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Electronic Supplementary Information

A method for designing a novel class of gold-containing molecules

Christian A. Celaya[a,b], Mesías Orozco-Ic[a], Maria Dimitrova[a], Lukas N. Wirz[a], Dage Sundholm*[a]

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Contents

[a] University of Helsinki, Department of Chemistry, P.O. Box 55 (A.I. Virtanens plats 1), FIN-00014 University of Helsinki, Finland Email: Dage.Sundholm@helsinki.fi
[b] Departamento de Materiales de Baja Dimensionalidad, Instituto de Investigacíones en Materiales, UNAM, Apartado Postal 70-360, Ciudad de México 04510, México.

1 Computational methods

The molecular structures were optimized at the B3LYP(D3-BJ)/def2-TZVP level of theory using Turbomole.[1–5] The integration grid 6 was used.[6] Excitation energies were calculated at the time-dependent density functional theory level using the B3LYP and M06-2X functionals and the def2-TZVP basis set.[1,5,7–9]

The calculations on infinite one-dimensional (1D) nanotubes with periodic boundary conditions (PBC) were performed at the PBE[10] level with the SIESTA *ab initio* package[11] using the Troullier-Martins pseudopotentials[12] and the corresponding double-ζ polarization (DZP) basis sets. Dispersion interaction was considered employing the semi-empirical D2 correction.[13] The convergence criteria of the 1D PBC calculations were 10^{-5} eV for the energy, 10^{-5} e for the electron density, and 0.04 eV/Å for the structure optimizations. The real-space mesh cut-off energy is set to 250 Ry and a $1 \times 1 \times 3$ k point grid were employed.[14] The starting structures of the single-wall nanotubes were generated by using our own code which is available for free.[15]

Calculations on the two-dimensional (2D) structures with PBC were performed with the Quantum ESPRESSO 6.2 code at the PBE level using a plane-wave basis set with a cut-off at 680 eV.[10,16] The USPP ultrasoft pseudopotentials were used for all atoms.[17] The D3-BJ semi-empirical correction was used to account for van-der-Waals interactions.[4] In the structure optimization, we used $6 \times 6 \times 1$ k points for the primitive cell. A primitive cell consisting of $12 \times 12 \times 2$ k points were used in the calculation of electronic properties and density of states.[14] The convergence criteria of the 2D PBC calculations were 10^{-5} eV for the energy, 10^{-5} eV and 0.025 eV/Å for the structure optimizations using the Broyden-Fletcher-Goldfarb-Shannon (BFGS) quasi-Newton algorithm.[18]

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2 Molecular coordinates in Å

2.1 Molecule in Figure 1(a)

27

C	−2.61555700	−4.36408400	0.00000000
C	5.08718700	−0.08309700	0.00000000
H	−3.48924800	−5.00845900	0.00000000
H	6.08207600	−0.51754800	0.00000000
C	−2.47162900	4.44718100	0.00000000
H	−2.59282800	5.52600700	0.00000000
C	−1.75491700	−2.25043200	0.00000000
C	2.82639000	−0.39458700	0.00000000
C	−1.07147200	2.64501900	0.00000000
C	−0.39918300	−4.13747400	0.00000000
H	0.60269700	−4.55136600	0.00000000
C	3.78275000	1.72303400	0.00000000
H	3.64025000	2.79763400	0.00000000
C	−3.38356600	2.41444000	0.00000000
H	−4.24294700	1.75373200	0.00000000
N	2.67929100	0.96592500	0.00000000
N	5.01440600	1.25113200	0.00000000
N	4.06217300	−0.92094500	0.00000000
N	−2.17616100	1.83737200	0.00000000
N	−1.23352400	3.97841700	0.00000000
N	−3.59071500	3.71703700	0.00000000
N	−0.50313000	−2.80329700	0.00000000
N	−2.82864800	−3.05747200	0.00000000
N	−1.42369000	−4.96816900	0.00000000
Au	0.75355000	1.81979000	0.00000000
Au	−1.95276000	−0.25730100	0.00000000
Au	1.19920900	−1.56248900	0.00000000

2.2 Molecule in Figure 1(b)

63

C	0.68327400	1.18346600	0.00000000
C	−6.15669100	1.17810600	0.00000000
C	−2.71900100	−4.70944700	0.00000000
C	−2.71900100	4.70944700	0.00000000
C	0.68327400	−1.18346600	0.00000000
C	2.05807600	−5.92090400	0.00000000
C	−1.36654900	0.00000000	0.00000000
C	5.43800100	0.00000000	0.00000000
C	2.05807600	5.92090400	0.00000000
C	4.04521300	7.00651500	0.00000000
H	4.58854400	7.94759100	0.00000000
C	7.47820000	1.11492000	0.00000000
H	8.00306800	2.06264000	0.00000000
C	7.47820000	−1.11492000	0.00000000
H	8.00306800	−2.06264000	0.00000000
C	4.04521300	−7.00651500	0.00000000
H	4.58854400	−7.94759100	0.00000000
C	−2.77355100	−7.03377100	0.00000000
H	−2.21523600	−7.96218000	0.00000000
C	−4.70464900	−5.91885100	0.00000000
H	−5.78783200	−5.89954000	0.00000000
C	−8.09042700	0.00000000	0.00000000
H	−9.17708700	0.00000000	0.00000000
C	−4.70464900	5.91885100	0.00000000
H	−5.78783200	5.89954000	0.00000000
C	−2.77355100	7.03377100	0.00000000
H	−2.21523600	7.96218000	0.00000000
N	−0.67122300	1.16259300	0.00000000
N	1.34244700	0.00000000	0.00000000
N	−0.67122300	−1.16259300	0.00000000
Au	−1.71977100	2.97873000	0.00000000
Au	1.68744500	2.92274000	0.00000000
Au	−3.37488900	0.00000000	0.00000000
N	−5.47393100	0.00000000	0.00000000
N	−7.49277500	−1.18594200	0.00000000
N	−7.49277500	1.18594200	0.00000000
N	−4.09577200	7.09408500	0.00000000
C	4.09861500	−4.74279800	0.00000000
C	4.09861500	4.74279800	0.00000000
Au	0.05571800	−5.89955800	0.00000000
Au	0.05571800	5.89955800	0.00000000
Au	5.08130800	−2.99803200	0.00000000
C	−6.15669100	−1.17810600	0.00000000
Au	−5.13702600	−2.90152600	0.00000000
Au	−5.13702600	2.90152600	0.00000000
N	−4.07847400	4.73991700	0.00000000
N	−4.07847400	−4.73991700	0.00000000
N	−2.06565200	−5.90202100	0.00000000
N	−4.09577200	−7.09408500	0.00000000
N	2.73696500	−4.74056300	0.00000000
N	4.77344300	−5.89596300	0.00000000
N	2.71933200	−7.08190400	0.00000000
N	6.14412600	−1.16210400	0.00000000
N	8.19154300	0.00000000	0.00000000
N	2.73696500	4.74056300	0.00000000
N	−2.06565200	5.90202100	0.00000000
N	6.14412600	1.16210400	0.00000000
N	4.77344300	5.89596300	0.00000000
N	2.71933200	7.08190400	0.00000000
Au	−1.71977100	−2.97873000	0.00000000
Au	1.68744500	−2.92274000	0.00000000
Au	3.43954100	0.00000000	0.00000000

```
Au      5.08130800      2.99803200      0.00000000
```

2.3 Unit cell in Figure 2(b)

```
9
cell parameters a=b=6.75 \AA, c= 20.0 \AA
C        2.437723469   0.676291798   2.000024761
C        3.761748928   5.338629238   2.000026795
N        1.742568268   1.841875116   2.000044039
C        7.137399391   1.860560851   2.000023699
Au       6.152447481   3.565208292   1.999923222
N        6.475568317   0.675761325   2.000040163
N        5.118748213   5.357768749   2.000045212
Au       4.406411157   0.676783463   1.999927049
Au       2.777716040   3.633520945   1.999945058
```

2.4 Molecule in Figure 3(a)

```
66
Energy =
C    -1.9389457    3.3583525    0.0000000
C    -1.9389457   -3.3583525    0.0000000
C     3.8778914    0.0000000    0.0000000
C    -7.7136406    0.0000000    0.0000000
C     3.8568203    6.6802087    0.0000000
C     3.8568203   -6.6802087    0.0000000
C    -1.8511369   10.1584711    0.0000000
C     9.7230625    3.4761040    0.0000000
C     9.7230625   -3.4761040    0.0000000
H     8.0512160   -7.6992870    0.0000000
C    -1.8511369  -10.1584711    0.0000000
C    -7.8719256   -6.6823671    0.0000000
C    -7.8719256    6.6823671    0.0000000
H    10.8163171   -3.5027050    0.0000000
H    10.8163171    3.5027050    0.0000000
H     8.0512160    7.6992870    0.0000000
H     2.6421701   10.8222011    0.0000000
H    -2.3747270   11.1185579    0.0000000
H    -8.4415900    7.6158529    0.0000000
H   -10.6933861    3.1229141    0.0000000
H   -10.6933861   -3.1229141    0.0000000
H    -8.4415900   -7.6158529    0.0000000
H    -2.3747270  -11.1185579    0.0000000
H     2.6421701  -10.8222011    0.0000000
Au    2.4897560    1.3596719    0.0000000
Au   -2.4223884   -1.4763560    0.0000000
Au   -0.0673676   -2.8360278    0.0000000
Au    2.4897560   -1.3596719    0.0000000
Au   -0.0673676    2.8360278    0.0000000
Au   -2.4223884    1.4763560    0.0000000
Au   -2.9040480    5.0299587    0.0000000
Au   -2.8958286    8.4630429    0.0000000
Au    0.0779237   10.0730779    0.0000000
Au    2.6860923    8.1505421    0.0000000
Au    2.8520408    4.9398795    0.0000000
Au    5.7155303    6.4014952    0.0000000
Au    8.6845795    5.1040228    0.0000000
Au    8.7771244    1.7236603    0.0000000
Au    5.8080960    0.0000000    0.0000000
Au    8.7771244   -1.7236603    0.0000000
Au    8.6845795   -5.1040228    0.0000000
Au    5.7155303   -6.4014952    0.0000000
Au    2.8520408   -4.9398795    0.0000000
Au    2.6860923   -8.1505421    0.0000000
Au    0.0779237  -10.0730779    0.0000000
Au   -2.8958286   -8.4630429    0.0000000
Au   -2.9040480   -5.0299587    0.0000000
Au   -5.8812958   -6.7393826    0.0000000
Au   -8.7625032   -4.9690551    0.0000000
Au   -8.4016227   -1.7490468    0.0000000
Au   -5.7040815    0.0000000    0.0000000
Au   -8.4016227    1.7490468    0.0000000
Au   -8.7625032    4.9690551    0.0000000
Au   -5.8812958    6.7393826    0.0000000
N    -3.7025158    0.0000000    0.0000000
N     1.8512579    3.2064727    0.0000000
N     1.8512579   -3.2064727    0.0000000
N    -3.8927635   -6.7424642    0.0000000
N     7.7855270    0.0000000    0.0000000
N     7.6309295    6.7788733    0.0000000
N     7.6309295   -6.7788733    0.0000000
N     2.0552118   -9.9980154    0.0000000
N    -9.6861412   -3.2191421    0.0000000
N    -9.6861412    3.2191421    0.0000000
N    -3.8927635    6.7424642    0.0000000
N     2.0552118    9.9980154    0.0000000
```

2.5 Molecule in Figure 3(b)

```
54
Energy =
C    -2.0676535    3.5812809    0.0000000
C    -2.0676535   -3.5812809    0.0000000
C     4.1353070    0.0000000    0.0000000
C     2.5598769   -4.4338369    0.0000000
C     2.5598769    4.4338369    0.0000000
C    -5.1197539    0.0000000    0.0000000
C    -6.7754602    4.6221594    0.0000000
H    -7.4322313    5.4972516    0.0000000
H    -8.3669558    3.4843592    0.0000000
H     1.1659343    8.9881759    0.0000000
C    -0.6151774    8.1788004    0.0000000
H    -1.0446439    9.1851269    0.0000000
H     7.2010215    5.5038167    0.0000000
C     7.3906376    3.5566409    0.0000000
H     8.4768751    3.6878753    0.0000000
H     7.2010215   -5.5038167    0.0000000
C     7.3906376   -3.5566409    0.0000000
H     8.4768751   -3.6878753    0.0000000
C    -0.6151774   -8.1788004    0.0000000
H    -1.0446439   -9.1851269    0.0000000
H     1.1659343   -8.9881759    0.0000000
H    -8.3669558   -3.4843592    0.0000000
C    -6.7754602   -4.6221594    0.0000000
H    -7.4322313   -5.4972516    0.0000000
N     0.6679295   -8.1008951    0.0000000
N    -2.6705256   -4.6254860    0.0000000
N    -7.3495457   -3.4720037    0.0000000
N    -3.8546908    0.0000000    0.0000000
N    -2.6705256    4.6254860    0.0000000
N    -7.3495457    3.4720037    0.0000000
N     0.6679295    8.1008951    0.0000000
N     1.9273454    3.3382601    0.0000000
N     5.3410512    0.0000000    0.0000000
N     6.6816163    4.6288915    0.0000000
N     6.6816163   -4.6288915    0.0000000
N     1.9273454   -3.3382601    0.0000000
Au    4.5746869    4.5682162    0.0000000
Au    1.6688478    6.2459031    0.0000000
Au   -0.1052225    3.0688419    0.0000000
Au   -1.7211560    6.5029752    0.0000000
Au    6.4923197   -1.7609228    0.0000000
Au    6.4923197    1.7609228    0.0000000
Au    2.7103063   -1.4432956    0.0000000
Au    4.5746869   -4.5682162    0.0000000
Au    2.7103063    1.4432956    0.0000000
Au    1.6688478   -6.2459031    0.0000000
Au   -0.1052225   -3.0688419    0.0000000
```

```
Au   -1.7211560   -6.5029752    0.0000000
Au   -4.7711637   -4.7420524    0.0000000
Au   -2.6050838   -1.6255463    0.0000000
Au   -6.2435347   -1.6776869    0.0000000
Au   -4.7711637    4.7420524    0.0000000
Au   -6.2435347    1.6776869    0.0000000
Au   -2.6050838    1.6255463    0.0000000
```

2.6 Unit cell in Figure 4(b)

```
24
 cell parameters a=16.47 \AA, b =9.5 \AA, c= 20.0 \AA
C       4.269560449     3.39785566      14.99997376
C       7.881636671     9.663058801     14.9999886
C       11.50764107     3.393180791     15.00000146
C       3.277608753     8.134620242     15.00002531
C       12.49227735     8.13992732      15.00000766
C       16.12233198     4.919128976     15.00004748
N       4.363464354     7.508718973     15.00003583
N       3.187824911     2.773363163     14.99996511
N       7.881420744     1.414937089     14.9999625
N       12.59334286     2.771750797     15.00001447
N       16.1219111      6.170739898     15.00006643
N       11.40827132     7.514703006     15.0000021
Au      14.34890926     7.317673249     15.00003795
Au      9.524379541     8.468144517     14.99999214
Au      6.243257751     8.465940396     15.00001146
Au      4.519459013     5.411255441     15.00000167
Au      1.423747528     7.305387517     14.99998029
Au      1.295841604     3.723857847     14.99993782
Au      11.27628144     5.409773012     15.00000606
Au      14.47907733     3.726744273     15.00002741
Au      12.69854094     0.659872981     14.99997896
Au      9.652956971     2.565560723     14.99998097
Au      6.133277434     2.592628002     14.99998024
Au      3.090367878     0.658226367     14.9999743
```

2.7 Molecule in Figure 5(a)

```
20

Au      1.72649900      1.78577100      -0.00703300
Au      1.70916200      -1.85110200     0.00454400
Au      -1.74012100     1.78185900      -0.00631800
Au      -1.69357500     -1.85466700     0.00527700
C       -3.38599800     0.63926800      -0.00112400
N       -3.39221400     -0.65226900     0.00000600
H       -4.38212600     1.09847800      0.00180700
H       -4.31412800     -1.08146900     0.00299200
C       3.37974100      0.65442700      -0.00993500
C       0.00913900      -2.90063500     0.01344000
N       -0.00833400     2.92619100      -0.00946500
N       3.39880800      -0.63694300     -0.00569600
H       4.32478900      -1.05723700     -0.00955900
H       4.37103000      1.12356500      -0.01774200
C       -0.00874700     4.19222900      -0.01500700
N       0.00824300      -4.21253200     0.02599200
H       -0.85025300     -4.74705800     0.03173100
H       0.86565700      -4.74876000     0.03131000
H       -0.93612400     4.77042400      -0.02118200
H       0.91855300      4.77046000      -0.01403700
```

Bent version of 5(a)

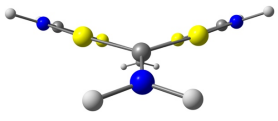

Fig. S1 The bent molecular structure of 5(a), which is 0.5 kJ/mol higher in energy than the planar 5(a) structure in the main article.

```
20

H      -1.0505337   -1.0710050   -4.2426966
H       1.1297425   -0.8572257   -4.2066744
C      -0.6030182   -0.7246237   -3.3035243
N       0.6835795   -0.6133431   -3.3261063
Au     -1.7341610   -0.2965046   -1.7053524
Au      1.8101481   -0.0022735   -1.6839711
C       2.7497276    0.5188619    0.0000000
N      -2.8268719    0.1482013    0.0000000
N       3.8931157    1.1600364    0.0000000
C      -3.9832507    0.6615824    0.0000000
Au     -1.7341610   -0.2965046    1.7053524
Au      1.8101481   -0.0022735    1.6839711
C       2.7497276    0.5188619    0.0000000
N      -2.8268719    0.1482013    0.0000000
N       3.8931157    1.1600364    0.0000000
C      -3.9832507    0.6615824    0.0000000
Au     -1.7341610   -0.2965046    1.7053524
Au      1.8101481   -0.0022735    1.6839711
C      -0.6030182   -0.7246237    3.3035243
N       0.6835795   -0.6133431    3.3261063
H      -1.0505337   -1.0710050    4.2426966
H       1.1297425   -0.8572257    4.2066744
H       4.3592167    1.4239441   -0.8579512
H       4.3592167    1.4239441    0.8579512
H      -4.5113340    0.8966906    0.9274117
H      -4.5113340    0.8966906   -0.9274117
```

2.8 Molecule in Figure 5(b)

```
28

C       5.8058894    0.0000000   -0.7354113
N       5.8945714    0.0000000    0.6002915
N       4.6914573   -0.0000000   -1.4451596
C       4.7268070    0.0000000    1.2108587
C       3.5178561   -0.0000000   -0.7806435
N       3.5422876    0.0000000    0.5897635
Au      1.7724203    0.0000000   -1.7726536
Au      1.7290968    0.0000000    1.6621529
C       0.0000000    0.0000000    2.6607620
N       0.0000000    0.0000000   -2.8431585
N       0.0000000    0.0000000    3.9724674
C       0.0000000    0.0000000   -4.1111781
Au     -1.7724203    0.0000000   -1.7726536
Au     -1.7290968    0.0000000    1.6621529
C      -3.5178561    0.0000000   -0.7806435
N      -3.5422876   -0.0000000    0.5897635
N      -4.6914573    0.0000000   -1.4451596
C      -5.8058894    0.0000000   -0.7354113
C      -4.7268070    0.0000000    1.2108587
N      -5.8945714    0.0000000    0.6002915
H       0.8581620    0.0000000    4.5075704
H      -0.8581620    0.0000000    4.5075704
H      -0.9275969    0.0000000   -4.6876737
H       0.9275969    0.0000000   -4.6876737
H       6.7433985    0.0000000   -1.2837141
H       4.7116118   -0.0000000    2.2951723
H      -4.7116118    0.0000000    2.2951723
H      -6.7433985    0.0000000   -1.2837141
```

Bent version of 5(b)

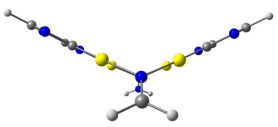

Fig. S2 The bent molecular structure of 5(a), which is 3 kJ/mol lower in energy than the planar 5(b) structure in the main article.

```
28
```

```
C     0.3581612   -1.5581299    5.3699089
N    -0.9380203   -1.2402132    5.4653119
N     1.1640477   -1.2699703    4.3617158
C    -1.4037456   -0.5772634    4.4246205
C     0.6460483   -0.5977818    3.3165688
N    -0.6785448   -0.2420744    3.3544004
Au    1.7332808   -0.0976265    1.7020856
Au   -1.4448019    0.7830511    1.6775587
C    -2.0869762    1.6489423    0.0000000
N     2.7974737    0.3984018    0.0000000
N    -2.8422571    2.7179335    0.0000000
C     3.9438877    0.9344659    0.0000000
Au    1.7332808   -0.0976265   -1.7020856
Au   -1.4448019    0.7830511   -1.6775587
C     0.6460483   -0.5977818   -3.3165688
N    -0.6785448   -0.2420744   -3.3544004
N     1.1640477   -1.2699703   -4.3617158
C     0.3581612   -1.5581299   -5.3699089
C    -1.4037456   -0.5772634   -4.4246205
N    -0.9380203   -1.2402132   -5.4653119
H    -3.1481211    3.1573618    0.8582708
H    -3.1481211    3.1573618   -0.8582708
H     4.4665074    1.1780682   -0.9276918
H     4.4665074    1.1780682    0.9276918
H     0.7856699   -2.1058785    6.2044480
H    -2.4465456   -0.2794148    4.4256525
H    -2.4465456   -0.2794148   -4.4256525
H     0.7856699   -2.1058785   -6.2044480
```

2.9 Molecule in Figure 6(a)

```
84

C       8.86554300      5.86202800      0.00000000
C       8.86554300      -5.86202800     0.00000000
C       4.05837400      -7.02931000     0.00000000
C       2.05095900      -5.88015100     0.00000000
C       0.64389300      -10.60880000    0.00000000
C       4.06688100      -4.71625800     0.00000000
H       4.59961000      -7.96675800     0.00000000
C       4.05837400      7.02931000      0.00000000
C       2.05095900      5.88015100      0.00000000
C       -9.50943700     -4.74677200     0.00000000
C       0.64389300      10.60880000     0.00000000
C       4.06688100      4.71625800      0.00000000
C       -8.11674900     0.00000000      0.00000000
C       -6.11783900     1.16389300      0.00000000
C       -6.11783900     -1.16389300     0.00000000
C       -9.50943700     4.74677200      0.00000000
H       -9.19922000     0.00000000      0.00000000
N       -5.46241200     0.00000000      0.00000000
N       2.73120600      4.73058800      0.00000000
N       2.73120600      -4.73058800     0.00000000
N       -7.49407600     1.16869000      0.00000000
N       -7.49407600     -1.16869000     0.00000000
N       2.73492300      7.07440600      0.00000000
N       4.75915300      5.90571600      0.00000000
N       4.75915300      -5.90571600     0.00000000
N       2.73492300      -7.07440600     0.00000000
Au      5.09376600      2.99435900      0.00000000
Au      6.86877400      5.92579900      0.00000000
Au      8.53258800      2.89989400      0.00000000
Au      5.09376600      -2.99435900     0.00000000
Au      8.53258800      -2.89989400     0.00000000
Au      6.86877400      -5.92579900     0.00000000
Au      0.04630800      -5.90851000     0.00000000
Au      1.69750600      -8.91143200     0.00000000
Au      -1.75491200     -8.83938500     0.00000000
Au      -5.14007400     -2.91415200     0.00000000
Au      -6.77767600     -5.93949100     0.00000000
Au      -8.56628000     -2.98563300     0.00000000
Au      -5.14007400     2.91415200      0.00000000
Au      -6.77767600     5.93949100      0.00000000
Au      -8.56628000     2.98563300      0.00000000
Au      0.04630800      5.90851000      0.00000000
Au      1.69750600      8.91143200      0.00000000
Au      -1.75491200     8.83938500      0.00000000
C       -2.76905900     -4.79615200     0.00000000
H       -2.22768200     -3.85845800     0.00000000
C       -2.76905900     4.79615200      0.00000000
H       -2.22768200     3.85845800      0.00000000
C       5.53811900      0.00000000      0.00000000
H       4.45536300      0.00000000      0.00000000
C       7.53943400      -1.16361400     0.00000000
C       7.53943400      1.16361400      0.00000000
C       -2.76199800     7.11114900      0.00000000
C       -4.77743600     5.94753400      0.00000000
C       -4.77743600     -5.94753400     0.00000000
C       -2.76199800     -7.11114900     0.00000000
N       -4.09435300     -4.75078600     0.00000000
N       -2.06712500     -5.92120700     0.00000000
N       -4.09631700     -7.09502900     0.00000000
N       -0.64391800     -10.60089200    0.00000000
N       -4.09435300     4.75078600      0.00000000
N       -4.09631700     7.09502900      0.00000000
N       -2.06712500     5.92120700      0.00000000
N       -0.64391800     10.60089200     0.00000000
N       6.16147800      1.17042100      0.00000000
N       6.16147800      -1.17042100     0.00000000
N       8.19263400      0.00000000      0.00000000
N       9.50260000      4.74279700      0.00000000
N       9.50260000      -4.74279700     0.00000000
N       -8.85868300     -5.85809500     0.00000000
H       4.59961000      7.96675800      0.00000000
N       -8.85868300     5.85809500      0.00000000
H       1.11806700      11.59530400     0.00000000
H       -1.08967200     11.51510500     0.00000000
H       -9.42753700     6.70123600      0.00000000
H       -10.60086100    4.82937800      0.00000000
H       -10.60086100    -4.82937800     0.00000000
H       -9.42753700     -6.70123600     0.00000000
H       9.48279500      6.76592600      0.00000000
H       10.51720900     4.81386900      0.00000000
H       10.51720900     -4.81386900     0.00000000
H       9.48279500      -6.76592600     0.00000000
H       1.11806700      -11.59530400    0.00000000
H       -1.08967200     -11.51510500    0.00000000
```

2.10 Unit cell in Figure 6(b)

```
81
cell parameters a=21.35 \AA, b =24.35 \AA, c= 20.0 \AA
C       19.96300890     18.03830572     13.85659327
C       19.96713818     6.50025180      13.85627287
C       14.89156279     5.08362952      13.85726054
C       12.82292107     6.16635861      13.85646315
C       11.38194126     1.27936677      13.85960273
C       14.85010991     7.40697050      13.85617625
H       15.46016649     4.15230926      13.85630975
C       14.88883689     19.44768613     13.85631210
C       12.82075971     18.36430015     13.85805241
C       0.70154637      7.70495479      13.85838500
C       11.38282547     23.25568292     13.85975078
C       14.84798258     17.12413485     13.85807372
C       2.44056308      12.26976525     13.85416306
C       4.45406363      13.45758870     13.85426209
C       4.45614297      11.08537616     13.85487919
```

C	0.69909536	16.83456044	13.85649351
H	1.34824852	12.26904630	13.85211357
N	5.09854969	12.27184792	13.85372811
N	13.49663690	17.19620811	13.85793261
N	13.49879754	7.33466405	13.85533562
N	3.05498193	13.45772241	13.85343067
N	3.05681699	11.08270492	13.85503262
N	13.54017559	19.56034522	13.85714679
N	15.59854496	18.30004954	13.85644463
N	15.60105461	6.23134908	13.85647423
N	13.54276151	4.97071256	13.85706689
Au	15.85839225	15.36754035	13.85774697
Au	17.90442287	18.09213711	13.85623590
Au	19.44672990	15.11043841	13.85909170
Au	15.86139921	9.16443411	13.85623160
Au	19.45064022	9.42982889	13.85978719
Au	17.90852216	6.44320248	13.85592649
Au	10.77803322	6.10651288	13.85570877
Au	12.39979329	3.04897788	13.85816890
Au	8.83958931	3.21161593	13.85960547
Au	5.42148663	9.30581123	13.85395818
Au	3.69703436	6.38376996	13.85902353
Au	1.83155443	9.35579817	13.85718833
Au	5.41912575	15.23621845	13.85351033
Au	3.69598541	18.15641656	13.85463984
Au	1.82960864	15.18418142	13.85454216
Au	10.77625315	18.42631167	13.85641045
Au	12.39859884	21.48435726	13.85856805
Au	8.84010849	21.32510722	13.85733752
C	7.82348583	7.28988536	13.85375812
H	8.38888102	8.22326774	13.84885931
C	7.82240907	17.24729659	13.85425303
H	8.38720252	16.31361626	13.85135403
C	16.32770094	12.26683499	13.85722689
H	15.23656503	12.26573253	13.85443242
C	18.33524715	11.08837519	13.86095854
C	18.33242572	13.45091028	13.86073218
C	7.78645281	19.57520839	13.85768521
C	5.75125948	18.33470415	13.85610225
C	5.75167120	6.20437765	13.86028942
C	7.78620095	4.96198772	13.86114157
N	6.47916106	7.39712949	13.85527289
N	8.53188328	6.14497700	13.85652655
N	6.43072149	5.03654607	13.86218252
N	9.98294978	1.29396675	13.85778814
N	6.47795249	17.14151162	13.85417607
N	6.43089398	19.50198103	13.85711153
N	8.53124164	18.39172106	13.85580377
N	9.98378843	23.24185268	13.85734023
N	16.93793618	13.46630021	13.85812006
N	16.94060915	11.06911943	13.85806295
N	18.97727097	12.27044978	13.86182705
N	20.67441698	16.84763850	13.85745417
N	20.67700992	7.69222870	13.85801328
N	1.39366074	6.51543691	13.85677894
H	15.45734344	20.37905242	13.85409979
N	20.65984265	5.34157637	13.85286865
N	12.02047324	0.08772677	13.86005909
N	20.65396213	19.19802991	13.85332999
N	1.38973529	18.02485846	13.85412999
C	0.62712564	19.14585224	13.85245005
C	0.63299161	5.39316643	13.85356512
H	1.17609841	4.44522455	13.85004768
C	9.37767950	0.08845380	13.85675953
H	1.16838560	20.09491545	13.84933192
H	8.28643569	0.08882391	13.85392658

2.11 Molecule in Figure 7(a)

54

Energy =

C	2.3348862	-4.5195257	-1.6564914
C	2.7465810	4.2818336	-1.6564914
H	2.4188238	-5.6016578	-1.6438545
H	3.6417661	4.8955918	-1.6438545
C	-5.0814671	0.2376921	-1.6564914
H	-6.0605899	0.7060661	-1.6438545
C	0.9947912	-2.6720142	-1.6330123
C	1.8166366	2.1975215	-1.6330123
C	-2.8114278	0.4744927	-1.6330123
C	3.3116640	-2.5168098	-1.6914158
H	4.1918032	-1.8849901	-1.6987510
C	0.5237892	4.1263900	-1.6914158
H	-0.4634523	4.5727031	-1.6987510
C	-3.8354532	-1.6095802	-1.6914158
H	-3.7283509	-2.6877131	-1.6987510
N	0.5853366	2.7912052	-1.6646274
N	1.5762794	4.9226621	-1.7037642
N	2.9154774	2.9686280	-1.6122748
N	-2.7099230	-0.8886862	-1.6646274
N	-4.0286460	1.0405635	-1.6122748
N	-5.0512901	-1.0962331	-1.7037642
N	2.1245863	-1.9025190	-1.6646274
N	1.1131686	-4.0091915	-1.6122748
N	3.4750107	-3.8264290	-1.7037642
Au	-1.1507081	1.5944124	-1.6042618
Au	-0.8054476	-1.7937486	-1.6042618
Au	1.9561557	0.1993363	-1.6042618
C	2.3348862	4.5195257	1.6564914
C	2.7465810	-4.2818336	1.6564914
H	2.4188238	5.6016578	1.6438545
H	3.6417661	-4.8955918	1.6438545
C	-5.0814671	-0.2376921	1.6564914
H	-6.0605899	-0.7060661	1.6438545
C	0.9947912	2.6720142	1.6330123
C	1.8166366	-2.1975215	1.6330123
C	-2.8114278	-0.4744927	1.6330123
C	3.3116640	2.5168098	1.6914158
H	4.1918032	1.8849901	1.6987510
C	0.5237892	-4.1263900	1.6914158
H	-0.4634523	-4.5727031	1.6987510
C	-3.8354532	1.6095802	1.6914158
H	-3.7283509	2.6877131	1.6987510
N	0.5853366	-2.7912052	1.6646274
N	1.5762794	-4.9226621	1.7037642
N	2.9154774	-2.9686280	1.6122748
N	-2.7099230	0.8886862	1.6646274
N	-4.0286460	-1.0405635	1.6122748
N	-5.0512901	1.0962331	1.7037642
N	2.1245863	1.9025190	1.6646274
N	1.1131686	4.0091915	1.6122748
N	3.4750107	3.8264290	1.7037642
Au	-1.1507081	-1.5944124	1.6042618
Au	-0.8054476	1.7937486	1.6042618
Au	1.9561557	-0.1993363	1.6042618

7(a) of C_{3h} symmetry

54

C	-2.61555700	-4.36408400	0.00000000
C	5.08718700	-0.08309700	0.00000000
H	-3.48924800	-5.00845900	0.00000000
H	6.08207600	-0.51754800	0.00000000
C	-2.47162900	4.44718100	0.00000000
H	-2.59282800	5.52600700	0.00000000
C	-1.75491700	-2.25043200	0.00000000

C	2.82639000	-0.39458700	0.00000000
C	-1.07147200	2.64501900	0.00000000
C	-0.39918300	-4.13747400	0.00000000
H	0.60269700	-4.55136600	0.00000000
C	3.78275000	1.72303400	0.00000000
H	3.64025000	2.79763400	0.00000000
C	-3.38356600	2.41444000	0.00000000
H	-4.24294700	1.75373200	0.00000000
N	2.67929100	0.96592500	0.00000000
N	5.01440600	1.25113200	0.00000000
N	4.06217300	-0.92094500	0.00000000
N	-2.17616100	1.83737200	0.00000000
N	-1.23352400	3.97841700	0.00000000
N	-3.59071500	3.71703700	0.00000000
N	-0.50313000	-2.80329700	0.00000000
N	-2.82864800	-3.05747200	0.00000000
N	-1.42369000	-4.96816900	0.00000000
Au	0.75355000	1.81979000	0.00000000
Au	-1.95276000	-0.25730100	0.00000000
Au	1.19920900	-1.56248900	0.00000000
C	-2.61555700	-4.36408400	3.00000000
C	5.08718700	-0.08309700	3.00000000
H	-3.48924800	-5.00845900	3.00000000
H	6.08207600	-0.51754800	3.00000000
C	-2.47162900	4.44718100	3.00000000
H	-2.59282800	5.52600700	3.00000000
C	-1.75491700	-2.25043200	3.00000000
C	2.82639000	-0.39458700	3.00000000
C	-1.07147200	2.64501900	3.00000000
C	-0.39918300	-4.13747400	3.00000000
H	0.60269700	-4.55136600	3.00000000
C	3.78275000	1.72303400	3.00000000
H	3.64025000	2.79763400	3.00000000
C	-3.38356600	2.41444000	3.00000000
H	-4.24294700	1.75373200	3.00000000
N	2.67929100	0.96592500	3.00000000
N	5.01440600	1.25113200	3.00000000
N	4.06217300	-0.92094500	3.00000000
N	-2.17616100	1.83737200	3.00000000
N	-1.23352400	3.97841700	3.00000000
N	-3.59071500	3.71703700	3.00000000
N	-0.50313000	-2.80329700	3.00000000
N	-2.82864800	-3.05747200	3.00000000
N	-1.42369000	-4.96816900	3.00000000
Au	0.75355000	1.81979000	3.00000000
Au	-1.95276000	-0.25730100	3.00000000
Au	1.19920900	-1.56248900	3.00000000

2.12 Molecule in Figure 7(b)

126
Energy =

C	-1.1815111	0.6821458	-1.6312444
C	-1.1792983	-6.1528626	-1.6678615
C	4.7126682	-2.7208603	-1.6276899
C	-4.7126682	-2.7208603	-1.6276899
C	1.1815111	0.6821458	-1.6312444
C	5.9181845	2.0551291	-1.6678615
C	0.0000000	-1.3642915	-1.6312444
C	-0.0000000	5.4417206	-1.6276899
C	-5.9181845	2.0551291	-1.6678615
C	-7.0055498	4.0446561	-1.7014387
H	-7.9463648	4.5878358	-1.7146149
C	-1.1155874	7.4801242	-1.6083436
H	-2.0626014	8.0045720	-1.5882266
C	1.1155874	7.4801242	-1.6083436
H	2.0626014	8.0045720	-1.5882266
C	7.0055498	4.0446561	-1.7014387
H	7.9463648	4.5878358	-1.7146149
C	7.0357713	-2.7739351	-1.6083436
H	7.9634634	-2.2160208	-1.5882266
C	5.9201839	-4.7061892	-1.6083436
H	5.9008620	-5.7885512	-1.5882266
C	0.0000000	-8.0893121	-1.7014387
H	0.0000000	-9.1756717	-1.7146149
C	-5.9201839	-4.7061892	-1.6083436
H	-5.9008620	-5.7885512	-1.5882266
C	-7.0357713	-2.7739351	-1.6083436
H	-7.9634634	-2.2160208	-1.5882266
N	-1.1618726	-0.6708075	-1.6308424
N	0.0000000	1.3416149	-1.6308424
N	1.1618726	-0.6708075	-1.6308424
Au	-2.9822103	-1.7217799	-1.5877946
Au	-2.9192088	1.6854060	-1.6069331
Au	0.0000000	-3.3708120	-1.6069331
N	0.0000000	-5.4730987	-1.6675712
N	1.1852677	-7.4910234	-1.6826074
N	-1.1852677	-7.4910234	-1.6826074
N	-7.0942736	-4.0958808	-1.6054554
C	4.7388862	4.0977336	-1.6678615
C	-4.7388862	4.0977336	-1.6678615
Au	5.8983165	0.0542856	-1.6022430
Au	-5.8983165	0.0542856	-1.6022430
Au	2.9961709	5.0809491	-1.6022430
C	1.1792983	-6.1528626	-1.6678615
Au	2.9021455	-5.1352347	-1.6022430
Au	-2.9021455	-5.1352347	-1.6022430
N	-4.7421288	-4.0787209	-1.6238966
N	4.7421288	-4.0787209	-1.6238966
N	5.9033403	-2.0674435	-1.6238966
N	7.0942736	-4.0958808	-1.6054554
N	4.7398425	2.7365493	-1.6675712
N	5.8947827	4.7719836	-1.6826074
N	7.0800504	2.7190398	-1.6826074
N	1.1612116	6.1461644	-1.6238966
N	0.0000000	8.1917616	-1.6054554
N	-4.7398425	2.7365493	-1.6675712
N	-5.9033403	-2.0674435	-1.6238966
N	-1.1612116	6.1461644	-1.6238966
N	-5.8947827	4.7719836	-1.6826074
N	-7.0800504	2.7190398	-1.6826074
Au	2.9822103	-1.7217799	-1.5877946
Au	2.9192088	1.6854060	-1.6069331
Au	-0.0000000	3.4435598	-1.5877946
Au	-2.9961709	5.0809491	-1.6022430
C	-1.1815111	-0.6821458	1.6312444
C	-1.1792983	6.1528626	1.6678615
C	4.7126682	2.7208603	1.6276899
C	-4.7126682	2.7208603	1.6276899
C	1.1815111	-0.6821458	1.6312444
C	5.9181845	-2.0551291	1.6678615
C	0.0000000	1.3642915	1.6312444
C	-0.0000000	-5.4417206	1.6276899
C	-5.9181845	-2.0551291	1.6678615
C	-7.0055498	-4.0446561	1.7014387
H	-7.9463648	-4.5878358	1.7146149
C	-1.1155874	-7.4801242	1.6083436
H	-2.0626014	-8.0045720	1.5882266
C	1.1155874	-7.4801242	1.6083436
H	2.0626014	-8.0045720	1.5882266
C	7.0055498	-4.0446561	1.7014387
H	7.9463648	-4.5878358	1.7146149
C	7.0357713	2.7739351	1.6083436
H	7.9634634	2.2160208	1.5882266
C	5.9201839	4.7061892	1.6083436
H	5.9008620	5.7885512	1.5882266
C	-0.0000000	8.0893121	1.7014387

H	0.0000000	9.1756717	1.7146149
C	−5.9201839	4.7061892	1.6083436
H	−5.9008620	5.7885512	1.5882266
C	−7.0357713	2.7739351	1.6083436
H	−7.9634634	2.2160208	1.5882266
N	−1.1618726	0.6708075	1.6308424
N	0.0000000	−1.3416149	1.6308424
N	1.1618726	0.6708075	1.6308424
Au	−2.9822103	1.7217799	1.5877946
Au	−2.9192088	−1.6854060	1.6069331
Au	0.0000000	3.3708120	1.6069331
N	0.0000000	5.4730987	1.6675712
N	1.1852677	7.4910234	1.6826074
N	−1.1852677	7.4910234	1.6826074
N	−7.0942736	4.0958808	1.6054554
C	4.7388862	−4.0977336	1.6678615
C	−4.7388862	−4.0977336	1.6678615
Au	5.8983165	−0.0542856	1.6022430
Au	−5.8983165	−0.0542856	1.6022430
Au	2.9961709	−5.0809491	1.6022430
C	1.1792983	6.1528626	1.6678615
Au	2.9021455	5.1352347	1.6022430
Au	−2.9021455	5.1352347	1.6022430
N	−4.7421288	4.0787209	1.6238966
N	4.7421288	4.0787209	1.6238966
N	5.9033403	2.0674435	1.6238966
N	7.0942736	4.0958808	1.6054554
N	4.7398425	−2.7365493	1.6675712
N	5.8947827	−4.7719836	1.6826074
N	7.0800504	−2.7190398	1.6826074
N	1.1612116	−6.1461644	1.6238966
N	−0.0000000	−8.1917616	1.6054554
N	−4.7398425	−2.7365493	1.6675712
N	−5.9033403	2.0674435	1.6238966
N	−1.1612116	−6.1461644	1.6238966
N	−5.8947827	−4.7719836	1.6826074
N	−7.0800504	−2.7190398	1.6826074
Au	2.9822103	1.7217799	1.5877946
Au	2.9192088	−1.6854060	1.6069331
Au	0.0000000	−3.4435598	1.5877946
Au	−2.9961709	−5.0809491	1.6022430

7(b) of D_{3h} symmetry

126

C	0.68327400	1.18346600	0.00000000
C	−6.15669100	1.17810600	0.00000000
C	−2.71900100	−4.70944700	0.00000000
C	−2.71900100	4.70944700	0.00000000
C	0.68327400	−1.18346600	0.00000000
C	2.05807600	−5.92090400	0.00000000
C	−1.36654900	0.00000000	0.00000000
C	5.43800100	0.00000000	0.00000000
C	2.05807600	5.92090400	0.00000000
C	4.04521300	7.00651500	0.00000000
H	4.58854400	7.94759100	0.00000000
C	7.47820000	1.11492000	0.00000000
H	8.00306800	2.06264000	0.00000000
C	7.47820000	−1.11492000	0.00000000
H	8.00306800	−2.06264000	0.00000000
C	4.04521300	−7.00651500	0.00000000
H	4.58854400	−7.94759100	0.00000000
C	−2.77355100	−7.03377100	0.00000000
H	−2.21523600	−7.96218000	0.00000000
C	−4.70464900	−5.91885100	0.00000000
H	−5.78783200	−5.89954000	0.00000000
C	−8.09042700	0.00000000	0.00000000
H	−9.17708700	0.00000000	0.00000000
C	−4.70464900	5.91885100	0.00000000
H	−5.78783200	5.89954000	0.00000000
C	−2.77355100	7.03377100	0.00000000
H	−2.21523600	7.96218000	0.00000000
N	−0.67122300	1.16259300	0.00000000
N	1.34244700	0.00000000	0.00000000
N	−0.67122300	−1.16259300	0.00000000
Au	−1.71977100	2.97873000	0.00000000
Au	1.68744500	2.92274000	0.00000000
Au	−3.37488900	0.00000000	0.00000000
N	−5.47393100	0.00000000	0.00000000
N	−7.49277500	−1.18594200	0.00000000
N	−7.49277500	1.18594200	0.00000000
N	−4.09577200	7.09408500	0.00000000
C	4.09861500	−4.74279800	0.00000000
C	4.09861500	4.74279800	0.00000000
Au	0.05571800	−5.89955800	0.00000000
Au	0.05571800	5.89955800	0.00000000
Au	5.08130800	−2.99803200	0.00000000
C	−6.15669100	−1.17810600	0.00000000
Au	−5.13702600	−2.90152600	0.00000000
Au	−5.13702600	2.90152600	0.00000000
N	−4.07847400	4.73991700	0.00000000
N	−4.07847400	−4.73991700	0.00000000
N	−2.06565200	−5.90202100	0.00000000
N	−4.09577200	−7.09408500	0.00000000
N	2.73696500	−4.74056300	0.00000000
N	4.77344300	−5.89596300	0.00000000
N	2.71933200	−7.08190400	0.00000000
N	6.14412600	−1.16210400	0.00000000
N	8.19154300	0.00000000	0.00000000
N	2.73696500	4.74056300	0.00000000
N	−2.06565200	5.90202100	0.00000000
N	6.14412600	1.16210400	0.00000000
N	4.77344300	5.89596300	0.00000000
N	2.71933200	7.08190400	0.00000000
Au	−1.71977100	−2.97873000	0.00000000
Au	1.68744500	−2.92274000	0.00000000
Au	3.43954100	0.00000000	0.00000000
Au	5.08130800	2.99803200	0.00000000
C	0.68327400	1.18346600	3.00000000
C	−6.15669100	1.17810600	3.00000000
C	−2.71900100	−4.70944700	3.00000000
C	−2.71900100	4.70944700	3.00000000
C	0.68327400	−1.18346600	3.00000000
C	2.05807600	−5.92090400	3.00000000
C	−1.36654900	0.00000000	3.00000000
C	5.43800100	0.00000000	3.00000000
C	2.05807600	5.92090400	3.00000000
C	4.04521300	7.00651500	3.00000000
H	4.58854400	7.94759100	3.00000000
C	7.47820000	1.11492000	3.00000000
H	8.00306800	2.06264000	3.00000000
C	7.47820000	−1.11492000	3.00000000
H	8.00306800	−2.06264000	3.00000000
C	4.04521300	−7.00651500	3.00000000
H	4.58854400	−7.94759100	3.00000000
C	−2.77355100	−7.03377100	3.00000000
H	−2.21523600	−7.96218000	3.00000000
C	−4.70464900	−5.91885100	3.00000000
H	−5.78783200	−5.89954000	3.00000000
C	−8.09042700	0.00000000	3.00000000
H	−9.17708700	0.00000000	3.00000000
C	−4.70464900	5.91885100	3.00000000
H	−5.78783200	5.89954000	3.00000000
C	−2.77355100	7.03377100	3.00000000
H	−2.21523600	7.96218000	3.00000000
N	−0.67122300	1.16259300	3.00000000

N	1.34244700	0.00000000	3.00000000
N	-0.67122300	-1.16259300	3.00000000
Au	-1.71977100	2.97873000	3.00000000
Au	1.68744500	2.92274000	3.00000000
Au	-3.37488900	0.00000000	3.00000000
N	-5.47393100	0.00000000	3.00000000
N	-7.49277500	-1.18594200	3.00000000
N	-7.49277500	1.18594200	3.00000000
N	-4.09577200	7.09408500	3.00000000
C	4.09861500	-4.74279800	3.00000000
C	4.09861500	4.74279800	3.00000000
Au	0.05571800	-5.89955800	3.00000000
Au	0.05571800	5.89955800	3.00000000
Au	5.08130800	-2.99803200	3.00000000
C	-6.15669100	-1.17810600	3.00000000
Au	-5.13702600	-2.90152600	3.00000000
Au	-5.13702600	2.90152600	3.00000000
N	-4.07847400	4.73991700	3.00000000
N	-4.07847400	-4.73991700	3.00000000
N	-2.06565200	-5.90202100	3.00000000
N	-4.09577200	-7.09408500	3.00000000
N	2.73696500	-4.74056300	3.00000000
N	4.77344300	-5.89596300	3.00000000
N	2.71933200	-7.08190400	3.00000000
N	6.14412600	-1.16210400	3.00000000
N	8.19154300	0.00000000	3.00000000
N	2.73696500	4.74056300	3.00000000
N	-2.06565200	5.90202100	3.00000000
N	6.14412600	1.16210400	3.00000000
N	4.77344300	5.89596300	3.00000000
N	2.71933200	7.08190400	3.00000000
Au	-1.71977100	-2.97873000	3.00000000
Au	1.68744500	-2.92274000	3.00000000
Au	3.43954100	0.00000000	3.00000000
Au	5.08130800	2.99803200	3.00000000

2.13 Molecule in Figure 8

180

C	1.11598100	7.83643600	-7.40456200
N	1.16532500	7.62695400	-6.08750400
N	-0.00045200	7.98264300	-8.10207600
C	-0.00033500	7.57118100	-5.38632700
C	-1.11681100	7.83582400	-7.40455600
N	-1.16602100	7.62640600	-6.08748200
Au	-2.91535400	6.95714000	-5.05817300
Au	-6.95800900	2.91484300	-5.05823100
H	-2.06224200	7.88293100	-7.93162700
H	-7.88413800	2.06138600	-7.93163500
C	-7.83643600	1.11598100	-7.40456200
N	-7.62695400	1.16532500	-6.08750400
N	-7.98264300	-0.00045200	-8.10207600
C	-7.57118100	-0.00033500	-5.38632700
C	-7.83582400	-1.11681100	-7.40455600
N	-7.62640600	-1.16602100	-6.08748200
Au	-6.95714000	-2.91535400	-5.05817300
Au	-2.91484300	-6.95800900	-5.05823100
H	-7.88293100	-2.06224200	-7.93162700
H	-2.06138600	-7.88413800	-7.93163500
C	-1.11598100	-7.83643600	-7.40456200
N	-1.16532500	-7.62695400	-6.08750400
N	0.00045200	-7.98264300	-8.10207600
C	0.00033500	-7.57118100	-5.38632700
C	1.11681100	-7.83582400	-7.40455600
N	1.16602100	-7.62640600	-6.08748200
Au	2.91535400	-6.95714000	-5.05817300
Au	6.95800900	-2.91484300	-5.05823100
H	2.06224200	-7.88293100	-7.93162700
H	7.88413800	-2.06138600	-7.93163500
C	7.83643600	-1.11598100	-7.40456200
N	7.62695400	-1.16532500	-6.08750400
N	7.98264300	0.00045200	-8.10207600
C	7.57118100	0.00033500	-5.38632700
C	7.83582400	1.11681100	-7.40455600
N	7.62640600	1.16602100	-6.08748200
Au	6.95714000	2.91535400	-5.05817300
Au	2.91484300	6.95800900	-5.05823100
H	7.88293100	2.06224200	-7.93162700
H	2.06138600	7.88413800	-7.93163500
C	-4.42337000	6.04880800	-4.09259900
N	-4.44393400	6.08498700	-2.72900800
N	-5.27250500	5.27183800	-4.76605700
C	-5.30348200	5.30278600	-2.04150100
C	-6.04967500	4.42285800	-4.09263200
N	-6.08592600	4.44347500	-2.72904300
Au	-7.45767300	-0.00029700	-3.39688100
Au	-6.91571600	2.83968000	-1.66261800
Au	-6.91473300	-2.84010900	-1.66257300
C	-6.04880800	-4.42337000	-4.09259900
N	-6.08498700	-4.44393400	-2.72900800
N	-5.27183800	-5.27250500	-4.76605700
C	-5.30278600	-5.30348200	-2.04150100
C	-4.42285800	-6.04967500	-4.09263200
N	-4.44347500	-6.08592600	-2.72904300
Au	0.00029700	-7.45767300	-3.39688100
Au	-2.83968000	-6.91571600	-1.66261800
Au	2.84010900	-6.91473300	-1.66257300
C	4.42337000	-6.04880800	-4.09259900
N	4.44393400	-6.08498700	-2.72900800
N	5.27250500	-5.27183800	-4.76605700
C	5.30348200	-5.30278600	-2.04150100
C	6.04967500	-4.42285800	-4.09263200
N	6.08592600	-4.44347500	-2.72904300
Au	7.45767300	0.00029700	-3.39688100
Au	6.91571600	-2.83968000	-1.66261800
Au	6.91473300	2.84010900	-1.66257300
C	6.04880800	4.42337000	-4.09259900
N	6.08498700	4.44393400	-2.72900800
N	5.27183800	5.27250500	-4.76605700
C	5.30278600	5.30348200	-2.04150100
C	4.42285800	6.04967500	-4.09263200
N	4.44347500	6.08592600	-2.72904300
Au	-0.00029700	7.45767300	-3.39688100
Au	2.83968000	6.91571600	-1.66261800
Au	-2.84010900	6.91473300	-1.66257300
C	1.17982000	7.38496500	-0.64912000
N	1.16280800	7.41299000	0.70108600
N	-0.00027800	7.45089100	-1.30837200
C	-0.00023600	7.45609300	1.39472800
C	-1.18032000	7.38434500	-0.64909200
N	-1.16326500	7.41227700	0.70111700
Au	-5.31119600	5.31051400	-0.03015100
Au	-2.90584200	6.90631100	1.75236200
Au	-6.90744800	2.90555600	1.75232000
C	-7.38496500	1.17982000	-0.64912000
N	-7.41299000	1.16280800	0.70108600
N	-7.45089100	-0.00027800	-1.30837200
C	-7.45609300	-0.00023600	1.39472800
C	-7.38434500	-1.18032000	-0.64909200
N	-7.41227700	-1.16326500	0.70111700
Au	-5.31051400	-5.31119600	-0.03015100
Au	-6.90631100	-2.90584200	1.75236200
Au	-2.90555600	-6.90744800	1.75232000
C	-1.17982000	-7.38496500	-0.64912000
N	-1.16280800	-7.41299000	0.70108600
N	0.00027800	-7.45089100	-1.30837200

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C       0.00023600      -7.45609300     1.39472800
C       1.18032000      -7.38434500     -0.64909200
N       1.16326500      -7.41227700     0.70111700
Au      5.31119600      -5.31051400     -0.03015100
Au      2.90584200      -6.90631100     1.75236200
Au      6.90744800      -2.90555600     1.75232000
C       7.38496500      -1.17982000     -0.64912000
N       7.41299000      -1.16280800     0.70108600
N       7.45089100      0.00027800      -1.30837200
C       7.45609300      0.00023600      1.39472800
C       7.38434500      1.18032000      -0.64909200
N       7.41227700      1.16326500      0.70111700
Au      5.31051400      5.31119600      -0.03015100
Au      6.90631100      2.90584200      1.75236200
Au      2.90555600      6.90744800      1.75232000
C       -4.43941600     6.11201100      2.74939800
N       -4.49742400     6.15378200      4.10892900
N       -5.32142100     5.32076700      2.09317900
C       -5.38467900     5.38401200      4.72831000
C       -6.11303100     4.43906200      2.74937600
N       -6.15485000     4.49712900      4.10889400
Au      -7.43795200     -0.00020200     3.39480000
Au      -7.00510600     2.84571500      5.17078600
Au      -7.00393400     -2.84596200     5.17082500
C       -6.11201100     -4.43941600     2.74939800
N       -6.15378200     -4.49742400     4.10892900
N       -5.32076700     -5.32142100     2.09317900
C       -5.38401200     -5.38467900     4.72831000
C       -4.43906200     -6.11303100     2.74937600
N       -4.49712900     -6.15485000     4.10889400
Au      0.00020200      -7.43795200     3.39480000
Au      -2.84571500     -7.00510600     5.17078600
Au      2.84596200      -7.00393400     5.17082500
C       4.43941600      -6.11201100     2.74939800
N       4.49742400      -6.15378200     4.10892900
N       5.32142100      -5.32076700     2.09317900
C       5.38467900      -5.38401200     4.72831000
C       6.11303100      -4.43906200     2.74937600
N       6.15485000      -4.49712900     4.10889400
Au      7.43795200      0.00020200      3.39480000
Au      7.00510600      -2.84571500     5.17078600
Au      7.00393400      2.84596200      5.17082500
C       6.11201100      4.43941600      2.74939800
N       6.15378200      4.49742400      4.10892900
N       5.32076700      5.32142100      2.09317900
C       5.38401200      5.38467900      4.72831000
C       4.43906200      6.11303100      2.74937600
N       4.49712900      6.15485000      4.10889400
Au      -0.00020200     7.43795200      3.39480000
Au      2.84571500      7.00510600      5.17078600
Au      -2.84596200     7.00393400      5.17082500
C       1.17962000      7.53522300      6.16126600
N       1.18690800      7.79879900      7.46938500
N       -0.00019100     7.48329000      5.48132700
C       -0.00029200     7.96855400      8.04318000
C       -1.18000600     7.53453500      6.16129900
N       -1.18740200     7.79802700      7.46943800
H       -0.00036400     8.24918700      9.09283100
H       -5.44697900     5.44631800      5.80698300
C       -7.53522300     1.17962000      6.16126600
N       -7.79879900     1.18690800      7.46938500
N       -7.48329000     -0.00019100     5.48132700
C       -7.96855400     -0.00029200     8.04318000
C       -7.53453500     -1.18000600     6.16129900
N       -7.79802700     -1.18740200     7.46943800
H       -8.24918700     -0.00036400     9.09283100
H       -5.44631800     -5.44697900     5.80698300
C       -1.17962000     -7.53522300     6.16126600
N       -1.18690800     -7.79879900     7.46938500
N       0.00019100      -7.48329000     5.48132700
C       0.00029200      -7.96855400     8.04318000
C       1.18000600      -7.53453500     6.16129900
N       1.18740200      -7.79802700     7.46943800
H       0.00036400      -8.24918700     9.09283100
H       5.44697900      -5.44631800     5.80698300
C       7.53522300      -1.17962000     6.16126600
N       7.79879900      -1.18690800     7.46938500
N       7.48329000      0.00019100      5.48132700
C       7.96855400      0.00029200      8.04318000
C       7.53453500      1.18000600      6.16129900
N       7.79802700      1.18740200      7.46943800
H       8.24918700      0.00036400      9.09283100
H       5.44631800      5.44697900      5.80698300
```

2.14 Unit cell in Figure 9

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108
cell parameters a= 7.15 \AA, b= 40 \AA and c=40 \AA
N       0.17424700      9.85925400      14.06563900
C       0.87271800      10.51909100     13.11218900
N       0.17324800      11.21882700     12.18844000
Au      1.33194100      12.59095200     10.87690700
Au      1.33403200      18.07775100     8.42437500
N       0.17491100      19.96906800     8.27143800
C       0.87403600      21.12394600     8.36951300
N       0.17484600      22.27358500     8.51650600
Au      1.33522500      24.09455500     9.04870500
Au      1.33308700      28.96524400     12.57471600
N       0.17336000      30.04092600     14.13765100
C       0.87287300      30.53799600     15.18400600
N       0.17408900      30.98906600     16.25196900
Au      1.33240900      31.43461600     18.09717400
Au      1.33327300      30.81407200     24.07556100
N       0.17430700      29.99708200     25.78935100
C       0.87278100      29.33724700     26.74280400
N       0.17331300      28.63750800     27.66654800
Au      1.33200500      27.26538400     28.97808500
Au      1.33408800      21.77858600     31.43061800
N       0.17496200      19.88726600     31.58355100
C       0.87408100      18.73239200     31.48547900
N       0.17488500      17.58274900     31.33848200
Au      1.33525500      15.76178300     30.80628800
Au      1.33308500      10.89109500     27.28027900
N       0.17334900      9.81540700      25.71733700
C       0.87287100      9.31834900      24.67101000
N       0.17406400      8.86726700      23.60301900
Au      1.33237400      8.42172100      21.75781900
Au      1.33321400      9.04226300      15.77943300
C       2.42601800      8.27372900      19.90984400
N       3.81232300      8.27209000      19.88611500
N       1.75926600      8.34691300      18.72943400
C       4.51148700      8.36992200      18.73177100
C       2.42606400      8.51966700      17.55940200
N       3.81245000      8.51706700      17.58277700
Au      3.08648300      10.58326900     13.16134900
Au      4.96149000      9.04997800      15.75729600
Au      4.95974900      12.57204400     10.89253200
C       2.42461400      14.11831600     9.82539200
N       3.81069800      14.13856400     9.81508400
N       1.75840600      15.17623700     9.29607400
C       4.51088500      15.18433400     9.31816900
C       2.42605900      16.27512700     8.86018000
N       3.81211100      16.25195700     8.86743000
Au      3.08754600      21.11441100     8.45170700
Au      4.96403300      18.09868400     8.42032600
Au      4.96163000      24.07368600     9.03964300
```

C	2.42631900	25.76888000	9.84850200
N	3.81261700	25.79041600	9.85943500
N	1.75905800	26.75357700	10.50291400
C	4.51106600	26.74377400	10.51875200
C	2.42523900	27.68348400	11.23445000
N	3.81133000	27.66697600	11.21790800
Au	3.08656300	30.46115600	15.21772100
Au	4.96203400	28.97996200	12.59192100
Au	4.96225500	31.43185500	18.07398100
C	2.42606100	31.58261300	19.94515600
N	3.81236500	31.58425600	19.96888900
N	1.75931400	31.50942500	21.12556100
C	4.51153500	31.48642700	21.12323700
C	2.42611700	31.33667500	22.29559700
N	3.81250200	31.33928100	22.27222700
Au	3.08654600	29.27307400	26.69365100
Au	4.96154800	30.80637200	24.09771300
Au	4.95981400	27.28430600	28.96247500
C	2.42467700	25.73802600	30.02960700
N	3.81076000	25.71778400	30.03992000
N	1.75846800	24.68010200	30.55892200
C	4.51094700	24.67201700	30.53683800
C	2.42611900	23.58121600	30.99481800
N	3.81217100	23.60439100	30.98757400
Au	3.08759100	18.74193200	31.40329200
Au	4.96408800	21.75766500	31.43468100
Au	4.96166100	15.78266500	30.81536700
C	2.42634600	14.08747200	30.00650300
N	3.81262800	14.06591300	29.99555400
N	1.75908000	13.10276300	29.35208500
C	4.51108100	13.11257900	29.33626000
C	2.42525000	12.17286500	28.62055500
N	3.81133500	12.18936800	28.63709300
Au	3.08654400	9.39518700	24.63727900
Au	4.96203100	10.87639000	27.26308700
Au	4.96222100	8.42449500	21.78102800
C	6.05538800	9.84762700	14.08585400
N	5.38880800	10.50147300	13.10067100
C	6.05425400	11.23352700	12.17146600
Au	6.72449000	15.21834900	9.39273000
C	6.05608700	19.94579800	8.27192500
N	5.38965300	21.12617400	8.34424300
C	6.05578700	22.29633000	8.51738200
Au	6.72501500	26.69502600	10.58134700
C	6.05463500	30.03151100	14.11698800
N	5.38864900	30.56144600	15.17458800
C	6.05525700	30.99718500	16.27341000
Au	6.72549300	31.40599800	21.11419300
C	6.05544900	30.00873000	25.76916000
N	5.38887200	29.35488000	26.75434000
C	6.05431900	28.62282900	27.68354800
Au	6.72455200	24.63800800	30.46228500
C	6.05613600	19.91055900	31.58309000
N	5.38969800	18.73017700	31.51076900
C	6.05582700	17.56002600	31.33763300
Au	6.72503100	13.16133000	29.27366800
C	6.05462400	9.82484500	25.73802600
N	5.38863100	9.29490600	24.68042100
C	6.05523200	8.85917100	23.58160500
Au	6.72544400	8.45035700	18.74082200

2.15 Molecule in Figure 10(a)

144

C	-2.03109000	-2.03109000	8.46511000
C	2.03109000	2.03109000	8.46511000
C	-0.63883000	-5.54905000	5.54905000
C	2.63593000	-2.63593000	7.58628000
C	-2.03109000	-8.46511000	2.03109000
C	2.63593000	-7.58628000	2.63593000
C	2.03109000	-8.46511000	-2.03109000
C	-5.54905000	-0.63883000	5.54905000
C	-2.63593000	2.63593000	7.58628000
C	-5.54905000	-5.54905000	0.63883000
C	-2.63593000	-7.58628000	-2.63593000
C	0.63883000	-5.54905000	-5.54905000
C	-8.46511000	-2.03109000	2.03109000
C	-7.58628000	2.63593000	2.63593000
C	-7.58628000	-2.63593000	-2.63593000
C	-2.63593000	-2.63593000	-7.58628000
C	2.03109000	-2.03109000	-8.46511000
C	-8.46511000	2.03109000	-2.03109000
C	-5.54905000	0.63883000	-5.54905000
C	-2.03109000	2.03109000	-8.46511000
C	-5.54905000	5.54905000	-0.63883000
C	-0.63883000	5.54905000	-5.54905000
C	2.63593000	2.63593000	-7.58628000
C	5.54905000	-0.63883000	-5.54905000
C	5.54905000	-5.54905000	-0.63883000
C	-2.63593000	7.58628000	2.63593000
C	-2.03109000	8.46511000	-2.03109000
C	2.63593000	7.58628000	-2.63593000
C	7.58628000	2.63593000	-2.63593000
C	8.46511000	-2.03109000	-2.03109000
C	7.58628000	-2.63593000	2.63593000
C	0.63883000	5.54905000	5.54905000
C	2.03109000	8.46511000	2.03109000
C	5.54905000	5.54905000	0.63883000
C	8.46511000	2.03109000	2.03109000
C	5.54905000	0.63883000	5.54905000
Au	-6.52316000	4.18737000	1.85351000
Au	-4.18737000	6.52316000	1.85351000
Au	-1.85351000	6.52316000	4.18737000
Au	-1.85351000	4.18737000	6.52316000
Au	-4.18737000	1.85351000	6.52316000
Au	-6.52316000	1.85351000	4.18737000
Au	6.52316000	-1.85351000	4.18737000
Au	6.52316000	-4.18737000	1.85351000
Au	4.18737000	-6.52316000	1.85351000
Au	1.85351000	-6.52316000	4.18737000
Au	1.85351000	-4.18737000	6.52316000
Au	4.18737000	-1.85351000	6.52316000
Au	-4.18737000	-6.52316000	-1.85351000
Au	-6.52316000	-4.18737000	-1.85351000
Au	-6.52316000	-1.85351000	-4.18737000
Au	-4.18737000	-1.85351000	-6.52316000
Au	-1.85351000	-4.18737000	-6.52316000
Au	-1.85351000	-6.52316000	-4.18737000
Au	6.61185000	1.84346000	4.29652000
Au	6.61185000	4.29652000	1.84346000
Au	4.29652000	6.61185000	1.84346000
Au	1.84346000	6.61185000	4.29652000
Au	1.84346000	4.29652000	6.61185000
Au	4.29652000	1.84346000	6.61185000
Au	6.61185000	-1.84346000	-4.29652000
Au	4.29652000	-1.84346000	-6.61185000
Au	1.84346000	-4.29652000	-6.61185000
Au	1.84346000	-6.61185000	-4.29652000
Au	4.29652000	-6.61185000	-1.84346000
Au	6.61185000	-4.29652000	-1.84346000
Au	-1.84346000	4.29652000	-6.61185000
Au	-1.84346000	6.61185000	-4.29652000
Au	-4.29652000	6.61185000	-1.84346000
Au	-6.61185000	4.29652000	-1.84346000
Au	-6.61185000	1.84346000	-4.29652000
Au	-4.29652000	1.84346000	-6.61185000

Au	-4.29652000	-1.84346000	6.61185000
Au	-1.84346000	-6.61185000	4.29652000
Au	-4.29652000	-6.61185000	1.84346000
Au	-6.61185000	-4.29652000	1.84346000
Au	-6.61185000	-1.84346000	4.29652000
Au	6.52316000	4.18737000	-1.85351000
Au	4.18737000	6.52316000	-1.85351000
Au	1.85351000	6.52316000	-4.18737000
Au	1.85351000	4.18737000	-6.52316000
Au	4.18737000	1.85351000	-6.52316000
Au	6.52316000	1.85351000	-4.18737000
Au	2.15510000	-0.02433000	-8.81422000
Au	-0.02433000	2.15510000	-8.81422000
Au	-2.15510000	0.02433000	-8.81422000
Au	0.02433000	-2.15510000	-8.81422000
Au	8.81422000	-0.02433000	-2.15510000
Au	8.81422000	2.15510000	0.02433000
Au	8.81422000	0.02433000	2.15510000
Au	8.81422000	-2.15510000	-0.02433000
Au	-8.81422000	-2.15510000	0.02433000
Au	-8.81422000	-0.02433000	2.15510000
Au	-8.81422000	2.15510000	-0.02433000
Au	-8.81422000	0.02433000	-2.15510000
Au	-2.15510000	-0.02433000	8.81422000
Au	-0.02433000	-2.15510000	8.81422000
Au	2.15510000	0.02433000	8.81422000
Au	0.02433000	2.15510000	8.81422000
Au	-2.15510000	8.81422000	-0.02433000
Au	-0.02433000	8.81422000	-2.15510000
Au	0.02433000	8.81422000	2.15510000
Au	2.15510000	8.81422000	0.02433000
Au	-1.84346000	-4.29652000	6.61185000
Au	-0.02433000	-8.81422000	2.15510000
Au	-2.15510000	-8.81422000	0.02433000
Au	0.02433000	-8.81422000	-2.15510000
Au	2.15510000	-8.81422000	-0.02433000
N	2.06532000	-2.06532000	8.50856000
N	-2.06532000	2.06532000	8.50856000
N	2.70988000	2.70988000	7.71619000
N	-2.70988000	-2.70988000	7.71619000
N	5.54205000	-0.59415000	5.54205000
N	-5.54205000	0.59415000	5.54205000
N	0.59415000	-5.54205000	5.54205000
N	-0.59415000	5.54205000	5.54205000
N	-7.71619000	-2.70988000	2.70988000
N	-8.50856000	2.06532000	2.06532000
N	-2.70988000	-7.71619000	2.70988000
N	-2.06532000	8.50856000	2.06532000
N	2.70988000	7.71619000	2.70988000
N	2.06532000	-8.50856000	2.06532000
N	5.54205000	-5.54205000	0.59415000
N	5.54205000	5.54205000	-0.59415000
N	7.71619000	2.70988000	2.70988000
N	8.50856000	-2.06532000	2.06532000
N	2.06532000	8.50856000	-2.06532000
N	2.70988000	-7.71619000	-2.70988000
N	8.50856000	2.06532000	-2.06532000
N	7.71619000	-2.70988000	-2.70988000
N	5.54205000	0.59415000	-5.54205000
N	2.70988000	-2.70988000	-7.71619000
N	2.06532000	2.06532000	-8.50856000
N	-2.70988000	7.71619000	-2.70988000
N	-5.54205000	5.54205000	0.59415000
N	-7.71619000	2.70988000	-2.70988000
N	0.59415000	5.54205000	-5.54205000
N	-2.70988000	2.70988000	-7.71619000
N	-8.50856000	-2.06532000	-2.06532000
N	-5.54205000	-5.54205000	-0.59415000
N	-2.06532000	-8.50856000	-2.06532000
N	-5.54205000	-0.59415000	-5.54205000
N	-2.06532000	-2.06532000	-8.50856000
N	-0.59415000	-5.54205000	-5.54205000

2.16 Molecule in Figure 10(b)

144

C	-1.60643500	-1.60643500	8.03311200
C	1.60643500	1.60643500	8.03311200
C	-0.11808900	-5.28759900	5.28759900
C	2.99357400	-2.99357400	8.10060700
C	-1.60643500	-8.03311200	1.60643500
C	2.99357400	-8.10060700	2.99357400
C	1.60643500	-8.03311200	-1.60643500
C	-5.28759900	-0.11808900	5.28759900
C	-2.99357400	2.99357400	8.10060700
C	-5.28759900	-5.28759900	0.11808900
C	-2.99357400	-8.10060700	-2.99357400
C	0.11808900	-5.28759900	-5.28759900
C	-8.03311200	-1.60643500	1.60643500
C	-8.10060700	2.99357400	2.99357400
C	-8.10060700	-2.99357400	-2.99357400
C	-2.99357400	-2.99357400	-8.10060700
C	1.60643500	-1.60643500	-8.03311200
C	-8.03311200	1.60643500	-1.60643500
C	-5.28759900	0.11808900	-5.28759900
C	-1.60643500	1.60643500	-8.03311200
C	-5.28759900	5.28759900	-0.11808900
C	-0.11808900	5.28759900	-5.28759900
C	2.99357400	2.99357400	-8.10060700
C	5.28759900	-0.11808900	-5.28759900
C	5.28759900	-5.28759900	-0.11808900
C	-2.99357400	8.10060700	2.99357400
C	-1.60643500	8.03311200	-1.60643500
C	2.99357400	8.10060700	-2.99357400
C	8.10060700	2.99357400	-2.99357400
C	8.03311200	-1.60643500	-1.60643500
C	8.10060700	-2.99357400	2.99357400
C	0.11808900	5.28759900	5.28759900
C	1.60643500	8.03311200	1.60643500
C	5.28759900	5.28759900	0.11808900
C	8.03311200	1.60643500	1.60643500
C	5.28759900	0.11808900	5.28759900
Au	-6.64302700	4.27314900	2.30687600
Au	-4.27314900	6.64302700	2.30687600
Au	-2.30687600	6.64302700	4.27314900
Au	-2.30687600	4.27314900	6.64302700
Au	-4.27314900	2.30687600	6.64302700
Au	-6.64302700	2.30687600	4.27314900
Au	6.64302700	-2.30687600	4.27314900
Au	6.64302700	-4.27314900	2.30687600
Au	4.27314900	-6.64302700	2.30687600
Au	2.30687600	-6.64302700	4.27314900
Au	2.30687600	-4.27314900	6.64302700
Au	4.27314900	-2.30687600	6.64302700
Au	-4.27314900	-6.64302700	-2.30687600
Au	-6.64302700	-4.27314900	-2.30687600
Au	-6.64302700	-2.30687600	-4.27314900
Au	-4.27314900	-2.30687600	-6.64302700
Au	-2.30687600	-4.27314900	-6.64302700
Au	-2.30687600	-6.64302700	-4.27314900
Au	6.27178200	1.17123700	3.85175300
Au	6.27178200	3.85175300	1.17123700
Au	3.85175300	6.27178200	1.17123700
Au	1.17123700	6.27178200	3.85175300
Au	1.17123700	3.85175300	6.27178200
Au	3.85175300	1.17123700	6.27178200

Au	6.27178200	-1.17123700	-3.85175300
Au	3.85175300	-1.17123700	-6.27178200
Au	1.17123700	-3.85175300	-6.27178200
Au	1.17123700	-6.27178200	-3.85175300
Au	3.85175300	-6.27178200	-1.17123700
Au	6.27178200	-3.85175300	-1.17123700
Au	-1.17123700	3.85175300	-6.27178200
Au	-1.17123700	6.27178200	-3.85175300
Au	-3.85175300	6.27178200	-1.17123700
Au	-6.27178200	3.85175300	-1.17123700
Au	-6.27178200	1.17123700	-3.85175300
Au	-3.85175300	1.17123700	-6.27178200
Au	-3.85175300	-1.17123700	6.27178200
Au	-1.17123700	-6.27178200	3.85175300
Au	-3.85175300	-6.27178200	1.17123700
Au	-6.27178200	-3.85175300	1.17123700
Au	-6.27178200	-1.17123700	3.85175300
Au	6.64302700	4.27314900	-2.30687600
Au	4.27314900	6.64302700	-2.30687600
Au	2.30687600	6.64302700	-4.27314900
Au	2.30687600	4.27314900	-6.64302700
Au	4.27314900	2.30687600	-6.64302700
Au	6.64302700	2.30687600	-4.27314900
Au	2.19901500	0.24141800	-8.63535900
Au	0.24141800	2.19901500	-8.63535900
Au	-2.19901500	-0.24141800	-8.63535900
Au	-0.24141800	-2.19901500	-8.63535900
Au	8.63535900	0.24141800	-2.19901500
Au	8.63535900	2.19901500	-0.24141800
Au	8.63535900	-0.24141800	2.19901500
Au	8.63535900	-2.19901500	0.24141800
Au	-8.63535900	-2.19901500	-0.24141800
Au	-8.63535900	0.24141800	2.19901500
Au	-8.63535900	2.19901500	0.24141800
Au	-8.63535900	-0.24141800	-2.19901500
Au	-2.19901500	0.24141800	8.63535900
Au	0.24141800	-2.19901500	8.63535900
Au	2.19901500	-0.24141800	8.63535900
Au	-0.24141800	2.19901500	8.63535900
Au	-2.19901500	8.63535900	0.24141800
Au	0.24141800	8.63535900	-2.19901500
Au	-0.24141800	8.63535900	2.19901500
Au	2.19901500	8.63535900	-0.24141800
Au	-1.17123700	-3.85175300	6.27178200
Au	0.24141800	-8.63535900	2.19901500
Au	-2.19901500	-8.63535900	-0.24141800
Au	-0.24141800	-8.63535900	-2.19901500
Au	2.19901500	-8.63535900	0.24141800
N	2.51382500	-2.51382500	9.07810400
N	-2.51382500	2.51382500	9.07810400
N	2.23041800	2.23041800	7.18675700
N	-2.23041800	-2.23041800	7.18675700
N	5.46673800	-1.13722300	5.46673800
N	-5.46673800	1.13722300	5.46673800
N	1.13722300	-5.46673800	5.46673800
N	-1.13722300	5.46673800	5.46673800
N	-7.18675700	-2.23041800	2.23041800
N	-9.07810400	2.51382500	2.51382500
N	-2.23041800	-7.18675700	2.23041800
N	-2.51382500	9.07810400	2.51382500
N	2.23041800	7.18675700	2.23041800
N	2.51382500	-9.07810400	2.51382500
N	5.46673800	-5.46673800	1.13722300
N	5.46673800	5.46673800	-1.13722300
N	7.18675700	2.23041800	2.23041800
N	9.07810400	-2.51382500	2.51382500
N	2.51382500	9.07810400	-2.51382500
N	2.23041800	-7.18675700	-2.23041800
N	9.07810400	2.51382500	-2.51382500
N	7.18675700	-2.23041800	-2.23041800
N	5.46673800	1.13722300	-5.46673800
N	2.23041800	-2.23041800	-7.18675700
N	2.51382500	2.51382500	-9.07810400
N	-2.23041800	7.18675700	-2.23041800
N	-5.46673800	5.46673800	1.13722300
N	-7.18675700	2.23041800	-2.23041800
N	1.13722300	5.46673800	-5.46673800
N	-2.23041800	2.23041800	-7.18675700
N	-9.07810400	-2.51382500	-2.51382500
N	-5.46673800	-5.46673800	-1.13722300
N	-2.51382500	-9.07810400	-2.51382500
N	-5.46673800	-1.13722300	-5.46673800
N	-2.51382500	-2.51382500	-9.07810400
N	-1.13722300	-5.46673800	-5.46673800

2.17 Molecule in Figure 11

36

C	2.40524500	0.55931400	2.47309400
C	0.34971700	1.47588100	3.14860400
C	0.71563600	-0.83919400	3.31630300
C	2.73331000	-0.14993300	-2.17275900
C	1.27825100	-1.94276100	-2.60883200
C	2.73629300	-2.03386500	-0.76834100
C	-2.90415500	-1.41033600	1.33843000
C	-3.09819300	-1.27157900	-0.99924000
C	-1.81777800	-2.98487000	-0.02620700
C	-2.04333100	2.74613300	-0.70550000
C	-0.54482200	2.39946000	-2.48198600
C	0.18979100	3.45176300	-0.51358100
N	1.78663200	-0.75344400	-2.97236200
N	3.26373200	-0.81342600	-1.13183800
N	1.81460800	-2.63130900	-1.54205600
N	-2.36413800	-2.38777600	-1.14189600
N	-2.14892500	-2.55536000	1.20299600
N	-3.44277700	-0.82199500	0.25731100
N	-1.79420000	2.32390400	-1.99369400
N	0.44248000	3.04474000	-1.76879700
N	-1.08827000	3.37792300	-0.00280600
N	1.63779700	1.64119100	2.68675000
N	1.97325500	-0.68849500	2.86824000
N	-0.08022600	0.26406500	3.53813000
Au	0.21325900	0.79928500	-3.48278100
Au	-0.73418700	-2.21937500	-2.71093700
Au	-2.76139500	0.28900000	-2.25939500
Au	3.47297900	0.44242800	0.74592000
Au	2.35270100	1.83822400	-1.97476300
Au	1.57017700	3.07864900	0.93285200
Au	-0.93759400	2.69884400	2.15662100
Au	-2.17728000	-0.23602700	2.83158000
Au	-0.38866400	-2.40151000	2.62598300
Au	-3.26687700	1.43987100	0.26067700
Au	2.55532700	-2.17131900	1.25285000
Au	0.10162200	-3.55810200	-0.37857100