

*Supplementary information for*

**Ligand Effects on the Stability of Thiol-  
Stabilized Gold Nanoclusters:  $\text{Au}_{25}(\text{SR})_{18}^-$ ,  
 $\text{Au}_{38}(\text{SR})_{24}$  and  $\text{Au}_{102}(\text{SR})_{44}$**

*Jaehoon Jung,<sup>†</sup> Sunwoo Kang,<sup>‡</sup> and Young-Kyu Han<sup>\*,‡</sup>*

<sup>†</sup> RIKEN Advanced Science Institute, Wako, Saitama 351-0198, Japan

<sup>‡</sup> Division of Materials Science, Korea Basic Science Institute, Daejeon 305-333, Republic of  
Korea

\* Authors to whom correspondence should be addressed.

Fax: +82-42-865-3610; E-mail Address: ykhan@kbsi.re.kr

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Figure S1. Radial distribution functions (RDF) of  $\text{Au}_{25}(\text{SR})_{18}^-$ ,  $\text{Au}_{38}(\text{SR})_{24}$ , and  $\text{Au}_{102}(\text{SR})_{44}$  clusters ( $\text{R} = \text{CH}_3$ ,  $\text{C}_6\text{H}_{13}$ ,  $\text{CH}_2\text{CH}_2\text{Ph}$ ,  $\text{Ph}$ ,  $\text{PhF}$ , and  $\text{PhCOOH}$ ).

Table S2. Optimized geometries of  $\text{Au}_{25}(\text{SR})_{18}^-$ ,  $\text{Au}_{38}(\text{SR})_{24}$ , and  $\text{Au}_{102}(\text{SR})_{44}$  clusters ( $\text{R} = \text{CH}_3$ ,  $\text{C}_6\text{H}_{13}$ ,  $\text{CH}_2\text{CH}_2\text{Ph}$ ,  $\text{Ph}$ ,  $\text{PhF}$ , and  $\text{PhCOOH}$ ).

Table S1. HOMO, LUMO, and HOMO–LUMO gaps for thiol (SR)-stabilized  $\text{Au}_{25}^-$ ,  $\text{Au}_{38}$ , and  $\text{Au}_{102}$  nanoclusters ( $\text{R} = \text{CH}_3$ ,  $\text{C}_6\text{H}_{13}$ ,  $\text{CH}_2\text{CH}_2\text{Ph}$ ,  $\text{Ph}$ ,  $\text{PhF}$ , and  $\text{PhCOOH}$ ). Units are in eV.

|                                                           | HOMO  | LUMO  | H–L gap |
|-----------------------------------------------------------|-------|-------|---------|
| $\text{Au}_{25}(\text{SCH}_3)_{18}^-$                     | –1.57 | –0.27 | 1.29    |
| $\text{Au}_{25}(\text{SC}_6\text{H}_{13})_{18}^-$         | –1.48 | –0.27 | 1.21    |
| $\text{Au}_{25}(\text{SCH}_2\text{CH}_2\text{Ph})_{18}^-$ | –1.77 | –0.47 | 1.30    |
| $\text{Au}_{25}(\text{SPh})_{18}^-$                       | –2.13 | –0.98 | 1.15    |
| $\text{Au}_{25}(\text{SPhF})_{18}^-$                      | –2.74 | –1.59 | 1.15    |
| $\text{Au}_{25}(\text{SPhCOOH})_{18}^-$                   | –3.30 | –2.23 | 1.07    |
| $\text{Au}_{38}(\text{SCH}_3)_{24}$                       | –3.82 | –2.90 | 0.92    |
| $\text{Au}_{38}(\text{SC}_6\text{H}_{13})_{24}$           | –3.53 | –2.61 | 0.92    |
| $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$   | –3.74 | –2.79 | 0.95    |
| $\text{Au}_{38}(\text{SPh})_{24}$                         | –3.96 | –3.13 | 0.83    |
| $\text{Au}_{38}(\text{SPhF})_{24}$                        | –4.61 | –3.77 | 0.84    |
| $\text{Au}_{38}(\text{SPhCOOH})_{24}$                     | –4.90 | –4.12 | 0.78    |
| $\text{Au}_{102}(\text{SCH}_3)_{44}$                      | –3.82 | –3.27 | 0.56    |
| $\text{Au}_{102}(\text{SC}_6\text{H}_{13})_{44}$          | –3.34 | –2.80 | 0.54    |
| $\text{Au}_{102}(\text{SCH}_2\text{CH}_2\text{Ph})_{44}$  | –3.67 | –3.16 | 0.51    |
| $\text{Au}_{102}(\text{SPh})_{44}$                        | –3.87 | –3.34 | 0.53    |
| $\text{Au}_{102}(\text{SPhF})_{44}$                       | –4.80 | –4.29 | 0.51    |
| $\text{Au}_{102}(\text{SPhCOOH})_{44}$                    | –4.88 | –4.40 | 0.48    |

Figure S1. Radial distribution functions (RDF) of  $\text{Au}_{25}(\text{SR})_{18}^-$ ,  $\text{Au}_{38}(\text{SR})_{24}$ , and  $\text{Au}_{102}(\text{SR})_{44}$  clusters ( $\text{R} = \text{CH}_3$ ,  $\text{C}_6\text{H}_{13}$ ,  $\text{CH}_2\text{CH}_2\text{Ph}$ ,  $\text{Ph}$ ,  $\text{PhF}$ , and  $\text{PhCOOH}$ ).

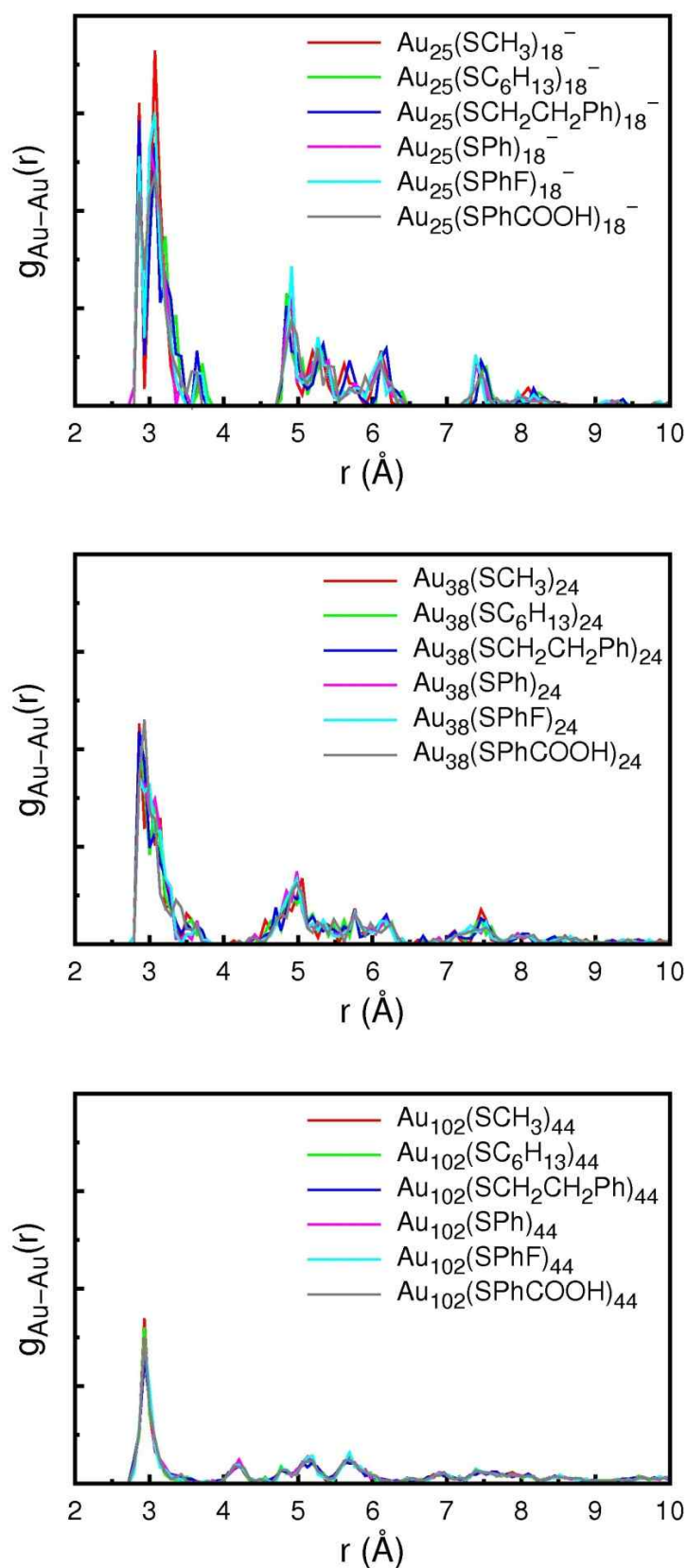


Table S2. Optimized geometries of Au<sub>25</sub>(SR)<sub>18</sub><sup>-</sup>, Au<sub>38</sub>(SR)<sub>24</sub>, and Au<sub>102</sub>(SR)<sub>44</sub> clusters (R = CH<sub>3</sub>, C<sub>6</sub>H<sub>13</sub>, CH<sub>2</sub>CH<sub>2</sub>Ph, Ph, PhF, and PhCOOH).

| Au <sub>25</sub> (SCH <sub>3</sub> ) <sub>18</sub> <sup>-</sup> |             |             |            |      |             |             |            |
|-----------------------------------------------------------------|-------------|-------------|------------|------|-------------|-------------|------------|
| Atom                                                            | x           | y           | z          | Atom | x           | y           | z          |
| Au                                                              | 7.75990000  | 10.41420000 | 4.30780000 | H    | 4.12740000  | 3.34690000  | 6.73210000 |
| Au                                                              | 10.65920000 | 11.49480000 | 5.32470000 | H    | 5.32900000  | 4.18160000  | 7.75410000 |
| Au                                                              | 12.55080000 | 8.46700000  | 5.99060000 | S    | 6.93870000  | 2.52300000  | 4.27160000 |
| Au                                                              | 10.07200000 | 6.27470000  | 5.79730000 | S    | 2.63620000  | 4.40740000  | 3.86850000 |
| Au                                                              | 6.22400000  | 9.16070000  | 6.55630000 | S    | 3.02370000  | 8.99370000  | 2.85200000 |
| Au                                                              | 4.97720000  | 11.64140000 | 5.01250000 | S    | 10.27570000 | 2.49910000  | 6.56070000 |
| Au                                                              | 6.33120000  | 11.08500000 | 1.53280000 | S    | 7.94410000  | 5.32680000  | 9.53930000 |
| Au                                                              | 7.94100000  | 8.43900000  | 1.98770000 | S    | 10.85560000 | 4.18730000  | 2.21000000 |
| Au                                                              | 9.26660000  | 9.06950000  | 6.64740000 | S    | 5.70350000  | 5.26150000  | 0.45960000 |
| Au                                                              | 7.55600000  | 9.26950000  | 9.38030000 | S    | 10.17740000 | 6.33690000  | 0.58860000 |
| Au                                                              | 4.56330000  | 7.24690000  | 8.41870000 | S    | 11.96800000 | 9.57580000  | 2.33710000 |
| Au                                                              | 5.24810000  | 6.45360000  | 5.45340000 | C    | 6.69170000  | 1.36880000  | 5.68890000 |
| Au                                                              | 7.72690000  | 4.74300000  | 5.12700000 | H    | 6.28740000  | 1.90220000  | 6.55170000 |
| Au                                                              | 4.87200000  | 3.63260000  | 4.07100000 | H    | 7.66850000  | 0.95080000  | 5.94580000 |
| Au                                                              | 2.95380000  | 6.68840000  | 3.39140000 | C    | 2.10930000  | 3.65220000  | 2.26930000 |
| Au                                                              | 5.41610000  | 8.89440000  | 3.62760000 | H    | 2.21620000  | 2.56520000  | 2.35030000 |
| Au                                                              | 9.26850000  | 6.01960000  | 2.86960000 | H    | 2.72510000  | 4.02890000  | 1.45000000 |
| Au                                                              | 10.50120000 | 3.54620000  | 4.46660000 | C    | 3.09120000  | 8.93410000  | 1.00950000 |
| Au                                                              | 9.14290000  | 4.10280000  | 7.89320000 | H    | 3.62080000  | 8.04000000  | 0.67380000 |
| Au                                                              | 7.54000000  | 6.71960000  | 7.42590000 | H    | 3.62150000  | 9.82330000  | 0.65060000 |
| Au                                                              | 6.23120000  | 6.08180000  | 2.78570000 | C    | 11.99800000 | 2.49610000  | 7.20870000 |
| Au                                                              | 7.96170000  | 5.88100000  | 0.05540000 | H    | 11.97220000 | 2.22480000  | 8.26860000 |
| Au                                                              | 10.93820000 | 7.93810000  | 0.98060000 | H    | 12.45370000 | 3.48240000  | 7.07620000 |
| Au                                                              | 10.23510000 | 8.71330000  | 3.97890000 | C    | 9.17200000  | 6.33860000  | 0.46080000 |
| Au                                                              | 7.74580000  | 7.57930000  | 4.70340000 | H    | 8.60430000  | 7.03980000  | 1.08250000 |
| S                                                               | 8.59440000  | 12.61120000 | 5.18770000 | H    | 9.79480000  | 6.91660000  | 9.77780000 |
| S                                                               | 12.90470000 | 10.74940000 | 5.46340000 | C    | 9.85290000  | 2.88940000  | 1.35850000 |
| S                                                               | 12.47770000 | 6.17420000  | 6.57700000 | H    | 9.59810000  | 3.24110000  | 0.35300000 |
| S                                                               | 5.19620000  | 12.68090000 | 2.89700000 | H    | 8.94190000  | 2.68530000  | 1.92600000 |
| S                                                               | 7.52330000  | 9.83620000  | 0.10070000 | C    | 5.79210000  | 3.41960000  | 0.48460000 |
| S                                                               | 4.64110000  | 10.98710000 | 7.26640000 | H    | 4.86830000  | 3.03860000  | 0.92990000 |
| S                                                               | 9.81340000  | 9.86300000  | 8.94950000 | H    | 6.63350000  | 3.08600000  | 1.09420000 |
| S                                                               | 5.31920000  | 8.81380000  | 0.02230000 | C    | 9.94050000  | 7.38600000  | 2.08750000 |
| S                                                               | 3.48080000  | 5.63540000  | 7.06690000 | H    | 9.34240000  | 8.26580000  | 1.83550000 |
| C                                                               | 8.76360000  | 13.78100000 | 3.77340000 | H    | 9.43630000  | 6.79160000  | 2.85700000 |
| H                                                               | 9.16580000  | 13.26520000 | 2.89940000 | C    | 11.12230000 | 11.13690000 | 1.83530000 |
| H                                                               | 7.76640000  | 14.16470000 | 3.54120000 | H    | 11.26240000 | 11.85130000 | 2.65650000 |
| C                                                               | 13.47810000 | 11.47140000 | 7.06260000 | H    | 10.05290000 | 10.96410000 | 1.69020000 |
| H                                                               | 13.39070000 | 12.56110000 | 6.99700000 | H    | 4.54300000  | 7.44360000  | 1.86320000 |
| H                                                               | 12.87290000 | 11.09720000 | 7.89070000 | H    | 3.76440000  | 3.66060000  | 8.46860000 |
| C                                                               | 12.38250000 | 6.22620000  | 8.41730000 | H    | 1.05870000  | 3.90770000  | 2.09340000 |
| H                                                               | 11.81620000 | 7.09950000  | 8.74780000 | H    | 5.89790000  | 3.04900000  | 0.54110000 |
| H                                                               | 11.88210000 | 5.31670000  | 8.76850000 | H    | 10.92620000 | 7.70090000  | 2.44530000 |
| C                                                               | 3.49290000  | 12.68850000 | 2.19700000 | H    | 5.68800000  | 9.48040000  | 1.65940000 |
| H                                                               | 3.55640000  | 12.88910000 | 1.12320000 | H    | 11.57940000 | 11.51550000 | 0.91550000 |
| H                                                               | 3.00350000  | 11.72640000 | 2.37530000 | H    | 14.52670000 | 11.19480000 | 7.21400000 |
| C                                                               | 6.29310000  | 8.82750000  | 1.02450000 | H    | 13.40120000 | 6.26890000  | 8.81850000 |
| H                                                               | 6.86120000  | 8.11640000  | 1.63370000 | H    | 9.65010000  | 12.04580000 | 0.01030000 |
| H                                                               | 5.66000000  | 8.25960000  | 0.34260000 | H    | 9.42740000  | 14.60160000 | 4.06310000 |
| C                                                               | 5.67620000  | 12.23340000 | 8.15360000 | H    | 5.09360000  | 13.15810000 | 8.24920000 |
| H                                                               | 5.92010000  | 11.84150000 | 9.14690000 | H    | 9.78650000  | 5.68280000  | 1.08310000 |

|   |             |             |            |    |             |             |            |
|---|-------------|-------------|------------|----|-------------|-------------|------------|
| H | 6.59230000  | 12.43600000 | 7.59370000 | H  | 6.00630000  | 0.56900000  | 5.39010000 |
| C | 9.78480000  | 11.70790000 | 8.97610000 | H  | 10.45390000 | 1.97390000  | 1.29290000 |
| H | 10.73690000 | 12.07850000 | 8.58270000 | H  | 12.56330000 | 1.74860000  | 6.64340000 |
| H | 8.97900000  | 12.09060000 | 8.34820000 | H  | 2.93210000  | 13.48510000 | 2.69500000 |
| C | 5.53500000  | 7.74750000  | 1.51330000 | H  | 2.06700000  | 8.93080000  | 0.61920000 |
| H | 6.12100000  | 6.86020000  | 1.25750000 | Au | 7.75990000  | 10.41420000 | 4.30780000 |
| H | 6.04270000  | 8.32780000  | 2.29140000 | Au | 10.65920000 | 11.49480000 | 5.32470000 |
| C | 4.26110000  | 4.04220000  | 7.57070000 |    |             |             |            |

| Au <sub>25</sub> (SC <sub>6</sub> H <sub>13</sub> ) <sub>18</sub> <sup>-</sup> |             |             |             |      |             |             |             |
|--------------------------------------------------------------------------------|-------------|-------------|-------------|------|-------------|-------------|-------------|
| Atom                                                                           | x           | y           | z           | Atom | x           | y           | z           |
| Au                                                                             | 7.81970000  | 10.39880000 | 4.23250000  | H    | 9.26220000  | 8.92880000  | -4.12540000 |
| Au                                                                             | 10.72730000 | 11.50720000 | 5.22860000  | C    | 10.57850000 | 10.37330000 | -6.00040000 |
| Au                                                                             | 12.58510000 | 8.45130000  | 5.95030000  | H    | 12.19150000 | 9.46540000  | -4.86980000 |
| Au                                                                             | 10.06090000 | 6.20440000  | 5.72080000  | H    | 11.14390000 | 8.30840000  | -5.68010000 |
| Au                                                                             | 6.24960000  | 9.17410000  | 6.54020000  | C    | 11.33150000 | 10.57680000 | -7.31320000 |
| Au                                                                             | 5.06190000  | 11.74820000 | 4.97310000  | H    | 9.52040000  | 10.15540000 | -6.21590000 |
| Au                                                                             | 6.54360000  | 11.32820000 | 1.52600000  | H    | 10.57600000 | 11.31210000 | -5.42510000 |
| Au                                                                             | 7.84680000  | 8.39920000  | 1.93880000  | H    | 10.89370000 | 11.39490000 | -7.89990000 |
| Au                                                                             | 9.30430000  | 9.04460000  | 6.57910000  | H    | 12.38790000 | 10.82060000 | -7.13350000 |
| Au                                                                             | 7.58420000  | 9.33770000  | 9.39130000  | H    | 11.30370000 | 9.66720000  | -7.93080000 |
| Au                                                                             | 4.56210000  | 7.36060000  | 8.57110000  | C    | 11.38260000 | 12.75670000 | 0.03690000  |
| Au                                                                             | 5.22110000  | 6.52590000  | 5.52410000  | C    | 12.44730000 | 13.39640000 | -0.85330000 |
| Au                                                                             | 7.70940000  | 4.71050000  | 5.16430000  | H    | 11.25840000 | 13.35540000 | 0.95500000  |
| Au                                                                             | 4.77960000  | 3.62320000  | 4.15660000  | H    | 10.40480000 | 12.78140000 | -0.46760000 |
| Au                                                                             | 2.87810000  | 6.71310000  | 3.48670000  | C    | 12.16400000 | 14.83700000 | -1.27820000 |
| Au                                                                             | 5.43280000  | 8.92790000  | 3.62390000  | H    | 13.41590000 | 13.35820000 | -0.32750000 |
| Au                                                                             | 9.17290000  | 5.93260000  | 2.85790000  | H    | 12.57940000 | 12.77650000 | -1.75640000 |
| Au                                                                             | 10.57350000 | 3.36310000  | 4.57020000  | C    | 13.28290000 | 15.40400000 | -2.14840000 |
| Au                                                                             | 9.03540000  | 3.85250000  | 7.89640000  | H    | 11.20670000 | 14.88260000 | -1.82080000 |
| Au                                                                             | 7.52740000  | 6.74900000  | 7.41110000  | H    | 12.03090000 | 15.46210000 | -0.38070000 |
| Au                                                                             | 6.18560000  | 6.09230000  | 2.81050000  | H    | 13.08960000 | 16.44420000 | -2.43970000 |
| Au                                                                             | 7.89520000  | 5.80340000  | 0.06260000  | H    | 14.24490000 | 15.37700000 | -1.61780000 |
| Au                                                                             | 10.94850000 | 7.74260000  | 0.83460000  | H    | 13.40510000 | 14.81480000 | -3.06800000 |
| Au                                                                             | 10.24600000 | 8.62750000  | 3.85930000  | C    | 15.17200000 | 11.65120000 | 8.89940000  |
| Au                                                                             | 7.74490000  | 7.57270000  | 4.68970000  | C    | 16.60600000 | 12.14860000 | 9.06360000  |
| S                                                                              | 8.68030000  | 12.64750000 | 5.04540000  | H    | 14.97760000 | 10.82380000 | 9.60120000  |
| S                                                                              | 12.95260000 | 10.72850000 | 5.45960000  | H    | 14.47850000 | 12.45600000 | 9.19700000  |
| S                                                                              | 12.42190000 | 6.21410000  | 6.59810000  | C    | 16.94180000 | 12.58500000 | 10.48950000 |
| S                                                                              | 5.26640000  | 12.81480000 | 2.85250000  | H    | 17.31230000 | 11.36540000 | 8.74230000  |
| S                                                                              | 7.71370000  | 9.98800000  | -0.06530000 | H    | 16.76510000 | 12.99620000 | 8.37600000  |
| S                                                                              | 4.74040000  | 11.03390000 | 7.22640000  | C    | 18.36240000 | 13.12470000 | 10.61840000 |
| S                                                                              | 9.85500000  | 9.80720000  | 8.86400000  | H    | 16.22110000 | 13.35150000 | 10.81640000 |
| S                                                                              | 5.39680000  | 8.88720000  | 10.20740000 | H    | 16.80090000 | 11.73150000 | 11.17250000 |
| S                                                                              | 3.43720000  | 5.79940000  | 7.16050000  | H    | 18.58990000 | 13.41080000 | 11.65270000 |
| C                                                                              | 8.80540000  | 13.76320000 | 3.56470000  | H    | 19.10310000 | 12.37480000 | 10.30610000 |
| H                                                                              | 9.32600000  | 13.23160000 | 2.76020000  | H    | 18.50650000 | 14.01300000 | 9.98710000  |
| H                                                                              | 7.77680000  | 13.94050000 | 3.23140000  | C    | 10.94490000 | 14.96570000 | 4.25000000  |
| C                                                                              | 9.46680000  | 15.08420000 | 3.90540000  | C    | 11.58530000 | 16.33850000 | 4.39410000  |
| H                                                                              | 8.92400000  | 15.55260000 | 4.74160000  | H    | 11.46700000 | 14.37460000 | 3.47950000  |
| H                                                                              | 9.34040000  | 15.75830000 | 3.04010000  | H    | 11.05820000 | 14.39130000 | 5.18150000  |
| C                                                                              | 13.38870000 | 11.41040000 | 7.13010000  | C    | 13.05960000 | 16.27630000 | 4.77890000  |
| H                                                                              | 13.14470000 | 12.48100000 | 7.10560000  | H    | 11.47600000 | 16.89940000 | 3.45060000  |
| H                                                                              | 12.74650000 | 10.92950000 | 7.87720000  | H    | 11.03340000 | 16.91990000 | 5.15150000  |
| C                                                                              | 14.85930000 | 11.20280000 | 7.46100000  | C    | 13.66220000 | 17.66900000 | 4.92460000  |
| H                                                                              | 15.11240000 | 10.14130000 | 7.31990000  | H    | 13.16240000 | 15.71820000 | 5.72220000  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 15.47940000 | 11.76690000 | 6.74720000  | H | 13.61380000 | 15.69490000 | 4.02570000  |
| C | 12.25610000 | 6.41170000  | 8.43540000  | H | 14.72310000 | 17.63230000 | 5.20200000  |
| H | 11.50290000 | 7.18150000  | 8.63430000  | H | 13.58140000 | 18.23050000 | 3.98360000  |
| H | 11.87300000 | 5.45200000  | 8.81040000  | H | 13.13170000 | 18.24450000 | 5.69640000  |
| C | 13.59500000 | 6.75190000  | 9.08090000  | C | 13.55850000 | 6.78620000  | 10.61720000 |
| H | 14.34410000 | 6.01370000  | 8.75410000  | C | 14.94980000 | 6.60120000  | 11.22640000 |
| H | 13.93300000 | 7.72200000  | 8.68620000  | H | 12.88750000 | 5.99560000  | 10.99150000 |
| C | 3.58170000  | 12.69880000 | 2.11470000  | H | 13.12270000 | 7.73510000  | 10.96520000 |
| H | 3.65950000  | 13.10410000 | 1.09620000  | C | 14.98450000 | 6.58560000  | 12.75490000 |
| H | 3.31130000  | 11.63880000 | 2.05770000  | H | 15.38090000 | 5.66020000  | 10.84690000 |
| C | 2.53660000  | 13.46020000 | 2.91420000  | H | 15.61310000 | 7.40240000  | 10.86000000 |
| H | 2.76270000  | 14.53830000 | 2.94810000  | C | 16.39650000 | 6.38780000  | 13.30230000 |
| H | 2.54050000  | 13.11490000 | 3.95830000  | H | 14.55990000 | 7.52440000  | 13.14340000 |
| C | 6.31250000  | 9.31790000  | -1.10820000 | H | 14.32670000 | 5.78300000  | 13.12380000 |
| H | 6.59530000  | 8.29660000  | -1.39390000 | H | 16.41220000 | 6.38390000  | 14.39940000 |
| H | 5.43660000  | 9.24280000  | -0.46140000 | H | 16.82360000 | 5.43670000  | 12.95600000 |
| C | 6.00040000  | 10.15530000 | -2.34410000 | H | 17.06710000 | 7.18910000  | 12.96190000 |
| H | 6.88720000  | 10.21040000 | -2.99610000 | C | 10.56560000 | 13.70030000 | 10.11630000 |
| H | 5.23730000  | 9.59370000  | -2.91020000 | C | 10.83840000 | 14.27230000 | 11.50420000 |
| C | 5.74280000  | 12.35500000 | 8.08090000  | H | 9.83620000  | 14.32950000 | 9.58210000  |
| H | 5.98870000  | 11.95990000 | 9.07670000  | H | 11.49410000 | 13.74400000 | 9.52220000  |
| H | 6.67000000  | 12.48120000 | 7.51290000  | C | 11.41680000 | 15.68610000 | 11.47890000 |
| C | 4.95680000  | 13.66360000 | 8.16040000  | H | 9.91010000  | 14.26260000 | 12.09860000 |
| H | 4.61110000  | 13.88890000 | 7.14160000  | H | 11.54040000 | 13.60780000 | 12.03390000 |
| H | 4.05370000  | 13.49750000 | 8.76690000  | C | 11.69950000 | 16.23040000 | 12.87530000 |
| C | 9.89050000  | 11.65130000 | 8.77350000  | H | 12.34680000 | 15.68440000 | 10.88780000 |
| H | 10.73080000 | 11.89890000 | 8.11270000  | H | 10.72270000 | 16.35270000 | 10.94540000 |
| H | 8.98420000  | 12.00680000 | 8.27440000  | H | 12.12950000 | 17.23960000 | 12.84210000 |
| C | 10.07780000 | 12.25190000 | 10.15910000 | H | 10.78180000 | 16.27360000 | 13.47860000 |
| H | 9.13540000  | 12.17430000 | 10.71920000 | H | 12.41020000 | 15.58400000 | 13.40880000 |
| H | 10.80690000 | 11.64240000 | 10.71320000 | C | 9.93170000  | 3.90050000  | 11.64580000 |
| C | 5.85490000  | 7.66730000  | 11.52680000 | C | 10.23550000 | 3.18600000  | 12.95950000 |
| H | 6.36390000  | 6.83990000  | 11.02040000 | H | 10.87390000 | 4.07100000  | 11.09710000 |
| H | 6.57610000  | 8.18170000  | 12.17340000 | H | 9.32820000  | 3.24520000  | 11.00130000 |
| C | 4.68230000  | 7.13730000  | 12.34060000 | C | 10.96070000 | 1.85600000  | 12.74450000 |
| H | 4.23680000  | 7.95350000  | 12.92750000 | H | 10.85220000 | 3.83860000  | 13.59990000 |
| H | 3.89800000  | 6.78460000  | 11.65580000 | H | 9.29900000  | 3.01570000  | 13.51830000 |
| C | 4.19340000  | 4.18330000  | 7.67970000  | C | 11.29030000 | 1.13210000  | 14.04590000 |
| H | 3.84580000  | 3.46500000  | 6.92400000  | H | 10.33900000 | 1.20970000  | 12.10730000 |
| H | 5.28250000  | 4.27290000  | 7.58620000  | H | 11.88630000 | 2.03800000  | 12.17350000 |
| C | 3.76440000  | 3.75970000  | 9.07710000  | H | 11.81450000 | 0.18550000  | 13.86220000 |
| H | 4.19850000  | 4.46720000  | 9.79860000  | H | 11.93520000 | 1.74920000  | 14.68650000 |
| H | 2.67400000  | 3.88160000  | 9.15060000  | H | 10.37850000 | 0.90730000  | 14.61870000 |
| S | 6.85230000  | 2.48660000  | 4.29470000  | C | 14.60360000 | 2.11710000  | 7.27410000  |
| S | 2.56540000  | 4.41160000  | 3.97780000  | C | 15.40100000 | 0.81600000  | 7.38810000  |
| S | 3.02310000  | 9.01660000  | 2.88120000  | H | 14.55170000 | 2.59240000  | 8.26770000  |
| S | 10.41980000 | 2.32600000  | 6.70520000  | H | 15.14960000 | 2.83080000  | 6.64070000  |
| S | 7.73020000  | 5.23710000  | 9.38280000  | C | 16.82730000 | 0.95720000  | 7.91820000  |
| S | 10.82800000 | 4.12100000  | 2.35050000  | H | 14.84140000 | 0.12500000  | 8.03870000  |
| S | 5.64530000  | 5.31950000  | 0.52930000  | H | 15.43500000 | 0.32880000  | 6.40060000  |
| S | 10.04360000 | 6.25020000  | -0.77770000 | C | 17.53030000 | -0.39420000 | 8.03650000  |
| S | 12.07400000 | 9.24980000  | 2.28740000  | H | 17.40180000 | 1.62280000  | 7.25680000  |
| C | 6.66940000  | 1.40810000  | 5.79900000  | H | 16.81110000 | 1.45300000  | 8.90080000  |
| H | 6.13680000  | 1.97500000  | 6.57020000  | H | 18.55750000 | -0.29860000 | 8.41380000  |
| H | 7.69740000  | 1.26030000  | 6.15350000  | H | 16.98350000 | -1.05640000 | 8.72190000  |
| C | 5.99080000  | 0.07060000  | 5.52090000  | H | 17.57440000 | -0.90190000 | 7.06290000  |
| H | 6.56110000  | -0.45870000 | 4.74190000  | C | 9.86130000  | 0.29120000  | 0.82130000  |
| H | 6.07650000  | -0.53920000 | 6.43730000  | C | 10.77000000 | -0.78340000 | 0.21920000  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 2.08010000  | 3.64870000  | 2.35720000  | H | 9.16110000  | 0.64740000  | 0.04880000  |
| H | 2.23710000  | 2.56640000  | 2.46240000  | H | 9.23700000  | -0.15700000 | 1.61000000  |
| H | 2.76320000  | 4.02110000  | 1.58670000  | C | 10.05020000 | -2.02330000 | -0.31430000 |
| C | 0.63610000  | 3.95510000  | 1.98870000  | H | 11.35460000 | -0.33120000 | -0.59780000 |
| H | 0.48360000  | 5.04150000  | 2.06490000  | H | 11.50460000 | -1.09740000 | 0.97800000  |
| H | -0.04440000 | 3.49450000  | 2.72230000  | C | 11.00410000 | -3.04150000 | -0.93640000 |
| C | 3.09650000  | 8.84230000  | 1.03090000  | H | 9.48710000  | -2.49410000 | 0.50600000  |
| H | 3.89860000  | 8.13340000  | 0.79880000  | H | 9.30010000  | -1.71820000 | -1.05970000 |
| H | 3.39480000  | 9.83240000  | 0.66310000  | H | 10.47110000 | -3.92590000 | -1.30890000 |
| C | 1.79160000  | 8.40870000  | 0.36800000  | H | 11.54860000 | -2.60040000 | -1.78290000 |
| H | 0.97430000  | 9.06780000  | 0.69980000  | H | 11.75300000 | -3.37990000 | -0.20710000 |
| H | 1.54350000  | 7.39980000  | 0.73020000  | C | 4.89820000  | 1.42980000  | -0.75520000 |
| C | 12.08970000 | 2.64790000  | 7.44660000  | C | 4.70550000  | 0.81920000  | -2.14070000 |
| H | 12.03410000 | 2.33510000  | 8.49850000  | H | 3.92110000  | 1.46350000  | -0.24480000 |
| H | 12.27890000 | 3.72630000  | 7.40040000  | H | 5.53490000  | 0.77110000  | -0.14410000 |
| C | 13.18350000 | 1.89180000  | 6.70160000  | C | 3.99990000  | -0.53610000 | -2.11200000 |
| H | 12.94530000 | 0.81830000  | 6.72050000  | H | 4.11480000  | 1.51290000  | -2.76080000 |
| H | 13.14680000 | 2.19710000  | 5.64640000  | H | 5.68190000  | 0.72340000  | -2.64290000 |
| C | 8.99820000  | 5.99830000  | 10.51340000 | C | 3.78050000  | -1.13500000 | -3.49730000 |
| H | 8.63550000  | 7.01530000  | 10.70860000 | H | 4.58030000  | -1.23310000 | -1.48890000 |
| H | 9.93440000  | 6.08460000  | 9.95620000  | H | 3.02900000  | -0.41660000 | -1.60500000 |
| C | 9.21050000  | 5.23690000  | 11.81940000 | H | 3.25190000  | -2.09600000 | -3.44770000 |
| H | 8.23870000  | 5.08070000  | 12.31430000 | H | 3.18380000  | -0.46100000 | -4.12740000 |
| H | 9.79940000  | 5.88050000  | 12.49540000 | H | 4.73750000  | -1.30320000 | -4.01130000 |
| C | 9.85810000  | 2.76930000  | 1.51690000  | C | 4.51950000  | 0.14180000  | 5.10660000  |
| H | 9.60510000  | 3.16010000  | 0.52260000  | C | 3.81030000  | -1.21060000 | 5.15000000  |
| H | 8.93340000  | 2.62640000  | 2.08770000  | H | 4.45840000  | 0.55910000  | 4.09200000  |
| C | 10.65520000 | 1.47130000  | 1.41070000  | H | 3.98390000  | 0.85860000  | 5.74860000  |
| H | 11.00850000 | 1.21030000  | 2.41860000  | C | 2.36680000  | -1.16210000 | 4.64680000  |
| H | 11.55210000 | 1.65500000  | 0.79980000  | H | 4.37740000  | -1.94180000 | 4.55070000  |
| C | 5.55180000  | 3.47360000  | 0.61180000  | H | 3.82280000  | -1.59760000 | 6.18290000  |
| H | 4.65190000  | 3.25590000  | 1.19970000  | C | 1.66380000  | -2.51560000 | 4.69840000  |
| H | 6.40220000  | 3.09850000  | 1.18950000  | H | 1.80070000  | -0.42800000 | 5.24030000  |
| C | 5.47260000  | 2.84710000  | -0.77520000 | H | 2.36070000  | -0.78290000 | 3.61340000  |
| H | 6.47320000  | 2.86060000  | -1.22900000 | H | 0.62940000  | -2.45840000 | 4.33490000  |
| H | 4.84270000  | 3.47790000  | -1.41900000 | H | 2.19250000  | -3.25580000 | 4.08130000  |
| C | 9.55490000  | 7.43950000  | -2.11040000 | H | 1.63530000  | -2.90560000 | 5.72520000  |
| H | 9.02670000  | 8.27180000  | -1.62950000 | C | 1.19300000  | 13.18010000 | 2.22970000  |
| H | 8.85090000  | 6.90630000  | -2.76090000 | C | 0.23100000  | 14.36390000 | 2.23370000  |
| C | 10.75300000 | 7.95270000  | -2.90260000 | H | 0.71910000  | 12.30240000 | 2.69530000  |
| H | 11.21060000 | 7.12980000  | -3.47120000 | H | 1.37780000  | 12.88950000 | 1.18060000  |
| H | 11.51520000 | 8.30010000  | -2.19160000 | C | -1.03340000 | 14.03070000 | 1.44490000  |
| C | 11.35610000 | 10.89350000 | 1.80350000  | H | -0.02290000 | 14.65260000 | 3.26710000  |
| H | 11.74260000 | 11.59350000 | 2.55840000  | H | 0.72890000  | 15.24200000 | 1.78770000  |
| H | 10.26710000 | 10.84190000 | 1.92000000  | C | -2.04220000 | 15.17420000 | 1.39410000  |
| C | 11.75610000 | 11.30350000 | 0.39580000  | H | -0.74780000 | 13.74610000 | 0.41920000  |
| H | 11.28580000 | 10.60020000 | -0.30600000 | H | -1.50170000 | 13.13630000 | 1.88620000  |
| H | 12.84160000 | 11.16240000 | 0.28530000  | H | -2.92580000 | 14.89830000 | 0.80370000  |
| C | 0.30860000  | 3.45670000  | 0.56930000  | H | -2.37850000 | 15.45010000 | 2.40220000  |
| C | -1.13300000 | 2.99050000  | 0.37910000  | H | -1.60150000 | 16.07030000 | 0.93440000  |
| H | 0.98730000  | 2.62730000  | 0.30840000  | C | 5.71810000  | 14.89030000 | 8.69660000  |
| H | 0.52750000  | 4.25540000  | -0.15730000 | C | 4.78090000  | 16.00390000 | 9.17810000  |
| C | -1.42540000 | 2.53820000  | -1.05180000 | H | 6.35740000  | 15.28450000 | 7.89190000  |
| H | -1.34030000 | 2.16440000  | 1.08010000  | H | 6.39860000  | 14.60120000 | 9.51310000  |
| H | -1.82650000 | 3.80030000  | 0.66010000  | C | 5.46620000  | 17.31060000 | 9.58250000  |
| C | -2.85440000 | 2.04570000  | -1.25650000 | H | 4.05390000  | 16.22230000 | 8.37850000  |
| H | -1.22420000 | 3.37560000  | -1.73950000 | H | 4.18650000  | 15.62830000 | 10.02600000 |
| H | -0.71550000 | 1.74380000  | -1.33200000 | C | 4.48280000  | 18.37700000 | 10.06650000 |



|   |             |             |             |   |            |             |             |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| H | -3.03070000 | 1.75270000  | -2.29890000 | H | 6.20490000 | 17.10760000 | 10.37310000 |
| H | -3.06870000 | 1.17300000  | -0.62360000 | H | 6.03710000 | 17.69840000 | 8.72470000  |
| H | -3.58430000 | 2.82670000  | -0.99980000 | H | 4.99480000 | 19.30650000 | 10.34970000 |
| C | 1.86750000  | 8.42350000  | -1.16870000 | H | 3.75140000 | 18.62430000 | 9.28480000  |
| C | 0.49100000  | 8.48270000  | -1.83450000 | H | 3.91890000 | 18.02710000 | 10.94200000 |
| H | 2.41340000  | 7.53810000  | -1.52980000 | C | 5.16350000 | 5.99900000  | 13.25670000 |
| H | 2.46330000  | 9.29000000  | -1.49810000 | C | 4.36420000 | 5.84500000  | 14.54910000 |
| C | 0.51810000  | 8.55000000  | -3.36190000 | H | 6.22200000 | 6.16470000  | 13.51750000 |
| H | -0.10080000 | 7.60650000  | -1.52340000 | H | 5.14730000 | 5.05000000  | 12.69850000 |
| H | -0.05140000 | 9.36040000  | -1.44520000 | C | 4.89870000 | 4.73440000  | 15.45100000 |
| C | -0.88180000 | 8.62490000  | -3.96930000 | H | 4.38050000 | 6.80170000  | 15.09700000 |
| H | 1.10440000  | 9.42810000  | -3.67560000 | H | 3.30470000 | 5.65250000  | 14.31280000 |
| H | 1.05440000  | 7.67550000  | -3.76370000 | C | 4.12750000 | 4.59810000  | 16.76160000 |
| H | -0.84790000 | 8.67670000  | -5.06460000 | H | 4.87500000 | 3.78080000  | 14.90100000 |
| H | -1.47890000 | 7.74520000  | -3.69230000 | H | 5.96190000 | 4.92630000  | 15.66700000 |
| H | -1.42220000 | 9.51050000  | -3.60590000 | H | 4.52700000 | 3.78620000  | 17.38200000 |
| C | 5.47010000  | 11.57330000 | -2.09610000 | H | 4.18070000 | 5.52800000  | 17.34600000 |
| C | 4.94930000  | 12.18920000 | -3.40100000 | H | 3.06450000 | 4.38800000  | 16.57640000 |
| H | 6.26380000  | 12.18890000 | -1.64680000 | C | 4.14900000 | 2.31410000  | 9.45340000  |
| H | 4.66110000  | 11.54880000 | -1.34790000 | C | 3.12080000 | 1.66650000  | 10.38090000 |
| C | 4.46620000  | 13.64020000 | -3.34790000 | H | 5.14100000 | 2.30660000  | 9.92890000  |
| H | 5.73950000  | 12.11440000 | -4.16540000 | H | 4.24580000 | 1.70210000  | 8.54090000  |
| H | 4.12210000  | 11.55910000 | -3.77200000 | C | 3.44400000 | 0.24210000  | 10.83410000 |
| C | 3.90780000  | 14.10860000 | -4.69420000 | H | 2.99140000 | 2.30010000  | 11.27520000 |
| H | 3.69260000  | 13.74750000 | -2.57050000 | H | 2.14420000 | 1.66830000  | 9.86990000  |
| H | 5.29540000  | 14.29640000 | -3.04090000 | C | 2.35350000 | -0.34060000 | 11.72940000 |
| H | 3.57200000  | 15.15300000 | -4.65900000 | H | 3.57550000 | -0.39910000 | 9.94710000  |
| H | 4.66610000  | 14.02890000 | -5.48690000 | H | 4.41050000 | 0.23330000  | 11.36100000 |
| H | 3.05040000  | 13.49250000 | -5.00270000 | H | 2.57670000 | -1.37180000 | 12.03110000 |
| C | 10.31500000 | 9.09000000  | -3.84020000 | H | 2.22940000 | 0.25510000  | 12.64520000 |
| C | 11.13750000 | 9.25730000  | -5.11840000 | H | 1.38540000 | -0.34610000 | 11.20940000 |
| H | 10.32260000 | 10.03950000 | -3.28320000 |   |            |             |             |

| Au <sub>25</sub> (SCH <sub>2</sub> H <sub>2</sub> Ph) <sub>18</sub> <sup>-</sup> |             |             |            |      |             |             |             |
|----------------------------------------------------------------------------------|-------------|-------------|------------|------|-------------|-------------|-------------|
| Atom                                                                             | x           | y           | z          | Atom | x           | y           | z           |
| Au                                                                               | 7.80640000  | 10.42610000 | 4.25300000 | H    | 2.83830000  | 4.03840000  | 9.33690000  |
| Au                                                                               | 10.70610000 | 11.53410000 | 5.28330000 | C    | 4.16160000  | 2.34880000  | 9.43210000  |
| Au                                                                               | 12.56020000 | 8.46630000  | 5.96460000 | C    | 3.10530000  | 1.46060000  | 9.68310000  |
| Au                                                                               | 10.11620000 | 6.24800000  | 5.68800000 | H    | 2.08340000  | 1.84140000  | 9.68910000  |
| Au                                                                               | 6.26400000  | 9.11090000  | 6.60160000 | C    | 3.34530000  | 0.10650000  | 9.92920000  |
| Au                                                                               | 5.02160000  | 11.76890000 | 4.89310000 | H    | 2.51050000  | -0.56320000 | 10.13490000 |
| Au                                                                               | 6.47900000  | 11.38010000 | 1.56180000 | C    | 4.65260000  | -0.38250000 | 9.91740000  |
| Au                                                                               | 7.95760000  | 8.41480000  | 1.96720000 | H    | 4.84280000  | -1.43810000 | 10.10930000 |
| Au                                                                               | 9.32240000  | 9.06690000  | 6.57010000 | C    | 5.71520000  | 0.49080000  | 9.66860000  |
| Au                                                                               | 7.55670000  | 9.27450000  | 9.39960000 | H    | 6.73980000  | 0.12020000  | 9.65530000  |
| Au                                                                               | 4.58490000  | 7.28180000  | 8.59130000 | C    | 5.47280000  | 1.84640000  | 9.43250000  |
| Au                                                                               | 5.23850000  | 6.50550000  | 5.49300000 | H    | 6.31340000  | 2.51880000  | 9.24470000  |
| Au                                                                               | 7.70050000  | 4.71760000  | 5.13770000 | S    | 6.87400000  | 2.50820000  | 4.33410000  |
| Au                                                                               | 4.78710000  | 3.59660000  | 4.18330000 | S    | 2.55380000  | 4.35910000  | 3.97930000  |
| Au                                                                               | 2.91130000  | 6.65240000  | 3.52530000 | S    | 3.05900000  | 8.94860000  | 2.91600000  |
| Au                                                                               | 5.44720000  | 8.84710000  | 3.60560000 | S    | 10.31680000 | 2.34910000  | 6.56560000  |
| Au                                                                               | 9.15540000  | 5.93030000  | 2.81630000 | S    | 7.74540000  | 5.18520000  | 9.36200000  |
| Au                                                                               | 10.50230000 | 3.44900000  | 4.47880000 | S    | 10.82750000 | 4.17990000  | 2.23320000  |
| Au                                                                               | 8.99660000  | 3.82360000  | 7.86670000 | S    | 5.69180000  | 5.32170000  | 0.50380000  |
| Au                                                                               | 7.64380000  | 6.74610000  | 7.41210000 | S    | 10.09340000 | 6.37230000  | -0.84430000 |
| Au                                                                               | 6.22620000  | 6.09050000  | 2.80180000 | S    | 12.04690000 | 9.29220000  | 2.28390000  |

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Au | 7.94300000  | 5.85700000  | 0.00140000  | C | 6.68980000  | 1.37770000  | 5.79050000  |
| Au | 10.90660000 | 7.81790000  | 0.84610000  | H | 6.14000000  | 1.88650000  | 6.58810000  |
| Au | 10.24770000 | 8.69160000  | 3.91190000  | H | 7.70910000  | 1.19790000  | 6.15310000  |
| Au | 7.76730000  | 7.57620000  | 4.70180000  | C | 6.02760000  | 0.05310000  | 5.39940000  |
| S  | 8.62660000  | 12.63200000 | 5.10860000  | H | 6.59910000  | -0.40330000 | 4.57860000  |
| S  | 12.92520000 | 10.75190000 | 5.50390000  | H | 6.11750000  | -0.62610000 | 6.26350000  |
| S  | 12.41300000 | 6.19280000  | 6.60470000  | C | 4.57770000  | 0.17840000  | 5.00570000  |
| S  | 5.14990000  | 12.86970000 | 2.81920000  | C | 3.59440000  | 0.36930000  | 5.98670000  |
| S  | 7.70960000  | 10.02990000 | 0.05370000  | H | 3.88150000  | 0.41600000  | 7.03840000  |
| S  | 4.75620000  | 11.01040000 | 7.11580000  | C | 2.25280000  | 0.50840000  | 5.63300000  |
| S  | 9.81760000  | 9.80390000  | 8.89680000  | H | 1.50550000  | 0.66320000  | 6.41040000  |
| S  | 5.39800000  | 8.76600000  | 10.25170000 | C | 1.86730000  | 0.44160000  | 4.29280000  |
| S  | 3.48730000  | 5.77180000  | 7.15130000  | H | 0.81700000  | 0.54190000  | 4.01870000  |
| C  | 8.79230000  | 13.76220000 | 3.64930000  | C | 2.83620000  | 0.24100000  | 3.30750000  |
| H  | 9.34100000  | 13.23920000 | 2.85930000  | H | 2.55560000  | 0.18150000  | 2.25550000  |
| H  | 7.77110000  | 13.94460000 | 3.29440000  | C | 4.18070000  | 0.12430000  | 3.66380000  |
| C  | 9.47310000  | 15.09030000 | 4.00520000  | H | 4.93300000  | -0.00510000 | 2.88750000  |
| H  | 8.90990000  | 15.56860000 | 4.81830000  | C | 2.11260000  | 3.68410000  | 2.30450000  |
| H  | 9.38490000  | 15.73620000 | 3.11670000  | H | 2.23540000  | 2.59720000  | 2.36140000  |
| C  | 10.92400000 | 14.99240000 | 4.40900000  | H | 2.82950000  | 4.07680000  | 1.57840000  |
| C  | 11.93230000 | 14.77840000 | 3.45730000  | C | 0.68220000  | 4.05660000  | 1.90630000  |
| H  | 11.67300000 | 14.69140000 | 2.40100000  | H | 0.57110000  | 5.14620000  | 1.99370000  |
| C  | 13.26580000 | 14.66670000 | 3.85330000  | H | -0.02570000 | 3.60190000  | 2.61360000  |
| H  | 14.03450000 | 14.49440000 | 3.10230000  | C | 0.37650000  | 3.60690000  | 0.49980000  |
| C  | 13.61610000 | 14.78310000 | 5.20000000  | C | -0.19480000 | 2.35480000  | 0.23740000  |
| H  | 14.66060000 | 14.70540000 | 5.50340000  | H | -0.45650000 | 1.70130000  | 1.07120000  |
| C  | 12.62220000 | 15.00300000 | 6.15390000  | C | -0.44090000 | 1.93840000  | -1.07230000 |
| H  | 12.87580000 | 15.10000000 | 7.20930000  | H | -0.89600000 | 0.96450000  | -1.25140000 |
| C  | 11.28760000 | 15.09430000 | 5.75610000  | C | -0.11520000 | 2.77100000  | -2.14430000 |
| H  | 10.51470000 | 15.23670000 | 6.50730000  | H | -0.31180000 | 2.45380000  | -3.16720000 |
| C  | 13.38380000 | 11.40960000 | 7.17970000  | C | 0.45960000  | 4.01890000  | -1.89700000 |
| H  | 13.17670000 | 12.48500000 | 7.17070000  | H | 0.71630000  | 4.68190000  | -2.72210000 |
| H  | 12.73410000 | 10.93290000 | 7.92080000  | C | 0.70150000  | 4.43020000  | -0.58680000 |
| C  | 14.85260000 | 11.13470000 | 7.50980000  | H | 1.14260000  | 5.41160000  | -0.41020000 |
| H  | 15.04120000 | 10.05750000 | 7.39550000  | C | 3.20980000  | 8.77320000  | 1.06770000  |
| H  | 15.49910000 | 11.65640000 | 6.79020000  | H | 4.01820000  | 8.06310000  | 0.86450000  |
| C  | 15.15650000 | 11.57510000 | 8.91970000  | H | 3.50740000  | 9.75310000  | 0.67370000  |
| C  | 15.63180000 | 12.86270000 | 9.20030000  | C | 1.89930000  | 8.30150000  | 0.42840000  |
| H  | 15.83360000 | 13.54800000 | 8.37530000  | H | 1.07790000  | 8.95450000  | 0.75170000  |
| C  | 15.85150000 | 13.27580000 | 10.51570000 | H | 1.68320000  | 7.29750000  | 0.82690000  |
| H  | 16.22170000 | 14.28200000 | 10.71060000 | C | 1.95230000  | 8.26990000  | -1.07980000 |
| C  | 15.59140000 | 12.40730000 | 11.57780000 | C | 1.10870000  | 9.09100000  | -1.84330000 |
| H  | 15.76280000 | 12.72530000 | 12.60450000 | H | 0.40610000  | 9.74880000  | -1.33000000 |
| C  | 15.11900000 | 11.12080000 | 11.31080000 | C | 1.16610000  | 9.08260000  | -3.23840000 |
| H  | 14.91450000 | 10.42770000 | 12.12640000 | H | 0.50470000  | 9.72840000  | -3.81290000 |
| C  | 14.90210000 | 10.71280000 | 9.99500000  | C | 2.07700000  | 8.25420000  | -3.89490000 |
| H  | 14.53540000 | 9.70370000  | 9.80210000  | H | 2.12730000  | 8.24660000  | -4.98240000 |
| C  | 12.27210000 | 6.35960000  | 8.43980000  | C | 2.92600000  | 7.43270000  | -3.14770000 |
| H  | 11.45990000 | 7.06240000  | 8.65110000  | H | 3.64200000  | 6.78250000  | -3.65050000 |
| H  | 11.99070000 | 5.37420000  | 8.82940000  | C | 2.86510000  | 7.44000000  | -1.75310000 |
| C  | 13.59350000 | 6.83820000  | 9.05000000  | H | 3.53950000  | 6.79830000  | -1.18370000 |
| H  | 14.40890000 | 6.18180000  | 8.71770000  | C | 11.97800000 | 2.58440000  | 7.34400000  |
| H  | 13.80070000 | 7.83800000  | 8.63530000  | H | 11.90190000 | 2.20140000  | 8.36830000  |
| C  | 13.56260000 | 6.87430000  | 10.55660000 | H | 12.18300000 | 3.65890000  | 7.37810000  |
| C  | 14.40490000 | 6.03380000  | 11.29960000 | C | 13.08030000 | 1.88380000  | 6.55100000  |
| H  | 15.08420000 | 5.36510000  | 10.77000000 | H | 12.87550000 | 0.80690000  | 6.48410000  |
| C  | 14.37230000 | 6.03610000  | 12.69420000 | H | 13.06310000 | 2.27920000  | 5.52450000  |
| H  | 15.02960000 | 5.37130000  | 13.25300000 | C | 14.42980000 | 2.12300000  | 7.17810000  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 13.49030000 | 6.88040000  | 13.37090000 | C | 15.07920000 | 1.12600000  | 7.91600000  |
| H | 13.45950000 | 6.88040000  | 14.45910000 | H | 14.60840000 | 0.14750000  | 8.01430000  |
| C | 12.64520000 | 7.72450000  | 12.64410000 | C | 16.31860000 | 1.37040000  | 8.51040000  |
| H | 11.95420000 | 8.38530000  | 13.16550000 | H | 16.81740000 | 0.57760000  | 9.06580000  |
| C | 12.67890000 | 7.72110000  | 11.24810000 | C | 16.92070000 | 2.62360000  | 8.38340000  |
| H | 12.00790000 | 8.37770000  | 10.69000000 | H | 17.89060000 | 2.81060000  | 8.84100000  |
| C | 3.48140000  | 12.60550000 | 2.05420000  | C | 16.27740000 | 3.62920000  | 7.65880000  |
| H | 3.54250000  | 12.99570000 | 1.03240000  | H | 16.74170000 | 4.60850000  | 7.55620000  |
| H | 3.29930000  | 11.52780000 | 2.01730000  | C | 15.04300000 | 3.38040000  | 7.05970000  |
| C | 2.36890000  | 13.29470000 | 2.84700000  | H | 14.53460000 | 4.17600000  | 6.51300000  |
| H | 2.56360000  | 14.37480000 | 2.90450000  | C | 9.02390000  | 5.89070000  | 10.51690000 |
| H | 2.37470000  | 12.91200000 | 3.87870000  | H | 8.67820000  | 6.90390000  | 10.75430000 |
| C | 1.03200000  | 13.03580000 | 2.19880000  | H | 9.96280000  | 5.98170000  | 9.96810000  |
| C | 0.39000000  | 14.02790000 | 1.45050000  | C | 9.21790000  | 5.08520000  | 11.80990000 |
| H | 0.86150000  | 15.00800000 | 1.36360000  | H | 8.24270000  | 4.91110000  | 12.28590000 |
| C | -0.83480000 | 13.78410000 | 0.82810000  | H | 9.79690000  | 5.72570000  | 12.49210000 |
| H | -1.32160000 | 14.57770000 | 0.26280000  | C | 9.95980000  | 3.78650000  | 11.62650000 |
| C | -1.43590000 | 12.53090000 | 0.94240000  | C | 9.27150000  | 2.57880000  | 11.44960000 |
| H | -2.39470000 | 12.33740000 | 0.46470000  | H | 8.18320000  | 2.57800000  | 11.47630000 |
| C | -0.80430000 | 11.52990000 | 1.68230000  | C | 9.96650000  | 1.38600000  | 11.24670000 |
| H | -1.27290000 | 10.55100000 | 1.77910000  | H | 9.41310000  | 0.45690000  | 11.11490000 |
| C | 0.41640000  | 11.77920000 | 2.30790000  | C | 11.36150000 | 1.37920000  | 11.22080000 |
| H | 0.90520000  | 10.98740000 | 2.87580000  | H | 11.90310000 | 0.44790000  | 11.06440000 |
| C | 6.38530000  | 9.30140000  | -1.03150000 | C | 12.06000000 | 2.57690000  | 11.39940000 |
| H | 6.72500000  | 8.28930000  | -1.28720000 | H | 13.14890000 | 2.58710000  | 11.37970000 |
| H | 5.46890000  | 9.20180000  | -0.44490000 | C | 11.36200000 | 3.76680000  | 11.60520000 |
| C | 6.14530000  | 10.12260000 | -2.30660000 | H | 11.91590000 | 4.69510000  | 11.75140000 |
| H | 7.10180000  | 10.28430000 | -2.82490000 | C | 9.84450000  | 2.84840000  | 1.37930000  |
| H | 5.52670000  | 9.49640000  | -2.96570000 | H | 9.63640000  | 3.19470000  | 0.35890000  |
| C | 5.42700000  | 11.43070000 | -2.08970000 | H | 8.88840000  | 2.72400000  | 1.89900000  |
| C | 6.11320000  | 12.64250000 | -1.92680000 | C | 10.65100000 | 1.54290000  | 1.40930000  |
| H | 7.20000000  | 12.65260000 | -1.98990000 | H | 10.96040000 | 1.38760000  | 2.45360000  |
| C | 5.41190000  | 13.82670000 | -1.69080000 | H | 11.56570000 | 1.66420000  | 0.81160000  |
| H | 5.95520000  | 14.76240000 | -1.56790000 | C | 9.87560000  | 0.34150000  | 0.93180000  |
| C | 4.01870000  | 13.81760000 | -1.61570000 | C | 9.84180000  | -0.02400000 | -0.42100000 |
| H | 3.47140000  | 14.74210000 | -1.43430000 | H | 10.39900000 | 0.56630000  | -1.14850000 |
| C | 3.32550000  | 12.61550000 | -1.77890000 | C | 9.11930000  | -1.14140000 | -0.84150000 |
| H | 2.23830000  | 12.59520000 | -1.72120000 | H | 9.10240000  | -1.41060000 | -1.89710000 |
| C | 4.02820000  | 11.43510000 | -2.01540000 | C | 8.41910000  | -1.91400000 | 0.08590000  |
| H | 3.48540000  | 10.49900000 | -2.14690000 | H | 7.86080000  | -2.78750000 | -0.24560000 |
| C | 5.70430000  | 12.35220000 | 7.96740000  | C | 8.42830000  | -1.55170000 | -1.43430000 |
| H | 5.88750000  | 12.01530000 | 8.99580000  | H | 7.87260000  | -2.13660000 | 2.16600000  |
| H | 6.66630000  | 12.47940000 | 7.45980000  | C | 9.14810000  | -0.43110000 | 1.84840000  |
| C | 4.88180000  | 13.64620000 | 7.91800000  | H | 9.15150000  | -0.14550000 | 2.90080000  |
| H | 4.58110000  | 13.79890000 | 6.87190000  | C | 5.59490000  | 3.47470000  | 0.58450000  |
| H | 3.96050000  | 13.51610000 | 8.50270000  | H | 4.70900000  | 3.25060000  | 1.18870000  |
| C | 5.65150000  | 14.84700000 | 8.40320000  | H | 6.45640000  | 3.09330000  | 1.13900000  |
| C | 5.66260000  | 15.21370000 | 9.75480000  | C | 5.48040000  | 2.84160000  | -0.80860000 |
| H | 5.08990000  | 14.62300000 | 10.46850000 | H | 6.47780000  | 2.81920000  | -1.26810000 |
| C | 6.37900000  | 16.33050000 | 10.18910000 | H | 4.85440000  | 3.48050000  | -1.44310000 |
| H | 6.37640000  | 16.60220000 | 11.24430000 | C | 4.86860000  | 1.46440000  | -0.72340000 |
| C | 7.09560000  | 17.10300000 | 9.27230000  | C | 3.52560000  | 1.26320000  | -1.07600000 |
| H | 7.64960000  | 17.97690000 | 9.61310000  | H | 2.93960000  | 2.09740000  | -1.46160000 |
| C | 7.10550000  | 16.74070000 | 7.92340000  | C | 2.92400000  | 0.01250000  | -0.92350000 |
| H | 7.67230000  | 17.32820000 | 7.20350000  | H | 1.87850000  | -0.11450000 | -1.20170000 |
| C | 6.38970000  | 15.62120000 | 7.49550000  | C | 3.65630000  | -1.05750000 | -0.40740000 |
| H | 6.39560000  | 15.33430000 | 6.44380000  | H | 3.18640000  | -2.03250000 | -0.28350000 |
| C | 9.91950000  | 11.64910000 | 8.80840000  | C | 4.99440000  | -0.86880000 | -0.05480000 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 10.81630000 | 11.86180000 | 8.21720000  | H | 5.57660000  | -1.69470000 | 0.34750000  |
| H | 9.07020000  | 12.03690000 | 8.23960000  | C | 5.59680000  | 0.37920000  | -0.21610000 |
| C | 10.01410000 | 12.28550000 | 10.20140000 | C | 9.61750000  | 7.60530000  | -2.15210000 |
| H | 9.01080000  | 12.30810000 | 10.64640000 | H | 9.10450000  | 8.42670000  | -1.64240000 |
| H | 10.63110000 | 11.64820000 | 10.84590000 | H | 8.90870000  | 7.09910000  | -2.81770000 |
| C | 10.63470000 | 13.66010000 | 10.12480000 | C | 10.81000000 | 8.15710000  | -2.94590000 |
| C | 11.97950000 | 13.84630000 | 10.48140000 | H | 11.25510000 | 7.35320000  | -3.54750000 |
| H | 12.56070000 | 13.00720000 | 10.86530000 | H | 11.57900000 | 8.49630000  | -2.23930000 |
| C | 12.58920000 | 15.09450000 | 10.33910000 | C | 10.35140000 | 9.30610000  | -3.81340000 |
| H | 13.63400000 | 15.21210000 | 10.62160000 | C | 10.55950000 | 10.63370000 | -3.41550000 |
| C | 11.87200000 | 16.17530000 | 9.82630000  | H | 11.12540000 | 10.83390000 | -2.50840000 |
| H | 12.35560000 | 17.14430000 | 9.71020000  | C | 10.04240000 | 11.69930000 | -4.15330000 |
| C | 10.53270000 | 16.00330000 | 9.46860000  | H | 10.21340000 | 12.72050000 | -3.81710000 |
| H | 9.95730000  | 16.83650000 | 9.06970000  | C | 9.31280000  | 11.45320000 | -5.31690000 |
| C | 9.92080000  | 14.75770000 | 9.62290000  | H | 8.89870000  | 12.28210000 | -5.89010000 |
| H | 8.87370000  | 14.64140000 | 9.34440000  | C | 9.10850000  | 10.13600000 | -5.73400000 |
| C | 5.92110000  | 7.54080000  | 11.54360000 | H | 8.54210000  | 9.93550000  | -6.64240000 |
| H | 6.43720000  | 6.71690000  | 11.04100000 | C | 9.62590000  | 9.07460000  | -4.99090000 |
| H | 6.63890000  | 8.04870000  | 12.19800000 | H | 9.45420000  | 8.04840000  | -5.31550000 |
| C | 4.72070000  | 7.00130000  | 12.32560000 | C | 11.36240000 | 10.95540000 | 1.82980000  |
| H | 4.28290000  | 7.80540000  | 12.93230000 | H | 11.84570000 | 11.66980000 | 2.50930000  |
| H | 3.95840000  | 6.68000000  | 11.60420000 | H | 10.28750000 | 10.96750000 | 2.04320000  |
| C | 5.14970000  | 5.84550000  | 13.19390000 | C | 11.64390000 | 11.28420000 | 0.36370000  |
| C | 4.92540000  | 4.51990000  | 12.79730000 | H | 11.02210000 | 10.61390000 | -0.24510000 |
| H | 4.36420000  | 4.32010000  | 11.88570000 | H | 12.69330000 | 11.04660000 | 0.14490000  |
| C | 5.42430000  | 3.45500000  | 13.54970000 | C | 11.36490000 | 12.72680000 | 0.02510000  |
| H | 5.24430000  | 2.43320000  | 13.22070000 | C | 12.41920000 | 13.61520000 | -0.22980000 |
| C | 6.14920000  | 3.69980000  | 14.71680000 | H | 13.44320000 | 13.23880000 | -0.22730000 |
| H | 6.54680000  | 2.86960000  | 15.29920000 | C | 12.17510000 | 14.96580000 | -0.48740000 |
| C | 6.37050000  | 5.01570000  | 15.12950000 | H | 13.00880000 | 15.63660000 | -0.69210000 |
| H | 6.93380000  | 5.21770000  | 16.03970000 | C | 10.86800000 | 15.45450000 | -0.48420000 |
| C | 5.87030000  | 6.07510000  | 14.37390000 | H | 10.67710000 | 16.50860000 | -0.68200000 |
| H | 6.05270000  | 7.10190000  | 14.69130000 | C | 9.80670000  | 14.57990000 | -0.23400000 |
| C | 4.17750000  | 4.12960000  | 7.65580000  | H | 8.78010000  | 14.94580000 | -0.22270000 |
| H | 3.69770000  | 3.40870000  | 6.97980000  | C | 10.05280000 | 13.22750000 | 0.01270000  |
| H | 5.25480000  | 4.13240000  | 7.45590000  | H | 9.21380000  | 12.55590000 | 0.20280000  |
| C | 3.88790000  | 3.79850000  | 9.12220000  | H | 6.64410000  | 0.50480000  | 0.05930000  |
| H | 4.50360000  | 4.46300000  | 9.74520000  |   |             |             |             |

| Au <sub>25</sub> (SPh) <sub>18</sub> <sup>-</sup> |             |             |            |      |             |             |             |
|---------------------------------------------------|-------------|-------------|------------|------|-------------|-------------|-------------|
| Atom                                              | x           | y           | z          | Atom | x           | y           | z           |
| Au                                                | 7.63360000  | 10.44380000 | 4.14860000 | C    | 4.30010000  | 12.34100000 | 9.42540000  |
| Au                                                | 10.56160000 | 11.59070000 | 4.95710000 | C    | 6.17920000  | 12.70730000 | 7.93850000  |
| Au                                                | 12.54870000 | 8.61490000  | 5.72380000 | C    | 4.75260000  | 13.38130000 | 10.23960000 |
| Au                                                | 10.17170000 | 6.41220000  | 5.68700000 | H    | 3.40410000  | 11.77970000 | 9.68890000  |
| Au                                                | 6.26730000  | 9.13580000  | 6.48470000 | C    | 6.62330000  | 13.74070000 | 8.75780000  |
| Au                                                | 4.72330000  | 11.46700000 | 5.03470000 | H    | 6.74160000  | 12.43000000 | 7.04980000  |
| Au                                                | 6.02110000  | 11.22750000 | 1.66750000 | C    | 5.91120000  | 14.08520000 | 9.90860000  |
| Au                                                | 7.80550000  | 8.31670000  | 1.88720000 | H    | 4.19090000  | 13.63930000 | 11.13620000 |
| Au                                                | 9.22220000  | 9.28450000  | 6.47190000 | H    | 7.54240000  | 14.26540000 | 8.50340000  |
| Au                                                | 7.47970000  | 9.35450000  | 9.24300000 | H    | 6.26390000  | 14.89200000 | 10.54850000 |
| Au                                                | 4.54050000  | 7.36180000  | 8.51440000 | C    | 9.80070000  | 11.72650000 | 9.30480000  |
| Au                                                | 5.38330000  | 6.30570000  | 5.58760000 | C    | 10.50560000 | 12.64860000 | 8.52530000  |
| Au                                                | 7.89030000  | 4.73460000  | 5.17830000 | C    | 9.25360000  | 12.13390000 | 10.53030000 |
| Au                                                | 4.98460000  | 3.53490000  | 4.27580000 | C    | 10.67260000 | 13.95860000 | 8.97440000  |
| Au                                                | 3.13210000  | 6.61430000  | 3.42100000 | H    | 10.91230000 | 12.33990000 | 7.56440000  |

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Au | 5.39080000  | 8.79350000  | 3.59360000  | C | 9.42050000  | 13.44320000 | 10.97000000 |
| Au | 9.27270000  | 5.97830000  | 2.81470000  | H | 8.69500000  | 11.41280000 | 11.12290000 |
| Au | 10.81260000 | 3.80030000  | 4.30520000  | C | 10.13410000 | 14.36270000 | 10.19720000 |
| Au | 9.40070000  | 4.06010000  | 7.71910000  | H | 11.23270000 | 14.65970000 | 8.35880000  |
| Au | 7.72960000  | 6.85090000  | 7.43730000  | H | 8.98980000  | 13.74650000 | 11.92250000 |
| Au | 6.25240000  | 5.93540000  | 2.87960000  | H | 10.26390000 | 15.38700000 | 10.54550000 |
| Au | 7.97630000  | 5.74750000  | 0.11200000  | C | 13.49060000 | 11.84410000 | 6.45060000  |
| Au | 10.91890000 | 7.83130000  | 0.89430000  | C | 13.43730000 | 13.24390000 | 6.37680000  |
| Au | 10.15170000 | 8.85180000  | 3.75240000  | C | 14.11010000 | 11.22900000 | 7.54470000  |
| Au | 7.78030000  | 7.59070000  | 4.66620000  | C | 13.97750000 | 14.01720000 | 7.40210000  |
| S  | 8.46590000  | 12.67800000 | 4.94580000  | H | 12.94850000 | 13.71550000 | 5.52420000  |
| S  | 12.82480000 | 10.88150000 | 5.08750000  | C | 14.64920000 | 12.01190000 | 8.56450000  |
| S  | 12.63620000 | 6.30760000  | 6.28620000  | H | 14.15470000 | 10.14190000 | 7.59980000  |
| S  | 4.76150000  | 12.69510000 | 3.01450000  | C | 14.58350000 | 13.40330000 | 8.50190000  |
| S  | 7.46120000  | 10.10760000 | 0.17080000  | H | 13.92190000 | 15.10310000 | 7.34060000  |
| S  | 4.38450000  | 10.67830000 | 7.23840000  | H | 15.11810000 | 11.52490000 | 9.41840000  |
| S  | 9.73040000  | 9.98770000  | 8.85320000  | H | 15.00020000 | 14.00580000 | 9.30750000  |
| S  | 5.28820000  | 8.97180000  | 10.06200000 | C | 12.79150000 | 6.24860000  | 8.07820000  |
| S  | 3.34220000  | 5.90090000  | 7.08850000  | C | 11.89330000 | 6.89380000  | 8.93450000  |
| S  | 7.06140000  | 2.42730000  | 4.57150000  | C | 13.85260000 | 5.50800000  | 8.61430000  |
| S  | 2.77390000  | 4.34940000  | 3.96350000  | C | 12.06270000 | 6.81610000  | 10.31410000 |
| S  | 2.94080000  | 8.93350000  | 2.97310000  | H | 11.06350000 | 7.45400000  | 8.51230000  |
| S  | 10.75710000 | 2.66260000  | 6.38340000  | C | 14.00800000 | 5.42310000  | 9.99860000  |
| S  | 7.84170000  | 5.05300000  | 9.20190000  | H | 14.53340000 | 4.98250000  | 7.94890000  |
| S  | 11.14360000 | 4.30220000  | 1.99940000  | C | 13.11960000 | 6.07760000  | 10.85230000 |
| S  | 5.74010000  | 5.07500000  | 0.56460000  | H | 11.35460000 | 7.32540000  | 10.96520000 |
| S  | 10.17020000 | 6.24550000  | -0.67550000 | H | 14.82570000 | 4.83060000  | 10.40740000 |
| S  | 12.16490000 | 9.35210000  | 2.23740000  | H | 13.23650000 | 6.00210000  | 11.93250000 |
| C  | 12.42910000 | 2.54160000  | 7.00910000  | C | 8.76720000  | 5.34710000  | 10.71080000 |
| C  | 13.51530000 | 2.84050000  | 6.17900000  | C | 9.51080000  | 4.30060000  | 11.27630000 |
| C  | 12.65530000 | 1.99240000  | 8.27990000  | C | 8.63320000  | 6.55030000  | 11.40980000 |
| C  | 14.81460000 | 2.56970000  | 6.60830000  | C | 10.10290000 | 4.46030000  | 12.52710000 |
| H  | 13.32790000 | 3.28620000  | 5.20250000  | H | 9.61050000  | 3.36550000  | 10.72760000 |
| C  | 13.95710000 | 1.73530000  | 8.70400000  | C | 9.22860000  | 6.70410000  | 12.66130000 |
| H  | 11.80810000 | 1.75830000  | 8.92440000  | H | 8.07690000  | 7.37330000  | 10.96400000 |
| C  | 15.04220000 | 2.01380000  | 7.86860000  | C | 9.96010000  | 5.65960000  | 13.22860000 |
| H  | 15.65320000 | 2.80240000  | 5.95250000  | H | 10.67180000 | 3.63700000  | 12.95660000 |
| H  | 14.11940000 | 1.30740000  | 9.69260000  | H | 9.11150000  | 7.64720000  | 13.19220000 |
| H  | 16.05700000 | 1.79910000  | 8.19570000  | H | 10.42210000 | 5.77590000  | 14.20740000 |
| C  | 6.91540000  | 1.32150000  | 5.97370000  | C | 5.48600000  | 8.18410000  | 11.66140000 |
| C  | 8.01920000  | 0.50180000  | 6.25350000  | C | 6.10210000  | 8.91570000  | 12.68580000 |
| C  | 5.74220000  | 1.17240000  | 6.72420000  | C | 5.00250000  | 6.89820000  | 11.92520000 |
| C  | 7.95220000  | -0.44910000 | 7.26750000  | C | 6.25180000  | 8.35750000  | 13.95420000 |
| H  | 8.93520000  | 0.62270000  | 5.67890000  | H | 6.46660000  | 9.91920000  | 12.47430000 |
| C  | 5.68110000  | 0.21100000  | 7.73130000  | C | 5.15050000  | 6.34910000  | 13.19930000 |
| H  | 4.88060000  | 1.80760000  | 6.51720000  | H | 4.51920000  | 6.33710000  | 11.12590000 |
| C  | 6.77920000  | -0.60410000 | 8.00990000  | C | 5.78020000  | 7.06810000  | 14.21550000 |
| H  | 8.82560000  | -1.06740000 | 7.47740000  | H | 6.73700000  | 8.93210000  | 14.74190000 |
| H  | 4.75830000  | 0.11270000  | 8.30190000  | H | 4.78460000  | 5.34150000  | 13.38880000 |
| H  | 6.72220000  | -1.35120000 | 8.79900000  | H | 5.90090000  | 6.62480000  | 15.20250000 |
| C  | 10.75470000 | 2.72340000  | 1.22490000  | C | 8.51690000  | 13.95350000 | 3.69310000  |
| C  | 10.41670000 | 2.67370000  | -0.13550000 | C | 7.50160000  | 14.91920000 | 3.74560000  |
| C  | 10.90590000 | 1.51600000  | 1.92840000  | C | 9.52470000  | 14.05950000 | 2.72790000  |
| C  | 10.23540000 | 1.44720000  | -0.77450000 | C | 7.49560000  | 15.97770000 | 2.84070000  |
| H  | 10.29310000 | 3.60340000  | -0.68630000 | H | 6.72180000  | 14.82960000 | 4.49820000  |
| C  | 10.72770000 | 0.29450000  | 1.28140000  | C | 9.51390000  | 15.12720000 | 1.83290000  |
| H  | 11.18440000 | 1.54600000  | 2.98110000  | H | 10.30850000 | 13.30690000 | 2.67800000  |
| C  | 10.39320000 | 0.25010000  | -0.07300000 | C | 8.50410000  | 16.08860000 | 1.88330000  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 9.96280000  | 1.43210000  | -1.82860000 | H | 6.69890000  | 16.71740000 | 2.88730000  |
| H | 10.85630000 | -0.63050000 | 1.84280000  | H | 10.29930000 | 15.19130000 | 1.08290000  |
| H | 10.25740000 | -0.70410000 | -0.57990000 | H | 8.49700000  | 16.91300000 | 1.17260000  |
| C | 5.77180000  | 3.28200000  | 0.63270000  | C | 11.98170000 | 10.87820000 | 1.31930000  |
| C | 4.66580000  | 2.60040000  | 0.11160000  | C | 12.95900000 | 11.87120000 | 1.48530000  |
| C | 6.83550000  | 2.55900000  | 1.18510000  | C | 10.94900000 | 11.07680000 | 0.39130000  |
| C | 4.63890000  | 1.20610000  | 0.12770000  | C | 12.92680000 | 13.01890000 | 0.68930000  |
| H | 3.82550000  | 3.16160000  | -0.29060000 | H | 13.73440000 | 11.73390000 | 2.23630000  |
| C | 6.79840000  | 1.16780000  | 1.20070000  | C | 10.92080000 | 12.22620000 | -0.39490000 |
| H | 7.67460000  | 3.09190000  | 1.62770000  | H | 10.16330000 | 10.33000000 | 0.29650000  |
| C | 5.70440000  | 0.48310000  | 0.66550000  | C | 11.92140000 | 13.19290000 | -0.26550000 |
| H | 3.77170000  | 0.68980000  | -0.28120000 | H | 13.69970000 | 13.77610000 | 0.81220000  |
| H | 7.62880000  | 0.62460000  | 1.64640000  | H | 10.10490000 | 12.36280000 | -1.10380000 |
| H | 5.67870000  | -0.60520000 | 0.68010000  | H | 11.91230000 | 14.08480000 | -0.89190000 |
| C | 2.07190000  | 3.52100000  | 2.53300000  | C | 10.00470000 | 7.08330000  | -2.25270000 |
| C | 2.04740000  | 2.11990000  | 2.52570000  | C | 10.48930000 | 8.37650000  | -2.47260000 |
| C | 1.47810000  | 4.23090000  | 1.48140000  | C | 9.43110000  | 6.36550000  | -3.31040000 |
| C | 1.44290000  | 1.43510000  | 1.47430000  | C | 10.38580000 | 8.94860000  | -3.74130000 |
| H | 2.52960000  | 1.57550000  | 3.33730000  | H | 10.93400000 | 8.92870000  | -1.64480000 |
| C | 0.87850000  | 3.53690000  | 0.43000000  | C | 9.33650000  | 6.94270000  | -4.57520000 |
| H | 1.49190000  | 5.32000000  | 1.48990000  | H | 9.04880000  | 5.36270000  | -3.12860000 |
| C | 0.85600000  | 2.14200000  | 0.42080000  | C | 9.81250000  | 8.23770000  | -4.79570000 |
| H | 1.44210000  | 0.34640000  | 1.47400000  | H | 10.74750000 | 9.96360000  | -3.89600000 |
| H | 0.42330000  | 4.09630000  | -0.38680000 | H | 8.88940000  | 6.37920000  | -5.39290000 |
| H | 0.38340000  | 1.60950000  | -0.40350000 | H | 9.73170000  | 8.69610000  | -5.77990000 |
| C | 2.68240000  | 8.99060000  | 1.19410000  | C | 6.57040000  | 9.79980000  | -1.35360000 |
| C | 1.65800000  | 9.82670000  | 0.73250000  | C | 5.84850000  | 10.84020000 | -1.95710000 |
| C | 3.41630000  | 8.22620000  | 0.27800000  | C | 6.72380000  | 8.58430000  | -2.02880000 |
| C | 1.36650000  | 9.88460000  | -0.63060000 | C | 5.28970000  | 10.65830000 | -3.22010000 |
| H | 1.08870000  | 10.42440000 | 1.43960000  | H | 5.73410000  | 11.78610000 | -1.43060000 |
| C | 3.10990000  | 8.28100000  | -1.07910000 | C | 6.16660000  | 8.41270000  | -3.29650000 |
| H | 4.22570000  | 7.59390000  | 0.63450000  | H | 7.26960000  | 7.76970000  | -1.55320000 |
| C | 2.08490000  | 9.10940000  | -1.54140000 | C | 5.44990000  | 9.44720000  | -3.89870000 |
| H | 0.57380000  | 10.54950000 | -0.97320000 | H | 4.73420000  | 11.47450000 | -3.67980000 |
| H | 3.69560000  | 7.68940000  | -1.77730000 | H | 6.29860000  | 7.46390000  | -3.81290000 |
| H | 1.86430000  | 9.16200000  | -2.60600000 | H | 5.01490000  | 9.31520000  | -4.88770000 |
| C | 3.08580000  | 12.83430000 | 2.39810000  | C | 3.27930000  | 4.29190000  | 7.86690000  |
| C | 2.86060000  | 13.39570000 | 1.13300000  | C | 2.22500000  | 3.46040000  | 7.45490000  |
| C | 1.99920000  | 12.53080000 | 3.22610000  | C | 4.13380000  | 3.86410000  | 8.89370000  |
| C | 1.55720000  | 13.65040000 | 0.71010000  | C | 2.00460000  | 2.24030000  | 8.08960000  |
| H | 3.70720000  | 13.63800000 | 0.49030000  | H | 1.58320000  | 3.77940000  | 6.63720000  |
| C | 0.69860000  | 12.79550000 | 2.79640000  | C | 3.90450000  | 2.64120000  | 9.52170000  |
| H | 2.18470000  | 12.08680000 | 4.20390000  | H | 4.98220000  | 4.48270000  | 9.18340000  |
| C | 0.47180000  | 13.35860000 | 1.54020000  | C | 2.83320000  | 1.83060000  | 9.13600000  |
| H | 1.39340000  | 14.08570000 | -0.27510000 | H | 1.17550000  | 1.61200000  | 7.76890000  |
| H | -0.14030000 | 12.55370000 | 3.44820000  | H | 4.57950000  | 2.31850000  | 10.31220000 |
| H | -0.54370000 | 13.56960000 | 1.21210000  | H | 2.65160000  | 0.88520000  | 9.64410000  |
| C | 5.01080000  | 12.00940000 | 8.26400000  |   |             |             |             |

| Au <sub>25</sub> (SPhF) <sub>18</sub> <sup>-</sup> |             |             |            |      |             |             |             |
|----------------------------------------------------|-------------|-------------|------------|------|-------------|-------------|-------------|
| Atom                                               | x           | y           | z          | Atom | x           | y           | z           |
| Au                                                 | 7.64750000  | 10.46720000 | 4.12340000 | H    | 4.21770000  | 13.79900000 | 11.04060000 |
| Au                                                 | 10.58300000 | 11.58580000 | 4.90140000 | H    | 7.58250000  | 14.34330000 | 8.43030000  |
| Au                                                 | 12.49720000 | 8.62240000  | 5.68750000 | C    | 9.88830000  | 11.62960000 | 9.38120000  |
| Au                                                 | 10.14600000 | 6.40520000  | 5.66950000 | C    | 10.61320000 | 12.55820000 | 8.62890000  |
| Au                                                 | 6.25780000  | 9.15960000  | 6.50370000 | C    | 9.35930000  | 12.00970000 | 10.62330000 |



|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Au | 4.72550000  | 11.46620000 | 5.02530000  | C | 10.82600000 | 13.84790000 | 9.11620000  |
| Au | 6.02850000  | 11.23000000 | 1.64110000  | H | 11.00490000 | 12.27480000 | 7.65430000  |
| Au | 7.77990000  | 8.32560000  | 1.88230000  | C | 9.56140000  | 13.29460000 | 11.11570000 |
| Au | 9.27350000  | 9.27100000  | 6.45760000  | H | 8.78710000  | 11.28380000 | 11.19670000 |
| Au | 7.49450000  | 9.35770000  | 9.25520000  | C | 10.29740000 | 14.19320000 | 10.35160000 |
| Au | 4.57670000  | 7.35780000  | 8.43370000  | H | 11.39740000 | 14.57740000 | 8.54790000  |
| Au | 5.37920000  | 6.33930000  | 5.57740000  | H | 9.15890000  | 13.60810000 | 12.07440000 |
| Au | 7.85290000  | 4.73830000  | 5.19130000  | C | 13.52630000 | 11.78360000 | 6.42610000  |
| Au | 4.96040000  | 3.56970000  | 4.33470000  | C | 13.51690000 | 13.18380000 | 6.34600000  |
| Au | 3.07430000  | 6.65380000  | 3.49180000  | C | 14.11610000 | 11.15710000 | 7.53090000  |
| Au | 5.38260000  | 8.81340000  | 3.61890000  | C | 14.07070000 | 13.95730000 | 7.36330000  |
| Au | 9.24010000  | 5.98430000  | 2.80860000  | H | 13.05440000 | 13.66630000 | 5.48560000  |
| Au | 10.77860000 | 3.79000000  | 4.28820000  | C | 14.67590000 | 11.92540000 | 8.55300000  |
| Au | 9.39280000  | 4.02860000  | 7.70040000  | H | 14.13140000 | 10.06970000 | 7.59610000  |
| Au | 7.74150000  | 6.85510000  | 7.45120000  | C | 14.63870000 | 13.30870000 | 8.45370000  |
| Au | 6.21760000  | 5.95320000  | 2.87960000  | H | 14.06690000 | 15.04360000 | 7.32050000  |
| Au | 7.93990000  | 5.77340000  | 0.11140000  | H | 15.13270000 | 11.45970000 | 9.42260000  |
| Au | 10.89830000 | 7.83180000  | 0.89780000  | C | 12.79810000 | 6.29590000  | 8.02300000  |
| Au | 10.13750000 | 8.84930000  | 3.74270000  | C | 11.89320000 | 6.91850000  | 8.88970000  |
| Au | 7.77210000  | 7.59870000  | 4.66150000  | C | 13.90020000 | 5.60580000  | 8.54500000  |
| S  | 8.50260000  | 12.70780000 | 4.88760000  | C | 12.09170000 | 6.87180000  | 10.26720000 |
| S  | 12.84050000 | 10.86860000 | 5.03920000  | H | 11.03110000 | 7.44110000  | 8.48060000  |
| S  | 12.60260000 | 6.32360000  | 6.23700000  | C | 14.10070000 | 5.54240000  | 9.92420000  |
| S  | 4.75980000  | 12.67480000 | 2.99840000  | H | 14.59070000 | 5.10380000  | 7.87120000  |
| S  | 7.45100000  | 10.08600000 | 0.14760000  | C | 13.19360000 | 6.18040000  | 10.75750000 |
| S  | 4.38540000  | 10.70160000 | 7.24540000  | H | 11.39920000 | 7.35790000  | 10.95000000 |
| S  | 9.78060000  | 9.91170000  | 8.86320000  | H | 14.94390000 | 5.00460000  | 10.35150000 |
| S  | 5.25540000  | 8.99540000  | 9.97930000  | C | 8.78110000  | 5.35030000  | 10.68880000 |
| S  | 3.34380000  | 5.92560000  | 7.03120000  | C | 9.55440000  | 4.33910000  | 11.27750000 |
| S  | 7.01350000  | 2.43050000  | 4.62900000  | C | 8.61850000  | 6.56930000  | 11.35730000 |
| S  | 2.74980000  | 4.37260000  | 4.02520000  | C | 10.15120000 | 4.54000000  | 12.52270000 |
| S  | 2.94190000  | 8.98030000  | 3.03090000  | H | 9.67840000  | 3.39410000  | 10.75290000 |
| S  | 10.74040000 | 2.63460000  | 6.35110000  | C | 9.20860000  | 6.77890000  | 12.60390000 |
| S  | 7.85060000  | 5.03170000  | 9.18920000  | H | 8.04060000  | 7.36740000  | 10.89380000 |
| S  | 11.09460000 | 4.29780000  | 1.98610000  | C | 9.96210000  | 5.75800000  | 13.16790000 |
| S  | 5.69910000  | 5.11590000  | 0.55580000  | H | 10.74910000 | 3.76510000  | 12.99550000 |
| S  | 10.13510000 | 6.25620000  | -0.67630000 | H | 9.08600000  | 7.72140000  | 13.13090000 |
| S  | 12.13790000 | 9.35420000  | 2.24130000  | C | 5.34860000  | 8.21650000  | 11.59400000 |
| C  | 12.41510000 | 2.53360000  | 6.97630000  | C | 5.87770000  | 8.98540000  | 12.63980000 |
| C  | 13.49700000 | 2.85470000  | 6.14780000  | C | 4.87780000  | 6.92510000  | 11.85840000 |
| C  | 12.65050000 | 1.97990000  | 8.24290000  | C | 5.95220000  | 8.47280000  | 13.93290000 |
| C  | 14.80530000 | 2.61230000  | 6.56840000  | H | 6.23260000  | 9.99270000  | 12.43160000 |
| H  | 13.30370000 | 3.29660000  | 5.17060000  | C | 4.94900000  | 6.40220000  | 13.15030000 |
| C  | 13.95350000 | 1.74220000  | 8.67350000  | H | 4.46840000  | 6.33000000  | 11.04340000 |
| H  | 11.81080000 | 1.72540000  | 8.88840000  | C | 5.48780000  | 7.18270000  | 14.16270000 |
| C  | 15.00940000 | 2.05830000  | 7.82530000  | H | 6.36210000  | 9.05290000  | 14.75630000 |
| H  | 15.65810000 | 2.85310000  | 5.93710000  | H | 4.60860000  | 5.39460000  | 13.37170000 |
| H  | 14.15680000 | 1.31900000  | 9.65450000  | C | 8.57260000  | 13.98920000 | 3.64210000  |
| C  | 6.88460000  | 1.30770000  | 6.01840000  | C | 7.61630000  | 15.01530000 | 3.67790000  |
| C  | 7.98630000  | 0.48710000  | 6.30570000  | C | 9.59210000  | 14.02710000 | 2.68270000  |
| C  | 5.70130000  | 1.14960000  | 6.75080000  | C | 7.68440000  | 16.06880000 | 2.76690000  |
| C  | 7.91420000  | -0.47140000 | 7.31160000  | H | 6.82600000  | 14.98750000 | 4.42440000  |
| H  | 8.90840000  | 0.60540000  | 5.74180000  | C | 9.67170000  | 15.07780000 | 1.77380000  |
| C  | 5.61760000  | 0.18740000  | 7.75690000  | H | 10.32990000 | 13.22870000 | 2.65010000  |
| H  | 4.83860000  | 1.77800000  | 6.53240000  | C | 8.71260000  | 16.07910000 | 1.83250000  |
| C  | 6.72630000  | -0.60380000 | 8.01950000  | H | 6.95430000  | 16.87300000 | 2.77720000  |
| H  | 8.76470000  | -1.10710000 | 7.55090000  | H | 10.45480000 | 15.12340000 | 1.02220000  |
| H  | 4.70580000  | 0.05010000  | 8.33530000  | C | 11.87390000 | 10.91590000 | 1.40390000  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 10.67470000 | 2.72300000  | 1.21770000  | C | 12.84430000 | 11.91300000 | 1.57570000  |
| C | 10.33280000 | 2.67290000  | -0.14240000 | C | 10.79400000 | 11.15090000 | 0.54130000  |
| C | 10.80840000 | 1.51550000  | 1.92410000  | C | 12.76990000 | 13.10250000 | 0.84780000  |
| C | 10.13010000 | 1.45430000  | -0.78760000 | H | 13.65680000 | 11.74930000 | 2.27970000  |
| H | 10.22510000 | 3.60030000  | -0.69860000 | C | 10.70610000 | 12.33690000 | -0.18360000 |
| C | 10.60830000 | 0.29080000  | 1.28880000  | H | 10.00890000 | 10.40440000 | 0.44610000  |
| H | 11.09150000 | 1.54230000  | 2.97540000  | C | 11.71340000 | 13.28190000 | -0.03500000 |
| C | 10.27670000 | 0.28130000  | -0.05910000 | H | 13.52610000 | 13.87630000 | 0.94980000  |
| H | 9.85610000  | 1.41000000  | -1.83870000 | H | 9.86720000  | 12.52640000 | -0.84940000 |
| H | 10.71050000 | -0.64860000 | 1.82680000  | C | 9.93140000  | 7.08720000  | -2.25360000 |
| C | 5.77190000  | 3.32230000  | 0.57190000  | C | 10.41820000 | 8.38760000  | -2.41870000 |
| C | 4.71710000  | 2.64060000  | -0.04560000 | C | 9.34750000  | 6.41710000  | -3.33870000 |
| C | 6.81250000  | 2.59430000  | 1.16080000  | C | 10.31980000 | 9.02540000  | -3.65410000 |
| C | 4.70620000  | 1.24750000  | -0.09310000 | H | 10.87010000 | 8.89800000  | -1.56710000 |
| H | 3.89440000  | 3.20150000  | -0.48270000 | C | 9.24420000  | 7.04730000  | -4.57700000 |
| C | 6.80650000  | 1.20290000  | 1.12660000  | H | 8.96280000  | 5.40870000  | -3.20490000 |
| H | 7.61900000  | 3.11810000  | 1.67000000  | C | 9.73330000  | 8.34410000  | -4.71030000 |
| C | 5.75550000  | 0.55120000  | 0.49170000  | H | 10.67710000 | 10.04100000 | -3.79690000 |
| H | 3.89250000  | 0.70860000  | -0.57290000 | H | 8.79340000  | 6.55240000  | -5.43490000 |
| H | 7.60390000  | 0.63330000  | 1.59720000  | C | 6.52170000  | 9.70510000  | -1.33790000 |
| C | 2.13030000  | 3.46120000  | 2.61170000  | C | 5.77450000  | 10.71380000 | -1.96340000 |
| C | 2.13870000  | 2.05960000  | 2.63120000  | C | 6.66610000  | 8.46330000  | -1.96730000 |
| C | 1.55560000  | 4.14030000  | 1.53120000  | C | 5.17980000  | 10.48900000 | -3.20340000 |
| C | 1.58100000  | 1.33750000  | 1.57910000  | H | 5.66930000  | 11.68090000 | -1.47490000 |
| H | 2.60460000  | 1.53590000  | 3.46510000  | C | 6.07860000  | 8.23030000  | -3.21120000 |
| C | 1.00070000  | 3.42430000  | 0.47000000  | H | 7.23110000  | 7.67060000  | -1.47620000 |
| H | 1.54370000  | 5.22920000  | 1.52270000  | C | 5.34710000  | 9.24830000  | -3.80830000 |
| C | 1.02430000  | 2.03740000  | 0.51300000  | H | 4.60210000  | 11.26180000 | -3.70350000 |
| H | 1.58740000  | 0.25070000  | 1.57150000  | H | 6.18520000  | 7.27370000  | -3.71640000 |
| H | 0.54940000  | 3.93380000  | -0.37880000 | C | 3.27240000  | 4.30830000  | 7.79140000  |
| C | 2.79150000  | 9.05640000  | 1.24610000  | C | 2.21260000  | 3.47840000  | 7.39130000  |
| C | 1.79580000  | 9.88660000  | 0.71840000  | C | 4.14490000  | 3.87170000  | 8.79810000  |
| C | 3.59860000  | 8.30480000  | 0.38080000  | C | 2.00390000  | 2.24830000  | 8.01260000  |
| C | 1.59040000  | 9.95410000  | -0.65970000 | H | 1.55200000  | 3.80080000  | 6.58970000  |
| H | 1.17350000  | 10.47560000 | 1.38700000  | C | 3.94260000  | 2.64260000  | 9.42460000  |
| C | 3.39200000  | 8.35790000  | -0.99600000 | H | 4.99740000  | 4.48760000  | 9.07870000  |
| H | 4.38870000  | 7.67900000  | 0.79220000  | C | 2.86520000  | 1.85930000  | 9.03140000  |
| C | 2.38830000  | 9.18130000  | -1.49300000 | H | 1.18050000  | 1.60050000  | 7.72410000  |
| H | 0.82100000  | 10.59450000 | -1.08330000 | H | 4.61890000  | 2.29460000  | 10.20080000 |
| H | 4.01570000  | 7.78640000  | -1.67740000 | F | -0.86440000 | 13.32420000 | 1.25020000  |
| C | 3.06180000  | 12.74410000 | 2.42340000  | F | 2.18020000  | 9.23500000  | -2.84300000 |
| C | 2.77460000  | 13.27060000 | 1.15500000  | F | 0.48530000  | 1.33280000  | -0.52650000 |
| C | 2.01140000  | 12.41490000 | 3.28790000  | F | 5.74640000  | -0.81440000 | 0.45190000  |
| C | 1.45340000  | 13.46300000 | 0.75730000  | F | 10.08490000 | -0.91710000 | -0.68530000 |
| H | 3.58750000  | 13.53830000 | 0.48090000  | F | 9.62970000  | 8.96560000  | -5.92000000 |
| C | 0.68610000  | 12.61380000 | 2.90170000  | F | 4.77160000  | 9.02420000  | -5.02520000 |
| H | 2.23650000  | 11.99940000 | 4.27010000  | F | 8.78280000  | 17.10870000 | 0.93570000  |
| C | 0.43090000  | 13.13420000 | 1.63960000  | F | 11.65310000 | 14.43750000 | -0.76650000 |
| H | 1.21270000  | 13.86580000 | -0.22410000 | F | 16.28720000 | 1.82330000  | 8.24670000  |
| H | -0.14070000 | 12.36390000 | 3.56290000  | F | 13.39260000 | 6.12550000  | 12.10860000 |
| C | 5.04970000  | 12.05790000 | 8.21970000  | F | 10.53770000 | 5.95710000  | 14.38860000 |
| C | 4.33070000  | 12.42940000 | 9.36210000  | F | 5.56630000  | 6.67190000  | 15.42480000 |
| C | 6.22510000  | 12.74490000 | 7.88940000  | F | 2.65400000  | 0.65660000  | 9.65060000  |
| C | 4.76730000  | 13.49130000 | 10.15390000 | F | 6.65020000  | -1.54480000 | 9.00770000  |
| H | 3.42890000  | 11.88220000 | 9.63380000  | F | 15.18060000 | 14.06040000 | 9.45480000  |
| C | 6.66790000  | 13.80700000 | 8.67260000  | F | 10.50910000 | 15.45310000 | 10.83450000 |
| H | 6.79660000  | 12.44620000 | 7.01350000  | F | 6.35230000  | 15.20490000 | 10.56900000 |
| C | 5.92640000  | 14.16320000 | 9.79240000  |   |             |             |             |



| Au <sub>25</sub> (SPhCOOH) <sub>18</sub> <sup>-</sup> |             |             |             |      |             |             |             |
|-------------------------------------------------------|-------------|-------------|-------------|------|-------------|-------------|-------------|
| Atom                                                  | x           | y           | z           | Atom | x           | y           | z           |
| Au                                                    | 7.65510000  | 10.44120000 | 4.11500000  | H    | 13.17100000 | 4.37970000  | 8.42960000  |
| Au                                                    | 10.60940000 | 11.57230000 | 4.95170000  | C    | 12.91860000 | 6.63190000  | 10.97530000 |
| Au                                                    | 12.53660000 | 8.60890000  | 5.73490000  | H    | 12.33330000 | 8.69870000  | 10.73460000 |
| Au                                                    | 10.13510000 | 6.36270000  | 5.65520000  | H    | 13.43160000 | 4.54310000  | 10.89950000 |
| Au                                                    | 6.19600000  | 9.15510000  | 6.42970000  | C    | 8.97920000  | 5.52820000  | 10.67820000 |
| Au                                                    | 4.70460000  | 11.38840000 | 4.91770000  | C    | 9.63660000  | 4.50730000  | 11.38370000 |
| Au                                                    | 6.15960000  | 11.23500000 | 1.65460000  | C    | 8.82310000  | 6.78830000  | 11.26510000 |
| Au                                                    | 7.91370000  | 8.30890000  | 1.81190000  | C    | 10.09600000 | 4.74040000  | 12.67660000 |
| Au                                                    | 9.23520000  | 9.28670000  | 6.40760000  | H    | 9.75390000  | 3.52820000  | 10.92320000 |
| Au                                                    | 7.45000000  | 9.41930000  | 9.24780000  | C    | 9.25220000  | 7.00510000  | 12.56590000 |
| Au                                                    | 4.55390000  | 7.48040000  | 8.50240000  | H    | 8.34470000  | 7.58980000  | 10.70090000 |
| Au                                                    | 5.33790000  | 6.41840000  | 5.59960000  | C    | 9.88160000  | 5.98500000  | 13.29190000 |
| Au                                                    | 7.83740000  | 4.71690000  | 5.20800000  | H    | 10.57960000 | 3.93230000  | 13.22320000 |
| Au                                                    | 4.80740000  | 3.56080000  | 4.44830000  | H    | 9.10600000  | 7.97090000  | 13.04180000 |
| Au                                                    | 3.18050000  | 6.64720000  | 3.46740000  | C    | 5.52000000  | 7.99980000  | 11.61650000 |
| Au                                                    | 5.43840000  | 8.78780000  | 3.34110000  | C    | 6.21380000  | 8.56340000  | 12.69580000 |
| Au                                                    | 9.24570000  | 5.93280000  | 2.81860000  | C    | 4.95230000  | 6.72600000  | 11.74020000 |
| Au                                                    | 10.72380000 | 3.64040000  | 4.27740000  | C    | 6.37280000  | 7.83930000  | 13.87490000 |
| Au                                                    | 9.46670000  | 3.93330000  | 7.67740000  | H    | 6.63210000  | 9.56410000  | 12.60300000 |
| Au                                                    | 7.70510000  | 6.90820000  | 7.43710000  | C    | 5.08620000  | 6.02370000  | 12.93300000 |
| Au                                                    | 6.22040000  | 5.92860000  | 2.89690000  | H    | 4.41430000  | 6.29260000  | 10.89750000 |
| Au                                                    | 8.01990000  | 5.79650000  | 0.13740000  | C    | 5.80860000  | 6.56220000  | 14.00570000 |
| Au                                                    | 10.90960000 | 7.81710000  | 0.77440000  | H    | 6.91430000  | 8.28290000  | 14.70850000 |
| Au                                                    | 10.18360000 | 8.76890000  | 3.70560000  | H    | 4.63380000  | 5.04160000  | 13.05000000 |
| Au                                                    | 7.75310000  | 7.58550000  | 4.64000000  | C    | 8.67690000  | 13.96100000 | 3.59700000  |
| S                                                     | 8.54100000  | 12.70270000 | 4.85260000  | C    | 7.55360000  | 14.76830000 | 3.35090000  |
| S                                                     | 12.88250000 | 10.87210000 | 5.14330000  | C    | 9.87620000  | 14.23260000 | 2.92290000  |
| S                                                     | 12.53870000 | 6.33250000  | 6.41670000  | C    | 7.62140000  | 15.80580000 | 2.43170000  |
| S                                                     | 4.72310000  | 12.62160000 | 2.89640000  | H    | 6.62180000  | 14.57910000 | 3.88050000  |
| S                                                     | 7.64930000  | 10.16710000 | 0.14050000  | C    | 9.94560000  | 15.28330000 | 2.02130000  |
| S                                                     | 4.42720000  | 10.80980000 | 7.21470000  | H    | 10.75780000 | 13.62310000 | 3.12100000  |
| S                                                     | 9.69640000  | 10.00110000 | 8.78230000  | C    | 8.81890000  | 16.07250000 | 1.75070000  |
| S                                                     | 5.29250000  | 9.00190000  | 10.14200000 | H    | 6.74210000  | 16.41710000 | 2.24090000  |
| S                                                     | 3.37530000  | 5.94390000  | 7.16570000  | H    | 10.88090000 | 15.51710000 | 1.51830000  |
| S                                                     | 6.88490000  | 2.45240000  | 4.53790000  | C    | 12.03100000 | 10.84920000 | 1.24700000  |
| S                                                     | 2.62760000  | 4.46790000  | 4.32570000  | C    | 12.97660000 | 11.85830000 | 1.49920000  |
| S                                                     | 3.02340000  | 8.75940000  | 2.39740000  | C    | 11.06760000 | 11.04860000 | 0.24740000  |
| S                                                     | 10.74390000 | 2.47180000  | 6.35120000  | C    | 12.94810000 | 13.03870000 | 0.75820000  |
| S                                                     | 8.12010000  | 5.15420000  | 9.15790000  | H    | 13.73100000 | 11.70740000 | 2.26840000  |
| S                                                     | 11.03170000 | 4.14720000  | 1.97980000  | C    | 11.04400000 | 12.22130000 | -0.49150000 |
| S                                                     | 5.74970000  | 5.19870000  | 0.52590000  | H    | 10.32390000 | 10.27420000 | 0.06640000  |
| S                                                     | 10.19790000 | 6.21270000  | -0.77590000 | C    | 11.98590000 | 13.23130000 | -0.24700000 |
| S                                                     | 12.16460000 | 9.30660000  | 2.13640000  | H    | 13.68230000 | 13.81730000 | 0.95490000  |
| C                                                     | 12.37760000 | 2.38070000  | 7.06470000  | H    | 10.29000000 | 12.37870000 | -1.25990000 |
| C                                                     | 13.49630000 | 2.86830000  | 6.37620000  | C    | 9.62810000  | 6.95910000  | -2.30930000 |
| C                                                     | 12.54500000 | 1.73470000  | 8.30190000  | C    | 9.83650000  | 8.29700000  | -2.65860000 |
| C                                                     | 14.76630000 | 2.73120000  | 6.92860000  | C    | 8.86470000  | 6.12060000  | -3.13880000 |
| H                                                     | 13.35490000 | 3.37030000  | 5.42030000  | C    | 9.16860000  | 8.82150000  | -3.76660000 |
| C                                                     | 13.81490000 | 1.60130000  | 8.84910000  | H    | 10.45940000 | 8.92660000  | -2.02800000 |
| H                                                     | 11.67420000 | 1.34110000  | 8.82460000  | C    | 8.19610000  | 6.65200000  | -4.23060000 |
| C                                                     | 14.93830000 | 2.10400000  | 8.16950000  | H    | 8.73140000  | 5.07300000  | -2.87010000 |
| H                                                     | 15.63140000 | 3.12580000  | 6.40120000  | C    | 8.30240000  | 8.01910000  | -4.52270000 |
| H                                                     | 13.96020000 | 1.10340000  | 9.80530000  | H    | 9.23970000  | 9.88000000  | -4.01130000 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 6.80700000  | 1.18960000  | 5.79210000  | H | 7.54130000  | 6.02620000  | -4.82940000 |
| C | 7.95700000  | 0.40990000  | 6.00060000  | C | 6.49490000  | 9.91690000  | -1.20720000 |
| C | 5.63560000  | 0.89580000  | 6.50290000  | C | 5.81910000  | 11.04530000 | -1.70010000 |
| C | 7.95130000  | -0.60800000 | 6.94400000  | C | 6.29290000  | 8.66720000  | -1.79650000 |
| H | 8.85760000  | 0.61900000  | 5.42840000  | C | 4.91430000  | 10.91460000 | -2.74060000 |
| C | 5.62820000  | -0.13700000 | 7.42700000  | H | 5.99710000  | 12.01590000 | -1.24070000 |
| H | 4.72930000  | 1.47320000  | 6.32680000  | C | 5.41250000  | 8.54630000  | -2.86670000 |
| C | 6.78660000  | -0.88390000 | 7.68050000  | H | 6.81600000  | 7.79460000  | -1.40370000 |
| H | 8.85360000  | -1.18940000 | 7.11740000  | C | 4.71180000  | 9.66390000  | -3.33930000 |
| H | 4.71920000  | -0.38370000 | 7.96930000  | H | 4.35830000  | 11.77920000 | -3.09530000 |
| C | 10.61560000 | 2.63380000  | 1.11890000  | H | 5.24560000  | 7.57660000  | -3.33150000 |
| C | 10.45670000 | 2.68870000  | -0.27600000 | C | 3.57470000  | 4.39460000  | 8.03300000  |
| C | 10.56840000 | 1.37700000  | 1.75400000  | C | 2.53800000  | 3.45490000  | 7.91380000  |
| C | 10.25780000 | 1.52780000  | -1.01150000 | C | 4.67800000  | 4.11180000  | 8.84990000  |
| H | 10.50450000 | 3.64810000  | -0.78410000 | C | 2.60540000  | 2.25750000  | 8.62040000  |
| C | 10.36960000 | 0.21870000  | 1.01520000  | H | 1.68660000  | 3.67690000  | 7.27300000  |
| H | 10.71440000 | 1.31570000  | 2.83060000  | C | 4.74710000  | 2.90990000  | 9.54380000  |
| C | 10.21260000 | 0.27610000  | -0.37720000 | H | 5.48910000  | 4.83150000  | 8.92310000  |
| H | 10.13760000 | 1.58990000  | -2.08970000 | C | 3.70960000  | 1.97200000  | 9.43730000  |
| H | 10.33180000 | -0.75150000 | 1.50580000  | H | 1.81450000  | 1.51520000  | 8.54210000  |
| C | 5.82020000  | 3.42260000  | 0.28660000  | H | 5.62070000  | 2.68820000  | 10.15240000 |
| C | 5.05250000  | 2.88700000  | -0.76010000 | C | 11.88930000 | 14.47660000 | -1.03800000 |
| C | 6.59510000  | 2.57510000  | 1.08730000  | O | 11.19320000 | 14.62810000 | -2.02830000 |
| C | 5.07290000  | 1.51820000  | -1.00430000 | O | 12.65110000 | 15.48990000 | -0.51890000 |
| H | 4.46380000  | 3.55250000  | -1.38780000 | H | 12.39070000 | 16.28820000 | -1.02200000 |
| C | 6.60010000  | 1.20690000  | 0.85180000  | C | 8.94500000  | 17.16960000 | 0.77240000  |
| H | 7.20650000  | 2.99690000  | 1.88090000  | O | 9.97470000  | 17.49980000 | 0.19940000  |
| C | 5.84230000  | 0.66690000  | -0.19770000 | O | 7.76540000  | 17.82710000 | 0.54460000  |
| H | 7.20290000  | 0.55590000  | 1.47610000  | H | 7.99160000  | 18.50890000 | -0.11770000 |
| C | 1.80360000  | 3.97690000  | 2.80930000  | C | 0.80380000  | 7.64580000  | -3.15520000 |
| C | 0.43630000  | 4.27620000  | 2.71660000  | O | 0.55370000  | 8.55060000  | -3.94600000 |
| C | 2.47990000  | 3.43600000  | 1.70590000  | O | 0.43430000  | 6.39030000  | -3.49360000 |
| C | -0.23080000 | 4.12080000  | 1.50850000  | H | 0.62270000  | 5.71820000  | -2.80150000 |
| H | -0.08490000 | 4.67930000  | 3.58270000  | C | 3.69110000  | 9.47000000  | -4.39150000 |
| C | 1.82100000  | 3.32100000  | 0.48830000  | O | 3.74010000  | 8.61340000  | -5.27230000 |
| H | 3.52800000  | 3.15850000  | 1.79270000  | O | 2.64160000  | 10.30500000 | -4.24500000 |
| C | 0.47280000  | 3.69450000  | 0.37040000  | H | 1.86070000  | 9.85590000  | -4.65220000 |
| H | -1.27930000 | 4.39580000  | 1.42940000  | C | 7.35600000  | 8.67460000  | -5.46630000 |
| H | 2.35290000  | 2.95200000  | -0.38570000 | O | 7.38450000  | 9.85890000  | -5.76250000 |
| C | 2.59710000  | 8.35740000  | 0.70550000  | O | 6.39000000  | 7.81200000  | -5.88320000 |
| C | 2.03480000  | 9.40390000  | -0.04700000 | H | 5.56220000  | 8.32710000  | -6.04530000 |
| C | 2.64650000  | 7.07270000  | 0.14320000  | C | -0.12630000 | 3.76680000  | -0.96850000 |
| C | 1.46820000  | 9.15820000  | -1.29180000 | O | 0.51180000  | 3.91610000  | -2.01080000 |
| H | 2.01180000  | 10.40710000 | 0.36880000  | O | -1.48380000 | 3.70590000  | -0.97340000 |
| C | 2.08300000  | 6.83330000  | -1.10670000 | H | -1.74420000 | 3.83980000  | -1.90640000 |
| H | 3.11800000  | 6.25780000  | 0.68820000  | C | 9.99950000  | -0.98230000 | -1.11470000 |
| C | 1.46170000  | 7.86080000  | -1.83550000 | O | 9.88590000  | -2.09050000 | -0.60870000 |
| H | 1.01590000  | 9.97210000  | -1.85290000 | O | 9.93930000  | -0.80650000 | -2.47130000 |
| H | 2.13550000  | 5.82120000  | -1.50710000 | H | 9.76740000  | -1.69930000 | -2.82830000 |
| C | 3.08830000  | 12.58100000 | 2.16470000  | C | 6.72870000  | -1.90940000 | 8.73730000  |
| C | 2.90600000  | 13.15870000 | 0.90370000  | O | 5.77770000  | -2.10860000 | 9.48510000  |
| C | 1.98570000  | 12.10080000 | 2.88130000  | O | 7.87050000  | -2.65690000 | 8.84300000  |
| C | 1.61650000  | 13.26050000 | 0.36480000  | H | 7.68850000  | -3.26690000 | 9.58490000  |
| H | 3.75940000  | 13.53160000 | 0.34310000  | C | 3.78010000  | 0.63920000  | 10.07760000 |
| C | 0.70250000  | 12.20820000 | 2.34040000  | O | 2.91700000  | -0.22340000 | 9.99370000  |
| H | 2.14670000  | 11.64630000 | 3.85800000  | O | 4.95970000  | 0.42870000  | 10.72550000 |
| C | 0.51160000  | 12.78870000 | 1.09080000  | H | 5.01790000  | -0.54070000 | 10.86490000 |
| H | -0.14860000 | 11.82280000 | 2.89890000  | C | 5.88610000  | 5.77160000  | 15.27380000 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.47640000 | 12.87010000 | 0.64470000  | O | 5.01830000  | 4.97730000  | 15.59310000 |
| C | 5.25800000  | 12.15740000 | 8.05150000  | O | 6.94300000  | 5.99160000  | 16.09220000 |
| C | 5.01610000  | 12.25880000 | 9.43070000  | H | 7.71410000  | 6.41880000  | 15.64310000 |
| C | 6.09440000  | 13.09230000 | 7.42780000  | C | 10.23560000 | 6.25530000  | 14.70950000 |
| C | 5.63140000  | 13.25810000 | 10.17700000 | O | 9.52550000  | 6.93680000  | 15.44640000 |
| H | 4.36830000  | 11.53410000 | 9.91710000  | O | 11.38080000 | 5.73040000  | 15.19440000 |
| C | 6.68910000  | 14.10060000 | 8.17320000  | H | 11.99390000 | 5.44550000  | 14.46090000 |
| H | 6.30750000  | 13.00060000 | 6.36490000  | C | 14.54760000 | 13.79920000 | 10.17140000 |
| C | 6.48020000  | 14.18240000 | 9.55680000  | O | 14.12930000 | 14.92740000 | 10.43420000 |
| H | 5.46790000  | 13.31500000 | 11.25120000 | O | 15.33930000 | 13.12210000 | 11.04070000 |
| H | 7.36160000  | 14.81830000 | 7.70770000  | H | 15.42000000 | 13.70110000 | 11.82430000 |
| C | 9.84440000  | 11.67400000 | 9.41920000  | C | 10.51490000 | 15.48840000 | 11.30130000 |
| C | 10.44740000 | 12.70660000 | 8.69370000  | O | 9.74530000  | 15.93430000 | 12.15070000 |
| C | 9.45410000  | 11.90710000 | 10.75050000 | O | 11.59220000 | 16.21860000 | 10.96100000 |
| C | 10.69170000 | 13.93660000 | 9.30220000  | H | 12.27760000 | 15.69390000 | 10.48120000 |
| H | 10.70480000 | 12.55130000 | 7.64610000  | C | 7.26200000  | 15.18580000 | 10.31880000 |
| C | 9.67230000  | 13.14270000 | 11.34100000 | O | 7.95670000  | 16.04630000 | 9.79150000  |
| H | 8.98940000  | 11.10060000 | 11.31410000 | O | 7.18470000  | 15.00530000 | 11.65860000 |
| C | 10.31240000 | 14.17240000 | 10.63180000 | H | 7.97490000  | 15.47110000 | 12.05660000 |
| H | 11.13360000 | 14.74100000 | 8.71740000  | C | 13.03930000 | 6.68350000  | 12.43140000 |
| H | 9.35750000  | 13.32490000 | 12.36510000 | O | 13.22120000 | 5.70050000  | 13.16080000 |
| C | 13.43660000 | 11.71620000 | 6.62440000  | O | 12.90280000 | 7.93230000  | 12.95170000 |
| C | 13.40580000 | 13.12050000 | 6.66670000  | H | 12.97450000 | 7.83290000  | 13.92240000 |
| C | 13.93000000 | 10.99610000 | 7.72060000  | H | 4.50310000  | 1.08660000  | -1.82570000 |
| C | 13.79520000 | 13.78290000 | 7.82040000  | C | 5.87300000  | -0.77640000 | -0.52200000 |
| H | 13.03750000 | 13.67820000 | 5.80650000  | O | 5.36250000  | -1.29020000 | -1.50670000 |
| C | 14.34450000 | 11.66470000 | 8.86650000  | O | 6.56460000  | -1.50310000 | 0.40200000  |
| H | 13.97180000 | 9.90900000  | 7.67300000  | H | 6.62200000  | -2.40850000 | 0.03870000  |
| C | 14.25280000 | 13.06200000 | 8.93530000  | C | 16.26590000 | 1.95410000  | 8.80040000  |
| H | 13.74320000 | 14.86740000 | 7.88130000  | O | 16.47850000 | 1.41070000  | 9.87360000  |
| H | 14.71160000 | 11.10270000 | 9.72220000  | O | 17.27510000 | 2.49850000  | 8.05190000  |
| C | 12.60440000 | 6.44840000  | 8.19580000  | H | 18.08480000 | 2.34680000  | 8.57740000  |
| C | 12.36740000 | 7.66120000  | 8.85940000  | C | 1.36740000  | 13.85540000 | -0.97120000 |
| C | 12.98430000 | 5.31820000  | 8.93920000  | O | 0.26570000  | 14.03960000 | -1.46130000 |
| C | 12.52920000 | 7.75590000  | 10.23120000 | O | 2.51740000  | 14.18940000 | -1.63140000 |
| H | 12.02580000 | 8.52490000  | 8.29300000  | H | 2.21720000  | 14.56130000 | -2.48400000 |
| C | 13.13510000 | 5.41060000  | 10.31450000 |   |             |             |             |

\* All the optimized geometries of  $\text{Au}_{25}(\text{SR})_{18}^-$ ,  $\text{Au}_{38}(\text{SR})_{24}$ , and  $\text{Au}_{102}(\text{SR})_{44}$  clusters ( $\text{R} = \text{CH}_3$ ,  $\text{C}_6\text{H}_{13}$ ,  $\text{CH}_2\text{CH}_2\text{Ph}$ ,  $\text{Ph}$ ,  $\text{PhF}$ , and  $\text{PhCOOH}$ ) are on the website:

[http://sites.google.com/site/jjung2008/achievements/thiol-stabilized\\_gold\\_nanoclusters](http://sites.google.com/site/jjung2008/achievements/thiol-stabilized_gold_nanoclusters)