

# On Heteronuclear Alternatives to $\text{Au}_{13}(\text{dppe})_5\text{Cl}_2$ : Electronic and Optical Properties of the *18-electron* $\text{Os}@Au_{12}(\text{dppe})_5\text{Cl}_2$ Cluster from Relativistic DFT Computations

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## Content:

**Table S1.** Energy decomposition analysis between the  $[\text{Cl}_2(\text{dppe})_5]^{2-}$  ligand shell and the  $[\text{M}@Au_{12}]^{n+}$  ( $\text{M} = \text{Au}$ ,  $n = 5$ ;  $\text{M} = \text{Os}$ ,  $\text{Ru}$ ,  $\text{Fe}$ ,  $n = 2$ ) fragment. Values in  $\text{kcal.mol}^{-1}$ . Page 2

**Table S2.** Energy decomposition analysis between a single  $\text{Cl}^-$  anion and the  $[\text{M}@Au_{12}\text{Cl}(\text{dppe})_5]^{n+}$  fragment ( $\text{M} = \text{Au}$ ,  $n = 4$ ;  $\text{M} = \text{Os}$ ,  $\text{Ru}$ ,  $\text{Fe}$ ,  $n = 1$ ). Values in  $\text{kcal.mol}^{-1}$ . Page 2

**Table S3.** Relative energy of isomers **I**, **II**, and **III**, for  $[\text{Fe}@Au_{12}(\text{dppe})_5\text{Cl}_2]$ ,  $[\text{Ru}@Au_{12}(\text{dppe})_5\text{Cl}_2]$ , and  $[\text{Os}@Au_{12}(\text{dppe})_5\text{Cl}_2]$ . Values in  $\text{kcal.mol}^{-1}$ . Page 2

**Figure S1.** Isosurface for the 1P and 1D levels of  $[\text{Au}_{13}\text{Cl}_2(\text{dppe})_5]^{3+}$ . Page 3

**Figure S2** Isosurface for the 1P and 1D occupied levels of  $[\text{Os}@Au_{12}\text{Cl}_2(\text{dppe})_5]$ , as well as the lowest unoccupied levels, which are of ligand character. Page 4

**Figure S3.** Relative energy for isomers **I**, **II**, and **III**, of  $[\text{Hg}@Au_{12}(\text{dppe})_5\text{Cl}_2]^{4+}$ . Values in  $\text{kcal.mol}^{-1}$ . Page 5

**Table S4.** Optimized Cartesian coordinates for isomers **I**, **II**, and **III** of  $[\text{Au}@Au_{12}(\text{dppe})_5\text{Cl}_2]^{3+}$ , and  $[\text{M}@Au_{12}(\text{dppe})_5\text{Cl}_2]$  ( $\text{M} = \text{Os}$ ,  $\text{Ru}$ ,  $\text{Fe}$ ). Values in Angstroms (Å). Page 6

**Table S1.** Energy decomposition analysis between the  $[\text{Cl}_2(\text{dppe})_5]^{2-}$  ligand shell and the  $[\text{M}@\text{Au}_{12}]^{n+}$  ( $\text{M} = \text{Au}, n = 5$ ;  $\text{M} = \text{Os}, \text{Ru}, \text{Fe}, n = 2$ ) fragment. Values in  $\text{kcal.mol}^{-1}$ .

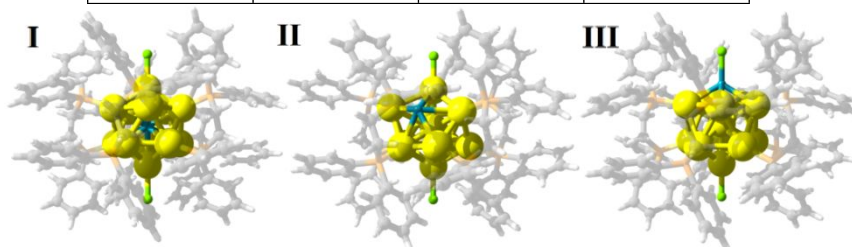
|                            | <b>1</b> |       | <b>2</b> |       | <b>3</b> |       | <b>4</b> |       |
|----------------------------|----------|-------|----------|-------|----------|-------|----------|-------|
|                            | Au       |       | Os       |       | Ru       |       | Fe       |       |
| $\Delta E_{\text{Pauli}}$  | 2005.8   |       | 2099.7   |       | 2005.2   |       | 1911.5   |       |
| $\Delta E_{\text{elstat}}$ | -2218.2  | 61.4% | -1911.8  | 66.3% | -1834.3  | 65.8% | -1725.7  | 64.7% |
| $\Delta E_{\text{orb}}$    | -1278.6  | 35.4% | -861.5   | 29.9% | -842.2   | 30.2% | -827.0   | 31.0% |
| $\Delta E_{\text{disp}}$   | -113.1   | 3.1%  | -111.2   | 3.9%  | -109.6   | 3.9%  | -114.4   | 4.3%  |
| $\Delta E_{\text{int}}$    | -1604.1  |       | -784.8   |       | -780.9   |       | -755.7   |       |

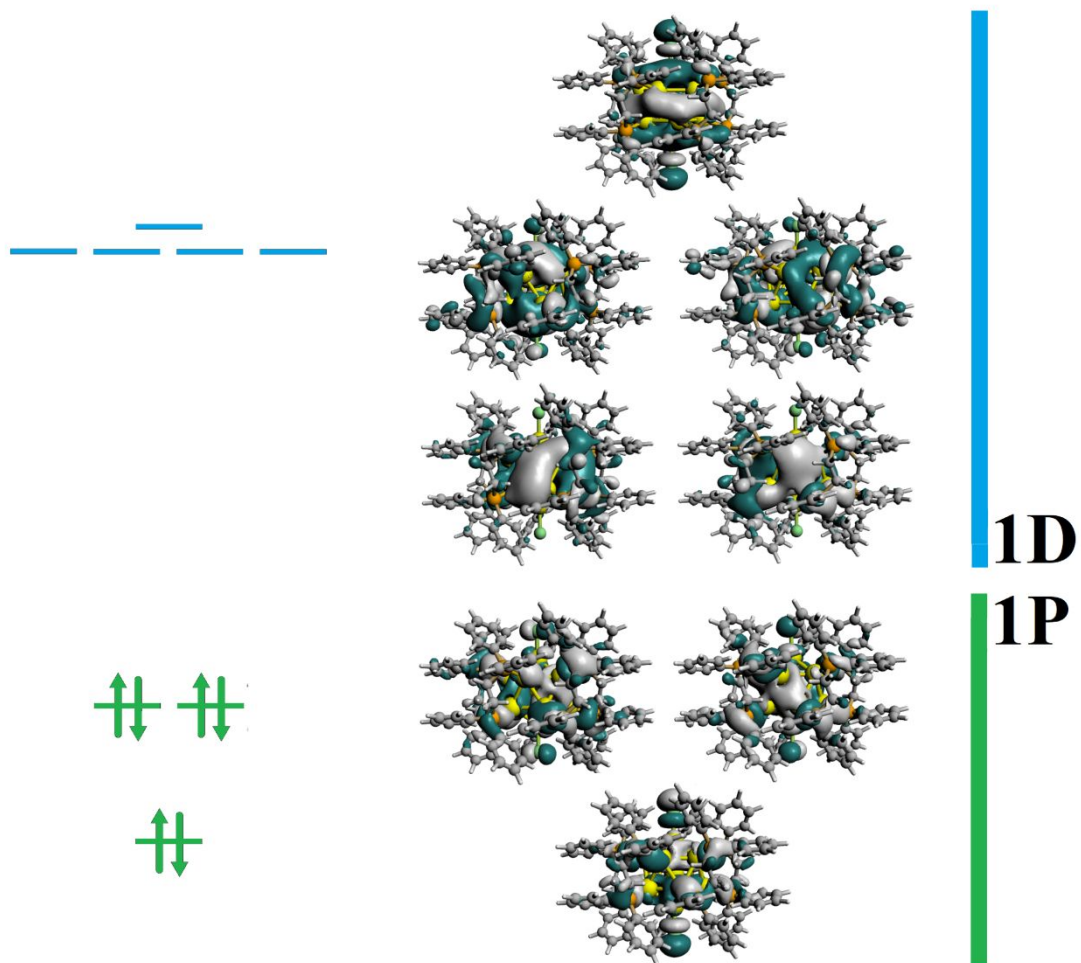
**Table S2.** Energy decomposition analysis between a single  $\text{Cl}^-$  anion and the  $[\text{M}@\text{Au}_{12}\text{Cl}(\text{dppe})_5]^{n+}$  fragment ( $\text{M} = \text{Au}, n = 4$ ;  $\text{M} = \text{Os}, \text{Ru}, \text{Fe}, n = 1$ ). Values in  $\text{kcal.mol}^{-1}$ .

|                            | <b>1</b> |       | <b>2</b> |       | <b>3</b> |       | <b>4</b> |       |
|----------------------------|----------|-------|----------|-------|----------|-------|----------|-------|
|                            | Au       |       | Os       |       | Ru       |       | Fe       |       |
| $\Delta E_{\text{Pauli}}$  | 157.1    |       | 119.1    |       | 116.7    |       | 110.9    |       |
| $\Delta E_{\text{elstat}}$ | -286.0   | 72.0% | -130.0   | 59.0% | -127.4   | 59.5% | -119.5   | 59.2% |
| $\Delta E_{\text{orb}}$    | -104.7   | 26.4% | -83.9    | 38.1% | -80.1    | 37.5% | -76.1    | 37.7% |
| $\Delta E_{\text{disp}}$   | -6.7     | 1.7%  | -6.3     | 2.9%  | -6.4     | 3.0%  | -6.3     | 3.1%  |
| $\Delta E_{\text{int}}$    | -240.3   |       | -101.1   |       | -97.3    |       | -91.0    |       |

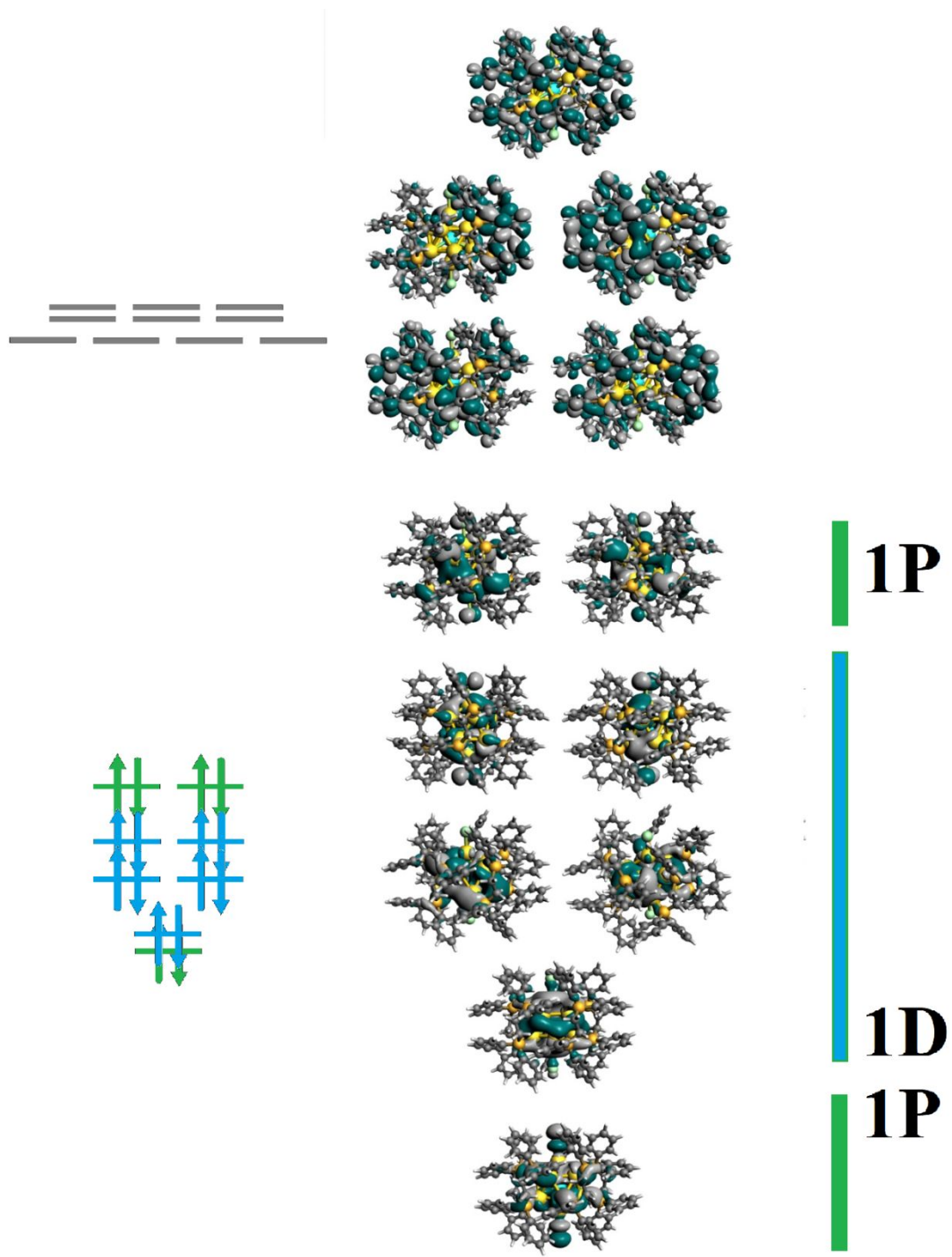
**Table S3.** Relative energy of isomers **I**, **II**, and **III**, for  $[\text{Fe}@\text{Au}_{12}(\text{dppe})_5\text{Cl}_2]$ ,  $[\text{Ru}@\text{Au}_{12}(\text{dppe})_5\text{Cl}_2]$ , and  $[\text{Os}@\text{Au}_{12}(\text{dppe})_5\text{Cl}_2]$ . Values in  $\text{kcal.mol}^{-1}$ .

|            | Fe         | Ru         | Os         |
|------------|------------|------------|------------|
| Isomer I   | <b>0.0</b> | <b>0.0</b> | <b>0.0</b> |
| Isomer II  | +253.5     | +129.8     | +99.1      |
| Isomer III | +128.4     | +88.7      | +101.0     |

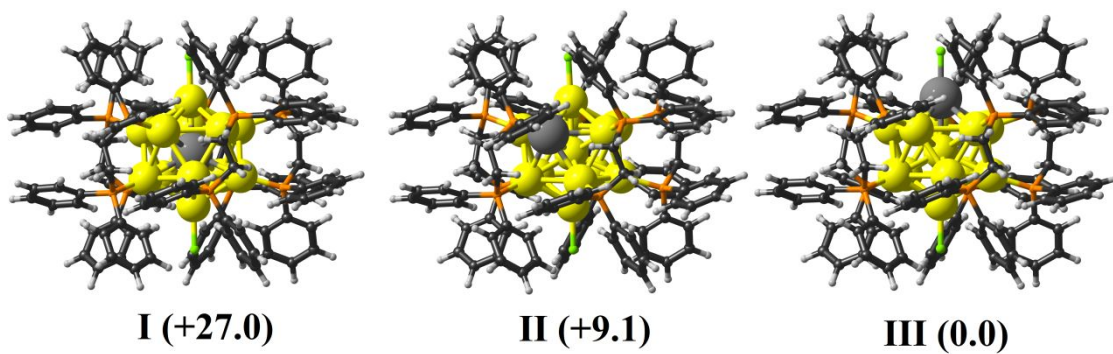




**Figure S1.** Isosurface for the 1P and 1D levels of  $[\text{Au}_{13}\text{Cl}_2(\text{dppe})_5]^{3+}$ .



**Figure S2.** Isosurface for the 1P and 1D occupied levels of [Os@Au<sub>12</sub>Cl<sub>2</sub>(dppe)<sub>5</sub>], as well as the lowest unoccupied levels, which are of ligand character.



**Figure S3.** Relative energy for isomers I, II, and III, of  $[\text{Hg}@Au_{12}(\text{dppe})_5\text{Cl}_2]^{4+}$ . Values in  $\text{kcal.mol}^{-1}$ .

**Table S4.** Optimized Cartesian coordinates for isomers **I**, **II**, and **III** of  $[\text{Au}@\text{Au}_{12}(\text{dppe})_5\text{Cl}_2]^{3+}$ ,  $[\text{M}@\text{Au}_{12}(\text{dppe})_5\text{Cl}_2]$  (M = Os, Ru, Fe), and  $[\text{HgAu}_{12}\text{Cl}_2(\text{dppe})_5]^{4+}$ . Values in Angstroms (Å).

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275
[Au13Cl12(dppe)5]3+
Au  0.  0.  -2.54804
Au -1.38449  1.92445  1.15492
Au  1.40243  1.91142  1.15492
Au -0.01108  2.37070  -1.15492
Au -0.01108  -2.37070  1.15492
Au  0.  0.  0.
Au -1.38449  -1.92445  -1.15492
Au  2.25124  0.74313  -1.15492
Au  2.25124  -0.74313  1.15492
Au -2.25809  0.72205  -1.15492
Au -2.25809  -0.72205  1.15492
Au  1.40243  -1.91142  -1.15492
Au  0.  0.  2.54804
P -1.95522  -3.92642  -1.81865
P  3.13005  3.07286  1.81865
P -0.72608  4.32579  -1.81865
P  3.13005  -3.07286  -1.81865
P  3.88970  -2.02729  1.81865
P -0.72608  -4.32579  1.81865
Cl  0.  0.  -4.74877
Cl  0.  0.  4.74877
P -4.33845  0.64620  -1.81865
P -4.33845  -0.64620  1.81865
P  3.88970  2.02729  -1.81865
P -1.95522  3.92642  1.81865
C  3.07957  4.78530  1.90449
C -3.59945  4.40758  1.90449
C -4.74442  3.20986  -2.24533
C -6.60123  2.01659  -1.64067
C -4.74442  -3.20986  2.24533
C -1.64147  -3.02013  3.90585
C -6.76597  -4.25362  2.05450
C -2.39292  -5.17458  3.69250
C -3.37956  0.62786  3.90585
C -6.76597  4.25362  -2.05450
C -1.64147  3.02013  -3.90585
C  4.15518  5.51156  1.64067
C -6.60123  -2.01659  1.64067
C  5.50273  1.45011  -1.90449
C  1.95161  5.38553  2.24533
C -5.30415  2.06126  -1.90449
C -5.47632  -4.30086  2.31865
C  5.72503  -0.19187  2.24533
C -1.90366  -4.83309  0.65043
C -0.44722  3.40817  3.90585
C -3.95779  5.65498  1.64067
C  4.97745  -2.77980  -3.69250
C  2.97357  7.41819  2.05450
C -2.39292  5.17458  -3.69250
C -5.73475  1.46953  4.73898
C  4.00828  -3.30399  0.65043
C -5.30415  -2.06126  1.90449
C -4.47764  0.26635  3.26385
C  4.10086  6.82332  1.71801
C  1.90245  6.69837  2.31865
C -5.66077  0.67676  3.69250
C -1.13036  -4.34079  -3.26385
C  3.46593  2.84737  -3.26385
C -0.44722  -3.40817  -3.90585
C  3.77904  2.41641  3.26385
C -1.90366  4.83309  -0.65043
C -5.47632  4.30086  -2.31865
C -1.30073  5.02899  0.65043
C  4.00828  3.30399  -0.65043
C  5.72503  0.19187  -2.24533
C -5.18480  -0.31698  -0.65043
C  3.77904  -2.41641  -3.26385
C  3.10316  1.47851  3.90585
C -1.30073  -5.02899  -0.65043
C -0.37453  5.90819  4.73898

```

|   |          |          |          |
|---|----------|----------|----------|
| C | -3.16975 | -4.99996 | 4.73898  |
| C | -1.63698 | -4.17618 | 3.26385  |
| C | 5.50273  | -1.45011 | 1.90449  |
| C | -1.13036 | 4.34079  | 3.26385  |
| C | -7.32831 | -3.10976 | 1.71801  |
| C | 0.28014  | 3.72760  | 4.95449  |
| C | -3.45859 | 1.41832  | 4.95449  |
| C | -3.16975 | 4.99996  | -4.73898 |
| C | 4.18187  | -3.87483 | 3.69250  |
| C | 3.10316  | -1.47851 | -3.90585 |
| C | -5.18480 | 0.31698  | 0.65043  |
| C | 4.38091  | 2.79111  | 0.65043  |
| C | 3.46593  | -2.84737 | 3.26385  |
| C | 4.97745  | 2.77980  | 3.69250  |
| C | 4.18187  | 3.87483  | -3.69250 |
| C | 1.58665  | -5.50412 | 2.24533  |
| C | -1.63698 | 4.17618  | -3.26385 |
| C | 5.50328  | -2.18193 | -4.73898 |
| C | 6.95842  | 0.26057  | 2.31865  |
| C | -4.51886 | 3.52032  | 2.24533  |
| C | 5.50328  | 2.18193  | 4.73898  |
| C | 4.83475  | -1.23098 | -5.36450 |
| C | -4.63494 | 1.84591  | 5.36450  |
| C | 4.83475  | 1.23098  | 5.36450  |
| C | -3.18784 | -3.83768 | 5.36450  |
| C | 6.95842  | -0.26057 | -2.31865 |
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| C | 7.75660  | -1.79162 | 1.71801  |
| C | 3.77574  | -4.55968 | 4.73898  |
| C | 1.96439  | -3.18035 | 4.95449  |
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| C | 7.97400  | 0.53569  | -2.05450 |
| C | 1.96439  | 3.18035  | -4.95449 |
| C | 7.97400  | -0.53569 | 2.05450  |
| C | 0.32130  | -5.68151 | 1.90449  |
| C | 6.52583  | -2.24864 | 1.64067  |
| C | 7.75660  | 1.79162  | -1.71801 |
| C | 4.10086  | -6.82332 | -1.71801 |
| C | -4.47764 | -0.26635 | -3.26385 |
| C | -6.13623 | -5.12038 | -2.05450 |
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| C | 0.69299  | -7.93060 | 1.71801  |
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| C | -5.78264 | -3.87925 | -2.31865 |
| C | 6.52583  | 2.24864  | -1.64067 |
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| C | 3.63173  | 0.88547  | 4.95449  |
| C | -4.63494 | -1.84591 | -5.36450 |
| C | 1.58665  | 5.50412  | -2.24533 |
| C | 0.69299  | 7.93060  | -1.71801 |
| C | -0.12200 | 6.90130  | -1.64067 |
| C | -0.12200 | -6.90130 | 1.64067  |
| C | 2.36508  | -2.49440 | 3.90585  |
| C | 0.32130  | 5.68151  | -1.90449 |
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| C | -5.78264 | 3.87925  | 2.31865  |
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| C | 0.32329  | 4.97851  | 5.36450  |

|   |          |          |          |
|---|----------|----------|----------|
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| C | 1.95463  | 7.74926  | -2.05450 |
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| C | -1.10563 | 5.59284  | 3.69250  |
| H | -0.35160 | 6.89035  | 5.07854  |
| H | 0.90165  | 5.23529  | 6.18923  |
| H | 0.81587  | 2.98496  | 5.44908  |
| H | -0.48024 | 2.41672  | 3.57965  |
| H | -1.67042 | 6.32520  | 3.21247  |
| H | 1.10570  | 4.81505  | 2.46887  |
| H | 1.01340  | 7.16119  | 2.59746  |
| H | 2.93431  | 8.45527  | 2.11740  |
| H | 4.95033  | 7.38835  | 1.51772  |
| H | 5.05165  | 5.05692  | 1.37042  |
| H | 2.59598  | 8.56520  | -2.11740 |
| H | 3.38939  | 6.38919  | -2.59746 |
| H | 0.33786  | 8.88703  | -1.51772 |
| H | -1.11449 | 7.06042  | -1.37042 |
| H | 1.93568  | 4.54537  | -2.46887 |
| H | 7.12386  | 1.24913  | 2.59746  |
| H | 8.94819  | -0.17787 | 2.11740  |
| H | 5.49944  | 3.54326  | 3.21247  |
| H | 6.44446  | 2.46363  | 5.07854  |
| H | 2.15003  | 1.20354  | 3.57965  |
| H | 3.09098  | 0.14646  | 5.44908  |
| H | 5.25768  | 0.76028  | 6.18923  |
| H | 8.55647  | -2.42492 | 1.51772  |
| H | 6.37046  | -3.24173 | 1.37042  |
| H | 4.92107  | 0.43635  | 2.46887  |
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| H | 8.55647  | 2.42492  | -1.51772 |
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| H | -2.41457 | -1.93532 | 5.44908  |
| H | -3.80667 | -3.70546 | 6.18923  |
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| H | -2.36646 | -6.09905 | 3.21247  |
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| H | -8.34766 | 3.06757  | -1.51772 |
| H | -7.34378 | 5.11571  | -2.11740 |
| H | -5.02910 | 5.19787  | -2.59746 |
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| H | -6.66177 | -1.79484 | -5.07854 |
| H | -6.53182 | -0.36593 | -3.21247 |
| H | -4.23770 | -2.53952 | -2.46887 |
| H | -3.24837 | -6.36708 | -1.37042 |
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| H | -7.13469 | -5.40351 | -2.11740 |



|   |          |          |          |
|---|----------|----------|----------|
| H | -6.49754 | -3.17673 | -2.59746 |
| H | -8.34766 | -3.06757 | 1.51772  |
| H | -7.05926 | -1.12185 | 1.37042  |
| H | -5.02910 | -5.19787 | 2.59746  |
| H | -7.34378 | -5.11571 | 2.11740  |
| H | -3.72475 | -3.24554 | 2.46887  |
| H | -1.11449 | -7.06042 | 1.37042  |
| H | 0.33786  | -8.88703 | 1.51772  |
| H | 2.59598  | -8.56520 | 2.11740  |
| H | 3.38939  | -6.38919 | 2.59746  |
| H | 1.93568  | -4.54537 | 2.46887  |
| H | 5.05165  | -5.05692 | -1.37042 |
| H | 4.95033  | -7.38835 | -1.51772 |
| H | 2.93431  | -8.45527 | -2.11740 |
| H | 1.01340  | -7.16119 | -2.59746 |
| H | 1.10570  | -4.81505 | -2.46887 |
| H | -0.48024 | -2.41672 | -3.57965 |
| H | 0.81587  | -2.98496 | -5.44908 |
| H | 0.90165  | -5.23529 | -6.18923 |
| H | -0.35160 | -6.89035 | -5.07854 |
| H | -1.67042 | -6.32520 | -3.21247 |
| H | 2.15003  | -1.20354 | -3.57965 |
| H | 3.09098  | -0.14646 | -5.44908 |
| H | 5.25768  | -0.76028 | -6.18923 |
| H | 6.44446  | -2.46363 | -5.07854 |
| H | 5.49944  | -3.54326 | -3.21247 |
| H | 5.06926  | 4.13535  | -3.21247 |
| H | 1.80903  | 1.67289  | -3.57965 |
| H | 1.09446  | 2.89444  | -5.44908 |
| H | 2.34778  | 4.76541  | -6.18923 |
| H | 4.33450  | 5.36775  | -5.07854 |
| H | 3.07353  | -3.78880 | 0.64041  |
| H | 4.68709  | -4.02247 | 1.00096  |
| H | 4.55313  | -1.75230 | -0.64041 |
| H | 5.27399  | -3.21467 | -1.00096 |
| H | -1.42758 | -6.00925 | -1.00096 |
| H | -2.65359 | -4.09390 | 0.64041  |
| H | -6.15628 | -0.49925 | -1.00096 |
| H | -4.71354 | 1.25862  | 0.64041  |
| H | -2.65359 | 4.09390  | -0.64041 |
| H | -1.42758 | 6.00925  | 1.00096  |
| H | 3.07353  | 3.78880  | -0.64041 |
| H | 4.55313  | 1.75230  | 0.64041  |
| H | 4.68709  | 4.02247  | -1.00096 |
| H | 5.27399  | 3.21467  | 1.00096  |
| H | -0.25954 | -4.87177 | -0.64041 |
| H | -2.37721 | -5.70070 | 1.00096  |
| H | -4.71354 | -1.25862 | -0.64041 |
| H | -6.15628 | 0.49925  | 1.00096  |
| H | -2.37721 | 5.70070  | -1.00096 |
| H | -0.25954 | 4.87177  | 0.64041  |

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|    | [OsAu12Cl12(dppe)5] | Isomer I | (S0)     |
|----|---------------------|----------|----------|
| Au | 0.                  | 0.       | -2.59680 |
| Au | -1.41705            | 1.86957  | 1.14848  |
| Au | 1.34016             | 1.92540  | 1.14848  |
| Au | 0.04752             | 2.34541  | -1.14848 |
| Au | 0.04752             | -2.34541 | 1.14848  |
| Os | 0.                  | 0.       | 0.       |
| Au | -1.41705            | -1.86957 | -1.14848 |
| Au | 2.24537             | 0.67962  | -1.14848 |
| Au | 2.24537             | -0.67962 | 1.14848  |
| Au | -2.21599            | 0.76993  | -1.14848 |
| Au | -2.21599            | -0.76993 | 1.14848  |
| Au | 1.34016             | -1.92540 | -1.14848 |
| Au | 0.                  | 0.       | 2.59680  |
| P  | -2.02998            | -3.83446 | -1.80599 |
| P  | 3.01946             | 3.11554  | 1.80599  |
| P  | -0.61151            | 4.29538  | -1.80599 |
| P  | 3.01946             | -3.11554 | -1.80599 |
| P  | 3.89614             | -1.90896 | 1.80599  |
| P  | -0.61151            | -4.29538 | 1.80599  |
| Cl | 0.                  | 0.       | -4.88487 |
| Cl | 0.                  | 0.       | 4.88487  |
| P  | -4.27412            | 0.74575  | -1.80599 |
| P  | -4.27412            | -0.74575 | 1.80599  |
| P  | 3.89614             | 1.90896  | -1.80599 |

|   |          |          |          |
|---|----------|----------|----------|
| P | -2.02998 | 3.83446  | 1.80599  |
| C | 2.95569  | 4.84510  | 1.86966  |
| C | -3.69464 | 4.30822  | 1.86966  |
| C | -4.64841 | 3.28417  | -2.31348 |
| C | -6.49077 | 2.25028  | -1.43784 |
| C | -4.64841 | -3.28417 | 2.31348  |
| C | -1.48526 | -3.09286 | 3.97720  |
| C | -6.54075 | -4.49197 | 1.88912  |
| C | -2.17291 | -5.26757 | 3.76407  |
| C | -3.40046 | 0.45676  | 3.97720  |
| C | -6.54075 | 4.49197  | -1.88912 |
| C | -1.48526 | 3.09286  | -3.97720 |
| C | 3.92845  | 5.63572  | 1.43784  |
| C | -6.49077 | -2.25028 | 1.43784  |
| C | 5.52132  | 1.31380  | -1.86966 |
| C | 1.83027  | 5.38925  | 2.31348  |
| C | -5.23913 | 2.18245  | -1.86966 |
| C | -5.29789 | -4.42915 | 2.33077  |
| C | 5.69108  | -0.07529 | 2.31348  |
| C | -1.85304 | -4.80448 | 0.67650  |
| C | -0.61632 | 3.37514  | 3.97720  |
| C | -4.14592 | 5.47777  | 1.43784  |
| C | 4.85417  | -2.98432 | -3.76407 |
| C | 2.65121  | 7.47855  | 1.88912  |
| C | -2.17291 | 5.26757  | -3.76407 |
| C | -5.78309 | 1.17275  | 4.85388  |
| C | 3.99676  | -3.24704 | 0.67650  |
| C | -5.23913 | -2.18245 | 1.86966  |
| C | -4.48583 | 0.08937  | 3.31014  |
| C | 3.77381  | 6.94574  | 1.44407  |
| C | 1.68271  | 6.69719  | 2.33077  |
| C | -5.68126 | 0.43881  | 3.76407  |
| C | -1.30123 | -4.29396 | -3.31014 |
| C | 3.57665  | 2.70903  | -3.31014 |
| C | -0.61632 | -3.37514 | -3.97720 |
| C | 3.68170  | 2.56440  | 3.31014  |
| C | -1.85304 | 4.80448  | -0.67650 |
| C | -5.29789 | 4.42915  | -2.33077 |
| C | -1.32485 | 4.97613  | 0.67650  |
| C | 3.99676  | 3.24704  | -0.67650 |
| C | 5.69108  | 0.07529  | -2.31348 |
| C | -5.14202 | -0.27774 | -0.67650 |
| C | 3.68170  | -2.56440 | -3.31014 |
| C | 3.01946  | 1.62914  | 3.97720  |
| C | -1.32485 | -4.97613 | -0.67650 |
| C | -0.67178 | 5.86245  | 4.85388  |
| C | -2.90241 | -5.13767 | 4.85388  |
| C | -1.47119 | -4.23869 | 3.31014  |
| C | 5.52132  | -1.31380 | 1.86966  |
| C | -1.30123 | 4.29396  | 3.31014  |
| C | -7.13563 | -3.40103 | 1.44407  |
| C | 0.04790  | 3.70050  | 5.06739  |
| C | -3.50456 | 1.18910  | 5.06739  |
| C | -2.90241 | 5.13767  | -4.85388 |
| C | 4.33827  | -3.69436 | 3.76407  |
| C | 3.01946  | -1.62914 | -3.97720 |
| C | -5.14202 | 0.27774  | 0.67650  |
| C | 4.32324  | 2.79774  | 0.67650  |
| C | 3.57665  | -2.70903 | 3.31014  |
| C | 4.85417  | 2.98432  | 3.76407  |
| C | 4.33827  | 3.69436  | -3.76407 |
| C | 1.68705  | -5.43582 | 2.31348  |
| C | -1.47119 | 4.23869  | -3.31014 |
| C | 5.36790  | -2.45047 | -4.85388 |
| C | 6.88944  | 0.46923  | 2.33077  |
| C | -4.55989 | 3.40603  | 2.31348  |
| C | 5.36790  | 2.45047  | 4.85388  |
| C | 4.71246  | -1.50142 | -5.50119 |
| C | -4.69499 | 1.55526  | 5.50119  |
| C | 4.71246  | 1.50142  | 5.50119  |
| C | -2.93000 | -3.98466 | 5.50119  |
| C | 6.88944  | -0.46923 | -2.33077 |
| C | -2.93000 | 3.98466  | -5.50119 |
| C | 2.25094  | -7.60864 | 1.88912  |
| C | 7.77198  | -1.44275 | 1.44407  |
| C | 3.98929  | -4.34800 | 4.85388  |
| C | 2.13635  | -3.02192 | 5.06739  |

|   |          |          |          |
|---|----------|----------|----------|
| C | -2.21391 | 2.96561  | -5.06739 |
| C | 2.88418  | -4.01782 | 5.50119  |
| C | 3.98929  | 4.34800  | -4.85388 |
| C | 7.93182  | 0.21048  | -1.88912 |
| C | 2.13635  | 3.02192  | -5.06739 |
| C | 7.93182  | -0.21048 | 1.88912  |
| C | 0.45667  | -5.65707 | 1.86966  |
| C | 6.57381  | -1.99465 | 1.43784  |
| C | 7.77198  | 1.44275  | -1.44407 |
| C | 3.77381  | -6.94574 | -1.44407 |
| C | -4.48583 | -0.08937 | -3.31014 |
| C | -6.29333 | -4.83253 | -1.88912 |
| C | -3.40046 | -0.45676 | -3.97720 |
| C | -5.78309 | -1.17275 | -4.85388 |
| C | -4.14592 | -5.47777 | -1.43784 |
| C | 1.68271  | -6.69719 | -2.33077 |
| C | -5.43960 | -5.73548 | -1.44407 |
| C | -4.55989 | -3.40603 | -2.31348 |
| C | 1.83027  | -5.38925 | -2.31348 |
| C | 2.95569  | -4.84510 | -1.86966 |
| C | 2.65121  | -7.47855 | -1.88912 |
| C | 3.92845  | -5.63572 | -1.43784 |
| C | -3.50456 | -1.18910 | -5.06739 |
| C | -5.68126 | -0.43881 | -3.76407 |
| C | 1.02954  | -7.83735 | 1.44407  |
| C | -3.69464 | -4.30822 | -1.86966 |
| C | -5.84941 | -3.66989 | -2.33077 |
| C | 6.57381  | 1.99465  | -1.43784 |
| C | 3.53423  | -1.09793 | -5.06739 |
| C | 3.53423  | 1.09793  | 5.06739  |
| C | -4.69499 | -1.55526 | -5.50119 |
| C | 1.68705  | 5.43582  | -2.31348 |
| C | 1.02954  | 7.83735  | -1.44407 |
| C | 0.13443  | 6.86846  | -1.43784 |
| C | 0.13443  | -6.86846 | 1.43784  |
| C | 2.48249  | -2.36828 | 3.97720  |
| C | 0.45667  | 5.65707  | -1.86966 |
| C | 4.32324  | -2.79774 | -0.67650 |
| C | -5.43960 | 5.73548  | 1.44407  |
| C | 2.57517  | -6.40726 | 2.33077  |
| C | -5.84941 | 3.66989  | 2.33077  |
| C | -6.29333 | 4.83253  | 1.88912  |
| C | -7.13563 | 3.40103  | -1.44407 |
| C | -2.21391 | -2.96561 | 5.06739  |
| C | 2.48249  | 2.36828  | -3.97720 |
| C | 0.02825  | 4.94580  | 5.50119  |
| C | 0.04790  | -3.70050 | -5.06739 |
| C | 0.02825  | -4.94580 | -5.50119 |
| C | 2.57517  | 6.40726  | -2.33077 |
| C | 2.88418  | 4.01782  | -5.50119 |
| C | -1.33827 | -5.53879 | -3.76407 |
| C | 2.25094  | 7.60864  | -1.88912 |
| C | -0.67178 | -5.86245 | -4.85388 |
| C | -1.33827 | 5.53879  | 3.76407  |
| H | -0.69332 | 6.83228  | 5.19889  |
| H | 0.55605  | 5.20607  | 6.34623  |
| H | 0.57976  | 2.96986  | 5.55996  |
| H | -0.58430 | 2.40257  | 3.63985  |
| H | -1.88818 | 6.25478  | 3.26650  |
| H | 1.06619  | 4.77755  | 2.63818  |
| H | 0.80309  | 7.09944  | 2.68286  |
| H | 2.53001  | 8.50138  | 1.88610  |
| H | 4.53061  | 7.55092  | 1.09472  |
| H | 4.80835  | 5.23677  | 1.08187  |
| H | 2.95012  | 8.36487  | -1.88610 |
| H | 3.52327  | 6.21558  | -2.68286 |
| H | 0.77296  | 8.77185  | -1.09472 |
| H | -0.81197 | 7.06298  | -1.08187 |
| H | 1.94562  | 4.49187  | -2.63818 |
| H | 7.00016  | 1.43009  | 2.68286  |
| H | 8.86708  | 0.22087  | 1.88610  |
| H | 5.36516  | 3.72865  | 3.26650  |
| H | 6.28369  | 2.77072  | 5.19889  |
| H | 2.10442  | 1.29821  | 3.63985  |
| H | 3.00368  | 0.36636  | 5.55996  |
| H | 5.12312  | 1.07998  | 6.34623  |
| H | 8.58140  | -1.97556 | 1.09472  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 6.46630  | -2.95475 | 1.08187  |
| H | 4.87325  | 0.46234  | 2.63818  |
| H | 6.46630  | 2.95475  | -1.08187 |
| H | 8.58140  | 1.97556  | -1.09472 |
| H | 8.86708  | -0.22087 | -1.88610 |
| H | 7.00016  | -1.43009 | -2.68286 |
| H | 4.87325  | -0.46234 | -2.63818 |
| H | 1.88487  | -1.60023 | 3.63985  |
| H | 1.27667  | -2.74342 | 5.55996  |
| H | 2.61021  | -4.53864 | 6.34623  |
| H | 4.57690  | -5.11991 | 5.19889  |
| H | 5.20409  | -3.95037 | 3.26650  |
| H | -0.93941 | -2.28713 | 3.63985  |
| H | -2.21467 | -2.06191 | 5.55996  |
| H | -3.50986 | -3.88500 | 6.34623  |
| H | -3.45497 | -5.93500 | 5.19889  |
| H | -2.14882 | -6.17004 | 3.26650  |
| H | -2.46549 | 0.18667  | 3.63985  |
| H | -2.64536 | 1.46911  | 5.55996  |
| H | -4.77944 | 2.13758  | 6.34623  |
| H | -6.71221 | 1.45191  | 5.19889  |
| H | -6.53215 | 0.13698  | 3.26650  |
| H | -4.21432 | 2.49033  | 2.63818  |
| H | -3.49465 | 6.19130  | 1.08187  |
| H | -5.78130 | 6.64221  | 1.09472  |
| H | -7.30350 | 5.03328  | 1.88610  |
| H | -6.50381 | 2.95758  | 2.68286  |
| H | -6.96813 | 1.41035  | -1.08187 |
| H | -8.10366 | 3.44580  | -1.09472 |
| H | -7.04380 | 5.39066  | -1.88610 |
| H | -4.82261 | 5.27154  | -2.68286 |
| H | -3.67074 | 3.23844  | -2.63818 |
| H | -0.93941 | 2.28713  | -3.63985 |
| H | -2.14882 | 6.17004  | -3.26650 |
| H | -2.21467 | 2.06191  | -5.55996 |
| H | -3.50986 | 3.88500  | -6.34623 |
| H | -3.45497 | 5.93500  | -5.19889 |
| H | -2.46549 | -0.18667 | -3.63985 |
| H | -2.64536 | -1.46911 | -5.55996 |
| H | -4.77944 | -2.13758 | -6.34623 |
| H | -6.71221 | -1.45191 | -5.19889 |
| H | -6.53215 | -0.13698 | -3.26650 |
| H | -4.21432 | -2.49033 | -2.63818 |
| H | -3.49465 | -6.19130 | -1.08187 |
| H | -5.78130 | -6.64221 | -1.09472 |
| H | -7.30350 | -5.03328 | -1.88610 |
| H | -6.50381 | -2.95758 | -2.68286 |
| H | -8.10366 | -3.44580 | 1.09472  |
| H | -6.96813 | -1.41035 | 1.08187  |
| H | -4.82261 | -5.27154 | 2.68286  |
| H | -7.04380 | -5.39066 | 1.88610  |
| H | -3.67074 | -3.23844 | 2.63818  |
| H | -0.81197 | -7.06298 | 1.08187  |
| H | 0.77296  | -8.77185 | 1.09472  |
| H | 2.95012  | -8.36487 | 1.88610  |
| H | 3.52327  | -6.21558 | 2.68286  |
| H | 1.94562  | -4.49187 | 2.63818  |
| H | 4.80835  | -5.23677 | -1.08187 |
| H | 4.53061  | -7.55092 | -1.09472 |
| H | 2.53001  | -8.50138 | -1.88610 |
| H | 0.80309  | -7.09944 | -2.68286 |
| H | 1.06619  | -4.77755 | -2.63818 |
| H | -0.58430 | -2.40257 | -3.63985 |
| H | 0.57976  | -2.96986 | -5.55996 |
| H | 0.55605  | -5.20607 | -6.34623 |
| H | -0.69332 | -6.83228 | -5.19889 |
| H | -1.88818 | -6.25478 | -3.26650 |
| H | 2.10442  | -1.29821 | -3.63985 |
| H | 3.00368  | -0.36636 | -5.55996 |
| H | 5.12312  | -1.07998 | -6.34623 |
| H | 6.28369  | -2.77072 | -5.19889 |
| H | 5.36516  | -3.72865 | -3.26650 |
| H | 5.20409  | 3.95037  | -3.26650 |
| H | 1.88487  | 1.60023  | -3.63985 |
| H | 1.27667  | 2.74342  | -5.55996 |
| H | 2.61021  | 4.53864  | -6.34623 |
| H | 4.57690  | 5.11991  | -5.19889 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 3.05611  | -3.68944 | 0.71826  |
| H | 4.66731  | -3.96208 | 1.01584  |
| H | 4.45324  | -1.76641 | -0.71826 |
| H | 5.21042  | -3.21454 | -1.01584 |
| H | -1.44710 | -5.94880 | -1.01584 |
| H | -2.56449 | -4.04664 | 0.71826  |
| H | -6.10477 | -0.46205 | -1.01584 |
| H | -4.64104 | 1.18853  | 0.71826  |
| H | -2.56449 | 4.04664  | -0.71826 |
| H | -1.44710 | 5.94880  | 1.01584  |
| H | 3.05611  | 3.68944  | -0.71826 |
| H | 4.45324  | 1.76641  | 0.71826  |
| H | 4.66731  | 3.96208  | -1.01584 |
| H | 5.21042  | 3.21454  | 1.01584  |
| H | -0.30382 | -4.78114 | -0.71826 |
| H | -2.32586 | -5.66321 | 1.01584  |
| H | -4.64104 | -1.18853 | -0.71826 |
| H | -6.10477 | 0.46205  | 1.01584  |
| H | -2.32586 | 5.66321  | -1.01584 |
| H | -0.30382 | 4.78114  | 0.71826  |

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[OsAu12Cl2(dppe)5] Isomer II

|    |          |          |          |
|----|----------|----------|----------|
| Au | 0.03775  | -0.03955 | -2.64939 |
| Au | -1.64871 | 1.93928  | 1.11014  |
| Au | 1.60769  | 1.75290  | 1.00710  |
| Au | 0.05349  | 2.57670  | -0.93977 |
| Au | 0.54701  | -2.80854 | 0.90661  |
| Au | -0.02852 | 0.03370  | -0.08566 |
| Au | -1.24832 | -2.04949 | -1.20254 |
| Au | 2.84788  | 0.19141  | -1.43954 |
| Au | 2.34593  | -0.83776 | 1.09569  |
| Au | -2.26867 | 0.70297  | -1.18190 |
| Au | -2.25765 | -0.85715 | 1.07992  |
| Os | 1.56644  | -1.93391 | -1.29211 |
| Au | 0.01904  | -0.05355 | 2.46644  |
| P  | -2.02073 | -4.03160 | -1.76263 |
| P  | 3.23021  | 3.04585  | 1.72582  |
| P  | -0.63104 | 4.54116  | -1.70314 |
| P  | 3.22779  | -3.10366 | -1.74423 |
| P  | 4.00516  | -2.06998 | 1.84746  |
| P  | -0.59630 | -4.43233 | 1.84037  |
| Cl | 0.00055  | 0.07900  | -4.91980 |
| Cl | -0.00182 | 0.05105  | 4.76514  |
| P  | -4.33147 | 0.65523  | -1.87940 |
| P  | -4.37825 | -0.88375 | 1.73632  |
| P  | 4.04777  | 1.96304  | -1.93388 |
| P  | -2.12200 | 3.97501  | 1.85663  |
| C  | 3.06520  | 4.77550  | 1.79588  |
| C  | -3.78029 | 4.47826  | 1.97537  |
| C  | -4.66646 | 3.22459  | -2.33048 |
| C  | -6.53600 | 2.17839  | -1.52409 |
| C  | -4.87798 | -3.34024 | 2.52358  |
| C  | -1.45599 | -3.00005 | 3.88549  |
| C  | -6.76864 | -4.55275 | 2.07702  |
| C  | -2.13329 | -5.18878 | 3.91494  |
| C  | -3.50365 | 0.40202  | 3.87985  |
| C  | -6.58057 | 4.42373  | -1.96844 |
| C  | -1.45021 | 3.27191  | -3.86898 |
| C  | 3.98827  | 5.61147  | 1.33504  |
| C  | -6.58789 | -2.39696 | 1.32720  |
| C  | 5.72519  | 1.62274  | -2.24968 |
| C  | 1.94097  | 5.26996  | 2.30045  |
| C  | -5.26903 | 2.11662  | -1.91599 |
| C  | -5.56984 | -4.45696 | 2.62862  |
| C  | 5.78968  | -0.29268 | 2.64378  |
| C  | -1.90644 | -4.88448 | 0.76343  |
| C  | -0.65134 | 3.42189  | 3.97155  |
| C  | -4.21949 | 5.65987  | 1.55820  |
| C  | 5.24042  | -3.01691 | -3.61130 |
| C  | 2.66855  | 7.39961  | 1.88028  |
| C  | -2.07002 | 5.47869  | -3.77211 |
| C  | -5.90087 | 1.01739  | 4.79839  |
| C  | 4.21540  | -3.40231 | 0.72910  |
| C  | -5.38322 | -2.29467 | 1.87723  |
| C  | -4.58494 | -0.00537 | 3.22697  |
| C  | 3.78819  | 6.91568  | 1.37405  |
| C  | 1.74929  | 6.57365  | 2.34950  |

|   |          |          |          |
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| C | -5.78740 | 0.29648  | 3.70054  |
| C | -1.34671 | -4.57273 | -3.26742 |
| C | 3.50139  | 2.85719  | -3.32643 |
| C | -0.49257 | -3.78557 | -3.90801 |
| C | 3.83596  | 2.57105  | 3.28217  |
| C | -1.90955 | 5.02711  | -0.60315 |
| C | -5.32046 | 4.36942  | -2.36139 |
| C | -1.41741 | 5.15897  | 0.76725  |
| C | 4.11225  | 3.24666  | -0.73739 |
| C | 6.01783  | 0.46254  | -2.82595 |
| C | -5.21971 | -0.38766 | -0.77830 |
| C | 4.00270  | -2.68532 | -3.27282 |
| C | 3.14213  | 1.68093  | 3.97937  |
| C | -1.44999 | -5.20030 | -0.58833 |
| C | -0.74381 | 5.85172  | 5.00352  |
| C | -2.83071 | -4.95373 | 5.00963  |
| C | -1.45276 | -4.20555 | 3.33814  |
| C | 5.62805  | -1.46720 | 2.04667  |
| C | -1.35835 | 4.36724  | 3.36728  |
| C | -7.27383 | -3.52159 | 1.42472  |
| C | 0.01078  | 3.69174  | 5.08179  |
| C | -3.61974 | 1.11920  | 4.98077  |
| C | -2.72064 | 5.34082  | -4.91159 |
| C | 4.38025  | -3.82903 | 3.84453  |
| C | 3.29138  | -1.93967 | -4.11248 |
| C | -5.23490 | 0.13512  | 0.58793  |
| C | 4.53930  | 2.80358  | 0.58896  |
| C | 3.61632  | -2.86269 | 3.34899  |
| C | 4.96716  | 3.05820  | 3.77972  |
| C | 4.19101  | 3.88569  | -3.80697 |
| C | 1.56006  | -5.80378 | 2.44828  |
| C | -1.44042 | 4.43895  | -3.23804 |
| C | 5.75793  | -2.60108 | -4.75407 |
| C | 6.99636  | 0.21374  | 2.80857  |
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| C | 5.40888  | 2.63581  | 4.94829  |
| C | 5.04556  | -1.84762 | -5.57356 |
| C | -4.81758 | 1.43424  | 5.43571  |
| C | 4.71955  | 1.73671  | 5.63278  |
| C | -2.84544 | -3.74122 | 5.54105  |
| C | 7.27132  | 0.15389  | -3.09936 |
| C | -2.74006 | 4.16937  | -5.52792 |
| C | 1.82514  | -8.06800 | 2.26050  |
| C | 7.90503  | -1.60206 | 1.75901  |
| C | 4.02589  | -4.44696 | 4.95502  |
| C | 2.15743  | -3.13065 | 5.09993  |
| C | -2.10038 | 3.13710  | -5.00999 |
| C | 2.91316  | -4.10085 | 5.58164  |
| C | 3.72170  | 4.57668  | -4.82751 |
| C | 8.24692  | 0.99066  | -2.79178 |
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| C | 8.05756  | -0.43778 | 2.36423  |
| C | 0.30698  | -5.90544 | 2.02272  |
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| C | 7.96513  | 2.14234  | -2.20918 |
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| C | -6.34637 | -4.74732 | -2.06819 |
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| C | -5.85642 | -1.02043 | -5.06439 |
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| C | -5.61305 | -5.55522 | -1.32417 |
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| C | 1.87659  | -5.35733 | -2.03059 |
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| C | 4.10229  | -5.70208 | -1.68413 |
| C | -3.57591 | -1.13271 | -5.23576 |
| C | -5.74449 | -0.37031 | -3.92277 |
| C | 0.57904  | -8.17795 | 1.83737  |
| C | -3.72415 | -4.36321 | -1.87000 |
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| C | -4.77292 | -1.40820 | -5.71811 |

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| C | 2.50859  | -2.51243 | 3.98773  |
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| C | 2.31109  | -6.87919 | 2.57122  |
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| C | -7.18634 | 3.32686  | -1.54902 |
| C | -2.14993 | -2.76743 | 4.98413  |
| C | 2.35329  | 2.51816  | -3.89558 |
| C | -0.02985 | 4.90724  | 5.59484  |
| C | 0.07464  | -4.19586 | -5.02653 |
| C | -0.21299 | -5.38782 | -5.51251 |
| C | 2.42721  | 6.81319  | -2.38777 |
| C | 2.56647  | 4.24287  | -5.38116 |
| C | -1.64419 | -5.76683 | -3.76641 |
| C | 2.07007  | 7.99431  | -1.91434 |
| C | -1.07354 | -6.17262 | -4.88310 |
| C | -1.40931 | 5.58410  | 3.89627  |
| H | -0.78359 | 6.79990  | 5.40930  |
| H | 0.49251  | 5.12261  | 6.45845  |
| H | 0.55573  | 2.94029  | 5.53057  |
| H | -0.60871 | 2.46985  | 3.57348  |
| H | -1.97535 | 6.32227  | 3.44900  |
| H | 1.21267  | 4.62951  | 2.65426  |
| H | 0.87133  | 6.93818  | 2.75033  |
| H | 2.51219  | 8.41917  | 1.90440  |
| H | 4.50854  | 7.55510  | 1.00228  |
| H | 4.86789  | 5.25293  | 0.93339  |
| H | 2.72526  | 8.79070  | -1.95629 |
| H | 3.35880  | 6.67669  | -2.80970 |
| H | 0.58854  | 9.07087  | -1.00344 |
| H | -0.89629 | 7.27844  | -0.89657 |
| H | 1.88868  | 4.86815  | -2.67512 |
| H | 7.09998  | 1.12480  | 3.28205  |
| H | 9.00094  | -0.03683 | 2.48368  |
| H | 5.50245  | 3.76921  | 3.25690  |
| H | 6.29311  | 3.00887  | 5.32807  |
| H | 2.26255  | 1.29425  | 3.60163  |
| H | 3.03295  | 0.56572  | 5.67210  |
| H | 5.07310  | 1.40292  | 6.54208  |
| H | 8.72754  | -2.11247 | 1.40320  |
| H | 6.60210  | -3.02102 | 1.11910  |
| H | 4.96336  | 0.22890  | 2.97729  |
| H | 6.51294  | 3.35969  | -1.48062 |
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| H | 9.22771  | 0.74424  | -2.99793 |
| H | 7.47764  | -0.74999 | -3.55161 |
| H | 5.26064  | -0.20372 | -3.05353 |
| H | 1.91556  | -1.75512 | 3.61104  |
| H | 1.28927  | -2.84703 | 5.57821  |
| H | 2.63713  | -4.58893 | 6.44800  |
| H | 4.62047  | -5.20079 | 5.33414  |
| H | 5.25474  | -4.09718 | 3.36750  |
| H | -0.91583 | -2.23429 | 3.45116  |
| H | -2.13274 | -1.82126 | 5.39269  |
| H | -3.39810 | -3.55983 | 6.39308  |
| H | -3.36403 | -5.71803 | 5.45257  |
| H | -2.11184 | -6.13998 | 3.51486  |
| H | -2.56306 | 0.16996  | 3.52456  |
| H | -2.76435 | 1.42664  | 5.46931  |
| H | -4.91103 | 2.00295  | 6.29102  |
| H | -6.83790 | 1.25098  | 5.16157  |
| H | -6.63691 | -0.03856 | 3.21794  |
| H | -4.32305 | 2.66834  | 2.76118  |
| H | -3.56565 | 6.35794  | 1.17295  |
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| H | -4.83508 | 5.21863  | -2.68974 |

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| H | -3.67845 | 3.18669  | -2.62718 |
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| H | -2.04224 | 6.39926  | -3.30463 |
| H | -2.09431 | 2.21980  | -5.48106 |
| H | -3.25469 | 4.06619  | -6.41596 |
| H | -3.21153 | 6.15025  | -5.32293 |
| H | -2.52136 | -0.28030 | -3.71653 |
| H | -2.72086 | -1.42040 | -5.73506 |
| H | -4.86569 | -1.92408 | -6.60684 |
| H | -6.79213 | -1.22627 | -5.44712 |
| H | -6.59407 | -0.06206 | -3.42427 |
| H | -4.03141 | -2.76530 | -3.11369 |
| H | -3.75734 | -6.00936 | -0.64029 |
| H | -6.05616 | -6.33344 | -0.81218 |
| H | -7.36530 | -4.89430 | -2.14147 |
| H | -6.33085 | -3.11054 | -3.29932 |
| H | -8.20563 | -3.59002 | 0.98697  |
| H | -7.00035 | -1.60415 | 0.81387  |
| H | -5.16325 | -5.25511 | 3.14067  |
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| H | 0.19456  | -9.10242 | 1.59008  |
| H | 2.41853  | -8.90770 | 2.34073  |
| H | 3.28337  | -6.78074 | 2.90138  |
| H | 1.94972  | -4.87377 | 2.67013  |
| H | 5.05913  | -5.35091 | -1.52696 |
| H | 4.70742  | -7.64971 | -1.62466 |
| H | 2.54544  | -8.50973 | -1.99297 |
| H | 0.72782  | -7.02491 | -2.26546 |
| H | 1.09171  | -4.69764 | -2.14653 |
| H | -0.25117 | -2.85868 | -3.51708 |
| H | 0.74754  | -3.57869 | -5.50570 |
| H | 0.23499  | -5.71062 | -6.38335 |
| H | -1.30014 | -7.10239 | -5.26536 |
| H | -2.32885 | -6.37316 | -3.28777 |
| H | 2.32698  | -1.67017 | -3.85468 |
| H | 3.23807  | -0.92535 | -5.87516 |
| H | 5.45781  | -1.51317 | -6.45860 |
| H | 6.72405  | -2.86383 | -5.00403 |
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| H | 5.10131  | 4.14155  | -3.39294 |
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| H | 0.99356  | 2.92607  | -5.34733 |
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| H | 4.90729  | -4.07151 | 1.12290  |
| H | 4.86277  | -1.96109 | -0.64174 |
| H | 5.40456  | -3.50692 | -0.95442 |
| H | -1.73947 | -6.15427 | -0.88259 |
| H | -2.54793 | -4.06339 | 0.77604  |
| H | -6.18160 | -0.54260 | -1.13949 |
| H | -4.74706 | 1.05360  | 0.65254  |
| H | -2.63033 | 4.28067  | -0.68458 |
| H | -1.57063 | 6.11684  | 1.13978  |
| H | 3.14133  | 3.62505  | -0.72190 |
| H | 4.73882  | 1.78180  | 0.61590  |
| H | 4.70726  | 4.02078  | -1.09214 |
| H | 5.40625  | 3.28505  | 0.89925  |
| H | -0.41233 | -5.17365 | -0.65778 |
| H | -2.44013 | -5.67030 | 1.18424  |
| H | -4.73921 | -1.30961 | -0.84133 |
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| H | -2.36151 | 5.90086  | -0.93841 |
| H | -0.39149 | 4.99304  | 0.82537  |

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[OsAu12Cl12(dppe)5] Isomer III

|    |          |          |          |
|----|----------|----------|----------|
| Os | 0.00615  | -0.01256 | -2.89834 |
| Au | -1.47247 | 1.86507  | 1.02343  |
| Au | 1.32545  | 1.97690  | 1.02609  |
| Au | -0.10228 | 2.34946  | -1.53588 |
| Au | 0.09676  | -2.38497 | 1.02551  |
| Au | 0.00454  | -0.00686 | -0.25973 |
| Au | -1.29324 | -1.97298 | -1.53350 |
| Au | 2.20397  | 0.81974  | -1.53258 |
| Au | 2.29381  | -0.65235 | 1.02656  |



|    |          |          |          |
|----|----------|----------|----------|
| Au | -2.26261 | 0.62362  | -1.53504 |
| Au | -2.22877 | -0.83006 | 1.02673  |
| Au | 1.47785  | -1.85299 | -1.53316 |
| Au | 0.00377  | -0.00279 | 2.44625  |
| P  | -1.97662 | -4.01464 | -1.84603 |
| P  | 3.01703  | 3.20534  | 1.74128  |
| P  | -0.74610 | 4.40873  | -1.83901 |
| P  | 3.20406  | -3.14776 | -1.82865 |
| P  | 3.96730  | -1.89405 | 1.75852  |
| P  | -0.56338 | -4.36459 | 1.74826  |
| Cl | 0.00218  | -0.01297 | -5.03537 |
| Cl | 0.00178  | 0.00340  | 4.78142  |
| P  | -4.41550 | 0.65431  | -1.84486 |
| P  | -4.31598 | -0.81152 | 1.74969  |
| P  | 3.94173  | 2.08342  | -1.84957 |
| P  | -2.10477 | 3.85202  | 1.75507  |
| C  | 2.96929  | 4.93773  | 1.88277  |
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| C  | -4.70247 | 3.22971  | -2.29984 |
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| C  | -3.39403 | 0.38572  | 3.92458  |
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| C  | 5.54454  | 1.40966  | -1.87500 |
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| C  | -5.31188 | 2.14460  | -1.84419 |
| C  | -5.47229 | -4.41164 | 2.60550  |
| C  | 5.79786  | -0.15818 | 2.50800  |
| C  | -1.81446 | -4.93418 | 0.66159  |
| C  | -0.67616 | 3.34741  | 3.92916  |
| C  | -4.22114 | 5.50057  | 1.40580  |
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| C  | -2.20167 | 5.66648  | -3.72521 |
| C  | -5.77313 | 0.97360  | 4.90647  |
| C  | 4.11404  | -3.26988 | 0.68320  |
| C  | -5.30540 | -2.23312 | 1.89191  |
| C  | -4.48608 | 0.00491  | 3.27692  |
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| C  | -5.68002 | 0.28907  | 3.78395  |
| C  | -1.35373 | -4.62259 | -3.36270 |
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| C  | 3.64004  | 2.65338  | 3.26995  |
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| C  | -5.32370 | 4.39407  | -2.31174 |
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| C  | -5.29012 | -0.33366 | -0.69112 |
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| C  | -2.72531 | -5.18554 | 4.90151  |
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| C  | -5.23357 | 0.21159  | 0.66239  |
| C  | 4.36296  | 2.92486  | 0.65400  |
| C  | 3.61968  | -2.64491 | 3.29068  |
| C  | 4.76944  | 3.13718  | 3.77442  |
| C  | 4.68075  | 3.85137  | -3.74382 |
| C  | 1.65143  | -5.55830 | 2.52589  |

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| C | -1.61542 | 4.53674  | -3.35042 |
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| C | -4.60785 | 3.52964  | 2.49710  |
| C | 5.25223  | 2.64856  | 4.89977  |
| C | 5.18119  | -2.03887 | -5.59521 |
| C | -4.67803 | 1.37101  | 5.53553  |
| C | 4.60792  | 1.68147  | 5.53462  |
| C | -2.75436 | -4.02360 | 5.53542  |
| C | 6.86306  | -0.40403 | -2.37287 |
| C | -3.01352 | 4.63151  | -5.59954 |
| C | 2.22231  | -7.74261 | 2.13899  |
| C | 7.86865  | -1.46619 | 1.52073  |
| C | 4.07315  | -4.18569 | 4.92380  |
| C | 2.18942  | -2.89292 | 5.06799  |
| C | -2.41808 | 3.51050  | -5.24002 |
| C | 2.96054  | -3.84531 | 5.55558  |
| C | 4.50725  | 4.52656  | -4.86379 |
| C | 7.93318  | 0.24945  | -1.95117 |
| C | 2.56127  | 3.38674  | -5.25303 |
| C | 8.05218  | -0.30667 | 2.12488  |
| C | 0.48875  | -5.74006 | 1.90975  |
| C | 6.65409  | -1.97614 | 1.41497  |
| C | 7.81182  | 1.48255  | -1.49317 |
| C | 3.81751  | -7.00453 | -1.39372 |
| C | -4.80853 | -0.11879 | -3.36424 |
| C | -6.28878 | -4.86504 | -1.89214 |
| C | -3.82085 | -0.56207 | -4.13051 |
| C | -6.32932 | -0.94096 | -4.87416 |
| C | -4.16293 | -5.54399 | -1.37383 |
| C | 1.77522  | -6.70849 | -2.38328 |
| C | -5.46518 | -5.76703 | -1.38754 |
| C | -4.50652 | -3.50650 | -2.35979 |
| C | 1.94600  | -5.40066 | -2.34544 |
| C | 3.05839  | -4.88006 | -1.84066 |
| C | 2.70993  | -7.51364 | -1.90571 |
| C | 3.99411  | -5.69567 | -1.36381 |
| C | -4.08708 | -1.20225 | -5.25448 |
| C | -6.06644 | -0.30025 | -3.75109 |
| C | 1.07069  | -7.93221 | 1.52001  |
| C | -3.67029 | -4.40803 | -1.85802 |
| C | -5.80566 | -3.73590 | -2.38355 |
| C | 6.62588  | 2.06271  | -1.45712 |
| C | 4.04877  | -1.46332 | -5.23800 |
| C | 3.47237  | 1.21535  | 5.05034  |
| C | -5.33960 | -1.39734 | -5.62485 |
| C | 1.59321  | 5.49917  | -2.35292 |
| C | 1.02129  | 7.88664  | -1.38272 |
| C | 0.10882  | 6.93288  | -1.36360 |
| C | 0.20710  | -6.93927 | 1.40950  |
| C | 2.51838  | -2.29444 | 3.93944  |
| C | 0.38697  | 5.72792  | -1.84860 |
| C | 4.48825  | -2.86920 | -0.67001 |
| C | -5.50090 | 5.80740  | 1.50630  |
| C | 2.50574  | -6.55492 | 2.64691  |
| C | -5.88252 | 3.84527  | 2.60776  |
| C | -6.33481 | 4.98177  | 2.10748  |
| C | -7.17215 | 3.41647  | -1.39762 |
| C | -2.09003 | -2.99175 | 5.05147  |
| C | 2.73197  | 2.71023  | -4.13181 |
| C | -0.15321 | 4.87224  | 5.54946  |
| C | -0.07568 | -4.27365 | -5.23807 |
| C | -0.28459 | -5.52153 | -5.61648 |
| C | 2.50043  | 6.45587  | -2.37903 |
| C | 3.44400  | 4.29840  | -5.61782 |
| C | -1.57634 | -5.87111 | -3.75687 |
| C | 2.21774  | 7.65106  | -1.89075 |
| C | -1.04015 | -6.31838 | -4.87715 |
| C | -1.49286 | 5.48570  | 3.79684  |
| H | -0.95897 | 6.73899  | 5.31350  |
| H | 0.33516  | 5.11455  | 6.42479  |
| H | 0.48684  | 2.92044  | 5.53574  |
| H | -0.59316 | 2.39167  | 3.54911  |
| H | -2.06695 | 6.19980  | 3.32113  |
| H | 1.17996  | 4.86877  | 2.87955  |
| H | 0.99493  | 7.18517  | 3.09248  |
| H | 2.65596  | 8.60289  | 2.17877  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 4.51790  | 7.65910  | 1.08368  |
| H | 4.72871  | 5.34782  | 0.90158  |
| H | 2.93157  | 8.39594  | -1.89874 |
| H | 3.42984  | 6.25756  | -2.78055 |
| H | 0.79677  | 8.81484  | -0.99294 |
| H | -0.81599 | 7.13633  | -0.95543 |
| H | 1.82048  | 4.56343  | -2.72393 |
| H | 7.14141  | 1.24630  | 3.10247  |
| H | 9.00226  | 0.09070  | 2.20585  |
| H | 5.26930  | 3.90121  | 3.29234  |
| H | 6.13361  | 3.02305  | 5.28424  |
| H | 2.10504  | 1.32346  | 3.54751  |
| H | 2.95022  | 0.47013  | 5.53584  |
| H | 4.99279  | 1.29469  | 6.40933  |
| H | 8.67402  | -1.97728 | 1.12694  |
| H | 6.53571  | -2.88323 | 0.94047  |
| H | 4.99047  | 0.36305  | 2.88677  |
| H | 6.55320  | 3.02356  | -1.08929 |
| H | 8.64437  | 1.99565  | -1.15678 |
| H | 8.86151  | -0.20346 | -1.97442 |
| H | 6.94342  | -1.36580 | -2.73613 |
| H | 4.83855  | -0.34413 | -2.64667 |
| H | 1.90376  | -1.55819 | 3.56201  |
| H | 1.32431  | -2.60462 | 5.54959  |
| H | 2.69906  | -4.32263 | 6.43096  |
| H | 4.68376  | -4.92131 | 5.31085  |
| H | 5.28207  | -3.84780 | 3.31903  |
| H | -0.90528 | -2.29890 | 3.54893  |
| H | -2.09201 | -2.08104 | 5.53562  |
| H | -3.29379 | -3.92667 | 6.40945  |
| H | -3.23409 | -5.99648 | 5.28560  |
| H | -2.01602 | -6.22427 | 3.29711  |
| H | -2.46114 | 0.16003  | 3.54873  |
| H | -2.62438 | 1.36008  | 5.52907  |
| H | -4.75473 | 1.91483  | 6.40722  |
| H | -6.70223 | 1.19802  | 5.29291  |
| H | -6.53802 | -0.02887 | 3.30549  |
| H | -4.26557 | 2.63337  | 2.87794  |
| H | -3.58792 | 6.16028  | 0.93441  |
| H | -5.84563 | 6.69459  | 1.10950  |
| H | -7.33518 | 5.22226  | 2.18249  |
| H | -6.52191 | 3.19178  | 3.08216  |
| H | -7.04985 | 1.42350  | -1.02771 |
| H | -8.13375 | 3.48755  | -1.03325 |
| H | -7.04200 | 5.40433  | -1.85092 |
| H | -4.83249 | 5.22406  | -2.67424 |
| H | -3.73276 | 3.15924  | -2.64296 |
| H | -1.26390 | 2.58074  | -3.83070 |
| H | -2.10363 | 6.51913  | -3.15046 |
| H | -2.49934 | 2.66277  | -5.82208 |
| H | -3.56330 | 4.66916  | -6.47178 |
| H | -3.35637 | 6.59099  | -5.12750 |
| H | -2.83946 | -0.42084 | -3.83161 |
| H | -3.30763 | -1.55284 | -5.83247 |
| H | -5.54845 | -1.90082 | -6.50107 |
| H | -7.30914 | -1.08134 | -5.16785 |
| H | -6.84475 | 0.06848  | -3.18088 |
| H | -4.13381 | -2.61737 | -2.72977 |
| H | -3.53894 | -6.25959 | -0.97054 |
| H | -5.83613 | -6.64801 | -0.99722 |
| H | -7.30692 | -5.03912 | -1.89664 |
| H | -6.43647 | -3.02288 | -2.78265 |
| H | -8.16166 | -3.50372 | 1.08022  |
| H | -6.96303 | -1.51641 | 0.91261  |
| H | -5.04935 | -5.22057 | 3.08610  |
| H | -7.22332 | -5.37423 | 2.16258  |
| H | -3.82733 | -3.24201 | 2.88901  |
| H | -0.68445 | -7.10992 | 0.92162  |
| H | 0.84250  | -8.85437 | 1.11485  |
| H | 2.89778  | -8.51818 | 2.22157  |
| H | 3.40023  | -6.39352 | 3.13506  |
| H | 1.88825  | -4.63013 | 2.91205  |
| H | 4.86471  | -5.32026 | -0.95639 |
| H | 4.54714  | -7.62832 | -1.01059 |
| H | 2.57372  | -8.53724 | -1.92525 |
| H | 0.90423  | -7.09092 | -2.78501 |
| H | 1.21019  | -4.77409 | -2.70945 |

|   |          |          |          |
|---|----------|----------|----------|
| H | -0.43782 | -2.84853 | -3.81364 |
| H | 0.51087  | -3.64310 | -5.80713 |
| H | 0.13628  | -5.87522 | -6.49050 |
| H | -1.21575 | -7.29052 | -5.17728 |
| H | -2.17938 | -6.49440 | -3.19522 |
| H | 2.56917  | -1.36180 | -3.82837 |
| H | 3.62653  | -0.72608 | -5.82360 |
| H | 5.65209  | -1.75596 | -6.46849 |
| H | 6.59205  | -3.44120 | -5.11728 |
| H | 5.52811  | -4.09398 | -3.13738 |
| H | 5.52285  | 4.02476  | -3.17125 |
| H | 2.03228  | 2.00592  | -3.83712 |
| H | 1.72896  | 3.19951  | -5.83359 |
| H | 3.30939  | 4.83008  | -6.49232 |
| H | 5.20579  | 5.23023  | -5.15219 |
| H | 3.18009  | -3.73176 | 0.70653  |
| H | 4.78613  | -3.95629 | 1.07972  |
| H | 4.69880  | -1.85195 | -0.73329 |
| H | 5.34760  | -3.35864 | -0.98843 |
| H | -1.51160 | -6.12365 | -1.01891 |
| H | -2.54729 | -4.19340 | 0.68792  |
| H | -6.27053 | -0.45250 | -1.01457 |
| H | -4.74621 | 1.13251  | 0.68875  |
| H | -2.71316 | 4.22897  | -0.74163 |
| H | -1.54458 | 5.99691  | 1.06439  |
| H | 3.17616  | 3.90621  | -0.75673 |
| H | 4.51731  | 1.89426  | 0.68132  |
| H | 4.80612  | 4.06472  | -1.02606 |
| H | 5.22564  | 3.35730  | 1.03979  |
| H | -0.28108 | -5.03950 | -0.75328 |
| H | -2.25677 | -5.78996 | 1.05193  |
| H | -4.85220 | -1.27619 | -0.75330 |
| H | -6.18382 | 0.37674  | 1.04976  |
| H | -2.36568 | 5.83176  | -0.99830 |
| H | -0.38606 | 4.86028  | 0.69842  |

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[RuAu12Cl12(dppe)5] Isomer I

|    |          |          |          |
|----|----------|----------|----------|
| Au | 0.       | 0.       | -2.60853 |
| Au | -1.44105 | 1.86257  | 1.15584  |
| Au | 1.32610  | 1.94608  | 1.15584  |
| Au | 0.07104  | 2.35387  | -1.15584 |
| Au | 0.07104  | -2.35387 | 1.15584  |
| Ru | 0.       | 0.       | 0.       |
| Au | -1.44105 | -1.86257 | -1.15584 |
| Au | 2.26062  | 0.65982  | -1.15584 |
| Au | 2.26062  | -0.65982 | 1.15584  |
| Au | -2.21671 | 0.79495  | -1.15584 |
| Au | -2.21671 | -0.79495 | 1.15584  |
| Au | 1.32610  | -1.94608 | -1.15584 |
| Au | 0.       | 0.       | 2.60853  |
| P  | -2.05085 | -3.85291 | -1.80791 |
| P  | 3.03059  | 3.14109  | 1.80791  |
| P  | -0.60551 | 4.32253  | -1.80791 |
| P  | 3.03059  | -3.14109 | -1.80791 |
| P  | 3.92386  | -1.91161 | 1.80791  |
| P  | -0.60551 | -4.32253 | 1.80791  |
| Cl | 0.       | 0.       | -4.91608 |
| Cl | 0.       | 0.       | 4.91608  |
| P  | -4.29809 | 0.75986  | -1.80791 |
| P  | -4.29809 | -0.75986 | 1.80791  |
| P  | 3.92386  | 1.91161  | -1.80791 |
| P  | -2.05085 | 3.85291  | 1.80791  |
| C  | 2.95230  | 4.87152  | 1.85164  |
| C  | -3.72078 | 4.31318  | 1.85164  |
| C  | -4.65071 | 3.30792  | -2.28374 |
| C  | -6.50055 | 2.27973  | -1.40729 |
| C  | -4.65071 | -3.30792 | 2.28374  |
| C  | -1.48201 | -3.11610 | 3.97955  |
| C  | -6.52686 | -4.53174 | 1.81932  |
| C  | -2.19953 | -5.28251 | 3.74928  |
| C  | -3.42156 | 0.44655  | 3.97955  |
| C  | -6.52686 | 4.53174  | -1.81932 |
| C  | -1.48201 | 3.11610  | -3.97955 |
| C  | 3.91906  | 5.66527  | 1.40729  |
| C  | -6.50055 | -2.27973 | 1.40729  |
| C  | 5.54540  | 1.30242  | -1.85164 |
| C  | 1.81816  | 5.40978  | 2.28374  |

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.25186 | 2.20583  | -1.85164 |
| C | -5.28776 | -4.46188 | 2.27389  |
| C | 5.70685  | -0.05746 | 2.28374  |
| C | -1.85357 | -4.81618 | 0.67705  |
| C | -0.63263 | 3.39209  | 3.97955  |
| C | -4.17693 | 5.47791  | 1.40729  |
| C | 4.88444  | -2.98079 | -3.74928 |
| C | 2.61665  | 7.50264  | 1.81932  |
| C | -2.19953 | 5.28251  | -3.74928 |
| C | -5.80184 | 1.22254  | 4.82087  |
| C | 4.00767  | -3.25113 | 0.67705  |
| C | -5.25186 | -2.20583 | 1.85164  |
| C | -4.50861 | 0.08197  | 3.31149  |
| C | 3.74864  | 6.97459  | 1.38846  |
| C | 1.65526  | 6.71780  | 2.27389  |
| C | -5.70366 | 0.45949  | 3.74928  |
| C | -1.31528 | -4.31328 | -3.31149 |
| C | 3.59936  | 2.71641  | -3.31149 |
| C | -0.63263 | -3.39209 | -3.97955 |
| C | 3.69573  | 2.58378  | 3.31149  |
| C | -1.85357 | 4.81618  | -0.67705 |
| C | -5.28776 | 4.46188  | -2.27389 |
| C | -1.33131 | 4.98587  | 0.67705  |
| C | 4.00767  | 3.25113  | -0.67705 |
| C | 5.70685  | 0.05746  | -2.28374 |
| C | -5.15324 | -0.27457 | -0.67705 |
| C | 3.69573  | -2.58378 | -3.31149 |
| C | 3.03057  | 1.64988  | 3.97955  |
| C | -1.33131 | -4.98587 | -0.67705 |
| C | -0.63016 | 5.89567  | 4.82087  |
| C | -2.95557 | -5.14010 | 4.82087  |
| C | -1.47120 | -4.26261 | 3.31149  |
| C | 5.54540  | -1.30242 | 1.85164  |
| C | -1.31528 | 4.31328  | 3.31149  |
| C | -7.13228 | -3.43916 | 1.38846  |
| C | 0.06082  | 3.72337  | 5.05152  |
| C | -3.52234 | 1.20843  | 5.05152  |
| C | -2.95557 | 5.14010  | -4.82087 |
| C | 4.34427  | -3.72426 | 3.74928  |
| C | 3.03057  | -1.64988 | -3.97955 |
| C | -5.15324 | 0.27457  | 0.67705  |
| C | 4.33045  | 2.80687  | 0.67705  |
| C | 3.59936  | -2.71641 | 3.31149  |
| C | 4.88444  | 2.98079  | 3.74928  |
| C | 4.34427  | 3.72426  | -3.74928 |
| C | 1.70887  | -5.44529 | 2.28374  |
| C | -1.47120 | 4.26261  | -3.31149 |
| C | 5.41238  | -2.42118 | -4.82087 |
| C | 6.90051  | 0.50167  | 2.27389  |
| C | -4.58316 | 3.40088  | 2.28374  |
| C | 5.41238  | 2.42118  | 4.82087  |
| C | 4.75584  | -1.46930 | -5.46588 |
| C | -4.71119 | 1.60673  | 5.46588  |
| C | 4.75584  | 1.46930  | 5.46588  |
| C | -2.98393 | -3.98410 | 5.46588  |
| C | 6.90051  | -0.50167 | -2.27389 |
| C | -2.98393 | 3.98410  | -5.46588 |
| C | 2.29303  | -7.60780 | 1.81932  |
| C | 7.79162  | -1.40991 | 1.38846  |
| C | 3.97520  | -4.39929 | 4.82087  |
| C | 2.13934  | -3.04802 | 5.05152  |
| C | -2.23775 | 2.97652  | -5.05152 |
| C | 2.86702  | -4.06904 | 5.46588  |
| C | 3.97520  | 4.39929  | -4.82087 |
| C | 7.94403  | 0.17014  | -1.81932 |
| C | 2.13934  | 3.04802  | -5.05152 |
| C | 7.94403  | -0.17014 | 1.81932  |
| C | 0.47495  | -5.67646 | 1.85164  |
| C | 6.59905  | -1.97659 | 1.40729  |
| C | 7.79162  | 1.40991  | -1.38846 |
| C | 3.74864  | -6.97459 | -1.38846 |
| C | -4.50861 | -0.08197 | -3.31149 |
| C | -6.32685 | -4.80703 | -1.81932 |
| C | -3.42156 | -0.44655 | -3.97955 |
| C | -5.80184 | -1.22254 | -4.82087 |
| C | -4.17693 | -5.47791 | -1.40729 |
| C | 1.65526  | -6.71780 | -2.27389 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.47483 | -5.72044 | -1.38846 |
| C | -4.58316 | -3.40088 | -2.28374 |
| C | 1.81816  | -5.40978 | -2.28374 |
| C | 2.95230  | -4.87152 | -1.85164 |
| C | 2.61665  | -7.50264 | -1.81932 |
| C | 3.91906  | -5.66527 | -1.40729 |
| C | -3.52234 | -1.20843 | -5.05152 |
| C | -5.70366 | -0.45949 | -3.74928 |
| C | 1.06684  | -7.84596 | 1.38846  |
| C | -3.72078 | -4.31318 | -1.85164 |
| C | -5.87750 | -3.65016 | -2.27389 |
| C | 6.59905  | 1.97659  | -1.40729 |
| C | 3.55993  | -1.09274 | -5.05152 |
| C | 3.55993  | 1.09274  | 5.05152  |
| C | -4.71119 | -1.60673 | -5.46588 |
| C | 1.70887  | 5.44529  | -2.28374 |
| C | 1.06684  | 7.84596  | -1.38846 |
| C | 0.15937  | 6.88686  | -1.40729 |
| C | 0.15937  | -6.88686 | 1.40729  |
| C | 2.50563  | -2.37241 | 3.97955  |
| C | 0.47495  | 5.67646  | -1.85164 |
| C | 4.33045  | -2.80687 | -0.67705 |
| C | -5.47483 | 5.72044  | 1.38846  |
| C | 2.60949  | -6.40775 | 2.27389  |
| C | -5.87750 | 3.65016  | 2.27389  |
| C | -6.32685 | 4.80703  | 1.81932  |
| C | -7.13228 | 3.43916  | -1.38846 |
| C | -2.23775 | -2.97652 | 5.05152  |
| C | 2.50563  | 2.37241  | -3.97955 |
| C | 0.07225  | 4.97711  | 5.46588  |
| C | 0.06082  | -3.72337 | -5.05152 |
| C | 0.07225  | -4.97711 | -5.46588 |
| C | 2.60949  | 6.40775  | -2.27389 |
| C | 2.86702  | 4.06904  | -5.46588 |
| C | -1.32552 | -5.56649 | -3.74928 |
| C | 2.29303  | 7.60780  | -1.81932 |
| C | -0.63016 | -5.89567 | -4.82087 |
| C | -1.32552 | 5.56649  | 3.74928  |
| H | -0.62836 | 6.87233  | 5.15104  |
| H | 0.62799  | 5.24257  | 6.29245  |
| H | 0.59411  | 2.99187  | 5.54399  |
| H | -0.62059 | 2.41454  | 3.65465  |
| H | -1.87242 | 6.28537  | 3.25063  |
| H | 1.05969  | 4.79556  | 2.61919  |
| H | 0.76787  | 7.11607  | 2.61417  |
| H | 2.48194  | 8.52485  | 1.79241  |
| H | 4.49888  | 7.58258  | 1.02737  |
| H | 4.80485  | 5.26899  | 1.05958  |
| H | 3.00285  | 8.35560  | -1.79241 |
| H | 3.56150  | 6.20836  | -2.61417 |
| H | 0.81726  | 8.77881  | -1.02737 |
| H | -0.79017 | 7.08692  | -1.05958 |
| H | 1.96145  | 4.50256  | -2.61919 |
| H | 7.00507  | 1.46870  | 2.61417  |
| H | 8.87458  | 0.27386  | 1.79241  |
| H | 5.39914  | 3.72307  | 3.25063  |
| H | 6.34180  | 2.72127  | 5.15104  |
| H | 2.10459  | 1.33635  | 3.65465  |
| H | 3.02903  | 0.35951  | 5.54399  |
| H | 5.18004  | 1.02279  | 6.29245  |
| H | 8.60169  | -1.93554 | 1.02737  |
| H | 6.49589  | -2.94148 | 1.05958  |
| H | 4.88831  | 0.47409  | 2.61919  |
| H | 6.49589  | 2.94148  | -1.05958 |
| H | 8.60169  | 1.93554  | -1.02737 |
| H | 8.87458  | -0.27386 | -1.79241 |
| H | 7.00507  | -1.46870 | -2.61417 |
| H | 4.88831  | -0.47409 | -2.61919 |
| H | 1.92130  | -1.58863 | 3.65465  |
| H | 1.27794  | -2.76968 | 5.54399  |
| H | 2.57345  | -4.61045 | 6.29245  |
| H | 4.54781  | -5.19049 | 5.15104  |
| H | 5.20927  | -3.98439 | 3.25063  |
| H | -0.91716 | -2.31818 | 3.65465  |
| H | -2.23922 | -2.07127 | 5.54399  |
| H | -3.58956 | -3.87221 | 6.29245  |
| H | -3.53110 | -5.92917 | 5.15104  |

|   |          |          |          |
|---|----------|----------|----------|
| H | -2.17963 | -6.18556 | 3.25063  |
| H | -2.48813 | 0.15591  | 3.65465  |
| H | -2.66185 | 1.48957  | 5.54399  |
| H | -4.79192 | 2.21730  | 6.29245  |
| H | -6.73015 | 1.52606  | 5.15104  |
| H | -6.55636 | 0.16151  | 3.25063  |
| H | -4.23339 | 2.48973  | 2.61919  |
| H | -3.52633 | 6.19789  | 1.05958  |
| H | -5.82123 | 6.62183  | 1.02737  |
| H | -7.34065 | 4.99479  | 1.79241  |
| H | -6.53050 | 2.92927  | 2.61417  |
| H | -6.98424 | 1.43848  | -1.05958 |
| H | -8.09660 | 3.49006  | -1.02737 |
| H | -7.01871 | 5.43790  | -1.79241 |
| H | -4.80394 | 5.30568  | -2.61417 |
| H | -3.67607 | 3.25682  | -2.61919 |
| H | -0.91716 | 2.31818  | -3.65465 |
| H | -2.17963 | 6.18556  | -3.25063 |
| H | -2.23922 | 2.07127  | -5.54399 |
| H | -3.58956 | 3.87221  | -6.29245 |
| H | -3.53110 | 5.92917  | -5.15104 |
| H | -2.48813 | -0.15591 | -3.65465 |
| H | -2.66185 | -1.48957 | -5.54399 |
| H | -4.79192 | -2.21730 | -6.29245 |
| H | -6.73015 | -1.52606 | -5.15104 |
| H | -6.55636 | -0.16151 | -3.25063 |
| H | -4.23339 | -2.48973 | -2.61919 |
| H | -3.52633 | -6.19789 | -1.05958 |
| H | -5.82123 | -6.62183 | -1.02737 |
| H | -7.34065 | -4.99479 | -1.79241 |
| H | -6.53050 | -2.92927 | -2.61417 |
| H | -8.09660 | -3.49006 | 1.02737  |
| H | -6.98424 | -1.43848 | 1.05958  |
| H | -4.80394 | -5.30568 | 2.61417  |
| H | -7.01871 | -5.43790 | 1.79241  |
| H | -3.67607 | -3.25682 | 2.61919  |
| H | -0.79017 | -7.08692 | 1.05958  |
| H | 0.81726  | -8.77881 | 1.02737  |
| H | 3.00285  | -8.35560 | 1.79241  |
| H | 3.56150  | -6.20836 | 2.61417  |
| H | 1.96145  | -4.50256 | 2.61919  |
| H | 4.80485  | -5.26899 | -1.05958 |
| H | 4.49888  | -7.58258 | -1.02737 |
| H | 2.48194  | -8.52485 | -1.79241 |
| H | 0.76787  | -7.11607 | -2.61417 |
| H | 1.05969  | -4.79556 | -2.61919 |
| H | -0.62059 | -2.41454 | -3.65465 |
| H | 0.59411  | -2.99187 | -5.54399 |
| H | 0.62799  | -5.24257 | -6.29245 |
| H | -0.62836 | -6.87233 | -5.15104 |
| H | -1.87242 | -6.28537 | -3.25063 |
| H | 2.10459  | -1.33635 | -3.65465 |
| H | 3.02903  | -0.35951 | -5.54399 |
| H | 5.18004  | -1.02279 | -6.29245 |
| H | 6.34180  | -2.72127 | -5.15104 |
| H | 5.39914  | -3.72307 | -3.25063 |
| H | 5.20927  | 3.98439  | -3.25063 |
| H | 1.92130  | 1.58863  | -3.65465 |
| H | 1.27794  | 2.76968  | -5.54399 |
| H | 2.57345  | 4.61045  | -6.29245 |
| H | 4.54781  | 5.19049  | -5.15104 |
| H | 3.06381  | -3.68695 | 0.72480  |
| H | 4.67462  | -3.97124 | 1.01500  |
| H | 4.45327  | -1.77453 | -0.72480 |
| H | 5.22141  | -3.21865 | -1.01500 |
| H | -1.44761 | -5.96047 | -1.01500 |
| H | -2.55973 | -4.05319 | 0.72480  |
| H | -6.11608 | -0.46513 | -1.01500 |
| H | -4.64581 | 1.18194  | 0.72480  |
| H | -2.55973 | 4.05319  | -0.72480 |
| H | -1.44761 | 5.96047  | 1.01500  |
| H | 3.06381  | 3.68695  | -0.72480 |
| H | 4.45327  | 1.77453  | 0.72480  |
| H | 4.67462  | 3.97124  | -1.01500 |
| H | 5.22141  | 3.21865  | 1.01500  |
| H | -0.31154 | -4.78367 | -0.72480 |
| H | -2.33234 | -5.67301 | 1.01500  |

|   |          |          |          |
|---|----------|----------|----------|
| H | -4.64581 | -1.18194 | -0.72480 |
| H | -6.11608 | 0.46513  | 1.01500  |
| H | -2.33234 | 5.67301  | -1.01500 |
| H | -0.31154 | 4.78367  | 0.72480  |

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[RuAu12Cl12(dppe)5] Isomer II

|    |          |          |          |
|----|----------|----------|----------|
| Au | 0.06433  | -0.08581 | -2.76432 |
| Au | -1.74813 | 1.85530  | 1.08972  |
| Au | 1.36836  | 1.78364  | 1.03204  |
| Au | 0.14912  | 2.50220  | -1.07875 |
| Au | 0.49385  | -2.65781 | 0.80456  |
| Au | -0.04638 | -0.00571 | -0.17151 |
| Au | -1.27422 | -1.93341 | -1.37708 |
| Au | 2.65271  | 0.22350  | -1.50823 |
| Au | 2.36530  | -0.85564 | 0.92222  |
| Au | -2.24886 | 0.85699  | -1.17426 |
| Au | -2.17050 | -1.03981 | 1.02035  |
| Ru | 1.53545  | -1.96922 | -1.43572 |
| Au | 0.07456  | -0.12239 | 2.40752  |
| P  | -1.92520 | -3.93541 | -1.89692 |
| P  | 3.05143  | 2.96671  | 1.72779  |
| P  | -0.67922 | 4.39367  | -1.76948 |
| P  | 3.22965  | -3.12691 | -1.71000 |
| P  | 3.97986  | -1.97569 | 1.81413  |
| P  | -0.64288 | -4.26762 | 1.71608  |
| Cl | -0.13250 | 0.28994  | -4.97480 |
| Cl | 0.02645  | 0.02767  | 4.70367  |
| P  | -4.29257 | 0.79832  | -1.85318 |
| P  | -4.22904 | -0.89785 | 1.71467  |
| P  | 3.86746  | 1.95517  | -1.95408 |
| P  | -2.08476 | 3.85110  | 1.87053  |
| C  | 2.96043  | 4.69615  | 1.75616  |
| C  | -3.72496 | 4.38579  | 1.99681  |
| C  | -4.71668 | 3.36442  | -2.15402 |
| C  | -6.49099 | 2.24910  | -1.23823 |
| C  | -4.75469 | -3.34887 | 2.42795  |
| C  | -1.42715 | -2.88884 | 3.81921  |
| C  | -6.65934 | -4.52376 | 1.96851  |
| C  | -2.13309 | -5.06604 | 3.79896  |
| C  | -3.26312 | 0.39380  | 3.80771  |
| C  | -6.59292 | 4.51558  | -1.53076 |
| C  | -1.60070 | 3.14222  | -3.88317 |
| C  | 3.95184  | 5.48466  | 1.36574  |
| C  | -6.48481 | -2.33667 | 1.31867  |
| C  | 5.52544  | 1.52164  | -2.24576 |
| C  | 1.80713  | 5.24101  | 2.12325  |
| C  | -5.26615 | 2.22846  | -1.74766 |
| C  | -5.45055 | -4.46239 | 2.49898  |
| C  | 5.66055  | -0.05374 | 2.42792  |
| C  | -1.97953 | -4.71504 | 0.67505  |
| C  | -0.51591 | 3.28158  | 3.88647  |
| C  | -4.13829 | 5.58078  | 1.60888  |
| C  | 5.18642  | -3.43725 | -3.59059 |
| C  | 2.63275  | 7.32535  | 1.69372  |
| C  | -2.33267 | 5.30341  | -3.68115 |
| C  | -5.61762 | 1.13124  | 4.74436  |
| C  | 4.26129  | -3.32976 | 0.74711  |
| C  | -5.26665 | -2.27243 | 1.84342  |
| C  | -4.36822 | -0.00768 | 3.19746  |
| C  | 3.78656  | 6.79174  | 1.33377  |
| C  | 1.64601  | 6.54675  | 2.09617  |
| C  | -5.55002 | 0.35437  | 3.68172  |
| C  | -1.05108 | -4.59393 | -3.23855 |
| C  | 3.35559  | 2.93250  | -3.29155 |
| C  | -0.09426 | -3.86205 | -3.79755 |
| C  | 3.65211  | 2.48005  | 3.27362  |
| C  | -1.93452 | 4.78558  | -0.61239 |
| C  | -5.37812 | 4.49888  | -2.05102 |
| C  | -1.37595 | 4.96174  | 0.72331  |
| C  | 3.97109  | 3.17738  | -0.70973 |
| C  | 5.76750  | 0.29853  | -2.70475 |
| C  | -5.09782 | -0.31906 | -0.76875 |
| C  | 4.02999  | -2.88670 | -3.25928 |
| C  | 2.99860  | 1.53239  | 3.92661  |
| C  | -1.49287 | -5.08026 | -0.64840 |
| C  | -0.44182 | 5.73723  | 4.85666  |
| C  | -2.81560 | -4.84940 | 4.90293  |



|   |          |          |          |
|---|----------|----------|----------|
| C | -1.44874 | -4.07619 | 3.24032  |
| C | 5.57080  | -1.31534 | 2.03399  |
| C | -1.24294 | 4.23865  | 3.32729  |
| C | -7.17410 | -3.45973 | 1.37918  |
| C | 0.25309  | 3.55391  | 4.92086  |
| C | -3.33187 | 1.17005  | 4.86951  |
| C | -3.11481 | 5.13116  | -4.72657 |
| C | 4.21025  | -3.80308 | 3.76885  |
| C | 3.43939  | -2.07386 | -4.13392 |
| C | -5.07044 | 0.16782  | 0.60928  |
| C | 4.34494  | 2.65093  | 0.59894  |
| C | 3.51779  | -2.78173 | 3.28426  |
| C | 4.76767  | 2.97777  | 3.78048  |
| C | 4.06086  | 3.97604  | -3.70544 |
| C | 1.54948  | -5.63053 | 2.17289  |
| C | -1.58033 | 4.30280  | -3.24510 |
| C | 5.74322  | -3.18556 | -4.76205 |
| C | 6.83348  | 0.53181  | 2.54775  |
| C | -4.61782 | 3.49746  | 2.41215  |
| C | 5.23879  | 2.50447  | 4.91794  |
| C | 5.14900  | -2.37303 | -5.62020 |
| C | -4.50820 | 1.54727  | 5.33320  |
| C | 4.59409  | 1.54262  | 5.55571  |
| C | -2.81120 | -3.64955 | 5.46017  |
| C | 7.00510  | -0.10422 | -2.91705 |
| C | -3.14517 | 3.96510  | -5.34732 |
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| C | 7.85675  | -1.38784 | 1.85517  |
| C | 3.74848  | -4.48195 | 4.79888  |
| C | 1.92082  | -3.11104 | 4.89389  |
| C | -2.37898 | 2.97517  | -4.93291 |
| C | 2.59949  | -4.14301 | 5.35499  |
| C | 3.56795  | 4.78020  | -4.62108 |
| C | 8.01528  | 0.70481  | -2.66148 |
| C | 1.68506  | 3.48919  | -4.75615 |
| C | 7.93570  | -0.13147 | 2.25499  |
| C | 0.26975  | -5.73984 | 1.84316  |
| C | 6.68275  | -1.97908 | 1.74670  |
| C | 7.78242  | 1.92057  | -2.19668 |
| C | 3.97530  | -7.01035 | -1.40055 |
| C | -4.55100 | 0.13673  | -3.42924 |
| C | -6.25380 | -4.42039 | -2.29140 |
| C | -3.49007 | -0.24808 | -4.12430 |
| C | -5.91598 | -0.56465 | -5.12526 |
| C | -4.22849 | -5.33477 | -1.77034 |
| C | 1.71797  | -6.71083 | -1.51738 |
| C | -5.53747 | -5.44155 | -1.86225 |
| C | -4.35097 | -3.18419 | -2.53702 |
| C | 1.90166  | -5.41077 | -1.61157 |
| C | 3.11742  | -4.88962 | -1.60935 |
| C | 2.75693  | -7.51549 | -1.41466 |
| C | 4.15098  | -5.70607 | -1.49096 |
| C | -3.64316 | -0.80307 | -5.30770 |
| C | -5.76638 | -0.01147 | -3.93998 |
| C | 0.53993  | -8.00960 | 1.62964  |
| C | -3.62299 | -4.20256 | -2.10345 |
| C | -5.65732 | -3.29317 | -2.63424 |
| C | 6.54391  | 2.32836  | -1.98949 |
| C | 3.99498  | -1.81776 | -5.30403 |
| C | 3.46983  | 1.06414  | 5.06586  |
| C | -4.85473 | -0.96462 | -5.80576 |
| C | 1.58252  | 5.69141  | -2.00935 |
| C | 0.61169  | 8.08144  | -1.45226 |
| C | -0.19541 | 7.03958  | -1.49842 |
| C | -0.22942 | -6.93866 | 1.57642  |
| C | 2.37871  | -2.43441 | 3.86129  |
| C | 0.28435  | 5.83354  | -1.77834 |
| C | 4.61153  | -2.91656 | -0.60981 |
| C | -5.42276 | 5.88086  | 1.63492  |
| C | 2.31253  | -6.70203 | 2.23511  |
| C | -5.89833 | 3.80338  | 2.44575  |
| C | -6.30424 | 4.99362  | 2.05179  |
| C | -7.14792 | 3.38882  | -1.12718 |
| C | -2.10884 | -2.67104 | 4.92311  |
| C | 2.17552  | 2.68357  | -3.83876 |
| C | 0.29793  | 4.78273  | 5.39838  |
| C | 0.72381  | -4.40738 | -4.67530 |

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| C | 0.58205  | -5.67579 | -5.00981 |
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| C | 1.90429  | 7.93009  | -1.68457 |
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| C | -1.21307 | 5.46773  | 3.82418  |
| H | -0.41068 | 6.69450  | 5.23597  |
| H | 0.91058  | 5.00259  | 6.19583  |
| H | 0.81402  | 2.79534  | 5.33375  |
| H | -0.53423 | 2.32254  | 3.51011  |
| H | -1.79044 | 6.21193  | 3.40337  |
| H | 1.03341  | 4.63181  | 2.42643  |
| H | 0.74301  | 6.94916  | 2.38575  |
| H | 2.50282  | 8.34575  | 1.65651  |
| H | 4.55998  | 7.39463  | 1.01709  |
| H | 4.85570  | 5.08539  | 1.07377  |
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| H | 3.39236  | 6.60327  | -2.14848 |
| H | 0.23203  | 9.01300  | -1.22758 |
| H | -1.19799 | 7.17296  | -1.30407 |
| H | 1.95885  | 4.75464  | -2.21993 |
| H | 6.87928  | 1.51025  | 2.86092  |
| H | 8.85386  | 0.32842  | 2.33176  |
| H | 5.26640  | 3.73327  | 3.28805  |
| H | 6.11233  | 2.88363  | 5.30771  |
| H | 2.13200  | 1.13942  | 3.54048  |
| H | 2.95097  | 0.32052  | 5.55104  |
| H | 4.97394  | 1.16660  | 6.43691  |
| H | 8.71259  | -1.90891 | 1.61925  |
| H | 6.64085  | -2.95496 | 1.42486  |
| H | 4.79578  | 0.46587  | 2.63193  |
| H | 6.38209  | 3.27811  | -1.61833 |
| H | 8.56720  | 2.55389  | -1.99224 |
| H | 8.98416  | 0.38846  | -2.82052 |
| H | 7.17085  | -1.05573 | -3.27763 |
| H | 4.98077  | -0.34416 | -2.88379 |
| H | 1.83861  | -1.63806 | 3.49434  |
| H | 1.02960  | -2.82532 | 5.32074  |
| H | 2.23418  | -4.68696 | 6.14773  |
| H | 4.28274  | -5.28155 | 5.16416  |
| H | 5.10743  | -4.07356 | 3.34114  |
| H | -0.87622 | -2.12395 | 3.40327  |
| H | -2.07343 | -1.73357 | 5.34769  |
| H | -3.35256 | -3.48287 | 6.31821  |
| H | -3.35400 | -5.61672 | 5.33003  |
| H | -2.13294 | -6.00426 | 3.37330  |
| H | -2.33773 | 0.11142  | 3.45492  |
| H | -2.45436 | 1.47109  | 5.31581  |
| H | -4.56450 | 2.16385  | 6.15598  |
| H | -6.53625 | 1.41520  | 5.11460  |
| H | -6.41679 | 0.02528  | 3.23083  |
| H | -4.30356 | 2.55664  | 2.69238  |
| H | -3.46418 | 6.28024  | 1.27129  |
| H | -5.73515 | 6.80867  | 1.32052  |
| H | -7.30763 | 5.22693  | 2.06029  |
| H | -6.57719 | 3.10148  | 2.77163  |
| H | -6.93836 | 1.38149  | -0.91147 |
| H | -8.09328 | 3.39761  | -0.71502 |
| H | -7.10580 | 5.40441  | -1.43354 |
| H | -4.93367 | 5.36884  | -2.37559 |
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| H | -1.01617 | 2.35724  | -3.56261 |
| H | -2.30801 | 6.21658  | -3.20487 |
| H | -2.37728 | 2.06319  | -5.40932 |
| H | -3.76716 | 3.83388  | -6.15658 |
| H | -3.70646 | 5.90661  | -5.05669 |
| H | -2.53899 | -0.12356 | -3.74279 |
| H | -2.80533 | -1.09805 | -5.82773 |
| H | -4.97601 | -1.40055 | -6.72852 |
| H | -6.86067 | -0.68082 | -5.52095 |
| H | -6.59118 | 0.31469  | -3.41399 |
| H | -3.88556 | -2.30081 | -2.78842 |
| H | -3.68815 | -6.13975 | -1.42042 |
| H | -5.99812 | -6.32267 | -1.58996 |
| H | -7.27679 | -4.50226 | -2.35251 |
| H | -6.20345 | -2.49027 | -2.97378 |

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|---|----------|----------|----------|
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| H | -6.90182 | -1.51841 | 0.85196  |
| H | -5.03811 | -5.28435 | 2.96314  |
| H | -7.19637 | -5.39995 | 2.01000  |
| H | -3.80135 | -3.31081 | 2.81695  |
| H | -1.21707 | -7.04760 | 1.31087  |
| H | 0.14789  | -8.93540 | 1.40717  |
| H | 2.41496  | -8.72534 | 1.98209  |
| H | 3.30379  | -6.60219 | 2.49051  |
| H | 1.94517  | -4.69746 | 2.36912  |
| H | 5.10683  | -5.33149 | -1.46265 |
| H | 4.79107  | -7.63380 | -1.31491 |
| H | 2.62163  | -8.53317 | -1.33823 |
| H | 0.76270  | -7.09090 | -1.51546 |
| H | 1.10162  | -4.76771 | -1.68904 |
| H | 0.03205  | -2.87159 | -3.52608 |
| H | 1.48286  | -3.83883 | -5.07928 |
| H | 1.23206  | -6.10561 | -5.68222 |
| H | -0.50769 | -7.38956 | -4.74805 |
| H | -1.95875 | -6.43288 | -3.18332 |
| H | 2.54381  | -1.62772 | -3.87998 |
| H | 3.52721  | -1.17761 | -5.96301 |
| H | 5.58477  | -2.17264 | -6.53330 |
| H | 6.64240  | -3.62353 | -5.00582 |
| H | 5.65845  | -4.07682 | -2.93626 |
| H | 4.99755  | 4.15927  | -3.31351 |
| H | 1.63486  | 1.85623  | -3.55055 |
| H | 0.76224  | 3.27960  | -5.16263 |
| H | 1.98538  | 5.18647  | -5.84264 |
| H | 4.11366  | 5.59548  | -4.93073 |
| H | 3.36056  | -3.85461 | 0.76081  |
| H | 4.97641  | -3.96427 | 1.15451  |
| H | 4.87536  | -1.91092 | -0.66453 |
| H | 5.42815  | -3.45692 | -0.95357 |
| H | -1.80329 | -6.02955 | -0.92823 |
| H | -2.60256 | -3.88107 | 0.65221  |
| H | -6.06433 | -0.50766 | -1.09797 |
| H | -4.54884 | 1.06566  | 0.69103  |
| H | -2.59145 | 3.97937  | -0.65228 |
| H | -1.45118 | 5.94100  | 1.05470  |
| H | 3.01459  | 3.58894  | -0.69375 |
| H | 4.45039  | 1.61651  | 0.58185  |
| H | 4.60422  | 3.94041  | -1.01333 |
| H | 5.24390  | 3.04126  | 0.93823  |
| H | -0.45534 | -5.10325 | -0.67078 |
| H | -2.52982 | -5.47924 | 1.11054  |
| H | -4.57663 | -1.21260 | -0.87027 |
| H | -6.02456 | 0.35766  | 0.96965  |
| H | -2.47631 | 5.61324  | -0.92226 |
| H | -0.36324 | 4.73006  | 0.74121  |

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[RuAu12Cl12(dppe)5] Isomer III

|    |          |          |          |
|----|----------|----------|----------|
| Ru | 0.00519  | -0.07807 | -2.77282 |
| Au | -1.59536 | 1.57475  | 1.02179  |
| Au | 1.11095  | 2.11518  | 1.06841  |
| Au | 0.21838  | 2.22708  | -1.49658 |
| Au | 0.27779  | -2.48802 | 1.15679  |
| Au | 0.12739  | -0.04729 | -0.20630 |
| Au | -1.27367 | -1.94638 | -1.50158 |
| Au | 2.62845  | 0.49186  | -1.42950 |
| Au | 2.31536  | -0.67638 | 1.06791  |
| Au | -2.15154 | 0.69937  | -1.54970 |
| Au | -2.15293 | -1.14161 | 0.99623  |
| Au | 1.47014  | -1.90691 | -1.42447 |
| Au | 0.08458  | -0.05604 | 2.49310  |
| P  | -2.00047 | -3.98757 | -1.68337 |
| P  | 2.93387  | 3.13654  | 1.73714  |
| P  | -0.57693 | 4.19675  | -1.92738 |
| P  | 3.23019  | -3.08178 | -1.84932 |
| P  | 3.92875  | -1.94801 | 1.78033  |
| P  | -0.70369 | -4.29330 | 1.94593  |
| Cl | 0.24686  | -0.00392 | -4.95192 |
| Cl | 0.06163  | -0.02530 | 4.82680  |
| P  | -4.29485 | 0.78765  | -1.82557 |
| P  | -4.22810 | -0.93986 | 1.71466  |
| P  | 4.00750  | 2.11729  | -1.96248 |
| P  | -2.19899 | 3.57987  | 1.66610  |

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.90343  | 4.86433  | 1.87010  |
| C | -3.84904 | 4.09362  | 1.78357  |
| C | -4.60511 | 3.31227  | -2.44631 |
| C | -6.29636 | 2.47785  | -1.14560 |
| C | -4.79406 | -3.36210 | 2.49706  |
| C | -1.50580 | -2.92646 | 4.05057  |
| C | -6.67297 | -4.56063 | 1.97327  |
| C | -2.20900 | -5.10974 | 4.00845  |
| C | -3.21605 | 0.28458  | 3.84185  |
| C | -6.33760 | 4.66743  | -1.81295 |
| C | -1.46669 | 3.09800  | -4.17442 |
| C | 3.93285  | 5.63562  | 1.54374  |
| C | -6.45980 | -2.39622 | 1.25312  |
| C | 5.69489  | 1.73241  | -1.89882 |
| C | 1.75999  | 5.42900  | 2.23722  |
| C | -5.15008 | 2.29404  | -1.78958 |
| C | -5.49254 | -4.47501 | 2.56683  |
| C | 5.77065  | -0.08841 | 1.96125  |
| C | -2.02586 | -4.76295 | 0.90165  |
| C | -0.68607 | 3.17410  | 3.80372  |
| C | -4.30810 | 5.22407  | 1.26061  |
| C | 5.35674  | -2.66285 | -3.47018 |
| C | 2.67629  | 7.50453  | 1.94477  |
| C | -2.07876 | 5.28586  | -3.86659 |
| C | -5.56200 | 0.95476  | 4.84798  |
| C | 4.01383  | -3.31774 | 0.69019  |
| C | -5.27161 | -2.30739 | 1.84152  |
| C | -4.32678 | -0.11142 | 3.23884  |
| C | 3.81837  | 6.94983  | 1.57988  |
| C | 1.65069  | 6.74202  | 2.27839  |
| C | -5.50458 | 0.21212  | 3.75948  |
| C | -1.24625 | -4.78702 | -3.03644 |
| C | 3.63551  | 2.97323  | -3.42186 |
| C | -0.31880 | -4.13790 | -3.72855 |
| C | 3.66333  | 2.46413  | 3.16025  |
| C | -1.90677 | 4.51303  | -0.82790 |
| C | -5.19863 | 4.48927  | -2.45911 |
| C | -1.45859 | 4.70151  | 0.54358  |
| C | 3.83140  | 3.36464  | -0.75303 |
| C | 6.03223  | 0.47039  | -2.13856 |
| C | -5.15606 | -0.25232 | -0.71200 |
| C | 4.05950  | -2.47166 | -3.25665 |
| C | 3.04253  | 1.46818  | 3.77612  |
| C | -1.53201 | -5.10532 | -0.42090 |
| C | -0.76111 | 5.68194  | 4.62115  |
| C | -2.92877 | -4.89347 | 5.09200  |
| C | -1.50684 | -4.11798 | 3.47180  |
| C | 5.57359  | -1.39095 | 1.81345  |
| C | -1.42948 | 4.05582  | 3.15076  |
| C | -7.15155 | -3.51959 | 1.31780  |
| C | 0.03370  | 3.54519  | 4.84517  |
| C | -3.27408 | 1.02642  | 4.93098  |
| C | -2.82103 | 5.22789  | -4.95620 |
| C | 4.28142  | -3.75886 | 3.73631  |
| C | 3.38506  | -1.66595 | -4.07040 |
| C | -5.05608 | 0.19562  | 0.67208  |
| C | 4.18787  | 2.84012  | 0.55553  |
| C | 3.56013  | -2.73939 | 3.28531  |
| C | 4.87740  | 2.82592  | 3.55932  |
| C | 4.30812  | 4.05496  | -3.79481 |
| C | 1.57873  | -5.53468 | 2.27557  |
| C | -1.41075 | 4.21364  | -3.45927 |
| C | 5.96665  | -2.04898 | -4.46669 |
| C | 6.98440  | 0.41694  | 1.87731  |
| C | -4.69318 | 3.27439  | 2.40082  |
| C | 5.47269  | 2.16814  | 4.53516  |
| C | 5.29133  | -1.23651 | -5.25954 |
| C | -4.44680 | 1.37234  | 5.42793  |
| C | 4.85987  | 1.15252  | 5.12384  |
| C | -2.94289 | -3.69297 | 5.65178  |
| C | 7.28040  | 0.07388  | -1.98493 |
| C | -2.89893 | 4.10223  | -5.64800 |
| C | 1.98338  | -7.75353 | 1.89882  |
| C | 7.82959  | -1.67486 | 1.49532  |
| C | 3.87541  | -4.43913 | 4.79138  |
| C | 2.04904  | -3.07036 | 4.98166  |
| C | -2.21224 | 3.04198  | -5.26224 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.75226  | -4.10434 | 5.40656  |
| C | 3.88019  | 4.77707  | -4.81076 |
| C | 8.20287  | 0.92822  | -1.57624 |
| C | 2.11976  | 3.33874  | -5.10321 |
| C | 8.01496  | -0.37343 | 1.63428  |
| C | 0.29017  | -5.71406 | 2.00607  |
| C | 6.61537  | -2.18383 | 1.58691  |
| C | 7.87516  | 2.18630  | -1.33488 |
| C | 3.85066  | -6.92160 | -2.30765 |
| C | -4.72848 | 0.09233  | -3.36427 |
| C | -6.36320 | -4.30175 | -1.90788 |
| C | -3.78687 | -0.41268 | -4.14966 |
| C | -6.32408 | -0.54289 | -4.88049 |
| C | -4.36804 | -5.23177 | -1.27802 |
| C | 1.71327  | -6.62101 | -1.57071 |
| C | -5.68589 | -5.27878 | -1.33090 |
| C | -4.40532 | -3.21974 | -2.36750 |
| C | 1.89865  | -5.31566 | -1.58287 |
| C | 3.05959  | -4.80463 | -1.95627 |
| C | 2.68868  | -7.42450 | -1.93734 |
| C | 4.03744  | -5.61532 | -2.31817 |
| C | -4.11602 | -0.99179 | -5.28767 |
| C | -5.99897 | 0.03614  | -3.74267 |
| C | 0.70098  | -7.94222 | 1.63866  |
| C | -3.71629 | -4.19980 | -1.79679 |
| C | -5.72057 | -3.27518 | -2.43252 |
| C | 6.62759  | 2.58780  | -1.49629 |
| C | 3.99730  | -1.05153 | -5.06327 |
| C | 3.63954  | 0.81226  | 4.75279  |
| C | -5.38246 | -1.06159 | -5.65208 |
| C | 1.64617  | 5.54320  | -2.24401 |
| C | 0.78512  | 7.79668  | -1.18124 |
| C | -0.03926 | 6.77443  | -1.31789 |
| C | -0.14354 | -6.92909 | 1.69433  |
| C | 2.45411  | -2.38979 | 3.92712  |
| C | 0.38784  | 5.63351  | -1.84164 |
| C | 4.48086  | -2.92531 | -0.63152 |
| C | -5.58902 | 5.53037  | 1.36015  |
| C | 2.41789  | -6.55023 | 2.22832  |
| C | -5.96898 | 3.58700  | 2.50458  |
| C | -6.42105 | 4.71558  | 1.98264  |
| C | -6.88440 | 3.66041  | -1.15731 |
| C | -2.22077 | -2.71385 | 5.13844  |
| C | 2.55044  | 2.60774  | -4.09314 |
| C | 0.00567  | 4.80247  | 5.24765  |
| C | 0.37342  | -4.76549 | -4.66107 |
| C | 0.13828  | -6.03997 | -4.91356 |
| C | 2.46423  | 6.56748  | -2.11405 |
| C | 2.77810  | 4.42691  | -5.45640 |
| C | -1.49523 | -6.06301 | -3.30859 |
| C | 2.03925  | 7.69385  | -1.57214 |
| C | -0.80232 | -6.68709 | -4.24147 |
| C | -1.47984 | 5.31177  | 3.57840  |
| H | -0.79185 | 6.66116  | 4.94245  |
| H | 0.58079  | 5.10140  | 6.04988  |
| H | 0.61331  | 2.83820  | 5.32222  |
| H | -0.65049 | 2.19215  | 3.49523  |
| H | -2.07729 | 6.00032  | 3.09468  |
| H | 0.95277  | 4.83391  | 2.48070  |
| H | 0.75538  | 7.16283  | 2.56453  |
| H | 2.58675  | 8.53141  | 1.96214  |
| H | 4.61893  | 7.54256  | 1.31487  |
| H | 4.82668  | 5.21693  | 1.24855  |
| H | 2.68354  | 8.48902  | -1.45054 |
| H | 3.43757  | 6.47600  | -2.43136 |
| H | 0.44860  | 8.67276  | -0.75896 |
| H | -1.01291 | 6.87066  | -1.00381 |
| H | 1.98263  | 4.65915  | -2.65195 |
| H | 7.11758  | 1.43272  | 1.98818  |
| H | 8.96176  | 0.02401  | 1.54517  |
| H | 5.36046  | 3.61533  | 3.10320  |
| H | 6.42151  | 2.43988  | 4.83186  |
| H | 2.09437  | 1.18757  | 3.48671  |
| H | 3.14092  | 0.03330  | 5.20727  |
| H | 5.33678  | 0.62871  | 5.87363  |
| H | 8.63129  | -2.29562 | 1.30541  |
| H | 6.48549  | -3.19890 | 1.46213  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 4.96104  | 0.52789  | 2.13300  |
| H | 6.38214  | 3.56856  | -1.29201 |
| H | 8.59176  | 2.85446  | -1.01294 |
| H | 9.17537  | 0.61416  | -1.43676 |
| H | 7.52444  | -0.90917 | -2.17088 |
| H | 5.30445  | -0.20325 | -2.42811 |
| H | 1.89140  | -1.59338 | 3.59635  |
| H | 1.17884  | -2.78257 | 5.45238  |
| H | 2.42834  | -4.65031 | 6.21858  |
| H | 4.43179  | -5.23800 | 5.12959  |
| H | 5.15864  | -4.02575 | 3.26446  |
| H | -0.95306 | -2.15445 | 3.65088  |
| H | -2.20336 | -1.77678 | 5.56551  |
| H | -3.51672 | -3.52581 | 6.49117  |
| H | -3.48437 | -5.66009 | 5.50028  |
| H | -2.19659 | -6.04695 | 3.57814  |
| H | -2.29543 | 0.02523  | 3.46020  |
| H | -2.39184 | 1.32334  | 5.37272  |
| H | -4.49612 | 1.96434  | 6.27026  |
| H | -6.47766 | 1.21227  | 5.24471  |
| H | -6.37364 | -0.11853 | 3.31287  |
| H | -4.34380 | 2.38855  | 2.79772  |
| H | -3.67464 | 5.86988  | 0.76869  |
| H | -5.93721 | 6.40559  | 0.94348  |
| H | -7.42113 | 4.95611  | 2.05449  |
| H | -6.60714 | 2.94138  | 2.99249  |
| H | -6.73789 | 1.70597  | -0.62575 |
| H | -7.76676 | 3.79590  | -0.64170 |
| H | -6.79599 | 5.59139  | -1.81389 |
| H | -4.76068 | 5.26456  | -2.97739 |
| H | -3.71340 | 3.17971  | -2.94832 |
| H | -0.94653 | 2.26078  | -3.86913 |
| H | -2.02072 | 6.16589  | -3.33120 |
| H | -2.25621 | 2.16059  | -5.79371 |
| H | -3.49439 | 4.05494  | -6.48815 |
| H | -3.34599 | 6.06028  | -5.26328 |
| H | -2.79581 | -0.36584 | -3.86180 |
| H | -3.37652 | -1.39035 | -5.88383 |
| H | -5.63861 | -1.51598 | -6.54082 |
| H | -7.31240 | -0.58629 | -5.16958 |
| H | -6.73274 | 0.45800  | -3.15254 |
| H | -3.90341 | -2.40519 | -2.75035 |
| H | -3.85764 | -5.99738 | -0.81417 |
| H | -6.18457 | -6.07359 | -0.90724 |
| H | -7.39311 | -4.33781 | -1.93917 |
| H | -6.23409 | -2.50343 | -2.88170 |
| H | -8.06891 | -3.57946 | 0.85099  |
| H | -6.85154 | -1.59604 | 0.73779  |
| H | -5.10816 | -5.27701 | 3.08684  |
| H | -7.21505 | -5.43707 | 2.01866  |
| H | -3.86806 | -3.30553 | 2.94859  |
| H | -1.13822 | -7.09047 | 1.47661  |
| H | 0.35858  | -8.87939 | 1.38169  |
| H | 2.64371  | -8.54244 | 1.83625  |
| H | 3.41508  | -6.39116 | 2.43496  |
| H | 1.92281  | -4.59007 | 2.50795  |
| H | 4.94173  | -5.23083 | -2.61529 |
| H | 4.61086  | -7.55001 | -2.59578 |
| H | 2.54643  | -8.44578 | -1.93435 |
| H | 0.80497  | -7.00619 | -1.28259 |
| H | 1.14936  | -4.66655 | -1.30440 |
| H | -0.12445 | -3.14540 | -3.52094 |
| H | 1.10210  | -4.25400 | -5.18155 |
| H | 0.68676  | -6.53324 | -5.63496 |
| H | -0.99331 | -7.67954 | -4.44533 |
| H | -2.23497 | -6.56991 | -2.79647 |
| H | 2.38295  | -1.48447 | -3.90405 |
| H | 3.45597  | -0.41442 | -5.66499 |
| H | 5.77654  | -0.73910 | -6.02139 |
| H | 6.97715  | -2.19056 | -4.61222 |
| H | 5.90933  | -3.26710 | -2.84561 |
| H | 5.16032  | 4.33603  | -3.28595 |
| H | 2.02169  | 1.76809  | -3.81252 |
| H | 1.26106  | 3.05375  | -5.59573 |
| H | 2.43302  | 5.00829  | -6.23397 |
| H | 4.39732  | 5.62269  | -5.09301 |
| H | 3.04411  | -3.69895 | 0.66551  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 4.61403  | -4.05600 | 1.10437  |
| H | 4.77867  | -1.92867 | -0.66375 |
| H | 5.29498  | -3.50222 | -0.91453 |
| H | -1.81968 | -6.06202 | -0.70083 |
| H | -2.66460 | -3.93979 | 0.88179  |
| H | -6.14401 | -0.34225 | -1.01998 |
| H | -4.48645 | 1.06483  | 0.75367  |
| H | -2.51592 | 3.67490  | -0.92430 |
| H | -1.59743 | 5.67745  | 0.86893  |
| H | 2.82318  | 3.61935  | -0.79705 |
| H | 4.26871  | 1.80133  | 0.53634  |
| H | 4.36166  | 4.22244  | -0.99583 |
| H | 5.10534  | 3.19739  | 0.88351  |
| H | -0.49436 | -5.10609 | -0.45197 |
| H | -2.56667 | -5.53914 | 1.33058  |
| H | -4.72364 | -1.18907 | -0.84902 |
| H | -5.98548 | 0.41847  | 1.07743  |
| H | -2.46704 | 5.31599  | -1.17246 |
| H | -0.44013 | 4.50207  | 0.63989  |

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[FeAu12Cl12(dppe)5] Isomer I

|    |          |          |          |
|----|----------|----------|----------|
| Au | 0.       | 0.       | -2.48357 |
| Au | -1.42152 | 1.90934  | 1.10435  |
| Au | 1.37662  | 1.94197  | 1.10435  |
| Au | 0.02775  | 2.38024  | -1.10435 |
| Au | 0.02775  | -2.38024 | 1.10435  |
| Fe | 0.       | 0.       | 0.       |
| Au | -1.42152 | -1.90934 | -1.10435 |
| Au | 2.27232  | 0.70914  | -1.10435 |
| Au | 2.27232  | -0.70914 | 1.10435  |
| Au | -2.25517 | 0.76193  | -1.10435 |
| Au | -2.25517 | -0.76193 | 1.10435  |
| Au | 1.37662  | -1.94197 | -1.10435 |
| Au | 0.       | 0.       | 2.48357  |
| P  | -1.71839 | -3.91923 | -1.87174 |
| P  | 3.19640  | 2.84540  | 1.87174  |
| P  | -0.91346 | 4.18077  | -1.87174 |
| P  | 3.19640  | -2.84540 | -1.87174 |
| P  | 3.69387  | -2.16068 | 1.87174  |
| P  | -0.91346 | -4.18077 | 1.87174  |
| Cl | 0.       | 0.       | -4.81437 |
| Cl | 0.       | 0.       | 4.81437  |
| P  | -4.25842 | 0.42318  | -1.87174 |
| P  | -4.25842 | -0.42318 | 1.87174  |
| P  | 3.69387  | 2.16068  | -1.87174 |
| P  | -1.71839 | 3.91923  | 1.87174  |
| C  | 3.16157  | 4.52098  | 2.30313  |
| C  | -3.32273 | 4.40389  | 2.30313  |
| C  | -5.00128 | 2.89680  | -1.59476 |
| C  | -6.14234 | 1.80500  | -3.24532 |
| C  | -5.00128 | -2.89680 | 1.59476  |
| C  | -1.80995 | -2.76161 | 3.86415  |
| C  | -6.68365 | -3.96001 | 2.69570  |
| C  | -3.07061 | -4.61948 | 3.43363  |
| C  | -3.18576 | 0.86798  | 3.86415  |
| C  | -6.68365 | 3.96001  | -2.69570 |
| C  | -1.80995 | 2.76161  | -3.86415 |
| C  | 3.90831  | 5.07066  | 3.24532  |
| C  | -6.14234 | -1.80500 | 3.24532  |
| C  | 5.27668  | 1.60977  | -2.30313 |
| C  | 2.34343  | 5.28324  | 1.59476  |
| C  | -5.21512 | 1.79923  | -2.30313 |
| C  | -5.74426 | -3.96550 | 1.77143  |
| C  | 5.74882  | -0.59612 | 1.59476  |
| C  | -1.95435 | -4.92194 | 0.64658  |
| C  | -0.15896 | 3.29805  | 3.86415  |
| C  | -3.61475 | 5.28394  | 3.24532  |
| C  | 5.19943  | -1.93238 | -3.43363 |
| C  | 3.07955  | 7.13226  | 2.69570  |
| C  | -3.07061 | 4.61948  | -3.43363 |
| C  | -5.24443 | 2.42758  | 4.35629  |
| C  | 4.07712  | -3.37966 | 0.64658  |
| C  | -5.21512 | -1.79923 | 2.30313  |
| C  | -4.30761 | 0.70939  | 3.17406  |
| C  | 3.85682  | 6.37211  | 3.44299  |
| C  | 2.31634  | 6.58455  | 1.77143  |
| C  | -5.34225 | 1.49282  | 3.43363  |

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.65645 | -4.31600 | -3.17406 |
| C | 3.06796  | 3.10586  | -3.17406 |
| C | -0.15896 | -3.29805 | -3.86415 |
| C | 3.90190  | 1.95804  | 3.17406  |
| C | -1.95435 | 4.92194  | -0.64658 |
| C | -5.74426 | 3.96550  | -1.77143 |
| C | -1.31194 | 5.13067  | 0.64658  |
| C | 4.07712  | 3.37966  | -0.64658 |
| C | 5.74882  | 0.59612  | -1.59476 |
| C | -5.28497 | -0.33773 | -0.64658 |
| C | 3.90190  | -1.95804 | -3.17406 |
| C | 3.08751  | 1.17033  | 3.86415  |
| C | -1.31194 | -5.13067 | -0.64658 |
| C | 0.68815  | 5.73791  | 4.35629  |
| C | -3.92938 | -4.23758 | 4.35629  |
| C | -2.00580 | -3.87757 | 3.17406  |
| C | 5.27668  | -1.60977 | 2.30313  |
| C | -0.65645 | 4.31600  | 3.17406  |
| C | -6.86566 | -2.88817 | 3.44299  |
| C | 0.76278  | 3.49648  | 4.77852  |
| C | -3.08964 | 1.80592  | 4.77852  |
| C | -3.92938 | 4.23758  | -4.35629 |
| C | 3.44451  | -4.34782 | 3.43363  |
| C | 3.08751  | -1.17033 | -3.86415 |
| C | -5.28497 | 0.33773  | 0.64658  |
| C | 4.47415  | 2.83320  | 0.64658  |
| C | 3.06796  | -3.10586 | 3.17406  |
| C | 5.19943  | 1.93238  | 3.43363  |
| C | 3.44451  | 4.34782  | -3.43363 |
| C | 1.20954  | -5.65166 | 1.59476  |
| C | -2.00580 | 3.87757  | -3.17406 |
| C | 5.66973  | -1.11864 | -4.35629 |
| C | 6.97807  | -0.16823 | 1.77143  |
| C | -4.30050 | 3.86134  | 1.59476  |
| C | 5.66973  | 1.11864  | 4.35629  |
| C | 4.85680  | -0.32064 | -5.01682 |
| C | -4.11770 | 2.59535  | 5.01682  |
| C | 4.85680  | 0.32064  | 5.01682  |
| C | -3.74076 | -3.11416 | 5.01682  |
| C | 6.97807  | 0.16823  | -1.77143 |
| C | -3.74076 | 3.11416  | -5.01682 |
| C | 1.70083  | -7.58024 | 2.69570  |
| C | 7.25206  | -1.69896 | 3.44299  |
| C | 2.81593  | -5.04655 | 4.35629  |
| C | 1.43808  | -3.27706 | 4.77852  |
| C | -2.67228 | 2.38036  | -4.77852 |
| C | 1.80578  | -4.52001 | 5.01682  |
| C | 2.81593  | 5.04655  | -4.35629 |
| C | 7.73482  | 0.72484  | -2.69570 |
| C | 1.43808  | 3.27706  | -4.77852 |
| C | 7.73482  | -0.72484 | 2.69570  |
| C | 0.09960  | -5.51587 | 2.30313  |
| C | 6.03022  | -2.15010 | 3.24532  |
| C | 7.25206  | 1.69896  | -3.44299 |
| C | 3.85682  | -6.37211 | -3.44299 |
| C | -4.30761 | -0.70939 | -3.17406 |
| C | -5.83155 | -5.13282 | -2.69570 |
| C | -3.18576 | -0.86798 | -3.86415 |
| C | -5.24443 | -2.42758 | -4.35629 |
| C | -3.61475 | -5.28394 | -3.24532 |
| C | 2.31634  | -6.58455 | -1.77143 |
| C | -4.86842 | -5.63714 | -3.44299 |
| C | -4.30050 | -3.86134 | -1.59476 |
| C | 2.34343  | -5.28324 | -1.59476 |
| C | 3.16157  | -4.52098 | -2.30313 |
| C | 3.07955  | -7.13226 | -2.69570 |
| C | 3.90831  | -5.07066 | -3.24532 |
| C | -3.08964 | -1.80592 | -4.77852 |
| C | -5.34225 | -1.49282 | -3.43363 |
| C | 0.62520  | -7.42213 | 3.44299  |
| C | -3.32273 | -4.40389 | -2.30313 |
| C | -5.54649 | -4.23771 | -1.77143 |
| C | 6.03022  | 2.15010  | -3.24532 |
| C | 3.56106  | -0.35503 | -4.77852 |
| C | 3.56106  | 0.35503  | 4.77852  |
| C | -4.11770 | -2.59535 | -5.01682 |
| C | 1.20954  | 5.65166  | -1.59476 |



|   |          |          |          |
|---|----------|----------|----------|
| C | 0.62520  | 7.42213  | -3.44299 |
| C | -0.18143 | 6.39949  | -3.24532 |
| C | -0.18143 | -6.39949 | 3.24532  |
| C | 2.06715  | -2.57475 | 3.86415  |
| C | 0.09960  | 5.51587  | -2.30313 |
| C | 4.47415  | -2.83320 | -0.64658 |
| C | -4.86842 | 5.63714  | 3.44299  |
| C | 1.99634  | -6.68852 | 1.77143  |
| C | -5.54649 | 4.23771  | 1.77143  |
| C | -5.83155 | 5.13282  | 2.69570  |
| C | -6.86566 | 2.88817  | -3.44299 |
| C | -2.67228 | -2.38036 | 4.77852  |
| C | 2.06715  | 2.57475  | -3.86415 |
| C | 1.19588  | 4.71817  | 5.01682  |
| C | 0.76278  | -3.49648 | -4.77852 |
| C | 1.19588  | -4.71817 | -5.01682 |
| C | 1.99634  | 6.68852  | -1.77143 |
| C | 1.80578  | 4.52001  | -5.01682 |
| C | -0.23109 | -5.54209 | -3.43363 |
| C | 1.70083  | 7.58024  | -2.69570 |
| C | 0.68815  | -5.73791 | -4.35629 |
| C | -0.23109 | 5.54209  | 3.43363  |
| H | 1.03238  | 6.69162  | 4.53629  |
| H | 1.93987  | 4.87515  | 5.71245  |
| H | 1.14556  | 2.68373  | 5.28386  |
| H | -0.46876 | 2.33744  | 3.66691  |
| H | -0.59169 | 6.34845  | 2.90284  |
| H | 1.70599  | 4.82755  | 0.92689  |
| H | 1.68106  | 7.16297  | 1.20162  |
| H | 3.05366  | 8.15086  | 2.85142  |
| H | 4.43137  | 6.79803  | 4.18517  |
| H | 4.51368  | 4.47925  | 3.83447  |
| H | 2.32049  | 8.38909  | -2.85142 |
| H | 2.85028  | 6.78307  | -1.20162 |
| H | 0.41073  | 8.10442  | -4.18517 |
| H | -1.01881 | 6.27687  | -3.83447 |
| H | 1.45738  | 4.90832  | -0.92689 |
| H | 7.33187  | 0.61469  | 1.20162  |
| H | 8.69557  | -0.38545 | 2.85142  |
| H | 5.85489  | 2.52451  | 2.90284  |
| H | 6.68313  | 1.08597  | 4.53629  |
| H | 2.07818  | 1.16812  | 3.66691  |
| H | 2.90638  | -0.26017 | 5.28386  |
| H | 5.23600  | -0.33842 | 5.71245  |
| H | 7.83468  | -2.11378 | 4.18517  |
| H | 5.65483  | -2.90860 | 3.83447  |
| H | 5.11845  | -0.13070 | 0.92689  |
| H | 5.65483  | 2.90860  | -3.83447 |
| H | 7.83468  | 2.11378  | -4.18517 |
| H | 8.69557  | 0.38545  | -2.85142 |
| H | 7.33187  | -0.61469 | -1.20162 |
| H | 5.11845  | 0.13070  | -0.92689 |
| H | 1.75314  | -1.61550 | 3.66691  |
| H | 0.65068  | -2.84453 | 5.28386  |
| H | 1.29616  | -5.08431 | 5.71245  |
| H | 3.09802  | -6.02045 | 4.53629  |
| H | 4.21022  | -4.78822 | 2.90284  |
| H | -0.99468 | -2.16656 | 3.66691  |
| H | -2.50423 | -1.49784 | 5.28386  |
| H | -4.43493 | -2.80386 | 5.71245  |
| H | -4.76845 | -4.80681 | 4.53629  |
| H | -3.25284 | -5.48380 | 2.90284  |
| H | -2.36789 | 0.27650  | 3.66691  |
| H | -2.19838 | 1.91881  | 5.28386  |
| H | -4.03709 | 3.35143  | 5.71245  |
| H | -6.04508 | 3.04967  | 4.53629  |
| H | -6.22058 | 1.39905  | 2.90284  |
| H | -4.06409 | 3.11429  | 0.92689  |
| H | -2.86522 | 5.67693  | 3.83447  |
| H | -5.09595 | 6.31519  | 4.18517  |
| H | -6.80830 | 5.42296  | 2.85142  |
| H | -6.29291 | 3.81227  | 1.20162  |
| H | -6.28448 | 0.97071  | -3.83447 |
| H | -7.58084 | 2.89503  | -4.18517 |
| H | -7.26142 | 4.79929  | -2.85142 |
| H | -5.57030 | 4.80686  | -1.20162 |
| H | -4.21774 | 2.90281  | -0.92689 |

|   |          |          |          |
|---|----------|----------|----------|
| H | -0.99468 | 2.16656  | -3.66691 |
| H | -3.25284 | 5.48380  | -2.90284 |
| H | -2.50423 | 1.49784  | -5.28386 |
| H | -4.43493 | 2.80386  | -5.71245 |
| H | -4.76845 | 4.80681  | -4.53629 |
| H | -2.36789 | -0.27650 | -3.66691 |
| H | -2.19838 | -1.91881 | -5.28386 |
| H | -4.03709 | -3.35143 | -5.71245 |
| H | -6.04508 | -3.04967 | -4.53629 |
| H | -6.22058 | -1.39905 | -2.90284 |
| H | -4.06409 | -3.11429 | -0.92689 |
| H | -2.86522 | -5.67693 | -3.83447 |
| H | -5.09595 | -6.31519 | -4.18517 |
| H | -6.80830 | -5.42296 | -2.85142 |
| H | -6.29291 | -3.81227 | -1.20162 |
| H | -7.58084 | -2.89503 | 4.18517  |
| H | -6.28448 | -0.97071 | 3.83447  |
| H | -5.57030 | -4.80686 | 1.20162  |
| H | -7.26142 | -4.79929 | 2.85142  |
| H | -4.21774 | -2.90281 | 0.92689  |
| H | -1.01881 | -6.27687 | 3.83447  |
| H | 0.41073  | -8.10442 | 4.18517  |
| H | 2.32049  | -8.38909 | 2.85142  |
| H | 2.85028  | -6.78307 | 1.20162  |
| H | 1.45738  | -4.90832 | 0.92689  |
| H | 4.51368  | -4.47925 | -3.83447 |
| H | 4.43137  | -6.79803 | -4.18517 |
| H | 3.05366  | -8.15086 | -2.85142 |
| H | 1.68106  | -7.16297 | -1.20162 |
| H | 1.70599  | -4.82755 | -0.92689 |
| H | -0.46876 | -2.33744 | -3.66691 |
| H | 1.14556  | -2.68373 | -5.28386 |
| H | 1.93987  | -4.87515 | -5.71245 |
| H | 1.03238  | -6.69162 | -4.53629 |
| H | -0.59169 | -6.34845 | -2.90284 |
| H | 2.07818  | -1.16812 | -3.66691 |
| H | 2.90638  | 0.26017  | -5.28386 |
| H | 5.23600  | 0.33842  | -5.71245 |
| H | 6.68313  | -1.08597 | -4.53629 |
| H | 5.85489  | -2.52451 | -2.90284 |
| H | 4.21022  | 4.78822  | -2.90284 |
| H | 1.75314  | 1.61550  | -3.66691 |
| H | 0.65068  | 2.84453  | -5.28386 |
| H | 1.29616  | 5.08431  | -5.71245 |
| H | 3.09802  | 6.02045  | -4.53629 |
| H | 3.22144  | -3.96687 | 0.57294  |
| H | 4.83803  | -3.98203 | 1.02137  |
| H | 4.76820  | -1.83795 | -0.57294 |
| H | 5.28216  | -3.37073 | -1.02137 |
| H | -1.57347 | -6.06525 | -1.02137 |
| H | -2.77724 | -4.28961 | 0.57294  |
| H | -6.25462 | -0.37780 | -1.02137 |
| H | -4.93787 | 1.31575  | 0.57294  |
| H | -2.77724 | 4.28961  | -0.57294 |
| H | -1.57347 | 6.06525  | 1.02137  |
| H | 3.22144  | 3.96687  | -0.57294 |
| H | 4.76820  | 1.83795  | 0.57294  |
| H | 4.83803  | 3.98203  | -1.02137 |
| H | 5.28216  | 3.37073  | 1.02137  |
| H | -0.27454 | -5.10278 | -0.57294 |
| H | -2.29210 | -5.83175 | 1.02137  |
| H | -4.93787 | -1.31575 | -0.57294 |
| H | -6.25462 | 0.37780  | 1.02137  |
| H | -2.29210 | 5.83175  | -1.02137 |
| H | -0.27454 | 5.10278  | 0.57294  |

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[FeAu12Cl12(dppe)5] Isomer II

|    |         |         |         |
|----|---------|---------|---------|
| Au | 0.0000  | 0.0000  | -2.5566 |
| Au | -1.3892 | 1.9309  | 1.1588  |
| Au | 1.4071  | 1.9178  | 1.1588  |
| Au | -0.0112 | 2.3787  | -1.1588 |
| Au | -0.0112 | -2.3787 | 1.1588  |
| Au | 0.0000  | 0.0000  | 0.0000  |
| Au | -1.3892 | -1.9309 | -1.1588 |
| Au | 2.2588  | 0.7456  | -1.1588 |
| Au | 2.2588  | -0.7456 | 1.1588  |
| Au | -2.2657 | 0.7244  | -1.1588 |

|    |         |         |         |
|----|---------|---------|---------|
| Au | -2.2657 | -0.7244 | 1.1588  |
| Fe | 1.4071  | -1.9178 | -1.1588 |
| Au | 0.0000  | 0.0000  | 2.5566  |
| P  | -1.9618 | -3.9397 | -1.8248 |
| P  | 3.1406  | 3.0832  | 1.8248  |
| P  | -0.7285 | 4.3404  | -1.8248 |
| P  | 3.1406  | -3.0832 | -1.8248 |
| P  | 3.9028  | -2.0341 | 1.8248  |
| P  | -0.7285 | -4.3404 | 1.8248  |
| Cl | 0.0000  | 0.0000  | -4.7648 |
| Cl | 0.0000  | 0.0000  | 4.7648  |
| P  | -4.3531 | 0.6484  | -1.8248 |
| P  | -4.3531 | -0.6484 | 1.8248  |
| P  | 3.9028  | 2.0341  | -1.8248 |
| P  | -1.9618 | 3.9397  | 1.8248  |
| C  | 3.0900  | 4.8015  | 1.9109  |
| C  | -3.6116 | 4.4225  | 1.9109  |
| C  | -4.7604 | 3.2207  | -2.2529 |
| C  | -6.6235 | 2.0234  | -1.6462 |
| C  | -4.7604 | -3.2207 | 2.2529  |
| C  | -1.6470 | -3.0303 | 3.9190  |
| C  | -6.7888 | -4.2680 | 2.0614  |
| C  | -2.4010 | -5.1920 | 3.7049  |
| C  | -3.3909 | 0.6300  | 3.9190  |
| C  | -6.7888 | 4.2680  | -2.0614 |
| C  | -1.6470 | 3.0303  | -3.9190 |
| C  | 4.1692  | 5.5301  | 1.6462  |
| C  | -6.6235 | -2.0234 | 1.6462  |
| C  | 5.5212  | 1.4550  | -1.9109 |
| C  | 1.9582  | 5.4037  | 2.2529  |
| C  | -5.3220 | 2.0682  | -1.9109 |
| C  | -5.4947 | -4.3153 | 2.3265  |
| C  | 5.7443  | -0.1925 | 2.2529  |
| C  | -1.9100 | -4.8494 | 0.6527  |
| C  | -0.4488 | 3.4196  | 3.9190  |
| C  | -3.9711 | 5.6740  | 1.6462  |
| C  | 4.9942  | -2.7892 | -3.7049 |
| C  | 2.9836  | 7.4432  | 2.0614  |
| C  | -2.4010 | 5.1920  | -3.7049 |
| C  | -5.7541 | 1.4745  | 4.7549  |
| C  | 4.0217  | -3.3151 | 0.6527  |
| C  | -5.3220 | -2.0682 | 1.9109  |
| C  | -4.4927 | 0.2673  | 3.2748  |
| C  | 4.1147  | 6.8463  | 1.7238  |
| C  | 1.9089  | 6.7209  | 2.3265  |
| C  | -5.6798 | 0.6791  | 3.7049  |
| C  | -1.1341 | -4.3555 | -3.2748 |
| C  | 3.4776  | 2.8569  | -3.2748 |
| C  | -0.4488 | -3.4196 | -3.9190 |
| C  | 3.7917  | 2.4246  | 3.2748  |
| C  | -1.9100 | 4.8494  | -0.6527 |
| C  | -5.4947 | 4.3153  | -2.3265 |
| C  | -1.3051 | 5.0460  | 0.6527  |
| C  | 4.0217  | 3.3151  | -0.6527 |
| C  | 5.7443  | 0.1925  | -2.2529 |
| C  | -5.2023 | -0.3181 | -0.6527 |
| C  | 3.7917  | -2.4246 | -3.2748 |
| C  | 3.1136  | 1.4835  | 3.9190  |
| C  | -1.3051 | -5.0460 | -0.6527 |
| C  | -0.3758 | 5.9280  | 4.7549  |
| C  | -3.1804 | -5.0168 | 4.7549  |
| C  | -1.6425 | -4.1903 | 3.2748  |
| C  | 5.5212  | -1.4550 | 1.9109  |
| C  | -1.1341 | 4.3555  | 3.2748  |
| C  | -7.3530 | -3.1202 | 1.7238  |
| C  | 0.2811  | 3.7402  | 4.9711  |
| C  | -3.4702 | 1.4231  | 4.9711  |
| C  | -3.1804 | 5.0168  | -4.7549 |
| C  | 4.1960  | -3.8879 | 3.7049  |
| C  | 3.1136  | -1.4835 | -3.9190 |
| C  | -5.2023 | 0.3181  | 0.6527  |
| C  | 4.3957  | 2.8005  | 0.6527  |
| C  | 3.4776  | -2.8569 | 3.2748  |
| C  | 4.9942  | 2.7892  | 3.7049  |
| C  | 4.1960  | 3.8879  | -3.7049 |
| C  | 1.5920  | -5.5227 | 2.2529  |
| C  | -1.6425 | 4.1903  | -3.2748 |

|   |         |         |         |
|---|---------|---------|---------|
| C | 5.5218  | -2.1893 | -4.7549 |
| C | 6.9819  | 0.2615  | 2.3265  |
| C | -4.5341 | 3.5322  | 2.2529  |
| C | 5.5218  | 2.1893  | 4.7549  |
| C | 4.8510  | -1.2352 | -5.3825 |
| C | -4.6506 | 1.8522  | 5.3825  |
| C | 4.8510  | 1.2352  | 5.3825  |
| C | -3.1986 | -3.8506 | 5.3825  |
| C | 6.9819  | -0.2615 | -2.3265 |
| C | -3.1986 | 3.8506  | -5.3825 |
| C | 1.9612  | -7.7753 | 2.0614  |
| C | 7.7827  | -1.7976 | 1.7238  |
| C | 3.7885  | -4.5751 | 4.7549  |
| C | 1.9710  | -3.1910 | 4.9711  |
| C | -2.4258 | 2.8606  | -4.9711 |
| C | 2.6737  | -4.2319 | 5.3825  |
| C | 3.7885  | 4.5751  | -4.7549 |
| C | 8.0009  | 0.5375  | -2.0614 |
| C | 1.9710  | 3.1910  | -4.9711 |
| C | 8.0009  | -0.5375 | 2.0614  |
| C | 0.3224  | -5.7006 | 1.9109  |
| C | 6.5478  | -2.2562 | 1.6462  |
| C | 7.7827  | 1.7976  | -1.7238 |
| C | 4.1147  | -6.8463 | -1.7238 |
| C | -4.4927 | -0.2673 | -3.2748 |
| C | -6.1569 | -5.1377 | -2.0614 |
| C | -3.3909 | -0.6300 | -3.9190 |
| C | -5.7541 | -1.4745 | -4.7549 |
| C | -3.9711 | -5.6740 | -1.6462 |
| C | 1.9089  | -6.7209 | -2.3265 |
| C | -5.2397 | -6.0289 | -1.7238 |
| C | -4.5341 | -3.5322 | -2.2529 |
| C | 1.9582  | -5.4037 | -2.2529 |
| C | 3.0900  | -4.8015 | -1.9109 |
| C | 2.9836  | -7.4432 | -2.0614 |
| C | 4.1692  | -5.5301 | -1.6462 |
| C | -3.4702 | -1.4231 | -4.9711 |
| C | -5.6798 | -0.6791 | -3.7049 |
| C | 0.6954  | -7.9573 | 1.7238  |
| C | -3.6116 | -4.4225 | -1.9109 |
| C | -5.8021 | -3.8923 | -2.3265 |
| C | 6.5478  | 2.2562  | -1.6462 |
| C | 3.6440  | -0.8885 | -4.9711 |
| C | 3.6440  | 0.8885  | 4.9711  |
| C | -4.6506 | -1.8522 | -5.3825 |
| C | 1.5920  | 5.5227  | -2.2529 |
| C | 0.6954  | 7.9573  | -1.7238 |
| C | -0.1224 | 6.9245  | -1.6462 |
| C | -0.1224 | -6.9245 | 1.6462  |
| C | 2.3731  | -2.5028 | 3.9190  |
| C | 0.3224  | 5.7006  | -1.9109 |
| C | 4.3957  | -2.8005 | -0.6527 |
| C | -5.2397 | 6.0289  | 1.7238  |
| C | 2.4062  | -6.5594 | 2.3265  |
| C | -5.8021 | 3.8923  | 2.3265  |
| C | -6.1569 | 5.1377  | 2.0614  |
| C | -7.3530 | 3.1202  | -1.7238 |
| C | -2.4258 | -2.8606 | 4.9711  |
| C | 2.3731  | 2.5028  | -3.9190 |
| C | 0.3244  | 4.9952  | 5.3825  |
| C | 0.2811  | -3.7402 | -4.9711 |
| C | 0.3244  | -4.9952 | -5.3825 |
| C | 2.4062  | 6.5594  | -2.3265 |
| C | 2.6737  | 4.2319  | -5.3825 |
| C | -1.1093 | -5.6117 | -3.7049 |
| C | 1.9612  | 7.7753  | -2.0614 |
| C | -0.3758 | -5.9280 | -4.7549 |
| C | -1.1093 | 5.6117  | 3.7049  |
| H | -0.3528 | 6.9136  | 5.0956  |
| H | 0.9047  | 5.2529  | 6.2101  |
| H | 0.8186  | 2.9950  | 5.4675  |
| H | -0.4818 | 2.4248  | 3.5917  |
| H | -1.6760 | 6.3465  | 3.2233  |
| H | 1.1094  | 4.8313  | 2.4772  |
| H | 1.0168  | 7.1853  | 2.6062  |
| H | 2.9441  | 8.4838  | 2.1245  |
| H | 4.9670  | 7.4132  | 1.5228  |

|   |         |         |         |
|---|---------|---------|---------|
| H | 5.0686  | 5.0740  | 1.3750  |
| H | 2.6047  | 8.5941  | -2.1245 |
| H | 3.4008  | 6.4107  | -2.6062 |
| H | 0.3390  | 8.9170  | -1.5228 |
| H | -1.1182 | 7.0842  | -1.3750 |
| H | 1.9422  | 4.5607  | -2.4772 |
| H | 7.1479  | 1.2534  | 2.6062  |
| H | 8.9783  | -0.1784 | 2.1245  |
| H | 5.5180  | 3.5552  | 3.2233  |
| H | 6.4661  | 2.4719  | 5.0956  |
| H | 2.1573  | 1.2076  | 3.5917  |
| H | 3.1014  | 0.1470  | 5.4675  |
| H | 5.2754  | 0.7628  | 6.2101  |
| H | 8.5853  | -2.4330 | 1.5228  |
| H | 6.3920  | -3.2526 | 1.3750  |
| H | 4.9377  | 0.4378  | 2.4772  |
| H | 6.3920  | 3.2526  | -1.3750 |
| H | 8.5853  | 2.4330  | -1.5228 |
| H | 8.9783  | 0.1784  | -2.1245 |
| H | 7.1479  | -1.2534 | -2.6062 |
| H | 4.9377  | -0.4378 | -2.4772 |
| H | 1.8151  | -1.6785 | 3.5917  |
| H | 1.0982  | -2.9042 | 5.4675  |
| H | 2.3556  | -4.7814 | 6.2101  |
| H | 4.3491  | -5.3859 | 5.0956  |
| H | 5.0864  | -4.1493 | 3.2233  |
| H | -1.0355 | -2.2450 | 3.5917  |
| H | -2.4227 | -1.9419 | 5.4675  |
| H | -3.8195 | -3.7180 | 6.2101  |
| H | -3.7783 | -5.8005 | 5.0956  |
| H | -2.3744 | -6.1195 | 3.2233  |
| H | -2.4551 | 0.2910  | 3.5917  |
| H | -2.5955 | 1.7040  | 5.4675  |
| H | -4.7162 | 2.4837  | 6.2101  |
| H | -6.6842 | 1.8009  | 5.0956  |
| H | -6.5538 | 0.3672  | 3.2233  |
| H | -4.2519 | 2.5481  | 2.4772  |
| H | -3.2593 | 6.3885  | 1.3750  |
| H | -5.5155 | 7.0147  | 1.5228  |
| H | -7.1587 | 5.4217  | 2.1245  |
| H | -6.5194 | 3.1874  | 2.6062  |
| H | -7.0830 | 1.1256  | -1.3750 |
| H | -8.3758 | 3.0779  | -1.5228 |
| H | -7.3685 | 5.1330  | -2.1245 |
| H | -5.0461 | 5.2153  | -2.6062 |
| H | -3.7373 | 3.2565  | -2.4772 |
| H | -1.0355 | 2.2450  | -3.5917 |
| H | -2.3744 | 6.1195  | -3.2233 |
| H | -2.4227 | 1.9419  | -5.4675 |
| H | -3.8195 | 3.7180  | -6.2101 |
| H | -3.7783 | 5.8005  | -5.0956 |
| H | -2.4551 | -0.2910 | -3.5917 |
| H | -2.5955 | -1.7040 | -5.4675 |
| H | -4.7162 | -2.4837 | -6.2101 |
| H | -6.6842 | -1.8009 | -5.0956 |
| H | -6.5538 | -0.3672 | -3.2233 |
| H | -4.2519 | -2.5481 | -2.4772 |
| H | -3.2593 | -6.3885 | -1.3750 |
| H | -5.5155 | -7.0147 | -1.5228 |
| H | -7.1587 | -5.4217 | -2.1245 |
| H | -6.5194 | -3.1874 | -2.6062 |
| H | -8.3758 | -3.0779 | 1.5228  |
| H | -7.0830 | -1.1256 | 1.3750  |
| H | -5.0461 | -5.2153 | 2.6062  |
| H | -7.3685 | -5.1330 | 2.1245  |
| H | -3.7373 | -3.2565 | 2.4772  |
| H | -1.1182 | -7.0842 | 1.3750  |
| H | 0.3390  | -8.9170 | 1.5228  |
| H | 2.6047  | -8.5941 | 2.1245  |
| H | 3.4008  | -6.4107 | 2.6062  |
| H | 1.9422  | -4.5607 | 2.4772  |
| H | 5.0686  | -5.0740 | -1.3750 |
| H | 4.9670  | -7.4132 | -1.5228 |
| H | 2.9441  | -8.4838 | -2.1245 |
| H | 1.0168  | -7.1853 | -2.6062 |
| H | 1.1094  | -4.8313 | -2.4772 |
| H | -0.4818 | -2.4248 | -3.5917 |

|                                |         |         |         |
|--------------------------------|---------|---------|---------|
| H                              | 0.8186  | -2.9950 | -5.4675 |
| H                              | 0.9047  | -5.2529 | -6.2101 |
| H                              | -0.3528 | -6.9136 | -5.0956 |
| H                              | -1.6760 | -6.3465 | -3.2233 |
| H                              | 2.1573  | -1.2076 | -3.5917 |
| H                              | 3.1014  | -0.1470 | -5.4675 |
| H                              | 5.2754  | -0.7628 | -6.2101 |
| H                              | 6.4661  | -2.4719 | -5.0956 |
| H                              | 5.5180  | -3.5552 | -3.2233 |
| H                              | 5.0864  | 4.1493  | -3.2233 |
| H                              | 1.8151  | 1.6785  | -3.5917 |
| H                              | 1.0982  | 2.9042  | -5.4675 |
| H                              | 2.3556  | 4.7814  | -6.2101 |
| H                              | 4.3491  | 5.3859  | -5.0956 |
| H                              | 3.0839  | -3.8016 | 0.6426  |
| H                              | 4.7029  | -4.0360 | 1.0043  |
| H                              | 4.5685  | -1.7582 | -0.6426 |
| H                              | 5.2918  | -3.2255 | -1.0043 |
| H                              | -1.4324 | -6.0295 | -1.0043 |
| H                              | -2.6625 | -4.1077 | 0.6426  |
| H                              | -6.1770 | -0.5009 | -1.0043 |
| H                              | -4.7294 | 1.2629  | 0.6426  |
| H                              | -2.6625 | 4.1077  | -0.6426 |
| H                              | -1.4324 | 6.0295  | 1.0043  |
| H                              | 3.0839  | 3.8016  | -0.6426 |
| H                              | 4.5685  | 1.7582  | 0.6426  |
| H                              | 4.7029  | 4.0360  | -1.0043 |
| H                              | 5.2918  | 3.2255  | 1.0043  |
| H                              | -0.2604 | -4.8882 | -0.6426 |
| H                              | -2.3852 | -5.7199 | 1.0043  |
| H                              | -4.7294 | -1.2629 | -0.6426 |
| H                              | -6.1770 | 0.5009  | 1.0043  |
| H                              | -2.3852 | 5.7199  | -1.0043 |
| H                              | -0.2604 | 4.8882  | 0.6426  |
| 275                            |         |         |         |
| [FeAu12Cl12(dppe)5] Isomer III |         |         |         |
| Fe                             | 0.0049  | -0.0735 | -2.6123 |
| Au                             | -1.5030 | 1.4836  | 0.9626  |
| Au                             | 1.0466  | 1.9927  | 1.0065  |
| Au                             | 0.2057  | 2.0981  | -1.4099 |
| Au                             | 0.2617  | -2.3440 | 1.0898  |
| Au                             | 0.1200  | -0.0446 | -0.1944 |
| Au                             | -1.1999 | -1.8337 | -1.4146 |
| Au                             | 2.4763  | 0.4634  | -1.3467 |
| Au                             | 2.1813  | -0.6372 | 1.0061  |
| Au                             | -2.0270 | 0.6589  | -1.4600 |
| Au                             | -2.0283 | -1.0755 | 0.9385  |
| Au                             | 1.3850  | -1.7965 | -1.3420 |
| Au                             | 0.0797  | -0.0528 | 2.3487  |
| P                              | -1.8846 | -3.7567 | -1.5859 |
| P                              | 2.7640  | 2.9549  | 1.6366  |
| P                              | -0.5435 | 3.9538  | -1.8158 |
| P                              | 3.0432  | -2.9033 | -1.7422 |
| P                              | 3.7013  | -1.8352 | 1.6772  |
| P                              | -0.6629 | -4.0447 | 1.8333  |
| Cl                             | 0.2326  | -0.0037 | -4.6652 |
| Cl                             | 0.0581  | -0.0238 | 4.5473  |
| P                              | -4.0462 | 0.7420  | -1.7199 |
| P                              | -3.9833 | -0.8854 | 1.6154  |
| P                              | 3.7755  | 1.9947  | -1.8489 |
| P                              | -2.0717 | 3.3726  | 1.5696  |
| C                              | 2.7353  | 4.5827  | 1.7618  |
| C                              | -3.6262 | 3.8566  | 1.6803  |
| C                              | -4.3385 | 3.1205  | -2.3047 |
| C                              | -5.9318 | 2.3344  | -1.0793 |
| C                              | -4.5165 | -3.1674 | 2.3525  |
| C                              | -1.4186 | -2.7570 | 3.8160  |
| C                              | -6.2866 | -4.2966 | 1.8590  |
| C                              | -2.0811 | -4.8139 | 3.7764  |
| C                              | -3.0298 | 0.2681  | 3.6194  |
| C                              | -5.9707 | 4.3972  | -1.7080 |
| C                              | -1.3818 | 2.9186  | -3.9327 |
| C                              | 3.7051  | 5.3093  | 1.4544  |
| C                              | -6.0858 | -2.2575 | 1.1806  |
| C                              | 5.3652  | 1.6321  | -1.7889 |
| C                              | 1.6581  | 5.1147  | 2.1077  |
| C                              | -4.8519 | 2.1612  | -1.6860 |

|   |         |         |         |
|---|---------|---------|---------|
| C | -5.1745 | -4.2159 | 2.4182  |
| C | 5.4365  | -0.0833 | 1.8477  |
| C | -1.9086 | -4.4872 | 0.8494  |
| C | -0.6463 | 2.9903  | 3.5835  |
| C | -4.0587 | 4.9216  | 1.1876  |
| C | 5.0466  | -2.5087 | -3.2693 |
| C | 2.5213  | 7.0700  | 1.8322  |
| C | -1.9584 | 4.9798  | -3.6427 |
| C | -5.2400 | 0.8995  | 4.5673  |
| C | 3.7814  | -3.1256 | 0.6502  |
| C | -4.9664 | -2.1738 | 1.7349  |
| C | -4.0763 | -0.1050 | 3.0513  |
| C | 3.5973  | 6.5474  | 1.4884  |
| C | 1.5551  | 6.3517  | 2.1465  |
| C | -5.1859 | 0.1998  | 3.5418  |
| C | -1.1741 | -4.5099 | -2.8606 |
| C | 3.4250  | 2.8011  | -3.2237 |
| C | -0.3003 | -3.8983 | -3.5127 |
| C | 3.4512  | 2.3215  | 2.9773  |
| C | -1.7964 | 4.2517  | -0.7800 |
| C | -4.8976 | 4.2293  | -2.3167 |
| C | -1.3741 | 4.4293  | 0.5121  |
| C | 3.6096  | 3.1698  | -0.7094 |
| C | 5.6830  | 0.4432  | -2.0147 |
| C | -4.8575 | -0.2377 | -0.6708 |
| C | 3.8245  | -2.3286 | -3.0681 |
| C | 2.8664  | 1.3832  | 3.5575  |
| C | -1.4433 | -4.8097 | -0.3965 |
| C | -0.7170 | 5.3530  | 4.3536  |
| C | -2.7592 | -4.6101 | 4.7972  |
| C | -1.4196 | -3.8795 | 3.2708  |
| C | 5.2509  | -1.3104 | 1.7085  |
| C | -1.3467 | 3.8210  | 2.9683  |
| C | -6.7375 | -3.3158 | 1.2415  |
| C | 0.0317  | 3.3399  | 4.5646  |
| C | -3.0845 | 0.9670  | 4.6455  |
| C | -2.6577 | 4.9252  | -4.6692 |
| C | 4.0335  | -3.5412 | 3.5200  |
| C | 3.1891  | -1.5695 | -3.8347 |
| C | -4.7633 | 0.1843  | 0.6332  |
| C | 3.9454  | 2.6757  | 0.5234  |
| C | 3.3540  | -2.5808 | 3.0951  |
| C | 4.5950  | 2.6623  | 3.3532  |
| C | 4.0587  | 3.8202  | -3.5751 |
| C | 1.4873  | -5.2142 | 2.1438  |
| C | -1.3291 | 3.9697  | -3.2590 |
| C | 5.6212  | -1.9303 | -4.2081 |
| C | 6.5800  | 0.3928  | 1.7686  |
| C | -4.4214 | 3.0848  | 2.2618  |
| C | 5.1558  | 2.0426  | 4.2726  |
| C | 4.9850  | -1.1649 | -4.9550 |
| C | -4.1893 | 1.2929  | 5.1137  |
| C | 4.5785  | 1.0858  | 4.8272  |
| C | -2.7725 | -3.4791 | 5.3245  |
| C | 6.8589  | 0.0696  | -1.8700 |
| C | -2.7311 | 3.8647  | -5.3210 |
| C | 1.8685  | -7.3046 | 1.7889  |
| C | 7.3763  | -1.5779 | 1.4087  |
| C | 3.6510  | -4.1821 | 4.5140  |
| C | 1.9304  | -2.8926 | 4.6932  |
| C | -2.0842 | 2.8658  | -4.9576 |
| C | 2.5929  | -3.8667 | 5.0935  |
| C | 3.6555  | 4.5005  | -4.5322 |
| C | 7.7279  | 0.8745  | -1.4850 |
| C | 1.9970  | 3.1454  | -4.8077 |
| C | 7.5509  | -0.3518 | 1.5397  |
| C | 0.2734  | -5.3832 | 1.8899  |
| C | 6.2323  | -2.0574 | 1.4950  |
| C | 7.4192  | 2.0597  | -1.2576 |
| C | 3.6277  | -6.5208 | -2.1740 |
| C | -4.4547 | 0.0870  | -3.1695 |
| C | -5.9948 | -4.0527 | -1.7974 |
| C | -3.5676 | -0.3888 | -3.9094 |
| C | -5.9579 | -0.5115 | -4.5979 |
| C | -4.1151 | -4.9289 | -1.2040 |
| C | 1.6141  | -6.2377 | -1.4798 |
| C | -5.3567 | -4.9731 | -1.2538 |

|   |         |         |         |
|---|---------|---------|---------|
| C | -4.1503 | -3.0333 | -2.2304 |
| C | 1.7887  | -5.0079 | -1.4912 |
| C | 2.8824  | -4.5264 | -1.8430 |
| C | 2.5330  | -6.9946 | -1.8252 |
| C | 3.8037  | -5.2902 | -2.1839 |
| C | -3.8777 | -0.9344 | -4.9815 |
| C | -5.6516 | 0.0340  | -3.5260 |
| C | 0.6604  | -7.4824 | 1.5438  |
| C | -3.5011 | -3.9566 | -1.6928 |
| C | -5.3893 | -3.0855 | -2.2917 |
| C | 6.2439  | 2.4380  | -1.4097 |
| C | 3.7659  | -0.9906 | -4.7701 |
| C | 3.4288  | 0.7652  | 4.4776  |
| C | -5.0708 | -1.0001 | -5.3248 |
| C | 1.5509  | 5.2222  | -2.1141 |
| C | 0.7397  | 7.3453  | -1.1128 |
| C | -0.0370 | 6.3822  | -1.2416 |
| C | -0.1352 | -6.5279 | 1.5962  |
| C | 2.3120  | -2.2514 | 3.6997  |
| C | 0.3654  | 5.3073  | -1.7350 |
| C | 4.2214  | -2.7559 | -0.5950 |
| C | -5.2654 | 5.2102  | 1.2814  |
| C | 2.2779  | -6.1710 | 2.0993  |
| C | -5.6234 | 3.3793  | 2.3596  |
| C | -6.0493 | 4.4425  | 1.8678  |
| C | -6.4858 | 3.4485  | -1.0903 |
| C | -2.0922 | -2.5567 | 4.8409  |
| C | 2.4028  | 2.4568  | -3.8561 |
| C | 0.0053  | 4.5244  | 4.9438  |
| C | 0.3518  | -4.4896 | -4.3912 |
| C | 0.1303  | -5.6903 | -4.6291 |
| C | 2.3216  | 6.1872  | -1.9916 |
| C | 2.6172  | 4.1706  | -5.1405 |
| C | -1.4087 | -5.7120 | -3.1170 |
| C | 1.9212  | 7.2484  | -1.4811 |
| C | -0.7559 | -6.2999 | -3.9959 |
| C | -1.3942 | 5.0042  | 3.3712  |
| H | -0.7460 | 6.2755  | 4.6563  |
| H | 0.5472  | 4.8060  | 5.6996  |
| H | 0.5778  | 2.6739  | 5.0141  |
| H | -0.6128 | 2.0652  | 3.2929  |
| H | -1.9570 | 5.6529  | 2.9155  |
| H | 0.8976  | 4.5540  | 2.3371  |
| H | 0.7116  | 6.7481  | 2.4160  |
| H | 2.4370  | 8.0374  | 1.8485  |
| H | 4.3515  | 7.1058  | 1.2387  |
| H | 4.5472  | 4.9149  | 1.1763  |
| H | 2.5282  | 7.9975  | -1.3666 |
| H | 3.2385  | 6.1010  | -2.2906 |
| H | 0.4226  | 8.1706  | -0.7150 |
| H | -0.9543 | 6.4728  | -0.9457 |
| H | 1.8678  | 4.3894  | -2.4984 |
| H | 6.7055  | 1.3498  | 1.8731  |
| H | 8.4429  | 0.0226  | 1.4557  |
| H | 5.0501  | 3.4060  | 2.9235  |
| H | 6.0497  | 2.2986  | 4.5521  |
| H | 1.9731  | 1.1188  | 3.2848  |
| H | 2.9591  | 0.0314  | 4.9058  |
| H | 5.0278  | 0.5923  | 5.5335  |
| H | 8.1315  | -2.1627 | 1.2298  |
| H | 6.1100  | -3.0137 | 1.3775  |
| H | 4.6738  | 0.4973  | 2.0095  |
| H | 6.0126  | 3.3619  | -1.2172 |
| H | 8.0943  | 2.6892  | -0.9543 |
| H | 8.6441  | 0.5786  | -1.3536 |
| H | 7.0888  | -0.8565 | -2.0452 |
| H | 4.9973  | -0.1915 | -2.2875 |
| H | 1.7819  | -1.5011 | 3.3881  |
| H | 1.1106  | -2.6215 | 5.1367  |
| H | 2.2877  | -4.3811 | 5.8585  |
| H | 4.1752  | -4.9347 | 4.8326  |
| H | 4.8600  | -3.7927 | 3.0754  |
| H | -0.8979 | -2.0297 | 3.4395  |
| H | -2.0758 | -1.6739 | 5.2433  |
| H | -3.3131 | -3.3217 | 6.1153  |
| H | -3.2826 | -5.3324 | 5.1818  |
| H | -2.0694 | -5.6968 | 3.3710  |



|   |         |         |         |
|---|---------|---------|---------|
| H | -2.1625 | 0.0238  | 3.2599  |
| H | -2.2534 | 1.2467  | 5.0616  |
| H | -4.2358 | 1.8506  | 5.9072  |
| H | -6.1026 | 1.1421  | 4.9410  |
| H | -6.0046 | -0.1117 | 3.1211  |
| H | -4.0923 | 2.2503  | 2.6357  |
| H | -3.4619 | 5.5300  | 0.7242  |
| H | -5.5934 | 6.0347  | 0.8889  |
| H | -6.9914 | 4.6692  | 1.9355  |
| H | -6.2246 | 2.7711  | 2.8192  |
| H | -6.3478 | 1.6072  | -0.5895 |
| H | -7.3171 | 3.5761  | -0.6045 |
| H | -6.4025 | 5.2676  | -1.7089 |
| H | -4.4850 | 4.9597  | -2.8050 |
| H | -3.4984 | 2.9956  | -2.7776 |
| H | -0.8917 | 2.1299  | -3.6451 |
| H | -1.9037 | 5.8089  | -3.1383 |
| H | -2.1256 | 2.0355  | -5.4583 |
| H | -3.2921 | 3.8202  | -6.1125 |
| H | -3.1523 | 5.7094  | -4.9585 |
| H | -2.6339 | -0.3447 | -3.6382 |
| H | -3.1810 | -1.3098 | -5.5432 |
| H | -5.3121 | -1.4282 | -6.1621 |
| H | -6.8890 | -0.5523 | -4.8703 |
| H | -6.3429 | 0.4315  | -2.9700 |
| H | -3.6774 | -2.2659 | -2.5911 |
| H | -3.6343 | -5.6501 | -0.7670 |
| H | -5.8265 | -5.7219 | -0.8547 |
| H | -6.9650 | -4.0867 | -1.8269 |
| H | -5.8731 | -2.3585 | -2.7148 |
| H | -7.6017 | -3.3722 | 0.8017  |
| H | -6.4548 | -1.5036 | 0.6951  |
| H | -4.8124 | -4.9715 | 2.9081  |
| H | -6.7973 | -5.1223 | 1.9018  |
| H | -3.6441 | -3.1141 | 2.7779  |
| H | -1.0723 | -6.6799 | 1.3911  |
| H | 0.3378  | -8.3653 | 1.3017  |
| H | 2.4906  | -8.0478 | 1.7299  |
| H | 3.2173  | -6.0211 | 2.2940  |
| H | 1.8115  | -4.3243 | 2.3627  |
| H | 4.6556  | -4.9280 | -2.4639 |
| H | 4.3439  | -7.1129 | -2.4455 |
| H | 2.3990  | -7.9568 | -1.8224 |
| H | 0.7584  | -6.6005 | -1.2083 |
| H | 1.0828  | -4.3964 | -1.2289 |
| H | -0.1172 | -2.9633 | -3.3171 |
| H | 1.0383  | -4.0077 | -4.8815 |
| H | 0.6470  | -6.1550 | -5.3087 |
| H | -0.9358 | -7.2349 | -4.1879 |
| H | -2.1056 | -6.1895 | -2.6346 |
| H | 2.2450  | -1.3985 | -3.6780 |
| H | 3.2559  | -0.3904 | -5.3370 |
| H | 5.4421  | -0.6963 | -5.6728 |
| H | 6.5732  | -2.0637 | -4.3452 |
| H | 5.5672  | -3.0779 | -2.6808 |
| H | 4.8615  | 4.0850  | -3.0957 |
| H | 1.9046  | 1.6657  | -3.5918 |
| H | 1.1880  | 2.8769  | -5.2717 |
| H | 2.2921  | 4.7183  | -5.8730 |
| H | 4.1427  | 5.2971  | -4.7981 |
| H | 2.8679  | -3.4848 | 0.6270  |
| H | 4.3469  | -3.8212 | 1.0404  |
| H | 4.5020  | -1.8170 | -0.6253 |
| H | 4.9884  | -3.2994 | -0.8616 |
| H | -1.7143 | -5.7110 | -0.6603 |
| H | -2.5103 | -3.7117 | 0.8307  |
| H | -5.7883 | -0.3224 | -0.9609 |
| H | -4.2267 | 1.0032  | 0.7100  |
| H | -2.3702 | 3.4621  | -0.8708 |
| H | -1.5049 | 5.3487  | 0.8186  |
| H | 2.6597  | 3.4098  | -0.7509 |
| H | 4.0216  | 1.6970  | 0.5053  |
| H | 4.1091  | 3.9780  | -0.9382 |
| H | 4.8097  | 3.0123  | 0.8324  |
| H | -0.4657 | -4.8104 | -0.4258 |
| H | -2.4181 | -5.2184 | 1.2535  |
| H | -4.4501 | -1.1202 | -0.7999 |

|   |         |        |         |
|---|---------|--------|---------|
| H | -5.6389 | 0.3942 | 1.0150  |
| H | -2.3242 | 5.0082 | -1.1046 |
| H | -0.4146 | 4.2414 | 0.6028  |

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[OsAu12Cl12(dppe)5] Isomer I Excited state T1

|    |         |         |         |
|----|---------|---------|---------|
| Au | -0.0150 | 0.0220  | -2.6145 |
| Au | -1.4784 | 1.8868  | 1.1285  |
| Au | 1.1107  | 2.2009  | 1.3090  |
| Au | 0.0651  | 2.3438  | -1.1723 |
| Au | 0.1082  | -2.3220 | 1.1862  |
| Os | 0.0113  | 0.0087  | -0.0066 |
| Au | -1.5217 | -1.7811 | -1.2748 |
| Au | 2.2347  | 0.6053  | -1.2003 |
| Au | 2.2652  | -0.6213 | 1.1417  |
| Au | -2.2264 | 0.8174  | -1.1526 |
| Au | -2.1940 | -0.7935 | 1.1623  |
| Au | 1.3083  | -1.9634 | -1.1355 |
| Au | 0.0065  | 0.0464  | 2.5691  |
| P  | -1.9744 | -3.8333 | -1.8180 |
| P  | 3.0303  | 3.0755  | 1.7952  |
| P  | -0.5774 | 4.3369  | -1.7684 |
| P  | 3.0155  | -3.1354 | -1.8109 |
| P  | 3.9318  | -1.8703 | 1.7947  |
| P  | -0.6459 | -4.2463 | 1.8439  |
| Cl | -0.0373 | -0.0023 | -4.9067 |
| Cl | -0.0067 | 0.0451  | 4.8630  |
| P  | -4.2892 | 0.7152  | -1.8237 |
| P  | -4.2697 | -0.7568 | 1.7890  |
| P  | 3.8323  | 1.9205  | -1.8412 |
| P  | -2.0592 | 3.8748  | 1.8141  |
| C  | 2.9762  | 4.7969  | 1.9075  |
| C  | -3.7209 | 4.3591  | 1.8069  |
| C  | -4.6347 | 3.2841  | -2.1531 |
| C  | -6.5180 | 2.1920  | -1.4608 |
| C  | -4.6499 | -3.2806 | 2.3700  |
| C  | -1.4914 | -3.0178 | 4.0069  |
| C  | -6.5290 | -4.4991 | 1.9311  |
| C  | -2.2160 | -5.1789 | 3.8020  |
| C  | -3.4063 | 0.5760  | 3.8911  |
| C  | -6.5431 | 4.4594  | -1.7280 |
| C  | -1.5253 | 3.1432  | -3.9194 |
| C  | 3.9208  | 5.5873  | 1.4205  |
| C  | -6.4704 | -2.2720 | 1.4291  |
| C  | 5.4529  | 1.3275  | -1.8961 |
| C  | 1.8859  | 5.3401  | 2.4357  |
| C  | -5.2464 | 2.1557  | -1.8300 |
| C  | -5.2976 | -4.4239 | 2.3975  |
| C  | 5.7847  | -0.0588 | 2.1333  |
| C  | -1.8891 | -4.6940 | 0.7018  |
| C  | -0.7349 | 3.3974  | 4.0342  |
| C  | -4.1339 | 5.5553  | 1.4151  |
| C  | 4.8331  | -2.9567 | -3.7770 |
| C  | 2.6855  | 7.4276  | 1.9702  |
| C  | -2.1965 | 5.3140  | -3.6666 |
| C  | -5.7978 | 1.3421  | 4.6864  |
| C  | 3.9782  | -3.1930 | 0.6505  |
| C  | -5.2294 | -2.1928 | 1.8856  |
| C  | -4.4817 | 0.1429  | 3.2537  |
| C  | 3.7734  | 6.8954  | 1.4489  |
| C  | 1.7474  | 6.6468  | 2.4693  |
| C  | -5.6822 | 0.5133  | 3.6715  |
| C  | -1.1351 | -4.3431 | -3.2437 |
| C  | 3.4852  | 2.7258  | -3.3318 |
| C  | -0.3916 | -3.4603 | -3.8919 |
| C  | 3.7108  | 2.4374  | 3.2479  |
| C  | -1.8144 | 4.8437  | -0.6399 |
| C  | -5.2811 | 4.4277  | -2.1105 |
| C  | -1.3123 | 5.0146  | 0.7165  |
| C  | 3.9097  | 3.2382  | -0.7022 |
| C  | 5.6280  | 0.0840  | -2.3167 |
| C  | -5.1372 | -0.3233 | -0.7010 |
| C  | 3.6497  | -2.5769 | -3.3225 |
| C  | 3.0782  | 1.4679  | 3.8888  |
| C  | -1.3048 | -4.9081 | -0.6144 |
| C  | -0.7647 | 5.8885  | 4.8919  |
| C  | -2.9479 | -5.0295 | 4.8847  |
| C  | -1.4948 | -4.1656 | 3.3478  |

|   |         |         |         |
|---|---------|---------|---------|
| C | 5.5728  | -1.3248 | 1.8124  |
| C | -1.3832 | 4.3226  | 3.3450  |
| C | -7.1139 | -3.4205 | 1.4504  |
| C | -0.0949 | 3.7177  | 5.1387  |
| C | -3.5252 | 1.4017  | 4.9081  |
| C | -2.9919 | 5.1835  | -4.7065 |
| C | 4.3003  | -3.7340 | 3.6890  |
| C | 2.9624  | -1.6581 | -3.9819 |
| C | -5.1341 | 0.2397  | 0.6419  |
| C | 4.2799  | 2.7568  | 0.6198  |
| C | 3.5762  | -2.7075 | 3.2700  |
| C | 4.9046  | 2.8291  | 3.6691  |
| C | 4.2491  | 3.7111  | -3.7784 |
| C | 1.6619  | -5.4280 | 2.1842  |
| C | -1.4722 | 4.2861  | -3.2536 |
| C | 5.3321  | -2.3974 | -4.8582 |
| C | 6.9958  | 0.4495  | 2.0802  |
| C | -4.6178 | 3.4438  | 2.1372  |
| C | 5.4704  | 2.2248  | 4.6915  |
| C | 4.6527  | -1.4616 | -5.4953 |
| C | -4.7194 | 1.7967  | 5.2968  |
| C | 4.8472  | 1.2378  | 5.3070  |
| C | -2.9613 | -3.8732 | 5.5224  |
| C | 6.8238  | -0.4610 | -2.3007 |
| C | -3.0641 | 4.0306  | -5.3459 |
| C | 2.1312  | -7.6203 | 1.7601  |
| C | 7.8092  | -1.5631 | 1.3792  |
| C | 3.8996  | -4.4436 | 4.7220  |
| C | 2.0694  | -3.0956 | 4.9504  |
| C | -2.3206 | 3.0152  | -4.9597 |
| C | 2.7774  | -4.1337 | 5.3449  |
| C | 3.8783  | 4.4009  | -4.8349 |
| C | 7.8573  | 0.2240  | -1.8501 |
| C | 2.0048  | 3.1076  | -5.0339 |
| C | 8.0102  | -0.2993 | 1.6961  |
| C | 0.3934  | -5.6273 | 1.8618  |
| C | 6.5982  | -2.0759 | 1.4383  |
| C | 7.6926  | 1.4635  | -1.4350 |
| C | 4.0194  | -6.8928 | -1.3813 |
| C | -4.5292 | -0.0989 | -3.3335 |
| C | -6.2053 | -4.9187 | -1.9907 |
| C | -3.4589 | -0.4600 | -4.0229 |
| C | -5.8559 | -1.1945 | -4.8379 |
| C | -4.0559 | -5.5116 | -1.5007 |
| C | 1.8159  | -6.7966 | -1.9658 |
| C | -5.3400 | -5.8002 | -1.5305 |
| C | -4.5009 | -3.4531 | -2.3872 |
| C | 1.8947  | -5.4864 | -2.0441 |
| C | 3.0358  | -4.8664 | -1.7938 |
| C | 2.8759  | -7.5022 | -1.6270 |
| C | 4.1013  | -5.5815 | -1.4652 |
| C | -3.5864 | -1.1994 | -5.1042 |
| C | -5.7317 | -0.4523 | -3.7585 |
| C | 0.8689  | -7.8287 | 1.4421  |
| C | -3.6248 | -4.3339 | -1.9268 |
| C | -5.7819 | -3.7484 | -2.4249 |
| C | 6.4977  | 2.0177  | -1.4616 |
| C | 3.4630  | -1.0994 | -5.0621 |
| C | 3.6458  | 0.8679  | 4.9112  |
| C | -4.7826 | -1.5780 | -5.5043 |
| C | 1.7244  | 5.4690  | -2.2777 |
| C | 1.0927  | 7.8500  | -1.3490 |
| C | 0.1902  | 6.8914  | -1.3634 |
| C | 0.0016  | -6.8390 | 1.4960  |
| C | 2.4701  | -2.3818 | 3.9204  |
| C | 0.5008  | 5.6885  | -1.8227 |
| C | 4.2982  | -2.7309 | -0.6927 |
| C | -5.4220 | 5.8221  | 1.3449  |
| C | 2.5235  | -6.4203 | 2.1393  |
| C | -5.9017 | 3.7178  | 2.0827  |
| C | -6.3075 | 4.9053  | 1.6762  |
| C | -7.1601 | 3.3407  | -1.4070 |
| C | -2.2254 | -2.8709 | 5.0882  |
| C | 2.3731  | 2.4154  | -3.9777 |
| C | -0.0981 | 4.9657  | 5.5603  |
| C | 0.3876  | -3.8481 | -4.8785 |
| C | 0.4244  | -5.1174 | -5.2285 |

|   |         |         |         |
|---|---------|---------|---------|
| C | 2.6206  | 6.4301  | -2.2711 |
| C | 2.7497  | 4.1082  | -5.4556 |
| C | -1.1209 | -5.6128 | -3.6214 |
| C | 2.3103  | 7.6210  | -1.7986 |
| C | -0.3397 | -5.9971 | -4.6080 |
| C | -1.4124 | 5.5677  | 3.7908  |
| H | -0.7750 | 6.8605  | 5.2265  |
| H | 0.4166  | 5.2227  | 6.4125  |
| H | 0.4092  | 2.9821  | 5.6492  |
| H | -0.7086 | 2.4261  | 3.7021  |
| H | -1.9376 | 6.2885  | 3.2780  |
| H | 1.1416  | 4.7334  | 2.8067  |
| H | 0.8967  | 7.0483  | 2.8831  |
| H | 2.5689  | 8.4497  | 1.9827  |
| H | 4.5057  | 7.4995  | 1.0533  |
| H | 4.7713  | 5.1896  | 1.0026  |
| H | 3.0154  | 8.3691  | -1.7762 |
| H | 3.5646  | 6.2382  | -2.6293 |
| H | 0.8466  | 8.7769  | -0.9784 |
| H | -0.7513 | 7.0861  | -1.0011 |
| H | 1.9726  | 4.5350  | -2.6291 |
| H | 7.1388  | 1.4354  | 2.3335  |
| H | 8.9560  | 0.1003  | 1.6377  |
| H | 5.3912  | 3.6027  | 3.1963  |
| H | 6.4025  | 2.5210  | 5.0072  |
| H | 2.1443  | 1.1675  | 3.5843  |
| H | 3.1412  | 0.1073  | 5.3830  |
| H | 5.2995  | 0.7585  | 6.0955  |
| H | 8.5986  | -2.1484 | 1.0759  |
| H | 6.4558  | -3.0595 | 1.1764  |
| H | 4.9899  | 0.5278  | 2.4180  |
| H | 6.3859  | 2.9839  | -1.1294 |
| H | 8.4949  | 1.9996  | -1.0804 |
| H | 8.7896  | -0.2085 | -1.8179 |
| H | 6.9391  | -1.4268 | -2.6322 |
| H | 4.8184  | -0.4587 | -2.6467 |
| H | 1.9026  | -1.5818 | 3.6125  |
| H | 1.1980  | -2.8332 | 5.4277  |
| H | 2.4578  | -4.7033 | 6.1391  |
| H | 4.4578  | -5.2472 | 5.0381  |
| H | 5.1741  | -3.9817 | 3.2058  |
| H | -0.9310 | -2.2253 | 3.6699  |
| H | -2.2159 | -1.9648 | 5.5726  |
| H | -3.5469 | -3.7571 | 6.3596  |
| H | -3.5167 | -5.8137 | 5.2297  |
| H | -2.2097 | -6.0811 | 3.3076  |
| H | -2.4692 | 0.2857  | 3.5858  |
| H | -2.6755 | 1.7367  | 5.3779  |
| H | -4.8141 | 2.4585  | 6.0775  |
| H | -6.7306 | 1.6423  | 4.9976  |
| H | -6.5254 | 0.1605  | 3.1993  |
| H | -4.3006 | 2.5105  | 2.4311  |
| H | -3.4571 | 6.2822  | 1.1518  |
| H | -5.7340 | 6.7480  | 1.0243  |
| H | -7.3123 | 5.1144  | 1.6119  |
| H | -6.5816 | 2.9948  | 2.3484  |
| H | -7.0118 | 1.3291  | -1.2005 |
| H | -8.1427 | 3.3630  | -1.1043 |
| H | -7.0440 | 5.3555  | -1.6733 |
| H | -4.7897 | 5.2926  | -2.3681 |
| H | -3.6445 | 3.2591  | -2.4317 |
| H | -0.9635 | 2.3384  | -3.6152 |
| H | -2.1440 | 6.2152  | -3.1728 |
| H | -2.3571 | 2.1122  | -5.4491 |
| H | -3.7020 | 3.9276  | -6.1456 |
| H | -3.5644 | 5.9797  | -5.0150 |
| H | -2.5202 | -0.1865 | -3.7061 |
| H | -2.7408 | -1.4810 | -5.6155 |
| H | -4.8829 | -2.1728 | -6.3369 |
| H | -6.7902 | -1.4814 | -5.1578 |
| H | -6.5709 | -0.1523 | -3.2447 |
| H | -4.1738 | -2.5307 | -2.7049 |
| H | -3.3961 | -6.2076 | -1.1314 |
| H | -5.6661 | -6.7130 | -1.1873 |
| H | -7.2089 | -5.1436 | -2.0050 |
| H | -6.4460 | -3.0530 | -2.7876 |
| H | -8.0735 | -3.4737 | 1.0844  |

|   |         |         |         |
|---|---------|---------|---------|
| H | -6.9406 | -1.4438 | 1.0434  |
| H | -4.8306 | -5.2568 | 2.7780  |
| H | -7.0308 | -5.3968 | 1.9373  |
| H | -3.6824 | -3.2272 | 2.7151  |
| H | -0.9782 | -7.0156 | 1.2392  |
| H | 0.5603  | -8.7634 | 1.1437  |
| H | 2.8084  | -8.3928 | 1.7072  |
| H | 3.5040  | -6.2463 | 2.3942  |
| H | 1.9710  | -4.4875 | 2.4652  |
| H | 4.9971  | -5.1206 | -1.2599 |
| H | 4.8490  | -7.4401 | -1.1159 |
| H | 2.8123  | -8.5259 | -1.5488 |
| H | 0.9196  | -7.2594 | -2.1642 |
| H | 1.0665  | -4.9321 | -2.2981 |
| H | -0.4057 | -2.4691 | -3.6193 |
| H | 0.9685  | -3.1501 | -5.3586 |
| H | 1.0464  | -5.4240 | -5.9879 |
| H | -0.3194 | -6.9856 | -4.8903 |
| H | -1.7159 | -6.3011 | -3.1412 |
| H | 2.0388  | -1.3581 | -3.6450 |
| H | 2.9133  | -0.3790 | -5.5467 |
| H | 5.0540  | -1.0164 | -6.3306 |
| H | 6.2571  | -2.6854 | -5.2026 |
| H | 5.3666  | -3.6853 | -3.2846 |
| H | 5.1292  | 3.9410  | -3.2980 |
| H | 1.7781  | 1.6443  | -3.6505 |
| H | 1.1296  | 2.8563  | -5.5096 |
| H | 2.4560  | 4.6622  | -6.2702 |
| H | 4.4647  | 5.1748  | -5.1726 |
| H | 3.0272  | -3.6067 | 0.6960  |
| H | 4.6277  | -3.9332 | 0.9691  |
| H | 4.3686  | -1.6959 | -0.7363 |
| H | 5.2090  | -3.0961 | -1.0216 |
| H | -1.3827 | -5.8954 | -0.9164 |
| H | -2.5527 | -3.8949 | 0.7073  |
| H | -6.0983 | -0.5086 | -1.0372 |
| H | -4.6356 | 1.1503  | 0.6720  |
| H | -2.5284 | 4.0913  | -0.6887 |
| H | -1.4487 | 5.9826  | 1.0562  |
| H | 2.9569  | 3.6516  | -0.7102 |
| H | 4.3824  | 1.7233  | 0.6338  |
| H | 4.5485  | 3.9781  | -1.0425 |
| H | 5.1885  | 3.1407  | 0.9350  |
| H | -0.2902 | -4.6865 | -0.6175 |
| H | -2.4228 | -5.5178 | 1.0308  |
| H | -4.6310 | -1.2284 | -0.7460 |
| H | -6.0932 | 0.4236  | 0.9843  |
| H | -2.2769 | 5.7013  | -0.9883 |
| H | -0.2957 | 4.8173  | 0.7868  |

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[RuAu12Cl12(dppe)5] Isomer I Excited state T1

|    |         |         |         |
|----|---------|---------|---------|
| Au | 0.0438  | -0.0419 | -2.5955 |
| Au | -1.4815 | 1.8086  | 1.1226  |
| Au | 1.2347  | 1.9480  | 1.2423  |
| Au | 0.1632  | 2.3236  | -1.1568 |
| Au | 0.1049  | -2.4127 | 1.1182  |
| Ru | -0.0018 | -0.0013 | 0.0051  |
| Au | -1.4389 | -1.8541 | -1.1126 |
| Au | 2.3695  | 0.4559  | -1.2988 |
| Au | 2.2487  | -0.6419 | 1.1443  |
| Au | -2.1350 | 0.8158  | -1.2229 |
| Au | -2.1772 | -1.1581 | 1.4170  |
| Au | 1.3176  | -1.9933 | -1.1594 |
| Au | -0.0139 | -0.0596 | 2.5845  |
| P  | -2.0804 | -3.8392 | -1.7445 |
| P  | 3.0093  | 3.0312  | 1.8755  |
| P  | -0.5487 | 4.2835  | -1.8274 |
| P  | 3.0519  | -3.1177 | -1.8387 |
| P  | 3.9057  | -1.9039 | 1.7684  |
| P  | -0.5946 | -4.3625 | 1.8148  |
| Cl | 0.0530  | -0.0351 | -4.8980 |
| Cl | -0.0379 | -0.0605 | 4.8893  |
| P  | -4.2096 | 0.6617  | -1.8491 |
| P  | -4.2609 | -0.6997 | 1.8488  |
| P  | 3.8873  | 1.9322  | -1.8102 |
| P  | -2.0815 | 3.8099  | 1.7832  |
| C  | 2.9799  | 4.7565  | 1.9148  |

|   |         |         |         |
|---|---------|---------|---------|
| C | -3.7129 | 4.3841  | 1.7626  |
| C | -4.6134 | 3.2096  | -2.2620 |
| C | -6.4638 | 2.0927  | -1.5175 |
| C | -4.7279 | -3.1986 | 2.4653  |
| C | -1.3937 | -3.2127 | 4.0409  |
| C | -6.6460 | -4.3537 | 2.0215  |
| C | -2.1898 | -5.3348 | 3.7395  |
| C | -3.3805 | 0.7217  | 3.8883  |
| C | -6.5448 | 4.3505  | -1.8462 |
| C | -1.4226 | 3.0238  | -3.9615 |
| C | 3.9979  | 5.5102  | 1.5269  |
| C | -6.5089 | -2.1336 | 1.5034  |
| C | 5.5252  | 1.3987  | -1.8954 |
| C | 1.8404  | 5.3346  | 2.2606  |
| C | -5.1950 | 2.0776  | -1.8985 |
| C | -5.4163 | -4.3181 | 2.4956  |
| C | 5.7314  | -0.1093 | 2.2954  |
| C | -1.8428 | -4.8746 | 0.7034  |
| C | -0.6557 | 3.3173  | 3.9358  |
| C | -4.0529 | 5.6071  | 1.3813  |
| C | 4.9396  | -2.9454 | -3.7384 |
| C | 2.7303  | 7.3872  | 1.8148  |
| C | -2.1863 | 5.1692  | -3.7606 |
| C | -5.7695 | 1.5564  | 4.6269  |
| C | 3.9806  | -3.2439 | 0.6493  |
| C | -5.2693 | -2.0939 | 1.9683  |
| C | -4.4574 | 0.2752  | 3.2622  |
| C | 3.8703  | 6.8195  | 1.4753  |
| C | 1.7190  | 6.6428  | 2.2162  |
| C | -5.6570 | 0.6818  | 3.6504  |
| C | -1.3676 | -4.2596 | -3.2687 |
| C | 3.4931  | 2.8219  | -3.2414 |
| C | -0.6905 | -3.3341 | -3.9277 |
| C | 3.6738  | 2.4291  | 3.3540  |
| C | -1.8175 | 4.6900  | -0.6956 |
| C | -5.2868 | 4.3386  | -2.2401 |
| C | -1.2880 | 4.8760  | 0.6465  |
| C | 3.9075  | 3.1876  | -0.5990 |
| C | 5.7402  | 0.1752  | -2.3587 |
| C | -5.0001 | -0.3589 | -0.6774 |
| C | 3.7389  | -2.5653 | -3.3303 |
| C | 3.0168  | 1.4772  | 3.9966  |
| C | -1.3401 | -4.9927 | -0.6593 |
| C | -0.5698 | 5.8160  | 4.7615  |
| C | -2.9298 | -5.2056 | 4.8211  |
| C | -1.4341 | -4.3283 | 3.3308  |
| C | 5.5364  | -1.3329 | 1.8302  |
| C | -1.3256 | 4.2499  | 3.2779  |
| C | -7.1915 | -3.2593 | 1.5284  |
| C | 0.0670  | 3.6336  | 4.9882  |
| C | -3.4975 | 1.5961  | 4.8644  |
| C | -2.9585 | 4.9857  | -4.8101 |
| C | 4.3069  | -3.6836 | 3.7276  |
| C | 3.0725  | -1.6543 | -4.0206 |
| C | -5.0136 | 0.2870  | 0.6251  |
| C | 4.2581  | 2.6648  | 0.7124  |
| C | 3.5598  | -2.6900 | 3.2726  |
| C | 4.8637  | 2.8127  | 3.7907  |
| C | 4.2144  | 3.8634  | -3.6280 |
| C | 1.7353  | -5.4498 | 2.2710  |
| C | -1.4254 | 4.1802  | -3.3183 |
| C | 5.4798  | -2.3882 | -4.8013 |
| C | 6.9381  | 0.4119  | 2.3121  |
| C | -4.6644 | 3.5124  | 2.0546  |
| C | 5.4004  | 2.2216  | 4.8363  |
| C | 4.8210  | -1.4590 | -5.4687 |
| C | -4.6895 | 2.0236  | 5.2256  |
| C | 4.7534  | 1.2501  | 5.4539  |
| C | -2.9092 | -4.0777 | 5.5065  |
| C | 6.9553  | -0.3263 | -2.3664 |
| C | -2.9741 | 3.8185  | -5.4272 |
| C | 2.3558  | -7.5897 | 1.7778  |
| C | 7.7776  | -1.4960 | 1.3865  |
| C | 3.9341  | -4.3472 | 4.8008  |
| C | 2.0940  | -3.0087 | 5.0021  |
| C | -2.1966 | 2.8414  | -5.0091 |
| C | 2.8227  | -4.0175 | 5.4325  |

|   |         |         |         |
|---|---------|---------|---------|
| C | 3.7962  | 4.6207  | -4.6190 |
| C | 7.9667  | 0.3793  | -1.8997 |
| C | 1.9583  | 3.2880  | -4.8733 |
| C | 7.9632  | -0.2769 | 1.8509  |
| C | 0.5068  | -5.6964 | 1.8411  |
| C | 6.5715  | -2.0248 | 1.3789  |
| C | 7.7604  | 1.5962  | -1.4361 |
| C | 3.7124  | -6.9554 | -1.4609 |
| C | -4.4024 | -0.2114 | -3.3275 |
| C | -6.3323 | -4.8613 | -1.7494 |
| C | -3.3176 | -0.6015 | -3.9762 |
| C | -5.6951 | -1.3763 | -4.8075 |
| C | -4.1782 | -5.4792 | -1.3093 |
| C | 1.6153  | -6.6610 | -2.3116 |
| C | -5.4683 | -5.7431 | -1.2892 |
| C | -4.6145 | -3.4445 | -2.2478 |
| C | 1.7960  | -5.3589 | -2.3096 |
| C | 2.9426  | -4.8425 | -1.8931 |
| C | 2.5701  | -7.4616 | -1.8794 |
| C | 3.9022  | -5.6517 | -1.4717 |
| C | -3.4200 | -1.3907 | -5.0232 |
| C | -5.5963 | -0.5872 | -3.7601 |
| C | 1.1369  | -7.8428 | 1.3467  |
| C | -3.7399 | -4.3232 | -1.7839 |
| C | -5.9006 | -3.7145 | -2.2358 |
| C | 6.5466  | 2.1064  | -1.4360 |
| C | 3.6128  | -1.1016 | -5.0852 |
| C | 3.5572  | 0.8864  | 5.0401  |
| C | -4.6070 | -1.7884 | -5.4318 |
| C | 1.7104  | 5.5742  | -2.0937 |
| C | 0.7732  | 7.9437  | -1.4284 |
| C | -0.0415 | 6.9116  | -1.4963 |
| C | 0.2127  | -6.9041 | 1.3828  |
| C | 2.4629  | -2.3473 | 3.9271  |
| C | 0.4226  | 5.7154  | -1.8277 |
| C | 4.3391  | -2.8142 | -0.6961 |
| C | -5.3222 | 5.9440  | 1.2881  |
| C | 2.6501  | -6.3930 | 2.2491  |
| C | -5.9313 | 3.8535  | 1.9690  |
| C | -6.2637 | 5.0671  | 1.5774  |
| C | -7.1332 | 3.2262  | -1.4904 |
| C | -2.1292 | -3.0873 | 5.1245  |
| C | 2.3745  | 2.5272  | -3.8843 |
| C | 0.1199  | 4.8850  | 5.3948  |
| C | -0.0273 | -3.6428 | -5.0205 |
| C | -0.0402 | -4.8819 | -5.4663 |
| C | 2.5213  | 6.6079  | -2.0330 |
| C | 2.6612  | 4.3416  | -5.2330 |
| C | -1.4031 | -5.4971 | -3.7379 |
| C | 2.0564  | 7.7928  | -1.6934 |
| C | -0.7372 | -5.8053 | -4.8305 |
| C | -1.2931 | 5.5014  | 3.7083  |
| H | -0.5346 | 6.7912  | 5.0845  |
| H | 0.6976  | 5.1385  | 6.2061  |
| H | 0.5885  | 2.8920  | 5.4721  |
| H | -0.6766 | 2.3406  | 3.6193  |
| H | -1.8276 | 6.2305  | 3.2169  |
| H | 1.0453  | 4.7504  | 2.5538  |
| H | 0.8260  | 7.0739  | 2.4859  |
| H | 2.6298  | 8.4091  | 1.7590  |
| H | 4.6604  | 7.3973  | 1.1596  |
| H | 4.8901  | 5.0808  | 1.2505  |
| H | 2.6915  | 8.5992  | -1.6303 |
| H | 3.5187  | 6.4783  | -2.2451 |
| H | 0.4072  | 8.8671  | -1.1615 |
| H | -1.0376 | 7.0444  | -1.2784 |
| H | 2.0737  | 4.6454  | -2.3452 |
| H | 7.0687  | 1.3624  | 2.6805  |
| H | 8.9055  | 0.1356  | 1.8485  |
| H | 5.3724  | 3.5666  | 3.3097  |
| H | 6.3297  | 2.5111  | 5.1664  |
| H | 2.0877  | 1.1789  | 3.6760  |
| H | 3.0343  | 0.1383  | 5.5122  |
| H | 5.1851  | 0.7787  | 6.2591  |
| H | 8.5733  | -2.0364 | 1.0231  |
| H | 6.4454  | -2.9750 | 1.0088  |
| H | 4.9286  | 0.4353  | 2.6373  |

|   |         |         |         |
|---|---------|---------|---------|
| H | 6.4007  | 3.0544  | -1.0659 |
| H | 8.5460  | 2.1480  | -1.0679 |
| H | 8.9149  | -0.0189 | -1.8916 |
| H | 7.1027  | -1.2761 | -2.7307 |
| H | 4.9475  | -0.3860 | -2.7006 |
| H | 1.8790  | -1.5725 | 3.5904  |
| H | 1.2311  | -2.7280 | 5.4844  |
| H | 2.5274  | -4.5496 | 6.2608  |
| H | 4.5069  | -5.1299 | 5.1418  |
| H | 5.1760  | -3.9420 | 3.2408  |
| H | -0.8086 | -2.4255 | 3.7378  |
| H | -2.0919 | -2.2039 | 5.6481  |
| H | -3.5032 | -3.9738 | 6.3391  |
| H | -3.5298 | -5.9827 | 5.1261  |
| H | -2.2080 | -6.2175 | 3.2111  |
| H | -2.4465 | 0.3964  | 3.6116  |
| H | -2.6485 | 1.9417  | 5.3287  |
| H | -4.7798 | 2.7197  | 5.9769  |
| H | -6.7004 | 1.8815  | 4.9172  |
| H | -6.5002 | 0.3191  | 3.1851  |
| H | -4.4038 | 2.5606  | 2.3442  |
| H | -3.3319 | 6.3007  | 1.1438  |
| H | -5.5773 | 6.8920  | 0.9812  |
| H | -7.2543 | 5.3300  | 1.4916  |
| H | -6.6553 | 3.1614  | 2.2009  |
| H | -6.9329 | 1.2246  | -1.2290 |
| H | -8.1138 | 3.2328  | -1.1814 |
| H | -7.0661 | 5.2360  | -1.8100 |
| H | -4.8191 | 5.2083  | -2.5241 |
| H | -3.6267 | 3.2011  | -2.5544 |
| H | -0.8300 | 2.2499  | -3.6381 |
| H | -2.1799 | 6.0802  | -3.2825 |
| H | -2.1834 | 1.9283  | -5.4808 |
| H | -3.5929 | 3.6739  | -6.2352 |
| H | -3.5583 | 5.7515  | -5.1428 |
| H | -2.3863 | -0.3076 | -3.6581 |
| H | -2.5623 | -1.6938 | -5.5011 |
| H | -4.6893 | -2.4205 | -6.2383 |
| H | -6.6213 | -1.6796 | -5.1341 |
| H | -6.4458 | -0.2699 | -3.2738 |
| H | -4.2801 | -2.5420 | -2.6100 |
| H | -3.5209 | -6.1776 | -0.9410 |
| H | -5.7986 | -6.6384 | -0.9065 |
| H | -7.3396 | -5.0669 | -1.7249 |
| H | -6.5630 | -3.0192 | -2.6019 |
| H | -8.1488 | -3.2835 | 1.1538  |
| H | -6.9456 | -1.2913 | 1.1076  |
| H | -4.9790 | -5.1635 | 2.8829  |
| H | -7.1784 | -5.2338 | 2.0300  |
| H | -3.7591 | -3.1803 | 2.8144  |
| H | -0.7319 | -7.1192 | 1.0390  |
| H | 0.9042  | -8.7725 | 0.9733  |
| H | 3.0770  | -8.3220 | 1.7409  |
| H | 3.5961  | -6.1826 | 2.5917  |
| H | 1.9726  | -4.5081 | 2.6121  |
| H | 4.7976  | -5.2730 | -1.1370 |
| H | 4.4568  | -7.5764 | -1.1178 |
| H | 2.4229  | -8.4792 | -1.8622 |
| H | 0.7206  | -7.0433 | -2.6431 |
| H | 1.0417  | -4.7319 | -2.6217 |
| H | -0.6595 | -2.3680 | -3.5809 |
| H | 0.4995  | -2.9043 | -5.5035 |
| H | 0.4922  | -5.1317 | -6.3097 |
| H | -0.7549 | -6.7707 | -5.1839 |
| H | -1.9482 | -6.2201 | -3.2490 |
| H | 2.1380  | -1.3550 | -3.7182 |
| H | 3.0815  | -0.3863 | -5.5969 |
| H | 5.2529  | -1.0145 | -6.2888 |
| H | 6.4189  | -2.6736 | -5.1073 |
| H | 5.4558  | -3.6715 | -3.2237 |
| H | 5.0983  | 4.0847  | -3.1502 |
| H | 1.8163  | 1.7102  | -3.6090 |
| H | 1.0786  | 3.0508  | -5.3481 |
| H | 2.3272  | 4.9463  | -5.9942 |
| H | 4.3507  | 5.4361  | -4.9085 |
| H | 3.0291  | -3.6593 | 0.6801  |
| H | 4.6267  | -3.9691 | 1.0067  |



|   |         |         |         |
|---|---------|---------|---------|
| H   | 4.4917  | -1.7888 | -0.7486 |
| H   | 5.2181  | -3.2567 | -1.0171 |
| H   | -1.4598 | -5.9512 | -1.0313 |
| H   | -2.5757 | -4.1439 | 0.7872  |
| H   | -5.9484 | -0.6288 | -0.9927 |
| H   | -4.4428 | 1.1560  | 0.6231  |
| H   | -2.4714 | 3.8853  | -0.7396 |
| H   | -1.3472 | 5.8624  | 0.9542  |
| H   | 2.9369  | 3.5595  | -0.6107 |
| H   | 4.3124  | 1.6273  | 0.7111  |
| H   | 4.5200  | 3.9726  | -0.8839 |
| H   | 5.1815  | 3.0034  | 1.0356  |
| H   | -0.3243 | -4.7836 | -0.7134 |
| H   | -2.2712 | -5.7587 | 1.0291  |
| H   | -4.4358 | -1.2313 | -0.6697 |
| H   | -5.9675 | 0.5716  | 0.9116  |
| H   | -2.3540 | 5.5136  | -1.0191 |
| H   | -0.2848 | 4.6156  | 0.7026  |
| 275   |         |         |         |
| [FeAu12Cl12(dppe)5] Isomer I Excited state T1 |         |         |         |
| Au  | 0.0172  | -0.0549 | -2.4515 |
| Au  | -1.3756 | 1.8222  | 1.1060  |
| Au  | 1.3685  | 1.8611  | 1.0935  |
| Au  | 0.0400  | 2.2881  | -1.0967 |
| Au  | 0.0382  | -2.4430 | 1.0775  |
| Fe  | 0.0248  | -0.1057 | -0.0028 |
| Au  | -1.4213 | -1.9466 | -1.0810 |
| Au  | 2.2601  | 0.6665  | -1.0996 |
| Au  | 2.2700  | -0.7334 | 1.0807  |
| Au  | -2.1848 | 0.7134  | -1.0943 |
| Au  | -2.2368 | -0.7995 | 1.0946  |
| Au  | 1.3791  | -1.9637 | -1.0737 |
| Au  | 0.0120  | -0.0621 | 2.4344  |
| P   | -1.7612 | -3.9496 | -1.8694 |
| P   | 3.1713  | 2.8967  | 1.8561  |
| P   | -0.8722 | 4.1800  | -1.8580 |
| P   | 3.2067  | -2.8489 | -1.8774 |
| P   | 3.7440  | -2.1328 | 1.8587  |
| P   | -0.9455 | -4.1989 | 1.8656  |
| Cl  | 0.0080  | -0.0044 | -4.8010 |
| Cl  | 0.0008  | -0.0151 | 4.7896  |
| P   | -4.2414 | 0.4728  | -1.8528 |
| P   | -4.2665 | -0.4244 | 1.8836  |
| P   | 3.6871  | 2.1723  | -1.8849 |
| P   | -1.7321 | 3.8957  | 1.8787  |
| C   | 3.1172  | 4.5845  | 2.2409  |
| C   | -3.3531 | 4.3676  | 2.2513  |
| C   | -4.8968 | 2.9727  | -1.5657 |
| C   | -6.1820 | 1.8884  | -3.1108 |
| C   | -4.9710 | -2.9135 | 1.5643  |
| C   | -1.7545 | -2.8448 | 3.9299  |
| C   | -6.6710 | -4.0086 | 2.6117  |
| C   | -3.0344 | -4.6952 | 3.5103  |
| C   | -3.2214 | 0.7538  | 3.9473  |
| C   | -6.6018 | 4.0771  | -2.5867 |
| C   | -1.6647 | 2.8139  | -3.9228 |
| C   | 3.9111  | 5.1824  | 3.1120  |
| C   | -6.1963 | -1.8384 | 3.1628  |
| C   | 5.2773  | 1.6075  | -2.2641 |
| C   | 2.2267  | 5.2981  | 1.5744  |
| C   | -5.1913 | 1.8724  | -2.2358 |
| C   | -5.6998 | -3.9966 | 1.7194  |
| C   | 5.7543  | -0.5012 | 1.5747  |
| C   | -1.9890 | -4.9385 | 0.6470  |
| C   | -0.2666 | 3.2644  | 3.9312  |
| C   | -3.6823 | 5.3078  | 3.1215  |
| C   | 5.1883  | -2.0320 | -3.5278 |
| C   | 2.9597  | 7.1966  | 2.5866  |
| C   | -2.9409 | 4.6655  | -3.5143 |
| C   | -5.3175 | 2.2241  | 4.5587  |
| C   | 4.1020  | -3.3580 | 0.6349  |
| C   | -5.2275 | -1.8173 | 2.2602  |
| C   | -4.3343 | 0.6396  | 3.2379  |
| C   | 3.8220  | 6.4846  | 3.2885  |
| C   | 2.1607  | 6.6004  | 1.7249  |
| C   | -5.3853 | 1.3806  | 3.5511  |
| C   | -0.7555 | -4.3445 | -3.2113 |

|   |         |         |         |
|---|---------|---------|---------|
| C | 3.1081  | 3.0706  | -3.2374 |
| C | -0.3075 | -3.3223 | -3.9294 |
| C | 3.8586  | 2.0591  | 3.1947  |
| C | -1.9392 | 4.8797  | -0.6345 |
| C | -5.6098 | 4.0648  | -1.7194 |
| C | -1.2889 | 5.0975  | 0.6584  |
| C | 4.0377  | 3.4029  | -0.6645 |
| C | 5.7063  | 0.5601  | -1.5796 |
| C | -5.2516 | -0.3128 | -0.6344 |
| C | 3.8970  | -2.0352 | -3.2321 |
| C | 3.0394  | 1.2986  | 3.9048  |
| C | -1.3404 | -5.1522 | -0.6436 |
| C | 0.4736  | 5.7147  | 4.5435  |
| C | -3.8319 | -4.3583 | 4.5024  |
| C | -1.9904 | -3.9353 | 3.2107  |
| C | 5.3309  | -1.5557 | 2.2521  |
| C | -0.7284 | 4.2848  | 3.2240  |
| C | -6.9062 | -2.9340 | 3.3412  |
| C | 0.5628  | 3.4668  | 4.9301  |
| C | -3.1550 | 1.6001  | 4.9482  |
| C | -3.7224 | 4.3408  | -4.5232 |
| C | 3.5805  | -4.2801 | 3.4867  |
| C | 3.0632  | -1.2985 | -3.9542 |
| C | -5.2653 | 0.3671  | 0.6584  |
| C | 4.4376  | 2.8484  | 0.6281  |
| C | 3.1722  | -3.0533 | 3.2004  |
| C | 5.1468  | 2.0811  | 3.4930  |
| C | 3.5096  | 4.2917  | -3.5513 |
| C | 1.2067  | -5.6527 | 1.5658  |
| C | -1.9082 | 3.8999  | -3.2059 |
| C | 5.6336  | -1.2908 | -4.5209 |
| C | 6.9717  | -0.0340 | 1.7435  |
| C | -4.3029 | 3.7447  | 1.5747  |
| C | 5.6061  | 1.3424  | 4.4823  |
| C | 4.7972  | -0.5513 | -5.2233 |
| C | -4.2028 | 2.3379  | 5.2526  |
| C | 4.7850  | 0.5760  | 5.1737  |
| C | -3.5933 | -3.2651 | 5.2038  |
| C | 6.9318  | 0.1107  | -1.7369 |
| C | -3.4796 | 3.2511  | -5.2248 |
| C | 1.7203  | -7.5820 | 2.6628  |
| C | 7.3399  | -1.6179 | 3.3447  |
| C | 3.0144  | -4.9503 | 4.4715  |
| C | 1.6374  | -3.1756 | 4.9014  |
| C | -2.4464 | 2.4901  | -4.9270 |
| C | 2.0372  | -4.4021 | 5.1732  |
| C | 2.9532  | 4.9281  | -4.5603 |
| C | 7.7289  | 0.6826  | -2.6163 |
| C | 1.5903  | 3.1385  | -4.9510 |
| C | 7.7670  | -0.5912 | 2.6339  |
| C | 0.0948  | -5.5256 | 2.2687  |
| C | 6.1318  | -2.1072 | 3.1506  |
| C | 7.2949  | 1.7017  | -3.3319 |
| C | 3.8436  | -6.4271 | -3.3535 |
| C | -4.3092 | -0.6021 | -3.2009 |
| C | -5.9249 | -5.0586 | -2.6326 |
| C | -3.2062 | -0.7186 | -3.9240 |
| C | -5.3007 | -2.2092 | -4.4894 |
| C | -3.7117 | -5.3332 | -3.1514 |
| C | 2.2837  | -6.5886 | -1.6988 |
| C | -4.9774 | -5.6472 | -3.3398 |
| C | -4.3461 | -3.7954 | -1.5871 |
| C | 2.3244  | -5.2836 | -1.5434 |
| C | 3.1537  | -4.5406 | -2.2562 |
| C | 3.0438  | -7.1642 | -2.6082 |
| C | 3.9073  | -5.1231 | -3.1742 |
| C | -3.1471 | -1.5786 | -4.9143 |
| C | -5.3615 | -1.3484 | -3.4932 |
| C | 0.6338  | -7.4443 | 3.3970  |
| C | -3.3867 | -4.4092 | -2.2607 |
| C | -5.6067 | -4.1308 | -1.7519 |
| C | 6.0780  | 2.1714  | -3.1543 |
| C | 3.5099  | -0.5612 | -4.9435 |
| C | 3.4992  | 0.5595  | 4.8873  |
| C | -4.1925 | -2.3302 | -5.1938 |
| C | 1.2931  | 5.5803  | -1.5597 |
| C | 0.7041  | 7.4725  | -3.2820 |

|   |         |         |         |
|---|---------|---------|---------|
| C | -0.1319 | 6.4695  | -3.1067 |
| C | -0.1807 | -6.4279 | 3.1957  |
| C | 2.2018  | -2.5069 | 3.9217  |
| C | 0.1572  | 5.5214  | -2.2329 |
| C | 4.4922  | -2.8129 | -0.6617 |
| C | -4.9496 | 5.6251  | 3.2910  |
| C | 2.0045  | -6.6827 | 1.7423  |
| C | -5.5630 | 4.0837  | 1.7184  |
| C | -5.8889 | 5.0261  | 2.5815  |
| C | -6.8772 | 2.9931  | -3.2897 |
| C | -2.5487 | -2.5119 | 4.9210  |
| C | 2.1467  | 2.4991  | -3.9480 |
| C | 0.9384  | 4.6929  | 5.2341  |
| C | 0.5410  | -3.5155 | -4.9121 |
| C | 0.9541  | -4.7361 | -5.1875 |
| C | 2.1112  | 6.5958  | -1.7100 |
| C | 1.9912  | 4.3552  | -5.2562 |
| C | -0.3492 | -5.5704 | -3.5017 |
| C | 1.8175  | 7.5449  | -2.5761 |
| C | 0.5035  | -5.7631 | -4.4878 |
| C | -0.3534 | 5.5140  | 3.5375  |
| H | 0.7737  | 6.6701  | 4.7713  |
| H | 1.6021  | 4.8528  | 6.0051  |
| H | 0.9184  | 2.6538  | 5.4496  |
| H | -0.5414 | 2.3038  | 3.6937  |
| H | -0.6863 | 6.3199  | 2.9876  |
| H | 1.5711  | 4.8031  | 0.9540  |
| H | 1.4768  | 7.1415  | 1.1815  |
| H | 2.9028  | 8.2155  | 2.7229  |
| H | 4.4314  | 6.9487  | 3.9757  |
| H | 4.5863  | 4.6306  | 3.6582  |
| H | 2.4623  | 8.3358  | -2.7123 |
| H | 2.9826  | 6.6343  | -1.1637 |
| H | 0.4849  | 8.2040  | -3.9724 |
| H | -1.0001 | 6.4159  | -3.6576 |
| H | 1.5309  | 4.7982  | -0.9340 |
| H | 7.2870  | 0.7735  | 1.1928  |
| H | 8.7146  | -0.2203 | 2.7841  |
| H | 5.8043  | 2.6534  | 2.9483  |
| H | 6.6107  | 1.3487  | 4.6984  |
| H | 2.0359  | 1.2633  | 3.6819  |
| H | 2.8446  | -0.0370 | 5.4092  |
| H | 5.1526  | -0.0160 | 5.9294  |
| H | 7.9523  | -2.0429 | 4.0530  |
| H | 5.8016  | -2.9066 | 3.7083  |
| H | 5.0964  | -0.0398 | 0.9364  |
| H | 5.7426  | 2.9655  | -3.7134 |
| H | 7.9100  | 2.1349  | -4.0318 |
| H | 8.6829  | 0.3239  | -2.7526 |
| H | 7.2498  | -0.6944 | -1.1824 |
| H | 5.0509  | 0.0909  | -0.9420 |
| H | 1.8663  | -1.5620 | 3.7047  |
| H | 0.8744  | -2.7323 | 5.4306  |
| H | 1.5806  | -4.9387 | 5.9252  |
| H | 3.3210  | -5.9113 | 4.6764  |
| H | 4.3278  | -4.7282 | 2.9341  |
| H | -0.9584 | -2.2395 | 3.7014  |
| H | -2.3484 | -1.6529 | 5.4480  |
| H | -4.2314 | -2.9970 | 5.9642  |
| H | -4.6535 | -4.9411 | 4.7136  |
| H | -3.2434 | -5.5417 | 2.9561  |
| H | -2.3947 | 0.1937  | 3.7053  |
| H | -2.2724 | 1.6809  | 5.4683  |
| H | -4.1491 | 3.0129  | 6.0259  |
| H | -6.1328 | 2.8064  | 4.7910  |
| H | -6.2520 | 1.3159  | 3.0032  |
| H | -4.0329 | 2.9709  | 0.9525  |
| H | -2.9511 | 5.7829  | 3.6695  |
| H | -5.2054 | 6.3483  | 3.9774  |
| H | -6.8762 | 5.2859  | 2.7126  |
| H | -6.2871 | 3.5998  | 1.1704  |
| H | -6.4002 | 1.0446  | -3.6576 |
| H | -7.6409 | 3.0066  | -3.9790 |
| H | -7.1545 | 4.9341  | -2.7258 |
| H | -5.3792 | 4.9059  | -1.1744 |
| H | -4.0806 | 2.9565  | -0.9405 |
| H | -0.8697 | 2.2050  | -3.6889 |

|   |         |         |         |
|---|---------|---------|---------|
| H | -3.1560 | 5.5062  | -2.9617 |
| H | -2.2436 | 1.6318  | -5.4553 |
| H | -4.1038 | 2.9915  | -5.9999 |
| H | -4.5347 | 4.9296  | -4.7498 |
| H | -2.3784 | -0.1509 | -3.7019 |
| H | -2.2720 | -1.6629 | -5.4471 |
| H | -4.1435 | -3.0197 | -5.9551 |
| H | -6.1134 | -2.8017 | -4.7002 |
| H | -6.2245 | -1.2812 | -2.9386 |
| H | -4.0834 | -3.0275 | -0.9561 |
| H | -2.9773 | -5.7930 | -3.7062 |
| H | -5.2253 | -6.3577 | -4.0410 |
| H | -6.9102 | -5.3144 | -2.7788 |
| H | -6.3352 | -3.6538 | -1.2057 |
| H | -7.6494 | -2.9483 | 4.0517  |
| H | -6.3831 | -1.0037 | 3.7321  |
| H | -5.4935 | -4.8320 | 1.1548  |
| H | -7.2344 | -4.8587 | 2.7498  |
| H | -4.1708 | -2.9040 | 0.9178  |
| H | -1.0328 | -6.3296 | 3.7698  |
| H | 0.4161  | -8.1358 | 4.1281  |
| H | 2.3504  | -8.3828 | 2.8181  |
| H | 2.8580  | -6.7666 | 1.1755  |
| H | 1.4447  | -4.9049 | 0.9021  |
| H | 4.5357  | -4.5520 | -3.7561 |
| H | 4.4247  | -6.8712 | -4.0760 |
| H | 3.0025  | -8.1837 | -2.7466 |
| H | 1.6414  | -7.1481 | -1.1236 |
| H | 1.6953  | -4.8059 | -0.8880 |
| H | -0.6052 | -2.3659 | -3.7062 |
| H | 0.8843  | -2.7024 | -5.4397 |
| H | 1.6379  | -4.8902 | -5.9402 |
| H | 0.8337  | -6.7148 | -4.6953 |
| H | -0.6776 | -6.3775 | -2.9502 |
| H | 2.0634  | -1.2800 | -3.7237 |
| H | 2.8419  | 0.0139  | -5.4723 |
| H | 5.1546  | 0.0401  | -5.9839 |
| H | 6.6394  | -1.2777 | -4.7308 |
| H | 5.8536  | -2.5885 | -2.9721 |
| H | 4.2443  | 4.7581  | -3.0026 |
| H | 1.8191  | 1.5543  | -3.7081 |
| H | 0.8340  | 2.6761  | -5.4722 |
| H | 1.5437  | 4.8640  | -6.0287 |
| H | 3.2595  | 5.8819  | -4.7893 |
| H | 3.2342  | -3.9267 | 0.5643  |
| H | 4.8511  | -3.9818 | 0.9997  |
| H | 4.7769  | -1.8177 | -0.5875 |
| H | 5.3084  | -3.3372 | -1.0366 |
| H | -1.5792 | -6.0966 | -1.0080 |
| H | -2.8093 | -4.3082 | 0.5638  |
| H | -6.2136 | -0.3767 | -1.0123 |
| H | -4.9067 | 1.3363  | 0.5848  |
| H | -2.7500 | 4.2359  | -0.5590 |
| H | -1.5357 | 6.0336  | 1.0326  |
| H | 3.1792  | 3.9786  | -0.5858 |
| H | 4.7061  | 1.8510  | 0.5482  |
| H | 4.7870  | 4.0150  | -1.0352 |
| H | 5.2588  | 3.3623  | 0.9953  |
| H | -0.3042 | -5.1054 | -0.5640 |
| H | -2.3388 | -5.8450 | 1.0230  |
| H | -4.8837 | -1.2781 | -0.5552 |
| H | -6.2339 | 0.4224  | 1.0205  |
| H | -2.3017 | 5.7748  | -1.0114 |
| H | -0.2530 | 5.0613  | 0.5813  |

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[HgAu12Cl2(dppe)5]4+ Isomer I

|    |              |              |              |
|----|--------------|--------------|--------------|
| Au | 0.00000000   | 0.00000000   | -2.737579000 |
| Au | -1.560797000 | 2.117097000  | 1.252369000  |
| Au | 1.531167000  | 2.138625000  | 1.252369000  |
| Au | 0.018312000  | 2.630181000  | -1.252369000 |
| Au | 0.018312000  | -2.630181000 | 1.252369000  |
| Hg | 0.000000000  | 0.000000000  | 0.000000000  |
| Au | -1.560797000 | -2.117097000 | -1.252369000 |
| Au | 2.507110000  | 0.795355000  | -1.252369000 |
| Au | 2.507110000  | -0.795355000 | 1.252369000  |
| Au | -2.495792000 | 0.830187000  | -1.252369000 |
| Au | -2.495792000 | -0.830187000 | 1.252369000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| Au | 1.531167000  | -2.138625000 | -1.252369000 |
| Au | 0.000000000  | 0.000000000  | 2.737579000  |
| P  | -2.196864000 | -4.260341000 | -1.930506000 |
| P  | 3.372957000  | 3.405859000  | 1.930506000  |
| P  | -0.726866000 | 4.737972000  | -1.930506000 |
| P  | 3.372957000  | -3.405859000 | -1.930506000 |
| P  | 4.281466000  | -2.155404000 | 1.930506000  |
| P  | -0.726866000 | -4.737972000 | 1.930506000  |
| Cl | 0.000000000  | 0.000000000  | -5.074705000 |
| Cl | 0.000000000  | 0.000000000  | 5.074705000  |
| P  | -4.730693000 | 0.772824000  | -1.930506000 |
| P  | -4.730693000 | -0.772824000 | 1.930506000  |
| P  | 4.281466000  | 2.155404000  | -1.930506000 |
| P  | -2.196864000 | 4.260341000  | 1.930506000  |
| C  | 3.191796000  | 5.219651000  | 1.964257000  |
| C  | -3.977864000 | 4.648539000  | 1.964257000  |
| C  | -4.997012000 | 3.494701000  | -2.443240000 |
| C  | -6.993167000 | 2.431348000  | -1.556199000 |
| C  | -4.997012000 | -3.494701000 | 2.443240000  |
| C  | -1.667508000 | -3.413397000 | 4.211984000  |
| C  | -7.014221000 | -4.790846000 | 2.102352000  |
| C  | -2.234470000 | -5.773855000 | 4.067871000  |
| C  | -3.761621000 | 0.531097000  | 4.211984000  |
| C  | -7.014221000 | 4.790846000  | -2.102352000 |
| C  | -1.667508000 | 3.413397000  | -4.211984000 |
| C  | 4.228481000  | 6.077483000  | 1.556199000  |
| C  | -6.993167000 | -2.431348000 | 1.556199000  |
| C  | 5.950503000  | 1.422617000  | -1.964257000 |
| C  | 1.988534000  | 5.764442000  | 2.443240000  |
| C  | -5.650251000 | 2.346696000  | -1.964257000 |
| C  | -5.680049000 | -4.709968000 | 2.511922000  |
| C  | 6.096801000  | -0.109898000 | 2.443240000  |
| C  | -2.019393000 | -5.279735000 | 0.716978000  |
| C  | -0.657302000 | 3.741633000  | 4.211984000  |
| C  | -4.473357000 | 5.899570000  | 1.556199000  |
| C  | 5.201510000  | -3.357758000 | -4.067871000 |
| C  | 2.858635000  | 7.998732000  | 2.102352000  |
| C  | -2.234470000 | 5.773855000  | -4.067871000 |
| C  | -6.299195000 | 1.054293000  | 5.261503000  |
| C  | 4.397300000  | -3.552085000 | 0.716978000  |
| C  | -5.650251000 | -2.346696000 | 1.964257000  |
| C  | -4.907169000 | 0.088915000  | 3.530123000  |
| C  | 4.058641000  | 7.461499000  | 1.627635000  |
| C  | 1.826806000  | 7.149093000  | 2.511922000  |
| C  | -6.181751000 | 0.340888000  | 4.067871000  |
| C  | -1.431836000 | -4.694472000 | -3.530123000 |
| C  | 3.917721000  | 2.956295000  | -3.530123000 |
| C  | -0.657302000 | -3.741633000 | -4.211984000 |
| C  | 4.022246000  | 2.812428000  | 3.530123000  |
| C  | -2.019393000 | 5.279735000  | -0.716978000 |
| C  | -5.680049000 | 4.709968000  | -2.511922000 |
| C  | -1.469627000 | 5.458365000  | 0.716978000  |
| C  | 4.397300000  | 3.552085000  | -0.716978000 |
| C  | 6.096801000  | 0.109898000  | -2.443240000 |
| C  | -5.645353000 | -0.289029000 | -0.716978000 |
| C  | 4.022246000  | -2.812428000 | -3.530123000 |
| C  | 3.355387000  | 1.781359000  | 4.211984000  |
| C  | -1.469627000 | -5.458365000 | -0.716978000 |
| C  | -0.943866000 | 6.316685000  | 5.261503000  |
| C  | -2.949251000 | -5.665096000 | 5.261503000  |
| C  | -1.600962000 | -4.639519000 | 3.530123000  |
| C  | 5.950503000  | -1.422617000 | 1.964257000  |
| C  | -1.431836000 | 4.694472000  | 3.530123000  |
| C  | -7.669269000 | -3.650871000 | 1.627635000  |
| C  | -0.018091000 | 4.080231000  | 5.405368000  |
| C  | -3.886120000 | 1.243655000  | 5.405368000  |
| C  | -2.949251000 | 5.665096000  | -5.261503000 |
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| C | 3.874939000  | 1.278066000  | 5.405368000  |
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| H | 2.732972000  | 9.081510000  | 2.159924000  |
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| H | 5.174340000  | 5.681643000  | 1.184554000  |

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| 275                             |              |              |              |
| [HgAu12Cl12(dppe)5]4+ Isomer II |              |              |              |
| Au                              | -0.044426000 | 0.046906000  | -2.722672000 |
| Au                              | -1.487608000 | 2.086209000  | 1.224662000  |
| Au                              | 1.538934000  | 2.102506000  | 1.239446000  |
| Au                              | -0.025333000 | 2.575577000  | -1.286586000 |
| Au                              | -0.126039000 | -2.575759000 | 1.297755000  |
| Au                              | 0.000526000  | -0.012527000 | 0.011384000  |
| Au                              | -1.616371000 | -2.074100000 | -1.217676000 |
| Au                              | 2.444386000  | 0.904878000  | -1.221628000 |
| Au                              | 2.460284000  | -0.768190000 | 1.254424000  |
| Au                              | -2.495408000 | 0.773073000  | -1.252466000 |
| Au                              | -2.513386000 | -0.749847000 | 1.249680000  |
| Hg                              | 1.472905000  | -2.175278000 | -1.222540000 |
| Au                              | -0.011500000 | -0.009448000 | 2.743168000  |
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| P                               | 3.357414000  | 3.408324000  | 1.913607000  |
| P                               | -0.720305000 | 4.705192000  | -1.948075000 |
| P                               | 3.451308000  | -3.531980000 | -1.983781000 |
| P                               | 4.249808000  | -2.123811000 | 1.912215000  |
| P                               | -0.806644000 | -4.709412000 | 1.967580000  |
| Cl                              | 0.049952000  | -0.080079000 | -5.067079000 |
| Cl                              | 0.000174000  | -0.028759000 | 5.087210000  |
| P                               | -4.743117000 | 0.806995000  | -1.917639000 |
| P                               | -4.750077000 | -0.723148000 | 1.931167000  |
| P                               | 4.272798000  | 2.184727000  | -1.939087000 |
| P                               | -2.175419000 | 4.204683000  | 1.899105000  |
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| C                               | -2.297532000 | -5.791341000 | 4.099167000  |
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| H                                | -0.377189000 | 5.302549000  | 0.745095000  |
| 275                              |              |              |              |
| [HgAu12Cl12(dppe)5]4+ Isomer III |              |              |              |
| Hg                               | 0.000624000  | 0.008873000  | -2.745068000 |
| Au                               | -1.516258000 | 2.139911000  | 1.224165000  |
| Au                               | 1.554818000  | 2.111353000  | 1.224536000  |
| Au                               | -0.011414000 | 2.648891000  | -1.193711000 |
| Au                               | -0.026959000 | -2.609828000 | 1.225157000  |
| Au                               | -0.001270000 | 0.008367000  | 0.020755000  |
| Au                               | -1.540175000 | -2.136192000 | -1.193642000 |
| Au                               | 2.501722000  | 0.837053000  | -1.193500000 |
| Au                               | 2.475565000  | -0.820071000 | 1.226476000  |
| Au                               | -2.509021000 | 0.806680000  | -1.193971000 |
| Au                               | -2.495509000 | -0.777581000 | 1.225353000  |
| Au                               | 1.557139000  | -2.118164000 | -1.192313000 |
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| P                                | -2.205612000 | -4.261589000 | -1.923781000 |
| P                                | 3.375531000  | 3.403887000  | 1.915901000  |
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