96523  | 1.44852  | 0.07527  |
| Au | -0.06842 | 0.96523  | -1.44852 | 0.07527  |
| Au | -0.06842 | -1.53590 | 2.50977  | -0.12311 |
| Au | -0.06842 | -1.53590 | -2.50977 | -0.12311 |

Pd1Au7\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.02346  | -1.20106 | -1.10923 | 0.07876  |
| Au   | 1.39108  | -1.40717 | 1.37490  | 0.00106  |
| Au   | 1.40873  | 1.17165  | -0.15953 | 0.12055  |
| Au   | -1.46916 | 1.11333  | -0.17018 | 0.12029  |
| Au   | -1.30932 | -1.45297 | 1.38227  | -0.00018 |
| Au   | 2.80745  | -0.98617 | -1.08748 | -0.10752 |
| Au   | -2.76717 | -1.11273 | -1.07281 | -0.10714 |
| Au   | -0.07527 | 3.37342  | 0.37871  | -0.10581 |

Pd1Au7\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | 0.00000  | 0.61804  | 0.00000 | -0.01972 |
| Au   | 2.77562  | 0.58677  | 0.00000 | -0.07889 |
| Au   | 1.35835  | 3.04347  | 0.00000 | 0.02251  |
| Au   | -1.35467 | 3.04404  | 0.00000 | 0.02211  |
| Au   | -2.77484 | 0.58866  | 0.00000 | -0.07884 |
| Au   | -1.45835 | -1.77372 | 0.00000 | 0.11074  |
| Au   | 1.45491  | -1.77335 | 0.00000 | 0.11047  |
| Au   | -0.00102 | -4.07574 | 0.00000 | -0.08839 |

Pd1Au7\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00142 | 2.11376  | 0.00059  | 0.27788  |
| Au   | 2.09332  | 0.10803  | -0.01772 | 0.05636  |
| Au   | 0.00235  | -1.84610 | -0.00094 | 0.07774  |
| Au   | -2.09450 | 0.10464  | 0.01784  | 0.05647  |
| Au   | 2.42662  | -2.33562 | 1.07774  | -0.07879 |
| Au   | 2.43407  | 2.54151  | -1.05683 | -0.15518 |
| Au   | -2.42206 | -2.34028 | -1.07694 | -0.07922 |
| Au   | -2.43898 | 2.53701  | 1.05652  | -0.15525 |

Pd1Au8\_A

| Atom | X       | Y       | Z       | Charges  |
|------|---------|---------|---------|----------|
| Pd   | 0.00256 | 0.00091 | 1.80855 | -0.08560 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.48025  | -1.43617 | -0.20668 | 0.12178  |
| Au | -1.48657 | -1.43227 | -0.20132 | 0.12146  |
| Au | -1.48361 | 1.43203  | -0.20116 | 0.12110  |
| Au | 1.48544  | 1.43093  | -0.20313 | 0.12122  |
| Au | -0.00215 | -2.82400 | 1.64545  | -0.06600 |
| Au | 0.00217  | 2.82865  | 1.64032  | -0.06615 |
| Au | -3.18175 | 0.00275  | -1.76525 | -0.13394 |
| Au | 3.18474  | -0.00243 | -1.76131 | -0.13387 |

Pd1Au8\_B

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | 0.00000  | 0.00089  | 0.00000 | -0.12271 |
| Au   | -2.33018 | 1.76145  | 0.00000 | -0.10219 |
| Au   | 0.20617  | 2.73984  | 0.00000 | 0.11453  |
| Au   | 2.57897  | 0.94486  | 0.00000 | 0.11465  |
| Au   | 2.32975  | -1.76207 | 0.00000 | -0.10217 |
| Au   | -0.20660 | -2.73803 | 0.00000 | 0.11442  |
| Au   | -2.57840 | -0.94522 | 0.00000 | 0.11471  |
| Au   | -2.76211 | -3.65540 | 0.00000 | -0.06568 |
| Au   | 2.76240  | 3.65406  | 0.00000 | -0.06556 |

Pd1Au9\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.00583 | -0.13558 | 1.03453  | -0.03200 |
| Au   | 1.22168  | 1.69789  | 0.80432  | 0.12292  |
| Au   | 1.65450  | -1.24744 | 0.88315  | 0.12083  |
| Au   | -0.03250 | -1.49641 | -1.45916 | 0.07265  |
| Au   | -0.41580 | 1.29499  | -1.54096 | 0.08489  |
| Au   | 0.94758  | 0.21550  | 3.09191  | -0.04321 |
| Au   | -2.57922 | -0.42232 | -1.26408 | 0.05775  |
| Au   | 2.21329  | -3.00645 | -1.09011 | -0.12236 |
| Au   | 1.28392  | 3.41451  | -1.28320 | -0.12422 |
| Au   | -3.70776 | -0.37132 | 1.25575  | -0.13726 |

Pd1Au9\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.04578 | -1.52785 | 0.09825  | -0.00158 |
| Au   | 1.69077  | -1.47674 | -0.65625 | 0.08577  |
| Au   | 0.88422  | -0.21789 | 1.96003  | 0.01144  |
| Au   | 1.42403  | 1.46016  | -0.34945 | 0.12055  |
| Au   | -1.77245 | -0.01720 | 2.26240  | 0.02884  |
| Au   | -1.41979 | 1.20960  | -0.52708 | 0.12448  |
| Au   | -3.57775 | -0.39888 | -0.03202 | -0.11702 |
| Au   | 3.47987  | 0.02045  | 0.83646  | -0.09725 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -0.03167 | -3.01404 | -1.97332 | -0.09297 |
| Au | -0.06830 | 3.32417  | -1.57798 | -0.06226 |

Pd1Au9\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -3.01993 | -0.23322 | 0.00000  | 0.03874  |
| Au   | 1.31104  | 1.00877  | 1.50144  | 0.12063  |
| Au   | -1.11435 | 1.68568  | 0.00000  | -0.06464 |
| Au   | 1.31104  | 1.00877  | -1.50144 | 0.12063  |
| Au   | -0.75277 | -0.98392 | 1.47239  | 0.09433  |
| Au   | -0.75277 | -0.98392 | -1.47239 | 0.09433  |
| Au   | -2.22020 | -2.88724 | 0.00000  | -0.09890 |
| Au   | 1.35437  | 3.30726  | 0.00000  | -0.11184 |
| Au   | 1.31104  | -1.00980 | 3.27220  | -0.09664 |
| Au   | 1.31104  | -1.00980 | -3.27220 | -0.09664 |

Pd1Au9\_D

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | -3.68112 | 0.26127  |
| Au   | 0.00000  | 1.42163  | -1.18493 | 0.04002  |
| Au   | -1.41190 | 0.00000  | 0.84905  | 0.07173  |
| Au   | 0.00000  | -1.42163 | -1.18493 | 0.04002  |
| Au   | 1.41190  | 0.00000  | 0.84905  | 0.07173  |
| Au   | 0.00000  | 0.00000  | 3.42119  | 0.11030  |
| Au   | -2.69690 | 0.00000  | 3.24690  | -0.11643 |
| Au   | 2.69690  | 0.00000  | 3.24690  | -0.11643 |
| Au   | 0.00000  | 2.70609  | -3.54989 | -0.18110 |
| Au   | 0.00000  | -2.70609 | -3.54989 | -0.18110 |

Pd1Au10\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.55253 | -0.44517 | 0.00000  | -0.07776 |
| Au   | 1.59654  | 0.73330  | 1.48198  | 0.10567  |
| Au   | -0.70653 | 1.72097  | 0.00000  | 0.03038  |
| Au   | 1.59654  | 0.73330  | -1.48198 | 0.10567  |
| Au   | -0.35923 | -1.34425 | 1.47592  | 0.10270  |
| Au   | -0.35923 | -1.34425 | -1.47592 | 0.10270  |
| Au   | -1.97316 | -3.10291 | 0.00000  | -0.04997 |
| Au   | 1.84666  | 3.03372  | 0.00000  | -0.04538 |
| Au   | 1.59654  | -1.16336 | 3.38060  | -0.09133 |
| Au   | 1.59654  | -1.16336 | -3.38060 | -0.09133 |
| Au   | -3.34836 | 2.15605  | 0.00000  | -0.09136 |

Pd1Au10\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.99980 | -0.10209 | 0.00219  | -0.20226 |
| Au   | 0.95084  | 1.50214  | 1.42991  | 0.14109  |
| Au   | 1.16305  | -1.37190 | 1.44772  | 0.13876  |
| Au   | 1.14871  | -1.39516 | -1.44205 | 0.13907  |
| Au   | 0.94933  | 1.48007  | -1.44390 | 0.14077  |
| Au   | -0.84462 | -0.06465 | 2.84868  | -0.01089 |
| Au   | -0.85829 | -0.08842 | -2.84437 | -0.01030 |
| Au   | 2.62444  | -3.16478 | 0.01101  | -0.16953 |
| Au   | 2.15061  | 3.46754  | -0.02204 | -0.16324 |
| Au   | -3.34572 | -0.14925 | 1.39001  | -0.00130 |
| Au   | -3.35620 | -0.15614 | -1.37625 | -0.00218 |

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.09602 | 0.12768  | 0.00000  | -0.15314 |
| Au   | -1.80807 | 2.42962  | 1.50797  | -0.09682 |
| Au   | 0.58500  | 2.44869  | 0.00000  | 0.17118  |
| Au   | 1.49469  | -0.01613 | -1.47107 | 0.12735  |
| Au   | -0.92616 | 0.06820  | 2.82311  | 0.06106  |
| Au   | 1.49469  | -0.01613 | 1.47107  | 0.12735  |
| Au   | -1.80807 | 2.42962  | -1.50797 | -0.09682 |
| Au   | -0.92616 | 0.06820  | -2.82311 | 0.06106  |
| Au   | -0.18915 | -2.27423 | 1.48451  | 0.03947  |
| Au   | -0.18915 | -2.27423 | -1.48451 | 0.03947  |
| Au   | -0.33045 | -4.55584 | 0.00000  | -0.18938 |
| Au   | 3.24101  | 1.61788  | 0.00000  | -0.09077 |

Pd1Au10\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.34295 | 1.04222  | 1.65461  | -0.10885 |
| Au   | 2.13157  | 0.97122  | 0.16051  | 0.11449  |
| Au   | -0.47095 | 1.33190  | -1.15395 | 0.15093  |
| Au   | -2.62510 | -0.05494 | 0.22786  | 0.14031  |
| Au   | 1.91265  | -1.79903 | -0.46010 | 0.06591  |
| Au   | -0.55798 | -1.55787 | -1.63009 | 0.00251  |
| Au   | 0.69251  | 3.30980  | 0.39243  | -0.00611 |
| Au   | -0.34908 | -1.75967 | 1.15487  | 0.06893  |
| Au   | -2.23980 | -0.62268 | 2.88395  | -0.06386 |
| Au   | -2.63609 | 0.18064  | -2.52623 | -0.14654 |
| Au   | 4.34198  | -0.60623 | -0.01269 | -0.21771 |

Pd1Au11\_C

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.29007 | -0.70285 | 0.00000  | -0.01435 |
| Au   | -0.35795 | -0.50658 | 2.92607  | 0.08301  |
| Au   | -1.59428 | 1.61448  | 1.40131  | 0.03888  |
| Au   | -1.59428 | 1.61448  | -1.40131 | 0.03888  |
| Au   | 2.19293  | -0.22916 | 1.35956  | 0.00868  |
| Au   | 0.84315  | 1.92330  | 0.00000  | 0.12742  |
| Au   | -2.61475 | -1.15161 | 1.46201  | -0.05268 |
| Au   | -2.61475 | -1.15161 | -1.46201 | -0.05268 |
| Au   | 2.19293  | -0.22916 | -1.35956 | 0.00868  |
| Au   | -0.35795 | -0.50658 | -2.92607 | 0.08301  |
| Au   | 2.03693  | -0.48416 | -4.12213 | -0.13443 |
| Au   | 2.03693  | -0.48416 | 4.12213  | -0.13443 |

Pd1Au11\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.40147  | 0.72660  | -0.08857 | -0.00891 |
| Au   | -0.53027 | -1.77335 | -1.27687 | 0.08500  |
| Au   | -0.47188 | -1.57701 | 1.51204  | 0.08961  |
| Au   | -2.13542 | 0.80690  | 1.42034  | 0.11899  |
| Au   | -2.20446 | 0.59919  | -1.47914 | 0.11402  |
| Au   | 1.89702  | -1.70658 | 0.06561  | 0.01062  |
| Au   | -1.37336 | 2.90016  | -0.20777 | 0.00886  |
| Au   | -2.38437 | -1.01104 | 3.39558  | -0.15009 |
| Au   | -2.51635 | -1.48738 | -3.15354 | -0.15087 |
| Au   | 3.23189  | 0.97994  | -0.07071 | 0.08780  |
| Au   | 1.63046  | 3.15620  | -0.17408 | -0.09502 |
| Au   | 4.62296  | -1.31011 | 0.02010  | -0.10998 |

Pd1Au12\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.91907 | 0.05845  | 0.00000  | -0.21836 |
| Au   | -2.13219 | -1.99005 | 1.53366  | -0.00512 |
| Au   | 0.63695  | -1.87654 | 1.49664  | 0.15288  |
| Au   | 2.01590  | 0.29365  | 0.00000  | 0.09263  |
| Au   | -2.13219 | -1.99005 | -1.53366 | -0.00512 |
| Au   | 0.63695  | -1.87654 | -1.49664 | 0.15288  |
| Au   | -0.90930 | 0.14242  | 2.86518  | 0.11377  |
| Au   | 0.54488  | 2.20682  | 1.39006  | 0.07297  |
| Au   | -0.90930 | 0.14242  | -2.86518 | 0.11377  |
| Au   | 0.54488  | 2.20682  | -1.39006 | 0.07297  |
| Au   | -0.34721 | 2.55197  | -3.96944 | -0.20469 |
| Au   | -0.34721 | 2.55197  | 3.96944  | -0.20469 |
| Au   | 2.93301  | -2.39694 | 0.00000  | -0.13386 |

Pd1Au11\_B

Pd1Au12\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.85664 | -0.35274 | 0.00000  | -0.18360 |
| Au   | 2.45635  | 1.00398  | 1.48433  | 0.10884  |
| Au   | 0.01597  | 1.71062  | 0.00000  | -0.00539 |
| Au   | 2.45635  | 1.00398  | -1.48433 | 0.10884  |
| Au   | 0.47353  | -1.07447 | 1.43310  | 0.09254  |
| Au   | 0.47353  | -1.07447 | -1.43310 | 0.09254  |
| Au   | -1.09025 | -2.98755 | 0.00000  | 0.03773  |
| Au   | 2.43613  | 3.31039  | 0.00000  | -0.04487 |
| Au   | 2.45635  | -0.93940 | 3.33016  | -0.09363 |
| Au   | 2.45635  | -0.93940 | -3.33016 | -0.09363 |
| Au   | -2.66408 | 2.29365  | 0.00000  | 0.01228  |
| Au   | -4.57333 | 0.27047  | 0.00000  | -0.00608 |
| Au   | -3.81580 | -2.37239 | 0.00000  | -0.02557 |

Pd1Au13\_A

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00337 | 0.00891  | -0.72560 | 0.05913  |
| Au   | -2.94922 | -0.03895 | -0.58808 | 0.03874  |
| Au   | -1.51839 | 0.72999  | 1.68221  | 0.13469  |
| Au   | 1.45802  | 0.87308  | 1.67941  | 0.13313  |
| Au   | -1.26731 | -2.54204 | -0.71302 | 0.05277  |
| Au   | 0.09689  | -1.79579 | 1.61464  | 0.12786  |
| Au   | -1.61523 | 2.39470  | -0.57262 | 0.07002  |
| Au   | 1.35842  | 2.53393  | -0.57844 | 0.07133  |
| Au   | 1.50797  | -2.41218 | -0.72188 | 0.04930  |
| Au   | 2.93206  | 0.24701  | -0.60481 | 0.03669  |
| Au   | 4.07531  | -2.01573 | -1.58208 | -0.18020 |
| Au   | -3.86378 | -2.40190 | -1.56998 | -0.18501 |
| Au   | -0.23061 | 4.55783  | -1.49587 | -0.22482 |
| Au   | 0.01782  | -0.13514 | 3.87301  | -0.18362 |

Pd1Au13\_B

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.28409  | 0.23943  | -0.84010 | -0.17806 |
| Au   | -1.74131 | -1.30254 | -2.04346 | -0.00668 |
| Au   | -1.69813 | -1.32298 | 0.87381  | 0.16292  |
| Au   | 0.48834  | 0.26262  | 2.06932  | 0.09196  |
| Au   | 0.90632  | -2.06129 | -2.33463 | 0.05009  |
| Au   | 1.14172  | -2.17397 | 0.47827  | 0.14084  |
| Au   | -2.54466 | 1.19203  | -0.40516 | 0.11972  |
| Au   | -0.17736 | -2.37235 | 2.93767  | -0.14514 |
| Au   | -0.24954 | 2.58720  | 0.70088  | 0.07053  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 3.03166  | -0.72770 | -1.01270 | 0.03652  |
| Au | 2.38018  | 1.66987  | 0.56959  | 0.07446  |
| Au | -2.40279 | 3.88844  | -0.38487 | -0.15064 |
| Au | -4.14345 | -1.04915 | -0.41461 | -0.06979 |
| Au | 4.84360  | 1.27042  | -0.54494 | -0.19676 |

**Pd<sub>n</sub>Au<sub>m</sub> clusters (n ≤ 2, m ≤ 2)**

Pd2Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.41933  | 0.00000  | 1.14880  | 0.01831  |
| Pd   | -1.41933 | 0.00000  | 1.14880  | 0.01831  |
| Au   | 0.00000  | 1.44712  | -0.66892 | -0.01831 |
| Au   | 0.00000  | -1.44712 | -0.66892 | -0.01831 |

Pd2Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.96800  | -0.89290 | -1.47956 | 0.17207  |
| Pd   | -0.96800 | 0.89290  | -1.47956 | 0.17207  |
| Au   | 0.00000  | 0.00000  | 0.97998  | 0.07414  |
| Au   | 0.00000  | 2.63977  | 0.37153  | -0.20914 |
| Au   | 0.00000  | -2.63977 | 0.37153  | -0.20914 |

Pd2Au4

| Atom | X        | Y        | Z       | Charges  |
|------|----------|----------|---------|----------|
| Pd   | -1.45237 | -0.97570 | 0.00000 | 0.23848  |
| Pd   | 1.45150  | -0.97478 | 0.00000 | 0.23822  |
| Au   | 0.00000  | 1.48018  | 0.00000 | 0.05032  |
| Au   | 2.67262  | 1.43450  | 0.00000 | -0.15820 |
| Au   | 0.00018  | -3.21360 | 0.00000 | -0.21051 |
| Au   | -2.67229 | 1.43464  | 0.00000 | -0.15832 |

Pd2Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.37184  | 0.00125  | -1.27595 | 0.17890  |
| Pd   | 1.37108  | 0.00146  | 1.27725  | 0.17934  |
| Au   | -0.85149 | 1.44850  | -0.00084 | 0.07122  |
| Au   | 1.62980  | -2.53714 | -0.00049 | -0.17726 |
| Au   | -0.84806 | -1.45063 | 0.00036  | 0.07134  |
| Au   | 1.62363  | 2.54099  | 0.00012  | -0.17737 |
| Au   | -3.15102 | -0.00330 | 0.00009  | -0.14618 |

| Pd2Au6 |          |          |          |          |
|--------|----------|----------|----------|----------|
| Atom   | X        | Y        | Z        | Charges  |
| Pd     | 0.48582  | 0.01860  | 1.43083  | 0.01365  |
| Pd     | -0.09777 | 0.02134  | -1.20707 | 0.00112  |
| Au     | 1.21110  | 2.44293  | 0.09274  | -0.04609 |
| Au     | 2.59161  | 0.13149  | -0.63257 | 0.03452  |
| Au     | 1.49582  | -2.31125 | 0.15218  | -0.04655 |
| Au     | -1.22822 | -2.02140 | 0.47441  | 0.03408  |
| Au     | -1.45092 | 1.87006  | 0.56730  | 0.03588  |
| Au     | -2.84534 | -0.13508 | -0.78434 | -0.02660 |

| Pd2Au7 |          |          |          |          |
|--------|----------|----------|----------|----------|
| Atom   | X        | Y        | Z        | Charges  |
| Pd     | -0.95073 | 1.80520  | -0.30402 | 0.08236  |
| Pd     | -0.15220 | 0.28385  | 1.74230  | 0.05792  |
| Au     | 0.91904  | -1.69137 | -0.10289 | 0.12008  |
| Au     | -3.07037 | 0.91110  | -1.81257 | -0.13872 |
| Au     | -0.91695 | -2.46055 | 1.78591  | -0.07957 |
| Au     | 2.98155  | -0.98026 | -1.69870 | -0.13011 |
| Au     | 0.83513  | 2.88040  | 1.49198  | -0.10710 |
| Au     | 1.82990  | 1.02973  | -0.26518 | 0.11269  |
| Au     | -1.93608 | -0.90545 | -0.23604 | 0.08246  |

| Pd2Au8 |          |          |          |          |
|--------|----------|----------|----------|----------|
| Atom   | X        | Y        | Z        | Charges  |
| Pd     | -0.00158 | 0.00015  | -2.00092 | -0.10223 |
| Pd     | 0.00129  | -0.00086 | 2.00099  | -0.10225 |
| Au     | 1.53105  | 2.35267  | 1.93369  | -0.09106 |
| Au     | -0.42946 | 2.03734  | -0.00104 | 0.14214  |
| Au     | -2.35434 | 1.53201  | -1.93153 | -0.09101 |
| Au     | 2.03757  | 0.42933  | 0.00126  | 0.14204  |
| Au     | 2.35320  | -1.52881 | -1.93468 | -0.09111 |
| Au     | 0.43047  | -2.03820 | -0.00154 | 0.14237  |
| Au     | -1.53087 | -2.35328 | 1.93253  | -0.09096 |
| Au     | -2.03745 | -0.43065 | 0.00128  | 0.14208  |

| Pd2Au9 |         |          |          |          |
|--------|---------|----------|----------|----------|
| Atom   | X       | Y        | Z        | Charges  |
| Pd     | 0.29677 | -0.18782 | 1.49726  | -0.04684 |
| Pd     | 2.61575 | 0.02716  | 0.06842  | 0.11733  |
| Au     | 0.58864 | -0.40031 | -1.95060 | 0.05892  |
| Au     | 0.43940 | 2.01460  | -0.28517 | 0.13713  |
| Au     | 0.88411 | -2.43232 | -0.02520 | 0.07866  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -1.63771 | -1.60369 | -0.85355 | 0.03596  |
| Au | -2.16843 | 0.86046  | 0.50631  | 0.11219  |
| Au | -0.62401 | 2.37651  | 2.22452  | -0.01155 |
| Au | 2.60899  | -1.79431 | 2.08070  | -0.16929 |
| Au | 2.41107  | 1.72468  | -2.17259 | -0.11775 |
| Au | -4.19796 | -0.65208 | -0.43610 | -0.19476 |

| Pd2Au10 |          |          |          |          |
|---------|----------|----------|----------|----------|
| Atom    | X        | Y        | Z        | Charges  |
| Pd      | 0.58143  | 1.34367  | -1.58418 | -0.12232 |
| Pd      | 0.57367  | -1.34151 | 1.58401  | -0.12234 |
| Au      | -2.00477 | -1.40510 | 0.24400  | 0.08958  |
| Au      | 0.45421  | -1.50443 | -1.27000 | 0.12893  |
| Au      | 2.60575  | -0.00299 | 0.00103  | 0.17822  |
| Au      | 0.45892  | 1.50694  | 1.27040  | 0.12900  |
| Au      | -1.99776 | 1.40383  | -0.24741 | 0.08963  |
| Au      | 2.46731  | -0.31437 | -2.76920 | -0.08829 |
| Au      | -4.30602 | 0.00534  | 0.00128  | -0.11069 |
| Au      | 2.46565  | 0.30858  | 2.77107  | -0.08825 |
| Au      | -0.41049 | -3.63130 | 0.32765  | -0.04175 |
| Au      | -0.40538 | 3.63226  | -0.32871 | -0.04171 |

| Pd2Au11 |          |          |          |          |
|---------|----------|----------|----------|----------|
| Atom    | X        | Y        | Z        | Charges  |
| Pd      | -1.19596 | -1.93706 | 0.66827  | 0.11057  |
| Pd      | -0.07492 | -0.06440 | -0.87394 | -0.10277 |
| Au      | -1.56447 | -2.28266 | -2.03852 | -0.08962 |
| Au      | 0.00168  | 0.40834  | 2.02478  | 0.09885  |
| Au      | 1.49172  | -2.11898 | -1.89889 | 0.03066  |
| Au      | 1.69309  | -1.76973 | 0.84789  | 0.13752  |
| Au      | -2.94994 | -0.20515 | -0.86987 | 0.11037  |
| Au      | -1.58557 | 2.05486  | 0.43392  | 0.07298  |
| Au      | 2.81508  | 0.15369  | -0.94665 | 0.08378  |
| Au      | 1.18811  | 2.28226  | 0.33133  | 0.04914  |
| Au      | 3.71522  | 2.68914  | -0.67730 | -0.18793 |
| Au      | -4.25222 | 2.08124  | -0.22425 | -0.19890 |
| Au      | 0.18731  | -2.12760 | 3.13732  | -0.11466 |

| Pd2Au12 |          |          |          |          |
|---------|----------|----------|----------|----------|
| Atom    | X        | Y        | Z        | Charges  |
| Pd      | -1.87560 | -1.29674 | 1.36838  | -0.11193 |
| Pd      | 0.30991  | 0.28478  | -1.11402 | -0.12942 |
| Au      | -1.59006 | -1.71567 | -1.42361 | 0.14783  |
| Au      | 0.33271  | 0.49719  | 1.82186  | 0.10941  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.03886  | -2.22853 | -2.33533 | -0.04273 |
| Au | 0.74641  | -2.08200 | 0.46910  | 0.17258  |
| Au | -2.57808 | 0.91699  | -0.30675 | 0.10694  |
| Au | 0.15721  | -1.94283 | 3.16936  | -0.09507 |
| Au | -0.36260 | 2.71572  | 0.24892  | 0.05531  |
| Au | 2.93782  | -0.65720 | -0.99442 | 0.10812  |
| Au | 2.26681  | 1.88941  | 0.33439  | 0.02787  |
| Au | -2.81733 | 3.60547  | -0.58559 | -0.18100 |
| Au | -4.08912 | -1.44683 | -0.32094 | -0.01201 |
| Au | 4.86904  | 1.03751  | -0.22509 | -0.15589 |

Pd3Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.11724 | -1.38248 | -0.68148 | 0.15274  |
| Pd   | -0.11782 | 1.38424  | -0.68052 | 0.15310  |
| Pd   | 0.24659  | -0.00012 | 1.53496  | 0.14507  |
| Au   | 2.35842  | -0.00035 | -0.11682 | -0.21938 |
| Au   | -2.36514 | -0.00061 | 0.01611  | -0.23152 |

Pd3Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.07593  | -1.14295 | -0.01919 | 0.03201  |
| Pd   | 1.06682  | 0.99656  | 1.33464  | 0.12304  |
| Pd   | 1.08437  | 1.03101  | -1.30623 | 0.11980  |
| Au   | -2.67829 | -1.05483 | 0.00049  | -0.08359 |
| Au   | -1.40201 | 1.32528  | -0.00339 | -0.00435 |
| Au   | 2.78350  | -0.78555 | -0.00248 | -0.18691 |

Pd3Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.24489 | 0.28483  | 1.28116  | 0.17572  |
| Pd   | 0.30619  | -1.68618 | -0.00293 | 0.15859  |
| Pd   | -1.24645 | 0.28799  | -1.27714 | 0.17424  |
| Au   | 1.34282  | 0.98406  | 0.00058  | 0.04890  |
| Au   | -0.66744 | 2.78186  | -0.00088 | -0.14831 |
| Au   | 2.96868  | -1.15023 | 0.00002  | -0.16891 |
| Au   | -2.37169 | -1.96740 | -0.00036 | -0.24023 |

Pd3Au5

| Atom | X       | Y       | Z        | Charges |
|------|---------|---------|----------|---------|
| Pd   | 3.03980 | 0.00099 | -0.01196 | 0.18224 |
| Pd   | 0.79945 | 0.00068 | -1.39275 | 0.06384 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 0.81643  | 0.00104  | 1.39398  | 0.06340  |
| Au | -3.36513 | -0.00306 | -0.00882 | -0.11962 |
| Au | -1.13653 | -1.56360 | 0.00884  | 0.06249  |
| Au | -1.14012 | 1.56275  | 0.00843  | 0.06267  |
| Au | 1.46782  | -2.44352 | -0.00117 | -0.15743 |
| Au | 1.46306  | 2.44585  | -0.00103 | -0.15760 |

Pd3Au6

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.74274 | 0.38104  | 1.27547  | 0.04849  |
| Pd   | 0.74438  | 0.37517  | -1.27738 | 0.04856  |
| Pd   | -0.00276 | -2.00024 | 0.00127  | 0.12008  |
| Au   | -2.43068 | -1.80321 | 1.19566  | -0.11042 |
| Au   | 2.42645  | -1.81239 | -1.19230 | -0.11046 |
| Au   | 2.09580  | -0.21087 | 1.14003  | 0.05620  |
| Au   | -2.09640 | -0.21026 | -1.13958 | 0.05621  |
| Au   | 1.07577  | 2.38135  | 0.98908  | -0.05415 |
| Au   | -1.07029 | 2.37974  | -0.99251 | -0.05450 |

Pd3Au7

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.07516 | 2.04956  | -0.25220 | 0.07829  |
| Pd   | 0.11179  | -0.22276 | -1.98956 | -0.09408 |
| Pd   | -0.12027 | 0.50431  | 1.91768  | 0.04953  |
| Au   | -2.26430 | 2.20677  | 1.50013  | -0.12430 |
| Au   | -2.10808 | 0.02687  | -0.16591 | 0.12907  |
| Au   | -1.78020 | -2.27182 | -1.68350 | -0.08977 |
| Au   | 2.02140  | 1.79614  | -2.13956 | -0.09262 |
| Au   | 2.14102  | 0.18538  | 0.04671  | 0.12028  |
| Au   | 1.94332  | -1.38741 | 2.31429  | -0.11531 |
| Au   | 0.09554  | -1.91328 | 0.31656  | 0.13892  |

Pd3Au8

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.72484  | 0.26843  | -1.79551 | -0.08490 |
| Pd   | -1.50668 | -0.28245 | 1.72712  | -0.08009 |
| Pd   | 1.13878  | -1.32131 | 1.13853  | -0.05696 |
| Au   | 1.68400  | -2.35002 | -1.41600 | -0.02664 |
| Au   | 0.63931  | 1.47752  | 0.81060  | 0.09984  |
| Au   | -0.95703 | -1.77144 | -0.67108 | 0.11242  |
| Au   | -1.82802 | 1.10950  | -0.77233 | 0.12676  |
| Au   | 0.06944  | 2.96233  | -1.52268 | -0.09314 |
| Au   | 0.68131  | 0.31650  | 3.31934  | -0.10287 |
| Au   | 3.03954  | 0.00308  | -0.32502 | 0.13160  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -3.53637 | -0.96994 | -0.04595 | -0.02604 |
|----|----------|----------|----------|----------|

Pd3Au9

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 2.59882  | -0.30060 | 0.10116  | 0.12534  |
| Pd   | 0.56072  | -1.22194 | 1.54821  | 0.03021  |
| Pd   | 0.81114  | 1.28102  | -1.62574 | -0.11811 |
| Au   | -1.70645 | 1.39444  | -0.25277 | 0.09096  |
| Au   | 0.83612  | 1.66432  | 1.18200  | 0.11488  |
| Au   | 0.37361  | -1.52639 | -1.32432 | 0.10140  |
| Au   | -2.05177 | -1.38958 | 0.22235  | 0.08208  |
| Au   | 2.47170  | 0.24662  | 2.86932  | -0.12360 |
| Au   | -4.16622 | 0.28002  | 0.11972  | -0.10337 |
| Au   | 2.51659  | -0.59102 | -2.72335 | -0.08619 |
| Au   | -0.15188 | 3.64468  | -0.51587 | -0.05443 |
| Au   | -0.43375 | -3.58246 | 0.40916  | -0.05917 |

Pd3Au10

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.42972  | -1.67242 | 0.00414  | -0.13122 |
| Pd   | 0.42958  | 0.83651  | 1.44192  | -0.13196 |
| Pd   | 0.43026  | 0.82914  | -1.44442 | -0.13226 |
| Au   | 0.33163  | -1.64591 | 2.86505  | -0.03093 |
| Au   | 0.33248  | 3.30388  | -0.00774 | -0.03090 |
| Au   | 0.33279  | -1.65909 | -2.85689 | -0.03088 |
| Au   | 2.70988  | -0.84034 | -1.44788 | 0.06866  |
| Au   | 2.71022  | 1.67635  | -0.00371 | 0.06849  |
| Au   | 2.70908  | -0.83350 | 1.45202  | 0.06896  |
| Au   | -1.90795 | -0.86082 | -1.48389 | 0.16658  |
| Au   | -1.90871 | 1.71654  | -0.00470 | 0.16656  |
| Au   | -1.90798 | -0.85360 | 1.48675  | 0.16654  |
| Au   | -4.15232 | 0.00041  | 0.00003  | -0.21765 |

Pd3Au11

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.48620  | 0.00007  | 1.84553  | 0.03786  |
| Pd   | -0.55272 | 2.32103  | 0.91410  | -0.07970 |
| Pd   | -0.55240 | -2.32078 | 0.91380  | -0.07963 |
| Au   | 1.97510  | -1.47000 | -0.17329 | 0.14553  |
| Au   | 1.97440  | 1.47020  | -0.17376 | 0.14554  |
| Au   | -2.32091 | 0.00002  | 0.82841  | 0.11416  |
| Au   | -1.38365 | -1.41349 | -1.64881 | 0.05822  |
| Au   | -1.38311 | 1.41338  | -1.64862 | 0.05824  |
| Au   | 0.83331  | -0.00046 | -2.46246 | 0.00819  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | 1.73915  | -2.48223 | 2.36866  | -0.03784 |
| Au | 1.73915  | 2.48240  | 2.36833  | -0.03785 |
| Au | -3.20338 | -2.55171 | 0.17183  | -0.07680 |
| Au | -3.20345 | 2.55163  | 0.17148  | -0.07674 |
| Au | 3.59378  | 0.00008  | -1.94073 | -0.17916 |

Pd4Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.31053  | 1.72821  | -0.00017 | 0.10581  |
| Pd   | -0.00022 | -0.46284 | -1.28362 | 0.11649  |
| Pd   | -0.00004 | -0.46256 | 1.28390  | 0.11655  |
| Pd   | -1.30997 | 1.72834  | 0.00000  | 0.10578  |
| Au   | -2.49562 | -0.73678 | -0.00003 | -0.22231 |
| Au   | 2.49545  | -0.73705 | -0.00003 | -0.22232 |

Pd4Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.95674  | 1.40607  | 0.00253  | 0.12289  |
| Pd   | -1.15534 | 0.00204  | 1.28414  | 0.18333  |
| Pd   | 0.95304  | -1.40703 | -0.00050 | 0.12261  |
| Pd   | -1.15303 | 0.00049  | -1.28086 | 0.18192  |
| Au   | -1.50026 | -2.50308 | -0.00062 | -0.21189 |
| Au   | -1.49539 | 2.50520  | -0.00208 | -0.21187 |
| Au   | 3.22774  | -0.00304 | -0.00039 | -0.18700 |

Pd4Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.31421 | 0.69475  | -1.35055 | 0.13511  |
| Pd   | 1.31427  | 0.69267  | 1.35243  | 0.13545  |
| Pd   | -1.31313 | 0.69643  | 1.34957  | 0.13449  |
| Pd   | 1.31394  | 0.69381  | -1.34898 | 0.13453  |
| Au   | -0.00166 | -1.59216 | -0.00013 | 0.05415  |
| Au   | 0.00375  | 2.83304  | -0.00082 | -0.25551 |
| Au   | 2.68596  | -1.43168 | -0.00108 | -0.16927 |
| Au   | -2.68856 | -1.42657 | 0.00059  | -0.16895 |

Pd4Au5

| Atom | X        | Y        | Z        | Charges |
|------|----------|----------|----------|---------|
| Pd   | 2.53318  | -0.00056 | 1.37036  | 0.04606 |
| Pd   | -0.18339 | 0.00020  | -1.30246 | 0.06532 |
| Pd   | 2.53266  | 0.01285  | -1.36896 | 0.04679 |
| Pd   | -0.18334 | -0.00154 | 1.30297  | 0.06578 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -1.34581 | -2.35472 | 0.00198  | -0.02117 |
| Au | 1.38550  | 2.14523  | 0.01007  | -0.05051 |
| Au | -2.81378 | -0.00781 | 0.00541  | -0.08068 |
| Au | 1.39725  | -2.13841 | -0.00863 | -0.05042 |
| Au | -1.35935 | 2.34934  | -0.00994 | -0.02116 |

|    |         |          |          |         |
|----|---------|----------|----------|---------|
| Au | 2.49107 | -0.00453 | 1.26705  | 0.10538 |
| Au | 2.03211 | 1.44366  | -1.22098 | 0.04787 |
| Au | 2.03166 | -1.43283 | -1.23220 | 0.04821 |

Pd4Au6

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.01339 | 1.43870  | 1.33138  | 0.06638  |
| Pd   | -0.01399 | -1.45035 | 1.32321  | 0.06701  |
| Pd   | -0.01314 | -1.44154 | -1.33376 | 0.06741  |
| Pd   | -0.01335 | 1.44847  | -1.32484 | 0.06717  |
| Au   | 2.04852  | 2.75180  | 0.00790  | -0.13880 |
| Au   | 2.12769  | 0.00055  | 0.00147  | 0.12063  |
| Au   | 2.05009  | -2.75004 | -0.00848 | -0.13901 |
| Au   | -1.99667 | -0.00804 | 2.70284  | -0.11033 |
| Au   | -2.20096 | -0.00016 | 0.00056  | 0.11028  |
| Au   | -1.99729 | 0.00864  | -2.70196 | -0.11075 |

Pd4Au9

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.26421 | 0.69455  | -1.49527 | -0.10383 |
| Pd   | -0.26589 | 0.83877  | 1.29811  | -0.05109 |
| Pd   | -0.46155 | -1.77264 | 0.20833  | -0.12483 |
| Pd   | 1.86527  | -0.77291 | 1.69993  | 0.11388  |
| Au   | -0.11377 | 3.26284  | -0.26435 | -0.05202 |
| Au   | -0.46597 | -1.44081 | 3.02122  | -0.09091 |
| Au   | -0.27115 | -1.93187 | -2.60872 | -0.02384 |
| Au   | -2.63589 | -0.83351 | -1.42074 | 0.05909  |
| Au   | -2.70042 | -0.57752 | 1.46885  | 0.11458  |
| Au   | -2.56816 | 1.76200  | -0.19519 | 0.01978  |
| Au   | 1.95418  | -1.11905 | -1.15852 | 0.14886  |
| Au   | 2.09476  | 1.63023  | -0.07558 | 0.15995  |
| Au   | 4.19773  | -0.16291 | 0.23670  | -0.16962 |

Pd4Au7

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.77269  | 0.66586  | 1.59927  | -0.03847 |
| Pd   | -1.65858 | -0.84404 | -1.33533 | 0.06999  |
| Pd   | -1.65477 | -0.83911 | 1.32874  | 0.07310  |
| Pd   | 0.78000  | 0.66371  | -1.60066 | -0.03765 |
| Au   | 1.19811  | 2.92659  | 0.00043  | -0.03972 |
| Au   | 0.84225  | -1.72740 | 0.00239  | 0.09889  |
| Au   | -1.32309 | 1.74828  | -0.00790 | 0.10173  |
| Au   | 0.52215  | -1.85510 | 2.73478  | -0.11562 |
| Au   | 0.52810  | -1.86153 | -2.72877 | -0.11441 |
| Au   | 2.99181  | 0.53964  | 0.00180  | 0.07822  |
| Au   | -3.73414 | 0.43540  | 0.00192  | -0.07607 |

Pd4Au10

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.00000  | 0.00000  | -4.54935 | 0.00249  |
| Pd   | 0.00000  | -1.67940 | -0.19901 | -0.12895 |
| Pd   | -1.45440 | 0.83970  | -0.19901 | -0.12895 |
| Pd   | 1.45440  | 0.83970  | -0.19901 | -0.12895 |
| Au   | 0.00000  | 0.00000  | 4.34957  | -0.16998 |
| Au   | 0.00000  | 1.71870  | 2.11776  | 0.16360  |
| Au   | 0.00000  | 1.74634  | -2.45890 | 0.06050  |
| Au   | 0.00000  | 3.32705  | -0.10984 | -0.03932 |
| Au   | 1.48844  | -0.85935 | 2.11776  | 0.16360  |
| Au   | 1.51237  | -0.87317 | -2.45890 | 0.06050  |
| Au   | -1.48844 | -0.85935 | 2.11776  | 0.16360  |
| Au   | -1.51237 | -0.87317 | -2.45890 | 0.06050  |
| Au   | 2.88131  | -1.66352 | -0.10984 | -0.03932 |
| Au   | -2.88131 | -1.66352 | -0.10984 | -0.03932 |

Pd4Au8

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.10187  | -1.45917 | 0.89594  | -0.12082 |
| Pd   | -0.41414 | 0.00595  | -1.57131 | -0.10345 |
| Pd   | 0.10111  | 1.45011  | 0.90603  | -0.12119 |
| Pd   | -2.06567 | -0.00767 | 2.15522  | -0.02844 |
| Au   | -0.39053 | -2.83148 | -1.53222 | 0.01013  |
| Au   | -0.39090 | 2.84283  | -1.51096 | 0.01023  |
| Au   | 0.51745  | -0.01324 | 3.26559  | -0.01199 |
| Au   | -2.48294 | 1.44766  | -0.20766 | 0.08202  |
| Au   | -2.48218 | -1.44581 | -0.21786 | 0.08203  |

Pd5Au2

| Atom | X        | Y        | Z        | Charges |
|------|----------|----------|----------|---------|
| Pd   | -0.44603 | -0.88597 | 1.24247  | 0.11546 |
| Pd   | -0.40316 | -0.72222 | -1.33153 | 0.10992 |
| Pd   | -0.85754 | 1.65375  | 0.03657  | 0.08593 |
| Pd   | 1.57029  | 1.25488  | -1.25516 | 0.05951 |
| Pd   | 1.40368  | 1.16616  | 1.38106  | 0.08132 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -2.87288 | -0.27796 | -0.02766 | -0.28917 |
| Au | 2.13499  | -1.15829 | -0.01508 | -0.16297 |

Pd5Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.76839  | 0.26510  | 1.44705  | 0.20032  |
| Pd   | 0.22920  | -1.74699 | -0.13070 | 0.11830  |
| Pd   | 1.62686  | 1.05248  | -0.86159 | 0.10007  |
| Pd   | -0.93736 | 0.21996  | -1.42050 | 0.16943  |
| Pd   | -1.80596 | 0.68050  | 1.04082  | 0.10775  |
| Au   | 2.88234  | -1.23268 | 0.09082  | -0.24148 |
| Au   | -2.46567 | -1.81246 | -0.09294 | -0.24499 |
| Au   | -0.34745 | 2.77085  | -0.04160 | -0.20940 |

Pd5Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -2.89134 | -0.00685 | -1.70579 | 0.07938  |
| Pd   | -0.68874 | -1.35384 | -1.01330 | 0.05345  |
| Pd   | -0.69851 | 1.35387  | -1.00834 | 0.05279  |
| Pd   | -0.09104 | -1.33853 | 1.59218  | 0.12586  |
| Pd   | -0.09551 | 1.33379  | 1.59595  | 0.12659  |
| Au   | 1.64444  | 2.71285  | -0.22897 | -0.18395 |
| Au   | 1.66014  | -2.70393 | -0.22923 | -0.18399 |
| Au   | 1.80866  | 0.00502  | -0.18910 | 0.07892  |
| Au   | -2.51329 | -0.00721 | 0.96131  | -0.14905 |

Pd5Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.13894 | 1.45513  | 1.34173  | 0.06761  |
| Pd   | -0.13711 | -1.45667 | 1.34018  | 0.06752  |
| Pd   | -2.24831 | -0.00092 | 0.00005  | 0.17623  |
| Pd   | -0.13722 | -1.45545 | -1.34157 | 0.06755  |
| Pd   | -0.13917 | 1.45648  | -1.34024 | 0.06756  |
| Au   | 1.90816  | 2.75770  | 0.00133  | -0.13853 |
| Au   | 1.98246  | 0.00120  | -0.00034 | 0.13279  |
| Au   | 1.91194  | -2.75540 | -0.00117 | -0.13855 |
| Au   | -2.08579 | -0.00271 | 2.68093  | -0.15109 |
| Au   | -2.08594 | 0.00002  | -2.68083 | -0.15108 |

Pd5Au6

| Atom | X        | Y       | Z        | Charges  |
|------|----------|---------|----------|----------|
| Pd   | -0.69088 | 0.92962 | -1.70930 | -0.03651 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 1.27139  | -1.15034 | 1.32882  | 0.07315  |
| Pd | 1.27064  | -1.15113 | -1.32789 | 0.07298  |
| Pd | -0.69049 | 0.93120  | 1.70878  | -0.03653 |
| Pd | -2.69571 | 1.11212  | -0.00010 | 0.22219  |
| Au | -0.64922 | 3.17453  | -0.00132 | -0.13420 |
| Au | -1.31835 | -1.40492 | 0.00067  | 0.05834  |
| Au | 1.52817  | 1.43409  | -0.00042 | 0.11602  |
| Au | -1.13030 | -1.60301 | -2.73175 | -0.11135 |
| Au | -1.12950 | -1.60059 | 2.73317  | -0.11143 |
| Au | 3.59303  | -0.39109 | -0.00054 | -0.11267 |

Pd5Au7

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00005 | -1.33322 | 0.98290  | -0.04038 |
| Pd   | -0.00103 | 0.00047  | -1.63406 | -0.07397 |
| Pd   | 0.00162  | 1.33299  | 0.98376  | -0.04032 |
| Pd   | -2.30257 | 0.00018  | 1.78634  | 0.04638  |
| Pd   | 2.30614  | -0.00170 | 1.78271  | 0.04631  |
| Au   | -0.00304 | -2.79402 | -1.48802 | 0.01174  |
| Au   | 0.00015  | 2.79485  | -1.48696 | 0.01166  |
| Au   | 0.00315  | -0.00056 | 3.44735  | -0.10117 |
| Au   | -2.33131 | 1.42189  | -0.68369 | 0.03499  |
| Au   | -2.33342 | -1.41893 | -0.68463 | 0.03489  |
| Au   | 2.33174  | 1.41928  | -0.68772 | 0.03500  |
| Au   | 2.33034  | -1.42176 | -0.68818 | 0.03485  |

Pd5Au8

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.45442  | -1.46256 | 0.97823  | -0.00109 |
| Pd   | 0.30433  | 1.32901  | 1.06335  | -0.02931 |
| Pd   | 0.53993  | 0.06887  | -1.49414 | -0.10195 |
| Pd   | 2.55030  | -0.08378 | 1.84393  | 0.12421  |
| Pd   | -1.98319 | -0.08047 | 1.70608  | 0.09393  |
| Au   | 0.17321  | -0.15132 | 3.43783  | -0.12661 |
| Au   | 0.38980  | 2.90769  | -1.30312 | -0.03393 |
| Au   | 0.52004  | -2.77566 | -1.54736 | -0.04468 |
| Au   | 2.87574  | -1.31331 | -0.71501 | 0.01902  |
| Au   | 2.78438  | 1.50481  | -0.50220 | -0.00470 |
| Au   | -1.80818 | -1.45253 | -0.87058 | 0.12914  |
| Au   | -1.90228 | 1.47996  | -0.80984 | 0.12295  |
| Au   | -4.11911 | -0.06632 | -0.07559 | -0.14699 |

Pd5Au9

| Atom | X | Y | Z | Charges |
|------|---|---|---|---------|
|------|---|---|---|---------|

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 0.16324  | 0.03101  | -1.71523 | -0.12087 |
| Pd | 0.00217  | 1.35182  | 0.77441  | -0.01369 |
| Pd | -0.16727 | -1.47312 | 0.89748  | -0.12174 |
| Pd | -2.09445 | 1.62833  | -0.94604 | 0.00479  |
| Pd | 2.09499  | 0.00391  | 1.87974  | 0.00486  |
| Au | 0.28111  | 2.88794  | -1.67481 | -0.07755 |
| Au | -0.27876 | 0.01349  | 3.33657  | -0.07774 |
| Au | -0.00176 | -2.81896 | -1.61499 | -0.03943 |
| Au | -2.25072 | -1.25184 | -1.03798 | 0.13595  |
| Au | -2.42862 | 0.16701  | 1.61364  | 0.15520  |
| Au | 2.24728  | -1.53010 | -0.55424 | 0.13579  |
| Au | 2.43151  | 1.47787  | -0.67467 | 0.15539  |
| Au | 4.46275  | -0.09497 | 0.34312  | -0.07060 |
| Au | -4.46203 | 0.25170  | -0.25509 | -0.07036 |

Pd6Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 2.52827  | 1.53743  | -0.55548 | 0.07783  |
| Pd   | 0.23135  | 0.25903  | -1.38404 | -0.00024 |
| Pd   | 0.77690  | 0.83602  | 1.30423  | 0.02825  |
| Pd   | -1.43451 | 1.88591  | -0.01052 | 0.07923  |
| Pd   | -0.24376 | -1.67737 | 0.36554  | 0.07835  |
| Pd   | -1.84020 | -0.01650 | 1.77656  | 0.05311  |
| Au   | 2.48380  | -1.09664 | 0.03771  | -0.17255 |
| Au   | -2.49431 | -0.54801 | -0.90897 | -0.14397 |

Pd6Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.15664  | -1.04122 | 1.71612  | 0.06262  |
| Pd   | -1.48548 | -0.48757 | 1.71553  | 0.06289  |
| Pd   | 0.31555  | 1.52316  | 1.71610  | 0.06263  |
| Pd   | -0.33869 | -1.62484 | -0.64901 | 0.09376  |
| Pd   | -1.23608 | 1.10853  | -0.64904 | 0.09397  |
| Pd   | 1.58041  | 0.51881  | -0.64566 | 0.09461  |
| Au   | -2.97508 | -0.97644 | -0.62526 | -0.15655 |
| Au   | 0.64354  | 3.06685  | -0.61988 | -0.15703 |
| Au   | 2.33601  | -2.08860 | -0.62050 | -0.15691 |

Pd6Au4

| Atom | X        | Y        | Z        | Charges |
|------|----------|----------|----------|---------|
| Pd   | 1.93722  | -0.82815 | 0.00031  | 0.13531 |
| Pd   | -1.86530 | 0.88618  | -0.00033 | 0.20424 |
| Pd   | 0.65374  | 1.26998  | 1.39493  | 0.08981 |
| Pd   | 0.65358  | 1.26867  | -1.39607 | 0.08978 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -0.63145 | -1.33646 | -1.32028 | 0.05603  |
| Pd | -0.63136 | -1.33525 | 1.32142  | 0.05600  |
| Au | 1.76356  | -0.84566 | 2.69908  | -0.14291 |
| Au | 1.76341  | -0.84808 | -2.69842 | -0.14291 |
| Au | -0.54423 | 3.28576  | -0.00143 | -0.16728 |
| Au | -3.05054 | -1.54833 | 0.00079  | -0.17808 |

Pd6Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.65659 | 1.04343  | -1.55428 | -0.00678 |
| Pd   | -1.61445 | -1.52990 | 0.00133  | -0.00931 |
| Pd   | 0.96037  | -1.31669 | 1.32276  | 0.07057  |
| Pd   | 0.96197  | -1.32066 | -1.31977 | 0.07081  |
| Pd   | -0.65769 | 1.04771  | 1.55184  | -0.00666 |
| Pd   | -2.73560 | 0.81703  | -0.00162 | 0.29126  |
| Au   | -0.01345 | 3.24944  | -0.00391 | -0.13298 |
| Au   | 1.77602  | 1.13655  | -0.00121 | 0.12404  |
| Au   | -1.49187 | -1.28965 | -2.70842 | -0.14496 |
| Au   | -1.49405 | -1.28275 | 2.71059  | -0.14494 |
| Au   | 3.40223  | -1.08044 | 0.00280  | -0.11104 |

Pd6Au6

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 1.13259  | 0.14805  | 1.22129  | -0.09876 |
| Pd   | -0.10015 | 0.76745  | -1.22787 | -0.08850 |
| Pd   | -0.94990 | -1.56901 | 0.16313  | -0.00650 |
| Pd   | 1.84028  | -2.23810 | 0.08862  | 0.11107  |
| Pd   | 0.65278  | -1.64324 | -2.23462 | 0.06753  |
| Pd   | -1.44016 | -0.08420 | 2.29872  | 0.09659  |
| Au   | 1.80507  | 2.52402  | -0.09679 | 0.04966  |
| Au   | -2.10402 | -0.90771 | -2.33025 | -0.05065 |
| Au   | 0.39345  | -2.21007 | 2.54451  | -0.11260 |
| Au   | 2.67837  | 0.10928  | -1.26879 | -0.01336 |
| Au   | -2.69171 | 0.77015  | -0.14631 | 0.08478  |
| Au   | -0.74231 | 2.40390  | 1.11755  | -0.03928 |

Pd6Au7

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.39460 | 0.44051  | -1.35190 | -0.01756 |
| Pd   | -0.07063 | 0.91382  | 1.35868  | -0.01735 |
| Pd   | -0.50216 | -1.78453 | 0.45845  | 0.01282  |
| Pd   | -2.43479 | -0.51180 | 1.76787  | 0.11440  |
| Pd   | 1.66889  | -1.26236 | -1.38484 | 0.08405  |
| Pd   | 2.02328  | -0.78491 | 1.41938  | 0.08511  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -0.07385 | 3.12084  | -0.42073 | -0.04173 |
| Au | -0.08160 | -1.24038 | 3.17515  | -0.12605 |
| Au | -0.80074 | -2.20246 | -2.32571 | -0.09765 |
| Au | -2.90589 | -0.80555 | -1.02357 | 0.08053  |
| Au | -2.58802 | 1.75642  | 0.06913  | -0.06279 |
| Au | 2.13905  | 1.49348  | -0.45988 | 0.10739  |
| Au | 4.14220  | -0.38176 | -0.33480 | -0.12116 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 1.62603  | 0.36815  | -0.92490 | 0.15150  |
| Pd | 0.48189  | 1.56650  | 1.41800  | 0.02622  |
| Au | 2.13068  | -2.30030 | -0.94771 | -0.17477 |
| Au | -3.05351 | -0.69193 | -0.95871 | -0.17474 |
| Au | 0.93154  | 2.99254  | -0.94906 | -0.17489 |

Pd6Au8

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.20355  | -1.57789 | 0.63033  | -0.02039 |
| Pd   | 0.18658  | 1.30271  | 0.95778  | -0.01349 |
| Pd   | 0.01629  | 0.19971  | -1.53413 | -0.00745 |
| Pd   | 2.21219  | -1.34782 | -1.22788 | 0.04646  |
| Pd   | 2.23301  | 1.64858  | -0.84775 | 0.02429  |
| Pd   | -1.95133 | -0.24475 | 1.84178  | -0.02435 |
| Au   | 0.44132  | -0.43010 | 3.25019  | -0.09800 |
| Au   | -0.13824 | 3.07966  | -1.29361 | -0.07890 |
| Au   | -0.13748 | -2.65622 | -2.01896 | -0.07820 |
| Au   | 2.55438  | -0.17829 | 1.44672  | 0.13862  |
| Au   | -2.26848 | -1.41835 | -0.79468 | 0.13427  |
| Au   | -2.28279 | 1.59120  | -0.41523 | 0.13856  |
| Au   | -4.36570 | -0.04204 | 0.38430  | -0.07595 |
| Au   | 4.50821  | 0.06548  | -0.45401 | -0.08546 |

Pd7Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.89316 | -1.76882 | -0.71426 | 0.02735  |
| Pd   | 1.89744  | 1.85698  | -0.46566 | 0.02817  |
| Pd   | 2.25170  | 0.24573  | 1.73616  | 0.01990  |
| Pd   | -2.25172 | -0.49236 | 1.68005  | 0.02051  |
| Pd   | -0.00248 | 0.11052  | -1.46390 | -0.00043 |
| Pd   | 0.32288  | -1.39059 | 0.80475  | 0.05188  |
| Pd   | -0.31409 | 1.25128  | 0.99058  | 0.04665  |
| Au   | 2.60171  | -0.80514 | -0.80962 | -0.09731 |
| Au   | -2.60786 | 0.91418  | -0.68551 | -0.09672 |

Pd7Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00836 | -0.00195 | 3.44068  | -0.00811 |
| Pd   | 1.10954  | -1.20437 | 1.41649  | 0.02564  |
| Pd   | -1.60537 | -0.36489 | 1.41287  | 0.02663  |
| Pd   | -0.49037 | -1.58705 | -0.93095 | 0.15117  |
| Pd   | -1.12832 | 1.22307  | -0.92821 | 0.15134  |

Pd7Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.79568  | 0.97077  | 1.54322  | -0.02296 |
| Pd   | 1.20430  | -1.69815 | 0.00934  | -0.00153 |
| Pd   | -1.28676 | -0.99924 | -1.31940 | 0.06952  |
| Pd   | -1.59628 | 1.51530  | -0.00836 | 0.20384  |
| Pd   | -1.28480 | -0.98203 | 1.33189  | 0.06909  |
| Pd   | 0.79398  | 0.95123  | -1.55424 | -0.02315 |
| Pd   | 2.80667  | 0.36479  | -0.00270 | 0.29126  |
| Au   | 0.56028  | 3.21358  | -0.01972 | -0.15245 |
| Au   | 1.10706  | -1.47112 | 2.72340  | -0.13756 |
| Au   | 1.10425  | -1.50364 | -2.70716 | -0.13765 |
| Au   | -3.60587 | -0.31025 | 0.00362  | -0.15841 |

Pd7Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.54942 | 0.48086  | 1.29392  | -0.04088 |
| Pd   | -0.62975 | -0.31118 | -1.30206 | -0.04888 |
| Pd   | 1.96874  | -0.36273 | 0.06920  | 0.01422  |
| Pd   | 1.27487  | 2.42983  | 0.59275  | 0.11114  |
| Pd   | 1.20850  | 1.61092  | -1.91482 | 0.11414  |
| Pd   | 0.70307  | -1.81457 | 1.86014  | 0.12366  |
| Pd   | 0.35780  | -2.70719 | -0.71549 | 0.08343  |
| Au   | -3.02466 | 0.42724  | -0.03556 | 0.07766  |
| Au   | 1.74643  | -1.11354 | -2.60742 | -0.12038 |
| Au   | 1.93149  | 0.61544  | 2.67685  | -0.12334 |
| Au   | -1.23462 | 2.50634  | -0.71551 | -0.10895 |
| Au   | -1.94214 | -2.04298 | 0.74939  | -0.08183 |

Pd7Au6

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.44151 | 0.70756  | -1.30368 | 0.01549  |
| Pd   | 1.87341  | 2.21803  | 1.31621  | 0.10921  |
| Pd   | 0.20359  | -2.05864 | 1.34399  | 0.11302  |
| Pd   | -0.44151 | 0.70756  | 1.30368  | 0.01549  |
| Pd   | 2.07275  | -0.32243 | 0.00000  | -0.01419 |
| Pd   | 1.87341  | 2.21803  | -1.31621 | 0.10921  |
| Pd   | 0.20359  | -2.05864 | -1.34399 | 0.11302  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -1.40237 | -3.85045 | 0.00000  | -0.14787 |
| Au | 1.87341  | -0.29428 | 2.70880  | -0.10577 |
| Au | -0.37673 | 3.29410  | 0.00000  | -0.10267 |
| Au | -2.25294 | -1.18002 | 0.00000  | 0.07263  |
| Au | 1.87341  | -0.29428 | -2.70880 | -0.10577 |
| Au | -2.82630 | 1.50308  | 0.00000  | -0.07178 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -1.67530 | 1.06828  | -0.18700 | 0.02476  |
| Pd | 0.02570  | 1.23323  | -2.13874 | 0.26460  |
| Pd | -0.02638 | -1.37648 | 3.32633  | -0.00394 |
| Au | 0.03661  | 3.15206  | 0.36630  | -0.16709 |
| Au | 2.71897  | -1.23267 | -1.31769 | -0.15979 |
| Au | -2.74114 | -1.16875 | -1.33215 | -0.15967 |

Pd7Au7

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.28194  | -1.66099 | 0.19941  | -0.03233 |
| Pd   | -0.08112 | 0.82163  | 1.37244  | 0.00876  |
| Pd   | -0.00245 | 0.71672  | -1.45416 | -0.08397 |
| Pd   | 2.04925  | 1.82189  | 0.12300  | 0.05254  |
| Pd   | 2.27703  | -0.68634 | 1.67422  | 0.08679  |
| Pd   | -2.09902 | -1.16133 | -1.31901 | 0.09222  |
| Pd   | -2.26320 | -1.04597 | 1.33652  | 0.10863  |
| Au   | -0.05132 | -1.55469 | 2.98400  | -0.12681 |
| Au   | -0.32764 | 3.26542  | -0.14846 | -0.09595 |
| Au   | 0.30313  | -1.85859 | -2.63543 | -0.09075 |
| Au   | 2.47002  | -0.67983 | -1.31919 | 0.13651  |
| Au   | -2.43746 | 1.48952  | -0.13290 | 0.13873  |
| Au   | -4.50119 | -0.33118 | -0.12137 | -0.10889 |
| Au   | 4.44989  | 0.36482  | 0.24813  | -0.08549 |

Pd8Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.18331 | 0.77409  | -1.32846 | 0.01000  |
| Pd   | 0.40084  | 0.76027  | 1.26391  | -0.00514 |
| Pd   | -0.22227 | -1.87915 | 0.00805  | 0.02527  |
| Pd   | 0.45785  | 3.04932  | -0.10158 | 0.12622  |
| Pd   | -2.61755 | -0.38860 | -0.77523 | 0.13188  |
| Pd   | -2.00486 | -0.43247 | 1.78738  | 0.13277  |
| Pd   | 1.70603  | -1.09400 | -1.64640 | 0.13732  |
| Pd   | 2.45963  | -0.92858 | 0.92533  | 0.12849  |
| Au   | 0.38558  | -1.72932 | 2.70011  | -0.18261 |
| Au   | -0.91119 | -1.69163 | -2.64698 | -0.17494 |
| Au   | -2.11892 | 2.09303  | 0.48280  | -0.17591 |
| Au   | 2.64665  | 1.40892  | -0.61337 | -0.15336 |

Pd8Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -1.42227 | 0.29046  | 1.39288  | 0.06559  |
| Pd   | -1.42227 | 0.29046  | -1.39022 | 0.06532  |
| Pd   | 1.42183  | 0.29101  | -1.39314 | 0.06559  |
| Pd   | 1.42175  | 0.28833  | 1.38946  | 0.06485  |
| Pd   | 0.00148  | 2.39290  | 0.00118  | -0.06118 |
| Pd   | -0.00032 | -1.78483 | -0.00048 | 0.13615  |
| Pd   | 0.00246  | 2.11313  | 2.62523  | 0.05232  |
| Pd   | -0.00192 | 2.11601  | -2.62337 | 0.05228  |
| Au   | 2.70653  | -1.74653 | -0.00293 | -0.22043 |
| Au   | -2.70696 | -1.74567 | 0.00205  | -0.22050 |

Pd8Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.26355  | 0.54756  | -1.38426 | -0.01740 |
| Pd   | 0.11654  | -1.97225 | -0.00490 | 0.02033  |
| Pd   | 0.35824  | 0.59042  | 1.35247  | -0.02614 |
| Pd   | 2.53288  | -0.94800 | 1.41113  | 0.07263  |
| Pd   | 2.27867  | -1.24227 | -1.34180 | 0.11849  |
| Pd   | -2.04386 | -0.74865 | 1.44402  | 0.01970  |
| Pd   | -2.19093 | -0.75223 | -1.28557 | 0.03313  |
| Pd   | -4.15901 | 0.29447  | 0.18183  | 0.10067  |
| Au   | -0.09134 | -1.88281 | -2.78310 | -0.12506 |
| Au   | 0.21159  | -1.82862 | 2.77732  | -0.11747 |
| Au   | 0.63271  | 3.02387  | -0.05557 | 0.02844  |
| Au   | 2.83654  | 1.30610  | -0.20112 | -0.02741 |
| Au   | -1.93355 | 1.84506  | 0.04532  | -0.07991 |

Pd8Au3

| Atom | X        | Y        | Z        | Charges |
|------|----------|----------|----------|---------|
| Pd   | 1.70481  | 1.02710  | -0.17018 | 0.02535 |
| Pd   | -0.01220 | -1.25513 | -1.29278 | 0.01028 |
| Pd   | -1.46907 | -1.42704 | 1.15558  | 0.06021 |
| Pd   | 0.00241  | 0.90552  | 2.06718  | 0.04496 |
| Pd   | 1.42523  | -1.46464 | 1.16135  | 0.06032 |

Pd8Au6

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.31885 | 1.54154  | 0.80561  | 0.03065  |
| Pd   | 0.06915  | -1.36080 | 0.97054  | -0.00794 |
| Pd   | -0.01513 | 0.05947  | -1.52991 | 0.00371  |
| Pd   | -2.39749 | 1.39516  | -0.88747 | 0.07916  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | -2.22653 | -1.49134 | -0.75527 | 0.05673  |
| Pd | -2.49031 | -0.20153 | 1.55053  | 0.10060  |
| Pd | 2.11167  | 1.57697  | -0.79566 | 0.04192  |
| Pd | 2.03367  | 0.25662  | 1.74424  | 0.07117  |
| Au | -0.30069 | 0.12308  | 3.28001  | -0.12326 |
| Au | 0.17964  | -2.80827 | -1.46875 | -0.09040 |
| Au | -0.17635 | 2.87888  | -1.66688 | -0.12918 |
| Au | 2.39377  | -1.33758 | -0.74501 | 0.13015  |
| Au | 4.37563  | 0.28725  | 0.17733  | -0.05978 |
| Au | -4.58901 | -0.17754 | -0.21873 | -0.10354 |

Pd9Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.79001  | -1.79877 | 1.52012  | 0.07885  |
| Pd   | -2.11695 | -1.82080 | 1.02085  | -0.01478 |
| Pd   | -1.14061 | 1.23805  | -1.26390 | 0.08611  |
| Pd   | 1.70342  | 0.82005  | -1.29076 | 0.06924  |
| Pd   | -0.64964 | 0.62982  | 1.29592  | 0.00940  |
| Pd   | -0.17040 | -1.21776 | -0.95747 | -0.02456 |
| Pd   | -3.24294 | 0.51992  | 0.59650  | 0.05511  |
| Pd   | 2.01989  | 0.56695  | 1.26826  | 0.12942  |
| Pd   | -2.78545 | -1.01333 | -1.50506 | 0.01427  |
| Au   | 2.61343  | -1.72381 | -0.58614 | -0.17610 |
| Au   | 0.64306  | 2.93255  | 0.18758  | -0.22696 |

Pd9Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.03471 | -0.08238 | -1.34228 | 0.00143  |
| Pd   | 0.21777  | 1.73552  | 1.05893  | -0.01335 |
| Pd   | -0.09026 | -1.25860 | 1.03675  | 0.02614  |
| Pd   | 0.01339  | 0.33551  | 3.23847  | -0.05825 |
| Pd   | -0.32663 | -2.73736 | -1.16281 | 0.07812  |
| Pd   | -2.19765 | 0.22591  | 1.73065  | 0.10189  |
| Pd   | -2.11646 | 1.47387  | -0.61244 | 0.14580  |
| Pd   | 2.31647  | -0.13024 | 1.66221  | 0.09904  |
| Pd   | 2.39288  | 1.00351  | -0.71966 | 0.13268  |
| Au   | 0.28028  | 2.76587  | -1.48837 | -0.18642 |
| Au   | -2.64946 | -1.28432 | -0.68448 | -0.16455 |
| Au   | 2.26740  | -1.81097 | -0.67439 | -0.16253 |

Pd9Au4

| Atom | X       | Y       | Z        | Charges  |
|------|---------|---------|----------|----------|
| Pd   | 0.31027 | 0.79206 | 1.35206  | -0.00404 |
| Pd   | 0.31027 | 0.79206 | -1.35224 | -0.00397 |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Pd | 0.17775  | -1.84519 | 0.00022  | 0.06094  |
| Pd | 0.40672  | 3.09336  | -0.00005 | 0.09005  |
| Pd | 2.54138  | -0.79497 | 1.32625  | 0.12768  |
| Pd | 2.54126  | -0.79514 | -1.32621 | 0.12766  |
| Pd | -2.04736 | -0.71979 | 1.39128  | 0.02757  |
| Pd | -2.04730 | -0.72007 | -1.39120 | 0.02756  |
| Pd | -4.16257 | 0.10097  | -0.00012 | 0.09448  |
| Au | 0.21817  | -1.73712 | -2.71073 | -0.15870 |
| Au | 0.21818  | -1.73658 | 2.71111  | -0.15868 |
| Au | 2.79551  | 1.67428  | -0.00014 | -0.12910 |
| Au | -2.08501 | 1.85572  | -0.00024 | -0.10146 |

Pd9Au5

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.12630  | -1.45534 | 0.80305  | 0.00728  |
| Pd   | -0.12621 | 1.45282  | 0.80556  | 0.00709  |
| Pd   | -0.00016 | 0.00164  | -1.60938 | 0.05527  |
| Pd   | 2.21457  | -1.46215 | -0.85102 | 0.08050  |
| Pd   | 2.32024  | 1.43728  | -0.71834 | 0.09358  |
| Pd   | 2.30625  | 0.16154  | 1.61944  | 0.09452  |
| Pd   | -2.31985 | -1.43552 | -0.72092 | 0.09343  |
| Pd   | -2.21482 | 1.46423  | -0.84823 | 0.08048  |
| Pd   | -2.30647 | -0.16431 | 1.61907  | 0.09451  |
| Au   | 0.00001  | -0.00345 | 3.21597  | -0.12234 |
| Au   | 0.07300  | 2.85747  | -1.59637 | -0.13506 |
| Au   | -0.07289 | -2.85410 | -1.60229 | -0.13507 |
| Au   | -4.48922 | 0.08324  | -0.03750 | -0.10708 |
| Au   | 4.48917  | -0.08328 | -0.03759 | -0.10710 |

Pd10Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | 0.68617  | -2.25339 | -0.63491 | -0.00490 |
| Pd   | -0.56449 | -2.18795 | 1.72429  | 0.10143  |
| Pd   | -1.94700 | 0.00485  | 0.99268  | 0.03583  |
| Pd   | 0.70215  | 2.25007  | -0.63018 | -0.00521 |
| Pd   | 2.22916  | -0.00389 | -1.70439 | -0.01413 |
| Pd   | 1.01699  | -0.00321 | 1.16034  | -0.14762 |
| Pd   | -0.61527 | 0.00202  | -1.24433 | 0.09089  |
| Pd   | -0.55533 | 2.19054  | 1.72362  | 0.10128  |
| Pd   | 3.17365  | -1.37346 | 0.34067  | 0.05560  |
| Pd   | 3.18421  | 1.35324  | 0.34573  | 0.05544  |
| Au   | -2.12022 | 2.35695  | -0.60469 | -0.13428 |
| Au   | -2.13638 | -2.34462 | -0.60268 | -0.13432 |

Pd10Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.32452 | 1.36028  | 0.84751  | -0.01401 |
| Pd   | -0.32489 | -1.36212 | 0.84537  | -0.01387 |
| Pd   | 0.12943  | 0.00170  | -1.73035 | 0.08345  |
| Pd   | -0.61781 | -0.00255 | 3.11577  | 0.08031  |
| Pd   | -2.35849 | 1.32683  | -1.00268 | 0.10681  |
| Pd   | -2.35882 | -1.32426 | -1.00523 | 0.10676  |
| Pd   | 2.21837  | 1.40510  | -0.35889 | 0.00661  |
| Pd   | 2.21793  | -1.40455 | -0.36196 | 0.00653  |
| Pd   | 1.92292  | -0.00240 | 2.08137  | -0.04294 |
| Pd   | 4.16148  | -0.00121 | 0.71344  | 0.09150  |
| Au   | 0.06674  | -2.71274 | -1.63611 | -0.15547 |
| Au   | 0.06751  | 2.71594  | -1.63122 | -0.15544 |
| Au   | -2.85094 | -0.00135 | 1.43643  | -0.10023 |

Pd10Au4

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.22696 | -1.64774 | 0.00138  | 0.02257  |
| Pd   | -0.17575 | 0.82935  | -1.40794 | 0.04212  |
| Pd   | -0.17571 | 0.83136  | 1.40657  | 0.04190  |
| Pd   | -2.48540 | -0.81662 | 1.42250  | 0.02954  |
| Pd   | -2.55940 | 1.61071  | -0.00093 | 0.05838  |
| Pd   | -2.48537 | -0.81826 | -1.42150 | 0.02958  |
| Pd   | 2.13920  | -0.88746 | 1.35057  | 0.10302  |
| Pd   | 1.99235  | 1.68634  | -0.00075 | 0.05228  |
| Pd   | 2.13879  | -0.88872 | -1.34950 | 0.10288  |
| Pd   | -4.55071 | -0.08589 | 0.00014  | 0.04128  |
| Au   | -0.14120 | -1.64279 | -2.78415 | -0.13358 |
| Au   | -0.29779 | 3.26770  | -0.00247 | -0.14099 |
| Au   | -0.14095 | -1.63818 | 2.78664  | -0.13352 |
| Au   | 4.30008  | 0.12213  | -0.00033 | -0.11546 |

Pd11Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.32460 | 1.44187  | 0.97801  | -0.00515 |
| Pd   | -0.32481 | -1.44363 | 0.97715  | -0.00487 |
| Pd   | -0.23140 | 0.00084  | -1.55452 | 0.07090  |
| Pd   | -0.51104 | -0.00158 | 3.17286  | 0.03773  |
| Pd   | -2.61484 | 1.31730  | -0.59483 | 0.08124  |
| Pd   | -2.61474 | -1.31638 | -0.59608 | 0.08124  |
| Pd   | -2.73888 | -0.00082 | 1.81421  | 0.00171  |
| Pd   | 2.07942  | 1.40894  | -0.58674 | -0.00194 |
| Pd   | 2.07930  | -1.40808 | -0.58796 | -0.00204 |
| Pd   | 1.95628  | -0.00109 | 1.83668  | -0.04732 |
| Pd   | 4.09981  | -0.00010 | 0.32018  | 0.08337  |

|    |          |          |          |          |
|----|----------|----------|----------|----------|
| Au | -0.24879 | -2.72402 | -1.50909 | -0.14748 |
| Au | -0.24877 | 2.72561  | -1.50651 | -0.14738 |

Pd11Au3

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00046 | -1.84066 | 0.00128  | 0.05802  |
| Pd   | 0.00017  | 0.79459  | -1.34714 | 0.02478  |
| Pd   | 0.00017  | 0.79702  | 1.34693  | 0.02506  |
| Pd   | -2.30659 | -0.78184 | 1.38661  | 0.01341  |
| Pd   | -2.32915 | 1.69607  | -0.00171 | 0.04496  |
| Pd   | -2.30702 | -0.78434 | -1.38547 | 0.01352  |
| Pd   | 2.30672  | -0.78220 | 1.38659  | 0.01349  |
| Pd   | 2.32953  | 1.69593  | -0.00148 | 0.04498  |
| Pd   | 2.30678  | -0.78448 | -1.38579 | 0.01358  |
| Pd   | 4.36563  | 0.05297  | -0.00022 | 0.07440  |
| Pd   | -4.36570 | 0.05357  | 0.00011  | 0.07448  |
| Au   | -0.00027 | -1.67234 | -2.74389 | -0.13312 |
| Au   | 0.00025  | 3.27278  | -0.00222 | -0.13444 |
| Au   | -0.00002 | -1.66834 | 2.74628  | -0.13311 |

Pd12Au2

| Atom | X        | Y        | Z        | Charges  |
|------|----------|----------|----------|----------|
| Pd   | -0.00013 | 1.44247  | 0.99565  | 0.00360  |
| Pd   | 0.00004  | 0.00073  | -1.55245 | 0.09097  |
| Pd   | -0.00001 | -1.44373 | 0.99478  | 0.00372  |
| Pd   | -0.00008 | -0.00133 | 3.20108  | 0.03273  |
| Pd   | 2.34168  | -0.00052 | 1.82883  | -0.02793 |
| Pd   | 2.32779  | -1.40037 | -0.61923 | 0.01610  |
| Pd   | 2.32778  | 1.40090  | -0.61844 | 0.01611  |
| Pd   | -2.34177 | -0.00062 | 1.82876  | -0.02794 |
| Pd   | -2.32768 | -1.40046 | -0.61927 | 0.01611  |
| Pd   | -2.32786 | 1.40088  | -0.61849 | 0.01613  |
| Pd   | -4.39824 | -0.00006 | 0.17887  | 0.08498  |
| Pd   | 4.39829  | 0.00006  | 0.17898  | 0.08498  |
| Au   | -0.00001 | 2.73675  | -1.50688 | -0.15474 |
| Au   | 0.00011  | -2.73556 | -1.50878 | -0.15479 |