# Phosphorescent Modulation of Metallophilic Cluster and Recognition of Solvents through Flexible Host-Guest Assembly: A Theoretical Investigation

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## 1. Figure 1S

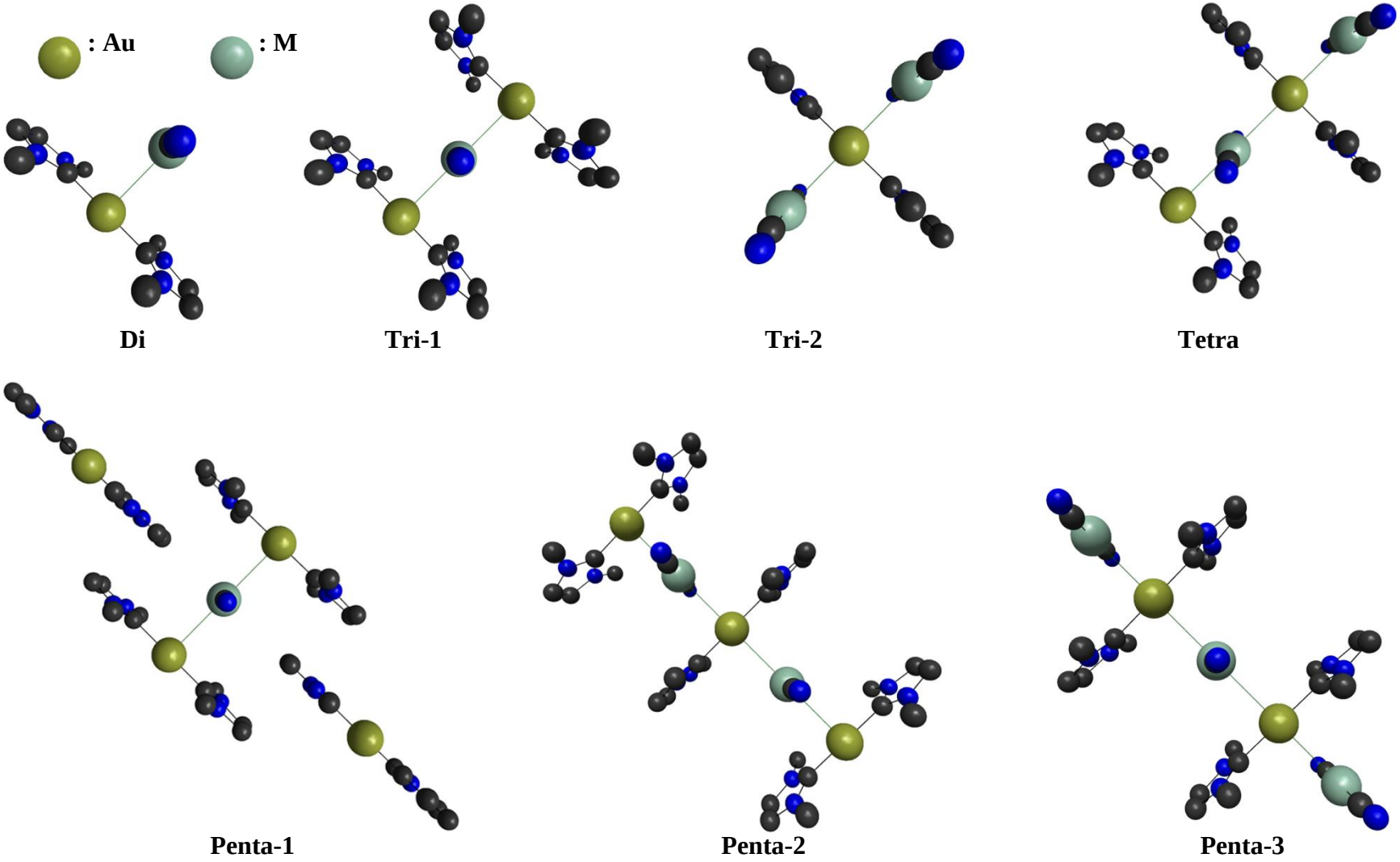



**Figure 1S.** Structure diagrams of clusters.

## 2. Table 1S

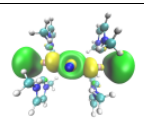
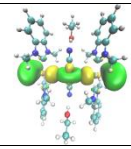
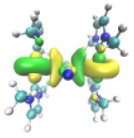
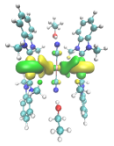
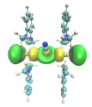
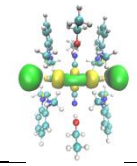
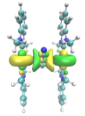
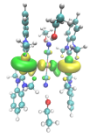
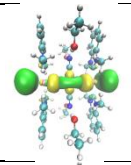
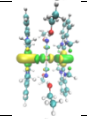
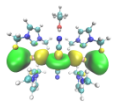
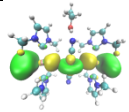
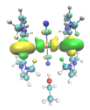
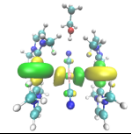
**Table 1S.** Comparing the calculated and experimental parameters for the different oligomeric I (bond length: Å, wavelength: nm).

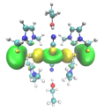
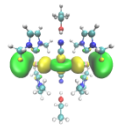
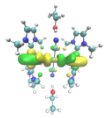
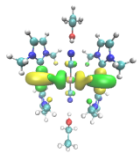
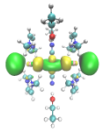
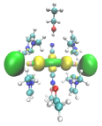
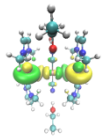
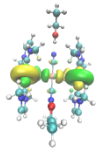
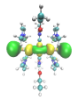
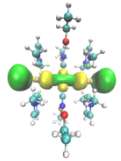
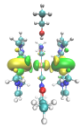
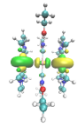
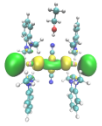
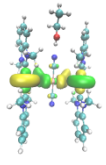
| Cluster | Methods | BS1 | | | BS2 | |
|---|---|---|---|---|---|---|
| | | $d^{cal}$ (Au···Au) | $d^{cal}$-$d^{exp}$* | $\lambda_{max}^{cal} - \lambda_{max}^{exp}$ ** | $d^{cal}$ (Au···Au) | $d^{cal}$-$d^{exp}$* |
| Di | B3LYP | 3.21 | 0.06 | −60.07 | 3.24 | 0.09 |
| | B3LYP-D3 | 3.11 | −0.04 | 57.91 | 3.12 | −0.03 |
| | PBE0 | 3.08 | -0.07 | −55.38 | 3.09 | −0.06 |
| | ωB97XD | 3.21 | 0.06 | −97.45 | 3.22 | 0.07 |
| | M062X | 3.20 | 0.05 | −99.38 | 3.23 | 0.08 |
| | MP2 | 2.99 | −0.16 | | - | - |
| Tri-1 | B3LYP | 3.37 | 0.22 | −11.39 | - | - |
| | B3LYP-D3 | 3.06 | −0.09 | | 3.06 | −0.09 |
| | PBE0 | 3.12 | −0.03 | 8.56 | 3.13 | −0.02 |
| | ωB97XD | 3.18 | 0.03 | −51.9 | 3.11 | −0.04 |
| | M062X | 3.32 | 0.17 | | 3.37 | 0.22 |
| | MP2 | 2.94 | −0.21 | | - | - |
| Tri-2 | B3LYP | 5.74 | 2.59 | | 5.84 | 2.69 |
| | B3LYP-D3 | 4.25 | 1.10 | | 4.20 | 1.05 |
| | PBE0 | 3.21 | 0.06 | | 3.23 | 0.08 |
| | ωB97XD | 4.26 | 1.11 | | 4.23 | 1.08 |
| | M062X | 4.29 | 1.14 | | 4.20 | 1.05 |
| Tetra | B3LYP | 3.26 | 0.11 | 88.17 | | |
| | PBE0 | 3.11 | −0.04 | 111.25 | | |
| Penta-1 | ωB97XD | 3.16 | 0.01 | −57.19 | | |
| | M062X | 3.23 | 0.08 | −76.66 | | |
| | B3LYP | >4.0 | - | | | |
| | B3LYP-D3 | - | - | | | |
| | PBE0 | - | - | | | |
| Penta-2 | B3LYP | 3.27 | 0.12 | | | |
| | B3LYP-D3 | - | - | | | |
| | PBE0 | 3.16 | 0.01 | 95.64 | | |
| | ωB97XD | - | - | | | |
| | M062X | 3.54 | 0.39 | | | |
| Penta-3 | B3LYP | - | - | | | |
| | B3LYP-D3 | >3.8 | - | | | |
| | PBE0 | >3.3 | - | | | |
| | ωB97XD | | | | | |
| | M062X | >3.7 | | | | |

*$d^{exp}$ = 3.15 Å, **$\lambda_{max}^{exp}$= 448 nm.

It can be seen from Table 1S, the Au-M distances of **Penta-1** at *ω*B97XD/BS1 and **Penta-2** at PBE0/BS1 are only beyond the experimental data 0.01 Å respectively as well as the **Tri-1** at PBE0/BS1 is shorter by 0.03 Å than the experiment. These cases indicate that the PBE0/BS1 is reliable for the complexes and the **Penta-1**, **Penta-2**, and **Tri-1** can act as plausible cluster unit with the geometrical parameters as the reference. In order to further verify which cluster is the most represented mode for studying, the calculated phosphorescent character of them are listed in Table S1 (ESI†). It can be seen that the calculated phosphorescent wavelength of **Tri-1** is the most close to the experiment and the difference only is only about 9 nm.

## 3. Table 2S

| complex | | | | | complex | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | donor | acceptor | Eij | | | donor | acceptor | Eij | |
| I | LP(5)(Au2) | LP(7)*(Au1) | 32.41 |  | II-2S2 | LP(3)(Au2) | LP(7)*(Au1) | 15.64 |  |
| | | LP(7)*(Au3) | 30.42 | | | | LP(7)*(Au3) | 15.64 | |
| | LP(4)(Au1) | LP(6)*(Au2) | 29.47 |  | | LP(3)(Au1) | LP(6)*(Au2) | 14.18 |  |
| | LP(4)(Au3) | | 26.36 | | | LP(3)(Au3) | | 14.18 | |
| II | LP(5)(Au2) | LP(6)*(Au1) | 31.78 |  | II-3S2 | LP(4)(Au2) | LP(7)*(Au1) | 16.43 |  |
| | | LP(7)*(Au3) | 31.84 | | | | LP(7)*(Au3) | 16.43 | |
| | LP(4)(Au1) | LP(6)*(Au2) | 24.39 |  | | LP(4)(Au1) | LP(7)*(Au2) | 16.08 |  |
| | LP(4)(Au3) | | 24.44 | | | LP(4)(Au3) | | 16.08 | |
| III | LP(5)(Ag2) | LP(7)*(Au1) | 16.87 |  | II-4S2 | LP(5)(Au2) | LP(7)*(Au1) | 25.07 |  |
| | | LP(7)*(Au3) | 16.87 | | | | LP(7)*(Au3) | 25.07 | |
| | LP(4)(Au1) | LP(6)*(Ag2) | 26.76 |  | | LP(4)(Au1) | LP(7)*(Au2) | 21.21 |  |
| | LP(4)(Au3) | | 26.76 | | | LP(4)(Au3) | | 21.21 | |
| I-S2 | LP(3)(Au2) | LP(7)*(Au1) | 12.87 |  | III-S2 | LP(5)(Ag2) | LP(7)*(Au1) | 4.49 |  |
| | | LP(7)*(Au3) | 12.87 | | | | LP(7)*(Au3) | 4.78 | |
| | LP(3)(Au1) | LP(6)*(Au2) | 13.86 |  | | LP(3)(Au1) | LP(6)*(Ag2) | 13.98 |  |
| | LP(3)(Au3) | | 13.85 | | | LP(3)(Au3) | | 13.14 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| I-2S2 | LP(3)(Au2) | LP(7)*(Au1) | 14.8 |  | III-2S2 | LP(5)(Ag2) | LP(7)*(Au1) | 5.39 |  |
| | | LP(7)*(Au3) | 14.81 | | | | LP(7)*(Au3) | 5.39 | |
| | LP(3)(Au1) | LP(6)*(Au2) | 15.78 |  | | LP(3)(Au1) | LP(6)*(Ag2) | 11.06 |  |
| | LP(3)(Au3) | | 15.75 | | | LP(3)(Au3) | | 11.06 | |
| I-3S2 | LP(3)(Au2) | LP(7)*(Au1) | 13.21 |  | III-3S2 | LP(5)(Ag2) | LP(7)*(Au1) | 4.52 |  |
| | | LP(7)*(Au3) | 13.72 | | | | LP(7)*(Au3) | 4.64 | |
| | LP(4)(Au1) | LP(7)*(Au2) | 13.04 |  | | LP(4)(Au1) | LP(6)*(Ag2) | 13.09 |  |
| | LP(4)(Au3) | | 14.32 | | | LP(4)(Au3) | | 14.9 | |
| I-4S2 | LP(4)(Au2) | LP(7)*(Au1) | 24.43 |  | II-4S2 | LP(5)(Ag2) | LP(7)*(Au1) | 10.46 |  |
| | | LP(7)*(Au3) | 24.41 | | | | LP(7)*(Au3) | 10.46 | |
| | LP(4)(Au1) | LP(7)*(Au2) | 22.14 |  | | LP(4)(Au1) | LP(6)*(Ag2) | 19.09 |  |
| | LP(4)(Au3) | | 22.14 | | | LP(4)(Au3) | | 19.09 | |
| II-S2 | LP(3)(Au2) | LP(7)*(Au1) | 13.01 |  | | | | | |
| | | LP(7)*(Au3) | 13.37 | | | | | | |
| | LP(3)(Au1) | LP(6)*(Au2) | 12.42 |  | | | | | |
| | LP(3)(Au3) | | 12.28 | | | | | | |

## 4. Figure 2S

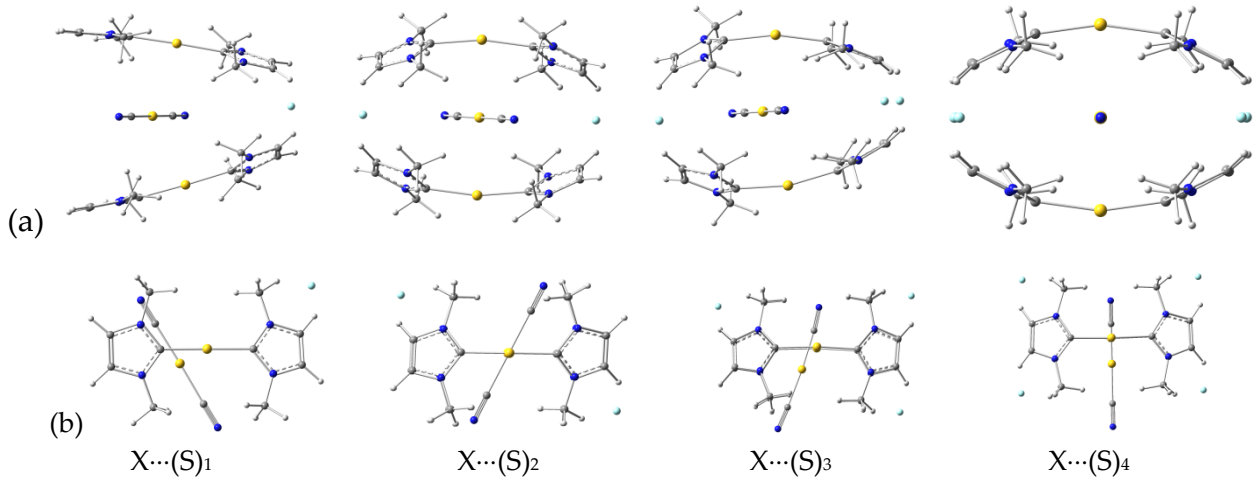



**Figure 2S**. Top view (**a**) and face view (**b**) of the representative cluster **X**···(**S**)$_x$ (X = I–III; $x$ = 1–4)

## 5. Table 3S

**Table 3S.** The key parameters and the phosphorescent character of complexes **X**···(**S**)$_x$ (bond length: Å, bond angle:°, wavelength: nm).

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | d0($S_0$) | | | | | | | | |
| | I | I-S1 | I-2S1 | I-3S1 | I-4S1 | II | II-S1 | II-2S1 | II-3S1 | II-4S1 | III | III-S1 | III-2S1 | III-3S1 | III-4S1 |
| Au1-M2 | 3.12 | 3.54 | 3.46 | 3.40 | 3.25 | 3.15 | 3.53 | 3.44 | 3.36 | 3.22 | 3.06 | 3.56 | 3.44 | 3.42 | 3.22 |
| M2-Au3 | 3.11 | 3.54 | 3.46 | 3.40 | 3.25 | 3.15 | 3.51 | 3.44 | 3.36 | 3.22 | 3.06 | 3.56 | 3.44 | 3.39 | 3.22 |
| Au-C1 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C2 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| M-C3 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.04 | 2.04 | 2.04 | 2.05 |
| M-C4 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.04 | 2.04 | 2.04 | 2.05 |
| Au-C5 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C6 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au1M2Au3 | 180.0 | 168.3 | 180.0 | 159.1 | 180.0 | 180.0 | 151.7 | 180.0 | 165.5 | 180.0 | 180.0 | 165.9 | 180.0 | 157.1 | 180.0 |
| | | | | | | | d1($T_1$) | | | | | | | | |
| Au1-M2 | 2.77 | 2.77 | 2.84 | 2.85 | 2.86 | 2.76 | 2.76 | 2.86 | 2.86 | 2.85 | 2.76 | 2.76 | 2.85 | 2.86 | 2.87 |
| M2-Au3 | 2.77 | 2.77 | 2.84 | 2.85 | 2.86 | 2.75 | 2.76 | 2.86 | 2.86 | 2.85 | 2.76 | 2.76 | 2.85 | 2.86 | 2.87 |
| Au-C1 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au-C2 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| M-C3 | 1.99 | 1.99 | 1.99 | 1.99 | 1.98 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 2.02 | 2.02 | 2.02 | 2.02 | 2.01 |
| M-C4 | 1.99 | 1.99 | 1.99 | 1.99 | 1.98 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 2.02 | 2.02 | 2.02 | 2.02 | 2.01 |
| Au-C5 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au-C6 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au1M2Au3 | 180.0 | 176.8 | 180.0 | 173.1 | 180.0 | 180.0 | 178.2 | 180.0 | 175.8 | 180.0 | 180.0 | 176.3 | 180.0 | 172.4 | 179.9 |
| λ | 457 | 444 | 419 | 418 | 412 | 483 | 478 | 437 | 439 | 443 | 417 | 409 | 383 | 379 | 371 |
| Δλ | | -13 | -38 | -39 | -45 | | -5 | -46 | -44 | -40 | | -8 | -34 | -38 | -46 |
| | | | | | | | d0($S_0$) | | | | | | | | |
| | I | I-S2 | I-2S2 | I-3S2 | I-4S2 | II | II-S2 | II-2S2 | II-3S2 | II-4S2 | III | III-S2 | III-2S2 | III-3S2 | III-4S2 |
| Au1-M2 | 3.12 | 3.50 | 3.45 | 3.41 | 3.25 | 3.15 | 3.51 | 3.45 | 3.35 | 3.22 | 3.06 | 3.54 | 3.44 | 3.42 | 3.24 |
| M2-Au3 | 3.11 | 3.50 | 3.45 | 3.41 | 3.25 | 3.15 | 3.54 | 3.45 | 3.35 | 3.22 | 3.06 | 3.55 | 3.44 | 3.39 | 3.24 |
| Au-C1 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C2 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| M-C3 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.05 | 2.04 | 2.05 | 2.05 |
| M-C4 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.05 | 2.04 | 2.05 | 2.05 |
| Au-C5 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C6 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au1M2Au3 | 180.0 | 170.3 | 180.0 | 159.1 | 180.0 | 180.0 | 152.2 | 179.9 | 166.0 | 180.0 | 180.0 | 166.8 | 180.0 | 157.2 | 179.9 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | d1($T_1$) | | | | | | | | |
| Au1-M2 | 2.77 | 2.77 | 2.84 | 2.85 | 2.85 | 2.76 | 2.76 | 2.86 | 2.85 | 2.85 | 2.76 | 2.76 | 2.85 | 2.86 | 2.87 |
| M2-Au3 | 2.77 | 2.77 | 2.84 | 2.85 | 2.85 | 2.75 | 2.76 | 2.86 | 2.85 | 2.85 | 2.76 | 2.76 | 2.85 | 2.86 | 2.87 |
| Au-C1 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au-C2 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| M-C3 | 1.99 | 1.99 | 1.99 | 1.99 | 1.98 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 2.02 | 2.02 | 2.02 | 2.02 | 2.01 |
| M-C4 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 2.02 | 2.02 | 2.02 | 2.02 | 2.01 |
| Au-C5 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au-C6 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 |
| Au1M2Au3 | 180.0 | 175.1 | 180.0 | 172.4 | 180.0 | 180.0 | 170.9 | 180.0 | 175.8 | 180.0 | 180.0 | 174.2 | 180.0 | 171.0 | 180.0 |
| λ | 457 | 444.00 | 420.00 | 418.00 | 412.00 | 483 | 476 | 437 | 440 | 443 | 417 | 408 | 383 | 378 | 372 |
| Δλ | | -13 | -37 | -39 | -45 | | -7 | -46 | -43 | -40 | | -9 | -34 | -39 | -45 |
| | | | | | | | d0($S_0$) | | | | | | | | |
| | I | I-S3 | I-2S3 | I-3S3 | I-4S3 | II | II-S3 | II-2S3 | II-3S3 | II-4S3 | III | III-S3 | III-2S3 | III-3S3 | III-4S3 |
| Au1-M2 | 3.12 | 3.52 | 3.49 | 3.42 | 3.21 | 3.15 | 3.55 | 3.44 | 3.57 | 3.22 | 3.06 | 3.56 | 3.47 | 3.41 | 3.20 |
| M2-Au3 | 3.11 | 3.52 | 3.49 | 3.42 | 3.21 | 3.15 | 3.55 | 3.44 | 3.57 | 3.22 | 3.06 | 3.56 | 3.47 | 3.41 | 3.20 |
| Au-C1 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.05 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C2 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.05 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| M-C3 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.05 | 2.04 | 2.04 | 2.05 |
| M-C4 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.00 | 1.99 | 1.99 | 1.99 | 1.99 | 2.05 | 2.04 | 2.04 | 2.04 | 2.05 |
| Au-C5 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.05 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au-C6 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 | 2.05 | 2.04 | 2.04 | 2.04 | 2.04 | 2.04 |
| Au1M2Au3 | 179.98 | 171.28 | 179.98 | 158.67 | 180.00 | 180.00 | 153.10 | 180.00 | 149.70 | 179.99 | 180.00 | 168.10 | 179.98 | 157.96 | 180.00 |
| | | | | | | | d1($T_1$) | | | | | | | | |
| Au1-M2 | 2.77 | 2.77 | 2.84 | 2.85 | 2.80 | 2.76 | 2.76 | 2.84 | 2.86 | 2.86 | 2.76 | 2.77 | 2.85 | 2.86 | 2.80 |
| M2-Au3 | 2.77 | 2.79 | 2.84 | 2.85 | 2.80 | 2.75 | 2.79 | 2.83 | 2.85 | 2.86 | 2.76 | 2.80 | 2.85 | 2.86 | 2.80 |
| Au-C1 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.02 | 2.03 | 2.03 | 2.03 |
| Au-C2 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.02 | 2.03 | 2.03 | 2.03 |
| M-C3 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.98 | 2.02 | 2.03 | 2.02 | 2.02 | 2.02 |
| M-C4 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.99 | 1.98 | 2.02 | 2.03 | 2.02 | 2.02 | 2.02 |
| Au-C5 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.04 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 |
| Au-C6 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.03 | 2.04 | 2.03 | 2.04 | 2.03 | 2.03 | 2.03 |
| Au1M2Au3 | 179.99 | 171.00 | 179.99 | 174.26 | 180.00 | 179.98 | 169.80 | 180.00 | 173.45 | 179.99 | 179.99 | 163.84 | 179.99 | 174.03 | 180.00 |
| λ | 457 | 450 | 421 | 419 | 435 | 483 | 475 | 444 | 441 | 444 | 417 | 429 | 383 | 380 | 391 |
| Δλ | | -7 | -36 | -38 | -22 | | -8 | -39 | -43 | -39 | | 12 | -34 | -37 | -26 |

## 6. Table 4S

**Table 4S**. Selected GKS-EDA results of **X**···(**S*n***)$_x$ (kcal/mol).

| | | | | | **II** | | | | | | | **I** | | | | **III** | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | S1 | (S1)2 | (S1)3 | (S1)4 | S2 | (S2)2 | (S2)3 | (S2)4 | S2 | (S2)2 | (S2)3 | (S2)4 | S2 | (S2)2 | (S2)3 | (S2)4 |
| $E^{CP1}$ | $E_{es}$ | -17.1 | -15.8 | -12.4 | -11.7 | -17.0 | -15.6 | -12.1 | -11.5 | -16.5 | -15.6 | -11.9 | -11.4 | -17.5 | -16.2 | -12.4 | -11.8 |
| | $E_{ex}$ | -36.1 | -34.3 | -26.2 | -24.5 | -36.9 | -35.1 | -26.3 | -24.8 | -32.9 | -31.3 | -24.7 | -23.3 | -34.9 | -32.7 | -25.8 | -24.1 |
| | $E_{rep}$ | 61.0 | 57.5 | 43.5 | 40.8 | 62.0 | 58.6 | 43.7 | 41.1 | 55.1 | 52.4 | 41.3 | 38.9 | 58.6 | 54.7 | 43.2 | 40.2 |
| | $E_{pol}$ | -11.2 | -10.4 | -7.5 | -7.1 | -11.2 | -10.4 | -7.4 | -7.1 | -11.0 | -10.1 | -7.5 | -7.1 | -12.0 | -10.9 | -8.0 | -7.6 |
| | $E_{disp}$ | -7.1 | -7.5 | -7.2 | -6.9 | -8.1 | -8.6 | -8.0 | -7.6 | -7.2 | -7.0 | -6.6 | -6.1 | -7.2 | -6.9 | -6.6 | -6.1 |
| | $E_{corr}$ | -4.7 | -4.6 | -3.9 | -3.5 | -4.7 | -4.7 | -3.8 | -3.5 | -3.9 | -3.9 | -3.6 | -3.3 | -3.9 | -3.9 | -3.6 | -3.1 |
| | $E_{tot}$ | -15.3 | -15.1 | -13.7 | -13.0 | -15.9 | -15.8 | -14.1 | -13.4 | -16.5 | -15.5 | -12.9 | -12.2 | -16.9 | -15.8 | -13.3 | -12.4 |
| $E^{CP2}$ | $E_{es}$ | | -31.8 | -29.2 | -23.6 | | -31.5 | -24.6 | -23.2 | | -31.3 | -24.0 | -23.7 | | -32.5 | -30.0 | -23.7 |
| | $E_{ex}$ | | -68.7 | -61.2 | -49.1 | | -70.4 | -52.8 | -49.6 | | -62.8 | -49.4 | -47.5 | | -65.5 | -60.2 | -48.1 |
| | $E_{rep}$ | | 115.1 | 102.2 | 81.7 | | 117.5 | 87.2 | 82.3 | | 105.0 | 82.3 | 79.0 | | 109.6 | 100.9 | 80.5 |
| | $E_{pol}$ | | -20.6 | -18.4 | -14.1 | | -20.6 | -15.1 | -14.0 | | -20.2 | -14.8 | -14.6 | | -21.7 | -19.8 | -15.0 |
| | $E_{disp}$ | | -15.0 | -14.6 | -13.7 | | -17.2 | -15.5 | -15.2 | | -13.9 | -13.0 | -12.0 | | -13.9 | -13.3 | -12.2 |
| | $E_{corr}$ | | -9.2 | -8.3 | -7.1 | | -9.4 | -7.6 | -7.1 | | -7.9 | -7.1 | -6.5 | | -7.9 | -7.5 | -6.3 |
| | $E_{tot}$ | | -30.2 | -29.6 | -25.9 | | -31.7 | -28.3 | -26.8 | | -31.1 | -26.0 | -25.4 | | -31.7 | -29.8 | -24.8 |
| $E^{CP3}$ | $E_{es}$ | | | -42.1 | -36.7 | | | -41.3 | -36.0 | | | -41.0 | -35.6 | | | -42.8 | -36.9 |
| | $E_{ex}$ | | | -87.4 | -74.7 | | | -88.7 | -75.4 | | | -82.0 | -71.0 | | | -85.9 | -73.4 |
| | $E_{rep}$ | | | 145.5 | 123.8 | | | 147.2 | 124.6 | | | 136.9 | 118.3 | | | 143.3 | 122.3 |
| | $E_{pol}$ | | | -26.0 | -21.9 | | | -25.8 | -21.6 | | | -25.4 | -21.7 | | | -27.8 | -23.1 |
| | $E_{disp}$ | | | -21.4 | -20.4 | | | -24.1 | -22.6 | | | -19.7 | -18.1 | | | -19.5 | -18.0 |
| | $E_{corr}$ | | | -12.1 | -10.6 | | | -12.2 | -10.6 | | | -11.0 | -9.8 | | | -10.7 | -9.4 |
| | $E_{tot}$ | | | -43.5 | -40.4 | | | -44.9 | -41.5 | | | -42.2 | -38.0 | | | -43.3 | -38.6 |
| $E^{CP4}$ | $E_{es}$ | | | | -49.9 | | | | -48.9 | | | | -48.5 | | | | -50.3 |
| | $E_{ex}$ | | | | -100.3 | | | | -101.2 | | | | -95.6 | | | | -98.8 |
| | $E_{rep}$ | | | | 166.1 | | | | 167.1 | | | | 159.0 | | | | 164.3 |
| | $E_{pol}$ | | | | -29.5 | | | | -29.2 | | | | -29.2 | | | | -31.2 |
| | $E_{disp}$ | | | | -27.0 | | | | -29.9 | | | | -24.0 | | | | -23.9 |
| | $E_{corr}$ | | | | -14.2 | | | | -14.2 | | | | -13.2 | | | | -12.6 |
| | $E_{tot}$ | | | | -54.8 | | | | -56.3 | | | | -51.5 | | | | -52.4 |

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $E^{CP}$ | $E_{es}$ | -99.7 | -112.8 | -124.4 | -135.5 | -99.4 | -112.3 | -123.7 | -134.5 | -101.5 | -114.8 | -125.7 | - | -101.7 | -114.7 | -126.0 | -137.7 |
| | $E_{ex}$ | -93.7 | -126.5 | -154.5 | -185.9 | -93.9 | -127.7 | -156.5 | -186.9 | -30.3 | -125.9 | -151.4 | - | -89.8 | -123.8 | -149.3 | -180.7 |
| | $E_{rep}$ | 149.8 | 203.3 | 248.9 | 300.2 | 150.0 | 204.8 | 251.7 | 301.5 | 100.6 | 201.4 | 243.5 | - | 142.6 | 197.9 | 239.7 | 290.9 |
| | $E_{pol}$ | -26.0 | -34.3 | -42.3 | -51.7 | -25.9 | -34.3 | -42.4 | -51.5 | -30.7 | -32.7 | -40.2 | - | -22.7 | -31.8 | -39.2 | -47.8 |
| | $E_{disp}$ | -33.3 | -41.5 | -48.7 | -55.4 | -34.3 | -43.8 | -51.4 | -58.4 | -34.6 | -42.0 | -47.7 | - | -31.6 | -38.9 | -44.9 | -49.4 |
| | $E_{corr}$ | -11.4 | -16.2 | -19.8 | -24.0 | -11.4 | -16.4 | -20.0 | -24.1 | -20.5 | -16.3 | -19.6 | - | -11.4 | -16.6 | -19.3 | -23.5 |
| | $E_{tot}$ | -114.3 | -128.1 | -140.8 | -152.2 | -114.8 | -129.5 | -142.3 | -153.8 | -117.1 | -130.3 | -141.1 | - | -114.6 | -127.9 | -139.0 | -148.3 |

.

## 7. Figure 3S

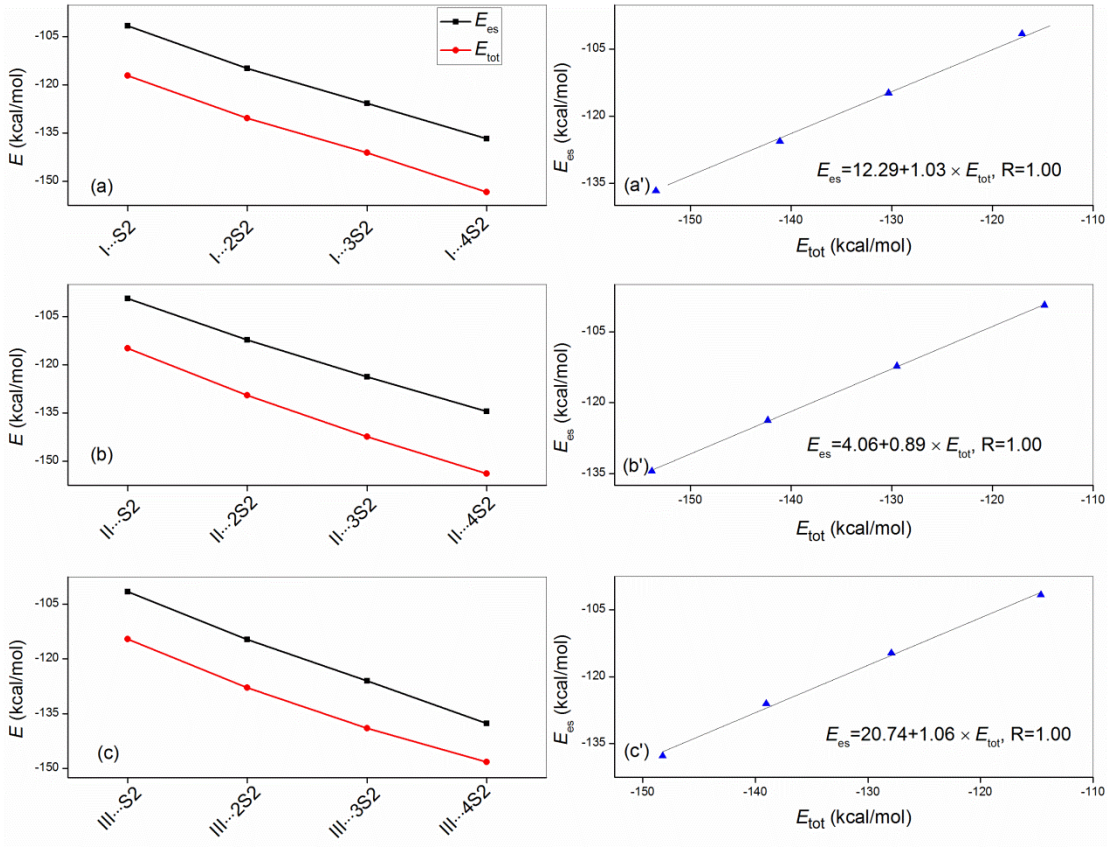



**Figure 3S.** Trends of interaction energies (**a**, **b**, **c**) and the relationships between the $E_{es}$ and $E_{tot}$ (**a'**, **b'**, **c'**).

## 8. Figure 4S

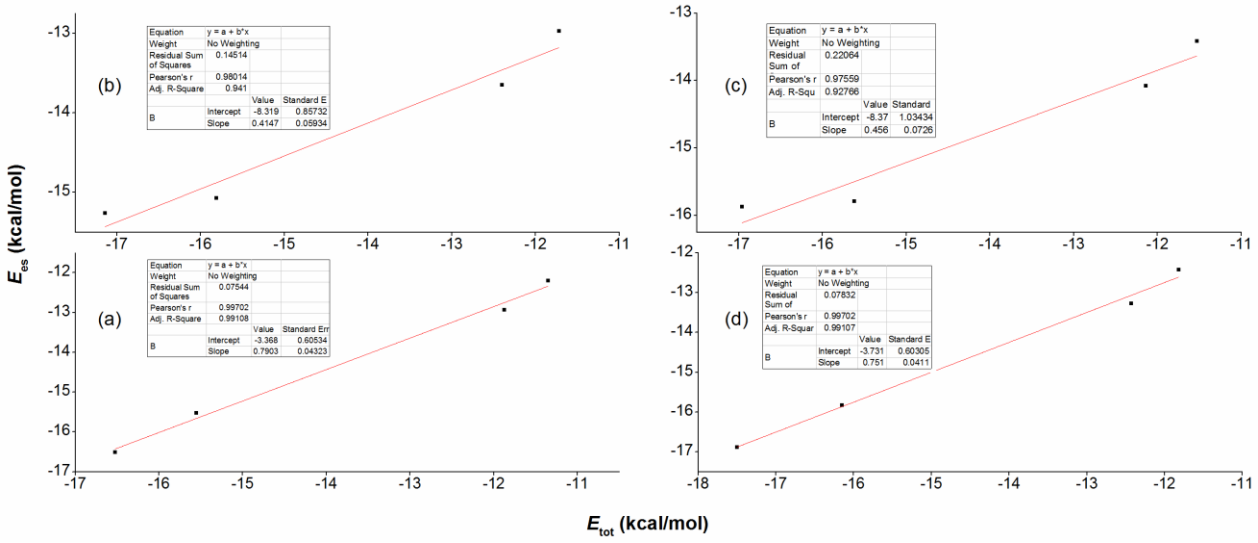



**Figure 4S**. The relationships between the $E_{es}$ and $E_{tot}$ (a) I···(**S2**)$_x$, (b) II···(**S1**)$_x$, (c) II···(**S2**)$_x$ and (d) III···(**S2**)$_x$ for the $E^{CP1}$ of clusters.

## 9. Table 5S

**Table 5S**. Molecular Orbitals and their main consist of natural atomic orbital and the characters.

| | HOMO (%) | d (%) | LUMO (%) | p (%) |
|---|---|---|---|---|
| I | 77.23 | 45.29 | 35.71 | 35.34 |
| II | 74.71 | 42.78 | 26.25 | 26.03 |
| III | 69.50 | 42.74 | 34.30 | 34.10 |
| I-S1 | 74.32 | 41.19 | 39.84 | 39.51 |
| I-(S1)2 | 75.24 | 43.13 | 41.21 | 40.77 |
| I-(S1)3 | 75.48 | 43.31 | 39.41 | 38.63 |
| I-(S1)4 | 76.02 | 45.16 | 38.39 | 37.86 |
| I-S2 | 75.44 | 42.33 | 39.94 | 38.30 |
| I-(S2)2 | 75.21 | 42.42 | 41.14 | 40.68 |
| I-(S2)3 | 75.54 | 43.64 | 39.45 | 38.46 |
| I-(S2)4 | 76.05 | 45.14 | 38.45 | 37.92 |
| II-S1 | 65.22 | 35.63 | 27.87 | 26.75 |
| II-(S1)2 | 60.31 | 34.28 | 29.47 | 29.61 |
| II-(S1)3 | 64.86 | 37.84 | 27.87 | 26.14 |
| II-(S1)4 | 70.06 | 41.03 | 26.34 | 25.99 |
| II-S2 | 65.05 | 34.85 | 27.93 | 24.02 |
| II-(S2)2 | 59.99 | 34.61 | 29.41 | 29.03 |
| II-(S2)3 | 65.38 | 37.80 | 27.82 | 27.43 |
| II-(S2)4 | 70.12 | 41.63 | 26.31 | 25.96 |
| III-S1 | 67.71 | 39.66 | 39.58 | 39.34 |
| III-(S1)2 | 68.44 | 41.19 | 41.28 | 40.94 |
| III-(S1)3 | 68.44 | 41.72 | 39.38 | 38.95 |
| III-(S1)4 | 68.68 | 43.02 | 37.89 | 37.51 |
| III-S2 | 67.97 | 40.20 | 39.69 | 39.24 |
| III-(S2)2 | 68.47 | 41.17 | 41.24 | 40.91 |
| III-(S2)3 | 68.44 | 41.69 | 39.43 | 39.17 |
| III-(S2)4 | 68.62 | 43.07 | 38.41 | 38.11 |

## 10. Table 6S

**Table 6S**. Calculated phosphorescent emission (in nm) of the studied complexes with the TDDFT method, along with experimental values.

| Complex | λ | E(eV) | Configuration | | Character | Exp | |
|---|---|---|---|---|---|---|---|
| I | 457 | 2.72 | HOMO-LUMO | 98% | MLCT | 448 | 9* |
| II | 483 | 2.57 | HOMO-LUMO | 97% | MLCT | 465 | 18* |
| III | 417 | 2.98 | HOMO-LUMO | 97% | MLCT | 446 | -29* |
| I-S1 | 450 | 2.76 | HOMO-LUMO | 98% | MLCT | | -7 |
| I-(S1)2 | 418.84 | 2.96 | HOMO-LUMO | 98% | MLCT | | -38 |
| I-(S1)3 | 417.98 | 2.97 | HOMO-LUMO | 98% | MLCT | | -39 |
| I-(S1)4 | 412.24 | 3.01 | HOMO-LUMO | 98% | MLCT | | -45 |
| I-S2 | 449.15 | 2.76 | HOMO-LUMO | 98% | MLCT | | -8 |
| I-(S2)2 | 420.38 | 2.95 | HOMO-LUMO | 98% | MLCT | | -37 |
| I-(S2)3 | 417.53 | 2.97 | HOMO-LUMO | 98% | MLCT | | -39 |
| I-(S2)4 | 412.2 | 3.01 | HOMO-LUMO | 98% | MLCT | | -45 |
| II-S1 | 478.46 | 2.59 | HOMO-LUMO | 97% | MLCT | | -5 |
| II-(S1)2 | 437.33 | 2.84 | HOMO-LUMO | 96% | MLCT | | -46 |
| II-(S1)3 | 439.21 | 2.82 | HOMO-LUMO | 96% | MLCT | | -44 |
| II-(S1)4 | 442.89 | 2.80 | HOMO-LUMO | 96% | MLCT | | -40 |
| II-S2 | 475.86 | 2.61 | HOMO-LUMO | 97% | MLCT | | -7 |
| II-(S2)2 | 436.66 | 2.84 | HOMO-LUMO | 96% | MLCT | | -46 |
| II-(S2)3 | 439.54 | 2.82 | HOMO-LUMO | 96% | MLCT | | -43 |
| II-(S2)4 | 443.04 | 2.80 | HOMO-LUMO | 96% | MLCT | | -40 |
| III-S1 | 408.98 | 3.03 | HOMO-LUMO | 97% | MLCT | | -8 |
| III-(S1)2 | 382.75 | 3.24 | HOMO-LUMO | 97% | MLCT | | -34 |
| III-(S1)3 | 379.18 | 3.27 | HOMO-LUMO | 97% | MLCT | | -38 |
| III-(S1)4 | 371.23 | 3.34 | HOMO-LUMO | 97% | MLCT | | -46 |
| III-S2 | 408.44 | 3.04 | HOMO-LUMO | 97% | MLCT | | -9 |
| III-(S2)2 | 383.08 | 3.24 | HOMO-LUMO | 97% | MLCT | | -34 |
| III-(S2)3 | 378.45 | 3.28 | HOMO-LUMO | 97% | MLCT | | -39 |
| III-(S2)4 | 371.68 | 3.34 | HOMO-LUMO | 97% | MLCT | | -45 |

$$\delta^* = \lambda^{cal}_{[X]} - \lambda^{\exp}_{[X]}$$

$$\delta = \lambda^{cal}_{[X\cdots(S)_n]} - \lambda^{cal}_{[X]}$$

## 11. Figure 5S

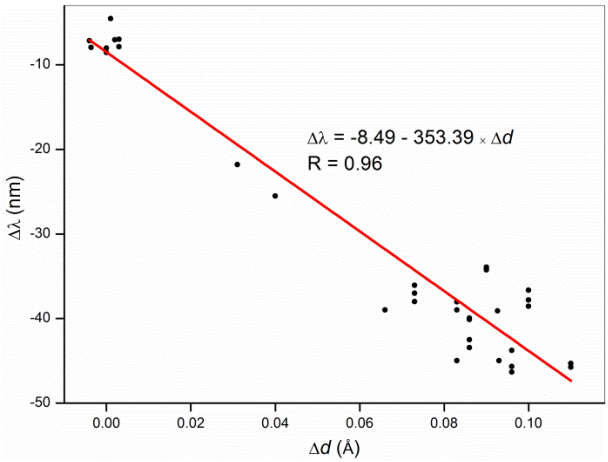



**Figure 5S.** The relationship between Δd and Δλ for complexes X···$(S)_x$ in T1 states.

## 12. Figure 6S

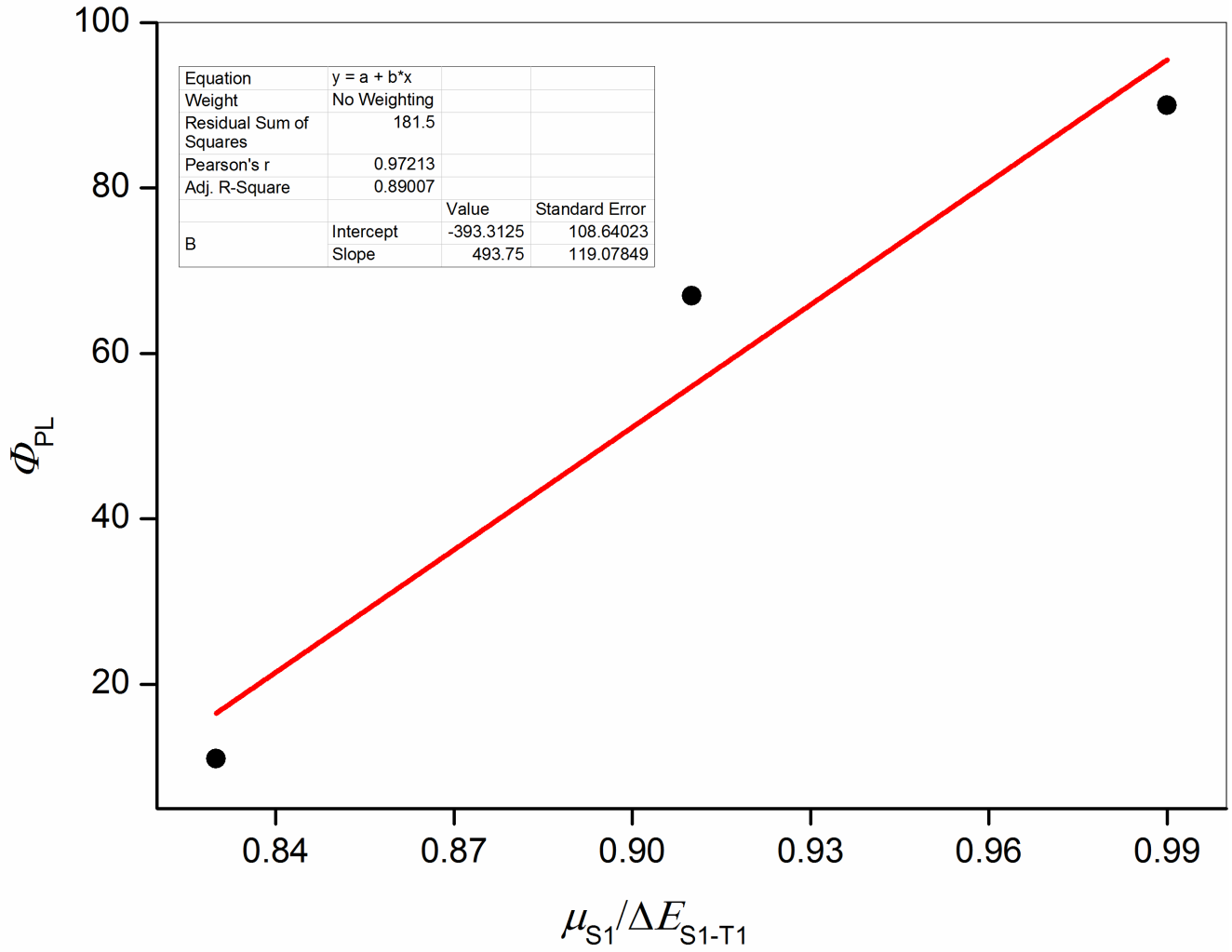



**Figure 6S**. The relationship betwwen $\mu_{S1}/\Delta E_{S1\text{-}T1}$ values in theory and the $\Phi_{PL}$ values in experiment.

## 13. Table 7S

**Table 7S**. The singlet-triplet splitting energy ($\Delta E_{S1\text{-}T1}$, in eV), transition electric dipole moment ($\mu_{S1}$, in atomics units), the $\mu_{S1}/\Delta E_{S1\text{-}T1}$, and the predicted $\Phi_{PL}$ (> 50%) for complexes X···$(S)_x$.

| complex | $\Delta E_{S1\text{-}T1}$ | $\mu_{S1}$ | $\mu_{S1}/\Delta E_{S1\text{-}T1}$ | $\Phi_{PL}$(%) |
|---|---|---|---|---|
| I-S1 | 2.85 | 2.81 | 0.99 | 94.6 |
| II-S1 | 2.73 | 2.53 | 0.92 | 63.0 |
| II-2S1 | 3.01 | 2.82 | 0.94 | 69.2 |
| II-3S1 | 3.00 | 2.77 | 0.92 | 62.9 |
| I-4S1 | 2.96 | 2.77 | 0.94 | 68.4 |
| II-4S1 | 2.97 | 2.72 | 0.92 | 59.1 |
| I-S2 | 2.85 | 2.80 | 0.98 | 92.5 |
| II-3S2 | 3.00 | 2.74 | 0.91 | 58.2 |
| I-4S2 | 2.96 | 2.73 | 0.92 | 61.7 |
| II-4S2 | 2.97 | 2.68 | 0.90 | 52.7 |
| I-S3 | 2.95 | 2.79 | 0.94 | 73.2 |
| II-S3 | 2.83 | 2.68 | 0.95 | 74.9 |
| I-2S3 | 3.12 | 2.83 | 0.91 | 55.1 |
| II-2S3 | 2.96 | 2.72 | 0.92 | 59.5 |

## 14. Table 8S

**Table 9S**. The $E^{CP}$ of cluster **I** at different calculated levels (kcal/mol).

| Mode | MP2 | | | PBE0-D3 | | PBE0 | | M06-2X | |
|---|---|---|---|---|---|---|---|---|---|
| | BS1 | BS3 | BS4 | BS3 | BS4 | BS3 | BS4 | BS3 | BS4 |
| $E^{CP}_{add}$ | -22.5 | -29.2 | -30.7 | -29.0 | -29.0 | -19.8 | -19.8 | -24.3 | -24.3 |
| $E^{CP}_{tot}$ | -88.8 | -102.3 | -105.1 | -102.5 | -102.6 | -85.9 | -85.9 | -94.9 | -97.1 |

The binding energies with BSSE corrections of cluster **I** at different calculated levels show that the $E^{CP}$ of the PBE0-D3/BS3 and PBE0-D3/BS4 are identical to each other, and they both close to the MP2/BS4 results and the PBE0-D3/BS3 are more financial than PBE0-D3/BS4 in time.

## 15. Table 9S

**Table 10S**. The EDA results of cluster I at different calculated levels (kcal/mol).

| | | $E_{es}$ | $E_{ex}$ | $E_{rep}$ | $E_{pol}$ | $E_{disp}$ | $E_{corr}$ | $E_{tot}$ | $E^{CP}$[a] |
|---|---|---|---|---|---|---|---|---|---|
| $E_{add}^{CP}$ | MP2/BS5[b] | -23.44 | -39.6 | 64.73 | -12.97 | -15.34 | | -26.62 | |
| | MP2/BS6[b] | -23.01 | -39.09 | 64.16 | -13.21 | -18.1 | | -29.25 | |
| | B3LYP-D3/BS5[c] | -23.29 | -46.03 | 74.84 | -15.55 | -13.99 | -5.56 | -29.57 | -30.65 |
| | B3LYP-D3/BS6[c] | -22.87 | -45.38 | 74.1 | -15.78 | -13.99 | -5.46 | -29.38 | |
| $E_{tot}^{CP}$ | MP2/BS5[b] | -95.48 | -85.14 | 137.53 | -25.19 | -28.66 | | -96.94 | |
| | MP2/BS6[b] | -95.11 | -84.03 | 136.16 | -25.34 | -33.97 | | -102.29 | |
| | B3LYP-D3/BS5[c] | -95.76 | -99.47 | 159.8 | -29.87 | -26.23 | -12.48 | -104.0 | -105.10 |
| | B3LYP-D3/BS6[c] | -95.23 | -97.97 | 157.93 | -30.19 | -26.23 | -12.01 | -103.69 | |

[a] Calculated at the MP2/BS4 with gaussian; [b]LMO-EDA; [c]GKS-EDA.

The LMO-EDA and GKS-EDA results at four calculated levels MP2/BS5, MP2/BS6, B3LYP-D3/BS5 and B3LYP-D3/BS6 show that the GKS-EDA total interaction energies ($E_{tot}$) at B3LYP-D3/BS5 and B3LYP-D3/BS6 levels are very close and they are also consistent with those in MP2/BS6 level with LMO-EDA scheme as well as the $E^{CP}$ at MP2/BS4 level.

## 16. The $S_0$ .xyz files of I and its complexes

I

| | | | |
|---|---|---|---|
| Au | 3.113900 | -0.000000 | -0.000500 |
| N | 2.946500 | -2.991000 | 0.564400 |
| N | 3.179300 | -2.639800 | -1.539700 |
| C | 3.107900 | -2.006500 | -0.348500 |
| C | 3.061100 | -4.001000 | -1.377600 |
| H | 3.091700 | -4.686000 | -2.210800 |
| C | 2.919100 | -4.224100 | -0.046300 |
| H | 2.814900 | -5.142700 | 0.510300 |
| C | 2.834600 | -2.769300 | 1.996300 |
| H | 2.125200 | -1.961300 | 2.190100 |
| H | 2.469800 | -3.684600 | 2.465600 |
| C | 3.270400 | -1.969200 | -2.826900 |
| H | 3.912100 | -1.092700 | -2.723200 |
| H | 3.715100 | -2.654200 | -3.551400 |
| H | 3.809700 | -2.513200 | 2.419300 |
| H | 2.277500 | -1.655900 | -3.163300 |
| N | 2.946000 | 2.990900 | -0.565200 |
| N | 3.180300 | 2.639700 | 1.538700 |
| C | 3.108100 | 2.006400 | 0.347500 |
| C | 3.061800 | 4.000800 | 1.376800 |
| H | 3.092800 | 4.685800 | 2.210000 |
| C | 2.918800 | 4.224000 | 0.045600 |
| H | 2.814000 | 5.142600 | -0.510900 |
| C | 2.833200 | 2.769200 | -1.997000 |
| H | 2.122700 | 1.962100 | -2.190400 |
| H | 2.469400 | 3.684900 | -2.466200 |
| C | 3.272600 | 1.969000 | 2.825900 |
| H | 3.915000 | 1.093100 | 2.721700 |
| H | 3.717100 | 2.654300 | 3.550100 |
| H | 3.807700 | 2.511800 | -2.420300 |
| H | 2.280100 | 1.654900 | 3.162800 |
| N | -0.006900 | 0.384600 | 3.142500 |
| C | -0.003100 | 0.237500 | 1.982300 |
| N | -0.010000 | -0.385700 | -3.141400 |
| C | -0.004800 | -0.238000 | -1.981300 |
| Au | -0.002300 | -0.000100 | 0.000500 |
| Au | -3.116700 | 0.000200 | 0.000200 |
| N | -3.114300 | -2.574500 | 1.639600 |
| N | -3.003100 | -3.012300 | -0.458200 |
| C | -3.107600 | -1.991200 | 0.421000 |
| C | -2.944400 | -4.219400 | 0.199900 |
| H | -2.872300 | -5.160100 | -0.323800 |
| C | -3.012800 | -3.942100 | 1.527200 |
| H | -3.008000 | -4.593500 | 2.387500 |
| C | -3.160200 | -1.843800 | 2.896600 |
| H | -2.221300 | -1.306700 | 3.058600 |
| H | -3.988800 | -1.133200 | 2.874000 |
| C | -2.938500 | -2.844500 | -1.901400 |
| H | -3.857200 | -2.377100 | -2.263200 |
| H | -2.079800 | -2.223800 | -2.170700 |
| H | -3.322300 | -2.554300 | 3.708800 |
| H | -2.833300 | -3.827800 | -2.362700 |
| N | -3.115200 | 2.574600 | -1.639300 |
| N | -3.001300 | 3.012800 | 0.458300 |
| C | -3.107100 | 1.991600 | -0.420600 |
| C | -2.943300 | 4.219700 | -0.200100 |
| H | -2.870400 | 5.160500 | 0.323400 |
| C | -3.013400 | 3.942300 | -1.527300 |
| H | -3.009400 | 4.593500 | -2.387700 |
| C | -3.162400 | 1.843600 | -2.896200 |
| H | -2.224100 | 1.305700 | -3.058500 |
| H | -3.991700 | 1.133900 | -2.872900 |
| C | -2.935800 | 2.845200 | 1.901500 |
| H | -3.857400 | 2.384800 | 2.265100 |
| H | -2.081200 | 2.218400 | 2.169600 |
| H | -3.324300 | 2.554200 | -3.708400 |
| H | -2.822500 | 3.827900 | 2.362000 |

I...S1

| | | | |
|---|---|---|---|
| Au | 3.521600 | -0.131500 | -0.027800 |
| N | 3.445700 | -2.960900 | 1.122000 |
| N | 3.338300 | -3.024400 | -1.018200 |
| C | 3.440100 | -2.170500 | 0.023200 |
| C | 3.263000 | -4.325200 | -0.581300 |
| H | 3.143600 | -5.154300 | -1.261000 |
| C | 3.339300 | -4.287800 | 0.771300 |
| H | 3.323600 | -5.079900 | 1.504000 |
| C | 3.558900 | -2.491700 | 2.488500 |
| H | 3.417200 | -1.410200 | 2.496900 |
| H | 2.783700 | -2.957000 | 3.102400 |
| C | 3.191600 | -2.637200 | -2.408100 |
| H | 3.453300 | -1.582500 | -2.503900 |
| H | 3.865600 | -3.233500 | -3.028200 |
| H | 4.544300 | -2.734800 | 2.897100 |
| H | 2.153900 | -2.792000 | -2.715000 |
| N | 2.977400 | 2.766200 | -0.852400 |
| N | 4.335400 | 2.695200 | 0.803800 |
| C | 3.630100 | 1.906700 | -0.040600 |
| C | 4.114900 | 4.026800 | 0.531000 |
| H | 4.576700 | 4.817000 | 1.102900 |
| C | 3.255000 | 4.070000 | -0.516100 |
| H | 2.803100 | 4.899600 | -1.036100 |
| C | 2.113900 | 2.391900 | -1.956700 |
| H | 1.687600 | 1.408100 | -1.753200 |
| H | 1.312500 | 3.130400 | -2.024900 |
| C | 5.171500 | 2.221300 | 1.889100 |
| H | 5.344300 | 1.152900 | 1.752800 |
| H | 6.130800 | 2.744600 | 1.870300 |
| H | 2.683600 | 2.363400 | -2.890600 |
| H | 4.680300 | 2.392100 | 2.851400 |
| N | -0.002500 | 2.533800 | 1.086100 |
| C | -0.001300 | 1.400900 | 0.802100 |
| N | 0.002900 | -3.314400 | -1.265400 |
| C | 0.002100 | -2.281200 | -0.718900 |
| Au | 0.000600 | -0.467700 | 0.107800 |
| Au | -3.521500 | -0.135500 | -0.027600 |
| N | -3.439200 | -2.963200 | 1.125800 |
| N | -3.333200 | -3.029300 | -1.014400 |
| C | -3.435900 | -2.174300 | 0.025900 |
| C | -3.255100 | -4.329400 | -0.575900 |

| | | | |
|---|---|---|---|
| H | -3.134500 | -5.159200 | -1.254500 |
| C | -3.330500 | -4.290400 | 0.776700 |
| H | -3.312800 | -5.081500 | 1.510500 |
| C | -3.552300 | -2.492400 | 2.491700 |
| H | -3.412000 | -1.410700 | 2.498700 |
| H | -4.537000 | -2.736400 | 2.901300 |
| C | -3.188500 | -2.643800 | -2.405000 |
| H | -3.451700 | -1.589500 | -2.501800 |
| H | -2.150800 | -2.797500 | -2.712700 |
| H | -2.776100 | -2.955900 | 3.105800 |
| H | -3.862300 | -3.241800 | -3.023600 |
| N | -2.981600 | 2.762200 | -0.854800 |
| N | -4.341800 | 2.690600 | 0.799500 |
| C | -3.633900 | 1.902500 | -0.043000 |
| C | -4.123400 | 4.022400 | 0.525500 |
| H | -4.587500 | 4.812300 | 1.095700 |
| C | -3.262100 | 4.065900 | -0.520500 |
| H | -2.811200 | 4.895700 | -1.041000 |
| C | -2.115900 | 2.388100 | -1.957500 |
| H | -1.688400 | 1.405200 | -1.752500 |
| H | -2.684100 | 2.357900 | -2.892300 |
| C | -5.178800 | 2.216600 | 1.884100 |
| H | -5.347800 | 1.147300 | 1.749800 |
| H | -4.690200 | 2.391000 | 2.847100 |
| H | -1.315500 | 3.127800 | -2.025100 |
| H | -6.139800 | 2.736700 | 1.862000 |
| O | -0.003300 | 4.675200 | -0.759600 |
| H | -0.003300 | 4.017000 | -0.030200 |
| C | -0.005500 | 5.960600 | -0.182300 |
| H | 0.882800 | 6.139900 | 0.441300 |
| H | -0.005700 | 6.692600 | -0.995800 |
| H | -0.895500 | 6.137600 | 0.439700 |

I···2S1

| | | | |
|---|---|---|---|
| Au | -3.455700 | -0.000900 | 0.000100 |
| N | -3.009100 | 2.942600 | 0.723300 |
| N | -3.982500 | 2.769100 | -1.178600 |
| C | -3.487900 | 2.035100 | -0.155000 |
| C | -3.804400 | 4.114300 | -0.947900 |
| H | -4.118400 | 4.867300 | -1.654200 |
| C | -3.188000 | 4.222200 | 0.254600 |
| H | -2.849000 | 5.083800 | 0.807700 |
| C | -2.372000 | 2.639100 | 1.991800 |
| H | -1.993800 | 1.616000 | 1.958500 |
| H | -1.540500 | 3.334000 | 2.132800 |
| C | -4.571900 | 2.227900 | -2.387500 |
| H | -4.724700 | 1.156800 | -2.248400 |
| H | -5.535700 | 2.707400 | -2.577100 |
| H | -3.090400 | 2.738900 | 2.811200 |
| H | -3.905900 | 2.392400 | -3.239300 |
| N | -3.006800 | -2.944100 | -0.723300 |
| N | -3.979800 | -2.771300 | 1.178900 |
| C | -3.486000 | -2.036900 | 0.155200 |
| C | -3.800800 | -4.116300 | 0.948200 |
| H | -4.114100 | -4.869600 | 1.654600 |
| C | -3.184600 | -4.223900 | -0.254500 |
| H | -2.845300 | -5.085200 | -0.807700 |
| C | -2.370300 | -2.640200 | -1.991900 |
| H | -1.993500 | -1.616600 | -1.959100 |
| H | -1.537800 | -3.334000 | -2.132700 |
| C | -4.569000 | -2.230500 | 2.388100 |
| H | -4.723900 | -1.159800 | 2.248500 |
| H | -5.531700 | -2.711700 | 2.578900 |
| H | -3.088600 | -2.741400 | -2.811300 |
| H | -3.901900 | -2.393200 | 3.239300 |
| N | 0.001600 | -3.006900 | 0.967200 |
| C | 0.001000 | -1.880300 | 0.658500 |
| N | -0.001600 | 3.006600 | -0.967300 |
| C | -0.001000 | 1.880000 | -0.658700 |
| Au | 0.000000 | -0.000200 | -0.000200 |
| Au | 3.455700 | 0.001000 | 0.000200 |
| N | 3.006400 | 2.944100 | 0.723600 |
| N | 3.981100 | 2.771600 | -1.177800 |
| C | 3.486400 | 2.037000 | -0.154600 |
| C | 3.801800 | 4.116600 | -0.947000 |
| H | 4.115700 | 4.869900 | -1.653000 |
| C | 3.184600 | 4.223900 | 0.255200 |
| H | 2.844700 | 5.085100 | 0.808200 |
| C | 2.369100 | 2.640000 | 1.991800 |
| H | 1.991300 | 1.616700 | 1.958200 |
| H | 3.087100 | 2.740000 | 2.811500 |
| C | 4.571200 | 2.230900 | -2.386600 |
| H | 4.726600 | 1.160300 | -2.246800 |
| H | 3.904600 | 2.393300 | -3.238200 |
| H | 1.537200 | 3.334400 | 2.132700 |
| H | 5.533900 | 2.712500 | -2.576800 |
| N | 3.009000 | -2.942300 | -0.723900 |
| N | 3.981700 | -2.769400 | 1.178500 |
| C | 3.487500 | -2.035000 | 0.154900 |
| C | 3.803700 | -4.114500 | 0.947400 |
| H | 4.117400 | -4.867700 | 1.653600 |
| C | 3.187700 | -4.222100 | -0.255400 |
| H | 2.848900 | -5.083500 | -0.808800 |
| C | 2.372300 | -2.638600 | -1.992500 |
| H | 1.995000 | -1.615100 | -1.959400 |
| H | 3.090700 | -2.739100 | -2.811800 |
| C | 4.570700 | -2.228500 | 2.387800 |
| H | 4.722300 | -1.157100 | 2.249400 |
| H | 3.905000 | -2.394300 | 3.239500 |
| H | 1.540300 | -3.332800 | -2.133400 |
| H | 5.535100 | -2.707100 | 2.576800 |
| O | 0.001900 | -4.907600 | -1.136500 |
| H | 0.001900 | -4.364200 | -0.320000 |
| C | 0.002000 | -6.266800 | -0.767700 |
| H | -0.885900 | -6.543900 | -0.179400 |
| H | 0.001700 | -6.860900 | -1.686100 |
| H | 0.890100 | -6.543900 | -0.179900 |
| O | -0.002100 | 4.908200 | 1.135600 |
| H | -0.002100 | 4.364200 | 0.319500 |
| C | -0.002200 | 6.267100 | 0.765800 |
| H | -0.001700 | 6.861800 | 1.683800 |
| H | 0.885500 | 6.543700 | 0.177100 |
| H | -0.890500 | 6.543800 | 0.178100 |

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| | | | |
|---|---|---|---|
| Au | -3.331000 | 0.312000 | 0.043900 |

| | | | |
|---|---|---|---|
| N | -3.419300 | -2.620700 | -0.840300 |
| N | -3.562100 | -2.468200 | 1.295100 |
| C | -3.442400 | -1.724400 | 0.172300 |
| C | -3.604800 | -3.808500 | 0.991200 |
| H | -3.698100 | -4.568300 | 1.751800 |
| C | -3.515500 | -3.904400 | -0.358300 |
| H | -3.517300 | -4.764800 | -1.009700 |
| C | -3.205000 | -2.308200 | -2.241700 |
| H | -3.072900 | -1.229700 | -2.337600 |
| H | -2.300600 | -2.816700 | -2.590900 |
| C | -3.524800 | -1.956100 | 2.653800 |
| H | -3.625200 | -0.870400 | 2.615900 |
| H | -4.356600 | -2.373100 | 3.227600 |
| H | -4.068100 | -2.623900 | -2.834800 |
| H | -2.569900 | -2.228800 | 3.115300 |
| N | -2.697500 | 3.213800 | 0.777900 |
| N | -3.800000 | 3.127200 | -1.057900 |
| C | -3.281000 | 2.349100 | -0.080100 |
| C | -3.533900 | 4.456600 | -0.819600 |
| H | -3.849300 | 5.238000 | -1.493700 |
| C | -2.835700 | 4.509600 | 0.341400 |
| H | -2.409200 | 5.339800 | 0.881700 |
| C | -2.011000 | 2.850000 | 2.003700 |
| H | -1.605500 | 1.842600 | 1.893700 |
| H | -1.195200 | 3.559500 | 2.161100 |
| C | -4.490800 | 2.640100 | -2.235700 |
| H | -4.735700 | 1.588000 | -2.083900 |
| H | -5.414500 | 3.205700 | -2.382400 |
| H | -2.703400 | 2.877100 | 2.850700 |
| H | -3.853700 | 2.742500 | -3.118800 |
| N | 0.296300 | 3.374100 | -0.985500 |
| C | 0.195600 | 2.215800 | -0.878900 |
| N | -0.243700 | -2.811600 | 0.148400 |
| C | -0.144800 | -1.674900 | -0.110400 |
| Au | 0.024600 | 0.262300 | -0.528900 |
| Au | 3.341100 | -0.149700 | 0.079700 |
| N | 2.956700 | -2.985300 | -1.006400 |
| N | 3.051500 | -3.006500 | 1.136800 |
| C | 3.101700 | -2.178400 | 0.069000 |
| C | 2.869800 | -4.309300 | 0.736000 |
| H | 2.799300 | -5.123700 | 1.440500 |
| C | 2.810800 | -4.295600 | -0.618700 |
| H | 2.677300 | -5.093000 | -1.333000 |
| C | 2.880300 | -2.550400 | -2.389500 |
| H | 2.811500 | -1.461700 | -2.406500 |
| H | 3.772000 | -2.868900 | -2.937700 |
| C | 3.048800 | -2.586600 | 2.527100 |
| H | 3.361900 | -1.542500 | 2.572600 |
| H | 2.039700 | -2.690900 | 2.940400 |
| H | 1.982900 | -2.981700 | -2.842000 |
| H | 3.754800 | -3.196800 | 3.096600 |
| N | 3.133100 | 2.778300 | 0.949400 |
| N | 4.348200 | 2.598100 | -0.806800 |
| C | 3.634700 | 1.870900 | 0.083800 |
| C | 4.282500 | 3.940400 | -0.508300 |
| H | 4.773200 | 4.689900 | -1.110000 |
| C | 3.512900 | 4.052800 | 0.602100 |
| H | 3.186600 | 4.915600 | 1.161000 |
| C | 2.303900 | 2.476100 | 2.101400 |
| H | 1.765000 | 1.546000 | 1.912100 |
| H | 2.922300 | 2.367000 | 2.997600 |
| C | 5.044500 | 2.060000 | -1.959000 |
| H | 5.091000 | 0.974700 | -1.860100 |
| H | 4.512800 | 2.319700 | -2.878900 |
| H | 1.591200 | 3.293600 | 2.232400 |
| H | 6.060600 | 2.460800 | -1.997100 |
| O | 0.366600 | 5.095000 | 1.252200 |
| H | 0.357600 | 4.615800 | 0.395500 |
| C | 0.493700 | 6.473700 | 0.988400 |
| H | -0.343600 | 6.866200 | 0.392200 |
| H | 1.425700 | 6.714800 | 0.455900 |
| H | 0.503500 | 6.997100 | 1.948800 |
| O | -0.132100 | -4.183600 | -2.403200 |
| H | -0.163300 | -3.853800 | -1.485300 |
| C | -0.362400 | -5.571800 | -2.390900 |
| H | 0.398300 | -6.123300 | -1.817000 |
| H | -1.348300 | -5.834200 | -1.977500 |
| H | -0.326600 | -5.921700 | -3.426000 |
| C | -0.415100 | -4.705900 | 3.284700 |
| O | -0.367100 | -3.331700 | 2.984100 |
| H | 0.473100 | -5.248600 | 2.925500 |
| H | -1.303600 | -5.200300 | 2.863100 |
| H | -0.345200 | -3.234900 | 2.012200 |
| H | -0.454500 | -4.805800 | 4.372800 |

I-4S1

| | | | |
|---|---|---|---|
| Au | -3.251900 | 0.000000 | 0.000000 |
| N | -3.281600 | 2.868300 | 1.072700 |
| N | -3.281600 | 2.868300 | -1.072700 |
| C | -3.279600 | 2.044200 | 0.000000 |
| C | -3.277300 | 4.185000 | -0.677800 |
| H | -3.277100 | 4.998300 | -1.387100 |
| C | -3.277300 | 4.185000 | 0.677800 |
| H | -3.277100 | 4.998300 | 1.387100 |
| C | -3.183900 | 2.452200 | 2.460400 |
| H | -3.248000 | 1.364200 | 2.498400 |
| H | -2.223400 | 2.780700 | 2.871500 |
| C | -3.183900 | 2.452200 | -2.460400 |
| H | -3.248000 | 1.364200 | -2.498400 |
| H | -4.009000 | 2.880900 | -3.035800 |
| H | -4.009000 | 2.880900 | 3.035800 |
| H | -2.223400 | 2.780700 | -2.871500 |
| N | -3.281600 | -2.868300 | -1.072700 |
| N | -3.281600 | -2.868300 | 1.072700 |
| C | -3.279600 | -2.044200 | 0.000000 |
| C | -3.277300 | -4.185000 | 0.677800 |
| H | -3.277100 | -4.998300 | 1.387100 |
| C | -3.277300 | -4.185000 | -0.677800 |
| H | -3.277100 | -4.998300 | -1.387100 |
| C | -3.183900 | -2.452200 | -2.460400 |
| H | -3.248000 | -1.364200 | -2.498400 |
| H | -2.223400 | -2.780700 | -2.871500 |
| C | -3.183900 | -2.452200 | 2.460400 |
| H | -3.248000 | -1.364200 | 2.498400 |
| H | -4.009000 | -2.880900 | 3.035800 |

| | | | |
|---|---|---|---|
| H | -4.009000 | -2.880900 | -3.035800 |
| H | -2.223400 | -2.780700 | 2.871500 |
| N | 0.000000 | -3.160200 | 0.000000 |
| C | 0.000000 | -1.990000 | 0.000000 |
| N | 0.000000 | 3.160200 | 0.000000 |
| C | 0.000000 | 1.990000 | 0.000000 |
| Au | 0.000000 | 0.000000 | 0.000000 |
| Au | 3.251900 | 0.000000 | 0.000000 |
| N | 3.281600 | 2.868300 | 1.072700 |
| N | 3.281600 | 2.868300 | -1.072700 |
| C | 3.279600 | 2.044200 | 0.000000 |
| C | 3.277300 | 4.185000 | -0.677800 |
| H | 3.277100 | 4.998300 | -1.387100 |
| C | 3.277300 | 4.185000 | 0.677800 |
| H | 3.277100 | 4.998300 | 1.387100 |
| C | 3.183900 | 2.452200 | 2.460400 |
| H | 3.248000 | 1.364200 | 2.498400 |
| H | 4.009000 | 2.880900 | 3.035800 |
| C | 3.183900 | 2.452200 | -2.460400 |
| H | 3.248000 | 1.364200 | -2.498400 |
| H | 2.223400 | 2.780700 | -2.871500 |
| H | 2.223400 | 2.780700 | 2.871500 |
| H | 4.009000 | 2.880900 | -3.035800 |
| N | 3.281600 | -2.868300 | -1.072700 |
| N | 3.281600 | -2.868300 | 1.072700 |
| C | 3.279600 | -2.044200 | 0.000000 |
| C | 3.277300 | -4.185000 | 0.677800 |
| H | 3.277100 | -4.998300 | 1.387100 |
| C | 3.277300 | -4.185000 | -0.677800 |
| H | 3.277100 | -4.998300 | -1.387100 |
| C | 3.183900 | -2.452200 | -2.460400 |
| H | 3.248000 | -1.364200 | -2.498400 |
| H | 4.009000 | -2.880900 | -3.035800 |
| C | 3.183900 | -2.452200 | 2.460400 |
| H | 3.248000 | -1.364200 | 2.498400 |
| H | 2.223400 | -2.780700 | 2.871500 |
| H | 2.223400 | -2.780700 | -2.871500 |
| H | 4.009000 | -2.880900 | 3.035800 |
| O | 0.000000 | -3.844500 | -2.832900 |
| H | 0.000000 | -3.724900 | -1.864700 |
| C | 0.000000 | -5.225600 | -3.107800 |
| H | -0.889600 | -5.735700 | -2.707700 |
| H | 0.889600 | -5.735700 | -2.707700 |
| H | 0.000000 | -5.345700 | -4.194300 |
| O | 0.000000 | 3.844500 | 2.832900 |
| H | 0.000000 | 3.724900 | 1.864700 |
| C | 0.000000 | 5.225600 | 3.107800 |
| H | 0.889600 | 5.735700 | 2.707700 |
| H | -0.889600 | 5.735700 | 2.707700 |
| H | 0.000000 | 5.345700 | 4.194300 |
| C | 0.000000 | 5.225600 | -3.107800 |
| O | 0.000000 | 3.844500 | -2.832900 |
| H | 0.889600 | 5.735700 | -2.707700 |
| H | -0.889600 | 5.735700 | -2.707700 |
| H | 0.000000 | 3.724900 | -1.864700 |
| H | 0.000000 | 5.345700 | -4.194300 |
| C | 0.000000 | -5.225600 | 3.107800 |
| O | 0.000000 | -3.844500 | 2.832900 |
| H | 0.889600 | -5.735700 | 2.707700 |
| H | -0.889600 | -5.735700 | 2.707700 |
| H | 0.000000 | -3.724900 | 1.864700 |
| H | 0.000000 | -5.345700 | 4.194300 |

I-S2

| | | | |
|---|---|---|---|
| N | -0.000200 | -3.317400 | -1.472900 |
| C | -0.000100 | -2.314700 | -0.872100 |
| N | 0.000100 | 2.392700 | 1.198700 |
| C | 0.000000 | 1.276800 | 0.852900 |
| Au | -0.000100 | -0.550600 | 0.055900 |
| Au | 3.486600 | -0.257000 | 0.009600 |
| N | 2.988800 | 2.671300 | -0.736400 |
| N | 4.296700 | 2.533800 | 0.955700 |
| C | 3.609300 | 1.779900 | 0.066100 |
| C | 4.097400 | 3.875600 | 0.719200 |
| C | 3.269100 | 3.960700 | -0.350500 |
| C | 2.148400 | 2.341500 | -1.872600 |
| C | 5.094000 | 2.017100 | 2.050600 |
| N | 3.357600 | -3.122500 | 1.063000 |
| N | 3.333900 | -3.116200 | -1.080700 |
| C | 3.397000 | -2.296900 | -0.009000 |
| C | 3.238000 | -4.430100 | -0.689600 |
| C | 3.261000 | -4.436900 | 0.665500 |
| C | 3.410600 | -2.697700 | 2.447400 |
| C | 3.245700 | -2.683500 | -2.462300 |
| H | 4.549600 | 4.642400 | 1.329200 |
| H | 2.843600 | 4.811700 | -0.858000 |
| H | 1.722000 | 1.348800 | -1.718900 |
| H | 1.345500 | 3.079800 | -1.924900 |
| H | 2.736500 | 2.353400 | -2.795400 |
| H | 5.254900 | 0.950400 | 1.888700 |
| H | 6.060900 | 2.525900 | 2.074800 |
| H | 4.576700 | 2.167900 | 3.002600 |
| H | 3.146000 | -5.236600 | -1.400200 |
| H | 3.215700 | -5.252400 | 1.370900 |
| H | 3.326000 | -1.610700 | 2.479200 |
| H | 2.576100 | -3.136300 | 3.000600 |
| H | 4.355300 | -3.004400 | 2.906000 |
| H | 3.514900 | -1.627600 | -2.512200 |
| H | 3.942500 | -3.262600 | -3.073400 |
| H | 2.220800 | -2.822400 | -2.816500 |
| Au | -3.486600 | -0.256700 | 0.009600 |
| N | -2.988600 | 2.671500 | -0.736200 |
| N | -4.296400 | 2.534100 | 0.955900 |
| C | -3.609100 | 1.780200 | 0.066200 |
| C | -4.096900 | 3.875900 | 0.719500 |
| C | -3.268700 | 3.960900 | -0.350300 |
| C | -2.148300 | 2.341800 | -1.872600 |
| C | -5.093600 | 2.017400 | 2.050800 |
| N | -3.357900 | -3.122300 | 1.062900 |
| N | -3.334200 | -3.115900 | -1.080900 |
| C | -3.397300 | -2.296700 | -0.009100 |
| C | -3.238400 | -4.429900 | -0.689800 |
| C | -3.261500 | -4.436800 | 0.665300 |
| C | -3.410900 | -2.697600 | 2.447200 |
| C | -3.245900 | -2.683100 | -2.462400 |

| | | | |
|---|---|---|---|
| H | -4.549000 | 4.642700 | 1.329500 |
| H | -2.843200 | 4.812000 | -0.857700 |
| H | -1.721900 | 1.348900 | -1.718900 |
| H | -2.736400 | 2.353700 | -2.795300 |
| H | -1.345300 | 3.079900 | -1.924900 |
| H | -5.254700 | 0.950700 | 1.888800 |
| H | -4.576300 | 2.168100 | 3.002800 |
| H | -6.060500 | 2.526400 | 2.075100 |
| H | -3.146500 | -5.236300 | -1.400500 |
| H | -3.216200 | -5.252200 | 1.370600 |
| H | -3.326200 | -1.610600 | 2.479100 |
| H | -4.355600 | -3.004200 | 2.905900 |
| H | -2.576400 | -3.136200 | 3.000400 |
| H | -3.515100 | -1.627200 | -2.512300 |
| H | -2.221100 | -2.822000 | -2.816600 |
| H | -3.942700 | -3.262100 | -3.073600 |
| C | 0.000300 | 5.851200 | -0.052700 |
| C | 0.000400 | 6.883900 | -1.159300 |
| O | 0.000200 | 4.561200 | -0.632700 |
| H | 0.884200 | 5.988400 | 0.590400 |
| H | -0.883600 | 5.988600 | 0.590400 |
| H | -0.884100 | 6.772100 | -1.796300 |
| H | 0.000500 | 7.897600 | -0.746000 |
| H | 0.884800 | 6.771900 | -1.796300 |
| H | 0.000200 | 3.898400 | 0.092400 |

I-2S2

| | | | |
|---|---|---|---|
| Au | 3.446300 | 0.206800 | -0.001700 |
| N | 2.813200 | 3.161200 | -0.513900 |
| N | 3.793700 | 2.912200 | 1.375900 |
| C | 3.347700 | 2.224400 | 0.299200 |
| C | 3.531400 | 4.256600 | 1.241700 |
| C | 2.910500 | 4.412200 | 0.046800 |
| C | 2.196000 | 2.910000 | -1.803400 |
| C | 4.413700 | 2.323300 | 2.546600 |
| N | 3.183400 | -2.800800 | 0.513600 |
| N | 4.153400 | -2.437200 | -1.363000 |
| C | 3.608100 | -1.807200 | -0.296800 |
| C | 4.059900 | -3.803600 | -1.225500 |
| C | 3.445500 | -4.031700 | -0.038800 |
| C | 2.523900 | -2.624600 | 1.794600 |
| C | 4.714800 | -1.778900 | -2.526300 |
| H | 3.795400 | 4.974800 | 2.002600 |
| H | 2.516800 | 5.288100 | -0.443800 |
| H | 1.863100 | 1.871200 | -1.836400 |
| H | 1.334700 | 3.574600 | -1.906000 |
| H | 2.912200 | 3.092500 | -2.610400 |
| H | 4.627600 | 1.274900 | 2.334300 |
| H | 5.348500 | 2.842900 | 2.772600 |
| H | 3.739400 | 2.390000 | 3.405000 |
| H | 4.424300 | -4.485600 | -1.978200 |
| H | 3.159200 | -4.948600 | 0.451400 |
| H | 2.063600 | -1.635500 | 1.819300 |
| H | 1.750800 | -3.391000 | 1.890000 |
| H | 3.247900 | -2.713800 | 2.610400 |
| H | 4.798700 | -0.712200 | -2.313600 |
| H | 5.708300 | -2.182800 | -2.737600 |
| H | 4.066100 | -1.926400 | -3.394300 |
| Au | -3.445900 | -0.206500 | 0.001500 |
| N | -3.183600 | 2.801200 | -0.513900 |
| N | -4.153300 | 2.437500 | 1.362800 |
| C | -3.607900 | 1.807600 | 0.296600 |
| C | -4.060100 | 3.803900 | 1.225300 |
| C | -3.445800 | 4.032000 | 0.038500 |
| C | -2.524100 | 2.625200 | -1.794900 |
| C | -4.714400 | 1.779000 | 2.526200 |
| N | -2.813400 | -3.161000 | 0.514000 |
| N | -3.793300 | -2.911800 | -1.376100 |
| C | -3.347400 | -2.224100 | -0.299300 |
| C | -3.531200 | -4.256300 | -1.241900 |
| C | -2.910700 | -4.412000 | -0.046700 |
| C | -2.196500 | -2.909900 | 1.803700 |
| C | -4.412600 | -2.322800 | -2.547000 |
| H | -4.424500 | 4.485900 | 1.978000 |
| H | -3.159800 | 4.949000 | -0.451700 |
| H | -2.064100 | 1.635800 | -1.819900 |
| H | -3.247900 | 2.714900 | -2.610700 |
| H | -1.750600 | 3.391300 | -1.890000 |
| H | -4.798400 | 0.712400 | 2.313400 |
| H | -4.065400 | 1.926500 | 3.394000 |
| H | -5.707800 | 2.183000 | 2.737800 |
| H | -3.795100 | -4.974400 | -2.002900 |
| H | -2.517400 | -5.288000 | 0.444000 |
| H | -1.863800 | -1.871100 | 1.837000 |
| H | -2.912800 | -3.092700 | 2.610400 |
| H | -1.335100 | -3.574400 | 1.906300 |
| H | -4.627400 | -1.274600 | -2.334500 |
| H | -3.737500 | -2.388700 | -3.404900 |
| H | -5.346900 | -2.842900 | -2.774100 |
| N | 0.179700 | -2.927400 | -1.175100 |
| C | 0.112400 | -1.827400 | -0.787800 |
| Au | -0.000100 | -0.000600 | -0.000300 |
| N | -0.179700 | 2.926200 | 1.174800 |
| C | -0.112500 | 1.826200 | 0.787300 |
| C | 0.493600 | -7.227200 | 1.531900 |
| C | 0.395700 | -6.308600 | 0.333200 |
| O | 0.305200 | -4.973200 | 0.789700 |
| H | 0.562700 | -8.273000 | 1.216100 |
| H | 1.378800 | -6.988200 | 2.131200 |
| H | -0.386000 | -7.118200 | 2.175300 |
| H | 1.275900 | -6.441400 | -0.316400 |
| H | -0.484200 | -6.575500 | -0.274600 |
| H | 0.265000 | -4.376800 | 0.011700 |
| C | -0.396300 | 6.308200 | -0.330900 |
| C | -0.495900 | 7.227800 | -1.528700 |
| O | -0.305800 | 4.973300 | -0.788700 |
| H | 0.484100 | 6.574900 | 0.276200 |
| H | -1.275900 | 6.440000 | 0.319700 |
| H | -1.381700 | 6.989000 | -2.127300 |
| H | -0.565100 | 8.273400 | -1.211900 |
| H | 0.383000 | 7.119800 | -2.173300 |
| H | -0.265300 | 4.376200 | -0.011200 |

I-3S2

| | | | |
|---|---|---|---|
| Au | -0.334500 | 3.336000 | -0.025200 |
| N | -3.254700 | 2.795800 | -0.780700 |
| N | -3.045200 | 2.988700 | 1.345800 |
| C | -2.341300 | 3.018000 | 0.191700 |
| C | -4.375700 | 2.743400 | 1.100800 |
| H | -5.104800 | 2.679500 | 1.893800 |
| C | -4.507800 | 2.622400 | -0.243100 |
| H | -5.375600 | 2.433400 | -0.856100 |
| C | -2.963600 | 2.639200 | -2.194200 |
| H | -1.886300 | 2.735100 | -2.336600 |
| H | -3.285400 | 1.645200 | -2.521200 |
| C | -2.479800 | 3.075700 | 2.680700 |
| H | -1.439300 | 3.392300 | 2.594300 |
| H | -3.031700 | 3.814900 | 3.267500 |
| H | -3.477800 | 3.411900 | -2.773000 |
| H | -2.534000 | 2.092300 | 3.159400 |
| N | 2.664600 | 3.313500 | 0.575000 |
| N | 2.271600 | 4.379700 | -1.242200 |
| C | 1.661100 | 3.709500 | -0.237600 |
| C | 3.636800 | 4.390700 | -1.065400 |
| H | 4.306000 | 4.860900 | -1.769400 |
| C | 3.883700 | 3.715000 | 0.083800 |
| H | 4.807100 | 3.465200 | 0.581700 |
| C | 2.503900 | 2.565300 | 1.808100 |
| H | 1.606100 | 1.949200 | 1.731200 |
| H | 3.379400 | 1.924100 | 1.934500 |
| C | 1.600700 | 4.960800 | -2.388400 |
| H | 0.528500 | 4.982200 | -2.188600 |
| H | 1.956500 | 5.982100 | -2.545900 |
| H | 2.409800 | 3.247800 | 2.658300 |
| H | 1.792900 | 4.363100 | -3.284000 |
| N | 3.370400 | 0.400800 | -1.184600 |
| C | 2.221900 | 0.262000 | -1.027100 |
| N | -2.738800 | -0.335000 | 0.222100 |
| C | -1.618300 | -0.199700 | -0.085800 |
| Au | 0.292200 | 0.030100 | -0.590300 |
| Au | 0.601900 | -3.295000 | 0.036500 |
| N | -2.299700 | -3.514800 | -0.910900 |
| N | -2.201300 | -3.577500 | 1.231300 |
| C | -1.431000 | -3.475500 | 0.124700 |
| C | -3.530900 | -3.670500 | 0.893700 |
| H | -4.309100 | -3.753700 | 1.636700 |
| C | -3.592700 | -3.631600 | -0.460400 |
| H | -4.433400 | -3.673100 | -1.135200 |
| C | -1.954200 | -3.372800 | -2.313900 |
| H | -0.904500 | -3.084100 | -2.384000 |
| H | -2.108900 | -4.319100 | -2.840800 |
| C | -1.726400 | -3.467900 | 2.599300 |
| H | -0.638500 | -3.549100 | 2.594000 |
| H | -2.025700 | -2.499500 | 3.014800 |
| H | -2.579900 | -2.588700 | -2.749800 |
| H | -2.142800 | -4.281400 | 3.199400 |
| N | 3.462300 | -2.479900 | 0.761000 |
| N | 3.452100 | -3.720200 | -0.986800 |
| C | 2.637300 | -3.165800 | -0.059500 |
| C | 4.764600 | -3.375200 | -0.755400 |
| H | 5.569000 | -3.704300 | -1.394900 |
| C | 4.769200 | -2.589900 | 0.349700 |
| H | 5.571900 | -2.087000 | 0.865400 |
| C | 3.051300 | -1.721800 | 1.928200 |
| H | 2.024100 | -1.382600 | 1.782900 |
| H | 3.109700 | -2.344000 | 2.826500 |
| C | 3.014200 | -4.521600 | -2.112800 |
| H | 1.969200 | -4.794100 | -1.958900 |
| H | 3.109700 | -3.953700 | -3.042600 |
| H | 3.713300 | -0.857900 | 2.024100 |
| H | 3.616800 | -5.431400 | -2.175300 |
| O | 5.171600 | 0.711000 | 0.975700 |
| H | 4.670200 | 0.612900 | 0.137300 |
| C | 6.543700 | 0.870900 | 0.667500 |
| H | 6.700300 | 1.756800 | 0.031400 |
| H | 6.919000 | 0.005100 | 0.098800 |
| C | 7.318800 | 1.017700 | 1.958900 |
| H | 7.188700 | 0.132900 | 2.591200 |
| H | 8.387500 | 1.143800 | 1.758200 |
| H | 6.968800 | 1.888700 | 2.523200 |
| O | -4.158100 | -0.748900 | -2.281400 |
| H | -3.812900 | -0.642500 | -1.374700 |
| C | -5.568900 | -0.814100 | -2.230400 |
| H | -5.902700 | -1.652900 | -1.597300 |
| H | -5.989700 | 0.102200 | -1.784100 |
| C | -6.096100 | -0.988400 | -3.637700 |
| H | -7.189600 | -1.041300 | -3.639900 |
| H | -5.787600 | -0.149400 | -4.269700 |
| H | -5.704400 | -1.908600 | -4.083600 |
| C | -4.515800 | -0.529800 | 3.450000 |
| O | -3.172700 | -0.293200 | 3.080000 |
| H | -4.861800 | -1.506300 | 3.071700 |
| H | -5.184100 | 0.230800 | 3.013400 |
| H | -3.116000 | -0.303900 | 2.104400 |
| C | -4.616400 | -0.499700 | 4.959300 |
| H | -4.298600 | 0.473900 | 5.347000 |
| H | -5.645600 | -0.682400 | 5.284700 |
| H | -3.971600 | -1.265400 | 5.402800 |

I-4S2

| | | | |
|---|---|---|---|
| C | 4.185000 | 3.265400 | 0.677800 |
| C | 2.451800 | 3.180100 | 2.460200 |
| C | 2.451800 | 3.180100 | -2.460200 |
| N | -2.868300 | 3.275500 | -1.072700 |
| N | -2.868300 | 3.275500 | 1.072700 |
| C | -2.044200 | 3.276800 | 0.000000 |
| C | -4.185000 | 3.265400 | 0.677800 |
| C | -4.185000 | 3.265400 | -0.677800 |
| C | -2.451800 | 3.180100 | -2.460200 |
| C | -2.451800 | 3.180100 | 2.460200 |
| Au | 0.000000 | 3.251800 | 0.000000 |
| N | 2.868300 | 3.275500 | 1.072700 |
| N | 2.868300 | 3.275500 | -1.072700 |
| C | 2.044200 | 3.276800 | 0.000000 |
| C | 4.185000 | 3.265400 | -0.677800 |
| H | 4.998300 | 3.259900 | 1.387100 |
| H | 1.363700 | 3.243000 | 2.497600 |
| H | 2.781400 | 2.220800 | 2.873200 |

| | | | |
|---|---|---|---|
| H | 2.879100 | 4.007000 | 3.034200 |
| H | 1.363700 | 3.243000 | -2.497600 |
| H | 2.879100 | 4.007000 | -3.034200 |
| H | 2.781400 | 2.220800 | -2.873200 |
| H | -4.998300 | 3.259900 | 1.387100 |
| H | -4.998300 | 3.259900 | -1.387100 |
| H | -1.363700 | 3.243000 | -2.497600 |
| H | -2.781400 | 2.220800 | -2.873200 |
| H | -2.879100 | 4.007000 | -3.034200 |
| H | -1.363700 | 3.243000 | 2.497600 |
| H | -2.879100 | 4.007000 | 3.034200 |
| H | -2.781400 | 2.220800 | 2.873200 |
| H | 4.998300 | 3.259900 | -1.387100 |
| N | -3.160300 | 0.000000 | 0.000000 |
| C | -1.990200 | 0.000000 | 0.000000 |
| N | 3.160300 | 0.000000 | 0.000000 |
| C | 1.990200 | 0.000000 | 0.000000 |
| Au | 0.000000 | 0.000000 | 0.000000 |
| Au | 0.000000 | -3.251800 | 0.000000 |
| N | 2.868300 | -3.275500 | 1.072700 |
| N | 2.868300 | -3.275500 | -1.072700 |
| C | 2.044200 | -3.276800 | 0.000000 |
| C | 4.185000 | -3.265400 | -0.677800 |
| C | 4.185000 | -3.265400 | 0.677800 |
| C | 2.451800 | -3.180100 | 2.460200 |
| C | 2.451800 | -3.180100 | -2.460200 |
| N | -2.868300 | -3.275500 | -1.072700 |
| N | -2.868300 | -3.275500 | 1.072700 |
| C | -2.044200 | -3.276800 | 0.000000 |
| C | -4.185000 | -3.265400 | 0.677800 |
| C | -4.185000 | -3.265400 | -0.677800 |
| C | -2.451800 | -3.180100 | -2.460200 |
| C | -2.451800 | -3.180100 | 2.460200 |
| H | 4.998300 | -3.259900 | -1.387100 |
| H | 4.998300 | -3.259900 | 1.387100 |
| H | 1.363700 | -3.243000 | 2.497600 |
| H | 2.879100 | -4.007000 | 3.034200 |
| H | 2.781400 | -2.220800 | 2.873200 |
| H | 1.363700 | -3.243000 | -2.497600 |
| H | 2.781400 | -2.220800 | -2.873200 |
| H | 2.879100 | -4.007000 | -3.034200 |
| H | -4.998300 | -3.259900 | 1.387100 |
| H | -4.998300 | -3.259900 | -1.387100 |
| H | -1.363700 | -3.243000 | -2.497600 |
| H | -2.879100 | -4.007000 | -3.034200 |
| H | -2.781400 | -2.220800 | -2.873200 |
| H | -1.363700 | -3.243000 | 2.497600 |
| H | -2.781400 | -2.220800 | 2.873200 |
| H | -2.879100 | -4.007000 | 3.034200 |
| O | -3.851600 | 0.000000 | 2.837700 |
| C | -5.424300 | 0.000000 | 4.621800 |
| C | -5.237100 | 0.000000 | 3.120700 |
| H | -3.733100 | 0.000000 | 1.869200 |
| H | -6.487900 | 0.000000 | 4.881100 |
| H | -4.959200 | -0.885600 | 5.067000 |
| H | -4.959200 | 0.885600 | 5.067000 |
| H | -5.727500 | -0.884200 | 2.681200 |
| H | -5.727500 | 0.884200 | 2.681200 |
| C | -5.424300 | 0.000000 | -4.621800 |
| O | -3.851600 | 0.000000 | -2.837700 |
| C | -5.237100 | 0.000000 | -3.120700 |
| H | -4.959200 | -0.885600 | -5.067000 |
| H | -6.487900 | 0.000000 | -4.881100 |
| H | -4.959200 | 0.885600 | -5.067000 |
| H | -3.733100 | 0.000000 | -1.869200 |
| H | -5.727500 | 0.884200 | -2.681200 |
| H | -5.727500 | -0.884200 | -2.681200 |
| C | 5.237100 | 0.000000 | -3.120700 |
| O | 3.851600 | 0.000000 | -2.837700 |
| C | 5.424300 | 0.000000 | -4.621800 |
| H | 5.727500 | -0.884200 | -2.681200 |
| H | 5.727500 | 0.884200 | -2.681200 |
| H | 3.733100 | 0.000000 | -1.869200 |
| H | 4.959200 | 0.885600 | -5.067000 |
| H | 6.487900 | 0.000000 | -4.881100 |
| H | 4.959200 | -0.885600 | -5.067000 |
| O | 3.851600 | 0.000000 | 2.837700 |
| C | 5.237100 | 0.000000 | 3.120700 |
| C | 5.424300 | 0.000000 | 4.621800 |
| H | 3.733100 | 0.000000 | 1.869200 |
| H | 5.727500 | 0.884200 | 2.681200 |
| H | 5.727500 | -0.884200 | 2.681200 |
| H | 6.487900 | 0.000000 | 4.881100 |
| H | 4.959200 | 0.885600 | 5.067000 |
| H | 4.959200 | -0.885600 | 5.067000 |

## 17. The $S_0$ .xyz files of II and its complexes

II

| | | | |
|---|---|---|---|
| Au | 0.003100 | -0.207200 | 0.009400 |
| N | 0.026700 | -0.287900 | 3.056500 |
| N | 2.041400 | -0.095600 | 2.274100 |
| C | 0.742300 | -0.174200 | 1.912300 |
| C | 0.867900 | -0.284700 | 4.156900 |
| C | 0.618300 | -0.365000 | 5.524200 |
| H | -0.389600 | -0.444100 | 5.919100 |
| C | 1.724500 | -0.333400 | 6.364200 |
| H | 1.576600 | -0.390600 | 7.438200 |
| C | 3.029500 | -0.227100 | 5.857200 |
| H | 3.866100 | -0.207800 | 6.548800 |
| C | 3.276500 | -0.144600 | 4.492700 |
| H | 4.287000 | -0.067600 | 4.105000 |
| C | 2.167200 | -0.170700 | 3.651800 |
| C | 3.165300 | -0.023200 | 1.360900 |
| H | 2.796800 | 0.308600 | 0.389200 |
| H | 3.628400 | -1.008500 | 1.251800 |
| H | 3.888000 | 0.706600 | 1.735200 |
| C | -1.412800 | -0.405300 | 3.140000 |
| H | -1.814800 | -0.497500 | 2.130400 |
| H | -1.840300 | 0.476400 | 3.627600 |
| H | -1.679600 | -1.301400 | 3.707900 |
| N | -0.020300 | -0.351400 | -3.035300 |
| N | -2.035600 | -0.149600 | -2.256900 |
| C | -0.736200 | -0.216300 | -1.893600 |
| C | -0.861500 | -0.374000 | -4.135500 |
| C | -0.611600 | -0.481900 | -5.500900 |
| H | 0.396600 | -0.565700 | -5.894100 |
| C | -1.717800 | -0.471600 | -6.341200 |
| H | -1.569800 | -0.550600 | -7.413800 |
| C | -3.023300 | -0.359100 | -5.836400 |
| H | -3.859900 | -0.357000 | -6.528200 |
| C | -3.270500 | -0.249000 | -4.473900 |
| H | -4.281300 | -0.167400 | -4.087800 |
| C | -2.161100 | -0.253800 | -3.632700 |
| C | -3.159700 | -0.062000 | -1.345300 |
| H | -2.792300 | 0.291200 | -0.380800 |
| H | -3.884800 | 0.657300 | -1.734800 |
| H | -3.619500 | -1.046400 | -1.215700 |
| C | 1.419600 | -0.465700 | -3.116400 |
| H | 1.821900 | -0.535200 | -2.105100 |
| H | 1.689500 | -1.372500 | -3.665400 |
| H | 1.844100 | 0.407000 | -3.622500 |
| N | -3.128300 | -3.370400 | -0.376800 |
| C | -1.971600 | -3.365400 | -0.209100 |
| N | 3.145000 | -3.351200 | 0.462100 |
| C | 1.988300 | -3.353500 | 0.294300 |
| Au | 0.008300 | -3.358600 | 0.042600 |
| Au | 0.013600 | -6.507500 | 0.075500 |
| N | -0.000600 | -6.359800 | 3.120000 |
| N | 2.024000 | -6.564600 | 2.366700 |
| C | 0.729100 | -6.497300 | 1.987500 |
| C | 0.827100 | -6.336500 | 4.230400 |
| C | 0.560500 | -6.226500 | 5.592500 |
| H | -0.452400 | -6.141400 | 5.973100 |
| C | 1.656300 | -6.236500 | 6.446400 |
| H | 1.495100 | -6.156000 | 7.516900 |
| C | 2.967800 | -6.350800 | 5.957800 |
| H | 3.795800 | -6.352600 | 6.659900 |
| C | 3.231700 | -6.463000 | 4.598600 |
| H | 4.247000 | -6.546100 | 4.225200 |
| C | 2.132700 | -6.458500 | 3.743800 |
| C | 3.158800 | -6.654500 | 1.468600 |
| H | 2.803400 | -7.013500 | 0.501800 |
| H | 3.880600 | -7.370500 | 1.870200 |
| H | 3.618500 | -5.670100 | 1.339200 |
| C | -1.441400 | -6.243900 | 3.183100 |
| H | -1.830900 | -6.172300 | 2.167000 |
| H | -1.716900 | -5.337300 | 3.729800 |
| H | -1.873300 | -7.116700 | 3.682700 |
| N | 0.027500 | -6.424200 | -2.971600 |
| N | -1.996500 | -6.619600 | -2.214000 |
| C | -0.701800 | -6.540100 | -1.836300 |
| C | -0.800300 | -6.427100 | -4.082100 |
| C | -0.534000 | -6.345000 | -5.446200 |
| H | 0.478600 | -6.264700 | -5.828700 |
| C | -1.629800 | -6.376700 | -6.299600 |
| H | -1.468900 | -6.318300 | -7.371700 |
| C | -2.940900 | -6.484900 | -5.808700 |
| H | -3.768900 | -6.504300 | -6.510500 |
| C | -3.204400 | -6.569200 | -4.447400 |
| H | -4.219500 | -6.647700 | -4.072200 |
| C | -2.105500 | -6.543000 | -3.593000 |
| C | -3.131000 | -6.694200 | -1.314100 |
| H | -2.774400 | -7.031600 | -0.339900 |
| H | -3.593900 | -5.708800 | -1.205300 |
| H | -3.850500 | -7.420800 | -1.700400 |
| C | 1.467800 | -6.304900 | -3.037200 |
| H | 1.857100 | -6.210600 | -2.022800 |
| H | 1.902600 | -7.186700 | -3.518200 |
| H | 1.740500 | -5.409300 | -3.602900 |

II-S1

97
Molecule Name

| | | | |
|---|---|---|---|
| Au | -0.304500 | 3.395200 | -0.068800 |
| N | 2.615700 | 3.682500 | 0.785600 |
| N | 2.426800 | 3.733300 | -1.373600 |
| C | 1.722100 | 3.606800 | -0.223000 |
| C | 3.777100 | 3.881000 | -1.102500 |
| C | 2.315300 | 3.569500 | 2.197400 |
| H | 1.245000 | 3.391700 | 2.308800 |
| H | 2.857700 | 2.717100 | 2.613200 |
| C | 1.872100 | 3.721900 | -2.708500 |
| H | 0.788000 | 3.626200 | -2.633000 |
| H | 2.115100 | 4.655400 | -3.225300 |
| H | 2.591500 | 4.495000 | 2.712100 |
| H | 2.273100 | 2.877100 | -3.277100 |
| N | -3.201200 | 2.919300 | -0.910100 |
| N | -3.099600 | 3.777000 | 1.079200 |
| C | -2.343400 | 3.333500 | 0.046500 |
| C | -4.446700 | 3.647500 | 0.785100 |
| C | -2.839000 | 2.333500 | -2.185300 |
| H | -1.773700 | 2.100100 | -2.167300 |
| H | -3.409400 | 1.411000 | -2.334500 |
| C | -2.597800 | 4.298700 | 2.331100 |
| H | -1.508800 | 4.333600 | 2.281100 |
| H | -2.982800 | 5.309300 | 2.497900 |
| H | -3.048500 | 3.038700 | -2.996500 |
| H | -2.901800 | 3.650600 | 3.158600 |
| C | 3.898200 | 3.841600 | 0.289200 |

| | | | |
|---|---|---|---|
| C | 5.134200 | 3.959100 | 0.918000 |
| C | 4.884300 | 4.046300 | -1.930100 |
| C | 6.240400 | 4.123900 | 0.094800 |
| H | 5.232400 | 3.916000 | 1.997600 |
| C | 6.118000 | 4.168800 | -1.303500 |
| H | 4.793200 | 4.080400 | -3.011100 |
| H | 7.224600 | 4.219200 | 0.542800 |
| H | 7.009200 | 4.301400 | -1.909000 |
| C | -4.510600 | 3.096700 | -0.497700 |
| C | -5.727300 | 2.842600 | -1.124400 |
| C | -5.596200 | 3.961400 | 1.505300 |
| C | -6.875600 | 3.158600 | -0.409000 |
| H | -5.775800 | 2.413100 | -2.119400 |
| C | -6.811400 | 3.706900 | 0.882500 |
| H | -5.550600 | 4.386100 | 2.503100 |
| H | -7.847000 | 2.979500 | -0.859700 |
| H | -7.733800 | 3.938600 | 1.405900 |
| N | -2.920900 | -0.352000 | 0.110300 |
| C | -1.793500 | -0.214500 | 0.377700 |
| N | 3.178800 | 0.416300 | 1.559900 |
| C | 2.061200 | 0.270700 | 1.251200 |
| Au | 0.138300 | 0.025900 | 0.795900 |
| Au | 0.640400 | -3.362000 | -0.060800 |
| N | 3.507000 | -2.890400 | 0.889300 |
| N | 3.411900 | -3.019900 | -1.272900 |
| C | 2.658900 | -3.058600 | -0.146900 |
| C | 4.745400 | -2.816000 | -0.958400 |
| C | 3.137800 | -2.834200 | 2.288100 |
| H | 2.054200 | -2.933300 | 2.362800 |
| H | 3.621900 | -3.649800 | 2.834200 |
| C | 2.918100 | -3.169300 | -2.623400 |
| H | 1.844100 | -3.356300 | -2.581500 |
| H | 3.106400 | -2.257000 | -3.197800 |
| H | 3.431000 | -1.865000 | 2.698200 |
| H | 3.411200 | -4.014900 | -3.112800 |
| N | -2.267300 | -3.547400 | -0.973900 |
| N | -1.994800 | -4.501800 | 0.954400 |
| C | -1.352200 | -3.810300 | -0.017100 |
| C | -3.326400 | -4.683800 | 0.620200 |
| C | -2.028600 | -2.810400 | -2.199100 |
| H | -1.083500 | -2.274800 | -2.101400 |
| H | -1.979600 | -3.498300 | -3.049800 |
| C | -1.403200 | -4.978800 | 2.184900 |
| H | -0.335700 | -4.755400 | 2.166700 |
| H | -1.863900 | -4.480900 | 3.043500 |
| H | -2.837600 | -2.089200 | -2.348800 |
| H | -1.542000 | -6.060600 | 2.272700 |
| C | 4.804400 | -2.726400 | 0.435000 |
| C | 6.007500 | -2.516600 | 1.102700 |
| C | 7.147000 | -2.407600 | 0.316400 |
| H | 6.054200 | -2.433600 | 2.183300 |
| C | 5.886100 | -2.707500 | -1.748900 |
| C | 7.088200 | -2.503300 | -1.083500 |
| H | 8.107200 | -2.242900 | 0.795300 |
| H | 5.843800 | -2.779800 | -2.831100 |
| H | 8.004400 | -2.414500 | -1.659100 |
| C | -3.500500 | -4.070000 | -0.623200 |
| C | -4.731200 | -4.072500 | -1.273600 |
| C | -5.778300 | -4.713600 | -0.623600 |
| H | -4.866700 | -3.586800 | -2.233800 |
| C | -4.375700 | -5.322500 | 1.275600 |
| C | -5.604500 | -5.326700 | 0.628200 |
| H | -6.755900 | -4.742500 | -1.095100 |
| H | -4.244800 | -5.796600 | 2.243100 |
| H | -6.450700 | -5.816000 | 1.100500 |
| O | -4.652200 | -0.581700 | -2.075000 |
| H | -4.182800 | -0.526200 | -1.214600 |
| C | -6.029700 | -0.736200 | -1.820300 |
| H | -6.445100 | 0.102700 | -1.243800 |
| H | -6.542900 | -0.774600 | -2.786600 |
| H | -6.253100 | -1.665000 | -1.275800 |

II-2S1

103

Molecule Name

| | | | |
|---|---|---|---|
| Au | -0.220000 | -3.436200 | -0.001800 |
| N | 2.733300 | -3.393100 | -0.798300 |
| N | 2.458800 | -4.267100 | 1.167700 |
| C | 1.804200 | -3.677000 | 0.138800 |
| C | 3.811700 | -4.364700 | 0.889500 |
| C | 2.493200 | -2.721700 | -2.060400 |
| H | 1.486800 | -2.300900 | -2.043400 |
| H | 3.223100 | -1.914600 | -2.179400 |
| C | 1.857200 | -4.726400 | 2.400300 |
| H | 0.778500 | -4.576300 | 2.337700 |
| H | 2.064400 | -5.791000 | 2.544900 |
| H | 2.582500 | -3.432400 | -2.888700 |
| H | 2.254600 | -4.159000 | 3.247400 |
| N | -3.148100 | -3.062300 | 0.801600 |
| N | -2.977400 | -3.930200 | -1.178800 |
| C | -2.258400 | -3.436100 | -0.142300 |
| C | -4.332300 | -3.876100 | -0.898800 |
| C | -2.832300 | -2.438200 | 2.071300 |
| H | -1.780300 | -2.149300 | 2.064000 |
| H | -3.454600 | -1.545900 | 2.194300 |
| C | -2.433900 | -4.435600 | -2.420200 |
| H | -1.345100 | -4.403300 | -2.361900 |
| H | -2.755300 | -5.469700 | -2.577500 |
| H | -3.016600 | -3.139300 | 2.892100 |
| H | -2.771000 | -3.817200 | -3.257700 |
| C | 3.987300 | -3.802800 | -0.377800 |
| C | 5.237800 | -3.750600 | -0.986700 |
| C | 4.878600 | -4.892700 | 1.611600 |
| C | 6.303100 | -4.282100 | -0.270500 |
| H | 5.373800 | -3.308100 | -1.967500 |
| C | 6.127400 | -4.841600 | 1.005800 |
| H | 4.745800 | -5.326400 | 2.597600 |
| H | 7.296500 | -4.266100 | -0.708400 |
| H | 6.988100 | -5.244800 | 1.530500 |
| C | -4.441100 | -3.318600 | 0.378000 |
| C | -5.676800 | -3.134300 | 0.991600 |
| C | -5.453500 | -4.266200 | -1.626300 |
| C | -6.796700 | -3.527900 | 0.269800 |
| H | -5.760600 | -2.697200 | 1.980700 |
| C | -6.687600 | -4.082300 | -1.016100 |
| H | -5.372300 | -4.696400 | -2.619400 |
| H | -7.781300 | -3.405900 | 0.711000 |
| H | -7.589300 | -4.375500 | -1.544700 |
| N | -3.116400 | 0.169700 | -0.484700 |
| C | -1.958600 | 0.107400 | -0.346400 |
| N | 3.116200 | -0.169400 | 0.483500 |
| C | 1.958500 | -0.107100 | 0.345100 |
| Au | -0.000100 | 0.000200 | -0.000700 |
| Au | 0.220300 | 3.436300 | 0.002400 |
| N | 3.148200 | 3.063500 | -0.802000 |
| N | 2.978000 | 3.929500 | 1.179300 |
| C | 2.258800 | 3.436400 | 0.142500 |

| | | | |
|---|---|---|---|
| C | 4.332800 | 3.875800 | 0.898900 |
| C | 2.832200 | 2.440300 | -2.072100 |
| H | 1.780600 | 2.149600 | -2.064000 |
| H | 3.014400 | 3.142500 | -2.892300 |
| C | 2.434800 | 4.433600 | 2.421400 |
| H | 1.346000 | 4.401500 | 2.363100 |
| H | 2.772000 | 3.814200 | 3.258000 |
| H | 3.455700 | 1.549100 | -2.196600 |
| H | 2.756300 | 5.467500 | 2.579700 |
| N | -2.733000 | 3.391900 | 0.799000 |
| N | -2.458700 | 4.267600 | -1.166300 |
| C | -1.803900 | 3.676800 | -0.137900 |
| C | -3.811600 | 4.364600 | -0.888100 |
| C | -2.492600 | 2.719800 | 2.060700 |
| H | -1.485500 | 2.300500 | 2.043900 |
| H | -2.583400 | 3.429600 | 2.889500 |
| C | -1.857300 | 4.728300 | -2.398400 |
| H | -0.778500 | 4.578400 | -2.336000 |
| H | -2.254500 | 4.161800 | -3.246100 |
| H | -3.221300 | 1.911600 | 2.178600 |
| H | -2.064600 | 5.793100 | -2.541800 |
| C | 4.441300 | 3.319600 | -0.378500 |
| C | 5.676800 | 3.136000 | -0.992600 |
| C | 6.797000 | 3.528800 | -0.270800 |
| H | 5.760500 | 2.699900 | -1.982200 |
| C | 5.454200 | 4.265300 | 1.626400 |
| C | 6.688200 | 4.081900 | 1.015700 |
| H | 7.781400 | 3.407200 | -0.712400 |
| H | 5.373300 | 4.694500 | 2.619900 |
| H | 7.590000 | 4.374600 | 1.544400 |
| C | -3.987000 | 3.801400 | 0.378800 |
| C | -5.237600 | 3.748100 | 0.987500 |
| C | -6.303000 | 4.279900 | 0.271700 |
| H | -5.373500 | 3.304400 | 1.967800 |
| C | -4.878700 | 4.892800 | -1.609700 |
| C | -6.127500 | 4.840700 | -1.004000 |
| H | -7.296500 | 4.263000 | 0.709600 |
| H | -4.746000 | 5.327400 | -2.595300 |
| H | -6.988300 | 5.244100 | -1.528400 |
| O | -4.901700 | 0.287200 | 1.707100 |
| H | -4.439300 | 0.256900 | 0.843800 |
| C | -6.289100 | 0.361400 | 1.466200 |
| H | -6.662400 | -0.508300 | 0.907700 |
| H | -6.791200 | 0.385500 | 2.438700 |
| H | -6.568600 | 1.268600 | 0.912200 |
| O | 4.898300 | -0.285900 | -1.709900 |
| H | 4.436200 | -0.255700 | -0.846300 |
| C | 6.285700 | -0.361700 | -1.469600 |
| H | 6.787300 | -0.387200 | -2.442300 |
| H | 6.660400 | 0.508000 | -0.912000 |
| H | 6.564300 | -1.268700 | -0.915000 |

II-3S1

109

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.005900 | 0.089300 | 3.329300 |
| N | -0.975600 | -2.799300 | 3.297900 |
| N | 1.192700 | -2.715700 | 3.344600 |
| C | 0.078300 | -1.952000 | 3.284900 |
| C | 0.856700 | -4.057000 | 3.397300 |
| C | -2.366900 | -2.427200 | 3.137600 |
| H | -2.427100 | -1.340400 | 3.063400 |
| H | -2.759000 | -2.875600 | 2.217700 |
| C | 2.555700 | -2.234100 | 3.239700 |
| H | 2.543200 | -1.145500 | 3.312400 |
| H | 3.156300 | -2.639600 | 4.059200 |
| H | -2.948800 | -2.765900 | 4.000500 |
| H | 2.974600 | -2.537100 | 2.273300 |
| N | 0.865600 | 3.021000 | 3.186600 |
| N | -1.006500 | 2.801800 | 4.259200 |
| C | -0.053400 | 2.115600 | 3.583500 |
| C | -0.698800 | 4.151400 | 4.295500 |
| C | 2.060500 | 2.739400 | 2.416100 |
| H | 1.977500 | 1.733200 | 2.002700 |
| H | 2.136500 | 3.464300 | 1.599800 |
| C | -2.196800 | 2.234200 | 4.852900 |
| H | -2.160800 | 1.150400 | 4.734800 |
| H | -2.236200 | 2.477800 | 5.918900 |
| H | 2.946200 | 2.803000 | 3.056900 |
| H | -3.089800 | 2.625100 | 4.355800 |
| C | -0.539900 | -4.110500 | 3.368600 |
| C | -1.226400 | -5.320400 | 3.431300 |
| C | 1.630100 | -5.211600 | 3.488100 |
| C | -0.456000 | -6.473500 | 3.519200 |
| H | -2.310700 | -5.362700 | 3.418800 |
| C | 0.947000 | -6.420100 | 3.547200 |
| H | 2.714300 | -5.172200 | 3.519100 |
| H | -0.950300 | -7.438500 | 3.575500 |
| H | 1.510600 | -7.344900 | 3.623800 |
| C | 0.507800 | 4.291700 | 3.604700 |
| C | 1.124400 | 5.530700 | 3.454700 |
| C | -1.349500 | 5.243700 | 4.863400 |
| C | 0.479300 | 6.621000 | 4.024600 |
| H | 2.055100 | 5.639500 | 2.908800 |
| C | -0.735400 | 6.480600 | 4.715800 |
| H | -2.288700 | 5.138800 | 5.396900 |
| H | 0.925300 | 7.606800 | 3.934700 |
| H | -1.205400 | 7.360200 | 5.144800 |
| N | -0.625600 | 3.343300 | 0.000000 |
| C | -0.597600 | 2.176700 | 0.000000 |
| N | 0.014300 | -2.937800 | 0.000000 |
| C | -0.149700 | -1.779400 | 0.000000 |
| Au | -0.404100 | 0.194700 | 0.000000 |
| Au | 0.005900 | 0.089300 | -3.329300 |
| N | -0.975600 | -2.799300 | -3.297900 |
| N | 1.192700 | -2.715700 | -3.344600 |
| C | 0.078300 | -1.952000 | -3.284900 |
| C | 0.856700 | -4.057000 | -3.397300 |
| C | -2.366900 | -2.427200 | -3.137600 |
| H | -2.427100 | -1.340400 | -3.063400 |
| H | -2.948800 | -2.765900 | -4.000500 |
| C | 2.555700 | -2.234100 | -3.239700 |
| H | 2.543200 | -1.145500 | -3.312400 |
| H | 2.974600 | -2.537100 | -2.273300 |
| H | -2.759000 | -2.875600 | -2.217700 |
| H | 3.156300 | -2.639600 | -4.059200 |
| N | 0.865600 | 3.021000 | -3.186600 |
| N | -1.006500 | 2.801800 | -4.259200 |
| C | -0.053400 | 2.115600 | -3.583500 |
| C | -0.698800 | 4.151400 | -4.295500 |
| C | 2.060500 | 2.739400 | -2.416100 |
| H | 1.977500 | 1.733200 | -2.002700 |
| H | 2.946200 | 2.803000 | -3.056900 |
| C | -2.196800 | 2.234200 | -4.852900 |
| H | -2.160800 | 1.150400 | -4.734800 |
| H | -3.089800 | 2.625100 | -4.355800 |
| H | 2.136500 | 3.464300 | -1.599800 |

| | | | |
|---|---|---|---|
| H | -2.236200 | 2.477800 | -5.918900 |
| C | -0.539900 | -4.110500 | -3.368600 |
| C | -1.226400 | -5.320400 | -3.431300 |
| C | -0.456000 | -6.473500 | -3.519200 |
| H | -2.310700 | -5.362700 | -3.418800 |
| C | 1.630100 | -5.211600 | -3.488100 |
| C | 0.947000 | -6.420100 | -3.547200 |
| H | -0.950300 | -7.438500 | -3.575500 |
| H | 2.714300 | -5.172200 | -3.519100 |
| H | 1.510600 | -7.344900 | -3.623800 |
| C | 0.507800 | 4.291700 | -3.604700 |
| C | 1.124400 | 5.530700 | -3.454700 |
| C | 0.479300 | 6.621000 | -4.024600 |
| H | 2.055100 | 5.639500 | -2.908800 |
| C | -1.349500 | 5.243700 | -4.863400 |
| C | -0.735400 | 6.480600 | -4.715800 |
| H | 0.925300 | 7.606800 | -3.934700 |
| H | -2.288700 | 5.138800 | -5.396900 |
| H | -1.205400 | 7.360200 | -5.144800 |
| O | 1.591000 | 5.095000 | 0.000000 |
| H | 0.723500 | 4.638300 | 0.000000 |
| C | 1.357200 | 6.486000 | 0.000000 |
| H | 0.802900 | 6.814200 | 0.890600 |
| H | 2.331800 | 6.984400 | 0.000000 |
| H | 0.802900 | 6.814200 | -0.890600 |
| O | -2.727000 | -3.984500 | 0.000000 |
| H | -1.769800 | -3.799900 | 0.000000 |
| C | -2.912100 | -5.382700 | 0.000000 |
| H | -3.989800 | -5.569200 | 0.000000 |
| H | -2.478100 | -5.862200 | -0.889100 |
| H | -2.478100 | -5.862200 | 0.889100 |
| H | 1.916600 | -3.416200 | 0.000000 |
| O | 2.890800 | -3.473800 | 0.000000 |
| C | 3.249900 | -4.837900 | 0.000000 |
| H | 4.342500 | -4.888600 | 0.000000 |
| H | 2.879200 | -5.368000 | 0.889100 |
| H | 2.879200 | -5.368000 | -0.889100 |

II-4S1

115

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000000 | 3.219900 | 0.000000 |
| N | 2.850200 | 3.334300 | 1.085000 |
| N | 2.850200 | 3.334300 | -1.085000 |
| C | 2.043800 | 3.286700 | 0.000000 |
| C | 4.176700 | 3.409800 | -0.698800 |
| C | 2.428500 | 3.200500 | 2.464700 |
| H | 1.338300 | 3.206800 | 2.494400 |
| H | 2.802100 | 2.253500 | 2.871100 |
| C | 2.428500 | 3.200500 | -2.464700 |
| H | 1.338300 | 3.206800 | -2.494400 |
| H | 2.807700 | 4.041300 | -3.053200 |
| H | 2.807700 | 4.041300 | 3.053200 |
| H | 2.802100 | 2.253500 | -2.871100 |
| N | -2.850200 | 3.334300 | -1.085000 |
| N | -2.850200 | 3.334300 | 1.085000 |
| C | -2.043800 | 3.286700 | 0.000000 |
| C | -4.176700 | 3.409800 | 0.698800 |
| C | -2.428500 | 3.200500 | -2.464700 |
| H | -1.338300 | 3.206800 | -2.494400 |
| H | -2.802100 | 2.253500 | -2.871100 |
| C | -2.428500 | 3.200500 | 2.464700 |
| H | -1.338300 | 3.206800 | 2.494400 |
| H | -2.807700 | 4.041300 | 3.053200 |
| H | -2.807700 | 4.041300 | -3.053200 |
| H | -2.802100 | 2.253500 | 2.871100 |
| C | 4.176700 | 3.409800 | 0.698800 |
| C | 5.359100 | 3.492700 | 1.429700 |
| C | 5.359100 | 3.492700 | -1.429700 |
| C | 6.540100 | 3.572800 | 0.702200 |
| H | 5.360700 | 3.499900 | 2.514900 |
| C | 6.540100 | 3.572800 | -0.702200 |
| H | 5.360700 | 3.499900 | -2.514900 |
| H | 7.485400 | 3.643500 | 1.231500 |
| H | 7.485400 | 3.643500 | -1.231500 |
| C | -4.176700 | 3.409800 | -0.698800 |
| C | -5.359100 | 3.492700 | -1.429700 |
| C | -5.359100 | 3.492700 | 1.429700 |
| C | -6.540100 | 3.572800 | -0.702200 |
| H | -5.360700 | 3.499900 | -2.514900 |
| C | -6.540100 | 3.572800 | 0.702200 |
| H | -5.360700 | 3.499900 | 2.514900 |
| H | -7.485400 | 3.643500 | -1.231500 |
| H | -7.485400 | 3.643500 | 1.231500 |
| N | -3.160000 | 0.000000 | 0.000000 |
| C | -1.990300 | 0.000000 | 0.000000 |
| N | 3.160000 | 0.000000 | 0.000000 |
| C | 1.990300 | 0.000000 | 0.000000 |
| Au | 0.000000 | 0.000000 | 0.000000 |
| Au | 0.000000 | -3.219900 | 0.000000 |
| N | 2.850200 | -3.334300 | 1.085000 |
| N | 2.850200 | -3.334300 | -1.085000 |
| C | 2.043800 | -3.286700 | 0.000000 |
| C | 4.176700 | -3.409800 | -0.698800 |
| C | 2.428500 | -3.200500 | 2.464700 |
| H | 1.338300 | -3.206800 | 2.494400 |
| H | 2.807700 | -4.041300 | 3.053200 |
| C | 2.428500 | -3.200500 | -2.464700 |
| H | 1.338300 | -3.206800 | -2.494400 |
| H | 2.802100 | -2.253500 | -2.871100 |
| H | 2.802100 | -2.253500 | 2.871100 |
| H | 2.807700 | -4.041300 | -3.053200 |
| N | -2.850200 | -3.334300 | -1.085000 |
| N | -2.850200 | -3.334300 | 1.085000 |
| C | -2.043800 | -3.286700 | 0.000000 |
| C | -4.176700 | -3.409800 | 0.698800 |
| C | -2.428500 | -3.200500 | -2.464700 |
| H | -1.338300 | -3.206800 | -2.494400 |
| H | -2.807700 | -4.041300 | -3.053200 |
| C | -2.428500 | -3.200500 | 2.464700 |
| H | -1.338300 | -3.206800 | 2.494400 |
| H | -2.802100 | -2.253500 | 2.871100 |
| H | -2.802100 | -2.253500 | -2.871100 |
| H | -2.807700 | -4.041300 | 3.053200 |
| C | 4.176700 | -3.409800 | 0.698800 |
| C | 5.359100 | -3.492700 | 1.429700 |
| C | 6.540100 | -3.572800 | 0.702200 |
| H | 5.360700 | -3.499900 | 2.514900 |
| C | 5.359100 | -3.492700 | -1.429700 |
| C | 6.540100 | -3.572800 | -0.702200 |
| H | 7.485400 | -3.643500 | 1.231500 |
| H | 5.360700 | -3.499900 | -2.514900 |
| H | 7.485400 | -3.643500 | -1.231500 |
| C | -4.176700 | -3.409800 | -0.698800 |
| C | -5.359100 | -3.492700 | -1.429700 |
| C | -6.540100 | -3.572800 | -0.702200 |
| H | -5.360700 | -3.499900 | -2.514900 |

| | | | |
|---|---|---|---|
| C | -5.359100 | -3.492700 | 1.429700 |
| C | -6.540100 | -3.572800 | 0.702200 |
| H | -7.485400 | -3.643500 | -1.231500 |
| H | -5.360700 | -3.499900 | 2.514900 |
| H | -7.485400 | -3.643500 | 1.231500 |
| O | -3.834500 | 0.000000 | -2.858700 |
| H | -3.744700 | 0.000000 | -1.888000 |
| C | -5.209900 | 0.000000 | -3.171800 |
| H | -5.726800 | 0.889300 | -2.783100 |
| H | -5.297300 | 0.000000 | -4.262000 |
| H | -5.726800 | -0.889300 | -2.783100 |
| O | 3.834500 | 0.000000 | 2.858700 |
| H | 3.744700 | 0.000000 | 1.888000 |
| C | 5.209900 | 0.000000 | 3.171800 |
| H | 5.297300 | 0.000000 | 4.262000 |
| H | 5.726800 | -0.889300 | 2.783100 |
| H | 5.726800 | 0.889300 | 2.783100 |
| H | 3.744700 | 0.000000 | -1.888000 |
| O | 3.834500 | 0.000000 | -2.858700 |
| C | 5.209900 | 0.000000 | -3.171800 |
| H | 5.297300 | 0.000000 | -4.262000 |
| H | 5.726800 | 0.889300 | -2.783100 |
| H | 5.726800 | -0.889300 | -2.783100 |
| H | -3.744700 | 0.000000 | 1.888000 |
| O | -3.834500 | 0.000000 | 2.858700 |
| C | -5.209900 | 0.000000 | 3.171800 |
| H | -5.726800 | -0.889300 | 2.783100 |
| H | -5.297300 | 0.000000 | 4.262000 |
| H | -5.726800 | 0.889300 | 2.783100 |

II-S2

100

Molecule Name

| | | | |
|---|---|---|---|
| Au | -0.620000 | 3.386100 | 0.019800 |
| N | -3.532800 | 3.002600 | -0.824300 |
| N | -3.356500 | 3.146500 | 1.332000 |
| C | -2.643400 | 3.152200 | 0.179600 |
| C | -4.706000 | 2.981300 | 1.066900 |
| C | -3.216300 | 2.924800 | -2.234900 |
| H | -2.134700 | 3.004300 | -2.350600 |
| H | -3.541900 | 1.956900 | -2.623500 |
| C | -2.810100 | 3.291400 | 2.662600 |
| H | -1.735200 | 3.458700 | 2.580000 |
| H | -3.269200 | 4.147900 | 3.165800 |
| H | -3.705800 | 3.743400 | -2.771600 |
| H | -2.993500 | 2.385000 | 3.247900 |
| N | 2.320500 | 3.478000 | 0.834600 |
| N | 2.016100 | 4.434700 | -1.087900 |
| C | 1.383700 | 3.766700 | -0.093500 |
| C | 3.362700 | 4.576200 | -0.797100 |
| C | 2.097800 | 2.752700 | 2.069600 |
| H | 1.134200 | 2.245900 | 2.003300 |
| H | 2.888800 | 2.007500 | 2.197100 |
| C | 1.400300 | 4.926000 | -2.300800 |
| H | 0.328100 | 4.732300 | -2.249300 |
| H | 1.566400 | 6.003400 | -2.395600 |
| H | 2.096100 | 3.444600 | 2.918500 |
| H | 1.820500 | 4.413800 | -3.171700 |
| C | -4.817500 | 2.882400 | -0.322700 |
| C | -6.049500 | 2.704900 | -0.945300 |
| C | -5.820700 | 2.914500 | 1.898200 |
| C | -7.163000 | 2.637500 | -0.118300 |
| H | -6.137200 | 2.614500 | -2.022800 |
| C | -7.051400 | 2.742500 | 1.277600 |
| H | -5.737800 | 2.993600 | 2.977500 |
| H | -8.144300 | 2.498600 | -0.561500 |
| H | -7.948700 | 2.686600 | 1.886200 |
| C | 3.557500 | 3.960600 | 0.442400 |
| C | 4.808100 | 3.927000 | 1.052800 |
| C | 4.409600 | 5.180500 | -1.488100 |
| C | 5.853000 | 4.534100 | 0.367500 |
| H | 4.959600 | 3.440400 | 2.010300 |
| C | 5.658000 | 5.148900 | -0.880200 |
| H | 4.262200 | 5.656000 | -2.452500 |
| H | 6.845700 | 4.533700 | 0.807300 |
| H | 6.503200 | 5.610600 | -1.381200 |
| N | 2.814600 | 0.245600 | -0.252300 |
| C | 1.673700 | 0.143000 | -0.474400 |
| N | -3.355700 | -0.322400 | -1.477100 |
| C | -2.224000 | -0.216000 | -1.206000 |
| Au | -0.279100 | -0.035900 | -0.819300 |
| Au | 0.111900 | -3.422000 | 0.034200 |
| N | -2.834800 | -3.604200 | -0.754500 |
| N | -2.599600 | -3.670300 | 1.399800 |
| C | -1.916900 | -3.563600 | 0.234000 |
| C | -3.959900 | -3.769900 | 1.158700 |
| C | -2.562400 | -3.495200 | -2.172200 |
| H | -1.490200 | -3.347500 | -2.306900 |
| H | -2.876600 | -4.410500 | -2.683400 |
| C | -2.014800 | -3.683500 | 2.721800 |
| H | -0.930200 | -3.622300 | 2.622200 |
| H | -2.375500 | -2.829200 | 3.302900 |
| H | -3.089700 | -2.626600 | -2.573600 |
| H | -2.276200 | -4.611400 | 3.239900 |
| N | 3.043700 | -3.023400 | 0.794200 |
| N | 2.863000 | -3.927000 | -1.169000 |
| C | 2.148500 | -3.431700 | -0.130000 |
| C | 4.220700 | -3.836500 | -0.911400 |
| C | 2.732900 | -2.396600 | 2.063600 |
| H | 1.679500 | -2.113800 | 2.059800 |
| H | 2.925000 | -3.094800 | 2.885100 |
| C | 2.312300 | -4.463100 | -2.394100 |
| H | 1.224600 | -4.465400 | -2.314000 |
| H | 2.612000 | -3.844000 | -3.245200 |
| H | 3.347500 | -1.498500 | 2.183100 |
| H | 2.663500 | -5.488200 | -2.546200 |
| C | -4.110600 | -3.720500 | -0.229800 |
| C | -5.363600 | -3.792000 | -0.831400 |
| C | -6.456300 | -3.921400 | 0.015700 |
| H | -5.484000 | -3.740500 | -1.908300 |
| C | -5.053600 | -3.900000 | 2.010200 |
| C | -6.304400 | -3.976500 | 1.410700 |
| H | -7.453000 | -3.980000 | -0.410400 |
| H | -4.940000 | -3.941900 | 3.088800 |
| H | -7.186000 | -4.080500 | 2.035600 |
| C | 4.335700 | -3.256400 | 0.354800 |
| C | 5.576200 | -3.029500 | 0.944400 |
| C | 6.694200 | -3.403000 | 0.209300 |
| H | 5.665200 | -2.577800 | 1.926800 |
| C | 5.339800 | -4.207900 | -1.651700 |
| C | 6.578600 | -3.980400 | -1.065800 |
| H | 7.682300 | -3.246200 | 0.631100 |
| H | 5.254000 | -4.655300 | -2.636700 |
| H | 7.479000 | -4.256600 | -1.605700 |
| O | 4.639300 | 0.444900 | 1.861300 |
| H | 4.137700 | 0.396500 | 1.018400 |
| C | 6.017800 | 0.548700 | 1.562100 |

H 6.224500 1.463200 0.984800
H 6.347700 -0.299900 0.943400
C 6.793600 0.572900 2.861900
H 6.611900 -0.340700 3.438900
H 7.869200 0.654900 2.673500
H 6.485900 1.422500 3.481600

II-2S2

109
Molecule Name
N 3.087400 0.002200 0.652800
C 1.937100 0.001400 0.452600
Au -0.002500 -0.000000 -0.000100
C -1.942200 -0.001400 -0.452500
N -3.092700 -0.002300 -0.652100
Au 0.003600 -3.448500 -0.000200
N -2.976200 -3.235300 0.659000
N -2.661900 -4.123800 -1.294400
C -2.022700 -3.571500 -0.235300
C -4.029400 -4.144500 -1.078800
C -2.756200 -2.577600 1.932000
C -2.031600 -4.616400 -2.499500
N 2.982900 -3.230900 -0.659800
N 2.670200 -4.120500 1.293400
C 2.030000 -3.568700 0.234600
C 4.037600 -4.139600 1.077400
C 2.761900 -2.572800 -1.932400
C 2.040800 -4.614200 2.498500
C -4.230800 -3.573600 0.180800
C -5.503000 -3.451900 0.732000
C -5.090200 -4.611300 -1.850300
C -6.562700 -3.922400 -0.033400
C -6.360600 -4.490400 -1.302000
C 4.238000 -3.568000 -0.182000
C 5.509900 -3.444800 -0.733700
C 5.099200 -4.605500 1.848400
C 6.570300 -3.914500 0.031200
C 6.369200 -4.483100 1.299700
H -1.728000 -2.213800 1.961200
H -3.444500 -1.730900 2.019300
H -2.922000 -3.281800 2.754100
H -0.950200 -4.526800 -2.387800
H -2.291200 -5.667800 -2.655800
H -2.357800 -4.027800 -3.362500
H 1.732900 -2.211400 -1.961800
H 3.448300 -1.724500 -2.018700
H 2.929800 -3.276000 -2.754900
H 0.959200 -4.526500 2.386800
H 2.302100 -5.665200 2.654700
H 2.365900 -4.025200 3.361500
H -5.658800 -3.003900 1.707600
H -4.937000 -5.051600 -2.830400
H -7.572500 -3.850300 0.358900
H -7.217600 -4.844300 -1.866600
H 5.665000 -2.996300 -1.709100
H 4.946800 -5.046300 2.828400
H 7.580000 -3.841300 -0.361400
H 7.226900 -4.836200 1.863900
Au -0.002500 3.448600 -0.000300
N -2.982100 3.231000 0.658500
N -2.668800 4.120000 -1.294900
C -2.028900 3.568700 -0.235700
C -4.036400 4.138700 -1.079400
C -2.761200 2.573700 1.931500
C -2.039100 4.613500 -2.499900
N 2.977300 3.235100 -0.659300
N 2.662900 4.124500 1.293800
C 2.023700 3.571700 0.234900
C 4.030400 4.145400 1.078000
C 2.757400 2.576700 -1.931900
C 2.032600 4.617600 2.498600
C -4.237100 3.567500 0.180100
C -5.509200 3.443900 0.731200
C -6.569500 3.912800 -0.034400
C -5.097800 4.603900 -1.851100
C -6.368000 4.481000 -1.302900
C 4.231800 3.574000 -0.181300
C 5.504000 3.452300 -0.732600
C 6.563600 3.923400 0.032500
C 5.091200 4.612800 1.849200
C 6.361500 4.491900 1.300800
H -1.732500 2.211600 1.961000
H -2.928500 3.277500 2.753600
H -3.448100 1.725700 2.018600
H -0.957500 4.525900 -2.387900
H -2.364000 4.024400 -3.362800
H -2.300500 5.664500 -2.656400
H 1.729000 2.213700 -1.961400
H 2.924300 3.280200 -2.754400
H 3.445100 1.729400 -2.018200
H 0.951100 4.528200 2.386800
H 2.358400 4.029200 3.361800
H 2.292400 5.669000 2.654700
H -5.664500 2.995800 1.706800
H -7.579300 3.839100 0.357800
H -4.945100 5.044400 -2.831200
H -7.225600 4.833600 -1.867700
H 5.659800 3.003800 -1.707900
H 7.573500 3.851500 -0.359800
H 4.937900 5.053500 2.829200
H 7.218500 4.846200 1.865200
O 4.983200 0.003700 -1.452300
C 6.366400 0.004700 -1.152500
C 7.141000 0.005000 -2.453000
H 4.480500 0.003300 -0.610900
H 6.635500 -0.879400 -0.555100
H 6.634200 0.889500 -0.555400
H 8.219600 0.005900 -2.264500
H 6.895800 -0.879300 -3.051800
H 6.894500 0.888700 -3.052200
O -4.983200 -0.004300 1.457700
C -6.367400 -0.004800 1.162800
C -7.137400 -0.004800 2.466000
H -4.483200 -0.003800 0.614600
H -6.638300 0.879400 0.566300
H -6.637700 -0.889400 0.566600
H -8.216700 -0.005300 2.281300
H -6.889100 -0.888600 3.064300
H -6.889800 0.879400 3.064000

II-3S2

118
Molecule Name
Au -0.132400 -3.324300 -0.041700
N 2.781800 -3.295200 -0.944100

| | | | |
|---|---|---|---|
| N | 2.639700 | -3.344100 | 1.221000 |
| C | 1.906400 | -3.282700 | 0.086600 |
| C | 3.989600 | -3.397300 | 0.921400 |
| C | 2.447100 | -3.132700 | -2.344600 |
| H | 1.362700 | -3.053000 | -2.433200 |
| H | 2.909900 | -2.214500 | -2.723900 |
| C | 2.121600 | -3.239900 | 2.570500 |
| H | 1.033400 | -3.308200 | 2.528300 |
| H | 2.507300 | -4.062100 | 3.180500 |
| H | 2.796900 | -3.996900 | -2.917900 |
| H | 2.416900 | -2.275500 | 2.999200 |
| N | -3.085000 | -3.189300 | 0.744000 |
| N | -2.818900 | -4.238400 | -1.135300 |
| C | -2.156800 | -3.575300 | -0.156800 |
| C | -4.175900 | -4.277600 | -0.862400 |
| C | -2.833000 | -2.432300 | 1.954100 |
| H | -1.824600 | -2.019300 | 1.900800 |
| H | -3.558500 | -1.615700 | 2.021100 |
| C | -2.221800 | -4.816900 | -2.318700 |
| H | -1.139000 | -4.703300 | -2.252300 |
| H | -2.467600 | -5.881300 | -2.379700 |
| H | -2.918900 | -3.082900 | 2.830800 |
| H | -2.587300 | -4.305600 | -3.214500 |
| C | 4.080700 | -3.367200 | -0.473300 |
| C | 5.308600 | -3.430300 | -1.126800 |
| C | 5.122800 | -3.489500 | 1.725500 |
| C | 6.440400 | -3.520300 | -0.325800 |
| H | 5.380400 | -3.416400 | -2.209600 |
| C | 6.349200 | -3.549300 | 1.075100 |
| H | 5.054500 | -3.520600 | 2.808200 |
| H | 7.418400 | -3.576600 | -0.794000 |
| H | 7.258300 | -3.626800 | 1.663500 |
| C | -4.346300 | -3.602300 | 0.349200 |
| C | -5.600500 | -3.461200 | 0.936400 |
| C | -5.251300 | -4.836800 | -1.547500 |
| C | -6.674200 | -4.022600 | 0.257100 |
| H | -5.732700 | -2.929300 | 1.872400 |
| C | -6.503300 | -4.697400 | -0.962900 |
| H | -5.122700 | -5.358200 | -2.490700 |
| H | -7.670900 | -3.938600 | 0.679600 |
| H | -7.370700 | -5.120200 | -1.460500 |
| N | -3.364700 | 0.000100 | -0.741900 |
| C | -2.199200 | 0.000000 | -0.683400 |
| N | 2.898300 | 0.000000 | 0.056100 |
| C | 1.744300 | 0.000000 | -0.135800 |
| Au | -0.222900 | 0.000000 | -0.439200 |
| Au | -0.131800 | 3.324300 | -0.041900 |
| N | 2.782400 | 3.294900 | -0.944100 |
| N | 2.640300 | 3.343900 | 1.221000 |
| C | 1.907000 | 3.282600 | 0.086500 |
| C | 3.990100 | 3.396800 | 0.921400 |
| C | 2.447800 | 3.132300 | -2.344600 |
| H | 1.363300 | 3.052900 | -2.433300 |
| H | 2.797900 | 3.996300 | -2.918100 |
| C | 2.122000 | 3.239900 | 2.570400 |
| H | 1.033900 | 3.308200 | 2.528100 |
| H | 2.417400 | 2.275500 | 2.999300 |
| H | 2.910400 | 2.213900 | -2.723800 |
| H | 2.507700 | 4.062100 | 3.180400 |
| N | -3.084300 | 3.189700 | 0.743900 |
| N | -2.818200 | 4.238600 | -1.135600 |
| C | -2.156100 | 3.575500 | -0.157000 |
| C | -4.175200 | 4.278000 | -0.862500 |
| C | -2.832400 | 2.432900 | 1.954100 |
| H | -1.824000 | 2.019900 | 1.901000 |
| H | -2.918500 | 3.083600 | 2.830700 |
| C | -2.221100 | 4.816800 | -2.319000 |
| H | -1.138300 | 4.703100 | -2.252700 |
| H | -2.586800 | 4.305500 | -3.214700 |
| H | -3.557900 | 1.616200 | 2.021100 |
| H | -2.466800 | 5.881300 | -2.380200 |
| C | 4.081300 | 3.366800 | -0.473200 |
| C | 5.309200 | 3.429600 | -1.126700 |
| C | 6.441100 | 3.519400 | -0.325700 |
| H | 5.381100 | 3.415700 | -2.209500 |
| C | 5.123300 | 3.488900 | 1.725600 |
| C | 6.349800 | 3.548400 | 1.075200 |
| H | 7.419100 | 3.575500 | -0.793800 |
| H | 5.055000 | 3.520000 | 2.808300 |
| H | 7.258900 | 3.625800 | 1.663700 |
| C | -4.345700 | 3.602900 | 0.349100 |
| C | -5.599800 | 3.461900 | 0.936400 |
| C | -6.673600 | 4.023400 | 0.257000 |
| H | -5.732100 | 2.930200 | 1.872400 |
| C | -5.250600 | 4.837200 | -1.547700 |
| C | -6.502600 | 4.698000 | -0.963000 |
| H | -7.670200 | 3.939500 | 0.679600 |
| H | -5.122000 | 5.358400 | -2.491000 |
| H | -7.369900 | 5.120800 | -1.460600 |
| O | -5.158800 | 0.000500 | 1.446000 |
| H | -4.687900 | 0.000500 | 0.585800 |
| C | -6.551800 | 0.000600 | 1.193900 |
| H | -6.839200 | -0.884500 | 0.606100 |
| H | -6.839100 | 0.885700 | 0.606100 |
| C | -7.283300 | 0.000500 | 2.518900 |
| H | -7.019200 | 0.884600 | 3.110100 |
| H | -8.367400 | 0.000600 | 2.365100 |
| H | -7.019200 | -0.883500 | 3.110100 |
| O | 4.025400 | -0.000300 | -2.657000 |
| H | 3.820000 | -0.000200 | -1.703600 |
| C | 5.432000 | -0.000400 | -2.819300 |
| H | 5.879800 | 0.883500 | -2.339500 |
| H | 5.879700 | -0.884100 | -2.339000 |
| C | 5.743100 | -0.000900 | -4.300100 |
| H | 5.316600 | 0.884100 | -4.784400 |
| H | 6.824700 | -0.000900 | -4.470300 |
| H | 5.316600 | -0.886100 | -4.783900 |
| H | 3.345300 | -0.000000 | 1.971200 |
| O | 3.376400 | -0.000100 | 2.947000 |
| C | 4.733600 | -0.000300 | 3.350800 |
| H | 5.257700 | -0.884200 | 2.955500 |
| H | 5.258100 | 0.883300 | 2.955200 |
| C | 4.784800 | -0.000000 | 4.863100 |
| H | 5.821000 | -0.000200 | 5.217200 |
| H | 4.281800 | 0.885100 | 5.266900 |
| H | 4.281400 | -0.884800 | 5.267200 |

II-4S2

127

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000000 | 0.000000 | -3.219300 |
| N | -1.084900 | 2.850200 | -3.333000 |
| N | 1.084900 | 2.850200 | -3.333000 |
| C | 0.000000 | 2.043700 | -3.285800 |
| C | 0.698800 | 4.176800 | -3.407400 |

| | | | |
|---|---|---|---|
| C | -2.464500 | 2.428000 | -3.199800 |
| H | -2.493900 | 1.337800 | -3.206600 |
| H | -2.871400 | 2.801100 | -2.252800 |
| C | 2.464500 | 2.428000 | -3.199800 |
| H | 2.493900 | 1.337800 | -3.206600 |
| H | 3.052700 | 2.807300 | -4.040800 |
| H | -3.052700 | 2.807300 | -4.040800 |
| H | 2.871400 | 2.801100 | -2.252800 |
| N | 1.084900 | -2.850200 | -3.333000 |
| N | -1.084900 | -2.850200 | -3.333000 |
| C | 0.000000 | -2.043700 | -3.285800 |
| C | -0.698800 | -4.176800 | -3.407400 |
| C | 2.464500 | -2.428000 | -3.199800 |
| H | 2.493900 | -1.337800 | -3.206600 |
| H | 2.871400 | -2.801100 | -2.252800 |
| C | -2.464500 | -2.428000 | -3.199800 |
| H | -2.493900 | -1.337800 | -3.206600 |
| H | -3.052700 | -2.807300 | -4.040800 |
| H | 3.052700 | -2.807300 | -4.040800 |
| H | -2.871400 | -2.801100 | -2.252800 |
| C | -0.698800 | 4.176800 | -3.407400 |
| C | -1.429700 | 5.359200 | -3.489100 |
| C | 1.429700 | 5.359200 | -3.489100 |
| C | -0.702200 | 6.540300 | -3.568300 |
| H | -2.514900 | 5.361100 | -3.495700 |
| C | 0.702200 | 6.540300 | -3.568300 |
| H | 2.514900 | 5.361100 | -3.495700 |
| H | -1.231500 | 7.485600 | -3.637600 |
| H | 1.231500 | 7.485600 | -3.637600 |
| C | 0.698800 | -4.176800 | -3.407400 |
| C | 1.429700 | -5.359200 | -3.489100 |
| C | -1.429700 | -5.359200 | -3.489100 |
| C | 0.702200 | -6.540300 | -3.568300 |
| H | 2.514900 | -5.361100 | -3.495700 |
| C | -0.702200 | -6.540300 | -3.568300 |
| H | -2.514900 | -5.361100 | -3.495700 |
| H | 1.231500 | -7.485600 | -3.637600 |
| H | -1.231500 | -7.485600 | -3.637600 |
| N | 0.000000 | -3.160200 | -0.000000 |
| C | 0.000000 | -1.990500 | -0.000000 |
| N | 0.000000 | 3.160200 | -0.000000 |
| C | 0.000000 | 1.990500 | -0.000000 |
| Au | 0.000000 | 0.000000 | -0.000000 |
| Au | 0.000000 | 0.000000 | 3.219300 |
| N | -1.084900 | 2.850200 | 3.332900 |
| N | 1.084900 | 2.850200 | 3.332900 |
| C | 0.000000 | 2.043700 | 3.285800 |
| C | 0.698800 | 4.176800 | 3.407400 |
| C | -2.464500 | 2.428000 | 3.199800 |
| H | -2.493900 | 1.337800 | 3.206600 |
| H | -3.052700 | 2.807300 | 4.040800 |
| C | 2.464500 | 2.428000 | 3.199800 |
| H | 2.493900 | 1.337800 | 3.206600 |
| H | 2.871500 | 2.801100 | 2.252800 |
| H | -2.871500 | 2.801100 | 2.252800 |
| H | 3.052700 | 2.807300 | 4.040800 |
| N | 1.084900 | -2.850200 | 3.332900 |
| N | -1.084900 | -2.850200 | 3.332900 |
| C | 0.000000 | -2.043700 | 3.285800 |
| C | -0.698800 | -4.176800 | 3.407400 |
| C | 2.464500 | -2.428000 | 3.199800 |
| H | 2.493900 | -1.337800 | 3.206600 |
| H | 3.052700 | -2.807300 | 4.040800 |
| C | -2.464500 | -2.428000 | 3.199800 |
| H | -2.493900 | -1.337800 | 3.206600 |
| H | -2.871500 | -2.801100 | 2.252800 |
| H | 2.871500 | -2.801100 | 2.252800 |
| H | -3.052700 | -2.807300 | 4.040800 |
| C | -0.698800 | 4.176800 | 3.407400 |
| C | -1.429700 | 5.359200 | 3.489100 |
| C | -0.702200 | 6.540300 | 3.568300 |
| H | -2.514900 | 5.361100 | 3.495600 |
| C | 1.429700 | 5.359200 | 3.489100 |
| C | 0.702200 | 6.540300 | 3.568300 |
| H | -1.231500 | 7.485600 | 3.637600 |
| H | 2.514900 | 5.361100 | 3.495600 |
| H | 1.231500 | 7.485600 | 3.637600 |
| C | 0.698800 | -4.176800 | 3.407400 |
| C | 1.429700 | -5.359200 | 3.489100 |
| C | 0.702200 | -6.540300 | 3.568300 |
| H | 2.514900 | -5.361100 | 3.495600 |
| C | -1.429700 | -5.359200 | 3.489100 |
| C | -0.702200 | -6.540300 | 3.568300 |
| H | 1.231500 | -7.485600 | 3.637600 |
| H | -2.514900 | -5.361100 | 3.495600 |
| H | -1.231500 | -7.485600 | 3.637600 |
| O | 2.863900 | -3.839800 | 0.000000 |
| H | 1.892500 | -3.753700 | 0.000000 |
| C | 3.189700 | -5.217900 | 0.000000 |
| H | 2.764400 | -5.718200 | -0.883900 |
| H | 2.764400 | -5.718200 | 0.883900 |
| C | 4.696500 | -5.354700 | 0.000000 |
| H | 5.127600 | -4.874900 | 0.885200 |
| H | 4.991500 | -6.409200 | 0.000000 |
| H | 5.127600 | -4.874900 | -0.885100 |
| O | -2.863900 | 3.839800 | 0.000000 |
| H | -1.892500 | 3.753700 | 0.000000 |
| C | -3.189700 | 5.217900 | 0.000000 |
| H | -2.764400 | 5.718200 | 0.883900 |
| H | -2.764400 | 5.718200 | -0.883900 |
| C | -4.696500 | 5.354700 | 0.000000 |
| H | -5.127600 | 4.874900 | 0.885200 |
| H | -4.991500 | 6.409200 | 0.000000 |
| H | -5.127600 | 4.874900 | -0.885100 |
| H | 1.892500 | 3.753700 | 0.000000 |
| O | 2.863900 | 3.839800 | 0.000000 |
| C | 3.189700 | 5.217900 | 0.000000 |
| H | 2.764400 | 5.718200 | -0.883900 |
| H | 2.764400 | 5.718200 | 0.883900 |
| C | 4.696500 | 5.354700 | 0.000000 |
| H | 4.991500 | 6.409200 | 0.000000 |
| H | 5.127600 | 4.874900 | 0.885200 |
| H | 5.127600 | 4.874900 | -0.885100 |
| H | -1.892500 | -3.753700 | 0.000000 |
| O | -2.863900 | -3.839800 | 0.000000 |
| C | -3.189700 | -5.217900 | 0.000000 |
| H | -2.764400 | -5.718200 | 0.883900 |
| H | -2.764400 | -5.718200 | -0.883900 |
| C | -4.696500 | -5.354700 | 0.000000 |
| H | -4.991500 | -6.409200 | 0.000000 |
| H | -5.127600 | -4.874900 | 0.885200 |
| H | -5.127600 | -4.874900 | -0.885100 |

## 18. The $S_0$ .xyz files of III and its complexes

III

| | | | |
|---|---|---|---|
| Au | 0.004700 | -0.078400 | 0.002000 |
| N | 0.035400 | -0.188900 | 3.050400 |
| N | 2.037000 | -0.185800 | 2.274700 |
| C | 0.740200 | -0.129700 | 1.898700 |
| C | 2.144500 | -0.278800 | 3.643000 |
| H | 3.098200 | -0.326400 | 4.145600 |
| C | 0.878300 | -0.280200 | 4.133800 |
| H | 0.512600 | -0.328000 | 5.147900 |
| C | -1.417800 | -0.179500 | 3.122800 |
| H | -1.829200 | -1.030400 | 2.573100 |
| H | -1.714700 | -0.247300 | 4.170600 |
| C | 3.159200 | -0.183600 | 1.348400 |
| H | 3.126100 | 0.717400 | 0.732000 |
| H | 4.086100 | -0.186900 | 1.924200 |
| H | -1.803900 | 0.752000 | 2.702600 |
| H | 3.123900 | -1.069300 | 0.707900 |
| N | -0.027900 | -0.101000 | -3.048400 |
| N | -2.028900 | -0.059700 | -2.272100 |
| C | -0.731100 | -0.053400 | -1.895200 |
| C | -2.138500 | -0.110400 | -3.642400 |
| H | -3.093000 | -0.115000 | -4.145700 |
| C | -0.872700 | -0.136000 | -4.133500 |
| H | -0.508200 | -0.165800 | -5.148700 |
| C | 1.424900 | -0.133300 | -3.121000 |
| H | 1.810400 | -1.011500 | -2.596000 |
| H | 1.720100 | -0.180100 | -4.170500 |
| C | -3.150900 | -0.050200 | -1.345600 |
| H | -3.091000 | 0.831400 | -0.703700 |
| H | -4.077200 | -0.009300 | -1.920800 |
| H | 1.838700 | 0.773800 | -2.674600 |
| H | -3.142500 | -0.954400 | -0.730600 |
| N | -3.065600 | -3.109100 | 1.062700 |
| C | -1.966300 | -3.119900 | 0.661300 |
| N | 2.983000 | -3.168700 | -1.146000 |
| C | 1.883700 | -3.157800 | -0.744600 |
| Ag | -0.041300 | -3.138900 | -0.041700 |
| Au | -0.087400 | -6.199400 | -0.085300 |
| N | -0.177300 | -6.197100 | 2.964100 |
| N | 1.853500 | -6.195500 | 2.268300 |
| C | 0.572000 | -6.223600 | 1.839800 |
| C | 1.907400 | -6.152800 | 3.642200 |
| H | 2.840800 | -6.135700 | 4.183500 |
| C | 0.622700 | -6.153200 | 4.082400 |
| H | 0.217400 | -6.135300 | 5.082300 |
| C | -1.632200 | -6.181300 | 2.978700 |
| H | -2.006400 | -5.273500 | 2.497300 |
| H | -2.015300 | -7.059800 | 2.454800 |
| C | 3.011600 | -6.189000 | 1.387500 |
| H | 3.024600 | -7.100300 | 0.785200 |
| H | 2.983300 | -5.314300 | 0.732100 |
| H | -1.970500 | -6.209800 | 4.015700 |
| H | 3.914300 | -6.154000 | 1.999500 |
| N | 0.003800 | -6.112900 | -3.133500 |
| N | -2.026200 | -6.070000 | -2.437000 |
| C | -0.746400 | -6.148900 | -2.010000 |
| C | -2.078300 | -5.986600 | -3.809100 |
| H | -3.010400 | -5.926000 | -4.349300 |
| C | -0.794000 | -6.013100 | -4.249700 |
| H | -0.387900 | -5.978800 | -5.248800 |
| C | 1.458600 | -6.140400 | -3.148200 |
| H | 1.859700 | -5.258400 | -2.641200 |
| H | 1.814900 | -7.044600 | -2.649700 |
| C | -3.184100 | -6.053800 | -1.555900 |
| H | -3.224700 | -6.981000 | -0.979800 |
| H | -3.129700 | -5.199300 | -0.875800 |
| H | 1.796300 | -6.149500 | -4.185700 |
| H | -4.085000 | -5.974200 | -2.166300 |

III-S1

73
Molecule Name

| | | | |
|---|---|---|---|
| N | 0.007000 | 2.541200 | 1.024800 |
| C | 0.003200 | 1.389800 | 0.825400 |
| N | -0.009700 | -3.414000 | -1.272400 |
| C | -0.007500 | -2.399900 | -0.689600 |
| Ag | -0.002900 | -0.549800 | 0.176300 |
| Au | 3.535300 | -0.166100 | -0.023800 |
| N | 3.464500 | -2.996500 | 1.122800 |
| N | 3.324700 | -3.056400 | -1.015900 |
| C | 3.444100 | -2.204500 | 0.025000 |
| C | 3.251400 | -4.357200 | -0.579800 |
| H | 3.116500 | -5.184500 | -1.258700 |
| C | 3.349000 | -4.322400 | 0.771600 |
| H | 3.341600 | -5.115600 | 1.503200 |
| C | 3.603000 | -2.530500 | 2.487900 |
| H | 3.458200 | -1.449400 | 2.502600 |
| H | 2.841700 | -3.000500 | 3.115600 |
| C | 3.155100 | -2.668200 | -2.403100 |
| H | 3.421500 | -1.615200 | -2.504100 |
| H | 3.814600 | -3.268600 | -3.034700 |
| H | 4.596900 | -2.771300 | 2.876800 |
| H | 2.110700 | -2.818400 | -2.689300 |
| N | 2.990600 | 2.730800 | -0.849600 |
| N | 4.340200 | 2.661800 | 0.813500 |
| C | 3.640800 | 1.872500 | -0.034900 |
| C | 4.118000 | 3.993100 | 0.540400 |
| H | 4.574800 | 4.783900 | 1.115300 |
| C | 3.263200 | 4.034900 | -0.511000 |
| H | 2.811300 | 4.863400 | -1.032600 |
| C | 2.130300 | 2.356000 | -1.956100 |
| H | 1.705200 | 1.371800 | -1.753700 |
| H | 1.328200 | 3.093500 | -2.026100 |
| C | 5.170900 | 2.189600 | 1.903600 |
| H | 5.342900 | 1.120600 | 1.771200 |
| H | 6.131200 | 2.711200 | 1.887700 |
| H | 2.702500 | 2.327900 | -2.888500 |
| H | 4.675600 | 2.363700 | 2.863200 |
| Au | -3.535700 | -0.153000 | -0.024500 |
| N | -3.484700 | -2.988200 | 1.111500 |
| N | -3.342000 | -3.040900 | -1.027200 |
| C | -3.457600 | -2.192200 | 0.016800 |
| C | -3.277500 | -4.343700 | -0.595900 |
| H | -3.146800 | -5.169300 | -1.277800 |
| C | -3.376900 | -4.313500 | 0.755400 |
| H | -3.375600 | -5.109500 | 1.484000 |
| C | -3.622200 | -2.526700 | 2.478200 |
| H | -3.473400 | -1.446100 | 2.496700 |
| H | -4.617200 | -2.765100 | 2.865700 |
| C | -3.167200 | -2.648400 | -2.412500 |
| H | -3.429600 | -1.594000 | -2.510600 |

| | | | |
|---|---|---|---|
| H | -2.122700 | -2.801300 | -2.696600 |
| H | -2.863000 | -3.001600 | 3.104600 |
| H | -3.827200 | -3.244200 | -3.048000 |
| N | -2.976700 | 2.743800 | -0.841600 |
| N | -4.319400 | 2.676400 | 0.827000 |
| C | -3.628600 | 1.886200 | -0.027600 |
| C | -4.090100 | 4.007400 | 0.558300 |
| H | -4.539400 | 4.798600 | 1.138400 |
| C | -3.239600 | 4.048100 | -0.496700 |
| H | -2.784600 | 4.875900 | -1.016800 |
| C | -2.123600 | 2.368100 | -1.953400 |
| H | -1.702100 | 1.381300 | -1.755800 |
| H | -2.700300 | 2.345200 | -2.883100 |
| C | -5.147300 | 2.204800 | 1.919500 |
| H | -5.333900 | 1.139200 | 1.779100 |
| H | -4.642300 | 2.364100 | 2.876700 |
| H | -1.318400 | 3.102100 | -2.025300 |
| H | -6.100900 | 2.738600 | 1.915800 |
| O | 0.011000 | 4.663000 | -0.813500 |
| H | 0.009800 | 4.006700 | -0.080200 |
| C | 0.017500 | 5.950900 | -0.242700 |
| H | 0.907800 | 6.128300 | 0.378900 |
| H | 0.019900 | 6.679700 | -1.059100 |
| H | -0.869900 | 6.136500 | 0.380700 |

III-2S1

79

Molecule Name

| | | | |
|---|---|---|---|
| Au | -3.435200 | -0.000200 | 0.000000 |
| N | -3.009800 | 2.949400 | 0.714700 |
| N | -3.925400 | 2.759900 | -1.214100 |
| C | -3.461100 | 2.034600 | -0.170400 |
| C | -3.754100 | 4.106700 | -0.989400 |
| H | -4.046000 | 4.853800 | -1.711300 |
| C | -3.174200 | 4.224800 | 0.230200 |
| H | -2.852300 | 5.091100 | 0.785800 |
| C | -2.402600 | 2.657900 | 2.000100 |
| H | -2.050400 | 1.625100 | 1.994300 |
| H | -1.557100 | 3.335700 | 2.142400 |
| C | -4.471800 | 2.208800 | -2.438700 |
| H | -4.651100 | 1.143100 | -2.290200 |
| H | -5.417300 | 2.702500 | -2.677200 |
| H | -3.132600 | 2.790900 | 2.804400 |
| H | -3.766700 | 2.347400 | -3.263100 |
| N | -3.009200 | -2.949800 | -0.714700 |
| N | -3.924800 | -2.760500 | 1.214200 |
| C | -3.460700 | -2.035100 | 0.170400 |
| C | -3.753100 | -4.107200 | 0.989500 |
| H | -4.044900 | -4.854400 | 1.711300 |
| C | -3.173300 | -4.225200 | -0.230100 |
| H | -2.851200 | -5.091500 | -0.785800 |
| C | -2.402100 | -2.658200 | -2.000100 |
| H | -2.050200 | -1.625300 | -1.994400 |
| H | -1.556500 | -3.335800 | -2.142500 |
| C | -4.471400 | -2.209500 | 2.438700 |
| H | -4.651000 | -1.143800 | 2.290200 |
| H | -5.416900 | -2.703300 | 2.677200 |
| H | -3.132200 | -2.791400 | -2.804400 |
| H | -3.766300 | -2.348000 | 3.263200 |
| N | 0.000300 | -3.064100 | 0.955300 |
| C | 0.000200 | -1.928100 | 0.679800 |
| N | -0.000400 | 3.064100 | -0.955300 |
| C | -0.000200 | 1.928100 | -0.679800 |
| Ag | 0.000000 | -0.000000 | -0.000000 |
| Au | 3.435200 | 0.000200 | 0.000000 |
| N | 3.009200 | 2.949800 | 0.714700 |
| N | 3.924800 | 2.760400 | -1.214100 |
| C | 3.460700 | 2.035100 | -0.170400 |
| C | 3.753200 | 4.107200 | -0.989400 |
| H | 4.044900 | 4.854400 | -1.711300 |
| C | 3.173300 | 4.225200 | 0.230200 |
| H | 2.851200 | 5.091500 | 0.785800 |
| C | 2.402000 | 2.658200 | 2.000100 |
| H | 2.050000 | 1.625400 | 1.994300 |
| H | 3.132000 | 2.791300 | 2.804400 |
| C | 4.471500 | 2.209500 | -2.438600 |
| H | 4.651000 | 1.143800 | -2.290100 |
| H | 3.766400 | 2.348000 | -3.263100 |
| H | 1.556400 | 3.335900 | 2.142400 |
| H | 5.417000 | 2.703300 | -2.677000 |
| N | 3.009800 | -2.949400 | -0.714800 |
| N | 3.925300 | -2.759900 | 1.214200 |
| C | 3.461100 | -2.034600 | 0.170400 |
| C | 3.753900 | -4.106700 | 0.989400 |
| H | 4.045800 | -4.853800 | 1.711300 |
| C | 3.174100 | -4.224800 | -0.230200 |
| H | 2.852200 | -5.091100 | -0.785800 |
| C | 2.402700 | -2.657900 | -2.000200 |
| H | 2.050600 | -1.625100 | -1.994500 |
| H | 3.132800 | -2.791000 | -2.804500 |
| C | 4.471700 | -2.208800 | 2.438700 |
| H | 4.651200 | -1.143100 | 2.290200 |
| H | 3.766600 | -2.347300 | 3.263100 |
| H | 1.557200 | -3.335600 | -2.142600 |
| H | 5.417200 | -2.702600 | 2.677300 |
| O | 0.000500 | -4.900000 | -1.184400 |
| H | 0.000400 | -4.370900 | -0.356900 |
| C | 0.000500 | -6.265400 | -0.840800 |
| H | -0.887200 | -6.553600 | -0.257700 |
| H | 0.000600 | -6.843400 | -1.769500 |
| H | 0.888200 | -6.553600 | -0.257600 |
| O | -0.000400 | 4.900100 | 1.184300 |
| H | -0.000400 | 4.370900 | 0.356900 |
| C | -0.000500 | 6.265400 | 0.840600 |
| H | -0.000500 | 6.843600 | 1.769100 |
| H | 0.887100 | 6.553600 | 0.257200 |
| H | -0.888300 | 6.553500 | 0.257300 |

III-3S1

85

Molecule Name

| | | | |
|---|---|---|---|
| Au | -3.313800 | 0.413400 | 0.007600 |
| N | -3.518700 | -2.526500 | -0.837600 |
| N | -3.637700 | -2.338200 | 1.296400 |
| C | -3.498100 | -1.615900 | 0.162100 |
| C | -3.734200 | -3.679900 | 1.012400 |
| H | -3.851000 | -4.424700 | 1.784500 |
| C | -3.659400 | -3.798400 | -0.336300 |
| H | -3.699000 | -4.667400 | -0.974900 |
| C | -3.295700 | -2.243300 | -2.243700 |
| H | -3.165100 | -1.166800 | -2.361800 |
| H | -2.389000 | -2.757900 | -2.578200 |
| C | -3.567000 | -1.809500 | 2.647400 |
| H | -3.628100 | -0.721500 | 2.595800 |

| | | | |
|---|---|---|---|
| H | -4.407000 | -2.188000 | 3.235700 |
| H | -4.155400 | -2.572100 | -2.834400 |
| H | -2.617300 | -2.110800 | 3.101700 |
| N | -2.583200 | 3.296700 | 0.721500 |
| N | -3.660700 | 3.231400 | -1.130100 |
| C | -3.182200 | 2.444900 | -0.138400 |
| C | -3.353900 | 4.553000 | -0.898200 |
| H | -3.631700 | 5.338700 | -1.583800 |
| C | -2.671200 | 4.592200 | 0.272400 |
| H | -2.224600 | 5.412400 | 0.811800 |
| C | -1.923000 | 2.921300 | 1.958300 |
| H | -1.557000 | 1.897300 | 1.864400 |
| H | -1.081100 | 3.600000 | 2.115400 |
| C | -4.351000 | 2.758600 | -2.313900 |
| H | -4.625300 | 1.713900 | -2.162000 |
| H | -5.258000 | 3.347400 | -2.472800 |
| H | -2.622100 | 2.985100 | 2.797700 |
| H | -3.701500 | 2.841600 | -3.190000 |
| N | 0.442600 | 3.460100 | -0.992800 |
| C | 0.297900 | 2.301600 | -0.945900 |
| N | -0.342100 | -2.807800 | 0.110900 |
| C | -0.204600 | -1.678600 | -0.165600 |
| Ag | 0.046300 | 0.301000 | -0.613200 |
| Au | 3.327900 | -0.228800 | 0.050400 |
| N | 2.876800 | -3.062800 | -1.014600 |
| N | 2.944500 | -3.065600 | 1.129800 |
| C | 3.031900 | -2.250000 | 0.055000 |
| C | 2.726600 | -4.365700 | 0.739100 |
| H | 2.622300 | -5.170500 | 1.450500 |
| C | 2.684400 | -4.363700 | -0.616300 |
| H | 2.534600 | -5.163700 | -1.324400 |
| C | 2.831800 | -2.640300 | -2.402700 |
| H | 2.822000 | -1.549800 | -2.431400 |
| H | 3.709300 | -3.011200 | -2.940500 |
| C | 2.941200 | -2.633900 | 2.516500 |
| H | 3.294200 | -1.602500 | 2.558200 |
| H | 1.924000 | -2.697700 | 2.918300 |
| H | 1.916300 | -3.029700 | -2.857400 |
| H | 3.617100 | -3.265900 | 3.098700 |
| N | 3.238300 | 2.706500 | 0.923100 |
| N | 4.350100 | 2.490000 | -0.896300 |
| C | 3.667200 | 1.784300 | 0.034600 |
| C | 4.336000 | 3.834000 | -0.600000 |
| H | 4.811300 | 4.568900 | -1.231100 |
| C | 3.631800 | 3.969400 | 0.550500 |
| H | 3.359800 | 4.842000 | 1.122800 |
| C | 2.455000 | 2.433900 | 2.113600 |
| H | 1.919800 | 1.493200 | 1.973600 |
| H | 3.106400 | 2.357100 | 2.989500 |
| C | 4.954000 | 1.933100 | -2.090800 |
| H | 5.026400 | 0.851100 | -1.972500 |
| H | 4.342300 | 2.163900 | -2.967700 |
| H | 1.740000 | 3.249500 | 2.246300 |
| H | 5.956600 | 2.346900 | -2.223500 |
| O | 0.544200 | 5.076300 | 1.300200 |
| H | 0.533300 | 4.626400 | 0.425900 |
| C | 0.695500 | 6.460900 | 1.087200 |
| H | -0.125600 | 6.887000 | 0.491400 |
| H | 1.639500 | 6.707100 | 0.578200 |
| H | 0.697100 | 6.951000 | 2.065000 |
| O | -0.229200 | -4.160600 | -2.447500 |
| H | -0.261000 | -3.827300 | -1.530400 |
| C | -0.511800 | -5.539000 | -2.434100 |
| H | 0.222000 | -6.117300 | -1.851500 |
| H | -1.510800 | -5.762500 | -2.029300 |
| H | -0.479700 | -5.893200 | -3.467900 |
| C | -0.558400 | -4.650400 | 3.261700 |
| O | -0.456100 | -3.282400 | 2.947800 |
| H | 0.309700 | -5.230700 | 2.912400 |
| H | -1.463000 | -5.114100 | 2.839800 |
| H | -0.433800 | -3.195800 | 1.974000 |
| H | -0.607200 | -4.738400 | 4.350500 |

III-4S1

91

Molecule Name

| | | | |
|---|---|---|---|
| Au | -3.224800 | -0.021700 | -0.000000 |
| N | -3.392700 | 2.973200 | 0.596700 |
| N | -3.095200 | 2.644700 | -1.502400 |
| C | -3.248500 | 1.995200 | -0.326400 |
| C | -3.132400 | 4.005900 | -1.317800 |
| H | -3.022500 | 4.699100 | -2.137100 |
| C | -3.319000 | 4.213700 | 0.009100 |
| H | -3.402100 | 5.126700 | 0.578300 |
| C | -3.463000 | 2.768400 | 2.032300 |
| H | -3.721500 | 1.725500 | 2.221300 |
| H | -2.494300 | 2.998900 | 2.489300 |
| C | -2.835300 | 2.023800 | -2.788700 |
| H | -2.705200 | 0.951800 | -2.634700 |
| H | -3.676100 | 2.193600 | -3.467600 |
| H | -4.240100 | 3.409900 | 2.455600 |
| H | -1.917700 | 2.450200 | -3.205300 |
| N | -3.351800 | -3.018800 | -0.596700 |
| N | -3.058900 | -2.686100 | 1.502400 |
| C | -3.221000 | -2.038900 | 0.326400 |
| C | -3.077600 | -4.047700 | 1.317900 |
| H | -2.958300 | -4.739400 | 2.137300 |
| C | -3.261300 | -4.258100 | -0.009000 |
| H | -3.332000 | -5.172200 | -0.578200 |
| C | -3.424700 | -2.815000 | -2.032300 |
| H | -3.697000 | -1.775700 | -2.221400 |
| H | -2.452900 | -3.032600 | -2.489200 |
| C | -2.807600 | -2.061800 | 2.788700 |
| H | -2.692000 | -0.988100 | 2.634600 |
| H | -3.646000 | -2.242900 | 3.467600 |
| H | -4.193100 | -3.466900 | -2.455600 |
| H | -1.884200 | -2.475600 | 3.205300 |
| N | 0.021900 | -3.218600 | 0.000000 |
| C | 0.014000 | -2.047500 | -0.000000 |
| N | -0.021900 | 3.218700 | 0.000000 |
| C | -0.013900 | 2.047600 | -0.000100 |
| Ag | 0.000000 | 0.000000 | -0.000100 |
| Au | 3.224800 | 0.021700 | 0.000000 |
| N | 3.058900 | 2.686100 | 1.502400 |
| N | 3.351800 | 3.018800 | -0.596700 |
| C | 3.221000 | 2.038900 | 0.326400 |
| C | 3.261300 | 4.258100 | -0.009000 |
| H | 3.332100 | 5.172100 | -0.578200 |
| C | 3.077700 | 4.047700 | 1.317900 |
| H | 2.958400 | 4.739400 | 2.137300 |
| C | 2.807500 | 2.061800 | 2.788800 |
| H | 2.691900 | 0.988100 | 2.634700 |
| H | 3.645900 | 2.242900 | 3.467700 |
| C | 3.424700 | 2.815000 | -2.032200 |
| H | 3.697100 | 1.775700 | -2.221400 |
| H | 2.453000 | 3.032600 | -2.489100 |
| H | 1.884200 | 2.475600 | 3.205300 |

| | | | |
|---|---|---|---|
| H | 4.193200 | 3.466900 | -2.455600 |
| N | 3.095200 | -2.644600 | -1.502400 |
| N | 3.392700 | -2.973300 | 0.596700 |
| C | 3.248500 | -1.995200 | -0.326400 |
| C | 3.319000 | -4.213700 | 0.009000 |
| H | 3.402200 | -5.126700 | 0.578300 |
| C | 3.132400 | -4.005900 | -1.317800 |
| H | 3.022500 | -4.699100 | -2.137200 |
| C | 2.835300 | -2.023800 | -2.788700 |
| H | 2.705200 | -0.951700 | -2.634600 |
| H | 3.676100 | -2.193600 | -3.467600 |
| C | 3.462900 | -2.768500 | 2.032300 |
| H | 3.721400 | -1.725600 | 2.221400 |
| H | 2.494200 | -2.999000 | 2.489300 |
| H | 1.917700 | -2.450100 | -3.205300 |
| H | 4.240100 | -3.409900 | 2.455600 |
| O | -0.067700 | -3.848100 | -2.843800 |
| H | -0.019500 | -3.736800 | -1.875500 |
| C | -0.178600 | -5.223500 | -3.124800 |
| H | -1.092600 | -5.668000 | -2.702000 |
| H | 0.680700 | -5.801900 | -2.752400 |
| H | -0.219600 | -5.336700 | -4.211400 |
| O | -0.120100 | 3.846700 | 2.843900 |
| H | -0.070400 | 3.736100 | 1.875600 |
| C | -0.249500 | 5.220500 | 3.124900 |
| H | 0.601800 | 5.810500 | 2.752400 |
| H | -1.169500 | 5.652500 | 2.702300 |
| H | -0.292000 | 5.333100 | 4.211500 |
| C | 0.178600 | 5.223500 | -3.124900 |
| O | 0.067700 | 3.848100 | -2.843800 |
| H | 1.092600 | 5.668000 | -2.702100 |
| H | -0.680700 | 5.801900 | -2.752600 |
| H | 0.019500 | 3.736800 | -1.875500 |
| H | 0.219700 | 5.336600 | -4.211500 |
| C | 0.249400 | -5.220600 | 3.124800 |
| O | 0.119900 | -3.846800 | 2.843800 |
| H | 1.169400 | -5.652600 | 2.702300 |
| H | -0.601900 | -5.810600 | 2.752300 |
| H | 0.070300 | -3.736200 | 1.875500 |
| H | 0.291700 | -5.333200 | 4.211400 |

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76

Molecule Name

| | | | |
|---|---|---|---|
| N | -0.215400 | -3.462600 | -1.411700 |
| C | -0.158300 | -2.473200 | -0.790400 |
| N | 0.169800 | 2.383900 | 1.125000 |
| C | 0.089800 | 1.244800 | 0.876700 |
| Ag | -0.042700 | -0.662600 | 0.149000 |
| Au | 3.499100 | -0.448900 | 0.008000 |
| N | 3.152100 | 2.482600 | -0.808700 |
| N | 4.504100 | 2.313100 | 0.845500 |
| C | 3.744300 | 1.578000 | 0.000000 |
| C | 4.377300 | 3.657400 | 0.575800 |
| C | 3.520800 | 3.762800 | -0.469700 |
| C | 2.254300 | 2.174800 | -1.906300 |
| C | 5.305500 | 1.779800 | 1.929300 |
| N | 3.214500 | -3.266000 | 1.155000 |
| N | 3.132000 | -3.323500 | -0.986900 |
| C | 3.275000 | -2.477600 | 0.056000 |
| C | 2.965100 | -4.615900 | -0.551300 |
| C | 3.025600 | -4.583100 | 0.802400 |
| C | 3.334700 | -2.804700 | 2.523500 |
| C | 3.035500 | -2.931000 | -2.379900 |
| H | 4.894400 | 4.412100 | 1.148300 |
| H | 3.131300 | 4.623700 | -0.989300 |
| H | 1.789600 | 1.205900 | -1.718400 |
| H | 1.484700 | 2.948800 | -1.941500 |
| H | 2.806900 | 2.143600 | -2.850400 |
| H | 5.387800 | 0.699700 | 1.800800 |
| H | 6.305000 | 2.221000 | 1.901000 |
| H | 4.835800 | 1.997900 | 2.892800 |
| H | 2.800200 | -5.435400 | -1.233100 |
| H | 2.948000 | -5.372100 | 1.534500 |
| H | 3.321600 | -1.713900 | 2.523900 |
| H | 2.490600 | -3.171700 | 3.112900 |
| H | 4.270800 | -3.158400 | 2.965700 |
| H | 3.344200 | -1.888400 | -2.467800 |
| H | 3.698300 | -3.555500 | -2.984100 |
| H | 1.999000 | -3.041500 | -2.709600 |
| Au | -3.540700 | -0.116700 | 0.001400 |
| N | -2.828500 | 2.790200 | -0.639800 |
| N | -4.087500 | 2.687100 | 1.091100 |
| C | -3.494200 | 1.918900 | 0.147900 |
| C | -3.784600 | 4.017000 | 0.902000 |
| C | -2.987200 | 4.080100 | -0.192400 |
| C | -2.053500 | 2.441500 | -1.815900 |
| C | -4.886600 | 2.190600 | 2.193700 |
| N | -3.709200 | -3.028500 | 0.915800 |
| N | -3.520900 | -2.926300 | -1.217300 |
| C | -3.602900 | -2.154300 | -0.112400 |
| C | -3.554200 | -4.259800 | -0.888300 |
| C | -3.682200 | -4.326800 | 0.459200 |
| C | -3.840000 | -2.666100 | 2.312500 |
| C | -3.292300 | -2.441300 | -2.564900 |
| H | -4.150000 | 4.790900 | 1.559300 |
| H | -2.504400 | 4.913000 | -0.678200 |
| H | -1.674800 | 1.424800 | -1.699100 |
| H | -2.676400 | 2.503800 | -2.713400 |
| H | -1.215300 | 3.137600 | -1.887500 |
| H | -5.146800 | 1.150400 | 1.992900 |
| H | -4.324100 | 2.252200 | 3.129700 |
| H | -5.803900 | 2.778800 | 2.278300 |
| H | -3.465900 | -5.037600 | -1.630600 |
| H | -3.751300 | -5.174600 | 1.123200 |
| H | -3.678300 | -1.591600 | 2.408000 |
| H | -4.838300 | -2.918800 | 2.681900 |
| H | -3.087300 | -3.194200 | 2.903500 |
| H | -3.470600 | -1.365200 | -2.580700 |
| H | -2.257600 | -2.651300 | -2.848300 |
| H | -3.984900 | -2.931500 | -3.253600 |
| C | 0.395800 | 5.825700 | -0.101000 |
| C | 0.441200 | 6.857700 | -1.207700 |
| O | 0.262700 | 4.542000 | -0.678500 |
| H | 1.312100 | 5.885600 | 0.507700 |
| H | -0.447200 | 6.037900 | 0.576200 |
| H | -0.473500 | 6.822800 | -1.809700 |
| H | 0.543600 | 7.866700 | -0.795700 |
| H | 1.287500 | 6.672100 | -1.878500 |
| H | 0.240000 | 3.877400 | 0.047000 |

III-2S2

85

Molecule Name

| | | | |
|---|---|---|---|
| Au | 3.446000 | 0.514200 | -0.030200 |

| | | | |
|---|---|---|---|
| N | 2.542400 | 3.426000 | -0.337600 |
| N | 3.510100 | 3.128300 | 1.551700 |
| C | 3.150400 | 2.485100 | 0.416600 |
| C | 3.119600 | 4.447800 | 1.511900 |
| H | 3.300100 | 5.128100 | 2.330000 |
| C | 2.506400 | 4.633800 | 0.317000 |
| H | 2.036200 | 5.502400 | -0.116500 |
| C | 1.975600 | 3.216900 | -1.657200 |
| H | 1.730700 | 2.159700 | -1.769900 |
| H | 1.064600 | 3.815000 | -1.737600 |
| C | 4.164500 | 2.513700 | 2.690300 |
| H | 4.506100 | 1.519200 | 2.399400 |
| H | 5.025900 | 3.115600 | 2.991600 |
| H | 2.691600 | 3.513100 | -2.430000 |
| H | 3.465700 | 2.427700 | 3.527600 |
| N | 3.577100 | -2.533700 | 0.291100 |
| N | 4.330600 | -1.934100 | -1.625100 |
| C | 3.802900 | -1.446400 | -0.477800 |
| C | 4.422400 | -3.306000 | -1.577800 |
| H | 4.804000 | -3.888700 | -2.402100 |
| C | 3.945000 | -3.682900 | -0.366600 |
| H | 3.829600 | -4.659900 | 0.076000 |
| C | 2.982700 | -2.526000 | 1.615600 |
| H | 2.555600 | -1.538400 | 1.796900 |
| H | 2.189400 | -3.278700 | 1.657400 |
| C | 4.705100 | -1.139900 | -2.778400 |
| H | 4.660400 | -0.085200 | -2.502100 |
| H | 5.724400 | -1.388100 | -3.085700 |
| H | 3.744300 | -2.738000 | 2.372100 |
| H | 4.015500 | -1.328500 | -3.606300 |
| N | 0.543300 | -3.195800 | -1.122200 |
| C | 0.360600 | -2.079100 | -0.827400 |
| N | -0.460900 | 2.759800 | 1.050000 |
| C | -0.272400 | 1.663100 | 0.693400 |
| Ag | 0.049300 | -0.200200 | -0.083500 |
| Au | -3.463600 | -0.446300 | -0.064900 |
| N | -3.432600 | 2.577100 | -0.568700 |
| N | -4.459000 | 2.122700 | 1.257600 |
| C | -3.812200 | 1.546700 | 0.217400 |
| C | -4.471900 | 3.493200 | 1.128500 |
| H | -4.928900 | 4.137800 | 1.863600 |
| C | -3.820600 | 3.778800 | -0.026000 |
| H | -3.584800 | 4.719000 | -0.498500 |
| C | -2.697800 | 2.465800 | -1.815300 |
| H | -2.173800 | 1.509100 | -1.828300 |
| H | -3.383700 | 2.521500 | -2.666400 |
| C | -5.025800 | 1.413300 | 2.388100 |
| H | -4.972500 | 0.342600 | 2.186600 |
| H | -4.461900 | 1.639700 | 3.297600 |
| H | -1.972600 | 3.281900 | -1.861200 |
| H | -6.071700 | 1.702600 | 2.522600 |
| N | -2.565300 | -3.315000 | 0.512000 |
| N | -3.475100 | -3.184500 | -1.425100 |
| C | -3.152500 | -2.445000 | -0.338700 |
| C | -3.083700 | -4.493700 | -1.259500 |
| H | -3.232500 | -5.240900 | -2.023800 |
| C | -2.507800 | -4.574400 | -0.034500 |
| H | -2.028200 | -5.392200 | 0.479600 |
| C | -2.050200 | -2.992200 | 1.830600 |
| H | -1.823700 | -1.925200 | 1.868300 |
| H | -2.792700 | -3.234400 | 2.597200 |
| C | -4.099400 | -2.674600 | -2.630200 |
| H | -4.415500 | -1.646300 | -2.448600 |
| H | -3.388600 | -2.694900 | -3.461500 |
| H | -1.138000 | -3.570400 | 1.995900 |
| H | -4.974200 | -3.281100 | -2.880400 |
| O | 0.534300 | -4.956900 | 1.096800 |
| H | 0.565800 | -4.492300 | 0.232800 |
| C | 1.032600 | -6.271100 | 0.943000 |
| H | 2.101100 | -6.258000 | 0.668100 |
| H | 0.505200 | -6.799500 | 0.132600 |
| C | 0.854200 | -7.012500 | 2.249900 |
| H | 1.255000 | -8.029000 | 2.179900 |
| H | 1.373400 | -6.489700 | 3.060600 |
| H | -0.206800 | -7.077700 | 2.514900 |
| O | -0.720300 | 4.979500 | -0.646900 |
| H | -0.653000 | 4.298000 | 0.058800 |
| C | -0.947500 | 6.236500 | -0.042000 |
| H | -1.868400 | 6.219100 | 0.563600 |
| H | -0.126900 | 6.495100 | 0.647700 |
| C | -1.061000 | 7.287800 | -1.125500 |
| H | -1.891100 | 7.057200 | -1.803000 |
| H | -1.234700 | 8.277500 | -0.689700 |
| H | -0.143100 | 7.329300 | -1.722900 |

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94

Molecule Name

| | | | |
|---|---|---|---|
| Au | -0.402400 | 3.318700 | -0.078200 |
| N | -3.324200 | 2.730700 | -0.790800 |
| N | -3.089500 | 2.948300 | 1.330800 |
| C | -2.401600 | 2.975800 | 0.167200 |
| C | -4.419100 | 2.679800 | 1.106000 |
| H | -5.136600 | 2.613000 | 1.909300 |
| C | -4.566900 | 2.542800 | -0.234800 |
| H | -5.439900 | 2.334200 | -0.833900 |
| C | -3.049100 | 2.560800 | -2.205900 |
| H | -1.980100 | 2.704700 | -2.368300 |
| H | -3.329300 | 1.547300 | -2.511200 |
| C | -2.507500 | 3.054000 | 2.657200 |
| H | -1.478400 | 3.401700 | 2.556000 |
| H | -3.072900 | 3.777400 | 3.250700 |
| H | -3.607700 | 3.298900 | -2.788700 |
| H | -2.526700 | 2.069900 | 3.137000 |
| N | 2.600600 | 3.365700 | 0.503000 |
| N | 2.178600 | 4.349600 | -1.353600 |
| C | 1.586100 | 3.708700 | -0.319800 |
| C | 3.543900 | 4.394200 | -1.184700 |
| H | 4.200800 | 4.846900 | -1.911200 |
| C | 3.809100 | 3.770200 | -0.010700 |
| H | 4.739700 | 3.556700 | 0.490600 |
| C | 2.463000 | 2.660100 | 1.763700 |
| H | 1.565500 | 2.040200 | 1.723500 |
| H | 3.342800 | 2.026100 | 1.897800 |
| C | 1.492500 | 4.868000 | -2.520700 |
| H | 0.421600 | 4.889400 | -2.313900 |
| H | 1.836800 | 5.883900 | -2.729900 |
| H | 2.379900 | 3.371300 | 2.591200 |
| H | 1.684000 | 4.229800 | -3.388100 |
| N | 3.467600 | 0.463800 | -1.212400 |
| C | 2.314900 | 0.301800 | -1.110400 |
| N | -2.728300 | -0.388000 | 0.203300 |
| C | -1.616600 | -0.234500 | -0.129700 |
| Ag | 0.335700 | 0.028900 | -0.679000 |
| Au | 0.690600 | -3.273400 | 0.009700 |
| N | -2.216000 | -3.594400 | -0.895000 |

| | | | |
|---|---|---|---|
| N | -2.088800 | -3.593900 | 1.246700 |
| C | -1.335700 | -3.503400 | 0.127300 |
| C | -3.419700 | -3.728100 | 0.929600 |
| H | -4.186000 | -3.809200 | 1.685000 |
| C | -3.499800 | -3.728900 | -0.424100 |
| H | -4.348000 | -3.810600 | -1.085700 |
| C | -1.894000 | -3.480100 | -2.306000 |
| H | -0.840700 | -3.211800 | -2.399400 |
| H | -2.073100 | -4.432500 | -2.813700 |
| C | -1.600800 | -3.434600 | 2.605100 |
| H | -0.511400 | -3.491200 | 2.589400 |
| H | -1.918900 | -2.462200 | 2.996800 |
| H | -2.515200 | -2.693500 | -2.744600 |
| H | -1.991100 | -4.240300 | 3.232500 |
| N | 3.540200 | -2.406500 | 0.717800 |
| N | 3.533300 | -3.589600 | -1.069200 |
| C | 2.719600 | -3.084500 | -0.113300 |
| C | 4.840300 | -3.221300 | -0.844800 |
| H | 5.642600 | -3.509300 | -1.506500 |
| C | 4.842700 | -2.472100 | 0.284900 |
| H | 5.641400 | -1.967200 | 0.804800 |
| C | 3.129700 | -1.688300 | 1.910000 |
| H | 2.084800 | -1.393500 | 1.799400 |
| H | 3.239200 | -2.324000 | 2.794100 |
| C | 3.098300 | -4.361400 | -2.216600 |
| H | 2.063500 | -4.667500 | -2.057400 |
| H | 3.164300 | -3.757800 | -3.126200 |
| H | 3.755900 | -0.797900 | 2.004900 |
| H | 3.723300 | -5.252000 | -2.321000 |
| O | 5.157900 | 0.830900 | 1.008100 |
| H | 4.689600 | 0.709900 | 0.151900 |
| C | 6.536000 | 1.021300 | 0.750800 |
| H | 6.692900 | 1.881900 | 0.080900 |
| H | 6.963100 | 0.143800 | 0.238800 |
| C | 7.250600 | 1.251000 | 2.064900 |
| H | 7.117100 | 0.393000 | 2.732300 |
| H | 8.323200 | 1.398500 | 1.903400 |
| H | 6.853100 | 2.136900 | 2.571600 |
| O | -4.099400 | -0.863600 | -2.323100 |
| H | -3.754300 | -0.738900 | -1.418400 |
| C | -5.508500 | -0.953500 | -2.265400 |
| H | -5.824400 | -1.792200 | -1.623100 |
| H | -5.943300 | -0.040600 | -1.825600 |
| C | -6.039300 | -1.150200 | -3.668400 |
| H | -7.131700 | -1.221700 | -3.664700 |
| H | -5.748200 | -0.312100 | -4.309800 |
| H | -5.634200 | -2.067800 | -4.107600 |
| C | -4.461300 | -0.580000 | 3.438200 |
| O | -3.127900 | -0.310100 | 3.056900 |
| H | -4.780400 | -1.572300 | 3.077700 |
| H | -5.154200 | 0.152800 | 2.992800 |
| H | -3.077600 | -0.331800 | 2.080300 |
| C | -4.555800 | -0.528600 | 4.947400 |
| H | -4.268200 | 0.460800 | 5.318200 |
| H | -5.577000 | -0.739400 | 5.281100 |
| H | -3.884400 | -1.265800 | 5.399800 |

III-4S2

103

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000700 | 3.239700 | -0.000600 |
| N | 2.867600 | 3.265700 | 1.073700 |
| N | 2.868700 | 3.266600 | -1.071800 |
| C | 2.044400 | 3.262700 | 0.000500 |
| C | 4.184900 | 3.261800 | -0.676200 |
| H | 4.998800 | 3.258900 | -1.384900 |
| C | 4.184200 | 3.261300 | 0.679500 |
| H | 4.997300 | 3.257800 | 1.389000 |
| C | 2.451200 | 3.164700 | 2.460800 |
| H | 1.363000 | 3.227000 | 2.498800 |
| H | 2.781600 | 2.203900 | 2.870000 |
| C | 2.453800 | 3.166300 | -2.459500 |
| H | 1.365700 | 3.229900 | -2.498600 |
| H | 2.882200 | 3.990900 | -3.035900 |
| H | 2.878000 | 3.989700 | 3.037900 |
| H | 2.783500 | 2.205200 | -2.868400 |
| N | -2.866300 | 3.265000 | -1.074800 |
| N | -2.867300 | 3.267200 | 1.070700 |
| C | -2.043100 | 3.262700 | -0.001700 |
| C | -4.183500 | 3.262200 | 0.675100 |
| H | -4.997400 | 3.259500 | 1.383800 |
| C | -4.182900 | 3.260900 | -0.680600 |
| H | -4.996000 | 3.256800 | -1.390100 |
| C | -2.449900 | 3.163900 | -2.462000 |
| H | -1.361600 | 3.225200 | -2.499800 |
| H | -2.781100 | 2.203500 | -2.871300 |
| C | -2.452300 | 3.168200 | 2.458400 |
| H | -1.364200 | 3.230200 | 2.497300 |
| H | -2.879400 | 3.994200 | 3.033800 |
| H | -2.875900 | 3.989400 | -3.038900 |
| H | -2.783300 | 2.208100 | 2.868800 |
| N | -3.221800 | 0.000100 | 0.002900 |
| C | -2.050700 | 0.000100 | 0.001900 |
| N | 3.215500 | -0.000100 | -0.001400 |
| C | 2.044400 | -0.000100 | -0.000500 |
| Ag | -0.003200 | 0.000000 | 0.000700 |
| Au | 0.000300 | -3.239700 | -0.000600 |
| N | 2.867300 | -3.265900 | 1.073700 |
| N | 2.868400 | -3.266700 | -1.071800 |
| C | 2.044100 | -3.262800 | 0.000500 |
| C | 4.184600 | -3.262100 | -0.676200 |
| H | 4.998400 | -3.259200 | -1.384900 |
| C | 4.183900 | -3.261600 | 0.679500 |
| H | 4.997000 | -3.258200 | 1.389000 |
| C | 2.450900 | -3.164900 | 2.460800 |
| H | 1.362700 | -3.227100 | 2.498800 |
| H | 2.877600 | -3.989900 | 3.037900 |
| C | 2.453400 | -3.166500 | -2.459400 |
| H | 1.365400 | -3.230000 | -2.498600 |
| H | 2.783300 | -2.205400 | -2.868400 |
| H | 2.781400 | -2.204100 | 2.870000 |
| H | 2.881800 | -3.991100 | -3.035900 |
| N | -2.866600 | -3.264800 | -1.074800 |
| N | -2.867700 | -3.267000 | 1.070700 |
| C | -2.043400 | -3.262600 | -0.001700 |
| C | -4.183900 | -3.261900 | 0.675100 |
| H | -4.997700 | -3.259100 | 1.383800 |
| C | -4.183200 | -3.260600 | -0.680600 |
| H | -4.996300 | -3.256500 | -1.390100 |
| C | -2.450100 | -3.163800 | -2.461900 |
| H | -1.361900 | -3.225200 | -2.499800 |
| H | -2.876200 | -3.989200 | -3.038900 |
| C | -2.452700 | -3.168000 | 2.458400 |
| H | -1.364500 | -3.230100 | 2.497300 |
| H | -2.783600 | -2.207900 | 2.868800 |
| H | -2.781300 | -2.203300 | -2.871300 |

| | | | |
|---|---|---|---|
| H | -2.879800 | -3.994000 | 3.033800 |
| O | -3.853000 | 0.000100 | -2.848800 |
| H | -3.741400 | 0.000100 | -1.878800 |
| C | -5.236600 | 0.000200 | -3.140200 |
| H | -5.729500 | 0.884300 | -2.703400 |
| H | -5.729600 | -0.884000 | -2.703500 |
| C | -5.415500 | 0.000200 | -4.642300 |
| H | -4.948000 | -0.885400 | -5.085000 |
| H | -6.477700 | 0.000200 | -4.907700 |
| H | -4.947900 | 0.885800 | -5.085000 |
| O | 3.850300 | -0.000200 | 2.849400 |
| H | 3.737600 | -0.000200 | 1.879600 |
| C | 5.234300 | -0.000200 | 3.139300 |
| H | 5.726600 | -0.884400 | 2.702000 |
| H | 5.726700 | 0.883900 | 2.702000 |
| C | 5.414800 | -0.000200 | 4.641200 |
| H | 6.477300 | -0.000200 | 4.905400 |
| H | 4.947800 | 0.885400 | 5.084400 |
| H | 4.947700 | -0.885800 | 5.084400 |
| C | 5.232100 | -0.000300 | -3.143300 |
| O | 3.848600 | -0.000200 | -2.851600 |
| H | 5.725000 | -0.884400 | -2.706500 |
| H | 5.725200 | 0.883900 | -2.706500 |
| H | 3.737000 | -0.000200 | -1.881600 |
| C | 5.410900 | -0.000300 | -4.645400 |
| H | 4.943300 | 0.885300 | -5.088000 |
| H | 6.473000 | -0.000300 | -4.910900 |
| H | 4.943200 | -0.885800 | -5.088000 |
| C | -5.229100 | 0.000300 | 3.150400 |
| O | -3.846000 | 0.000100 | 2.856700 |
| H | -5.722800 | -0.883800 | 2.714400 |
| H | -5.722600 | 0.884500 | 2.714300 |
| H | -3.736000 | 0.000100 | 1.886500 |
| C | -5.405600 | 0.000400 | 4.652700 |
| H | -6.467300 | 0.000600 | 4.919800 |
| H | -4.937400 | -0.885200 | 5.094700 |
| H | -4.937200 | 0.886000 | 5.094600 |

## 19. The $T_1$ .xyz files of I and its complexes

I

67
Molecule Name

| | | | |
|---|---|---|---|
| Au | 2.767000 | 0.000000 | 0.000000 |
| N | 2.863400 | -2.868900 | 1.031100 |
| N | 2.883200 | -2.832400 | -1.122500 |
| C | 2.856900 | -2.025900 | -0.031900 |
| C | 2.921200 | -4.155900 | -0.746000 |
| H | 2.957300 | -4.958700 | -1.466200 |
| C | 2.909100 | -4.178900 | 0.610800 |
| H | 2.933200 | -5.005600 | 1.303900 |
| C | 2.866700 | -2.435200 | 2.416300 |
| H | 2.008800 | -1.786800 | 2.612100 |
| H | 2.806500 | -3.314800 | 3.059300 |
| C | 2.907400 | -2.351500 | -2.491900 |
| H | 3.821700 | -1.777500 | -2.669300 |
| H | 2.889800 | -3.209800 | -3.165300 |
| N | 0.001000 | -0.006500 | 3.161400 |
| C | 0.000700 | -0.003900 | 1.991000 |
| H | 3.791900 | -1.894500 | 2.637100 |
| H | 2.036000 | -1.721300 | -2.687800 |
| N | 2.862900 | 2.868900 | -1.031200 |
| N | 2.882800 | 2.832500 | 1.122400 |
| C | 2.856600 | 2.026000 | 0.031900 |
| C | 2.920500 | 4.156000 | 0.745900 |
| H | 2.956500 | 4.958800 | 1.466000 |
| C | 2.908300 | 4.178900 | -0.610900 |
| H | 2.932300 | 5.005600 | -1.304000 |
| C | 2.866100 | 2.435100 | -2.416300 |
| H | 2.008000 | 1.786900 | -2.612100 |
| H | 2.806100 | 3.314700 | -3.059300 |
| C | 2.907200 | 2.351700 | 2.491900 |
| H | 3.821600 | 1.777800 | 2.669200 |
| H | 2.889800 | 3.210100 | 3.165300 |
| N | 0.000500 | 0.006400 | -3.161600 |
| C | 0.000400 | 0.003700 | -1.991200 |
| H | 3.791100 | 1.894200 | -2.637000 |
| H | 2.035900 | 1.721600 | 2.688100 |
| Au | -2.766100 | 0.000000 | 0.000100 |
| N | -2.887600 | -2.832500 | 1.121400 |
| N | -2.859600 | -2.868900 | -1.032100 |
| C | -2.856500 | -2.025900 | 0.031000 |
| C | -2.908900 | -4.178900 | -0.611900 |
| H | -2.931400 | -5.005600 | -1.305200 |
| C | -2.925800 | -4.155900 | 0.744700 |
| H | -2.964300 | -4.958700 | 1.464800 |
| C | -2.914700 | -2.351700 | 2.490800 |
| H | -2.041900 | -1.724600 | 2.690000 |
| H | -3.827800 | -1.774700 | 2.665200 |
| C | -2.862800 | -2.435600 | -2.417300 |
| H | -3.805800 | -1.932400 | -2.651400 |
| H | -2.028500 | -1.754100 | -2.601000 |
| H | -2.902500 | -3.210300 | 3.164100 |
| H | -2.757600 | -3.311700 | -3.059300 |
| N | -2.887200 | 2.832500 | -1.121300 |
| N | -2.858900 | 2.869000 | 1.032200 |
| C | -2.856100 | 2.026000 | -0.030800 |
| C | -2.908000 | 4.179000 | 0.612000 |
| H | -2.930200 | 5.005700 | 1.305300 |
| C | -2.925100 | 4.155900 | -0.744600 |
| H | -2.963500 | 4.958700 | -1.464700 |
| C | -2.914800 | 2.351700 | -2.490700 |
| H | -2.042200 | 1.724300 | -2.689900 |
| H | -3.828000 | 1.775100 | -2.664900 |
| C | -2.862100 | 2.435800 | 2.417400 |
| H | -3.805500 | 1.933400 | 2.651900 |
| H | -2.028300 | 1.753500 | 2.601000 |
| H | -2.902300 | 3.210300 | -3.164000 |
| H | -2.755900 | 3.311900 | 3.059400 |
| Au | 0.000500 | -0.000100 | -0.000100 |

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73
Molecule Name

| | | | |
|---|---|---|---|
| Au | 2.767500 | -0.138400 | -0.150900 |
| N | 2.962300 | -2.639100 | 1.587600 |
| N | 3.004400 | -3.157900 | -0.502400 |
| C | 2.935100 | -2.098900 | 0.342900 |
| C | 3.090300 | -4.337000 | 0.202700 |
| H | 3.162000 | -5.296400 | -0.286000 |
| C | 3.065000 | -4.010600 | 1.519400 |
| H | 3.112800 | -4.629500 | 2.402100 |
| C | 2.944500 | -1.863600 | 2.813000 |
| H | 2.123400 | -1.142800 | 2.786000 |
| H | 2.796800 | -2.540300 | 3.656400 |
| C | 3.025000 | -3.045400 | -1.949300 |
| H | 3.931400 | -2.523300 | -2.270400 |
| H | 3.020400 | -4.048300 | -2.379200 |
| N | 0.000200 | 0.774900 | 2.901800 |
| C | 0.000100 | 0.385200 | 1.798200 |
| H | 3.893600 | -1.334000 | 2.940800 |
| H | 2.144000 | -2.500900 | -2.298100 |
| N | 2.758300 | 2.342200 | -1.915500 |
| N | 2.776400 | 2.907700 | 0.162600 |
| C | 2.787700 | 1.829900 | -0.659100 |
| C | 2.751400 | 4.073900 | -0.567300 |
| H | 2.740900 | 5.045100 | -0.097000 |
| C | 2.743300 | 3.718200 | -1.876600 |
| H | 2.731600 | 4.319400 | -2.772800 |
| C | 2.795400 | 1.541900 | -3.125700 |
| H | 2.013500 | 0.779100 | -3.096900 |
| H | 2.624300 | 2.194700 | -3.983300 |
| C | 2.818700 | 2.858300 | 1.613200 |
| H | 3.753300 | 3.301800 | 1.970200 |
| H | 1.958800 | 3.384700 | 2.039900 |
| N | -0.000300 | -1.099400 | -3.136200 |
| C | -0.000100 | -0.769500 | -2.013100 |
| H | 3.773300 | 1.062500 | -3.231500 |
| H | 2.775400 | 1.813600 | 1.922900 |
| Au | -2.767500 | -0.137800 | -0.150800 |
| N | -2.963000 | -2.638300 | 1.588000 |
| N | -3.005400 | -3.157200 | -0.501900 |
| C | -2.935700 | -2.098200 | 0.343200 |
| C | -3.091700 | -4.336200 | 0.203300 |
| H | -3.163800 | -5.295700 | -0.285300 |
| C | -3.066300 | -4.009700 | 1.519900 |
| H | -3.114300 | -4.628600 | 2.402700 |
| C | -2.944900 | -1.862700 | 2.813300 |
| H | -2.124100 | -1.141700 | 2.785900 |
| H | -3.894100 | -1.333400 | 2.941600 |
| C | -3.026100 | -3.044900 | -1.948900 |

H -3.932300 -2.522600 -2.270000
H -2.144900 -2.500600 -2.297700
H -2.796600 -2.539300 3.656700
H -3.021600 -4.047800 -2.378700
N -2.757800 2.342500 -1.915800
N -2.775500 2.908400 0.162200
C -2.787200 1.830400 -0.659300
C -2.750400 4.074400 -0.567900
H -2.739700 5.045700 -0.097800
C -2.742500 3.718500 -1.877100
H -2.730800 4.319500 -2.773400
C -2.795500 1.542100 -3.125800
H -3.774000 1.063900 -3.232000
H -2.623200 2.194500 -3.983500
C -2.817500 2.859200 1.612900
H -3.751700 3.303400 1.970000
H -2.774800 1.814600 1.922800
H -2.014500 0.778300 -3.096600
H -1.957200 3.385300 2.039300
Au 0.000000 -0.201600 -0.105400
O 0.000700 3.651200 3.178700
H 0.000400 2.677100 3.253200
C 0.000700 4.194400 4.482000
H 0.891500 3.901400 5.055500
H 0.001500 5.283300 4.383300
H -0.890900 3.902600 5.055000

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79
Molecule Name
Au -2.847800 0.003400 -0.000200
N -2.774300 -2.934100 -0.902400
N -3.437100 -2.751500 1.133500
C -3.033500 -2.022800 0.064700
C -3.430700 -4.095400 0.837700
H -3.714100 -4.845600 1.559500
C -3.017800 -4.209700 -0.448300
H -2.871500 -5.076400 -1.072700
C -2.269800 -2.631900 -2.225600
H -1.834100 -1.630000 -2.207800
H -1.493400 -3.360500 -2.470700
C -3.726100 -2.198200 2.439400
H -4.205300 -1.223500 2.316800
H -4.408800 -2.865200 2.970000
H -3.074500 -2.666900 -2.966700
H -2.802800 -2.085300 3.015500
N -2.767000 2.940300 0.902700
N -3.430900 2.760100 -1.133000
C -3.028500 2.030000 -0.064700
C -3.421400 4.103800 -0.836600
H -3.703600 4.854900 -1.558000
C -3.007800 4.216600 0.449300
H -2.859400 5.082700 1.073900
C -2.262500 2.636500 2.225500
H -1.829500 1.633400 2.207300
H -1.483900 3.362900 2.470400
C -3.721700 2.207900 -2.439100
H -4.202400 1.233900 -2.316600
H -4.403700 2.876300 -2.968800
H -3.066600 2.673500 2.967100
H -2.799000 2.093800 -3.015800
N -0.017500 2.922000 -1.202500
C -0.010300 1.820700 -0.804700
N -0.025100 -2.922300 1.202800
C -0.015200 -1.820900 0.805100
Au -0.004700 -0.000100 0.000200
Au 2.841200 -0.003300 0.000100
N 2.873400 -2.987500 -0.720800
N 3.318500 -2.677400 1.358800
C 3.024000 -2.017800 0.212200
C 3.353200 -4.036000 1.144300
H 3.564000 -4.738800 1.935400
C 3.077900 -4.231100 -0.168600
H 3.006200 -5.134900 -0.752200
C 2.515200 -2.769100 -2.106500
H 2.098300 -1.764000 -2.201100
H 3.392800 -2.861800 -2.754000
C 3.458100 -2.040600 2.650700
H 4.028700 -1.115000 2.538600
H 2.471700 -1.818800 3.069400
H 1.755000 -3.503000 -2.384400
H 3.997200 -2.710000 3.323800
N 2.881100 2.981100 0.720200
N 3.324500 2.669500 -1.359400
C 3.029000 2.010900 -0.212600
C 3.362100 4.028100 -1.145400
H 3.574100 4.730200 -1.936800
C 3.088000 4.224100 0.167600
H 3.018700 5.128200 0.751100
C 2.523200 2.764000 2.106200
H 2.104300 1.759800 2.201500
H 3.401400 2.855100 2.753200
C 3.461200 2.032300 -2.651500
H 4.025200 1.102700 -2.538800
H 2.473900 1.817500 -3.071500
H 1.764700 3.499600 2.384300
H 4.006000 2.698100 -3.323600
O 0.065100 4.778300 1.080400
H 0.039800 4.234400 0.268700
C 0.044800 6.133300 0.694400
H -0.867100 6.396800 0.138600
H 0.077600 6.737700 1.605500
H 0.909000 6.403900 0.070100
O 0.053200 -4.778800 -1.080300
H 0.029100 -4.235100 -0.268500
C 0.030500 -6.133900 -0.694700
H 0.061600 -6.738100 -1.606100
H 0.894500 -6.406400 -0.071000
H -0.881600 -6.395800 -0.138500

I-3S1

85
Molecule Name
Au -0.119800 2.843900 0.090800
N 2.772700 2.922400 1.108900
N 2.689100 3.251200 -1.014700
C 1.909400 3.024000 0.070000
C 4.017000 3.292700 -0.657400
H 4.801800 3.463100 -1.378300
C 4.069300 3.089300 0.682300
H 4.905300 3.052300 1.363000
C 2.404500 2.625800 2.478300
H 1.385800 2.231200 2.482200
H 3.086600 1.863400 2.863500
C 2.208000 3.316700 -2.381700
H 1.174000 3.669200 -2.372600

| | | | |
|---|---|---|---|
| H | 2.816700 | 4.029700 | -2.943200 |
| H | 2.448700 | 3.527900 | 3.096300 |
| H | 2.262100 | 2.328900 | -2.852900 |
| N | -3.009800 | 2.794300 | -0.937600 |
| N | -2.922500 | 3.425000 | 1.115000 |
| C | -2.145400 | 3.033000 | 0.076400 |
| C | -4.250500 | 3.432400 | 0.753800 |
| H | -5.033500 | 3.709300 | 1.442600 |
| C | -4.304300 | 3.039400 | -0.542500 |
| H | -5.140300 | 2.906700 | -1.210200 |
| C | -2.644200 | 2.318200 | -2.255800 |
| H | -1.657100 | 1.854100 | -2.195600 |
| H | -3.377500 | 1.569700 | -2.565100 |
| C | -2.428100 | 3.694300 | 2.448400 |
| H | -1.482100 | 4.237500 | 2.380400 |
| H | -3.153400 | 4.311800 | 2.981800 |
| H | -2.614700 | 3.144400 | -2.973100 |
| H | -2.276700 | 2.757600 | 2.993400 |
| N | -3.215500 | -0.000500 | 0.980600 |
| C | -2.066800 | -0.000300 | 0.756400 |
| N | 2.923400 | 0.000300 | -0.503500 |
| C | 1.783000 | 0.000100 | -0.231500 |
| Au | -0.140500 | -0.000200 | 0.261800 |
| Au | -0.119100 | -2.844200 | 0.090600 |
| N | 2.773100 | -2.921300 | 1.109700 |
| N | 2.690400 | -3.251000 | -1.013800 |
| C | 1.910200 | -3.023700 | 0.070500 |
| C | 4.018200 | -3.291900 | -0.656000 |
| H | 4.803200 | -3.462200 | -1.376600 |
| C | 4.069900 | -3.088000 | 0.683700 |
| H | 4.905700 | -3.050600 | 1.364600 |
| C | 2.404200 | -2.624500 | 2.478900 |
| H | 1.385900 | -2.228900 | 2.482000 |
| H | 2.447300 | -3.526600 | 3.096900 |
| C | 2.209700 | -3.317400 | -2.380900 |
| H | 1.176300 | -3.671700 | -2.372100 |
| H | 2.262200 | -2.329500 | -2.852200 |
| H | 3.086700 | -1.862600 | 2.864600 |
| H | 2.819900 | -4.029200 | -2.942200 |
| N | -3.008900 | -2.794300 | -0.938600 |
| N | -2.922000 | -3.426100 | 1.113800 |
| C | -2.144700 | -3.033500 | 0.075500 |
| C | -4.249800 | -3.433300 | 0.752300 |
| H | -5.033000 | -3.710500 | 1.440900 |
| C | -4.303500 | -3.039500 | -0.543700 |
| H | -5.139400 | -2.906500 | -1.211600 |
| C | -2.643000 | -2.317900 | -2.256500 |
| H | -1.655900 | -1.853900 | -2.196000 |
| H | -2.613400 | -3.143900 | -2.974100 |
| C | -2.427800 | -3.695900 | 2.447100 |
| H | -1.482200 | -4.239800 | 2.379100 |
| H | -2.275700 | -2.759400 | 2.992200 |
| H | -3.376200 | -1.569200 | -2.565800 |
| H | -3.153600 | -4.313000 | 2.980400 |
| O | -4.885600 | 0.000100 | -1.393500 |
| H | -4.409900 | 0.000100 | -0.538500 |
| C | -6.268000 | -0.000100 | -1.120900 |
| H | -6.583600 | 0.888600 | -0.554600 |
| H | -6.583200 | -0.888600 | -0.554200 |
| H | -6.795200 | -0.000400 | -2.079200 |
| O | 4.493500 | 0.000700 | 1.959400 |
| H | 4.071200 | 0.000400 | 1.079300 |
| C | 5.890400 | 0.000800 | 1.777500 |
| H | 6.244000 | -0.888000 | 1.234000 |
| H | 6.243900 | 0.889400 | 1.233500 |
| H | 6.353000 | 0.001100 | 2.768400 |
| C | 4.159100 | 0.001700 | -4.046900 |
| O | 2.908000 | 0.001400 | -3.398000 |
| H | 4.758100 | -0.889600 | -3.806500 |
| H | 4.758700 | 0.892100 | -3.804800 |
| H | 3.061500 | 0.001300 | -2.435200 |
| H | 3.970900 | 0.002800 | -5.123700 |

I-4S1

91

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000000 | 2.853600 | 0.000000 |
| N | 2.853600 | 3.106000 | 1.075200 |
| N | 2.853600 | 3.106000 | -1.075200 |
| C | 2.031800 | 3.036300 | 0.000000 |
| C | 4.165300 | 3.222200 | -0.677800 |
| H | 4.975500 | 3.297400 | -1.386700 |
| C | 4.165300 | 3.222200 | 0.677800 |
| H | 4.975500 | 3.297400 | 1.386700 |
| C | 2.441800 | 2.985800 | 2.460400 |
| H | 1.356700 | 2.876300 | 2.489000 |
| H | 2.909900 | 2.099700 | 2.901400 |
| C | 2.441800 | 2.985800 | -2.460400 |
| H | 1.356700 | 2.876300 | -2.489000 |
| H | 2.724900 | 3.884100 | -3.016800 |
| H | 2.724900 | 3.884100 | 3.016800 |
| H | 2.909900 | 2.099700 | -2.901400 |
| N | -2.853600 | 3.106000 | -1.075200 |
| N | -2.853600 | 3.106000 | 1.075200 |
| C | -2.031800 | 3.036300 | 0.000000 |
| C | -4.165300 | 3.222200 | 0.677800 |
| H | -4.975500 | 3.297400 | 1.386700 |
| C | -4.165300 | 3.222200 | -0.677800 |
| H | -4.975500 | 3.297400 | -1.386700 |
| C | -2.441800 | 2.985800 | -2.460400 |
| H | -1.356700 | 2.876300 | -2.489000 |
| H | -2.909900 | 2.099700 | -2.901400 |
| C | -2.441800 | 2.985800 | 2.460400 |
| H | -1.356700 | 2.876300 | 2.489000 |
| H | -2.724900 | 3.884100 | 3.016800 |
| H | -2.724900 | 3.884100 | -3.016800 |
| H | -2.909900 | 2.099700 | 2.901400 |
| N | -3.153900 | 0.000000 | 0.000000 |
| C | -1.981900 | 0.000000 | 0.000000 |
| N | 3.153900 | 0.000000 | 0.000000 |
| C | 1.981900 | 0.000000 | 0.000000 |
| Au | 0.000000 | 0.000000 | 0.000000 |
| Au | 0.000000 | -2.853600 | 0.000000 |
| N | 2.853600 | -3.106000 | 1.075200 |
| N | 2.853600 | -3.106000 | -1.075200 |
| C | 2.031800 | -3.036300 | 0.000000 |
| C | 4.165300 | -3.222200 | -0.677800 |
| H | 4.975500 | -3.297400 | -1.386700 |
| C | 4.165300 | -3.222200 | 0.677800 |
| H | 4.975500 | -3.297400 | 1.386700 |
| C | 2.441800 | -2.985800 | 2.460400 |
| H | 1.356700 | -2.876300 | 2.489000 |
| H | 2.724900 | -3.884100 | 3.016800 |
| C | 2.441800 | -2.985800 | -2.460400 |
| H | 1.356700 | -2.876300 | -2.489000 |
| H | 2.909900 | -2.099700 | -2.901400 |
| H | 2.909900 | -2.099700 | 2.901400 |

| | | | |
|---|---|---|---|
| H | 2.724900 | -3.884100 | -3.016800 |
| N | -2.853600 | -3.106000 | -1.075200 |
| N | -2.853600 | -3.106000 | 1.075200 |
| C | -2.031800 | -3.036300 | 0.000000 |
| C | -4.165300 | -3.222200 | 0.677800 |
| H | -4.975500 | -3.297400 | 1.386700 |
| C | -4.165300 | -3.222200 | -0.677800 |
| H | -4.975500 | -3.297400 | -1.386700 |
| C | -2.441800 | -2.985800 | -2.460400 |
| H | -1.356700 | -2.876300 | -2.489000 |
| H | -2.724900 | -3.884100 | -3.016800 |
| C | -2.441800 | -2.985800 | 2.460400 |
| H | -1.356700 | -2.876300 | 2.489000 |
| H | -2.909900 | -2.099700 | 2.901400 |
| H | -2.909900 | -2.099700 | -2.901400 |
| H | -2.724900 | -3.884100 | 3.016800 |
| O | -4.108600 | 0.000000 | -2.725700 |
| H | -3.906700 | 0.000000 | -1.770600 |
| C | -5.508600 | 0.000000 | -2.881000 |
| H | -5.981400 | 0.889800 | -2.438300 |
| H | -5.981400 | -0.889800 | -2.438300 |
| H | -5.721800 | 0.000000 | -3.953200 |
| O | 4.108600 | 0.000000 | 2.725700 |
| H | 3.906700 | 0.000000 | 1.770600 |
| C | 5.508600 | 0.000000 | 2.881000 |
| H | 5.981400 | -0.889800 | 2.438300 |
| H | 5.981400 | 0.889800 | 2.438300 |
| H | 5.721800 | 0.000000 | 3.953200 |
| C | 5.508600 | 0.000000 | -2.881000 |
| O | 4.108600 | 0.000000 | -2.725700 |
| H | 5.981400 | -0.889800 | -2.438300 |
| H | 5.981400 | 0.889800 | -2.438300 |
| H | 3.906700 | 0.000000 | -1.770600 |
| H | 5.721800 | 0.000000 | -3.953200 |
| C | -5.508600 | 0.000000 | 2.881000 |
| O | -4.108600 | 0.000000 | 2.725700 |
| H | -5.981400 | -0.889800 | 2.438300 |
| H | -5.981400 | 0.889800 | 2.438300 |
| H | -3.906700 | 0.000000 | 1.770600 |
| H | -5.721800 | 0.000000 | 3.953200 |

## 20. The $T_1$ .xyz files of II and its complexes

II

91
Molecule Name
Au 0.000000 2.768000 -0.000600
N 2.983000 2.610500 0.611500
N 2.630300 3.009100 -1.499400
C 2.006500 2.826800 -0.308700
C 4.230500 2.668500 0.013900
C 5.517900 2.540400 0.527200
H 5.699100 2.365300 1.582700
C 6.567900 2.653000 -0.377900
H 7.588400 2.560700 -0.019200
C 6.339700 2.887100 -1.741900
H 7.187500 2.968600 -2.415000
C 5.053100 3.020300 -2.253200
H 4.881600 3.198400 -3.309800
C 4.002500 2.911300 -1.346700
C 1.963200 3.241600 -2.764300
H 0.960500 3.624000 -2.562800
H 1.884200 2.312600 -3.335900
H 2.518300 3.994000 -3.330700
C 2.767200 2.391300 2.024600
H 1.724000 2.115200 2.188900
H 3.004400 3.293700 2.597700
H 3.401900 1.568800 2.366200
N -2.983100 2.607700 -0.611900
N -2.630000 3.008400 1.498500
C -2.006500 2.825700 0.307800
C -4.230400 2.665000 -0.013900
C -5.517900 2.535200 -0.526600
H -5.699300 2.359100 -1.582000
C -6.567700 2.647500 0.378700
H -7.588200 2.553900 0.020500
C -6.339200 2.882900 1.742400
H -7.186800 2.964000 2.415800
C -5.052600 3.017800 2.253200
H -4.880900 3.196900 3.309500
C -4.002100 2.909100 1.346400
C -1.962400 3.242400 2.762900
H -0.961300 3.628600 2.560600
H -2.519700 3.992600 3.330300
H -1.879700 2.313400 3.333900
C -2.767700 2.387600 -2.025000
H -1.724100 2.113000 -2.189500
H -3.401200 1.563800 -2.365500
H -3.006600 3.289100 -2.598700
N -0.661900 0.016500 3.093200
C -0.412900 0.012800 1.951100
N 0.663200 0.015600 -3.092700
C 0.413600 0.012200 -1.950800
Au -0.000300 -2.750700 0.001500
N 2.608400 -2.756900 1.576500
N 2.982000 -2.851900 -0.567200
C 1.994400 -2.813700 0.364900
C 3.984000 -2.779800 1.422200
C 5.027600 -2.772500 2.343500
H 4.847300 -2.758100 3.413600
C 6.320200 -2.796100 1.829600
H 7.162300 -2.794600 2.514800
C 6.560500 -2.829100 0.448500
H 7.584400 -2.847400 0.088300
C 5.517600 -2.844200 -0.472000
H 5.708900 -2.869100 -1.539800
C 4.224300 -2.824800 0.042300
C 2.771100 -2.881600 -1.999300
H 1.774900 -3.280000 -2.199300
H 3.511500 -3.541400 -2.458700
H 2.843500 -1.878600 -2.429100
C 1.928000 -2.755300 2.854200
H 0.933400 -2.323200 2.734000
H 2.483700 -2.130800 3.557700
H 1.851000 -3.771700 3.254300
N -2.607200 -2.757100 -1.575600
N -2.984100 -2.845700 0.567700
C -1.995000 -2.811300 -0.363000
C -3.983100 -2.778200 -1.423400
C -5.025400 -2.772200 -2.346100
H -4.843700 -2.760700 -3.416000
C -6.318700 -2.793400 -1.833800
H -7.159900 -2.792900 -2.520200
C -6.560900 -2.822700 -0.452900
H -7.585400 -2.839300 -0.094200
C -5.519300 -2.836500 0.468900
H -5.711900 -2.858700 1.536600
C -4.225400 -2.819400 -0.043700
C -2.776600 -2.872100 2.000300
H -1.774200 -3.253000 2.203000
H -2.867000 -1.870300 2.429600
H -3.507100 -3.544200 2.458200
C -1.924800 -2.759100 -2.852300
H -0.930400 -2.326700 -2.731800
H -1.847200 -3.776700 -3.249400
H -2.479400 -2.136700 -3.558400
Au 0.000200 0.004100 0.000200

II-S1

97
Molecule Name
Au -0.104200 2.772000 -0.119700
N -2.998600 2.921800 -1.036900
N -2.873400 2.957300 1.136600
C -2.125300 2.895200 0.003900
C -4.217700 3.064800 0.823300
C -2.624800 2.887900 -2.435000
H -1.673800 2.363200 -2.542700
H -3.381700 2.334700 -2.995700
C -2.344900 2.968600 2.483700
H -1.369500 2.479800 2.491100
H -2.253600 3.993800 2.857500
N -0.171500 0.016400 -3.280400
C -0.162100 0.014000 -2.111400
H -2.542500 3.901900 -2.840300
H -3.012900 2.402400 3.137200
N 2.822600 2.726400 0.743500
N 2.636100 2.818000 -1.424400
C 1.921900 2.802900 -0.268400
C 3.991900 2.748700 -1.154500
C 2.507000 2.732600 2.157400
H 1.422400 2.757300 2.268600
H 2.888100 1.830700 2.648300
C 2.067300 2.885300 -2.753900

| | | | |
|---|---|---|---|
| H | 1.058900 | 3.297100 | -2.683400 |
| H | 2.675400 | 3.550400 | -3.372700 |
| N | 0.039100 | -0.008700 | 3.036300 |
| C | -0.056100 | -0.003200 | 1.870800 |
| H | 2.935700 | 3.624300 | 2.626600 |
| H | 2.011400 | 1.893300 | -3.210500 |
| Au | -0.068300 | -2.756000 | -0.151300 |
| N | -2.932300 | -2.956400 | -1.159700 |
| N | -2.869900 | -2.985100 | 1.016500 |
| C | -2.090300 | -2.911700 | -0.094200 |
| C | -4.202300 | -3.118300 | 0.664700 |
| C | -2.519800 | -2.920200 | -2.546900 |
| H | -1.579400 | -2.373100 | -2.630900 |
| H | -2.402900 | -3.933800 | -2.944500 |
| C | -2.381600 | -2.981100 | 2.378700 |
| H | -1.418200 | -2.469900 | 2.414400 |
| H | -3.082100 | -2.429200 | 3.010100 |
| H | -3.273300 | -2.387000 | -3.131200 |
| H | -2.278100 | -4.002900 | 2.758600 |
| N | 2.814400 | -2.761200 | 0.838100 |
| N | 2.732900 | -2.712600 | -1.337200 |
| C | 1.963300 | -2.766900 | -0.218400 |
| C | 4.074200 | -2.678900 | -0.998500 |
| C | 2.433600 | -2.839700 | 2.233900 |
| H | 1.344800 | -2.847900 | 2.296300 |
| H | 2.825000 | -3.764100 | 2.671600 |
| C | 2.240000 | -2.686500 | -2.697000 |
| H | 1.168000 | -2.884600 | -2.687700 |
| H | 2.406200 | -1.705400 | -3.150400 |
| H | 2.809700 | -1.971200 | 2.785700 |
| H | 2.743000 | -3.459500 | -3.285500 |
| Au | -0.126400 | 0.007400 | -0.120700 |
| C | -4.242600 | -3.100000 | -0.735600 |
| C | -5.442700 | -3.217800 | -1.430900 |
| C | -6.599700 | -3.350000 | -0.670300 |
| H | -5.479500 | -3.217100 | -2.515500 |
| C | -5.359500 | -3.255000 | 1.426000 |
| C | -6.559100 | -3.368200 | 0.731300 |
| H | -7.555900 | -3.449200 | -1.174600 |
| H | -5.332200 | -3.282200 | 2.510500 |
| H | -7.484500 | -3.481000 | 1.287400 |
| C | 4.126000 | -2.711900 | 0.400300 |
| C | 5.336500 | -2.704100 | 1.086900 |
| C | 6.492900 | -2.660200 | 0.315800 |
| H | 5.377500 | -2.727100 | 2.171000 |
| C | 5.231200 | -2.634500 | -1.771100 |
| C | 6.441400 | -2.626300 | -1.085900 |
| H | 7.459200 | -2.653500 | 0.810400 |
| H | 5.195200 | -2.608300 | -2.855500 |
| H | 7.368700 | -2.594400 | -1.649600 |
| C | -4.298400 | 3.042200 | -0.575200 |
| C | -5.520300 | 3.136200 | -1.235400 |
| C | -5.354600 | 3.182100 | 1.617700 |
| C | -6.656900 | 3.249000 | -0.441600 |
| H | -5.588600 | 3.131900 | -2.318400 |
| C | -6.575900 | 3.271600 | 0.958100 |
| H | -5.296000 | 3.212700 | 2.700900 |
| H | -7.629100 | 3.329200 | -0.918000 |
| H | -7.486600 | 3.368900 | 1.540800 |
| C | 4.110700 | 2.694800 | 0.240100 |
| C | 5.352200 | 2.636600 | 0.866500 |
| C | 5.111600 | 2.740900 | -1.981500 |
| C | 6.470800 | 2.630000 | 0.040500 |
| H | 5.444000 | 2.594200 | 1.946900 |
| C | 6.352700 | 2.681400 | -1.356400 |
| H | 5.026200 | 2.778000 | -3.062800 |
| H | 7.459100 | 2.585000 | 0.487400 |
| H | 7.251700 | 2.675300 | -1.965000 |
| H | 1.805600 | -0.027400 | 3.831000 |
| O | 2.769200 | -0.041200 | 3.988500 |
| C | 2.991200 | 0.013100 | 5.381400 |
| H | 2.594800 | 0.934500 | 5.831100 |
| H | 2.550900 | -0.845700 | 5.907700 |
| H | 4.072600 | -0.006500 | 5.541800 |

II-2S1

103

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000100 | -2.858500 | -0.000100 |
| N | 2.922000 | -3.061700 | -0.859100 |
| N | 2.713400 | -3.307200 | 1.290500 |
| C | 2.017100 | -3.071000 | 0.149000 |
| C | 4.060300 | -3.454900 | 1.014800 |
| C | 2.643300 | -2.758300 | -2.246300 |
| H | 1.587400 | -2.497300 | -2.337900 |
| H | 3.256400 | -1.903800 | -2.554200 |
| C | 2.151400 | -3.361700 | 2.619200 |
| H | 1.063000 | -3.363100 | 2.539300 |
| H | 2.470300 | -4.279000 | 3.123200 |
| H | 2.856800 | -3.628000 | -2.876300 |
| H | 2.470900 | -2.492700 | 3.203100 |
| N | -2.921900 | -3.061300 | 0.858900 |
| N | -2.713100 | -3.307300 | -1.290700 |
| C | -2.016900 | -3.070900 | -0.149100 |
| C | -4.060100 | -3.454800 | -1.015000 |
| C | -2.643100 | -2.757600 | 2.246000 |
| H | -1.587000 | -2.497500 | 2.337800 |
| H | -3.255700 | -1.902700 | 2.553600 |
| C | -2.151100 | -3.362400 | -2.619300 |
| H | -1.062700 | -3.361800 | -2.539500 |
| H | -2.468500 | -4.280800 | -3.122300 |
| H | -2.857400 | -3.627100 | 2.876200 |
| H | -2.472100 | -2.494500 | -3.204200 |
| C | 4.192600 | -3.303500 | -0.370200 |
| C | 5.425100 | -3.431200 | -1.003300 |
| C | 5.156300 | -3.724900 | 1.828200 |
| C | 6.521800 | -3.703400 | -0.191800 |
| H | 5.527400 | -3.322900 | -2.078100 |
| C | 6.390300 | -3.844800 | 1.197700 |
| H | 5.058700 | -3.837500 | 2.903200 |
| H | 7.502300 | -3.813100 | -0.645000 |
| H | 7.271700 | -4.057000 | 1.794800 |
| C | -4.192500 | -3.303000 | 0.370000 |
| C | -5.425000 | -3.430200 | 1.003000 |
| C | -5.156100 | -3.724800 | -1.828400 |
| C | -6.521700 | -3.702300 | 0.191500 |
| H | -5.527400 | -3.321600 | 2.077700 |
| C | -6.390100 | -3.844200 | -1.198000 |
| H | -5.058400 | -3.837800 | -2.903300 |
| H | -7.502300 | -3.811600 | 0.644600 |
| H | -7.271600 | -4.056400 | -1.795100 |
| N | -3.137800 | -0.000100 | -0.376300 |
| C | -1.972700 | -0.000100 | -0.273200 |
| N | 3.137500 | 0.000000 | 0.377500 |
| C | 1.972500 | 0.000000 | 0.273500 |
| Au | -0.000100 | 0.000000 | -0.000000 |
| Au | -0.000000 | 2.858500 | -0.000100 |
| N | 2.922000 | 3.061800 | -0.858800 |
| N | 2.713100 | 3.307200 | 1.290800 |

C 2.017000 3.071000 0.149100
C 4.060100 3.454900 1.015100
C 2.643300 2.758700 -2.246200
H 1.587500 2.497500 -2.337800
H 2.856500 3.628800 -2.875800
C 2.151000 3.361500 2.619400
H 1.062600 3.363000 2.539400
H 2.470500 2.492500 3.203300
H 3.256700 1.904600 -2.554400
H 2.469900 4.278900 3.123400
N -2.922100 3.061300 0.858600
N -2.713200 3.307100 -1.291000
C -2.017000 3.070900 -0.149300
C -4.060200 3.454600 -1.015300
C -2.643400 2.757900 2.245900
H -1.587300 2.497900 2.337700
H -2.857900 3.627400 2.875900
C -2.151100 3.361900 -2.619500
H -1.062700 3.361500 -2.539600
H -2.472000 2.494000 -3.204300
H -3.255900 1.902900 2.553500
H -2.468500 4.280200 -3.122700
C 4.192500 3.303600 -0.369800
C 5.425000 3.431300 -1.002800
C 6.521600 3.703500 -0.191200
H 5.527500 3.323100 -2.077500
C 5.156000 3.724900 1.828700
C 6.390000 3.844800 1.198300
H 7.502200 3.813300 -0.644300
H 5.058300 3.837400 2.903700
H 7.271400 4.057100 1.795500
C -4.192700 3.302900 0.369600
C -5.425200 3.430200 1.002500
C -6.521900 3.702200 0.190900
H -5.527700 3.321800 2.077200
C -5.156100 3.724400 -1.828900
C -6.390200 3.843900 -1.198600
H -7.502500 3.811500 0.643900
H -5.058300 3.837300 -2.903800
H -7.271600 4.056000 -1.795800
O -4.566800 -0.000200 2.123800
H -4.261000 -0.000300 1.195400
C -5.978400 -0.000000 2.130900
H -6.396200 -0.890000 1.640700
H -6.299600 0.000300 3.176800
H -6.396100 0.889800 1.640200
O 4.566700 0.000300 -2.122300
H 4.259900 0.000200 -1.194200
C 5.978300 0.000200 -2.127800
H 6.300700 0.000200 -3.173300
H 6.395600 0.890000 -1.636800
H 6.395400 -0.889800 -1.636800

II-3S1

109
Molecule Name
Au -0.074100 0.123000 2.853100
N -1.038300 -2.758200 3.111100
N 1.133900 -2.652500 3.147800
C 0.010400 -1.901400 3.032700
C 0.807800 -3.985600 3.311500
C -2.432000 -2.409300 2.938300
H -2.498800 -1.336700 2.748300
H -2.836600 -2.953600 2.077500
C 2.492900 -2.168700 3.029000
H 2.468700 -1.080000 2.957500
H 3.069400 -2.452600 3.914900
H -2.999000 -2.650800 3.843100
H 2.951900 -2.586900 2.125900
N 0.908100 3.003900 3.057200
N -1.241900 2.885200 3.353500
C -0.137100 2.142900 3.085500
C -0.905100 4.218100 3.503400
C 2.275500 2.668700 2.721100
H 2.315700 1.613800 2.444300
H 2.592400 3.280100 1.868800
C -2.592500 2.381600 3.433500
H -2.562000 1.291300 3.404000
H -3.055800 2.698000 4.373000
H 2.931400 2.842000 3.580400
H -3.185200 2.749700 2.590100
C -0.590200 -4.053400 3.289800
C -1.264800 -5.258900 3.459300
C 1.591100 -5.120500 3.500600
C -0.483000 -6.395000 3.644000
H -2.348700 -5.312100 3.452700
C 0.918200 -6.327200 3.664100
H 2.674800 -5.068400 3.524100
H -0.969000 -7.355700 3.784100
H 1.490600 -7.236800 3.818300
C 0.480000 4.292600 3.318300
C 1.167500 5.496600 3.436200
C -1.664800 5.345400 3.799700
C 0.409900 6.624500 3.734300
H 2.242500 5.554400 3.300700
C -0.980100 6.550800 3.910300
H -2.739800 5.292300 3.939000
H 0.906700 7.584400 3.837500
H -1.533800 7.455300 4.142100
N -0.347600 3.298900 0.000000
C -0.318700 2.129900 0.000000
N 0.061200 -3.005700 0.000000
C -0.022200 -1.837500 0.000000
Au -0.176000 0.145500 0.000000
Au -0.074100 0.123000 -2.853100
N -1.038300 -2.758200 -3.111100
N 1.133900 -2.652500 -3.147800
C 0.010400 -1.901400 -3.032700
C 0.807800 -3.985600 -3.311500
C -2.432000 -2.409300 -2.938300
H -2.498800 -1.336700 -2.748300
H -2.999000 -2.650800 -3.843100
C 2.492900 -2.168700 -3.029000
H 2.468700 -1.080000 -2.957500
H 2.951900 -2.586900 -2.125900
H -2.836600 -2.953600 -2.077500
H 3.069400 -2.452600 -3.914900
N 0.908100 3.003900 -3.057200
N -1.241900 2.885200 -3.353500
C -0.137100 2.142900 -3.085500
C -0.905100 4.218100 -3.503400
C 2.275500 2.668700 -2.721100
H 2.315700 1.613800 -2.444300
H 2.931400 2.842000 -3.580400
C -2.592500 2.381600 -3.433500
H -2.562000 1.291300 -3.404000
H -3.185200 2.749700 -2.590100
H 2.592400 3.280100 -1.868800
H -3.055800 2.698000 -4.373000

| | | | |
|---|---|---|---|
| C | -0.590200 | -4.053400 | -3.289800 |
| C | -1.264800 | -5.258900 | -3.459300 |
| C | -0.483000 | -6.395000 | -3.644000 |
| H | -2.348700 | -5.312100 | -3.452700 |
| C | 1.591100 | -5.120500 | -3.500600 |
| C | 0.918200 | -6.327200 | -3.664100 |
| H | -0.969000 | -7.355700 | -3.784100 |
| H | 2.674800 | -5.068400 | -3.524100 |
| H | 1.490600 | -7.236800 | -3.818300 |
| C | 0.480000 | 4.292600 | -3.318300 |
| C | 1.167500 | 5.496600 | -3.436200 |
| C | 0.409900 | 6.624500 | -3.734300 |
| H | 2.242500 | 5.554400 | -3.300700 |
| C | -1.664800 | 5.345400 | -3.799700 |
| C | -0.980100 | 6.550800 | -3.910300 |
| H | 0.906700 | 7.584400 | -3.837500 |
| H | -2.739800 | 5.292300 | -3.939000 |
| H | -1.533800 | 7.455300 | -4.142100 |
| O | 2.202600 | 4.637800 | 0.000000 |
| H | 1.263300 | 4.367800 | 0.000000 |
| C | 2.263800 | 6.048000 | 0.000000 |
| H | 1.789900 | 6.484200 | 0.890100 |
| H | 3.321300 | 6.328700 | 0.000000 |
| H | 1.789900 | 6.484200 | -0.890100 |
| O | -2.629600 | -4.142900 | 0.000000 |
| H | -1.676800 | -3.935200 | 0.000000 |
| C | -2.778100 | -5.546900 | 0.000000 |
| H | -3.850600 | -5.761000 | 0.000000 |
| H | -2.332000 | -6.012100 | -0.890200 |
| H | -2.332000 | -6.012100 | 0.890200 |
| H | 1.922000 | -3.635300 | 0.000000 |
| O | 2.894100 | -3.713100 | 0.000000 |
| C | 3.226800 | -5.085000 | 0.000000 |
| H | 4.318000 | -5.156100 | 0.000000 |
| H | 2.845800 | -5.605500 | 0.890100 |
| H | 2.845800 | -5.605500 | -0.890100 |

II-4S1

115

Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000000 | 2.848600 | 0.000000 |
| N | 2.830000 | 3.135000 | 1.087500 |
| N | 2.830000 | 3.135000 | -1.087500 |
| C | 2.025400 | 3.038800 | 0.000000 |
| C | 4.146000 | 3.302800 | -0.699900 |
| C | 2.413100 | 2.992300 | 2.466100 |
| H | 1.328700 | 2.873900 | 2.489900 |
| H | 2.886800 | 2.104200 | 2.899700 |
| C | 2.413100 | 2.992300 | -2.466100 |
| H | 1.328700 | 2.873900 | -2.489900 |
| H | 2.686500 | 3.886000 | -3.036000 |
| H | 2.686500 | 3.886000 | 3.036000 |
| H | 2.886800 | 2.104200 | -2.899700 |
| N | -2.830000 | 3.135000 | -1.087500 |
| N | -2.830000 | 3.135000 | 1.087500 |
| C | -2.025400 | 3.038800 | 0.000000 |
| C | -4.146000 | 3.302800 | 0.699900 |
| C | -2.413100 | 2.992300 | -2.466100 |
| H | -1.328700 | 2.873900 | -2.489900 |
| H | -2.886800 | 2.104200 | -2.899700 |
| C | -2.413100 | 2.992300 | 2.466100 |
| H | -1.328700 | 2.873900 | 2.489900 |
| H | -2.686500 | 3.886000 | 3.036000 |
| H | -2.686500 | 3.886000 | -3.036000 |
| H | -2.886800 | 2.104200 | 2.899700 |
| C | 4.146000 | 3.302800 | 0.699900 |
| C | 5.318100 | 3.477600 | 1.429900 |
| C | 5.318100 | 3.477600 | -1.429900 |
| C | 6.491300 | 3.647100 | 0.701600 |
| H | 5.318700 | 3.485500 | 2.515100 |
| C | 6.491300 | 3.647100 | -0.701600 |
| H | 5.318700 | 3.485500 | -2.515100 |
| H | 7.428000 | 3.790500 | 1.231300 |
| H | 7.428000 | 3.790500 | -1.231300 |
| C | -4.146000 | 3.302800 | -0.699900 |
| C | -5.318100 | 3.477600 | -1.429900 |
| C | -5.318100 | 3.477600 | 1.429900 |
| C | -6.491300 | 3.647100 | -0.701600 |
| H | -5.318700 | 3.485500 | -2.515100 |
| C | -6.491300 | 3.647100 | 0.701600 |
| H | -5.318700 | 3.485500 | 2.515100 |
| H | -7.428000 | 3.790500 | -1.231300 |
| H | -7.428000 | 3.790500 | 1.231300 |
| N | -3.158200 | 0.000000 | 0.000000 |
| C | -1.987200 | 0.000000 | 0.000000 |
| N | 3.158200 | 0.000000 | 0.000000 |
| C | 1.987200 | 0.000000 | 0.000000 |
| Au | 0.000000 | 0.000000 | 0.000000 |
| Au | 0.000000 | -2.848600 | 0.000000 |
| N | 2.830000 | -3.135000 | 1.087500 |
| N | 2.830000 | -3.135000 | -1.087500 |
| C | 2.025400 | -3.038800 | 0.000000 |
| C | 4.146000 | -3.302800 | -0.699900 |
| C | 2.413100 | -2.992300 | 2.466100 |
| H | 1.328700 | -2.873900 | 2.489900 |
| H | 2.686500 | -3.886000 | 3.036000 |
| C | 2.413100 | -2.992300 | -2.466100 |
| H | 1.328700 | -2.873900 | -2.489900 |
| H | 2.886800 | -2.104200 | -2.899700 |
| H | 2.886800 | -2.104200 | 2.899700 |
| H | 2.686500 | -3.886000 | -3.036000 |
| N | -2.830000 | -3.135000 | -1.087500 |
| N | -2.830000 | -3.135000 | 1.087500 |
| C | -2.025400 | -3.038800 | 0.000000 |
| C | -4.146000 | -3.302800 | 0.699900 |
| C | -2.413100 | -2.992300 | -2.466100 |
| H | -1.328700 | -2.873900 | -2.489900 |
| H | -2.686500 | -3.886000 | -3.036000 |
| C | -2.413100 | -2.992300 | 2.466100 |
| H | -1.328700 | -2.873900 | 2.489900 |
| H | -2.886800 | -2.104200 | 2.899700 |
| H | -2.886800 | -2.104200 | -2.899700 |
| H | -2.686500 | -3.886000 | 3.036000 |
| C | 4.146000 | -3.302800 | 0.699900 |
| C | 5.318100 | -3.477600 | 1.429900 |
| C | 6.491300 | -3.647100 | 0.701600 |
| H | 5.318700 | -3.485500 | 2.515100 |
| C | 5.318100 | -3.477600 | -1.429900 |
| C | 6.491300 | -3.647100 | -0.701600 |
| H | 7.428000 | -3.790500 | 1.231300 |
| H | 5.318700 | -3.485500 | -2.515100 |
| H | 7.428000 | -3.790500 | -1.231300 |
| C | -4.146000 | -3.302800 | -0.699900 |
| C | -5.318100 | -3.477600 | -1.429900 |
| C | -6.491300 | -3.647100 | -0.701600 |
| H | -5.318700 | -3.485500 | -2.515100 |
| C | -5.318100 | -3.477600 | 1.429900 |
| C | -6.491300 | -3.647100 | 0.701600 |
| H | -7.428000 | -3.790500 | -1.231300 |

H -5.318700 -3.485500 2.515100
H -7.428000 -3.790500 1.231300
O -4.053400 0.000000 -2.785000
H -3.926900 0.000000 -1.818500
C -5.440000 0.000000 -3.050200
H -5.941100 0.890100 -2.644200
H -5.564000 0.000000 -4.136700
H -5.941100 -0.890100 -2.644200
O 4.053400 0.000000 2.785000
H 3.926900 0.000000 1.818500
C 5.440000 0.000000 3.050200
H 5.564000 0.000000 4.136700
H 5.941100 -0.890100 2.644200
H 5.941100 0.890100 2.644200
H 3.926900 0.000000 -1.818500
O 4.053400 0.000000 -2.785000
C 5.440000 0.000000 -3.050200
H 5.564000 0.000000 -4.136700
H 5.941100 0.890100 -2.644200
H 5.941100 -0.890100 -2.644200
H -3.926900 0.000000 1.818500
O -4.053400 0.000000 2.785000
C -5.440000 0.000000 3.050200
H -5.941100 -0.890100 2.644200
H -5.564000 0.000000 4.136700
H -5.941100 0.890100 2.644200

II-S2

100
Molecule Name
Au -0.388500 2.739900 -0.446600
N -3.430000 2.658400 -0.635100
N -2.777400 3.199400 1.370400
C -2.329300 2.905600 0.122500
C -4.159800 3.141800 1.414900
C -3.415000 2.328100 -2.043600
H -2.431100 1.937800 -2.310100
H -4.157500 1.550700 -2.241700
C -1.930500 3.498200 2.506100
H -0.973400 3.873600 2.137900
H -2.401500 4.276500 3.111700
N -0.626200 -0.363900 -3.298600
C -0.519300 -0.230200 -2.142200
H -3.641900 3.209900 -2.651800
H -1.755600 2.603900 3.111100
N 2.643700 2.475600 -0.229200
N 2.000600 2.568400 -2.309300
C 1.556200 2.640500 -1.027200
C 3.366000 2.347200 -2.334600
C 2.643500 2.536900 1.218200
H 1.614100 2.638300 1.562800
H 3.062300 1.627300 1.657300
C 1.169500 2.695400 -3.489000
H 0.250200 3.215600 -3.212300
H 1.697300 3.292800 -4.237300
N -0.007200 0.360800 2.952800
C -0.151100 0.213800 1.801900
H 3.222500 3.403900 1.553200
H 0.914900 1.713200 -3.896700
Au 0.150600 -2.722300 0.005900
N -2.482300 -3.488200 -1.295300
N -2.769200 -3.075600 0.823100
C -1.828700 -3.149300 -0.154900
C -4.020000 -3.380200 0.313900
C -1.860200 -3.655100 -2.593100
H -0.801100 -3.876500 -2.445800
H -2.326100 -4.498900 -3.108600
C -2.508600 -2.768100 2.212200
H -1.540000 -2.272200 2.292800
H -3.276700 -2.084400 2.583400
H -1.953700 -2.745300 -3.192400
H -2.510100 -3.679900 2.818300
N 2.875000 -2.364100 1.308500
N 3.028500 -2.190000 -0.856000
C 2.156400 -2.424900 0.160500
C 4.307700 -2.005000 -0.360000
C 2.358400 -2.568100 2.647100
H 1.278100 -2.705700 2.584700
H 2.810100 -3.464300 3.085200
C 2.699400 -2.182500 -2.265000
H 1.619200 -2.088200 -2.383300
H 3.175200 -1.322700 -2.745000
H 2.577200 -1.687500 3.260000
H 3.045000 -3.103700 -2.745900
Au -0.331900 -0.007900 -0.171400
C -3.837400 -3.632100 -1.052100
C -4.906100 -3.962100 -1.880700
C -6.161200 -4.039600 -1.286100
H -4.772200 -4.148800 -2.941200
C -5.274700 -3.463800 0.910700
C -6.342100 -3.796600 0.083400
H -7.020900 -4.296900 -1.897000
H -5.418100 -3.283300 1.971200
H -7.337900 -3.873300 0.508600
C 4.205700 -2.106100 1.032600
C 5.315000 -1.959200 1.860200
C 6.533600 -1.717700 1.235300
H 5.232200 -2.023100 2.939900
C 5.527300 -1.765900 -0.986600
C 6.637800 -1.625500 -0.161000
H 7.426300 -1.602000 1.842300
H 5.612500 -1.690800 -2.065700
H 7.610100 -1.443900 -0.608900
C -4.580300 2.807600 0.120800
C -5.929500 2.689000 -0.200100
C -5.071800 3.354700 2.444700
C -6.841000 2.904900 0.828200
H -6.259900 2.444700 -1.204500
C -6.420000 3.230200 2.125800
H -4.752200 3.604900 3.451100
H -7.903200 2.823100 0.620100
H -7.163800 3.391300 2.899900
C 3.780400 2.295900 -0.996700
C 5.114600 2.102400 -0.651700
C 4.269400 2.197100 -3.383300
C 6.017700 1.954800 -1.699500
H 5.436100 2.057800 0.383700
C 5.603600 2.001200 -3.038800
H 3.953500 2.232200 -4.421000
H 7.068400 1.801100 -1.474000
H 6.341600 1.886100 -3.827000
H 1.784200 0.486100 3.703000
O 2.751400 0.458700 3.833400
C 3.041500 0.881700 5.154100
H 2.708500 1.919400 5.311600
H 2.512000 0.256300 5.889200
C 4.535100 0.783200 5.373200
H 4.802200 1.117800 6.380700
H 4.875000 -0.251300 5.254000

H 5.071400 1.405100 4.648700

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Molecule Name
Au -0.000100 -2.861000 -0.000200
N -2.969600 -3.035100 0.684100
N -2.627600 -3.361400 -1.437600
C -2.004100 -3.078500 -0.264800
C -3.988700 -3.505900 -1.240000
C -2.775700 -2.679000 2.073200
H -1.743500 -2.348400 2.203900
H -3.452100 -1.854900 2.325500
C -1.982900 -3.468100 -2.725100
H -0.902400 -3.503900 -2.574600
H -2.299500 -4.388500 -3.224700
H -2.966900 -3.541700 2.720000
H -2.234700 -2.606300 -3.351400
N 2.969500 -3.035100 -0.684400
N 2.627300 -3.362600 1.437100
C 2.003900 -3.078900 0.264400
C 3.988300 -3.507300 1.239400
C 2.775700 -2.677900 -2.073300
H 1.743800 -2.346400 -2.203700
H 3.452700 -1.854200 -2.325100
C 1.982400 -3.469900 2.724500
H 0.902000 -3.506400 2.573800
H 2.299700 -4.390000 3.224000
H 2.966200 -3.540400 -2.720700
H 2.233500 -2.607900 3.350800
C -4.206700 -3.303400 0.127600
C -5.475100 -3.415100 0.688400
C -5.031700 -3.812300 -2.108500
C -6.518600 -3.724400 -0.177800
H -5.643300 -3.266300 1.749900
C -6.301400 -3.916600 -1.550500
H -4.868300 -3.963800 -3.170600
H -7.524700 -3.823000 0.218200
H -7.143700 -4.156200 -2.192000
C 4.206400 -3.304000 -0.128000
C 5.474800 -3.415900 -0.688900
C 5.031300 -3.814500 2.107800
C 6.518200 -3.726100 0.177100
H 5.643000 -3.266700 -1.750400
C 6.300900 -3.919000 1.549700
H 4.867800 -3.966600 3.169800
H 7.524300 -3.825000 -0.218900
H 7.143100 -4.159300 2.191100
N 3.109600 -0.000100 0.564100
C 1.953000 -0.000000 0.392100
N -3.109900 0.000100 -0.563000
C -1.953200 0.000000 -0.391300
Au -0.000100 0.000000 0.000300
Au 0.000000 2.861100 -0.000100
N -2.970000 3.036200 0.681600
N -2.626200 3.360400 -1.440200
C -2.003700 3.078600 -0.266600
C -3.987500 3.505200 -1.243800
C -2.777400 2.681300 2.071200
H -1.745000 2.351800 2.203300
H -2.970000 3.544500 2.717000
C -1.980400 3.465800 -2.727200
H -0.900100 3.501600 -2.575900
H -2.231900 2.603500 -3.352900
H -3.453300 1.856900 2.323600
H -2.296500 4.385800 -3.227900
N 2.970100 3.035900 -0.681800
N 2.626300 3.361300 1.439700
C 2.003800 3.078800 0.266300
C 3.987500 3.506100 1.243200
C 2.777400 2.680300 -2.071200
H 1.745400 2.349500 -2.202900
H 2.968800 3.543400 -2.717600
C 1.980500 3.467200 2.726800
H 0.900200 3.503300 2.575400
H 2.231600 2.604900 3.352600
H 3.454200 1.856500 -2.323400
H 2.297000 4.387200 3.227300
C -4.206600 3.303900 0.123800
C -5.475500 3.416100 0.683500
C -6.518300 3.724700 -0.183900
H -5.644500 3.268500 1.745000
C -5.029800 3.810700 -2.113500
C -6.299900 3.915500 -1.556600
H -7.524700 3.823600 0.211100
H -4.865500 3.961200 -3.175600
H -7.141700 4.154600 -2.199100
C 4.206600 3.304300 -0.124300
C 5.475400 3.416800 -0.684100
C 6.518100 3.726100 0.183100
H 5.644400 3.268800 -1.745600
C 5.029800 3.812400 2.112700
C 6.299800 3.917400 1.555700
H 7.524500 3.825400 -0.212100
H 4.865600 3.963400 3.174800
H 7.141600 4.157100 2.198000
O 4.787900 0.000500 -1.775900
H 4.402900 0.000300 -0.876900
C 6.200800 0.000700 -1.670300
H 6.547700 -0.883700 -1.115800
H 6.547500 0.885300 -1.115900
C 6.784900 0.000600 -3.066200
H 7.879300 0.000800 -3.029500
H 6.458600 -0.884500 -3.623200
H 6.458300 0.885500 -3.623400
O -4.786600 0.000400 1.777700
H -4.402200 0.000200 0.878500
C -6.199600 0.000800 1.673000
H -6.546500 0.885500 1.118800
H -6.547000 -0.883600 1.118700
C -6.782900 0.000900 3.069300
H -7.877300 0.001200 3.033200
H -6.456300 -0.884300 3.626200
H -6.455800 0.885800 3.626300

II-3S2

118
Molecule Name
Au -0.175900 -2.852600 -0.131300
N 2.733900 -3.108700 -1.004400
N 2.561100 -3.152400 1.163300
C 1.845100 -3.033300 0.017400
C 3.903500 -3.315700 0.878200
C 2.428300 -2.928400 -2.407200
H 1.360400 -2.725300 -2.504400
H 2.994000 -2.072400 -2.792600
C 2.035900 -3.034800 2.506900
H 0.948500 -2.962200 2.449600

H 2.301200 -3.921700 3.090900
H 2.676000 -3.834100 -2.970100
H 2.440600 -2.132400 2.979200
N -3.088400 -3.055500 0.753600
N -2.897300 -3.350800 -1.391400
C -2.192600 -3.083700 -0.261900
C -4.240900 -3.499900 -1.100000
C -2.798500 -2.721400 2.131700
H -1.746800 -2.439800 2.205900
H -3.423500 -1.872800 2.431200
C -2.348200 -3.431200 -2.724100
H -1.259300 -3.412900 -2.656300
H -2.657500 -4.366200 -3.201000
H -2.988300 -3.583200 2.780000
H -2.687500 -2.582600 -3.326600
C 4.014500 -3.289900 -0.517000
C 5.240100 -3.457900 -1.154600
C 5.013800 -3.507700 1.695400
C 6.351500 -3.646000 -0.338900
H 5.326800 -3.447500 -2.236300
C 6.240600 -3.670200 1.059500
H 4.928700 -3.534100 2.777000
H 7.326700 -3.784700 -0.795600
H 7.131900 -3.826300 1.659300
C -4.361900 -3.315800 0.282000
C -5.588400 -3.433300 0.928500
C -5.342400 -3.794600 -1.897300
C -6.690500 -3.730100 0.133300
H -5.682400 -3.298600 2.001100
C -6.570200 -3.904900 -1.253500
H -5.253300 -3.932800 -2.970100
H -7.666700 -3.832500 0.597400
H -7.455800 -4.135400 -1.837600
N -3.345100 -0.000100 -0.499800
C -2.177700 -0.000000 -0.433700
N 2.944900 -0.000000 0.092400
C 1.779600 -0.000000 -0.023900
Au -0.198200 -0.000000 -0.233000
Au -0.175900 2.852600 -0.131400
N 2.733900 3.108700 -1.004300
N 2.561000 3.152400 1.163400
C 1.845100 3.033400 0.017400
C 3.903500 3.315800 0.878200
C 2.428300 2.928300 -2.407100
H 1.360400 2.725300 -2.504300
H 2.676100 3.834000 -2.970100
C 2.035800 3.034800 2.506900
H 0.948500 2.962200 2.449600
H 2.440600 2.132400 2.979300
H 2.994000 2.072400 -2.792500
H 2.301000 3.921700 3.090900
N -3.088400 3.055500 0.753500
N -2.897300 3.350700 -1.391500
C -2.192600 3.083700 -0.262000
C -4.240900 3.499900 -1.100100
C -2.798600 2.721600 2.131700
H -1.746800 2.440000 2.205900
H -2.988400 3.583300 2.779800
C -2.348200 3.431000 -2.724200
H -1.259300 3.412700 -2.656400
H -2.687500 2.582400 -3.326600
H -3.423600 1.872900 2.431200
H -2.657500 4.366000 -3.201200
C 4.014400 3.289900 -0.516900
C 5.240100 3.458000 -1.154500
C 6.351500 3.646100 -0.338800
H 5.326800 3.447600 -2.236200
C 5.013700 3.507800 1.695500
C 6.240500 3.670300 1.059600
H 7.326700 3.784800 -0.795400
H 4.928600 3.534200 2.777100
H 7.131800 3.826500 1.659400
C -4.361900 3.315800 0.281900
C -5.588500 3.433300 0.928400
C -6.690500 3.730100 0.133200
H -5.682500 3.298600 2.001000
C -5.342400 3.794500 -1.897500
C -6.570200 3.904800 -1.253700
H -7.666700 3.832500 0.597200
H -5.253300 3.932600 -2.970200
H -7.455800 4.135300 -1.837800
O -4.776800 0.000000 2.001400
H -4.476200 -0.000000 1.071100
C -6.193600 0.000000 2.022600
H -6.588300 -0.884500 1.501100
H -6.588300 0.884600 1.501000
C -6.651200 0.000100 3.465000
H -6.276400 0.885100 3.990700
H -7.744400 0.000100 3.525900
H -6.276400 -0.884900 3.990800
O 4.193500 -0.000000 -2.548200
H 3.950900 -0.000000 -1.603200
C 5.607200 -0.000000 -2.651100
H 6.031500 0.884800 -2.152800
H 6.031600 -0.884700 -2.152700
C 5.981000 -0.000100 -4.117200
H 5.576800 0.885200 -4.619700
H 7.069000 -0.000100 -4.239900
H 5.576900 -0.885500 -4.619600
H 3.525500 0.000000 1.975800
O 3.571400 0.000000 2.950200
C 4.935600 -0.000000 3.334800
H 5.451700 -0.884700 2.931500
H 5.451700 0.884700 2.931500
C 5.007600 -0.000000 4.846000
H 6.048800 -0.000000 5.184800
H 4.510800 0.885400 5.256800
H 4.510700 -0.885400 5.256800

II-4S2

127
Molecule Name
Au 0.000000 0.000000 -2.848500
N -1.087500 2.830000 -3.133900
N 1.087500 2.830000 -3.133900
C 0.000000 2.025300 -3.038100
C 0.699900 4.146100 -3.301200
C -2.465900 2.412800 -2.991600
H -2.489400 1.328400 -2.872600
H -2.900000 2.886800 -2.103900
C 2.465900 2.412800 -2.991600
H 2.489400 1.328400 -2.872600
H 3.035500 2.685400 -3.885700
H -3.035500 2.685400 -3.885700
H 2.900000 2.886800 -2.103900
N 1.087500 -2.830000 -3.133900
N -1.087500 -2.830000 -3.133900
C 0.000000 -2.025300 -3.038100
C -0.699900 -4.146100 -3.301200

| | | | |
|---|---|---|---|
| C | 2.465900 | -2.412800 | -2.991600 |
| H | 2.489400 | -1.328400 | -2.872600 |
| H | 2.900000 | -2.886800 | -2.103900 |
| C | -2.465900 | -2.412800 | -2.991600 |
| H | -2.489400 | -1.328400 | -2.872600 |
| H | -3.035500 | -2.685400 | -3.885700 |
| H | 3.035500 | -2.685400 | -3.885700 |
| H | -2.900000 | -2.886800 | -2.103900 |
| C | -0.699900 | 4.146100 | -3.301200 |
| C | -1.429900 | 5.318300 | -3.474800 |
| C | 1.429900 | 5.318300 | -3.474800 |
| C | -0.701500 | 6.491600 | -3.643700 |
| H | -2.515100 | 5.319100 | -3.482100 |
| C | 0.701500 | 6.491600 | -3.643700 |
| H | 2.515100 | 5.319100 | -3.482100 |
| H | -1.231300 | 7.428500 | -3.785900 |
| H | 1.231300 | 7.428500 | -3.785900 |
| C | 0.699900 | -4.146100 | -3.301200 |
| C | 1.429900 | -5.318300 | -3.474800 |
| C | -1.429900 | -5.318300 | -3.474800 |
| C | 0.701500 | -6.491600 | -3.643700 |
| H | 2.515100 | -5.319100 | -3.482100 |
| C | -0.701500 | -6.491600 | -3.643700 |
| H | -2.515100 | -5.319100 | -3.482100 |
| H | 1.231300 | -7.428500 | -3.785900 |
| H | -1.231300 | -7.428500 | -3.785900 |
| N | 0.000000 | -3.158400 | -0.000000 |
| C | 0.000000 | -1.987500 | -0.000100 |
| N | 0.000000 | 3.158400 | -0.000000 |
| C | 0.000000 | 1.987500 | -0.000100 |
| Au | 0.000000 | 0.000000 | -0.000100 |
| Au | 0.000000 | 0.000000 | 2.848400 |
| N | -1.087500 | 2.830000 | 3.133900 |
| N | 1.087500 | 2.830000 | 3.133900 |
| C | 0.000000 | 2.025300 | 3.038100 |
| C | 0.699900 | 4.146100 | 3.301300 |
| C | -2.465900 | 2.412800 | 2.991500 |
| H | -2.489400 | 1.328400 | 2.872500 |
| H | -3.035500 | 2.685400 | 3.885600 |
| C | 2.465900 | 2.412800 | 2.991500 |
| H | 2.489400 | 1.328400 | 2.872500 |
| H | 2.900000 | 2.886800 | 2.103800 |
| H | -2.900000 | 2.886800 | 2.103800 |
| H | 3.035500 | 2.685400 | 3.885600 |
| N | 1.087500 | -2.830000 | 3.133900 |
| N | -1.087500 | -2.830000 | 3.133900 |
| C | 0.000000 | -2.025300 | 3.038100 |
| C | -0.699900 | -4.146100 | 3.301300 |
| C | 2.465900 | -2.412800 | 2.991500 |
| H | 2.489400 | -1.328400 | 2.872500 |
| H | 3.035500 | -2.685400 | 3.885600 |
| C | -2.465900 | -2.412800 | 2.991500 |
| H | -2.489400 | -1.328400 | 2.872500 |
| H | -2.900000 | -2.886800 | 2.103800 |
| H | 2.900000 | -2.886800 | 2.103800 |
| H | -3.035500 | -2.685400 | 3.885600 |
| C | -0.699900 | 4.146100 | 3.301300 |
| C | -1.429900 | 5.318300 | 3.475100 |
| C | -0.701500 | 6.491500 | 3.644000 |
| H | -2.515100 | 5.319000 | 3.482400 |
| C | 1.429900 | 5.318300 | 3.475100 |
| C | 0.701500 | 6.491500 | 3.644000 |
| H | -1.231300 | 7.428400 | 3.786300 |
| H | 2.515100 | 5.319000 | 3.482400 |
| H | 1.231300 | 7.428400 | 3.786300 |
| C | 0.699900 | -4.146100 | 3.301300 |
| C | 1.429900 | -5.318300 | 3.475100 |
| C | 0.701500 | -6.491500 | 3.644000 |
| H | 2.515100 | -5.319000 | 3.482400 |
| C | -1.429900 | -5.318300 | 3.475100 |
| C | -0.701500 | -6.491500 | 3.644000 |
| H | 1.231300 | -7.428400 | 3.786300 |
| H | -2.515100 | -5.319000 | 3.482400 |
| H | -1.231300 | -7.428400 | 3.786300 |
| O | 2.789100 | -4.061200 | -0.000000 |
| H | 1.821700 | -3.939200 | -0.000100 |
| C | 3.068200 | -5.450900 | -0.000100 |
| H | 2.626500 | -5.934500 | -0.884700 |
| H | 2.626500 | -5.934600 | 0.884600 |
| C | 4.569400 | -5.637600 | -0.000100 |
| H | 5.016800 | -5.173300 | 0.885400 |
| H | 4.828300 | -6.701400 | -0.000100 |
| H | 5.016800 | -5.173300 | -0.885500 |
| O | -2.789100 | 4.061200 | -0.000000 |
| H | -1.821700 | 3.939200 | -0.000100 |
| C | -3.068200 | 5.450900 | -0.000100 |
| H | -2.626500 | 5.934600 | 0.884600 |
| H | -2.626500 | 5.934500 | -0.884700 |
| C | -4.569400 | 5.637600 | -0.000100 |
| H | -5.016800 | 5.173300 | 0.885400 |
| H | -4.828300 | 6.701400 | -0.000100 |
| H | -5.016800 | 5.173300 | -0.885500 |
| H | 1.821700 | 3.939200 | -0.000100 |
| O | 2.789100 | 4.061200 | -0.000000 |
| C | 3.068200 | 5.450900 | -0.000100 |
| H | 2.626500 | 5.934500 | -0.884700 |
| H | 2.626500 | 5.934600 | 0.884600 |
| C | 4.569400 | 5.637600 | -0.000100 |
| H | 4.828300 | 6.701400 | -0.000100 |
| H | 5.016800 | 5.173300 | 0.885400 |
| H | 5.016800 | 5.173300 | -0.885500 |
| H | -1.821700 | -3.939200 | -0.000100 |
| O | -2.789100 | -4.061200 | -0.000000 |
| C | -3.068200 | -5.450900 | -0.000100 |
| H | -2.626500 | -5.934600 | 0.884600 |
| H | -2.626500 | -5.934500 | -0.884700 |
| C | -4.569400 | -5.637600 | -0.000100 |
| H | -4.828300 | -6.701400 | -0.000100 |
| H | -5.016800 | -5.173300 | 0.885400 |
| H | -5.016800 | -5.173300 | -0.885500 |

## 21. The $T_1$ .xyz files of III and its complexes

III

67
Molecule Name
Au 2.755900 0.000100 0.000100
N 2.824700 2.899200 -0.948800
N 2.891900 2.797200 1.202900
C 2.833700 2.023300 0.088800
C 2.937700 4.130400 0.865000
H 2.995600 4.911000 1.607900
C 2.896800 4.194900 -0.490000
H 2.915100 5.042300 -1.158000
C 2.813200 2.510300 -2.346700
H 2.023800 1.775800 -2.524200
H 2.620600 3.394800 -2.956200
C 2.945700 2.276100 2.556700
H 3.863400 1.696800 2.696800
H 2.944100 3.114600 3.255000
N 0.000300 0.000200 -3.192000
C 0.000200 0.000100 -2.021400
H 3.781100 2.084400 -2.629100
H 2.077800 1.641600 2.753400
N 2.824600 -2.899100 0.948900
N 2.892100 -2.797100 -1.202700
C 2.833800 -2.023100 -0.088700
C 2.937900 -4.130300 -0.864800
H 2.995800 -4.910900 -1.607700
C 2.896800 -4.194800 0.490100
H 2.914900 -5.042100 1.158100
C 2.812900 -2.510100 2.346800
H 2.023200 -1.776000 2.524300
H 2.620800 -3.394700 2.956300
C 2.946200 -2.276000 -2.556500
H 3.863900 -1.696700 -2.696400
H 2.944600 -3.114500 -3.254800
N -0.000300 -0.000100 3.191700
C -0.000200 -0.000100 2.021100
H 3.780600 -2.083800 2.629200
H 2.078300 -1.641500 -2.753300
Au -2.755900 -0.000100 0.000000
N -2.892200 2.797100 -1.202700
N -2.824800 2.899000 0.948900
C -2.833900 2.023100 -0.088800
C -2.897100 4.194800 0.490100
H -2.915300 5.042100 1.158200
C -2.938000 4.130300 -0.864800
H -2.995900 4.910900 -1.607700
C -2.946000 2.276100 -2.556600
H -2.078100 1.641600 -2.753300
H -3.863700 1.696800 -2.696700
C -2.813300 2.510000 2.346800
H -3.781200 2.084100 2.629100
H -2.023900 1.775600 2.524300
H -2.944400 3.114600 -3.254900
H -2.620800 3.394600 2.956300
N -2.891800 -2.797400 1.202700
N -2.824500 -2.899100 -0.949000
C -2.833600 -2.023300 0.088800
C -2.896600 -4.194900 -0.490400
H -2.914700 -5.042100 -1.158500
C -2.937500 -4.130600 0.864600
H -2.995400 -4.911300 1.607400
C -2.945900 -2.276500 2.556600
H -2.078000 -1.642000 2.753500
H -3.863500 -1.697200 2.696500
C -2.812900 -2.509900 -2.346800
H -3.780800 -2.084000 -2.629200
H -2.023500 -1.775500 -2.524200
H -2.944400 -3.115100 3.254800
H -2.620400 -3.394400 -2.956500
Ag 0.000000 0.000000 -0.000200

III-S1

73
Molecule Name
Au 2.755900 -0.157300 -0.162700
N 2.943800 -2.655100 1.580400
N 2.971700 -3.178600 -0.509900
C 2.906100 -2.116600 0.333900
C 3.068400 -4.355200 0.197400
H 3.139700 -5.315600 -0.289400
C 3.051900 -4.026100 1.513700
H 3.107900 -4.643300 2.397200
C 2.940400 -1.878300 2.804900
H 2.123200 -1.152900 2.784100
H 2.796100 -2.553200 3.650300
C 2.992600 -3.069800 -1.956900
H 3.911700 -2.572200 -2.281600
H 2.960000 -4.073200 -2.384700
N 0.000500 0.762600 2.937400
C 0.000200 0.359600 1.838600
H 3.893500 -1.353500 2.924200
H 2.125500 -2.503000 -2.304900
N 2.740500 2.323800 -1.927800
N 2.760900 2.887100 0.151800
C 2.765300 1.809000 -0.671300
C 2.746800 4.053800 -0.577000
H 2.743600 5.024700 -0.105900
C 2.737500 3.699500 -1.886900
H 2.732000 4.302000 -2.782300
C 2.783000 1.526400 -3.139800
H 3.764000 1.053200 -3.246300
H 2.005800 0.758800 -3.113000
C 2.807400 2.836900 1.602400
H 3.745900 3.274700 1.956100
H 1.952200 3.368400 2.032400
N -0.002800 -1.090500 -3.171000
C -0.002000 -0.772600 -2.044200
H 2.608000 2.180200 -3.995900
H 2.758900 1.792500 1.912100
Au -2.757300 -0.149100 -0.161800
N -2.953400 -2.645200 1.582700
N -2.982800 -3.170000 -0.507200
C -2.914000 -2.107700 0.335800
C -3.083100 -4.345900 0.201000
H -3.157400 -5.306400 -0.285200
C -3.065600 -4.015800 1.517000
H -3.123500 -4.632200 2.400900
C -2.947300 -1.867400 2.806700
H -2.126500 -1.146000 2.786200
H -3.897900 -1.337900 2.924700
C -3.003600 -3.062400 -1.954300

| | | | |
|---|---|---|---|
| H | -3.921500 | -2.563000 | -2.279400 |
| H | -2.135200 | -2.497700 | -2.302700 |
| H | -2.807200 | -2.542500 | 3.652700 |
| H | -2.973100 | -4.066100 | -2.381300 |
| N | -2.733400 | 2.330400 | -1.928600 |
| N | -2.748700 | 2.895700 | 0.150600 |
| C | -2.759100 | 1.816900 | -0.671500 |
| C | -2.729900 | 4.061600 | -0.579200 |
| H | -2.721800 | 5.032900 | -0.109000 |
| C | -2.723800 | 3.706100 | -1.888800 |
| H | -2.716100 | 4.307800 | -2.784800 |
| C | -2.780200 | 1.532100 | -3.139800 |
| H | -3.762400 | 1.060800 | -3.243500 |
| H | -2.606200 | 2.184900 | -3.996900 |
| C | -2.794800 | 2.846800 | 1.601200 |
| H | -3.733300 | 3.284500 | 1.955000 |
| H | -2.745600 | 1.802800 | 1.912000 |
| H | -2.004500 | 0.763000 | -3.114400 |
| H | -1.939700 | 3.378900 | 2.030500 |
| Ag | -0.000700 | -0.218700 | -0.101700 |
| O | 0.007600 | 3.644700 | 3.185000 |
| H | 0.004800 | 2.671400 | 3.270400 |
| C | 0.013700 | 4.202100 | 4.482400 |
| H | 0.906500 | 3.913900 | 5.055200 |
| H | 0.015700 | 5.289800 | 4.371700 |
| H | -0.875900 | 3.917800 | 5.062000 |

III-2S1

79
Molecule Name

| | | | |
|---|---|---|---|
| Au | -2.935300 | -0.000100 | -0.000000 |
| N | -2.977900 | 2.986700 | 0.819100 |
| N | -3.427700 | 2.737200 | -1.280200 |
| C | -3.121900 | 2.038700 | -0.149400 |
| C | -3.475900 | 4.094100 | -1.018300 |
| H | -3.699600 | 4.819700 | -1.784500 |
| C | -3.197200 | 4.250600 | 0.301900 |
| H | -3.137900 | 5.136900 | 0.912700 |
| C | -2.599500 | 2.740100 | 2.205700 |
| H | -2.311400 | 1.692500 | 2.305600 |
| H | -1.747200 | 3.379100 | 2.450300 |
| C | -3.578500 | 2.145200 | -2.603400 |
| H | -4.152200 | 1.218400 | -2.523600 |
| H | -4.119500 | 2.843700 | -3.245000 |
| H | -3.439300 | 2.949700 | 2.875800 |
| H | -2.595900 | 1.938200 | -3.037200 |
| N | -2.977800 | -2.986800 | -0.819100 |
| N | -3.427500 | -2.737300 | 1.280200 |
| C | -3.121800 | -2.038800 | 0.149400 |
| C | -3.475600 | -4.094200 | 1.018300 |
| H | -3.699300 | -4.819800 | 1.784600 |
| C | -3.197000 | -4.250700 | -0.301800 |
| H | -3.137700 | -5.137100 | -0.912600 |
| C | -2.599400 | -2.740300 | -2.205700 |
| H | -2.311300 | -1.692700 | -2.305600 |
| H | -1.747100 | -3.379300 | -2.450300 |
| C | -3.578400 | -2.145300 | 2.603400 |
| H | -4.152200 | -1.218500 | 2.523500 |
| H | -4.119300 | -2.843700 | 3.245100 |
| H | -3.439300 | -2.949800 | -2.875800 |
| H | -2.595800 | -1.938100 | 3.037200 |
| N | 0.000000 | -2.911300 | 1.350200 |
| C | 0.000000 | -1.818800 | 0.924300 |
| N | -0.000200 | 2.911300 | -1.350200 |
| C | -0.000000 | 1.818800 | -0.924100 |
| Ag | 0.000100 | -0.000000 | 0.000100 |
| Au | 2.935500 | 0.000100 | 0.000000 |
| N | 2.977900 | 2.986900 | 0.818600 |
| N | 3.427700 | 2.737100 | -1.280500 |
| C | 3.121900 | 2.038800 | -0.149700 |
| C | 3.475800 | 4.094100 | -1.018900 |
| H | 3.699900 | 4.819500 | -1.785200 |
| C | 3.197100 | 4.250800 | 0.301200 |
| H | 3.137600 | 5.137200 | 0.912000 |
| C | 2.598900 | 2.740700 | 2.205200 |
| H | 2.310500 | 1.693200 | 2.305200 |
| H | 3.438500 | 2.950300 | 2.875600 |
| C | 3.578500 | 2.144900 | -2.603700 |
| H | 4.152800 | 1.218500 | -2.523900 |
| H | 2.595800 | 1.937200 | -3.037100 |
| H | 1.746500 | 3.379900 | 2.449100 |
| H | 4.118700 | 2.843600 | -3.245700 |
| N | 2.977900 | -2.986700 | -0.818800 |
| N | 3.427900 | -2.737000 | 1.280400 |
| C | 3.121900 | -2.038700 | 0.149600 |
| C | 3.476000 | -4.094000 | 1.018600 |
| H | 3.700100 | -4.819500 | 1.784900 |
| C | 3.197100 | -4.250600 | -0.301400 |
| H | 3.137600 | -5.137000 | -0.912200 |
| C | 2.598700 | -2.740500 | -2.205300 |
| H | 2.310200 | -1.693000 | -2.305200 |
| H | 3.438300 | -2.949800 | -2.875800 |
| C | 3.578600 | -2.145000 | 2.603500 |
| H | 4.152900 | -1.218500 | 2.523900 |
| H | 2.595900 | -1.937200 | 3.036900 |
| H | 1.746500 | -3.379800 | -2.449200 |
| H | 4.118800 | -2.843700 | 3.245600 |
| O | -0.000500 | -4.631300 | -1.130700 |
| H | -0.000600 | -4.137800 | -0.285800 |
| C | 0.000100 | -6.020100 | -0.831400 |
| H | -0.889400 | -6.323000 | -0.260400 |
| H | -0.000200 | -6.559700 | -1.783000 |
| H | 0.890200 | -6.322500 | -0.261100 |
| O | -0.000700 | 4.631200 | 1.130700 |
| H | -0.000600 | 4.137800 | 0.285900 |
| C | -0.000300 | 6.020000 | 0.831600 |
| H | -0.001000 | 6.559600 | 1.783200 |
| H | 0.890000 | 6.322600 | 0.261700 |
| H | -0.889500 | 6.322900 | 0.260300 |

III-3S1

85
Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.072000 | 2.856400 | -0.104700 |
| N | -2.844900 | 2.937000 | -1.057000 |
| N | -2.714200 | 3.169400 | 1.077300 |
| C | -1.957000 | 2.999900 | -0.034800 |
| C | -4.050200 | 3.210500 | 0.753500 |
| H | -4.819200 | 3.340700 | 1.499300 |
| C | -4.132600 | 3.067500 | -0.592400 |
| H | -4.984600 | 3.054300 | -1.254000 |
| C | -2.512500 | 2.712800 | -2.449200 |
| H | -1.449900 | 2.471100 | -2.516200 |
| H | -3.103300 | 1.869600 | -2.818400 |
| C | -2.201200 | 3.187600 | 2.433500 |
| H | -1.180900 | 3.578100 | 2.417800 |

| | | | |
|---|---|---|---|
| H | -2.820000 | 3.851500 | 3.042000 |
| H | -2.715500 | 3.610200 | -3.041500 |
| H | -2.209300 | 2.178500 | 2.860500 |
| N | 2.971000 | 2.905800 | 0.888000 |
| N | 2.855700 | 3.367500 | -1.209000 |
| C | 2.093000 | 3.050500 | -0.133800 |
| C | 4.186000 | 3.421100 | -0.863200 |
| H | 4.958700 | 3.651300 | -1.580300 |
| C | 4.258000 | 3.135300 | 0.460000 |
| H | 5.102400 | 3.072700 | 1.127600 |
| C | 2.628500 | 2.536500 | 2.245700 |
| H | 1.605300 | 2.155000 | 2.255200 |
| H | 3.312800 | 1.749100 | 2.571700 |
| C | 2.343500 | 3.509500 | -2.554500 |
| H | 1.425100 | 4.102300 | -2.534800 |
| H | 3.084900 | 4.026100 | -3.166800 |
| H | 2.696600 | 3.402900 | 2.911000 |
| H | 2.139500 | 2.524000 | -2.984500 |
| N | 3.246300 | 0.038800 | -1.120100 |
| C | 2.101300 | 0.027000 | -0.874800 |
| N | -2.909900 | -0.055900 | 0.554000 |
| C | -1.774900 | -0.032300 | 0.260400 |
| Ag | 0.164300 | 0.002100 | -0.298600 |
| Au | 0.175700 | -2.848400 | -0.123200 |
| N | -2.695200 | -2.947700 | -1.206600 |
| N | -2.643500 | -3.323500 | 0.910900 |
| C | -1.848000 | -3.056900 | -0.154100 |
| C | -3.963500 | -3.380400 | 0.528400 |
| H | -4.757800 | -3.582200 | 1.230400 |
| C | -3.995800 | -3.147500 | -0.807200 |
| H | -4.820200 | -3.111000 | -1.501800 |
| C | -2.310400 | -2.615900 | -2.562700 |
| H | -1.282800 | -2.245600 | -2.547600 |
| H | -2.368400 | -3.497200 | -3.208900 |
| C | -2.183800 | -3.419800 | 2.283200 |
| H | -1.159300 | -3.799800 | 2.284600 |
| H | -2.219600 | -2.438600 | 2.770000 |
| H | -2.973700 | -1.828000 | -2.929500 |
| H | -2.819200 | -4.124900 | 2.824600 |
| N | 3.034800 | -2.768400 | 0.989200 |
| N | 3.016300 | -3.306500 | -1.092400 |
| C | 2.202400 | -2.977500 | -0.059200 |
| C | 4.333000 | -3.304000 | -0.694900 |
| H | 5.139900 | -3.534900 | -1.373100 |
| C | 4.344100 | -2.969900 | 0.618900 |
| H | 5.159400 | -2.856300 | 1.315300 |
| C | 2.630700 | -2.351800 | 2.315900 |
| H | 1.583600 | -2.044500 | 2.280200 |
| H | 2.740500 | -3.174600 | 3.029100 |
| C | 2.564500 | -3.511100 | -2.451700 |
| H | 1.637000 | -4.089600 | -2.442700 |
| H | 2.395300 | -2.546700 | -2.940200 |
| H | 3.251600 | -1.503500 | 2.615600 |
| H | 3.324500 | -4.069500 | -3.001500 |
| O | 4.749600 | 0.110200 | 1.415300 |
| H | 4.319600 | 0.092600 | 0.538000 |
| C | 6.144400 | 0.114600 | 1.213900 |
| H | 6.484100 | 0.997800 | 0.653200 |
| H | 6.492400 | -0.778900 | 0.675500 |
| H | 6.621100 | 0.129500 | 2.198200 |
| O | -4.428600 | -0.029300 | -1.962000 |
| H | -4.021200 | -0.041300 | -1.075400 |
| C | -5.828400 | -0.056000 | -1.803100 |
| H | -6.175100 | -0.963000 | -1.286100 |
| H | -6.204700 | 0.813800 | -1.244700 |
| H | -6.274700 | -0.040200 | -2.801200 |
| C | -4.027100 | -0.158300 | 4.140300 |
| O | -2.800000 | -0.154400 | 3.446600 |
| H | -4.644400 | -1.036400 | 3.898300 |
| H | -4.624200 | 0.744800 | 3.943400 |
| H | -2.987900 | -0.127500 | 2.490300 |
| H | -3.800200 | -0.187800 | 5.209100 |

III-4S1

91

Molecule Name

| | | | |
|---|---|---|---|
| Au | -0.000000 | -2.867300 | -0.001000 |
| N | -2.852700 | -3.115000 | 1.073200 |
| N | -2.851900 | -3.112500 | -1.077900 |
| C | -2.029900 | -3.039800 | -0.001900 |
| C | -4.162800 | -3.235300 | -0.680800 |
| H | -4.972600 | -3.314300 | -1.389800 |
| C | -4.163300 | -3.236900 | 0.674900 |
| H | -4.973700 | -3.317400 | 1.383100 |
| C | -2.442100 | -2.996300 | 2.458600 |
| H | -1.354900 | -2.910000 | 2.489500 |
| H | -2.893400 | -2.099400 | 2.895900 |
| C | -2.440300 | -2.991600 | -2.462700 |
| H | -1.353200 | -2.902400 | -2.492600 |
| H | -2.739800 | -3.882000 | -3.023100 |
| H | -2.744400 | -3.886500 | 3.017800 |
| H | -2.893500 | -2.095500 | -2.899500 |
| N | 2.853000 | -3.112800 | -1.075000 |
| N | 2.851800 | -3.113100 | 1.076100 |
| C | 2.029900 | -3.039300 | 0.000100 |
| C | 4.162800 | -3.235000 | 0.679100 |
| H | 4.972500 | -3.314600 | 1.388100 |
| C | 4.163500 | -3.234800 | -0.676600 |
| H | 4.974000 | -3.314100 | -1.384800 |
| C | 2.442500 | -2.993100 | -2.460300 |
| H | 1.355500 | -2.904300 | -2.491200 |
| H | 2.895800 | -2.097200 | -2.897600 |
| C | 2.439900 | -2.993600 | 2.461000 |
| H | 1.352700 | -2.905800 | 2.490800 |
| H | 2.740400 | -3.884100 | 3.020800 |
| H | 2.742800 | -3.883900 | -3.019700 |
| H | 2.891900 | -2.097300 | 2.898500 |
| N | 3.185800 | 0.000000 | 0.000100 |
| C | 2.013700 | 0.000100 | -0.000200 |
| N | -3.186700 | -0.000100 | 0.003800 |
| C | -2.014500 | 0.000000 | 0.002200 |
| Ag | -0.000400 | -0.000200 | 0.000400 |
| Au | -0.000100 | 2.867500 | -0.000900 |
| N | -2.852900 | 3.114900 | 1.073200 |
| N | -2.852000 | 3.112300 | -1.077900 |
| C | -2.030000 | 3.039700 | -0.002000 |
| C | -4.162900 | 3.235100 | -0.680900 |
| H | -4.972700 | 3.313900 | -1.389900 |
| C | -4.163500 | 3.236700 | 0.674800 |
| H | -4.973900 | 3.317100 | 1.383000 |
| C | -2.442300 | 2.996300 | 2.458600 |
| H | -1.355100 | 2.910100 | 2.489500 |
| H | -2.744700 | 3.886500 | 3.017800 |
| C | -2.440300 | 2.991300 | -2.462800 |
| H | -1.353300 | 2.902200 | -2.492500 |
| H | -2.893500 | 2.095100 | -2.899500 |
| H | -2.893500 | 2.099400 | 2.895900 |

| | | | |
|---|---|---|---|
| H | -2.739900 | 3.881600 | -3.023300 |
| N | 2.852700 | 3.112700 | -1.075300 |
| N | 2.851800 | 3.113300 | 1.075900 |
| C | 2.029800 | 3.039300 | -0.000000 |
| C | 4.162700 | 3.235100 | 0.678700 |
| H | 4.972600 | 3.314700 | 1.387600 |
| C | 4.163300 | 3.234800 | -0.677000 |
| H | 4.973800 | 3.314000 | -1.385300 |
| C | 2.442200 | 2.992900 | -2.460500 |
| H | 1.355100 | 2.904200 | -2.491300 |
| H | 2.742400 | 3.883700 | -3.020000 |
| C | 2.440000 | 2.993800 | 2.460800 |
| H | 1.352900 | 2.906200 | 2.490700 |
| H | 2.892000 | 2.097400 | 2.898300 |
| H | 2.895400 | 2.097000 | -2.897700 |
| H | 2.740700 | 3.884300 | 3.020500 |
| O | 4.083500 | 0.000000 | -2.751000 |
| H | 3.899400 | 0.000000 | -1.792500 |
| C | 5.480800 | 0.000100 | -2.931400 |
| H | 5.961000 | -0.889700 | -2.497200 |
| H | 5.961000 | 0.889900 | -2.497200 |
| H | 5.674700 | 0.000100 | -4.007300 |
| O | -4.076200 | -0.000000 | 2.758300 |
| H | -3.895000 | -0.000000 | 1.799200 |
| C | -5.472900 | -0.000100 | 2.943100 |
| H | -5.954500 | 0.889700 | 2.510400 |
| H | -5.954400 | -0.890000 | 2.510400 |
| H | -5.663300 | -0.000100 | 4.019600 |
| C | -5.480200 | -0.000100 | -2.929400 |
| O | -4.083000 | -0.000200 | -2.748700 |
| H | -5.960500 | 0.889700 | -2.495300 |
| H | -5.960600 | -0.889900 | -2.495200 |
| H | -3.899100 | -0.000200 | -1.790100 |
| H | -5.673900 | -0.000100 | -4.005300 |
| C | 5.475300 | 0.000100 | 2.936400 |
| O | 4.078400 | 0.000100 | 2.753700 |
| H | 5.956300 | 0.889900 | 2.503000 |
| H | 5.956300 | -0.889800 | 2.503000 |
| H | 3.895800 | 0.000000 | 1.794900 |
| H | 5.667400 | 0.000100 | 4.012600 |

III-S2

76
Molecule Name

| | | | |
|---|---|---|---|
| Au | 2.754900 | -0.283700 | -0.206200 |
| N | 2.658700 | 1.873200 | -2.356000 |
| N | 2.706000 | 2.769400 | -0.396900 |
| C | 2.715000 | 1.571100 | -1.033000 |
| C | 2.657800 | 3.800700 | -1.306000 |
| H | 2.646800 | 4.835500 | -0.999900 |
| C | 2.631600 | 3.236900 | -2.540000 |
| H | 2.600300 | 3.684500 | -3.521500 |
| C | 2.699700 | 0.889800 | -3.422800 |
| H | 3.682600 | 0.409800 | -3.455100 |
| H | 1.926800 | 0.133100 | -3.268700 |
| C | 2.783200 | 2.959300 | 1.040800 |
| H | 3.701500 | 3.499800 | 1.290100 |
| H | 1.908100 | 3.506800 | 1.406200 |
| N | 0.000100 | -1.715500 | -2.990600 |
| C | 0.000100 | -1.222800 | -1.928500 |
| H | 2.519400 | 1.396000 | -4.372700 |
| H | 2.806600 | 1.978400 | 1.516700 |
| N | 3.040900 | -2.438600 | 1.931600 |
| N | 3.018800 | -3.319700 | -0.034700 |
| C | 2.957400 | -2.127600 | 0.612100 |
| C | 3.157600 | -4.352800 | 0.864100 |
| H | 3.233400 | -5.382600 | 0.550300 |
| C | 3.171800 | -3.798300 | 2.102500 |
| H | 3.263000 | -4.250300 | 3.078100 |
| C | 3.050200 | -1.457800 | 2.999800 |
| H | 2.198500 | -0.781100 | 2.893100 |
| H | 2.975400 | -1.977600 | 3.956500 |
| C | 3.000700 | -3.466600 | -1.478400 |
| H | 3.920100 | -3.058500 | -1.909600 |
| H | 2.932500 | -4.528100 | -1.722400 |
| N | -0.003300 | 1.055200 | 2.759200 |
| C | -0.001700 | 0.494100 | 1.732200 |
| H | 3.980800 | -0.882100 | 2.976300 |
| H | 2.136000 | -2.946700 | -1.898000 |
| Au | -2.755200 | -0.282200 | -0.206500 |
| N | -2.655400 | 1.877200 | -2.353500 |
| N | -2.707100 | 2.771200 | -0.393600 |
| C | -2.714300 | 1.573700 | -1.031100 |
| C | -2.657600 | 3.803600 | -1.301500 |
| H | -2.647400 | 4.838000 | -0.994100 |
| C | -2.628700 | 3.241200 | -2.536000 |
| H | -2.595700 | 3.689900 | -3.517000 |
| C | -2.694400 | 0.895000 | -3.421400 |
| H | -3.679000 | 0.418900 | -3.459900 |
| H | -2.506500 | 1.401200 | -4.369900 |
| C | -2.787100 | 2.959700 | 1.044100 |
| H | -3.706700 | 3.498600 | 1.292300 |
| H | -2.809800 | 1.978400 | 1.519100 |
| H | -1.925400 | 0.135100 | -3.263600 |
| H | -1.913400 | 3.508200 | 1.411400 |
| N | -3.042400 | -2.439300 | 1.928900 |
| N | -3.020200 | -3.318300 | -0.038300 |
| C | -2.958500 | -2.126900 | 0.609800 |
| C | -3.159500 | -4.352300 | 0.859400 |
| H | -3.235500 | -5.381700 | 0.544600 |
| C | -3.173700 | -3.799100 | 2.098400 |
| H | -3.265200 | -4.252100 | 3.073600 |
| C | -3.051900 | -1.459600 | 2.998200 |
| H | -2.200800 | -0.782100 | 2.891700 |
| H | -3.983000 | -0.884600 | 2.975900 |
| C | -3.001900 | -3.463800 | -1.482100 |
| H | -3.920700 | -3.053900 | -1.913100 |
| H | -2.136400 | -2.944600 | -1.900900 |
| H | -2.976100 | -1.980300 | 3.954200 |
| H | -2.935200 | -4.525100 | -1.727100 |
| Ag | -0.000100 | -0.370900 | -0.097600 |
| C | 0.004400 | 4.697700 | 3.758100 |
| C | 0.007100 | 6.167400 | 3.400600 |
| H | 0.891200 | 4.456200 | 4.363800 |
| H | -0.880000 | 4.460700 | 4.369000 |
| H | -0.881000 | 6.422700 | 2.812800 |
| H | 0.011100 | 6.785300 | 4.304200 |
| H | 0.893100 | 6.418400 | 2.807800 |
| O | -0.001100 | 3.941000 | 2.558800 |
| H | -0.001300 | 2.992000 | 2.792600 |

III-2S2

85
Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000700 | -2.938600 | 0.000100 |
| N | 3.045200 | -2.971300 | -0.568300 |

| | | | |
|---|---|---|---|
| N | 2.623200 | -3.432300 | 1.500600 |
| C | 2.020400 | -3.123300 | 0.316800 |
| C | 3.997500 | -3.473900 | 1.352800 |
| H | 4.657600 | -3.698000 | 2.176000 |
| C | 4.262500 | -3.188300 | 0.051700 |
| H | 5.196400 | -3.121500 | -0.482500 |
| C | 2.913200 | -2.589400 | -1.969600 |
| H | 1.881100 | -2.284400 | -2.150000 |
| H | 3.582900 | -1.747500 | -2.162400 |
| C | 1.922900 | -3.594700 | 2.768200 |
| H | 1.013000 | -4.178900 | 2.608900 |
| H | 2.570800 | -4.129400 | 3.465600 |
| H | 3.160500 | -3.432500 | -2.622600 |
| H | 1.667400 | -2.616500 | 3.186200 |
| N | -3.043900 | -2.972700 | 0.568300 |
| N | -2.621500 | -3.433400 | -1.500600 |
| C | -2.018900 | -3.124200 | -0.316800 |
| C | -3.995800 | -3.475600 | -1.353000 |
| H | -4.655700 | -3.700000 | -2.176200 |
| C | -4.261000 | -3.190200 | -0.051800 |
| H | -5.195000 | -3.123700 | 0.482200 |
| C | -2.912100 | -2.590700 | 1.969500 |
| H | -1.880200 | -2.285400 | 2.150100 |
| H | -3.582200 | -1.749000 | 2.162300 |
| C | -1.920900 | -3.595600 | -2.768200 |
| H | -1.010900 | -4.179400 | -2.608800 |
| H | -2.568600 | -4.130500 | -3.465700 |
| H | -3.159300 | -3.433900 | 2.622500 |
| H | -1.665800 | -2.617300 | -3.186100 |
| N | -2.828400 | -0.000500 | -1.515900 |
| C | -1.762600 | -0.000300 | -1.027400 |
| N | 2.828400 | 0.000800 | 1.515900 |
| C | 1.762600 | 0.000500 | 1.027500 |
| Ag | 0.000000 | -0.000000 | 0.000100 |
| Au | -0.000700 | 2.938600 | -0.000100 |
| N | 3.043500 | 2.972200 | -0.570400 |
| N | 2.622500 | 3.433700 | 1.498600 |
| C | 2.019100 | 3.124200 | 0.315300 |
| C | 3.996700 | 3.475700 | 1.350100 |
| H | 4.657200 | 3.700200 | 2.172800 |
| C | 4.261000 | 3.189800 | 0.048900 |
| H | 5.194700 | 3.122900 | -0.485800 |
| C | 2.910900 | 2.589700 | -1.971400 |
| H | 1.878900 | 2.284100 | -2.151200 |
| H | 3.157300 | 3.432800 | -2.624900 |
| C | 1.922900 | 3.596300 | 2.766600 |
| H | 1.012500 | 4.179800 | 2.607500 |
| H | 1.668300 | 2.618100 | 3.185200 |
| H | 3.581000 | 1.748300 | -2.164400 |
| H | 2.570900 | 4.131800 | 3.463400 |
| N | -3.044900 | 2.970900 | 0.570500 |
| N | -2.624200 | 3.432600 | -1.498600 |
| C | -2.020600 | 3.123300 | -0.315300 |
| C | -3.998400 | 3.474000 | -1.349900 |
| H | -4.659100 | 3.698300 | -2.172600 |
| C | -4.262500 | 3.188000 | -0.048700 |
| H | -5.196200 | 3.120700 | 0.486000 |
| C | -2.911900 | 2.588400 | 1.971400 |
| H | -1.879800 | 2.283100 | 2.151100 |
| H | -3.158500 | 3.431400 | 2.625000 |
| C | -1.924800 | 3.595500 | -2.766600 |
| H | -1.014600 | 4.179400 | -2.607600 |
| H | -1.669800 | 2.617500 | -3.185300 |
| H | -3.581700 | 1.746700 | 2.164500 |
| H | -2.573100 | 4.130800 | -3.463300 |
| O | -4.764000 | -0.001000 | 0.789300 |
| H | -4.202800 | -0.001000 | -0.012800 |
| C | -6.130900 | -0.001600 | 0.380800 |
| H | -6.348700 | -0.886500 | -0.236900 |
| H | -6.348900 | 0.882000 | -0.238800 |
| C | -7.011400 | -0.000500 | 1.620400 |
| H | -8.070500 | -0.001000 | 1.341400 |
| H | -6.817200 | -0.885500 | 2.236600 |
| H | -6.817600 | 0.886000 | 2.234800 |
| O | 4.764000 | 0.000800 | -0.789500 |
| H | 4.202800 | 0.000500 | 0.012700 |
| C | 6.130900 | 0.001000 | -0.381100 |
| H | 6.348600 | 0.884800 | 0.238300 |
| H | 6.349200 | -0.883700 | 0.236900 |
| C | 7.011300 | 0.002200 | -1.620700 |
| H | 6.817100 | 0.888300 | -2.235300 |
| H | 8.070500 | 0.002300 | -1.341800 |
| H | 6.817600 | -0.883100 | -2.236600 |

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Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.176100 | 2.853300 | -0.184600 |
| N | -2.766000 | 2.966100 | -1.050900 |
| N | -2.569700 | 3.231000 | 1.074600 |
| C | -1.848000 | 3.032000 | -0.055800 |
| C | -3.913900 | 3.287100 | 0.789000 |
| H | -4.658800 | 3.440200 | 1.554700 |
| C | -4.037500 | 3.123500 | -0.551400 |
| H | -4.908800 | 3.110900 | -1.187400 |
| C | -2.476700 | 2.709700 | -2.447100 |
| H | -1.424200 | 2.432900 | -2.535800 |
| H | -3.101800 | 1.879100 | -2.787000 |
| C | -2.019500 | 3.268600 | 2.415900 |
| H | -0.975800 | 3.585700 | 2.356400 |
| H | -2.573300 | 3.998400 | 3.011900 |
| H | -2.666600 | 3.603300 | -3.049600 |
| H | -2.084900 | 2.279800 | 2.883700 |
| N | 3.110200 | 2.825300 | 0.708100 |
| N | 2.927200 | 3.348000 | -1.369500 |
| C | 2.198400 | 3.013000 | -0.276400 |
| C | 4.269800 | 3.370700 | -1.071400 |
| H | 5.019900 | 3.608000 | -1.809800 |
| C | 4.384700 | 3.046300 | 0.239800 |
| H | 5.251700 | 2.949300 | 0.873400 |
| C | 2.811500 | 2.420200 | 2.065700 |
| H | 1.784200 | 2.051200 | 2.100500 |
| H | 3.497200 | 1.615900 | 2.343600 |
| C | 2.368800 | 3.539000 | -2.690500 |
| H | 1.463900 | 4.148500 | -2.619700 |
| H | 3.097700 | 4.058700 | -3.315000 |
| H | 2.914500 | 3.265400 | 2.753500 |
| H | 2.129200 | 2.570700 | -3.140400 |
| N | 3.267500 | -0.000500 | -1.338600 |
| C | 2.132500 | -0.000300 | -1.051200 |
| N | -2.823300 | 0.000500 | 0.559100 |
| C | -1.699700 | 0.000300 | 0.224500 |
| Ag | 0.217100 | -0.000100 | -0.405200 |
| Au | 0.174800 | -2.853400 | -0.184600 |
| N | -2.767700 | -2.965600 | -1.049800 |
| N | -2.570600 | -3.229800 | 1.075600 |
| C | -1.849300 | -3.031400 | -0.055100 |

| | | | |
|---|---|---|---|
| C | -3.914900 | -3.285700 | 0.790700 |
| H | -4.659500 | -3.438400 | 1.556700 |
| C | -4.039000 | -3.122500 | -0.549800 |
| H | -4.910600 | -3.110000 | -1.185400 |
| C | -2.479000 | -2.709500 | -2.446200 |
| H | -1.425800 | -2.435400 | -2.535800 |
| H | -2.671600 | -3.602600 | -3.048700 |
| C | -2.019900 | -3.267400 | 2.416800 |
| H | -0.975900 | -3.583600 | 2.356800 |
| H | -2.085900 | -2.278700 | 2.884900 |
| H | -3.102300 | -1.877300 | -2.785500 |
| H | -2.572900 | -3.997800 | 3.012700 |
| N | 3.109100 | -2.826600 | 0.707400 |
| N | 2.925600 | -3.348800 | -1.370300 |
| C | 2.197100 | -3.013900 | -0.277000 |
| C | 4.268300 | -3.371900 | -1.072400 |
| H | 5.018100 | -3.609300 | -1.811000 |
| C | 4.383400 | -3.047800 | 0.238900 |
| H | 5.250600 | -2.951100 | 0.872300 |
| C | 2.810700 | -2.421500 | 2.065100 |
| H | 1.783600 | -2.052200 | 2.100100 |
| H | 2.913600 | -3.266900 | 2.752700 |
| C | 2.366900 | -3.539400 | -2.691200 |
| H | 1.461400 | -4.147800 | -2.620200 |
| H | 2.128400 | -2.570900 | -3.141300 |
| H | 3.496800 | -1.617400 | 2.343000 |
| H | 3.095200 | -4.060000 | -3.315600 |
| O | 4.913800 | -0.000900 | 1.106700 |
| H | 4.444100 | -0.000800 | 0.249300 |
| C | 6.304700 | -0.001100 | 0.847100 |
| H | 6.590100 | 0.882000 | 0.253800 |
| H | 6.590000 | -0.884400 | 0.254200 |
| C | 7.045600 | -0.000800 | 2.166500 |
| H | 6.786400 | -0.885900 | 2.757600 |
| H | 8.128100 | -0.001000 | 2.003800 |
| H | 6.786700 | 0.884600 | 2.757200 |
| O | -4.441400 | 0.001400 | -1.895500 |
| H | -4.015100 | 0.001200 | -1.017400 |
| C | -5.844500 | 0.000900 | -1.715100 |
| H | -6.164100 | -0.882800 | -1.139800 |
| H | -6.164700 | 0.884300 | -1.139700 |
| C | -6.507900 | 0.000800 | -3.074600 |
| H | -7.598100 | 0.000400 | -2.974700 |
| H | -6.214300 | 0.886400 | -3.648000 |
| H | -6.213700 | -0.884700 | -3.648100 |
| C | -4.027400 | 0.000500 | 4.107800 |
| O | -2.775200 | 0.000500 | 3.448300 |
| H | -4.619000 | -0.885100 | 3.823700 |
| H | -4.619400 | 0.885600 | 3.822900 |
| H | -2.933300 | 0.000300 | 2.485400 |
| C | -3.786500 | 0.001200 | 5.601100 |
| H | -3.215900 | 0.887400 | 5.897200 |
| H | -4.735200 | 0.001200 | 6.147300 |
| H | -3.215400 | -0.884400 | 5.898000 |

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Molecule Name

| | | | |
|---|---|---|---|
| Au | 0.000300 | 2.868000 | -0.001200 |
| N | 2.853300 | 3.111300 | 1.073000 |
| N | 2.852500 | 3.108900 | -1.078100 |
| C | 2.030200 | 3.038500 | -0.002100 |
| C | 4.163700 | 3.227400 | -0.681000 |
| H | 4.974100 | 3.302200 | -1.389800 |
| C | 4.164200 | 3.228900 | 0.674700 |
| H | 4.975100 | 3.305300 | 1.382700 |
| C | 2.441900 | 2.994600 | 2.458200 |
| H | 1.354700 | 2.907200 | 2.488500 |
| H | 2.893600 | 2.098700 | 2.897100 |
| C | 2.440100 | 2.989500 | -2.462700 |
| H | 1.353100 | 2.899700 | -2.492000 |
| H | 2.738600 | 3.880900 | -3.022200 |
| H | 2.742900 | 3.886000 | 3.016200 |
| H | 2.893500 | 2.094100 | -2.900700 |
| N | -2.852900 | 3.109300 | -1.075600 |
| N | -2.851900 | 3.109800 | 1.075500 |
| C | -2.029700 | 3.038100 | -0.000400 |
| C | -4.163200 | 3.227500 | 0.678300 |
| H | -4.973600 | 3.303100 | 1.387100 |
| C | -4.163800 | 3.227100 | -0.677400 |
| H | -4.974800 | 3.302300 | -1.385500 |
| C | -2.441600 | 2.991000 | -2.460700 |
| H | -1.354600 | 2.901200 | -2.490900 |
| H | -2.895300 | 2.096000 | -2.899200 |
| C | -2.439500 | 2.992100 | 2.460300 |
| H | -1.352300 | 2.904000 | 2.489700 |
| H | -2.739400 | 3.883500 | 3.019000 |
| H | -2.740500 | 3.882900 | -3.019200 |
| H | -2.891500 | 2.096400 | 2.899100 |
| N | -3.185900 | -0.000000 | 0.000000 |
| C | -2.013900 | -0.000000 | -0.000300 |
| N | 3.186900 | -0.000000 | 0.002800 |
| C | 2.014900 | -0.000000 | 0.001400 |
| Ag | 0.000500 | -0.000000 | 0.000000 |
| Au | 0.000200 | -2.868000 | -0.001200 |
| N | 2.853200 | -3.111400 | 1.073100 |
| N | 2.852400 | -3.108900 | -1.078000 |
| C | 2.030100 | -3.038500 | -0.002000 |
| C | 4.163700 | -3.227400 | -0.680900 |
| H | 4.974000 | -3.302300 | -1.389700 |
| C | 4.164200 | -3.229000 | 0.674800 |
| H | 4.975000 | -3.305400 | 1.382900 |
| C | 2.441800 | -2.994600 | 2.458300 |
| H | 1.354600 | -2.907200 | 2.488600 |
| H | 2.742700 | -3.886100 | 3.016300 |
| C | 2.440200 | -2.989500 | -2.462600 |
| H | 1.353100 | -2.899700 | -2.491900 |
| H | 2.893500 | -2.094100 | -2.900600 |
| H | 2.893500 | -2.098700 | 2.897200 |
| H | 2.738700 | -3.880900 | -3.022100 |
| N | -2.852900 | -3.109300 | -1.075700 |
| N | -2.852000 | -3.109800 | 1.075400 |
| C | -2.029700 | -3.038100 | -0.000400 |
| C | -4.163300 | -3.227400 | 0.678200 |
| H | -4.973700 | -3.303000 | 1.387000 |
| C | -4.163900 | -3.227100 | -0.677500 |
| H | -4.974800 | -3.302400 | -1.385600 |
| C | -2.441600 | -2.991100 | -2.460700 |
| H | -1.354600 | -2.901300 | -2.490900 |
| H | -2.740500 | -3.883000 | -3.019200 |
| C | -2.439600 | -2.992000 | 2.460200 |
| H | -1.352500 | -2.904000 | 2.489700 |
| H | -2.891600 | -2.096200 | 2.898900 |
| H | -2.895200 | -2.096000 | -2.899200 |
| H | -2.739600 | -3.883300 | 3.019000 |
| O | -4.085600 | -0.000100 | -2.759000 |
| H | -3.907300 | -0.000100 | -1.799100 |

| | | | |
|---|---|---|---|
| C | -5.486700 | -0.000000 | -2.954800 |
| H | -5.947100 | 0.884500 | -2.485100 |
| H | -5.947200 | -0.884500 | -2.485100 |
| C | -5.768300 | 0.000000 | -4.441000 |
| H | -5.333000 | -0.885800 | -4.915100 |
| H | -6.846300 | 0.000000 | -4.631900 |
| H | -5.333000 | 0.885800 | -4.915100 |
| O | 4.076300 | -0.000100 | 2.766000 |
| H | 3.901000 | -0.000000 | 1.805600 |
| C | 5.476900 | -0.000000 | 2.966000 |
| H | 5.938700 | -0.884500 | 2.497600 |
| H | 5.938700 | 0.884500 | 2.497600 |
| C | 5.754000 | -0.000100 | 4.453000 |
| H | 6.831400 | -0.000000 | 4.647100 |
| H | 5.317300 | 0.885700 | 4.925800 |
| H | 5.317300 | -0.885900 | 4.925700 |
| C | 5.486400 | -0.000000 | -2.953700 |
| O | 4.085400 | 0.000000 | -2.757500 |
| H | 5.946900 | -0.884500 | -2.484100 |
| H | 5.947000 | 0.884400 | -2.484100 |
| H | 3.907300 | 0.000000 | -1.797600 |
| C | 5.767600 | 0.000000 | -4.440000 |
| H | 5.332200 | 0.885800 | -4.913900 |
| H | 6.845500 | -0.000000 | -4.631200 |
| H | 5.332100 | -0.885800 | -4.914000 |
| C | -5.480600 | 0.000100 | 2.960400 |
| O | -4.079800 | 0.000100 | 2.761700 |
| H | -5.942000 | -0.884400 | 2.491700 |
| H | -5.941900 | 0.884600 | 2.491600 |
| H | -3.903500 | 0.000100 | 1.801500 |
| C | -5.759000 | 0.000200 | 4.447200 |
| H | -6.836600 | 0.000200 | 4.640400 |
| H | -5.322700 | -0.885600 | 4.920400 |
| H | -5.322700 | 0.886000 | 4.920300 |