

# Electronic Supplementary Information: Revisiting the Ultrasmall Phosphine-Stabilized Rhodium-Doped Gold Clusters Au<sub>n</sub>Rh (n = 5,6,7,8): Geometric, Electronic, and Vibrational Properties

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## 1 Root Mean Square Deviations

|              | (A) Au <sub>5</sub> Rh | (B) Au <sub>7</sub> Rh | (C) Au <sub>8</sub> Rh |
|--------------|------------------------|------------------------|------------------------|
| AuRh         | 0.119                  | 0.095                  | 0.101                  |
| AuRh - P     | 0.202                  | 0.190                  | 0.229                  |
| full cluster | 0.488                  | 0.356                  | 0.529                  |

**Fig. S1** Root mean square deviations (RMSDs) over atomic positions of the gold-rhodium clusters for the AuRh core, AuRh-P/Cl atoms, and the full cluster. The overlap of experimental crystal structures<sup>1</sup> and DFT-optimized structures for gold-rhodium nanoclusters (A) Au<sub>5</sub>Rh (KOFVAC), (B) Au<sub>7</sub>Rh (KOFVAC), and (C) Au<sub>8</sub>Rh (JAPWOM).

## 2 Orbital Composition Analysis

**Table S1** The orbital contributions for key frontier orbitals of the Au<sub>5</sub>Rh and Au<sub>6</sub>Rh clusters in gas phase from the M06/LANL2DZ electron density, as predicted by Ros-Schuit, Hirshfeld, and Becke orbital partition methods.

| Partition Methods       | H-1         | HOMO        | LUMO        | L+1         |
|-------------------------|-------------|-------------|-------------|-------------|
| <b>Au<sub>5</sub>Rh</b> |             |             |             |             |
| Ros-Schuit (SCPA)       | Au 22.7%    | Au 27.2 %   | Au 31.7%    | Au 30.7%    |
|                         | Rh 28.2%    | Rh 26.6%    | Rh 13.4%    | Rh 9.3%     |
|                         | P 10.1%     | P 8.7%      | P 12.8%     | P 15.0%     |
|                         | C/H/N 39.0% | C/H/N 37.5% | C/H/N 42.4% | C/H/N 45.0% |
| Hirshfeld               | Au 28.2%    | Au 31.4%    | Au 39.7%    | Au 38.1%    |
|                         | Rh 29.0%    | Rh 30.2%    | Rh 12.6%    | Rh 10.7%    |
|                         | P 9.3%      | P 8.2%      | P 9.8%      | P 10.5%     |
|                         | C/H/N 33.5% | C/H/N 30.2% | C/H/N 37.9% | C/H/N 40.7% |
| Becke                   | Au 29.7%    | Au 33.2%    | Au 48.7%    | Au 47.1%    |
|                         | Rh 32.3%    | Rh 33.4%    | Rh 13.0%    | Rh 10.9%    |
|                         | P 9.4%      | P 8.1%      | P 9.5%      | P 10.5%     |
|                         | C/H/N 28.6% | C/H/N 25.3% | C/H/N 28.8% | C/H/N 31.5% |
| <b>Au<sub>6</sub>Rh</b> |             |             |             |             |
| Ros-Schuit (SCPA)       | Au 29.7%    | Au 34.9 %   | Au 24.4%    | Au 25.6%    |
|                         | Rh 28.9%    | Rh 16.6%    | Rh 5.9%     | Rh 5.5%     |
|                         | P 9.8%      | P 22.6%     | P 15.6%     | P 17.0%     |
|                         | C/H/O 31.6% | C/H/O 25.9% | C/H/O 54.1% | C/H/O 51.9% |
| Hirshfeld               | Au 37.1%    | Au 47.5%    | Au 36.9%    | Au 37.9%    |
|                         | Rh 29.8%    | Rh 11.4%    | Rh 8.0%     | Rh 7.4%     |
|                         | P 9.2%      | P 16.1%     | P 10.2%     | P 12.4%     |
|                         | C/H/O 24.0% | C/H/O 24.6% | C/H/O %     | C/H/O 42.3% |
| Becke                   | Au 38.8%    | Au 49.4%    | Au 46.6%    | Au 47.1%    |
|                         | Rh 33.0%    | Rh 14.4%    | Rh 8.2%     | Rh 7.3%     |
|                         | P 9.1%      | P 16.5%     | P 9.9%      | P 12.1%     |
|                         | C/H/O 19.1% | C/H/O 19.7% | C/H/O 35.3% | C/H/O 33.5% |

**Table S2** The orbital contributions for key frontier orbitals of the Au<sub>7</sub>Rh and Au<sub>8</sub>Rh clusters in gas phase from the M06/LANL2DZ electron density, as predicted by Ros-Schuit, Hirshfeld, and Becke orbital partition methods.

| Partition Methods       | H-1         | HOMO        | LUMO        | L+1         |
|-------------------------|-------------|-------------|-------------|-------------|
| <b>Au<sub>7</sub>Rh</b> |             |             |             |             |
| Ros-Schuit (SCPA)       | Au 31.5%    | Au 32.5 %   | Au 39.3%    | Au 42.1%    |
|                         | Rh 29.0%    | Rh 18.2%    | Rh 21.6%    | Rh 9.9%     |
|                         | P 11.4%     | P 22.6%     | P 10.5%     | P 14.0%     |
|                         | C/H/O 28.1% | C/H/O 26.7% | C/H/O 28.6% | C/H/O 34.0% |
| Hirshfeld               | Au 36.8%    | Au 45.6%    | Au 45.0%    | Au 49.4%    |
|                         | Rh 25.4%    | Rh 9.5%     | Rh 10.7%    | Rh 9.8%     |
|                         | P 12.0%     | P 18.1%     | P 10.4%     | P 12.3%     |
|                         | C/H/O 25.8% | C/H/O 26.8% | C/H/O 33.9% | C/H/O 28.5% |
| Becke                   | Au 38.5%    | Au 47.4%    | Au 54.6%    | Au 59.0%    |
|                         | Rh 28.0%    | Rh 12.2%    | Rh 11.1%    | Rh 9.8%     |
|                         | P 12.0%     | P 18.5%     | P 9.6%      | P 11.5%     |
|                         | C/H/N 21.5% | C/H/N 21.9% | C/H/N 24.7% | C/H/N 19.7% |
| <b>Au<sub>8</sub>Rh</b> |             |             |             |             |
| Ros-Schuit (SCPA)       | Au 39.1%    | Au 40.3 %   | Au 38.2%    | Au 33.3%    |
|                         | Rh 31.6%    | Rh 11.4%    | Rh 14.3%    | Rh 25.0%    |
|                         | P/Cl 10.1%  | P/Cl 21.6%  | P/Cl 15.7%  | P/Cl 9.9%   |
|                         | C/H/N 19.2% | C/H/N 26.7% | C/H/N 31.8% | C/H/N 31.8% |
| Hirshfeld               | Au 46.8%    | Au 47.1%    | Au 47.6%    | Au 36.7%    |
|                         | Rh 20.2%    | Rh 8.4%     | Rh 12.6%    | Rh 12.0%    |
|                         | P/Cl 15.7%  | P/Cl 18.0%  | P/Cl 12.7%  | P/Cl 10.1%  |
|                         | C/H/N 17.3% | C/H/N 26.5% | C/H/N 27.1% | C/H/N 41.2% |
| Becke                   | Au 48.5%    | Au 48.5%    | Au 55.3%    | Au 45.9%    |
|                         | Rh 22.4%    | Rh 10.6%    | Rh 12.8%    | Rh 12.4%    |
|                         | P/Cl 15.5%  | P/Cl 18.5%  | P/Cl 12.3%  | P/Cl 9.9%   |
|                         | C/H/N 13.6% | C/H/N 22.4% | C/H/N 19.6% | C/H/N 31.8% |

### 3 Vibration peak assignments for the AuRh clusters

**Table S3** The contributing transitions for the Au<sub>5</sub>Rh cluster and their assignment to the DFT-simulated far-IR spectral peaks.

| # | DFT Peak (cm <sup>-1</sup> ) | Contributing vibrations (cm <sup>-1</sup> ) | IR intensity (km mol <sup>-1</sup> ) | % Au motion | % Rh motion | % P motion | Mode description                           |
|---|------------------------------|---|--------------------------------------|-------------|-------------|------------|--|
| 1 | 160                          | 155.27                                      | 6.74                                 | 1.27        | 0.27        | 1.25       | Au core distortion                         |
|   |                              | 164.26                                      | 2.80                                 | 1.04        | 0.26        | 1.18       | AuRh breathing mode                        |
| 2 | 200                          | 191.69                                      | 9.00                                 | 1.11        | 0.81        | 0.36       | Rh-C stretching                            |
|   |                              | 210.89                                      | 13.57                                | 0.52        | 0.85        | 0.42       |  |
|   |                              | 215.17                                      | 9.48                                 | 0.39        | 0.91        | 0.42       | xylyl asymmetric stretching                |
| 3 | 225                          | 224.57                                      | 9.19                                 | 0.24        | 0.86        | 0.10       |  |
|   |                              | 254.80                                      | 3.86                                 | 0.00        | 0.14        | 0.43       |  |
|   |                              | 265.60                                      | 3.38                                 | 0.00        | 0.17        | 0.41       | PPh <sub>3</sub> stretch                   |
| 4 | 260                          | 295.15                                      | 6.87                                 | 0.00        | 0.26        | 0.00       | Rh-C wagging                               |
|   |                              | 332.11                                      | 17.32                                | 0.00        | 0.36        | 0.00       | Rh-C twisting                              |
| 5 | 300                          | 400.28                                      | 2.28                                 | 0.00        | 0.00        | 0.35       |  |
|   |                              | 403.10                                      | 2.79                                 | 0.00        | 0.00        | 0.19       | xylyl distortion                           |
| 6 | 330                          | 436.22                                      | 11.01                                | 0.00        | 0.20        | 2.63       | Rh-C twisting, PPh <sub>3</sub> distortion |
|   |                              |   |                                      |             |             |            |  |

**Table S4** The contributing transitions for the Au<sub>6</sub>Rh cluster and their assignment to the DFT-simulated far-IR spectral peaks.

| # | DFT Peak (cm <sup>-1</sup> ) | Contributing vibrations (cm <sup>-1</sup> ) | IR intensity (km mol <sup>-1</sup> ) | % Au motion | % Rh motion | % P motion | Mode description            |
|---|------------------------------|---|--------------------------------------|-------------|-------------|------------|-----------------------------|
| 1 | 100                          | 83.61                                       | 0.56                                 | 2.16        | 0.12        | 1.99       | Au core distortion          |
|   |                              | 84.93                                       | 0.33                                 | 1.92        | 0.25        | 1.80       |                             |
| 2 | 175                          | 156.03                                      | 5.75                                 | 2.59        | 0.7         | 2.04       | Au-Rh-Au symmetric stretch  |
|   |                              | 160.54                                      | 16.48                                | 2.72        | 0.83        | 1.88       |                             |
| 3 | 195                          | 182.50                                      | 6.99                                 | 3.25        | 1.58        | 0.94       | AuRh breathing mode         |
|   |                              | 208.02                                      | 15.73                                | 1.16        | 1.00        | 0.66       |                             |
| 4 | 220                          | 211.60                                      | 27.39                                | 2.97        | 2.90        | 0.45       | Au-Rh-Au asymmetric stretch |
|   |                              | 252.55                                      | 2.97                                 | 0.00        | 0.00        | 0.78       |                             |
| 5 | 260                          | 252.91                                      | 5.09                                 | 0.00        | 0.00        | 0.51       | PPh <sub>3</sub> distortion |
|   |                              | 256.57                                      | 4.17                                 | 0.00        | 0.00        | 0.58       |                             |
| 6 | 340                          | 342.52                                      | 12.11                                | 0.00        | 1.69        | 0.00       | Rh-C-O rocking              |
|   |                              | 425   | 52.51                                | 0.00        | 0.32        | 3.93       |                             |
| 7 | 425                          | 427.09                                      | 52.51                                | 0.00        | 0.32        | 3.93       | PPh <sub>3</sub> distortion |

**Table S5** The contributing transitions for the Au<sub>7</sub>Rh cluster and their assignment to the DFT-simulated far-IR spectral peaks.

| # | DFT Peak (cm <sup>-1</sup> ) | Contributing vibrations (cm <sup>-1</sup> ) | IR intensity (km mol <sup>-1</sup> ) | % Au motion | % Rh motion | % P motion | Mode description                            |
|---|------------------------------|---|--------------------------------------|-------------|-------------|------------|---|
| 1 | 100                          | 84.36                                       | 0.43                                 | 1.39        | 0.13        | 1.98       | Au core distortion                          |
| 2 | 175                          | 163.09                                      | 30.10                                | 3.46        | 0.99        | 1.90       | AuRh breathing mode                         |
| 3 | 185                          | 175.40                                      | 6.07                                 | 3.65        | 1.17        | 1.48       | Au-Rh-Au symmetric stretch                  |
|   |                              | 191.28                                      | 10.20                                | 0.90        | 0.82        | 0.82       |   |
| 4 | 209                          | 198.65                                      | 18.77                                | 1.39        | 1.26        | 0.80       | Au-Au stretch, PPh <sub>3</sub> distortion  |
|   |                              | 210.64                                      | 3.67                                 | 0.00        | 0.10        | 0.59       |   |
| 5 | 220                          | 210.64                                      | 3.67                                 | 0.00        | 0.10        | 0.59       | PPh <sub>3</sub> distortion                 |
| 6 | 260                          | 251.36                                      | 4.09                                 | 0.00        | 0.00        | 0.56       | PPh <sub>3</sub> distortion                 |
| 7 | 335                          | 332.96                                      | 11.34                                | 0.84        | 0.42        | 0.00       | Rh-C-O rocking                              |
| 8 | 430                          | 434.22                                      | 47.55                                | 0.10        | 0.73        | 4.51       | Rh-C-O wagging, PPh <sub>3</sub> distortion |

**Table S6** The contributing transitions for the Au<sub>6</sub>Rh cluster and their assignment to the DFT-simulated far-IR spectral peaks.

| # | DFT Peak (cm <sup>-1</sup> ) | Contributing vibrations (cm <sup>-1</sup> ) | IR intensity (km mol <sup>-1</sup> ) | % Au motion | % Rh motion | % P motion | % Cl motion | Mode description                 |
|---|------------------------------|---|--------------------------------------|-------------|-------------|------------|-------------|----------------------------------|
| 1 | 100                          | 76.46                                       | 1.00                                 | 2.69        | 0.08        | 1.99       | 1.31        | Au core distortion, Cl wagging   |
|   |                              | 79.42                                       | 1.70                                 | 1.71        | 0.11        | 1.62       | 1.20        |                                  |
|   |                              | 82.11                                       | 1.72                                 | 2.10        | 0.07        | 1.82       | 1.01        |                                  |
|   |                              | 119.36                                      | 3.16                                 | 1.35        | 0.19        | 0.68       | 2.26        |                                  |
| 2 | 180                          | 160.88                                      | 4.03                                 | 1.44        | 0.25        | 1.71       | 0.16        | Au core distortion               |
|   |                              | 192.83                                      | 19.03                                | 1.13        | 1.06        | 0.30       | 0.25        |                                  |
| 3 | 210                          | 196.17                                      | 18.02                                | 1.26        | 0.95        | 0.51       | 0.26        | Rh wagging                       |
|   |                              | 212.36                                      | 5.49                                 | 0.35        | 0.87        | 0.34       | 0.58        |                                  |
| 4 | 255                          | 233.46                                      | 4.21                                 | 0.11        | 0.11        | 0.26       | 0.68        | Au-Rh asymmetric stretching      |
|   |                              | 246.66                                      | 4.836                                | 1.61        | 0.49        | 0.20       | 7.66        |                                  |
| 5 | 310                          | 301.77                                      | 3.35                                 | 0.00        | 0.24        | 0.00       | 0.17        | PPh <sub>3</sub> wagging         |
|   |                              | 304.98                                      | 4.90                                 | 0.00        | 0.90        | 0.00       | 0.26        |                                  |
| 6 | 325                          | 320.56                                      | 19.01                                | 0.00        | 0.66        | 0.00       | 0.18        | Rh-Cl asymmetric stretching      |
|   |                              | 340.45                                      | 11.37                                | 0.00        | 0.80        | 0.00       | 0.19        |                                  |
| 7 | 350                          | 358.33                                      | 4.31                                 | 0.00        | 0.93        | 0.00       | 0.19        | xylyl distortion                 |
|   |                              | 430   | 437.74                               | 20.56       | 0.00        | 0.09       | 3.94        |                                  |
| 8 | 430                          | 437.74                                      | 20.56                                | 0.00        | 0.09        | 3.94       | 0.00        | Rh-C wagging                     |
| 8 | 430                          | 437.74                                      | 20.56                                | 0.00        | 0.09        | 3.94       | 0.00        | Rh-C-N rocking, xylyl distortion |
| 8 | 430                          | 437.74                                      | 20.56                                | 0.00        | 0.09        | 3.94       | 0.00        | PPh <sub>3</sub> distortion      |

## 4 Cartesian coordinates of the optimized structures

The optimized geometries of the Au<sub>n</sub>Rh (n=5,6,7,8) clusters are available as separate xyz files.

| Au <sub>5</sub> Rh |              |              |              |   |              |              |              |
|--------------------|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Au                 | -1.715522000 | 1.370522000  | -0.231004000 | C | -0.824374000 | 4.083337000  | 3.601167000  |
| Au                 | 1.160084000  | 1.917457000  | -0.381863000 | C | -0.993884000 | 5.451070000  | 3.864255000  |
| Au                 | -1.913541000 | -1.606936000 | -0.431000000 | C | -0.258894000 | 6.403045000  | 3.141423000  |
| Au                 | 0.181936000  | -0.430817000 | 1.192536000  | C | 0.651206000  | 5.990124000  | 2.156005000  |
| Au                 | 2.480367000  | -0.995057000 | -0.479140000 | C | 3.643705000  | 3.795203000  | 1.504826000  |
| Rh                 | 0.147224000  | -0.276248000 | -1.695476000 | C | 4.426258000  | 2.661324000  | 1.229524000  |
| P                  | -3.616778000 | 2.858692000  | 0.311538000  | C | 5.661566000  | 2.490379000  | 1.869683000  |
| P                  | 2.023048000  | 3.988138000  | 0.616021000  | C | 6.112295000  | 3.449976000  | 2.786888000  |
| P                  | -3.676565000 | -3.194430000 | 0.177914000  | C | 5.328954000  | 4.581980000  | 3.066754000  |
| P                  | 0.453072000  | -1.002044000 | 3.577284000  | C | 4.093434000  | 4.755428000  | 2.428247000  |
| P                  | 4.767657000  | -1.809730000 | -0.085419000 | C | -3.056706000 | -4.697514000 | 1.085870000  |
| N                  | -2.206589000 | 0.834383000  | -3.533871000 | C | -2.223040000 | -4.483405000 | 2.199362000  |
| N                  | 2.463866000  | 0.805713000  | -3.585141000 | C | -1.728680000 | -5.574747000 | 2.922511000  |
| N                  | 0.137258000  | -3.373341000 | -2.490034000 | C | -2.064709000 | -6.882716000 | 2.536817000  |
| C                  | -1.334650000 | 0.402140000  | -2.850473000 | C | -2.894325000 | -7.094895000 | 1.426405000  |
| C                  | 1.623618000  | 0.463698000  | -2.817350000 | C | -3.390681000 | -6.003533000 | 0.696696000  |
| C                  | 0.190467000  | -2.228539000 | -2.163306000 | C | -5.023472000 | -2.498339000 | 1.251127000  |
| C                  | -3.260001000 | 1.490052000  | -4.152891000 | C | -5.215655000 | -1.107532000 | 1.272106000  |
| C                  | -4.306460000 | 0.725847000  | -4.708152000 | C | -6.249718000 | -0.552089000 | 2.038977000  |
| C                  | -5.381350000 | 1.420984000  | -5.278684000 | C | -7.086024000 | -1.389795000 | 2.791907000  |
| C                  | -5.406359000 | 2.823127000  | -5.287377000 | C | -6.886781000 | -2.780621000 | 2.780227000  |
| C                  | -4.351049000 | 3.555516000  | -4.724437000 | C | -5.856761000 | -3.337787000 | 2.009691000  |
| C                  | -3.253065000 | 2.902512000  | -4.147258000 | C | -4.506517000 | -3.824768000 | -1.363025000 |
| C                  | -4.255026000 | -0.778025000 | -4.667593000 | C | -5.881215000 | -3.659019000 | -1.587084000 |
| C                  | -2.102826000 | 3.653714000  | -3.532894000 | C | -6.449146000 | -4.104088000 | -2.791217000 |
| C                  | 3.459673000  | 1.200866000  | -4.464284000 | C | -5.648390000 | -4.717020000 | -3.764764000 |
| C                  | 4.084428000  | 0.219302000  | -5.262365000 | C | -4.271579000 | -4.881239000 | -3.539610000 |
| C                  | 5.065535000  | 0.646166000  | -6.167162000 | C | -3.697828000 | -4.428806000 | -2.346176000 |
| C                  | 5.422706000  | 1.999182000  | -6.253203000 | C | -1.073132000 | -1.690591000 | 4.386927000  |
| C                  | 4.809813000  | 2.948607000  | -5.421585000 | C | -1.022177000 | -2.643283000 | 5.417739000  |
| C                  | 3.815120000  | 2.566654000  | -4.510843000 | C | -2.215570000 | -3.135422000 | 5.967594000  |
| C                  | 3.716914000  | -1.229660000 | -5.107623000 | C | -3.454803000 | -2.673362000 | 5.496961000  |
| C                  | 3.141879000  | 3.549042000  | -3.593013000 | C | -3.505394000 | -1.715752000 | 4.472823000  |
| C                  | -0.048620000 | -4.730691000 | -2.702118000 | C | -2.314501000 | -1.231805000 | 3.917113000  |
| C                  | -0.372678000 | -5.188366000 | -3.997500000 | C | 1.004254000  | 0.432863000  | 4.624989000  |
| C                  | -0.600165000 | -6.562143000 | -4.162403000 | C | 0.365759000  | 0.778279000  | 5.825738000  |
| C                  | -0.503942000 | -7.443132000 | -3.075470000 | C | 0.813422000  | 1.890719000  | 6.555946000  |
| C                  | -0.185317000 | -6.959943000 | -1.797894000 | C | 1.896599000  | 2.650117000  | 6.091465000  |
| C                  | 0.043631000  | -5.593407000 | -1.585332000 | C | 2.533353000  | 2.304376000  | 4.888465000  |
| C                  | -0.475384000 | -4.222687000 | -5.145530000 | C | 2.084704000  | 1.202521000  | 4.151746000  |
| C                  | 0.357140000  | -5.034401000 | -0.225837000 | C | 1.755985000  | -2.312609000 | 3.799917000  |
| C                  | -5.244919000 | 2.224198000  | -0.332150000 | C | 2.591266000  | -2.355771000 | 4.927761000  |
| C                  | -5.251754000 | 1.238471000  | -1.332210000 | C | 3.565216000  | -3.359908000 | 5.034460000  |
| C                  | -6.469816000 | 0.760026000  | -1.835101000 | C | 3.702563000  | -4.317311000 | 4.018778000  |
| C                  | -7.679210000 | 1.265220000  | -1.339183000 | C | 2.862617000  | -4.278630000 | 2.894871000  |
| C                  | -7.674044000 | 2.253000000  | -0.340959000 | C | 1.888153000  | -3.278739000 | 2.784918000  |
| C                  | -6.458909000 | 2.733717000  | 0.163002000  | C | 5.853450000  | -1.338415000 | -1.522274000 |
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| C                  | -4.273576000 | 4.292027000  | 2.721933000  | C | 7.568296000  | -1.828061000 | -3.168482000 |
| C                  | -4.481079000 | 4.369537000  | 4.107612000  | C | 7.460751000  | -0.522774000 | -3.668152000 |
| C                  | -4.315594000 | 3.232976000  | 4.912995000  | C | 6.549603000  | 0.378500000  | -3.095747000 |
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| C                  | -3.741582000 | 1.931211000  | 2.948884000  | C | 4.863667000  | -3.666899000 | -0.006189000 |
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| C                  | -2.330421000 | 5.336447000  | 0.068729000  | C | 4.094259000  | -5.802958000 | -0.878133000 |
| C                  | -2.130682000 | 6.630467000  | -0.425570000 | C | 4.963419000  | -6.470831000 | -0.000110000 |
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| C                  | -4.142589000 | 6.428501000  | -1.771984000 | C | 5.732821000  | -4.333758000 | 0.870890000  |
| C                  | -4.349460000 | 5.130928000  | -1.277478000 | C | 5.677046000  | -1.200500000 | 1.419589000  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 2.237656000  | 5.394117000  | -0.584113000 | C | 4.952136000  | -1.029829000 | 2.611143000  |
| C | 3.438893000  | 6.105499000  | -0.718330000 | C | 5.607846000  | -0.609705000 | 3.775851000  |
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| C | 2.439118000  | 7.448195000  | -2.484058000 | C | 7.713076000  | -0.530823000 | 2.562116000  |
| C | 1.237258000  | 6.732990000  | -2.349383000 | C | 7.059769000  | -0.949130000 | 1.393289000  |
| C | 1.139086000  | 5.702364000  | -1.408061000 | H | 2.054577000  | 3.562478000  | -3.750424000 |
| C | 0.819248000  | 4.620217000  | 1.891731000  | H | 5.096005000  | 3.995092000  | -5.483623000 |
| C | 0.076918000  | 3.667342000  | 2.613429000  | H | 6.179338000  | 2.314165000  | -6.964825000 |
| H | 5.555541000  | -0.089500000 | -6.799621000 | H | 6.854005000  | -3.251851000 | -1.704619000 |
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| H | 3.520193000  | 4.566307000  | -3.733218000 | H | 5.006931000  | -7.555412000 | -0.000046000 |
| H | 3.915047000  | -1.569700000 | -4.079204000 | H | 6.462377000  | -6.251451000 | 1.541880000  |
| H | 2.649520000  | -1.397526000 | -5.301486000 | H | 6.364315000  | -3.767161000 | 1.552794000  |
| H | -0.835871000 | -4.723053000 | -6.048759000 | H | 7.624408000  | -1.077664000 | 0.471814000  |
| H | -1.158133000 | -3.394086000 | -4.912690000 | H | 8.782151000  | -0.343848000 | 2.543450000  |
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| H | -5.175158000 | -1.214329000 | -5.068647000 | H | 0.321155000  | 2.157679000  | 7.485922000  |
| H | -6.200814000 | 0.858999000  | -5.719350000 | H | 2.239208000  | 3.509253000  | 6.659462000  |
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| H | -2.249667000 | 4.736421000  | -3.610005000 | H | -0.064344000 | -3.005945000 | 5.785663000  |
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| H | 0.210904000  | 5.135045000  | -1.321432000 | H | -3.645002000 | -5.363613000 | -4.284720000 |
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| H | 2.518909000  | 8.244558000  | -3.217381000 |   |              |              |              |
| H | 4.467456000  | 7.680606000  | -1.777388000 |   |              |              |              |
| H | 4.295953000  | 5.862525000  | -0.093970000 |   |              |              |              |
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| H | 6.267652000  | 1.613713000  | 1.651047000  |   |              |              |              |
| H | 7.070082000  | 3.316388000  | 3.281281000  |   |              |              |              |
| H | 5.680455000  | 5.325334000  | 3.775410000  |   |              |              |              |
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| H | 1.216653000  | 6.731614000  | 1.593110000  |   |              |              |              |
| H | -0.389890000 | 7.461517000  | 3.344364000  |   |              |              |              |
| H | -1.702364000 | 5.769355000  | 4.623832000  |   |              |              |              |
| H | -1.394009000 | 3.341028000  | 4.155781000  |   |              |              |              |
| H | 0.191289000  | 2.603054000  | 2.397633000  |   |              |              |              |
| H | 5.015078000  | 0.664020000  | -1.599184000 |   |              |              |              |
| H | 6.459249000  | 1.386863000  | -3.491138000 |   |              |              |              |
| H | 8.076917000  | -0.207387000 | -4.505036000 |   |              |              |              |
| H | 8.273248000  | -2.524731000 | -3.611076000 |   |              |              |              |

Au<sub>6</sub>Rh

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Au | -1.026271079 | -1.254788093 | 0.693925055  | C | 0.707438056  | 5.240191398  | 2.080383158  |
| Au | 1.712831130  | -1.760055135 | -0.297443023 | C | 0.803560061  | 6.465773490  | 1.400614108  |
| Au | 1.010533078  | 0.977844074  | 0.651136052  | C | 1.792320136  | 6.662141483  | 0.427921033  |
| Au | -1.739313133 | 1.552927116  | -0.241911019 | C | 2.688970206  | 5.624629425  | 0.121200009  |
| Au | -2.750213212 | -0.846884067 | -1.659135128 | C | 2.598102201  | 4.400764338  | 0.793117060  |
| Au | 2.513927193  | 0.610333047  | -1.852154144 | C | -2.898828223 | 4.860743370  | 1.431326111  |
| Rh | -0.096969007 | -0.173121013 | -1.674919125 | C | -2.979799227 | 4.373922336  | 2.746598211  |
| P  | -1.618298123 | -2.199284169 | 2.914765222  | C | -2.874545221 | 5.252063400  | 3.831686294  |
| P  | 3.446403261  | -3.403378262 | 0.284621022  | C | -2.698550208 | 6.626642527  | 3.606384275  |
| P  | 1.512030113  | 2.517439194  | 2.550879196  | C | -2.631428202 | 7.115687555  | 2.293802174  |
| P  | -3.086296238 | 3.624151275  | 0.041215003  | C | -2.726900207 | 6.234945474  | 1.205916092  |
| P  | -4.971151382 | -1.756710132 | -2.254681174 | C | -4.926641379 | 3.315860251  | 0.030163002  |
| P  | 4.815653367  | 1.303848100  | -2.396057184 | C | -5.399357400 | 2.007380151  | -0.165678013 |
| O  | 0.112765008  | -2.653608201 | -3.515720269 | C | -6.777559539 | 1.746859132  | -0.138073010 |
| O  | -0.351567027 | 2.098070161  | -3.765835287 | C | -7.683143582 | 2.794367211  | 0.077792006  |
| C  | 0.026658002  | -1.738268135 | -2.768254213 | C | -7.212953562 | 4.103496315  | 0.271907021  |
| C  | -0.258961020 | 1.279374097  | -2.918427223 | C | -5.837514469 | 4.364553332  | 0.252008019  |
| C  | -1.988387154 | -4.030086307 | 2.969421225  | C | -2.697477206 | 4.611117354  | -1.489135111 |
| C  | -1.841377142 | -4.788855366 | 4.143417314  | C | -3.649309276 | 4.884384374  | -2.481178191 |
| C  | -2.177859168 | -6.149168488 | 4.143816319  | C | -3.271423247 | 5.592748453  | -3.632282279 |
| C  | -2.662995202 | -6.754696542 | 2.973893228  | C | -1.949717151 | 6.030351474  | -3.788447290 |
| C  | -2.795214212 | -6.001903434 | 1.797440137  | C | -0.995896078 | 5.750422424  | -2.796789213 |
| C  | -2.454634189 | -4.641945352 | 1.792546137  | C | -1.363736105 | 5.033734387  | -1.653885129 |
| C  | -0.278476021 | -1.985086151 | 4.199340321  | C | -5.892884454 | -0.840404064 | -3.587711272 |
| C  | 0.945177074  | -2.643313200 | 3.970137303  | C | -5.668516422 | 0.541618042  | -3.715234284 |
| C  | 2.000783152  | -2.502226190 | 4.880160370  | C | -6.366801469 | 1.275889100  | -4.682551356 |
| C  | 1.848914139  | -1.688786131 | 6.015304477  | C | -7.279438545 | 0.631225049  | -5.530089422 |
| C  | 0.640203049  | -1.013260077 | 6.231389456  | C | -7.489756550 | -0.751304056 | -5.415419411 |
| C  | -0.423450032 | -1.165844087 | 5.328829397  | C | -6.798185545 | -1.488575115 | -4.444902341 |
| C  | -3.146757242 | -1.385779105 | 3.629180279  | C | -6.163962485 | -1.883481146 | -0.827931065 |
| C  | -3.726724283 | -1.805344140 | 4.840023371  | C | -5.624005419 | -2.085749158 | 0.453501035  |
| C  | -4.869825374 | -1.159414086 | 5.331453428  | C | -6.470929475 | -2.256613173 | 1.557032119  |
| C  | -5.446350403 | -0.099401007 | 4.610785353  | C | -7.862270609 | -2.207355170 | 1.382982107  |
| C  | -4.882560374 | 0.308533024  | 3.393651259  | C | -8.403698629 | -1.988919152 | 0.106066008  |
| C  | -3.735116283 | -0.333619026 | 2.904684220  | C | -7.556982592 | -1.831416142 | -1.000959076 |
| C  | 3.938648299  | -4.469208341 | -1.161718087 | C | -4.837109367 | -3.509491270 | -2.877767218 |
| C  | 4.844567369  | -5.534537421 | -1.013586076 | C | -5.700329447 | -4.532233346 | -2.453739187 |
| C  | 5.172646394  | -6.328781459 | -2.119445160 | C | -5.547055427 | -5.829818432 | -2.964322227 |
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| C  | 3.395220259  | -5.872357457 | 3.659964281  | C | 6.610958507  | 4.290057325  | -0.096846007 |
| C  | 3.816892292  | -4.935586379 | 2.702895209  | C | 6.079004453  | 3.589129276  | -1.191449090 |
| C  | 4.993915381  | -2.565873195 | 0.888996066  | C | 6.016164443  | -0.105307008 | -2.628249201 |
| C  | 6.222866474  | -2.679390203 | 0.223481017  | C | 7.385566577  | 0.033032003  | -2.342753180 |
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| C  | 4.391665337  | 0.914098071  | 5.024162385  | C | 6.293775485  | 3.334382253  | -5.718728411 |
| C  | 5.285309405  | 1.973828149  | 5.254487402  | C | 5.160210395  | 4.031990308  | -6.164047471 |
| C  | 5.072501388  | 3.212981245  | 4.633595353  | C | 3.940538303  | 3.897351296  | -5.485747438 |
| C  | 3.968681304  | 3.397887259  | 3.786722288  | C | 3.852416294  | 3.066807233  | -4.359921332 |
| C  | 0.244536019  | 2.625705203  | 3.921661302  | H | -1.444673109 | -4.329497329 | 5.047452386  |
| C  | 0.518099040  | 3.347945257  | 5.098608390  | H | -2.066489160 | -6.732460514 | 5.053007387  |
| C  | -0.398652030 | 3.342195254  | 6.155914493  | H | -2.930951224 | -7.807018578 | 2.978228227  |
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|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 2.661997205  | -1.587515120 | 6.728747489  | H | -2.669034204 | 6.619219493  | 0.189650014  |
| H | 0.518336040  | -0.367940028 | 7.096731527  | H | -4.689586360 | 1.192094089  | -0.332081025 |
| H | -1.358352103 | -0.641758047 | 5.512386432  | H | -7.136055535 | 0.730071057  | -0.282697022 |
| H | -3.294698251 | -2.635207199 | 5.396410412  | H | -8.749947664 | 2.592759199  | 0.098215007  |
| H | -5.312056383 | -1.484376114 | 6.268324493  | H | -7.914952586 | 4.914143376  | 0.442050034  |
| H | -6.334764496 | 0.395742030  | 4.990864383  | H | -5.471200408 | 5.376011423  | 0.420546032  |
| H | -5.335328381 | 1.113349085  | 2.819491213  | H | -4.676725358 | 4.544975347  | -2.362760182 |
| H | -3.300307250 | -0.022640002 | 1.951297147  | H | -4.007692303 | 5.799738463  | -4.403097338 |
| H | 5.280352406  | -5.752596443 | -0.039522003 | H | -1.661378125 | 6.577066503  | -4.681138357 |
| H | 5.870814429  | -7.152419547 | -2.005837155 | H | 0.034124003  | 6.073089469  | -2.918588220 |
| H | 4.833652368  | -6.695611521 | -4.222843321 | H | -0.611426046 | 4.795594364  | -0.899359071 |
| H | 3.198171246  | -4.827922368 | -4.472323343 | H | -4.937043379 | 1.037774080  | -3.076296233 |
| H | 2.625987201  | -3.405957260 | -2.516743194 | H | -6.188196474 | 2.342175181  | -4.782435366 |
| H | 1.106824086  | -5.053514387 | 0.615995047  | H | -7.814358584 | 1.199337091  | -6.285155505 |
| H | 0.390112030  | -6.742403490 | 2.290255173  | H | -8.185090639 | -1.253124095 | -6.081259489 |
| H | 1.835341140  | -7.243546569 | 4.257622327  | H | -6.949140552 | -2.564267195 | -4.367514333 |
| H | 4.033493309  | -6.101249477 | 4.508306343  | H | -4.540921346 | -2.100836160 | 0.586038043  |
| H | 4.783094366  | -4.445394338 | 2.810893215  | H | -6.041079484 | -2.422422186 | 2.542121196  |
| H | 6.312490473  | -3.298353252 | -0.667052053 | H | -8.521080674 | -2.336431179 | 2.236345171  |
| H | 8.285200656  | -2.057320158 | 0.157521012  | H | -9.480416742 | -1.948435150 | -0.028628002 |
| H | 8.106635614  | -0.614605047 | 2.186445165  | H | -7.979538616 | -1.662441126 | -1.989759152 |
| H | 5.916497454  | -0.394502030 | 3.359592257  | H | -6.482405478 | -4.324270328 | -1.725909132 |
| H | 3.916031300  | -1.590073121 | 2.503348194  | H | -6.216752466 | -6.619749517 | -2.637551201 |
| H | 2.590470200  | 0.270773021  | 4.012727309  | H | -4.419627338 | -7.110684555 | -4.289586326 |
| H | 4.545652350  | -0.046899004 | 5.509261429  | H | -3.126916238 | -3.002058232 | -4.110777312 |
| H | 6.133441446  | 1.836627141  | 5.918910449  | H | 5.199020397  | 0.693112053  | 0.412989032  |
| H | 5.756055463  | 4.037693309  | 4.814765365  | H | 6.140197452  | 1.937122150  | 2.337133181  |
| H | 3.806012291  | 4.362176331  | 3.308214253  | H | 7.045273537  | 4.240988322  | 2.021292152  |
| H | 1.452472113  | 3.898136298  | 5.196322398  | H | 7.005479514  | 5.291798420  | -0.239434018 |
| H | -0.179011014 | 3.894764296  | 7.064529556  | H | 6.061991458  | 4.049984308  | -2.177269168 |
| H | -2.304920177 | 2.602288199  | 6.865700519  | H | 7.766871593  | 0.966303073  | -1.931046147 |
| H | -2.804177215 | 1.346324105  | 4.771409365  | H | 9.318969738  | -0.924115073 | -2.366207179 |
| H | -1.161325088 | 1.347798102  | 2.891408222  | H | 8.446536639  | -3.078983236 | -3.263995250 |
| H | -0.078650006 | 5.097354388  | 2.823086216  | H | 6.009627464  | -3.339305253 | -3.726492286 |
| H | 0.099294008  | 7.259405534  | 1.634105124  | H | 4.458332341  | -1.433938109 | -3.330251252 |
| H | 1.861249145  | 7.612953564  | -0.092582007 | H | 7.088063550  | 1.955086151  | -4.259190326 |
| H | 3.451111261  | 5.765070421  | -0.640237049 | H | 7.235759567  | 3.431050263  | -6.249800485 |
| H | 3.283121250  | 3.588654276  | 0.538820039  | H | 5.225555398  | 4.667671357  | -7.041867541 |
| H | -3.122030239 | 3.307766252  | 2.926245225  | H | 3.058049233  | 4.422488340  | -5.837315445 |
| H | -2.930740226 | 4.863073369  | 4.844753369  | H | 2.899146222  | 2.941799226  | -3.845824296 |
| H | -2.622076200 | 7.310316566  | 4.446449338  | H | -2.874301218 | -5.295662419 | -5.022227385 |
| H | -2.512108194 | 8.180524633  | 2.114520160  |   |              |              |              |



Au<sub>7</sub>Rh

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Au | 1.081917000  | -0.022533000 | 1.196810000  | C | -0.897499000 | -3.100190000 | 3.938726000  |
| Au | -1.216965000 | 1.859783000  | 0.324014000  | C | -3.658585000 | -3.874834000 | 1.141000000  |
| Au | -1.714202000 | -0.998633000 | 0.813988000  | C | -3.452598000 | -5.232553000 | 1.425620000  |
| Au | 0.612892000  | -2.545119000 | -0.219420000 | C | -3.899368000 | -6.207406000 | 0.518355000  |
| Au | 2.574059000  | -0.662696000 | -1.474710000 | C | -4.550119000 | -5.830409000 | -0.664838000 |
| Au | 1.628856000  | 2.104431000  | -0.693358000 | C | -4.745112000 | -4.469393000 | -0.955597000 |
| Au | -2.890428000 | 0.240785000  | -1.524476000 | C | -4.290979000 | -3.495263000 | -0.059928000 |
| Rh | -0.098732000 | -0.058718000 | -1.388892000 | C | 0.144875000  | -6.176681000 | 0.834933000  |
| P  | 1.675616000  | 0.241201000  | 3.579981000  | C | 0.058783000  | -5.801227000 | 2.183573000  |
| P  | -2.448360000 | 3.901809000  | 0.973407000  | C | -0.476504000 | -6.685287000 | 3.128842000  |
| P  | -3.073968000 | -2.495741000 | 2.244348000  | C | -0.925270000 | -7.951365000 | 2.724410000  |
| P  | 0.954530000  | -4.981086000 | -0.344678000 | C | -0.833643000 | -8.329893000 | 1.375663000  |
| P  | 4.959970000  | -1.037312000 | -2.013227000 | C | -0.297324000 | -7.446339000 | 0.428927000  |
| P  | 3.009138000  | 4.136027000  | -0.486910000 | C | 2.756470000  | -5.443089000 | -0.254125000 |
| P  | -4.971780000 | 0.233492000  | -2.828955000 | C | 3.651371000  | -4.527829000 | 0.323200000  |
| O  | -0.209962000 | 2.076670000  | -3.614579000 | C | 4.999065000  | -4.874646000 | 0.497281000  |
| O  | -0.735889000 | -2.308817000 | -3.416342000 | C | 5.455181000  | -6.132295000 | 0.080540000  |
| C  | -0.114181000 | 1.311987000  | -2.715618000 | C | 4.561983000  | -7.047839000 | -0.501276000 |
| C  | -0.481361000 | -1.529600000 | -2.570052000 | C | 3.211802000  | -6.710607000 | -0.659364000 |
| C  | 2.768431000  | 1.682218000  | 4.041197000  | C | 0.326010000  | -5.443882000 | -2.030353000 |
| C  | 2.437098000  | 2.580804000  | 5.067839000  | C | 1.186211000  | -5.541135000 | -3.134228000 |
| C  | 3.327133000  | 3.612562000  | 5.404258000  | C | 0.656996000  | -5.785573000 | -4.409157000 |
| C  | 4.544309000  | 3.747016000  | 4.720767000  | C | -0.727201000 | -5.919318000 | -4.583242000 |
| C  | 4.868073000  | 2.855833000  | 3.685131000  | C | -1.588252000 | -5.795206000 | -3.481307000 |
| C  | 3.979163000  | 1.830952000  | 3.340935000  | C | -1.066479000 | -5.550271000 | -2.206567000 |
| C  | 0.138833000  | 0.486547000  | 4.602436000  | C | 5.452938000  | -2.334030000 | -3.255422000 |
| C  | -0.737596000 | 1.508721000  | 4.190502000  | C | 5.075108000  | -3.667196000 | -3.010689000 |
| C  | -1.898772000 | 1.778286000  | 4.924433000  | C | 5.423863000  | -4.668726000 | -3.923655000 |
| C  | -2.207285000 | 1.003499000  | 6.054788000  | C | 6.134842000  | -4.342604000 | -5.089616000 |
| C  | -1.350939000 | -0.034248000 | 6.447944000  | C | 6.496477000  | -3.012243000 | -5.338999000 |
| C  | -0.170538000 | -0.285169000 | 5.730867000  | C | 6.158568000  | -2.005272000 | -4.422681000 |
| C  | 2.575159000  | -1.241484000 | 4.262448000  | C | 5.895258000  | -1.491295000 | -0.460299000 |
| C  | 3.193743000  | -1.215188000 | 5.525251000  | C | 5.290168000  | -1.234842000 | 0.783483000  |
| C  | 3.874468000  | -2.348610000 | 5.991666000  | C | 5.974381000  | -1.519905000 | 1.974149000  |
| C  | 3.944417000  | -3.506206000 | 5.198366000  | C | 7.269605000  | -2.057851000 | 1.923682000  |
| C  | 3.337841000  | -3.530409000 | 3.933809000  | C | 7.869377000  | -2.330740000 | 0.683232000  |
| C  | 2.655898000  | -2.397720000 | 3.466347000  | C | 7.182302000  | -2.055239000 | -0.507780000 |
| C  | -2.108557000 | 5.298073000  | -0.207955000 | C | 5.733244000  | 0.549488000  | -2.614339000 |
| C  | -2.436284000 | 6.626427000  | 0.108959000  | C | 7.108127000  | 0.804272000  | -2.480883000 |
| C  | -2.194204000 | 7.644756000  | -0.824117000 | C | 7.639895000  | 2.025574000  | -2.915177000 |
| C  | -1.622665000 | 7.338653000  | -2.069767000 | C | 6.801486000  | 2.992639000  | -3.490341000 |
| C  | -1.291472000 | 6.011397000  | -2.384294000 | C | 5.432356000  | 2.732740000  | -3.642616000 |
| C  | -1.533412000 | 4.991748000  | -1.453353000 | C | 4.897252000  | 1.513917000  | -3.203690000 |
| C  | -2.308720000 | 4.642900000  | 2.675628000  | C | 4.746254000  | 3.820692000  | 0.114600000  |
| C  | -1.020276000 | 4.838051000  | 3.203378000  | C | 5.221375000  | 2.500468000  | 0.116652000  |
| C  | -0.868811000 | 5.383345000  | 4.484454000  | C | 6.535593000  | 2.223020000  | 0.518912000  |
| C  | -1.997339000 | 5.738062000  | 5.238855000  | C | 7.380399000  | 3.269038000  | 0.915095000  |
| C  | -3.282209000 | 5.553138000  | 4.706855000  | C | 6.904237000  | 4.590275000  | 0.925204000  |
| C  | -3.440622000 | 5.005545000  | 3.425295000  | C | 5.589107000  | 4.867336000  | 0.530910000  |
| C  | -4.252763000 | 3.493997000  | 0.768988000  | C | 2.350057000  | 5.445806000  | 0.662445000  |
| C  | -5.099713000 | 4.219798000  | -0.079714000 | C | 1.513137000  | 6.462436000  | 0.174724000  |
| C  | -6.437754000 | 3.825289000  | -0.234273000 | C | 0.999085000  | 7.424666000  | 1.055741000  |
| C  | -6.931972000 | 2.717881000  | 0.466228000  | C | 1.322515000  | 7.377785000  | 2.418601000  |
| C  | -6.086130000 | 1.997200000  | 1.326254000  | C | 2.145812000  | 6.350785000  | 2.905752000  |
| C  | -4.746798000 | 2.375397000  | 1.468280000  | C | 2.646964000  | 5.375293000  | 2.035901000  |
| C  | -4.621767000 | -1.734471000 | 2.954421000  | C | 3.158181000  | 4.987275000  | -2.141583000 |
| C  | -4.457614000 | -0.543885000 | 3.684417000  | C | 4.062051000  | 6.043565000  | -2.348084000 |
| C  | -5.557939000 | 0.052710000  | 4.310204000  | C | 4.155104000  | 6.648701000  | -3.607724000 |
| C  | -6.828589000 | -0.537058000 | 4.206398000  | C | 3.343444000  | 6.205402000  | -4.664905000 |
| C  | -6.992388000 | -1.719619000 | 3.470492000  | C | 2.435515000  | 5.157308000  | -4.458589000 |
| C  | -5.890569000 | -2.320986000 | 2.840136000  | C | 2.343975000  | 4.548330000  | -3.198254000 |
| C  | -2.276872000 | -3.260593000 | 3.744183000  | C | -6.398134000 | -0.758996000 | -2.163188000 |
| C  | -3.046223000 | -3.944558000 | 4.702876000  | C | -6.605505000 | -0.789031000 | -0.774052000 |
| C  | -2.431460000 | -4.471904000 | 5.845252000  | C | -7.703701000 | -1.480894000 | -0.246714000 |
| C  | -1.047305000 | -4.318400000 | 6.033676000  | C | -8.586075000 | -2.156540000 | -1.102585000 |
| C  | -0.280805000 | -3.635280000 | 5.079480000  | C | -8.367236000 | -2.143878000 | -2.488440000 |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | -7.276025000 | -1.443561000 | -3.021471000 | H | 0.403886000  | -4.816935000 | 2.499410000  |
| C | -5.644278000 | 1.925128000  | -3.208909000 | H | -0.539645000 | -6.383137000 | 4.171601000  |
| C | -7.015230000 | 2.156068000  | -3.403692000 | H | -1.336104000 | -8.641786000 | 3.454567000  |
| C | -7.463262000 | 3.440982000  | -3.743044000 | H | -1.169827000 | -9.313818000 | 1.063201000  |
| C | -6.544781000 | 4.492264000  | -3.886965000 | H | -0.232883000 | -7.745156000 | -0.615220000 |
| C | -5.175600000 | 4.261832000  | -3.682588000 | H | 3.303726000  | -3.535753000 | 0.619713000  |
| C | -4.725085000 | 2.980241000  | -3.340791000 | H | 5.684352000  | -4.161489000 | 0.951037000  |
| C | -4.608393000 | -0.539606000 | -4.483649000 | H | 6.498836000  | -6.401406000 | 0.209404000  |
| C | -5.082931000 | 0.002071000  | -5.687685000 | H | 4.914625000  | -8.024768000 | -0.816705000 |
| C | -4.779778000 | -0.632864000 | -6.901226000 | H | 2.520235000  | -7.432226000 | -1.090181000 |
| C | -4.003389000 | -1.800356000 | -6.912075000 | H | 2.260800000  | -5.420009000 | -3.008493000 |
| C | -3.524948000 | -2.337909000 | -5.707065000 | H | 1.323974000  | -5.863430000 | -5.261973000 |
| C | -3.828024000 | -1.709748000 | -4.494052000 | H | -1.132799000 | -6.113906000 | -5.571460000 |
| H | 1.499996000  | 2.475403000  | 5.611188000  | H | -2.663099000 | -5.884995000 | -3.611753000 |
| H | 3.076912000  | 4.296195000  | 6.210386000  | H | -1.743992000 | -5.437561000 | -1.357671000 |
| H | 5.236657000  | 4.538320000  | 4.991554000  | H | 4.514922000  | -3.924984000 | -2.110136000 |
| H | 5.806356000  | 2.956606000  | 3.144970000  | H | 5.144190000  | -5.699412000 | -3.724252000 |
| H | 4.232714000  | 1.148825000  | 2.527651000  | H | 6.403062000  | -5.119733000 | -5.798435000 |
| H | -0.509936000 | 2.102822000  | 3.302282000  | H | 7.041377000  | -2.756495000 | -6.242111000 |
| H | -2.552974000 | 2.592079000  | 4.613421000  | H | 6.442550000  | -0.974623000 | -4.623201000 |
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| H | 4.352157000  | -2.328245000 | 6.966066000  | H | 7.636876000  | -2.298392000 | -1.466829000 |
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| H | -2.455087000 | 8.670821000  | -0.583281000 | H | 3.828675000  | 1.319344000  | -3.311164000 |
| H | -1.438156000 | 8.129625000  | -2.790161000 | H | 4.561257000  | 1.688763000  | -0.195162000 |
| H | -0.848588000 | 5.768835000  | -3.346165000 | H | 6.893762000  | 1.194709000  | 0.518289000  |
| H | -1.272045000 | 3.959835000  | -1.693626000 | H | 8.401403000  | 3.058467000  | 1.218201000  |
| H | -0.136852000 | 4.571488000  | 2.617766000  | H | 7.554189000  | 5.400765000  | 1.239938000  |
| H | 0.128713000  | 5.528505000  | 4.890172000  | H | 5.218768000  | 5.889507000  | 0.577265000  |
| H | -1.877595000 | 6.159123000  | 6.232195000  | H | 1.266992000  | 6.516671000  | -0.885231000 |
| H | -4.156773000 | 5.839130000  | 5.282747000  | H | 0.358704000  | 8.212906000  | 0.671290000  |
| H | -4.437867000 | 4.863852000  | 3.013482000  | H | 0.935565000  | 8.133315000  | 3.095752000  |
| H | -4.724296000 | 5.078912000  | -0.632237000 | H | 2.410391000  | 6.312194000  | 3.959513000  |
| H | -7.087305000 | 4.383089000  | -0.902459000 | H | 3.281453000  | 4.579183000  | 2.427436000  |
| H | -7.966458000 | 2.411271000  | 0.339407000  | H | 4.695224000  | 6.396458000  | -1.537751000 |
| H | -6.463916000 | 1.139264000  | 1.881403000  | H | 4.854325000  | 7.463906000  | -3.764338000 |
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Au<sub>8</sub>Rh

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Au | -2.339531528 | 1.561527294  | -0.707908474 | C | 5.956342913  | -4.698206096 | 0.037708312  |
| Au | -2.543359550 | -1.320951548 | -0.658575311 | C | 6.150709717  | -5.625431128 | 1.070431799  |
| Au | 2.409632273  | -1.477562095 | -0.981001532 | C | 5.076800826  | -5.992864716 | 1.897693640  |
| Au | 2.483619228  | 1.398419827  | -0.790471316 | C | 3.804841206  | -5.441065986 | 1.689812105  |
| Au | 0.123345212  | 2.323003270  | 0.707349049  | C | 3.606174599  | -4.514902061 | 0.656987842  |
| Au | -0.042665203 | -2.398806492 | 0.600521630  | C | 3.635571930  | 4.768662793  | -1.276402592 |
| Au | 1.586855030  | -0.153784953 | 1.540799511  | C | 3.803895408  | 5.409139770  | -2.513967098 |
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| Rh | 0.001279960  | -0.020191330 | -0.910675437 | C | 2.445437666  | 7.265169068  | -1.722093002 |
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## Notes and references

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