Supplementary information for

Adatom Mediated Adsorption of N-Heterocyclic Carbenes On Cu(111) and Au(111)

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This Supplementary Material contains details of the DFT calculations including the influence of using different k-point meshes in computing adsorption energies and structural properties, different tested start geometries, a test on the role of adatoms in drastically reduction of the diffusion barriers, and a set of optimized structures. A movie can be downloaded showing the barrier-free extraction of an Au atom out of the surface layer, enabling the formation of the (NHC)_2Au dimer.

**Different k-point Meshes**

In the following, we show that using Gamma-only k-point meshes (Γ only) is sufficient for a proper description of the metallic surfaces with NHC molecules on top. For this purpose, other sampling: 2x2x1 and 3x3x1 have been tested for, e.g. NHC1 on both Cu(111) and Au(111) without and with an adatom (see Supplementary Tables I and II). Compared to the other meshes, using Γ-only k-point meshes leads to (i) tiny changes in the adsorption geometries, and (ii) to error bars for relative adsorption energies that are below 5 meV. However, it reduces the numerical costs, allowing for a systematic comparison of a large number of different structures.

**Supplementary Table I.** Calculated adsorption energies ($E_{ads}$ in eV) and the lengths of the carbene-Au covalent ($d_1$ in Å) of NHC1 in the surface-bound, ballbot, and (NHC1)_{2}Cu states in dependence on the k-point grid.

|         | Γ only | 2x2x1 | 3x3x1 |
|---------|--------|-------|-------|
|         | $E_{ads}$ (eV) | $d_1$ (Å) | $E_{ads}$ (eV) | $d_1$ (Å) | $E_{ads}$ (eV) | $d_1$ (Å) |
| Surface-bound | -1.961  | 2.049 | -2.012 | 2.041 | -2.014 | 2.040 |
| ballbot (flat-laying) | -3.124 | 1.964 | -3.131 | 1.965 | -3.128 | 1.964 |
| (NHC1)_{2}Cu | -2.969 | 1.968 | -3.012 | 1.969 | -3.017 | 1.969 |

**Supplementary Table II.** The same as Supplementary Table I, but for NHCs on Au(111).
| Surface-bound | -1.893  | 2.149  | -1.853  | 2.155  | -1.838  | 2.164  |
|---------------|---------|--------|---------|--------|---------|--------|
| ballbot (flat-laying) | -3.244  | 2.075  | -3.246  | 2.077  | -3.243  | 2.076  |
| (NHC1)₂Au     | -3.249  | 2.045  | -3.250  | 2.046  | -3.251  | 2.046  |

**Start configurations and most stable structures**

In order to determine the geometrical conformation of the studied NHCs on both M(111) surfaces (M = Cu and Au), we first allowed the carbene carbon atom (see its definition in the main text) to be above different registries of the surface (top, bridge, fcc and hcp hollows). Exemplarily, we discuss here the surface-bound state in detail. Irrespective of the molecular azimuthal or spatial orientation, all start structures were finally converged into on-top positions, i.e., the carbene carbon atom is atop of an atom from the surface, enabling a C-M covalent bond. Then, we considered the angle $\alpha$ to be a reference for the azimuthal orientation of the NHC ring with respect to the $<110>$ orientation of the surface (see, e.g., Figure S1 (a)). Three possibilities of $\alpha$ are tested ($\alpha = 0^\circ$, $15^\circ$, $30^\circ$). However, the case $\alpha = 15^\circ$ was unstable and converged to one of the other two cases. To express the molecular tilt angle with respect to the underlaying surface, the angle $\theta$ is considered as a reference between the central NHC ring and the underlaying surface (see main text and Figure S1 (b)). Three start configurations are typically tested for this parameter ($\theta = 0^\circ$, $45^\circ$, and $90^\circ$). Apart from this, one should carefully test the fashion of the molecular side-groups (in particular the methyl groups) with respect to the underlaying surface. As an example, the angle $\gamma$, which denotes the angle between the C-H1 bound and the underlying surface (H1 is the uppermost hydrogen atom in the outer methyl ring, see Figure S1 (c)), can be changed according to the values of $\alpha$ and $\theta$ (see Supplementary Tables III and IV). The values of $\gamma$ can be ranged between $30^\circ$ (two hydrogens in the methyl ring are pointing upwards, one downwards) and $90^\circ$ (one hydrogen in the methyl ring is pointing upwards, two downwards).

In our DFT-calculations, all tested start configurations are fully relaxed thereby converging into two distinct upright structures for each molecule. These two structures are mainly different in angle $\alpha$ (azimuthally rotated with respect to each other), providing energy difference of about 30-50 meV (see examples in Supplementary Tables III and IV). This indicates that the less stable structures can be thermally activated facilitating molecular rotations around the covalent bond.

![Figure S1](image)

**Figure S1**: Top- and side-views of NHCs on, e.g., Cu(111) to define the molecular geometries. (a) The angle $\alpha$ denotes the azimuthal orientation of the, e.g., NHC3 ring with respect to the $<110>$ direction of the surface. (b) The angle $\theta$ is defined between the, e.g., NHC2 ring plane and the surface normal. (c) $\gamma$ is the angle between the C-H1 bond and the underlying surface; H1 is the uppermost hydrogen atom in the outer methyl ring.

**Supplementary Table III.** A comparison between the geometries of the most stable structures (in bold) of the three NHCs on Cu(111) in the surface-bound state with slightly less stable structures
which result from variating the azimuthal orientation of each NHC on the surface. For definition of $E_{ads}$, $d_1$, $d_2$, $\alpha$, $\theta$, $\gamma$ see text.

| configuration | $E_{ads}$ (eV) | $d_1$ (Å) | $d_2$ (Å) | $\alpha$ (deg.) | $\theta$ (deg.) | $\gamma$ (deg.) |
|---------------|---------------|-----------|-----------|-----------------|-----------------|-----------------|
| NHC1          | upright       | -1.96     | 2.05      | 0.43            | 0               | 3               | 60              |
|               | upright       | -1.93     | 2.05      | 0.47            | 30              | 3               | 64              |
| NHC2          | upright       | -2.28     | 2.05      | 0.52            | 0               | 6.6             | 90              |
|               | upright       | -2.25     | 2.05      | 0.52            | 30              | 6.6             | 90              |
| NHC3          | upright       | -2.58     | 2.05      | 0.60            | 0               | 0               | 90              |
|               | upright       | -2.53     | 2.05      | 0.60            | 30              | 0               | 90              |

**Supplementary Table IV.** The same as Supplementary Table III, but for NHCs on Au(111).

| configuration | $E_{ads}$ (eV) | $d_1$ (Å) | $d_2$ (Å) | $\alpha$ (deg.) | $\theta$ (deg.) | $\gamma$ (deg.) |
|---------------|---------------|-----------|-----------|-----------------|-----------------|-----------------|
| NHC1          | upright       | -1.857    | 2.148     | 0.40            | 0               | 5               | 57              |
|               | upright       | -1.892    | 2.143     | 0.36            | 30              | 6               | 85              |
| NHC2          | upright       | 2.169     | 2.153     | 0.44            | 0               | 6               | 80              |
|               | upright       | 2.147     | 2.151     | 0.46            | 30              | 5               | 80              |
| NHC3          | upright       | -2.436    | 2.160     | 0.48            | 0               | 0               | 90              |
|               | upright       | -2.377    | 2.158     | 0.50            | 30              | 0               | 85              |

**Non-vertical geometries of NHCs in the surface-bound state**

In the previous paragraph, it is discussed that less stable upright structures (azimuthally rotated) might be thermally activated, due to their energies close to the most stable ones. The following data shows that such thermal effects alone are unable to give rise to stable flat-laying geometries.

Figure S2 presents the calculated adsorption energies (referenced to the most stable one) obtained by varying the tilting angle $\theta$ (see the previous paragraph) between 0° (vertical geometries) and 90° for NHC1 on Cu(111) and Au(111) in the bound-state. Thereby, the positions of the N atom in the z-direction (Figure S2) were kept fixed. The calculations indicate (i) no energetically local minima for NHC1 on both surfaces, and (ii) that flat-laying geometries are much higher in energy than the vertical ones, excluding their appearance at RT or above.
Figure S2: Spatial rotation of NHC1 on Cu(111) and Au(111) in the surface-bound state. The energies are calculated for different values of the angle θ, whereby the energies of the most stable structures are considered as references.

Figure S3: Side-views of the most stable structures of NHC1, NHC2, and NHC3 on Cu(111) and Au(111) in the surface-bound state. In all cases, upright geometries are calculated and a covalent bond between the carbene carbon atom and a surface atom is formed. The bond length \(d_1\) in Å is almost the same for the three NHCs on a given surface. The surface atom is lifted upwards by \(d_2\) (in Å).

**Diffusion barriers**

In order to show the role of the adatom to drastically reduce the diffusion barriers of the NHC molecules on planar surfaces, we exemplarily compare these barriers for an NHC in the surface-bound and the ballbot states. We select here NHC3 as an example and calculate the adsorption energies along
the <110> direction of the surface. The structures are optimized under the constraint that the carbene carbon atom is laterally fixed. The energy of the most stable structure is used as a reference.

Figure S4 shows two plots showing the calculated diffusion barriers for NHC3 molecule with (right) and without (left) adsorption on Au surface adatoms. The barriers in the latter case are apparently four times larger and the energy curves are completely different. For the surface-bound state, a steep increase of the energy curve around the saddle point reflects the fact that for movement breaking of the covalent Au-C(NHC) bond is required. However, the smooth saddle point in the ballbot state is given by the bridge-position of the Au adatom, connecting two adjacent hollow-site minima.

![Figure S4: The plots are showing the calculated diffusion barriers for NHC3 molecule without (left)/ with (right) adsorption on Au surface adatoms. The x-axis label shows the distance traveled by NHC3 along two equivalent sites along the <110> direction. The y-axis refers to the energy compared to the most stable structure, which is considered as a reference (0 eV). The structures in the saddle points, bridging between two equivalent points (dark Au atoms), and the characteristic distances are shown.](image)

**Optimized structures for NHCs on Cu(111) in ballbot states**

![NHC1/Cu(111) Upright Geometries: -2.80 eV](image)

![NHC2/Cu(111) Flat-laying Geometries: -3.09 eV](image)

![NHC3/Cu(111) Flat-laying Geometries: -3.25 eV](image)

![NHC1/Cu(111) Flat-laying Geometries: -3.12 eV](image)

![NHC2/Cu(111) Flat-laying Geometries: -3.29 eV](image)

![NHC3/Cu(111) Flat-laying Geometries: -3.08 eV](image)

**Figure S5: Side-views of NHC1, NHC2 and NHC3 molecules on, e.g. Cu(111) in the upright and flat-laying ballbot states. The adsorption energy of each structure is also depicted. Most stable states are given in bold. The**
geometries on Au(111) are similar to those on Cu(111). The respective adsorption energies are given in the main text in Table III.

**Charge density differences**

![Figure S6: Charge transfer (charge density difference plot) for NHC1 adsorbed on (a) Cu/ (c) Au plane surfaces and on (b)/(d) Cu/Au adatoms. The blue (red) regions represent electron density accumulation (depletion) for an isosurface value of 0.003 e/Å³. Upon formation of the covalent C-M bond (M=Ag, Au), the electron density mainly depletes on the carbene C and accumulates on the formed bond, i.e., parts of an electron are donated from the NHC1 molecule to the surface.](image)

**Supplementary video**

Supplementary Video shows the barrier-free extraction of an Au atom out of the surface layer, enabling the formation of the (NHC)₂Au dimer. The video was composed by considering two NHC molecules to be close to an Au surface atom. The Au surface atom is extracted from the surface, leaving a vacancy behind it and allowing the formation of a (NHC)₂Au complex.

**Optimized geometries**

a. **Optimized structure of the molecules in gas phase**

I. **NHC1 in xyz format (Å)**

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| C    | 9.422034216 | 9.726443947 | 9.941171416 |
| C    | 9.37684920 | 10.028107219 | 12.247629490 |
| C    | 10.730916668 | 10.025214446 | 11.841156819 |
| C    | 11.903580588 | 9.772558726 | 9.606286855 |
| C    | 7.166362006 | 9.784932132 | 11.026896203 |
| N    | 10.706533498 | 9.841144497 | 10.44711649 |
| N    | 8.629096457 | 9.845448901 | 11.071208840 |
| H    | 12.543581643 | 8.930607218 | 9.910758276 |
| H    | 12.481046381 | 10.706751457 | 9.677056840 |
| H    | 11.567404326 | 9.625028747 | 8.57462245 |
| H    | 6.794733231 | 8.945944639 | 11.634467922 |
| H    | 6.879362787 | 9.637228758 | 9.980842414 |
| H    | 6.72817803 | 10.722203822 | 11.40197117 |
| C    | 9.018312720 | 10.190905425 | 13.59197710 |
| C    | 11.771280859 | 10.184969730 | 12.765402528 |
| H    | 7.975144686 | 10.193385163 | 13.909097289 |
| H    | 12.81669384 | 10.183107167 | 12.455473424 |
| C    | 10.60548628 | 10.351284915 | 14.518877168 |
| C    | 11.412541853 | 10.348360331 | 14.112959227 |
| H    | 9.821247228 | 10.480677488 | 15.575082968 |
| H    | 12.194570747 | 10.475696171 | 14.862509136 |
## II. NHC2 in xyz format (Å)

| atom | x      | y      | z      |
|------|--------|--------|--------|
| C    | 9.966387462 | 9.701736251 | 10.022882920 |
| C    | 9.291189185  | 9.543012115  | 12.222196663 |
| C    | 12.448190745 | 9.722293260  | 10.366133695 |
| C    | 7.494877043  | 9.702967420  | 10.436893218 |
| N    | 11.064009306 | 9.641609600  | 10.864389170 |
| N    | 8.893572172  | 9.635559017  | 10.895153638 |
| C    | 13.065829346 | 11.117518516 | 10.558673970 |
| H    | 13.096017769 | 11.404735988 | 11.619215487 |
| H    | 12.47814852  | 11.870270150 | 10.015264174 |
| H    | 14.094711946 | 11.133531259 | 10.171065135 |
| H    | 13.39460524  | 9.463289688  | 9.301326271  |
| H    | 13.047082633 | 8.950243339  | 10.875428038 |
| C    | 6.866241077  | 11.089926106 | 10.652689360 |
| H    | 5.826736527  | 11.094386247 | 10.294101520 |
| H    | 7.428863324  | 11.85205319  | 10.096029704 |
| H    | 6.862046266  | 11.372851286 | 11.714770678 |
| H    | 6.919435598  | 8.922000155  | 10.959553756 |
| H    | 7.522217981  | 9.448769750  | 9.369865139  |
| C    | 8.579926384  | 9.436091600  | 13.445719356 |
| H    | 11.450949265 | 9.449335629  | 13.405107412 |
| H    | 7.489885936  | 9.434336758  | 13.467975354 |
| H    | 12.541188944 | 9.451659576  | 13.396653546 |
| C    | 9.326824040  | 9.342527952  | 14.629578239 |
| C    | 10.738390182 | 9.347500284  | 14.609645974 |
| H    | 8.806593695  | 9.262597783  | 15.584892228 |
| H    | 11.285868412 | 9.271458200  | 15.549925022 |

## III. NHC3 in xyz format (Å)

| atom | x      | y      | z      |
|------|--------|--------|--------|
| C    | 0.939380720 | 9.718126768 | 10.116267538 |
| C    | 0.936947050 | 9.772904758 | 13.643846838 |
| C    | 10.779390320 | 9.781864164 | 12.279319084 |
| C    | 12.426253234 | 9.746199014 | 10.275923267 |
| C    | 7.489402788  | 9.708970313  | 10.573249160 |
| N    | 11.077591705 | 9.747044600  | 10.901787636 |
| N    | 8.90306106   | 9.734784250  | 11.032579148 |
| C    | 13.186533765 | 11.05066115  | 10.566487475 |
| H    | 13.451119288 | 11.157129234 | 11.628331181 |
| C    | 12.577195710 | 11.922875877 | 10.279410628 |
| H    | 14.119064946 | 11.080044461 | 9.984698096  |
| H    | 12.637098753 | 7.578724100  | 10.414018544 |
| H    | 14.153993133 | 8.443853606  | 10.060621707 |
| C    | 13.493533531 | 8.450333685  | 11.708751603 |
| H    | 12.187399495 | 9.710636968  | 9.203234112  |
| C    | 13.222798213 | 8.479205139  | 10.64400055  |
| C    | 6.741285692  | 10.998821618 | 10.963131906 |
| H    | 5.746706830  | 11.006839324 | 10.494692643 |
| H    | 5.775059541  | 8.371028482  | 10.559220076 |
| H    | 6.632996549  | 8.380960568  | 12.113884565 |
| H    | 7.341553936  | 7.536654640  | 10.715777119 |
| H    | 7.294003839  | 11.881944501 | 10.614731588 |
| C    | 6.600431557  | 11.088063122 | 12.049414579 |
| C    | 6.769966597  | 8.422630822  | 11.024199346 |
| H    | 7.598272076  | 9.684218942  | 9.479398996  |
b. Optimized structure of single NHCs molecules on planar Au(111) surfaces

NHC1 in surface-bound state in xyz format (Å)

Au -1.47056 4.23127 9.57614
Au -5.87237 11.8571 9.57645
Au -10.2663 19.4799 9.5781
Au 7.33456 4.22755 9.57517
Au 2.89744 11.8535 9.57305
Au -1.47151 19.4834 9.5798
Au 16.1374 4.2347 9.5764
Au 11.7538 11.8577 9.57507
Au 7.33661 19.4911 9.57336
Au -2.93967 6.77129 9.5762
Au -7.33577 14.3991 9.57675
Au -11.7341 22.0199 9.5777
Au 5.86603 6.76457 9.5454
Au 1.44121 14.4042 9.57605
Au -2.93538 22.0205 9.57793
Au 14.6728 6.77323 9.57628
Au 10.2888 14.4035 9.57516
Au 5.86736 22.0252 9.57583
Au 5.86739 1.68968 9.5767
Au 1.43651 9.30881 9.57808
Au -2.94031 16.9419 9.57709
Au 14.6696 1.69589 9.57605
Au 10.2935 9.30906 9.57712
Au 5.86608 16.9634 9.54473
Au 23.469 1.69443 9.57592
Au 19.0683 9.31441 9.57675
Au 14.6733 16.9407 9.57691
Au 4.3994 4.22697 9.57519
Au -0.022019 11.8578 9.5763
Au -4.40356 19.4808 9.57835
Au 13.2047 4.23278 9.5764
Au 8.83457 11.853 9.5771
Au 4.3974 19.4917 9.5735
Au 22.0008 4.23383 9.57659
Au 17.6048 11.857 9.57651
Au 13.2054 19.4817 9.57688
Au 2.91863 6.75286 9.57307
Au -1.47995 14.4017 9.57691
Au -5.86826 22.0184 9.57795
Au 11.7425 6.76953 9.57387
Au 7.37816 14.436 9.50625
Au 2.93218 22.0256 9.57583
Au 20.5339 6.77355 9.57682
Au 16.139 14.3987 9.57659
Au 11.7367 22.0227 9.57762
| Element | Interval | Value | Interval | Value | Interval | Value |
|---------|----------|-------|----------|-------|----------|-------|
| Au 2.93298 | 1.68988 | 9.57658 | Au -1.4812 | 9.31296 | 9.57506 |
| Au -5.8705 | 16.9402 | 9.57831 | Au 11.7361 | 1.69238 | 9.57497 |
| Au 7.38347 | 9.28915 | 9.50562 | Au 2.91857 | 16.9631 | 9.57243 |
| Au 20.5355 | 1.69592 | 9.57641 | Au 16.1391 | 9.3151 | 9.57613 |
| Au 11.742 | 16.9438 | 9.57618 | Au 1.46068 | 4.22453 | 9.57568 |
| Au -2.94538 | 11.8576 | 9.57499 | Au -7.33481 | 4.22645 | 9.57552 |
| Au 19.0691 | 4.23452 | 9.57605 | Au 14.6776 | 11.8574 | 9.57483 |
| Au 10.2748 | 19.4882 | 9.57533 | Au -0.00983036 | 6.76844 | 9.57414 |
| Au -4.40659 | 14.3993 | 9.57669 | Au -8.80097 | 22.0178 | 9.57796 |
| Au 8.81295 | 6.75515 | 9.5729 | Au 4.34838 | 14.4358 | 9.49363 |
| Au -0.00217222 | 6.77388 | 9.57667 | Au 17.6033 | 11.401 | 9.57633 |
| Au 8.8026 | 22.0244 | 9.57564 | Au -0.0014839 | 1.6906 | 9.57758 |
| Au -4.40665 | 9.31484 | 9.57616 | Au -8.80017 | 16.9398 | 9.57807 |
| Au 8.80189 | 1.69108 | 9.57668 | Au 17.6032 | 11.401 | 9.57665 |
| Au 13.2116 | 14.401 | 9.57633 | Au 8.81325 | 16.9609 | 9.57212 |
| Au 7.33603 | 2.53537 | 7.16544 | Au 2.92114 | 10.1738 | 7.15095 |
| Au -1.47248 | 17.7887 | 7.16543 | Au 16.1358 | 2.54128 | 7.1654 |
| Au 11.7405 | 10.1644 | 7.16402 | Au 7.33996 | 17.7902 | 7.15746 |
| Au 24.9365 | 2.53963 | 7.1649 | Au 20.5345 | 10.1629 | 7.16479 |
| Au 16.1376 | 17.7863 | 7.16562 | Au 5.86742 | 5.06686 | 7.15857 |
| Au 1.46657 | 12.7101 | 7.16101 | Au -2.93621 | 20.3272 | 7.16566 |
| Au 14.6704 | 5.08073 | 7.16499 | Au 10.2635 | 12.7088 | 7.16134 |
| Au 5.86721 | 20.3291 | 7.16379 | Au 23.4681 | 5.08015 | 7.16496 |
| Au 19.0689 | 12.7044 | 7.16489 | Au 14.6707 | 20.3264 | 7.16558 |
| Au 1.462 | 7.62064 | 7.16334 | Au -2.93953 | 15.2461 | 7.16518 |
| Au -7.33461 | 22.8641 | 7.1655 | Au 10.2711 | 7.6214 | 7.16322 |
| Au 5.86722 | 15.2386 | 7.15066 | Au 1.46612 | 22.8688 | 7.16481 |
|        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|
| Au 19.0691 | 7.62175 | 7.16533 |
| Au 14.6727  | 15.2456  | 7.16504 |
| Au 10.2689  | 22.8679  | 7.16474 |
| Au 4.39882  | 2.53504  | 7.16535 |
| Au -0.00849893 | 10.1642 | 7.16412 |
| Au -4.40356  | 17.7869  | 7.16568 |
| Au 13.2025  | 2.54042  | 7.16503 |
| Au 8.80939  | 10.1739  | 7.15327 |
| Au 4.3941  | 17.7906  | 7.15755 |
| Au 22.0031  | 15.2456  | 7.16478 |
| Au 13.2062  | 22.8679  | 7.16525 |
| Au 2.93097  | 5.07657  | 7.16315 |
| Au -1.47062 | 12.7047  | 7.16429 |
| Au -5.86863 | 20.3258  | 7.16569 |
| Au 11.7369  | 5.07951  | 7.16402 |
| Au 7.29723  | 12.6744  | 7.22936 |
| Au 2.93101  | 20.3307  | 7.16431 |
| Au 20.5355  | 5.08105  | 7.16487 |
| Au 16.1372  | 12.7045  | 7.16491 |
| Au 11.7378  | 20.3287  | 7.16518 |
| Au -1.47087 | 17.62061 | 7.16441 |
| Au -5.86979 | 15.246  | 7.16553 |
| Au -10.2682 | 22.8642  | 7.16565 |
| Au 7.33232  | 7.61767  | 7.14636 |
| Au 2.9154  | 15.2481  | 7.14178 |
| Au -1.46792 | 22.8673  | 7.16525 |
| Au 16.137  | 7.62153  | 7.16497 |
| Au 11.7431  | 15.2468  | 7.16482 |
| Au 7.33442  | 22.8687  | 7.16462 |
| Au 1.46529  | 2.53756  | 7.16506 |
| Au -2.93913 | 10.1629  | 7.1643 |
| Au -7.33493 | 17.7861  | 7.16574 |
| Au 10.2695  | 2.53858  | 7.16508 |
| Au 5.86639  | 10.1962  | 7.21755 |
| Au 1.45867  | 17.7918  | 7.16341 |
| Au 19.0495  | 2.54184  | 7.16474 |
| Au 14.6723  | 10.1631  | 7.16417 |
| Au 10.2744  | 17.7897  | 7.16333 |
| Au -0.00267219 | 5.07875 | 7.16406 |
| Au -4.40381 | 12.7047  | 7.16499 |
| Au -8.80081 | 20.3255  | 7.1657 |
| Au 8.80309  | 5.07772  | 7.16326 |
| Au 4.43032  | 12.6755  | 7.22173 |
| Au -0.00336677 | 20.33  | 7.1653 |
| Au 17.6031  | 5.08121  | 7.16485 |
| Au 13.2031  | 12.7045  | 7.16399 |
| Au 8.80353  | 20.3299  | 7.16423 |
| Au 4.40123  | 7.6156  | 7.14464 |
| Au -0.0113303 | 5.12481 | 7.16502 |
| Au -4.40096 | 22.8649  | 7.16572 |
| Au 13.2045  | 7.62108  | 7.16425 |
| Au 8.81483  | 15.2448  | 7.14424 |
| Au 4.40043  | 22.8691  | 7.16466 |
| Au 26.4049  | -0.000348798 | 7.16515 |
| Au 22.001  | 7.62127  | 7.16501 |
| Au 17.6034  | 15.2458  | 7.16552 |
| Au -1.46689 | 5.92838  | 4.79085 |
| Au -5.86757 | 13.5506  | 4.79085 |
| Au -10.2683 | 21.1728  | 4.79085 |
|     | 7.33446 | 5.92838 | 4.79085 |
|-----|---------|---------|---------|
| Au  | 2.93379 | 13.5506 | 4.79085 |
| Au - | 1.46689 | 21.1728 | 4.79085 |
| Au  | 16.1358 | 5.92838 | 4.79085 |
| Au  | 11.7351 | 13.5506 | 4.79085 |
| Au  | 7.33446 | 21.1728 | 4.79085 |
| Au  | 7.33446 | 0.846911 | 4.79085 |
| Au  | 2.93379 | 8.46911 | 4.79085 |
| Au - | 1.46689 | 16.0913 | 4.79085 |
| Au  | 16.1358 | 0.846911 | 4.79085 |
| Au  | 11.7351 | 8.46911 | 4.79085 |
| Au  | 7.33446 | 16.0913 | 4.79085 |
| Au  | 24.9372 | 0.846911 | 4.79085 |
| Au  | 20.5365 | 8.46911 | 4.79085 |
| Au  | 16.1358 | 16.0913 | 4.79085 |
| Au  | 5.86757 | 3.38764 | 4.79085 |
| Au  | 1.46689 | 11.0098 | 4.79085 |
| Au - | 2.93379 | 18.632 | 4.79085 |
| Au  | 14.6689 | 3.38764 | 4.79085 |
| Au  | 10.2683 | 11.0098 | 4.79085 |
| Au  | 5.86757 | 18.632 | 4.79085 |
| Au  | 23.4703 | 3.38764 | 4.79085 |
| Au  | 19.0696 | 11.0098 | 4.79085 |
| Au  | 14.6689 | 18.632 | 4.79085 |
| Au  | 4.40068 | 5.92838 | 4.79085 |
| Au - | 4.9778e-08 | 13.5506 | 4.79085 |
| Au - | 4.40068 | 21.1728 | 4.79085 |
| Au  | 13.202 | 5.92838 | 4.79085 |
| Au  | 8.80136 | 13.5506 | 4.79085 |
| Au  | 4.40068 | 21.1728 | 4.79085 |
| Au  | 22.0034 | 5.92838 | 4.79085 |
| Au  | 17.6027 | 13.5506 | 4.79085 |
| Au  | 13.202 | 21.1728 | 4.79085 |
| Au  | 4.40068 | 0.846911 | 4.79085 |
| Au - | 4.9778e-08 | 8.46911 | 4.79085 |
| Au - | 4.40068 | 16.0913 | 4.79085 |
| Au  | 13.202 | 0.846911 | 4.79085 |
| Au  | 8.80136 | 8.46911 | 4.79085 |
| Au  | 4.40068 | 16.0913 | 4.79085 |
| Au  | 22.0034 | 0.846911 | 4.79085 |
| Au  | 17.6027 | 8.46911 | 4.79085 |
| Au  | 13.202 | 16.0913 | 4.79085 |

|     | 2.93379 | 3.38764 | 4.79085 |
|-----|---------|---------|---------|
| Au  | 11.7351 | 3.38764 | 4.79085 |
| Au  | 7.33446 | 11.0098 | 4.79085 |
| Au  | 2.93379 | 18.632 | 4.79085 |
| Au - | 1.46689 | 13.5506 | 4.79085 |
| Au  | 10.2683 | 11.0098 | 4.79085 |
| Au  | 5.86757 | 18.632 | 4.79085 |
| Au  | 23.4703 | 3.38764 | 4.79085 |
| Au  | 19.0696 | 11.0098 | 4.79085 |
| Au  | 14.6689 | 18.632 | 4.79085 |
| Au  | 4.40068 | 5.92838 | 4.79085 |
| Au - | 4.9778e-08 | 13.5506 | 4.79085 |
| Au - | 4.40068 | 21.1728 | 4.79085 |
| Au  | 13.202 | 5.92838 | 4.79085 |
| Au  | 8.80136 | 13.5506 | 4.79085 |
| Au  | 4.40068 | 21.1728 | 4.79085 |
| Au  | 22.0034 | 5.92838 | 4.79085 |
| Au  | 17.6027 | 13.5506 | 4.79085 |
| Au  | 13.202 | 21.1728 | 4.79085 |
| Au  | 4.40068 | 0.846911 | 4.79085 |
| Au - | 4.9778e-08 | 8.46911 | 4.79085 |
| Au - | 4.40068 | 16.0913 | 4.79085 |
| Au  | 13.202 | 0.846911 | 4.79085 |
| Au  | 8.80136 | 8.46911 | 4.79085 |
| Au  | 4.40068 | 16.0913 | 4.79085 |
| Au  | 22.0034 | 0.846911 | 4.79085 |
| Au  | 17.6027 | 8.46911 | 4.79085 |
| Au  | 13.202 | 16.0913 | 4.79085 |
Au 1.46689 0.846911 4.79085
Au -2.93379 8.469114 4.79085
Au -7.33447 16.0913 4.79085
Au 10.2683 0.846911 4.79085
Au 5.86757 8.469114 4.79085
Au 1.46689 16.0913 4.79085
Au 19.0696 0.846911 4.79085
Au 14.6689 8.469114 4.79085
Au 10.2683 16.0913 4.79085
Au 2.4894e-08 3.38764 4.79085
Au -4.40068 11.0098 4.79085
Au -8.80136 18.632 4.79085
Au 8.80136 3.38764 4.79085
Au 4.40068 11.0098 4.79085
Au 2.4894e-08 18.632 4.79085
Au 17.6027 3.38764 4.79085
Au 13.202 11.0098 4.79085
Au 8.80136 18.632 4.79085
Au -1.46689 4.23456 2.39543
Au -5.86757 11.8568 2.39543
Au -10.2683 19.479 2.39543
Au 7.33446 4.23456 2.39543
Au 2.93379 11.8568 2.39543
Au -1.46689 19.479 2.39543
Au 16.1358 4.23456 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
Au -7.33447 14.3975 2.39543
Au -11.7351 22.0197 2.39543
Au 5.86757 6.77529 2.39543
Au 1.46689 14.3975 2.39543
Au -2.93379 22.0197 2.39543
Au 14.6689 6.77529 2.39543
Au 10.2683 14.3975 2.39543
Au 5.86757 22.0197 2.39543
Au 5.86757 1.69382 2.39543
Au 1.46689 9.31602 2.39543
Au -2.93379 16.9382 2.39543
Au 14.6689 1.69382 2.39543
Au 10.2683 9.31602 2.39543
Au 5.86757 16.9382 2.39543
Au 23.4703 1.69382 2.39543
Au 19.0696 9.31602 2.39543
Au 14.6689 16.9382 2.39543
Au 4.40068 4.23456 2.39543
Au -7.4682e-08 11.8568 2.39543
Au -4.40068 19.479 2.39543
Au 13.202 4.23456 2.39543
Au 8.80136 11.8568 2.39543
Au 4.40068 19.479 2.39543
Au 22.0034 4.23456 2.39543
Au 17.6027 11.8568 2.39543
Au 13.202 19.479 2.39543
Au 2.93379 6.77529 2.39543
Au -1.46689 14.3975 2.39543
Au -5.86757 6.77529 2.39543
Au 14.6689 1.69382 2.39543
Au 10.2683 9.31602 2.39543
Au 5.86757 14.3975 2.39543
Au 22.0034 4.23456 2.39543
Au 17.6027 11.8568 2.39543
Au 13.202 19.479 2.39543
Au 2.93379 14.3975 2.39543
Au -1.46689 16.9382 2.39543
Au 23.4703 1.69382 2.39543
Au 19.0696 9.31602 2.39543
Au 14.6689 16.9382 2.39543
Au 4.40068 4.23456 2.39543
| Element | X-coordinate 1 | Y-coordinate 1 | Y-coordinate 2 | Z-coordinate |
|--------|---------------|---------------|---------------|-------------|
| Au     | 20.5365       | 6.77529       | 2.39543       |             |
| Au     | 16.1358       | 14.3975       | 2.39543       |             |
| Au     | 11.7351       | 22.0197       | 2.39543       |             |
| Au     | 2.93379       | 1.69382       | 2.39543       |             |
| Au     | -1.46689      | 9.31602       | 2.39543       |             |
| Au     | -5.86757      | 16.9382       | 2.39543       |             |
| Au     | 11.7351       | 1.69382       | 2.39543       |             |
| Au     | 7.33447       | 9.31602       | 2.39543       |             |
| Au     | 2.93379       | 16.9382       | 2.39543       |             |
| Au     | 20.5365       | 1.69382       | 2.39543       |             |
| Au     | 16.1358       | 9.31602       | 2.39543       |             |
| Au     | 11.7351       | 16.9382       | 2.39543       |             |
| Au     | 1.46689       | 4.23456       | 2.39543       |             |
| Au     | -2.93379      | 11.8568       | 2.39543       |             |
| Au     | -7.33447      | 19.479        | 2.39543       |             |
| Au     | 10.263        | 4.23456       | 2.39543       |             |
| Au     | 5.86757       | 11.8568       | 2.39543       |             |
| Au     | 1.46689       | 19.479        | 2.39543       |             |
| Au     | 19.0696       | 4.23456       | 2.39543       |             |
| Au     | 14.6689       | 11.8568       | 2.39543       |             |
| Au     | 10.263        | 19.479        | 2.39543       |             |
| Au     | 0.677529      | 2.39543       |             |             |
| Au     | -4.40068      | 14.3975       | 2.39543       |             |
| Au     | -8.80136      | 22.0197       | 2.39543       |             |
| Au     | 8.80136       | 6.77529       | 2.39543       |             |
| Au     | 4.40068       | 14.3975       | 2.39543       |             |
| Au     | 0.220197      | 2.39543       |             |             |
| Au     | 17.6027       | 6.77529       | 2.39543       |             |
| Au     | 13.202        | 14.3975       | 2.39543       |             |
| Au     | 8.80136       | 22.0197       | 2.39543       |             |
| Au     | 0.169382      | 2.39543       |             |             |
| Au     | -4.40068      | 9.31602       | 2.39543       |             |
| Au     | -8.80136      | 16.9382       | 2.39543       |             |
| Au     | 8.80136       | 1.69382       | 2.39543       |             |
| Au     | 4.40068       | 9.31602       | 2.39543       |             |
| Au     | 0.169382      | 2.39543       |             |             |
| Au     | 17.6027       | 1.69382       | 2.39543       |             |
| Au     | 13.202        | 9.31602       | 2.39543       |             |
| Au     | 8.80136       | 16.9382       | 2.39543       |             |
| C      | 5.77128       | 11.8734       | 12.0772       |             |
| C      | 5.47189       | 11.1793       | 14.2085       |             |
| C      | 5.46921       | 12.5754       | 14.2057       |             |
| C      | 5.76969       | 14.3532       | 12.5049       |             |
| C      | 5.77917       | 9.39596       | 12.5122       |             |
| N      | 5.66655       | 12.9624       | 12.8878       |             |
| N      | 5.67058       | 10.7875       | 12.8921       |             |
| H      | 5.88665       | 14.9614       | 13.4006       |             |
| H      | 4.87506       | 14.681        | 11.9608       |             |
| H      | 5.91433       | 11.8598       | 11.8598       |             |
| C      | 5.29941       | 10.4539       | 15.3835       |             |
| C      | 5.29267       | 13.3054       | 15.3773       |             |
| H      | 5.29158       | 9.37029       | 15.3972       |             |
| H      | 5.27943       | 14.3889       | 15.3863       |             |
| C      | 5.12516       | 11.181        | 16.5516       |             |
| C      | 5.12156       | 12.5826       | 16.5485       |             |
| H      | 4.9846        | 10.6523       | 17.4879       |             |
| H      | 4.97787       | 13.1147       | 17.4824       |             |
NHC2 in surface-bound state in xyz format (Å)

Au -1.47021 4.23088 9.57612
Au -5.87169 11.8562 9.57814
Au -10.2667 19.48 9.57729
Au 7.33516 4.22778 9.57696
Au 2.88356 11.8471 9.44538
Au -1.46974 19.4819 9.57673
Au 16.1377 4.23282 9.57656
Au 11.7606 11.8556 9.57134
Au 7.33575 19.4837 9.57508
Au -2.93788 6.77192 9.57619
Au -7.33494 14.3986 9.57749
Au -11.7341 22.0195 9.57652
Au 5.86731 6.76165 9.57848
Au 1.45383 14.4078 9.55284
Au -2.93551 22.0198 9.57652
Au 14.6726 6.77182 9.57635
Au 10.28 14.4069 9.55302
Au 5.86745 22.0212 9.57605
Au 5.86736 1.69018 9.57665
Au 1.45004 9.29909 9.57685
Au -2.93813 16.9409 9.57698
Au 14.6702 1.69302 9.57518
Au 10.284 9.29922 9.56634
Au 5.86727 16.9531 9.58229
Au 23.4686 1.69274 9.57495
Au 19.0692 9.31366 9.57617
Au 14.6723 16.9404 9.57696
Au 4.39959 4.22771 9.57693
Au -0.0268468 11.856 9.57115
Au -4.40302 19.4802 9.57731
Au 13.205 4.23101 9.57631
Au 8.84926 11.8464 9.44675
Au 4.39905 19.484 9.57512
Au 22.0012 4.23274 9.57635
Au 17.6059 11.8559 9.57813
Au 13.204 19.4814 9.57671
Au 2.92641 6.76041 9.57635
Au -1.47444 14.4002 9.57704
Au -5.86821 22.0186 9.57747
Au 11.7418 6.7669 9.57568
Au 7.34011 14.4248 9.56092
Au 2.93317 22.0209 9.57587
Au 20.535 6.77263 9.57655
Au 16.1391 14.3984 9.57718
Au 11.7364 22.0211 9.57641
Au 2.93285 1.69111 9.57653
Au -1.47566 9.31177 9.57498
Au -5.86954 16.9401 9.57758
Au 11.7364 1.69146 9.57661
Au 7.34364 9.28874 9.56092
Au 2.92477 16.9504 9.5775
Au 20.5358 1.69353 9.57633
Au 16.1391 9.3137 9.57633
Au 11.7409 16.9429 9.57733
Au 1.4634 4.227 9.57562
Au -2.9459 11.8565 9.57756
Au -7.33484 19.4796 9.57675
Au 10.2714 4.22718 9.57575
|   |   |   |   |
|---|---|---|---|
| Au | 5.8645 | 11.8721 | 10.0167 |
| Au | 1.46269 | 19.4845 | 9.57561 |
| Au | 19.0694 | 4.2302 | 9.57633 |
| Au | 14.6801 | 11.856 | 9.57756 |
| Au | 10.2718 | 19.4839 | 9.57551 |
| Au | -0.00715631 | 6.76679 | 9.57546 |
| Au | -4.40946 | 14.3989 | 9.57721 |
| Au | -8.80132 | 22.0186 | 9.57746 |
| Au | 8.80806 | 6.76067 | 9.57575 |
| Au | 4.39326 | 14.4257 | 9.5612 |
| Au | -0.00189588 | 22.0215 | 9.57551 |
| Au | 17.6036 | 6.77258 | 9.57658 |
| Au | 13.2085 | 14.3996 | 9.57699 |
| Au | 8.80161 | 22.0206 | 9.57575 |
| Au | -0.00173385 | 1.69123 | 9.57654 |
| Au | -4.40463 | 9.31395 | 9.5763 |
| Au | -8.80027 | 16.9398 | 9.57758 |
| Au | 8.80186 | 1.69125 | 9.57652 |
| Au | 4.39022 | 9.28804 | 9.56061 |
| Au | -0.0068375 | 16.9436 | 9.5774 |
| Au | 17.6032 | 2.53782 | 7.16529 |
| Au | 2.94237 | 10.1472 | 7.14429 |
| Au | -1.47062 | 17.7897 | 7.16572 |
| Au | 16.1363 | 2.5399 | 7.16522 |
| Au | 11.7385 | 10.1603 | 7.16138 |
| Au | 7.33505 | 17.7863 | 7.16569 |
| Au | 24.9361 | 2.53922 | 7.16475 |
| Au | 20.5352 | 10.162 | 7.16499 |
| Au | 16.1376 | 17.7867 | 7.16551 |
| Au | 5.86748 | 5.07568 | 7.1663 |
| Au | 1.45179 | 12.7149 | 7.13431 |
| Au | -2.95553 | 20.327 | 7.16537 |
| Au | 14.6704 | 5.07975 | 7.165 |
| Au | 10.2823 | 12.7143 | 7.13474 |
| Au | 5.86738 | 20.3265 | 7.16484 |
| Au | 23.4686 | 5.07983 | 7.16495 |
| Au | 19.0694 | 12.704 | 7.16519 |
| Au | 14.6703 | 20.3269 | 7.1654 |
| Au | 1.46513 | 7.61322 | 7.16193 |
| Au | -2.94001 | 15.2468 | 7.16561 |
| Au | -7.33471 | 22.8653 | 7.16541 |
| Au | 10.2696 | 7.61335 | 7.1621 |
| Au | 5.86729 | 15.2475 | 7.1634 |
| Au | 1.46682 | 22.8662 | 7.16488 |
| Au | 19.0695 | 7.6133 | 7.16559 |
| Au | 14.6745 | 15.2465 | 7.1656 |
| Au | 10.2682 | 22.8661 | 7.1648 |
| Au | 4.40011 | 2.53772 | 7.16529 |
| Au | -0.00406071 | 10.1606 | 7.16124 |
| Au | -4.40304 | 17.7868 | 7.16548 |
| Au | 13.203 | 2.53929 | 7.16483 |
| Au | 8.79204 | 10.1472 | 7.14452 |
| Au | 4.39965 | 17.7865 | 7.16571 |
| Au | 22.0027 | 2.53991 | 7.16512 |
| Au | 17.6037 | 10.162 | 7.16499 |
| Au | 13.2052 | 17.7893 | 7.16572 |
| Au | 2.93432 | 5.07842 | 7.16433 |
| Au  | 1.47721 | 12.7055 | 7.16315 |
|-----|---------|---------|---------|
| Au  | -5.86848 | 20.3261 | 7.16536 |
| Au  | 11.7372 | 5.07749 | 7.16473 |
| Au  | 7.29316 | 12.6935 | 7.21301 |
| Au  | 2.93278 | 20.3267 | 7.16443 |
| Au  | 20.5356 | 5.08043 | 7.1648 |
| Au  | 16.1397 | 12.7035 | 7.16573 |
| Au  | 11.7358 | 20.3266 | 7.1651 |
| Au  | -1.46941 | 7.61997 | 7.16471 |
| Au  | -5.8697 | 15.2457 | 7.16564 |
| Au  | -10.2681 | 22.8655 | 7.16538 |
| Au  | 7.32576 | 7.61903 | 7.15881 |
| Au  | 2.93428 | 15.2417 | 7.15679 |
| Au  | -1.4674 | 22.8662 | 7.16464 |
| Au  | 16.1372 | 7.62074 | 7.1686 |
| Au  | 11.746 | 15.2534 | 7.16099 |
| Au  | 7.33422 | 22.8666 | 7.16496 |
| Au  | 1.46624 | 2.53871 | 7.16511 |
| Au  | -2.93737 | 10.162 | 7.16459 |
| Au  | -7.33475 | 17.7863 | 7.16545 |
| Au  | 10.2687 | 2.53892 | 7.16513 |
| Au  | 5.86711 | 10.2071 | 7.23326 |
| Au  | 1.46606 | 17.7857 | 7.16449 |
| Au  | 19.0694 | 2.54028 | 7.16469 |
| Au  | 14.672 | 10.1618 | 7.16459 |
| Au  | 10.2686 | 17.7853 | 7.16445 |
| Au  | -0.00223354 | 5.0774 | 7.16464 |
| Au  | -4.40526 | 12.7036 | 7.16577 |
| Au  | -8.80999 | 20.3261 | 7.16537 |
| Au  | 8.8006 | 5.07862 | 7.16441 |
| Au  | 4.44148 | 12.6937 | 7.21307 |
| Au  | -0.000930608 | 20.3269 | 7.16514 |
| Au  | 17.6033 | 5.08036 | 7.16481 |
| Au  | 13.2115 | 12.7051 | 7.16321 |
| Au  | 8.80202 | 20.3264 | 7.16434 |
| Au  | 4.40903 | 7.6188 | 7.15867 |
| Au  | -0.0115735 | 15.2539 | 7.16096 |
| Au  | -4.40129 | 22.8656 | 7.16536 |
| Au  | 13.2041 | 7.61984 | 7.16479 |
| Au  | 8.80028 | 15.2412 | 7.15687 |
| Au  | 4.4006 | 22.8667 | 7.16503 |
| Au  | 26.4044 | -0.00053244 | 7.16461 |
| Au  | 22.0017 | 7.62088 | 7.16488 |
| Au  | 17.6043 | 15.2456 | 7.16563 |
| Au  | -1.46689 | 5.92838 | 4.79085 |
| Au  | -5.86757 | 13.5506 | 4.79085 |
| Au  | -10.2683 | 21.1728 | 4.79085 |
| Au  | 7.33446 | 5.92838 | 4.79085 |
| Au  | 2.93379 | 13.5506 | 4.79085 |
| Au  | -1.46689 | 21.1728 | 4.79085 |
| Au  | 16.1358 | 5.92838 | 4.79085 |
| Au  | 11.7351 | 13.5506 | 4.79085 |
| Au  | 7.33446 | 21.1728 | 4.79085 |
| Au  | 7.33446 | 0.846911 | 4.79085 |
| Au  | 2.93379 | 8.46911 | 4.79085 |
| Au  | -1.46689 | 16.0913 | 4.79085 |
| Au  | 16.1358 | 0.846911 | 4.79085 |
| Au  | 11.7351 | 8.46911 | 4.79085 |
| Au  | 7.33446 | 16.0913 | 4.79085 |
| Au  | 24.9372 | 0.846911 | 4.79085 |
|     |     |     |   |   |
|---|---|---|---|---|
| Au | 20.5365 | 8.46911 | 4.79085 |
| Au | 16.1358 | 16.0913 | 4.79085 |
| Au | 5.86757 | 3.38764 | 4.79085 |
| Au | 1.46689 | 11.0098 | 4.79085 |
| Au | -2.93379 | 18.632 | 4.79085 |
| Au | 14.6689 | 3.38764 | 4.79085 |
| Au | 10.2683 | 11.0098 | 4.79085 |
| Au | 5.86757 | 18.632 | 4.79085 |
| Au | 23.4703 | 3.38764 | 4.79085 |
| Au | 19.0696 | 11.0098 | 4.79085 |
| Au | 14.6689 | 18.632 | 4.79085 |
| Au | 4.40068 | 5.92838 | 4.79085 |
| Au | -4.9788e-08 | 13.5506 | 4.79085 |
| Au | -4.40068 | 21.1728 | 4.79085 |
| Au | 13.202 | 5.92838 | 4.79085 |
| Au | 8.80136 | 13.5506 | 4.79085 |
| Au | 4.40068 | 21.1728 | 4.79085 |
| Au | 22.0034 | 5.92838 | 4.79085 |
| Au | 17.6027 | 13.5506 | 4.79085 |
| Au | 13.202 | 21.1728 | 4.79085 |
| Au | 4.40068 | 0.846911 | 4.79085 |
| Au | -4.9788e-08 | 8.46911 | 4.79085 |
| Au | -4.40068 | 16.0913 | 4.79085 |
| Au | 13.202 | 0.846911 | 4.79085 |
| Au | 8.80136 | 8.46911 | 4.79085 |
| Au | 4.40068 | 16.0913 | 4.79085 |
| Au | 22.0034 | 0.846911 | 4.79085 |
| Au | 17.6027 | 8.46911 | 4.79085 |
| Au | 13.202 | 16.0913 | 4.79085 |
| Au | 2.93379 | 3.38764 | 4.79085 |
| Au | -1.46689 | 11.0098 | 4.79085 |
| Au | -5.86757 | 18.632 | 4.79085 |
| Au | 11.7351 | 3.38764 | 4.79085 |
| Au | 7.33447 | 11.0098 | 4.79085 |
| Au | 2.93379 | 18.632 | 4.79085 |
| Au | 20.5365 | 3.38764 | 4.79085 |
| Au | 11.7351 | 18.632 | 4.79085 |
| Au | 1.46689 | 5.92838 | 4.79085 |
| Au | -2.93379 | 13.5506 | 4.79085 |
| Au | -7.33447 | 21.1728 | 4.79085 |
| Au | 10.2683 | 5.92838 | 4.79085 |
| Au | 5.86757 | 13.5506 | 4.79085 |
| Au | 1.46689 | 21.1728 | 4.79085 |
| Au | 19.0696 | 5.92838 | 4.79085 |
| Au | 14.6689 | 13.5506 | 4.79085 |
| Au | 10.2683 | 11.0098 | 4.79085 |
| Au | 1.46689 | 0.846911 | 4.79085 |
| Au | -2.93379 | 8.46911 | 4.79085 |
| Au | -7.33447 | 16.0913 | 4.79085 |
| Au | 10.2683 | 0.846911 | 4.79085 |
| Au | 5.86757 | 8.46911 | 4.79085 |
| Au | 1.46689 | 16.0913 | 4.79085 |
| Au | 19.0696 | 0.846911 | 4.79085 |
| Au | 14.6689 | 8.46911 | 4.79085 |
| Au | 10.2683 | 16.0913 | 4.79085 |
| Au | 2.4894e-08 | 3.38764 | 4.79085 |
| Au | -4.40068 | 11.0098 | 4.79085 |
| Au | -8.80136 | 18.632 | 4.79085 |
| Au | 8.80136 | 3.38764 | 4.79085 |
Au 4.40068 11.0098 4.79085
Au 2.4894e-08 18.632 4.79085
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Au -1.46689 4.23456 2.39543
Au -5.86757 11.8568 2.39543
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Au -1.46689 19.479 2.39543
Au 16.1358 4.23456 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
Au -7.33447 14.3975 2.39543
Au -11.7351 22.0197 2.39543
Au 5.86757 6.77529 2.39543
Au 1.46689 14.3975 2.39543
Au -2.93379 22.0197 2.39543
Au 14.6689 6.77529 2.39543
Au 10.2683 14.3975 2.39543
Au 5.86757 22.0197 2.39543
Au 5.86757 1.69382 2.39543
Au 1.46689 9.31602 2.39543
Au -2.93379 16.9382 2.39543
Au 14.6689 1.69382 2.39543
Au 10.2683 9.31602 2.39543
Au 5.86757 16.9382 2.39543
Au 2.93379 6.77529 2.39543
Au -7.4682e-08 11.8568 2.39543
Au -4.40068 19.479 2.39543
Au 13.202 4.23456 2.39543
Au 8.80136 11.8568 2.39543
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Au 11.7351 22.0197 2.39543
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Au -1.46689 9.31602 2.39543
Au -5.86757 16.9382 2.39543
Au 10.2683 9.31602 2.39543
Au 5.86757 16.9382 2.39543
Au 23.4703 1.69382 2.39543
Au 19.0696 9.31602 2.39543
Au 14.6689 16.9382 2.39543
Au 4.40068 4.23456 2.39543
Au -7.4682e-08 11.8568 2.39543
Au -4.40068 19.479 2.39543
Au 13.202 4.23456 2.39543
Au 8.80136 11.8568 2.39543
Au 4.40068 19.479 2.39543
Au 22.0034 4.23456 2.39543
Au 17.6027 11.8568 2.39543
Au 13.202 19.479 2.39543
Au 2.93379 6.77529 2.39543
Au -1.46689 14.3975 2.39543
Au -5.86757 22.0197 2.39543
Au 11.7351 6.77529 2.39543
Au 7.33447 14.3975 2.39543
Au 2.93379 22.0197 2.39543
Au 20.5365 6.77529 2.39543
Au 16.1358 14.3975 2.39543
Au 11.7351 22.0197 2.39543
Au 2.93379 1.69382 2.39543
Au -1.46689 9.31602 2.39543
Au -5.86757 16.9382 2.39543
Au 10.2683 9.31602 2.39543
Au 5.86757 16.9382 2.39543
Au 23.4703 1.69382 2.39543
NHC3 in surface-bound state in xyz format (Å)

Au -2.93379 11.8568 2.39543
Au -7.33447 19.479 2.39543
Au 10.2683 4.23456 2.39543
Au 5.86757 11.8568 2.39543
Au 1.46689 19.479 2.39543
Au 19.0696 4.23456 2.39543
Au 14.6689 11.8568 2.39543
Au 10.2683 19.479 2.39543
Au 0 6.77529 2.39543
Au -4.40068 14.3975 2.39543
Au -8.80136 22.0197 2.39543
Au 8.80136 6.77529 2.39543
Au 4.40068 14.3975 2.39543
Au 0 22.0197 2.39543
Au 17.6027 6.77529 2.39543
Au 13.202 14.3975 2.39543
Au 8.80136 22.0197 2.39543
Au 0 1.69382 2.39543
Au -4.40068 9.31602 2.39543
Au -8.80136 16.9382 2.39543
Au 8.80136 1.69382 2.39543
Au 4.40068 9.31602 2.39543
Au 0 16.9382 2.39543
Au 17.6027 1.69382 2.39543
Au 13.202 9.31602 2.39543
Au 8.80136 16.9382 2.39543
C 5.86176 11.7722 12.1677
C 5.16413 11.4601 14.2959
C 6.55779 11.462 14.2968
C 8.3542 11.8425 12.643
C 3.36817 11.8344 12.6401
N 6.94957 11.6629 12.9808
N 4.77323 11.66 12.9796
C 8.86612 13.2382 12.9522
H 8.78233 13.4795 14.0156
H 8.30027 13.9857 12.3828
H 9.9117 13.3158 12.6571
H 8.46212 11.6227 11.5702
H 8.92463 11.0696 13.1657
C 2.85423 13.2271 12.9535
H 1.80476 13.3013 12.6553
H 3.41449 13.9788 12.3888
H 2.92883 13.4646 14.018
H 2.80057 11.0574 13.1607
H 3.26222 11.617 11.5675
C 4.43358 11.2702 15.4652
C 7.2873 11.2744 15.4671
H 3.3498 11.2675 15.4723
H 8.37107 11.275 15.4758
C 5.1588 11.0791 16.6324
C 6.56101 11.0812 16.6333
H 4.62853 10.9245 17.5657
H 7.09038 10.9281 17.5673
Au 20.5357 5.0809 7.16472
Au 16.1387 12.7028 7.16615
Au 11.7354 20.3263 7.1653
Au -1.46881 7.61997 7.16505
Au -5.86953 15.2447 7.16582
Au -10.2679 22.8647 7.16543
Au 7.324 7.62108 7.16063
Au 2.93411 15.2429 7.15751
Au -1.46743 22.8659 7.1647
Au 16.1363 7.62132 7.16492
Au 11.7452 15.2533 7.16155
Au 7.33425 22.8674 7.16498
Au 1.4666 2.53818 7.16518
Au -2.93682 10.1618 7.16501
Au -7.33476 17.7851 7.16539
Au 10.2682 2.53881 7.16518
Au 5.86686 10.2149 7.24195
Au 1.46653 17.7858 7.16476
Au 19.0693 2.54115 7.16475
Au 14.6707 10.1619 7.165
Au 10.2679 17.7854 7.16477
Au -0.00163485 5.0771 7.16478
Au -4.40478 12.7028 7.16619
Au -8.80105 20.3249 7.16543
Au 8.79962 5.07934 7.16465
Au 4.44051 12.6978 7.20685
Au -0.000703102 20.3268 7.16532
Au 17.6029 5.08099 7.16474
Au 13.2105 12.7048 7.16426
Au 8.80172 20.3269 7.16434
Au 4.41031 7.61998 7.15987
Au -0.0112581 15.2538 7.16164
Au -4.40136 22.865 7.16539
Au 13.203 7.6204 7.16513
Au 8.79998 15.2427 7.15722
Au 4.40037 22.8676 7.16503
Au 26.4043 -0.0011965 7.16469
Au 22.0021 7.62115 7.16494
Au 17.6039 15.2447 7.16581
Au -1.46689 5.92838 4.79085
Au -5.86757 13.5506 4.79085
Au -10.2683 21.1728 4.79085
Au 7.33446 5.92838 4.79085
Au 2.93379 13.5506 4.79085
Au -1.46689 21.1728 4.79085
Au 16.1358 5.92838 4.79085
Au 11.7351 13.5506 4.79085
Au 7.33446 21.1728 4.79085
Au 7.33446 0.846911 4.79085
Au 2.93379 8.46911 4.79085
Au -1.46689 11.0098 4.79085
Au -2.9372 18.632 4.79085
|     Au  14.6689  3.38764  4.79085 |
|-----|-----------------|-----------------|
|  Au 10.2683  11.0098  4.79085 |
|  Au  5.86757  18.632  4.79085 |
|  Au 23.4703  3.38764  4.79085 |
|  Au 19.0696  11.0098  4.79085 |
|  Au 14.6689  18.632  4.79085 |
|  Au  4.40068  5.92838  4.79085 |
| Au-4.9788e-08 13.5506  4.79085 |
| Au-4.40068  21.1728  4.79085 |
|  Au 13.202  5.92838  4.79085 |
|  Au  8.80136  13.5506  4.79085 |
|  Au  4.40068  21.1728  4.79085 |
|  Au 22.0034  5.92838  4.79085 |
|  Au 17.6027  13.5506  4.79085 |
|  Au 13.202  21.1728  4.79085 |
|  Au  4.40068  0.846911  4.79085 |
| Au-4.9788e-08  8.46911  4.79085 |
| Au-4.40068  16.0913  4.79085 |
|  Au 13.202  0.846911  4.79085 |
|  Au  8.80136  8.46911  4.79085 |
|  Au  4.40068  16.0913  4.79085 |
|  Au 22.0034  0.846911  4.79085 |
|  Au 17.6027  8.46911  4.79085 |
|  Au 13.202  16.0913  4.79085 |
|  Au  2.93379  3.38764  4.79085 |
| Au-1.46689  11.0098  4.79085 |
|  Au  5.86757  18.632  4.79085 |
|  Au 11.7351  3.38764  4.79085 |
|  Au  7.33447  11.0098  4.79085 |
|  Au  2.93379  18.632  4.79085 |
|  Au 20.5365  3.38764  4.79085 |
|  Au 16.1358  11.0098  4.79085 |
|  Au 11.7351  18.632  4.79085 |
|  Au  1.46689  5.92838  4.79085 |
| Au-2.93379  13.5506  4.79085 |
| Au-7.33447  21.1728  4.79085 |
|  Au 10.2683  5.92838  4.79085 |
|  Au  5.86757  13.5506  4.79085 |
|  Au 14.6689  21.1728  4.79085 |
|  Au 19.0696  5.92838  4.79085 |
|  Au 14.6689  13.5506  4.79085 |
|  Au 17.6027  3.38764  4.79085 |
|  Au 13.202  11.0098  4.79085 |
|  Au  8.80136  18.632  4.79085 |
| Au-4.40068  11.0098  4.79085 |
| Au-8.80136  18.632  4.79085 |
|  Au  8.80136  3.38764  4.79085 |
|  Au  4.40068  11.0098  4.79085 |
|  Au 2.4894e-08  3.38764  4.79085 |
| Au-4.40068  11.0098  4.79085 |
| Au-8.80136  18.632  4.79085 |
|  Au  8.80136  3.38764  4.79085 |
|  Au  4.40068  11.0098  4.79085 |
| Au | 1.46689 4.23456 2.39543 |
|----|----------------------------|
| Au | -5.86757 11.8568 2.39543 |
| Au | -10.2683 19.479 2.39543 |
| Au | 7.33446 4.23456 2.39543 |
| Au | 2.93379 11.8568 2.39543 |
| Au | -1.46689 19.479 2.39543 |
| Au | 16.1358 4.23456 2.39543 |
| Au | 11.7351 11.8568 2.39543 |
| Au | 7.33446 19.479 2.39543 |
| Au | -2.93379 6.77529 2.39543 |
| Au | -7.33447 14.3975 2.39543 |
| Au | -11.7351 22.0197 2.39543 |
| Au | 5.86757 6.77529 2.39543 |
| Au | 1.46689 14.3975 2.39543 |
| Au | -2.93379 22.0197 2.39543 |
| Au | 14.6689 6.77529 2.39543 |
| Au | 10.2683 14.3975 2.39543 |
| Au | 5.86757 22.0197 2.39543 |
| Au | 5.86757 1.69382 2.39543 |
| Au | 1.46689 9.31602 2.39543 |
| Au | -2.93379 16.9382 2.39543 |
| Au | 14.6689 1.69382 2.39543 |
| Au | 10.2683 9.31602 2.39543 |
| Au | 5.86757 16.9382 2.39543 |
| Au | 23.4703 1.69382 2.39543 |
| Au | 19.0696 9.31602 2.39543 |
| Au | 14.6689 16.9382 2.39543 |
| Au | 4.40068 4.23456 2.39543 |
| Au | -7.4682e-08 11.8568 2.39543 |
| Au | -4.40068 19.479 2.39543 |
| Au | 13.202 4.23456 2.39543 |
| Au | 8.80136 11.8568 2.39543 |
| Au | 4.40068 19.479 2.39543 |
| Au | 22.0034 4.23456 2.39543 |
| Au | 17.6027 11.8568 2.39543 |
| Au | 13.202 19.479 2.39543 |
| Au | 2.93379 6.77529 2.39543 |
| Au | -1.46689 14.3975 2.39543 |
| Au | -5.86757 22.0197 2.39543 |
| Au | 11.7351 6.77529 2.39543 |
| Au | 7.33447 14.3975 2.39543 |
| Au | 2.93379 22.0197 2.39543 |
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| Au | 11.7351 1.69382 2.39543 |
| Au | 7.33447 9.31602 2.39543 |
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| Au | 20.5365 1.69382 2.39543 |
| Au | 16.1358 9.31602 2.39543 |
| Au | 11.7351 16.9382 2.39543 |
| Au | 1.46689 4.23456 2.39543 |
| Au | -2.93379 11.8568 2.39543 |
| Au | -7.33447 19.479 2.39543 |
| Au | 10.2683 4.23456 2.39543 |
| Au | 5.86757 11.8568 2.39543 |
| Au | 1.46689 19.479 2.39543 |
Au 19.0696 4.23456 2.39543
Au 14.6689 11.8568 2.39543
Au 10.2683 19.479 2.39543
Au 0 6.77529 2.39543
Au -4.40068 14.3975 2.39543
Au -8.80136 22.0197 2.39543
Au 8.80136 6.77529 2.39543
Au 4.40068 14.3975 2.39543
Au 0 22.0197 2.39543
Au 17.6027 6.77529 2.39543
Au 13.202 14.3975 2.39543
Au 8.80136 22.0197 2.39543
Au 0 1.69382 2.39543
Au -4.40068 9.31602 2.39543
Au -8.80136 16.9382 2.39543
Au 8.80136 1.69382 2.39543
Au 4.40068 9.31602 2.39543
Au 0 16.9382 2.39543
Au 17.6027 1.69382 2.39543
Au 13.202 9.31602 2.39543
Au 8.80136 16.9382 2.39543
C 5.85394 11.8862 12.2144
C 5.15266 11.9113 14.3613
C 6.55015 11.9331 14.3626
C 8.35229 11.9236 12.6028
C 3.35379 11.8537 12.6002
N 6.94462 11.9171 13.0295
N 4.76106 11.8828 13.0275
C 9.05836 13.2167 12.9822
H 9.21004 13.3262 14.0583
H 8.49748 14.083 12.6205
H 10.0406 13.2331 12.5013
H 8.53534 9.76819 12.6512
H 10.0653 10.6426 12.542
H 9.21377 10.5569 14.0887
H 8.28368 11.9121 11.5013
C 9.07643 10.6485 13.0089
C 2.61362 13.1265 12.9843
H 1.62938 13.1165 12.5077
H 1.67687 10.5273 12.5274
H 2.52032 10.4627 14.0795
H 3.22878 9.69366 12.6457
H 3.14921 14.0083 12.6219
H 2.46328 13.23 14.0611
C 2.66234 10.5591 13.0007
H 3.42291 11.848 11.4986
C 4.42882 11.9183 15.5536
C 7.27147 11.9618 15.5561
H 3.34784 11.8997 15.5715
H 8.35247 11.9773 15.5757
C 5.14867 11.9481 16.7367
C 6.549 11.9695 16.7379
H 4.61422 11.9541 17.6804
H 7.08115 11.9921 17.6826
c. NHCs adsorption at Au adatoms
   NHC1 in ballbot state in xyz format (Å)
Au 19.0685 4.23377 9.57349
Au 14.676 11.853 9.58621
Au 10.279 19.4937 9.58139
Au -0.00434993 6.77071 9.57431
Au -4.41202 14.3972 9.57588
Au -8.80046 22.0193 9.57635
Au 8.80736 6.76815 9.58144
Au 4.30935 14.4166 9.61317
Au -0.00377301 22.0258 9.57522
Au 17.6014 6.77407 9.57505
Au 13.229 14.398 9.5873
Au 8.80124 22.0227 9.57444
Au -1.62848e-05 1.69398 9.57473
Au -4.40431 9.31292 9.57372
Au -8.8003 16.9385 9.57655
Au 8.80165 1.69322 9.57514
Au 4.38623 9.28171 9.57936
Au -0.0178067 16.948 9.57795
Au 17.6023 1.69425 9.57383
Au 13.2064 9.313 9.58553
Au 8.8314 16.9793 9.58666
Au 7.33457 2.53929 7.16502
Au 2.93129 10.1626 7.1667
Au -1.47248 17.7879 7.16528
Au 16.1353 2.54092 7.16459
Au 11.7394 10.1594 7.16669
Au 7.33186 17.7868 7.16167
Au 24.9369 2.54011 7.16417
Au 20.5345 10.162 7.1646
Au 16.1378 17.7858 7.16616
Au 5.86655 5.07649 7.16577
Au 1.46289 12.7043 7.1661
Au -2.93601 20.3277 7.16465
Au 14.6685 5.08188 7.16512
Au 10.2859 12.7068 7.15176
Au 5.86615 20.3257 7.1648
Au 23.4697 5.08061 7.1639
Au 19.0681 7.62196 7.16518
Au 14.6711 20.3272 7.16595
Au 1.46615 7.62027 7.1647
Au -2.93969 15.2452 7.16539
Au -7.33467 22.866 7.16503
Au 10.2708 7.61908 7.16683
Au 5.85058 15.2435 7.16773
Au 1.4662 22.8678 7.16464
Au 19.068 7.62196 7.16458
Au 14.6764 15.2452 7.1669
Au 10.2689 22.8664 7.16443
Au 4.40053 2.53865 7.16522
Au -0.00272042 10.1619 7.1644
Au -4.40392 17.7865 7.16478
Au 13.2017 2.54077 7.1648
Au 8.80569 10.1505 7.15237
Au 4.39375 17.7844 7.16435
Au 22.0029 2.53976 7.16408
Au 17.6011 10.1627 7.16579
Au 13.2094 17.789 7.16752
Au 2.93288 5.07841 7.16504
Au -1.47224 12.7034 7.16441
Au -5.86868 20.3265 7.16495
| Au 2.4894e-08 18.632 4.79085 |
| Au 17.6027 3.38764 4.79085 |
| Au 13.202 11.0098 4.79085 |
| Au 8.80136 18.632 4.79085 |
| Au -1.46689 4.23456 2.39543 |
| Au -5.86757 11.8568 2.39543 |
| Au -10.2683 19.479 2.39543 |
| Au 7.33446 4.23456 2.39543 |
| Au 2.93379 11.8568 2.39543 |
| Au -1.46689 19.479 2.39543 |
| Au 16.1358 4.23456 2.39543 |
| Au 11.7351 11.8568 2.39543 |
| Au 7.33446 19.479 2.39543 |
| Au -2.93379 6.77529 2.39543 |
| Au -7.33447 14.3975 2.39543 |
| Au -11.7351 22.0197 2.39543 |
| Au 5.86757 6.77529 2.39543 |
| Au 1.46689 14.3975 2.39543 |
| Au -2.93379 22.0197 2.39543 |
| Au 14.6689 6.77529 2.39543 |
| Au 10.2683 14.3975 2.39543 |
| Au 5.86757 22.0197 2.39543 |
| Au 5.86757 1.69382 2.39543 |
| Au 1.46689 9.31602 2.39543 |
| Au -2.93379 16.9382 2.39543 |
| Au 14.6689 1.69382 2.39543 |
| Au 10.2683 9.31602 2.39543 |
| Au 5.86757 16.9382 2.39543 |
| Au 23.4703 1.69382 2.39543 |
| Au 19.0696 9.31602 2.39543 |
| Au 14.6689 16.9382 2.39543 |
| Au 5.86757 1.69382 2.39543 |
| Au -2.93379 16.9382 2.39543 |
| Au 20.5365 1.69382 2.39543 |
| Au 16.1358 9.31602 2.39543 |
| Au 11.7351 16.9382 2.39543 |
| Au 1.46689 4.23456 2.39543 |
| Au -2.93379 11.8568 2.39543 |
Au  -7.33447 19.479 2.39543
Au  10.2683 4.23456 2.39543
Au  5.86757 11.8568 2.39543
Au  1.46689 19.479 2.39543
Au  19.0696 4.23456 2.39543
Au  14.6689 11.8568 2.39543
Au  10.2683 19.479 2.39543
Au   0.677529 2.39543
Au  -4.40068 14.3975 2.39543
Au  -8.80136 22.0197 2.39543
Au  8.80136 6.77529 2.39543
Au  4.40068 14.3975 2.39543
Au   0.220197 2.39543
Au  17.6027 6.77529 2.39543
Au  13.202 14.3975 2.39543
Au  8.80136 22.0197 2.39543
Au   0.169382 2.39543
Au  -4.40068 9.31602 2.39543
Au  -8.80136 16.9382 2.39543
Au  8.80136 1.69382 2.39543
Au  4.40068 9.31602 2.39543
Au   0.169382 2.39543
Au  13.202 9.31602 2.39543
Au  8.80136 16.9382 2.39543
Au   7.54561 13.286 12.8834
Au   9.50793 12.1985 13.0793
Au   9.76965 13.5754 13.0835
Au   8.35901 15.6442 12.9915
Au   7.43416 10.793 12.9868
Au   8.53956 14.2066 13.0021
Au   8.13029 12.0639 12.9966
Au   8.88432 16.0901 12.1381
Au   8.74092 16.0746 13.9211
Au   7.29599 15.8614 12.893
Au   7.75428 10.1874 12.1307
Au   6.36512 10.9811 12.8973
Au   7.63823 10.251 13.9141
Au  10.5354 11.2618 13.0667
Au  11.0692 14.0713 13.0795
Au  10.3397 10.1958 13.0302
Au  11.2769 15.1352 13.0535
Au  11.8341 11.7574 13.0418
Au  12.0956 13.1353 13.0516
Au  12.6647 11.0613 12.9922
Au  13.1241 13.478 13.0085

NHC2 in ballbot state in xyz format (Å)

Au  -1.46852 4.2337 9.57596
Au  -5.86787 11.8576 9.57568
Au  -10.2659 19.4791 9.5747
Au  7.33557 4.23025 9.57725
Au  2.8932 11.8567 9.54981
Au  -1.46774 19.4783 9.58032
Au  16.1366 4.23397 9.57431
Au  11.7603 11.8523 9.5749
Au  7.33202 19.4904 9.58171
Au  -2.93585 6.77458 9.57524
Au -7.33326 14.399 9.57504
Au -11.7334 22.0191 9.57289
Au 5.86661 6.76684 9.57803
Au 1.45031 14.3989 9.57568
Au -2.93386 22.0184 9.57565
Au 14.6733 6.7717 9.5748
Au 10.287 14.4041 9.58316
Au 5.86548 22.0244 9.57615
Au 5.86855 1.69147 9.57485
Au -1.45599 9.31162 9.5824
Au 14.6685 1.69378 9.57572
Au 10.2846 9.29787 9.57458
Au 5.84766 16.9713 9.55082
Au 23.4702 1.69503 9.57554
Au 19.0705 9.31601 9.57465
Au 14.6722 16.9401 9.57663
Au 4.40107 4.2298 9.57588
Au -0.0151428 11.8562 9.58773
Au -4.39997 19.4786 9.57638
Au 13.2048 4.23032 9.57461
Au 8.8441 11.8352 9.64662
Au 4.39292 19.4909 9.58611
Au 22.0025 4.23503 9.57394
Au 17.6077 11.8573 9.57491
Au 13.2054 19.4806 9.57562
Au 2.92653 6.76412 9.57866
Au -1.47355 14.4002 9.58677
Au -5.86654 22.0184 9.57487
Au 11.7425 6.76611 9.57738
Au 7.34302 14.4636 9.49667
Au 2.93082 22.0224 9.57699
Au 20.5358 6.77542 9.57511
Au 16.1399 14.3992 9.57695
Au 11.7364 22.0226 9.57427
Au 2.9346 1.69229 9.57329
Au -1.47202 9.31468 9.57642
Au -5.86633 16.9392 9.57519
Au 11.7351 1.69209 9.57515
Au 7.33908 9.29717 9.58132
Au 2.92538 16.9502 9.57602
Au 20.536 1.69563 9.57522
Au 16.141 9.31448 9.57493
Au 11.7393 16.944 9.57798
Au 1.46421 4.23092 9.57457
Au -2.93778 11.8578 9.57778
Au -7.33271 19.4786 9.57472
Au 10.2701 4.23024 9.577
Au 5.80777 11.8141 9.48681
Au 1.46146 19.4823 9.58539
Au 19.0694 4.23528 9.57476
Au 14.6808 11.8557 9.57747
Au 10.2721 19.4891 9.57885
Au -0.00421658 6.77248 9.5755
Au -4.40211 14.3987 9.57724
Au -8.79939 22.0184 9.57292
Au 8.80572 6.76583 9.57944
Au 4.3735 14.4125 9.50213
Au -0.00136809 22.0203 9.57714
Au 17.6039 6.77483 9.57418
| Au 13.2118 14.3996 9.57943 |
| Au 8.80125 22.0242 9.57568 |
| Au 0.00385994 1.69307 9.57422 |
| Au -4.40247 9.316 9.57498 |
| Au -8.79919 16.9395 9.57545 |
| Au 8.80187 1.69146 9.57587 |
| Au 4.38038 9.28672 9.56238 |
| Au -0.00277294 16.9401 9.58757 |
| Au 17.602 1.6956 9.57523 |
| Au 13.2131 9.30976 9.57713 |
| Au 8.81101 16.9674 9.56941 |
| Au 7.33543 2.539 7.16524 |
| Au 2.92484 10.1541 7.15854 |
| Au -1.46996 17.7871 7.16689 |
| Au 16.135 2.54087 7.16465 |
| Au 11.7372 10.162 7.16627 |
| Au 7.33744 17.7962 7.15945 |
| Au 24.9369 2.54057 7.16495 |
| Au 20.5359 10.1635 7.16464 |
| Au 16.1374 17.7853 7.16496 |
| Au 5.86938 5.07772 7.16588 |
| Au 1.45121 12.7068 7.15786 |
| Au -2.9337 20.3259 7.16576 |
| Au 14.6697 5.08113 7.16424 |
| Au 10.2688 12.6954 7.17697 |
| Au 5.86537 20.329 7.16614 |
| Au 23.4696 5.08131 7.16516 |
| Au 19.0699 12.7044 7.16488 |
| Au 14.6703 20.3258 7.1646 |
| Au 1.46373 7.619 7.16629 |
| Au -2.93592 15.2457 7.16668 |
| Au -7.33343 22.8658 7.16447 |
| Au 10.2694 7.61941 7.16528 |
| Au 5.87046 15.2514 7.14651 |
| Au 1.46589 22.8671 7.16526 |
| Au 19.0697 7.62236 7.16447 |
| Au 14.6711 15.2452 7.16602 |
| Au 10.2683 22.8681 7.1648 |
| Au 4.4015 2.53881 7.16469 |
| Au -0.00399731 10.1628 7.16619 |
| Au -4.40054 17.7854 7.16569 |
| Au 13.2016 2.53996 7.16486 |
| Au 8.80899 10.1677 7.17729 |
| Au 4.39079 17.7954 7.15743 |
| Au 22.0032 2.54127 7.16519 |
| Au 17.6035 10.1629 7.16452 |
| Au 13.2049 17.7853 7.16574 |
| Au 2.93232 5.07681 7.16532 |
| Au -1.4723 12.7053 7.16778 |
| Au -5.86662 20.3254 7.16506 |
| Au 11.7353 5.08027 7.16555 |
| Au 7.3479 12.6959 7.16296 |
| Au 7.28525 12.7106 11.7118 |
| Au 2.92961 20.3293 7.16708 |
| Au 20.5363 5.08166 7.16534 |
| Au 16.1371 12.7045 7.16568 |
| Au 11.7374 20.3286 7.16534 |
| Au -1.46856 7.62208 7.16477 |
| Au -5.86776 15.2451 7.16521 |
| Au -10.2674 22.8657 7.16444 |
Au 4.40068 5.92838 4.79085
Au -4.9788e-08 13.5506 4.79085
Au -4.40068 21.1728 4.79085
Au 13.202 5.92838 4.79085
Au 8.80136 13.5506 4.79085
Au 4.40068 21.1728 4.79085
Au 22.0034 5.92838 4.79085
Au 17.6027 13.5506 4.79085
Au 13.202 21.1728 4.79085
Au 4.40068 0.846911 4.79085
Au -4.9788e-08 8.46911 4.79085
Au -4.40068 16.0913 4.79085
Au 13.202 0.846911 4.79085
Au 8.80136 8.46911 4.79085
Au 4.40068 16.0913 4.79085
Au 22.0034 0.846911 4.79085
Au 17.6027 8.46911 4.79085
Au 13.202 16.0913 4.79085
Au 2.93379 3.38764 4.79085
Au -1.46689 11.0098 4.79085
Au -5.86757 18.632 4.79085
Au 11.7351 3.38764 4.79085
Au 7.33447 11.0098 4.79085
Au 2.93379 18.632 4.79085
Au 20.5365 3.38764 4.79085
Au 16.1358 11.0098 4.79085
Au 11.7351 18.632 4.79085
Au 1.46689 5.92838 4.79085
Au -2.93379 13.5506 4.79085
Au -7.33447 21.1728 4.79085
Au 10.2683 5.92838 4.79085
Au 5.86757 13.5506 4.79085
Au 1.46689 21.1728 4.79085
Au 19.0696 5.92838 4.79085
Au 14.6689 13.5506 4.79085
Au 10.2683 21.1728 4.79085
Au 1.46689 0.846911 4.79085
Au -2.93379 8.46911 4.79085
Au -7.33447 16.0913 4.79085
Au 10.2683 0.846911 4.79085
Au 5.86757 8.46911 4.79085
Au 1.46689 16.0913 4.79085
Au 19.0696 0.846911 4.79085
Au 14.6689 8.46911 4.79085
Au 10.2683 16.0913 4.79085
Au 2.4894e-08 3.38764 4.79085
Au -4.40068 11.0098 4.79085
Au -8.80136 18.632 4.79085
Au 8.80136 3.38764 4.79085
Au 4.40068 11.0098 4.79085
Au 2.4894e-08 18.632 4.79085
Au 17.6027 3.38764 4.79085
Au 13.202 11.0098 4.79085
Au 8.80136 18.632 4.79085
Au -1.46689 4.23456 2.39543
Au -5.86757 11.8568 2.39543
Au -10.2683 19.479 2.39543
Au 7.33446 4.23456 2.39543
Au 2.93379 11.8568 2.39543
Au -1.46689 19.479 2.39543
| Column 1 | Column 2 | Column 3 | Column 4 |
|---------|---------|---------|---------|
| Au 16.1358 | 4.23456 | 2.39543 |
| Au 11.7351 | 11.8568 | 2.39543 |
| Au 7.33446 | 19.479 | 2.39543 |
| Au -2.93379 | 6.77529 | 2.39543 |
| Au -7.33447 | 14.3975 | 2.39543 |
| Au -11.7351 | 22.0197 | 2.39543 |
| Au 5.86757 | 6.77529 | 2.39543 |
| Au 1.46689 | 14.3975 | 2.39543 |
| Au -2.93379 | 22.0197 | 2.39543 |
| Au 14.6689 | 6.77529 | 2.39543 |
| Au 10.2683 | 14.3975 | 2.39543 |
| Au 5.86757 | 22.0197 | 2.39543 |
| Au 5.86757 | 1.69382 | 2.39543 |
| Au 1.46689 | 9.31602 | 2.39543 |
| Au -2.93379 | 16.9382 | 2.39543 |
| Au 14.6689 | 1.69382 | 2.39543 |
| Au 10.2683 | 9.31602 | 2.39543 |
| Au 5.86757 | 16.9382 | 2.39543 |
| Au 23.4703 | 1.69382 | 2.39543 |
| Au 19.0696 | 9.31602 | 2.39543 |
| Au 14.6689 | 14.3975 | 2.39543 |
| Au 22.0034 | 4.23456 | 2.39543 |
| Au -7.4682e-08 | 11.8568 | 2.39543 |
| Au -4.40068 | 19.479 | 2.39543 |
| Au 13.202 | 4.23456 | 2.39543 |
| Au 8.80136 | 11.8568 | 2.39543 |
| Au 4.40068 | 19.479 | 2.39543 |
| Au 22.0034 | 4.23456 | 2.39543 |
| Au 17.6027 | 11.8568 | 2.39543 |
| Au 13.202 | 19.479 | 2.39543 |
| Au 2.93379 | 6.77529 | 2.39543 |
| Au -1.46689 | 14.3975 | 2.39543 |
| Au -5.86757 | 22.0197 | 2.39543 |
| Au 11.7351 | 6.77529 | 2.39543 |
| Au 7.33447 | 14.3975 | 2.39543 |
| Au 2.93379 | 22.0197 | 2.39543 |
| Au 20.5365 | 6.77529 | 2.39543 |
| Au 16.1358 | 14.3975 | 2.39543 |
| Au 11.7351 | 22.0197 | 2.39543 |
| Au 2.93379 | 1.69382 | 2.39543 |
| Au -1.46689 | 9.31602 | 2.39543 |
| Au -5.86757 | 16.9382 | 2.39543 |
| Au 11.7351 | 6.77529 | 2.39543 |
| Au 7.33447 | 14.3975 | 2.39543 |
| Au 2.93379 | 16.9382 | 2.39543 |
| Au 20.5365 | 6.77529 | 2.39543 |
| Au 16.1358 | 14.3975 | 2.39543 |
| Au 11.7351 | 16.9382 | 2.39543 |
| Au 1.46689 | 9.31602 | 2.39543 |
| Au -2.93379 | 11.8568 | 2.39543 |
| Au -7.33447 | 19.479 | 2.39543 |
| Au 10.2683 | 4.23456 | 2.39543 |
| Au 5.86757 | 11.8568 | 2.39543 |
| Au 1.46689 | 19.479 | 2.39543 |
| Au 19.0696 | 4.23456 | 2.39543 |
| Au 14.6689 | 11.8568 | 2.39543 |
| Au 10.2683 | 19.479 | 2.39543 |
| Au 0.677529 | 2.39543 |
| Au -4.40068 | 14.3975 | 2.39543 |
| Au -8.80136 | 22.0197 | 2.39543 |
NHC3 in ballbot state in xyz format (Å)

Au -1.46748 4.23473 9.5746
Au -5.86711 11.8584 9.57483
Au -10.2649 19.4799 9.5756
Au 7.33546 4.23072 9.57655
Au 2.91489 11.8536 9.56804
Au -1.46868 19.4801 9.57518
Au 16.1376 4.23519 9.57531
Au 11.7616 11.8501 9.5488
Au 7.33349 19.4939 9.58122
Au -2.93508 6.7754 9.5739
Au -7.33282 14.3989 9.57511
Au -11.7326 22.0214 9.57532
Au 5.86584 6.76509 9.57787
Au 1.4593 14.3979 9.57937
Au -2.93415 22.0196 9.57425

C 5.74891 13.5255 12.843
C 4.19527 15.1429 13.0306
C 3.53838 13.9048 13.0291
C 4.27913 11.4996 12.9308
C 6.6022 15.878 12.9283
N 4.52833 13.9048 13.0291
N 5.55147 14.8659 12.9467
C 3.92287 10.9446 12.9308
H 3.02048 11.4071 14.7069
H 4.73983 11.0302 12.5371
H 3.74136 9.87001 14.2167
H 5.184 11.0302 12.5371
H 3.48445 11.3081 12.1976
C 6.85352 16.499 14.2916
H 7.64298 17.2499 14.2062
H 7.17743 15.7418 15.0105
H 5.96296 16.9916 14.6897
H 6.32167 16.6355 12.1829
H 7.50071 15.3874 12.5461
C 3.48811 16.3423 13.0146
C 2.14899 13.8182 13.0071
H 3.98863 17.3035 12.985
H 1.6336 12.8652 12.9691
C 2.10205 16.2545 12.987
C 1.44425 15.0156 12.9808
H 1.51509 17.1658 12.9407
H 0.360733 14.9916 12.9317
Au 14.673 6.77363 9.57561
Au 10.2889 14.4115 9.56469
Au 5.86663 22.0265 9.57635
Au 5.86856 1.69189 9.57504
Au 1.45742 9.31092 9.57602
Au -2.93523 16.9397 9.57524
Au 14.6686 1.69528 9.57452
Au 10.2869 9.2952 9.58154
Au 5.84638 16.9741 9.55813
Au 23.4716 1.69689 9.57507
Au 19.0713 9.31713 9.57483
Au 14.673 16.94 9.57751
Au 4.4002 4.22994 9.57618
Au -0.00868238 11.8565 9.57689
Au -4.40087 19.4796 9.57528
Au 13.2053 4.23311 9.57441
Au 8.8535 11.822 9.53469
Au 4.39355 19.4928 9.58169
Au 22.0037 4.23614 9.5746
Au 17.6058 11.858 9.57517
Au 13.2079 19.4832 9.57627
Au 2.92731 6.76531 9.57507
Au -1.47047 14.3992 9.57623
Au -5.86683 22.0193 9.57496
Au 11.7418 6.76766 9.57975
Au 7.3385 14.4912 9.50469
Au 2.93192 22.0253 9.57505
Au 20.537 6.77646 9.57477
Au 16.1398 14.3997 9.57675
Au 11.7387 22.0248 9.57512
Au 2.93505 1.69254 9.57467
Au -1.47139 9.31527 9.57447
Au -5.86727 16.93999 9.57548
Au 11.7354 1.69366 9.57428
Au 7.33602 9.29247 9.57813
Au 2.92612 16.9452 9.58267
Au 20.537 1.69717 9.57462
Au 16.1404 9.31604 9.57591
Au 11.7438 16.9463 9.58279
Au 1.46443 4.23086 9.57449
Au -2.93742 11.8574 9.57437
Au -7.33292 19.4796 9.57616
Au 10.2699 4.23094 9.57639
Au 5.8363 11.8254 9.56415
Au 1.4627 19.4826 9.57735
Au 19.0707 4.23641 9.57514
Au 14.678 11.8569 9.57981
Au 10.2753 19.4933 9.58033
Au -0.00375131 6.77249 9.57458
Au -4.4016 14.3992 9.57463
Au -8.7995 22.0192 9.57534
Au 8.80618 6.76723 9.57941
Au 4.38379 14.407 9.57427
Au -0.000948511 22.0212 9.5745
Au 17.6047 6.77584 9.57457
Au 13.2097 14.3988 9.58209
Au 8.80313 22.0266 9.57621
Au 0.001538 1.69481 9.57526
Au -4.40157 9.31675 9.57453
Au -8.79906 16.9399 9.57566
Au 8.80211 1.69232 9.57495
Au 4.38569 9.29461 9.5676
Au -0.00330767 16.9403 9.57754
Au 17.6028 1.6972 9.57518
Au 13.2121 9.31114 9.582
Au 8.81892 16.9769 9.56913
Au 7.33499 2.53925 7.16498
Au 2.93112 10.161 7.16403
Au -1.46834 17.7862 7.16517
Au 16.1359 2.54163 7.16458
Au 11.7395 10.1562 7.16043
Au 7.33505 17.7959 7.16178
Au 24.9384 2.54122 7.16455
Au 20.5368 10.1643 7.1645
Au 16.138 17.7864 7.16548
Au 5.86831 5.07829 7.16554
Au 1.46211 12.7059 7.16432
Au -2.93413 20.3264 7.16472
Au 14.6703 5.08158 7.16469
Au 10.2703 12.7057 7.15993
Au 5.86607 20.3299 7.16609
Au 23.4702 5.08192 7.16432
Au 19.0705 12.7045 7.16488
Au 14.6712 20.327 7.16511
Au 1.46593 7.62067 7.16497
Au -2.9344 15.2454 7.16481
Au -7.33344 22.8663 7.16502
Au 10.2706 7.61527 7.16501
Au 5.85605 15.2529 7.15133
Au 1.46595 22.8682 7.16477
Au 19.0701 7.62302 7.16458
Au 14.6729 15.2466 7.16645
Au 10.2691 22.8684 7.16517
Au 4.40146 2.53949 7.1647
Au -0.00152645 10.1632 7.16498
Au -4.40055 17.7861 7.16499
Au 13.202 2.54055 7.1647
Au 8.80349 10.1522 7.15809
Au 4.39083 17.7951 7.16017
Au 22.0038 2.54169 7.16461
Au 17.6034 10.1634 7.16509
Au 13.2059 17.7875 7.16676
Au 2.93347 5.07904 7.1655
Au -1.46833 12.7046 7.16559
Au -5.86707 20.3261 7.16496
Au 11.7362 5.07974 7.16563
Au 7.33351 12.7036 7.16354
Au 7.27724 12.7418 11.6736
Au 2.9305 20.3299 7.1657
Au 20.5368 5.08232 7.16505
Au 16.139 12.7047 7.16566
Au 11.7388 20.3297 7.16546
Au -1.4677 7.62214 7.16428
Au -5.86711 15.2461 7.1649
Au -10.2664 22.8664 7.16488
Au 7.33474 7.61901 7.16747
Au 2.92862 15.2464 7.16653
Au -1.46737 22.8668 7.16474
Au 16.1369 7.62261 7.16475
Au 11.7443 15.2496 7.16319
| Au   | 7.33469 22.8685 7.16487 |
|------|-------------------------|
| Au   | 1.46775 2.53966 7.16476 |
| Au   | -2.93451 10.1631 7.16444 |
| Au   | -7.33353 17.7861 7.16494 |
| Au   | 10.2684 2.53997 7.16471 |
| Au   | 5.86356 10.1566 7.16055 |
| Au   | 1.46334 17.787 7.16665 |
| Au   | 19.07 2.54192 7.16464 |
| Au   | 14.6706 10.1629 7.16586 |
| Au   | 10.277 17.7946 7.16235 |
| Au   | -0.000657687 5.08119 7.16434 |
| Au   | -4.40129 12.7049 7.16474 |
| Au   | -8.79984 20.3264 7.16491 |
| Au   | 8.80173 5.07906 7.16595 |
| Au   | 4.39721 12.7007 7.16395 |
| Au   | -0.00151176 20.327 7.16502 |
| Au   | 17.6035 5.08235 7.16466 |
| Au   | 13.2107 12.707 7.16005 |
| Au   | 8.80284 20.3299 7.166 |
| Au   | 4.39957 7.61497 7.16399 |
| Au   | -0.00239735 15.2461 7.16617 |
| Au   | -4.40039 22.8664 7.16469 |
| Au   | 13.2039 7.62035 7.16595 |
| Au   | 8.80889 15.2553 7.15458 |
| Au   | 4.40054 22.8685 7.16495 |
| Au   | 26.4056 0.00127958 7.16473 |
| Au   | 22.0033 7.6229 7.16435 |
| Au   | 17.6041 15.2453 7.16522 |
| Au   | -1.46689 5.92838 4.79085 |
| Au   | -5.86757 13.5506 4.79085 |
| Au   | -10.2683 21.1728 4.79085 |
| Au   | 7.33446 5.92838 4.79085 |
| Au   | 2.93379 13.5506 4.79085 |
| Au   | -1.46689 21.1728 4.79085 |
| Au   | 16.1358 5.92838 4.79085 |
| Au   | 11.7351 13.5506 4.79085 |
| Au   | 7.33446 21.1728 4.79085 |
| Au   | 7.33446 0.846911 4.79085 |
| Au   | 2.93379 8.46911 4.79085 |
| Au   | -1.46689 16.0913 4.79085 |
| Au   | 16.1358 0.846911 4.79085 |
| Au   | 11.7351 8.46911 4.79085 |
| Au   | 7.33446 16.0913 4.79085 |
| Au   | 24.9372 0.846911 4.79085 |
| Au   | 20.5365 8.46911 4.79085 |
| Au   | 16.1358 16.0913 4.79085 |
| Au   | 5.86757 3.38764 4.79085 |
| Au   | 1.46689 11.0098 4.79085 |
| Au   | -2.93379 18.632 4.79085 |
| Au   | 14.6689 3.38764 4.79085 |
| Au   | 10.2683 11.0098 4.79085 |
| Au   | 5.86757 18.632 4.79085 |
| Au   | 23.4703 3.38764 4.79085 |
| Au   | 19.0696 11.0098 4.79085 |
| Au   | 14.6689 18.632 4.79085 |
| Au   | 4.40068 5.92838 4.79085 |
| Au   | -4.9788e-08 13.5506 4.79085 |
| Au   | -4.40068 21.1728 4.79085 |
| Au   | 13.202 5.92838 4.79085 |
| Au   | 8.80136 13.5506 4.79085 |
|   |   |   |   |
|---|---|---|---|
| Au | 4.40068 | 21.1728 | 4.79085 |
| Au | 22.0034 | 5.92838 | 4.79085 |
| Au | 17.6027 | 13.5506 | 4.79085 |
| Au | 13.202 | 21.1728 | 4.79085 |
| Au | 4.40068 | 0.846911 | 4.79085 |
| Au | -4.9788e-08 | 8.46911 | 4.79085 |
| Au | -4.40068 | 16.0913 | 4.79085 |
| Au | 13.202 | 0.846911 | 4.79085 |
| Au | 8.80136 | 8.46911 | 4.79085 |
| Au | 4.40068 | 16.0913 | 4.79085 |
| Au | 22.0034 | 0.846911 | 4.79085 |
| Au | 17.6027 | 8.46911 | 4.79085 |
| Au | 13.202 | 16.0913 | 4.79085 |
| Au | 2.93379 | 3.38764 | 4.79085 |
| Au | -1.46689 | 11.0098 | 4.79085 |
| Au | -5.86757 | 18.632 | 4.79085 |
| Au | 11.7351 | 3.38764 | 4.79085 |
| Au | 7.33447 | 11.0098 | 4.79085 |
| Au | 2.93379 | 18.632 | 4.79085 |
| Au | 20.5365 | 3.38764 | 4.79085 |
| Au | 16.1358 | 11.0098 | 4.79085 |
| Au | 11.7351 | 18.632 | 4.79085 |
| Au | 1.46689 | 5.92838 | 4.79085 |
| Au | -2.93379 | 13.5506 | 4.79085 |
| Au | -7.33447 | 21.1728 | 4.79085 |
| Au | 10.2683 | 5.92838 | 4.79085 |
| Au | 5.86757 | 13.5506 | 4.79085 |
| Au | 1.46689 | 21.1728 | 4.79085 |
| Au | 19.0696 | 5.92838 | 4.79085 |
| Au | 14.6689 | 13.5506 | 4.79085 |
| Au | 10.2683 | 21.1728 | 4.79085 |
| Au | 1.46689 | 0.846911 | 4.79085 |
| Au | -2.93379 | 8.46911 | 4.79085 |
| Au | -7.33447 | 16.0913 | 4.79085 |
| Au | 10.2683 | 0.846911 | 4.79085 |
| Au | 5.86757 | 8.46911 | 4.79085 |
| Au | 1.46689 | 16.0913 | 4.79085 |
| Au | 19.0696 | 0.846911 | 4.79085 |
| Au | 14.6689 | 8.46911 | 4.79085 |
| Au | 10.2683 | 16.0913 | 4.79085 |
| Au | 2.4894e-08 | 3.38764 | 4.79085 |
| Au | -4.40068 | 11.0098 | 4.79085 |
| Au | -8.80136 | 18.632 | 4.79085 |
| Au | 8.80136 | 3.38764 | 4.79085 |
| Au | 4.40068 | 11.0098 | 4.79085 |
| Au | 2.4894e-08 | 18.632 | 4.79085 |
| Au | 17.6027 | 3.38764 | 4.79085 |
| Au | 13.202 | 11.0098 | 4.79085 |
| Au | 2.93379 | 18.632 | 4.79085 |
| Au | 19.0696 | 5.92838 | 4.79085 |
| Au | 14.6689 | 13.5506 | 4.79085 |
| Au | 10.2683 | 19.479 | 2.39543 |
| Au | 7.33446 | 4.23456 | 2.39543 |
| Au | 2.93379 | 11.8568 | 2.39543 |
| Au | -2.93379 | 6.77529 | 2.39543 |
| Au | -7.33447 | 14.3975 | 2.39543 |
| Au | -11.7351 22.0197 2.39543 |
|----|-------------------------|
| Au | 5.86757 6.77529 2.39543 |
| Au | 1.46689 14.3975 2.39543 |
| Au | -2.93379 22.0197 2.39543 |
| Au | 14.6689 6.77529 2.39543 |
| Au | 10.2683 14.3975 2.39543 |
| Au | 5.86757 22.0197 2.39543 |
| Au | 5.86757 1.69382 2.39543 |
| Au | 5.86757 1.69382 2.39543 |
| Au | 1.46689 9.31602 2.39543 |
| Au | -2.93379 16.9382 2.39543 |
| Au | 14.6689 1.69382 2.39543 |
| Au | 10.2683 9.31602 2.39543 |
| Au | 5.86757 16.9382 2.39543 |
| Au | 23.4703 1.69382 2.39543 |
| Au | 19.0696 9.31602 2.39543 |
| Au | 14.6689 16.9382 2.39543 |
| Au | 4.40068 4.23456 2.39543 |
| Au | 7.4682e-08 11.8568 2.39543 |
| Au | -4.40068 19.479 2.39543 |
| Au | 13.202 4.23456 2.39543 |
| Au | 8.80136 11.8568 2.39543 |
| Au | 4.40068 19.479 2.39543 |
| Au | 22.0034 4.23456 2.39543 |
| Au | 17.6027 11.8568 2.39543 |
| Au | 13.202 19.479 2.39543 |
| Au | 2.93379 6.77529 2.39543 |
| Au | -1.46689 14.3975 2.39543 |
| Au | -5.86757 22.0197 2.39543 |
| Au | 11.7351 6.77529 2.39543 |
| Au | 7.33447 14.3975 2.39543 |
| Au | 2.93379 22.0197 2.39543 |
| Au | 20.5365 6.77529 2.39543 |
| Au | 16.1358 14.3975 2.39543 |
| Au | 11.7351 22.0197 2.39543 |
| Au | 2.93379 1.69382 2.39543 |
| Au | -1.46689 9.31602 2.39543 |
| Au | -5.86757 16.9382 2.39543 |
| Au | 11.7351 1.69382 2.39543 |
| Au | 7.33447 9.31602 2.39543 |
| Au | 2.93379 16.9382 2.39543 |
| Au | 20.5365 1.69382 2.39543 |
| Au | 16.1358 9.31602 2.39543 |
| Au | 11.7351 16.9382 2.39543 |
| Au | 1.46689 4.23456 2.39543 |
| Au | -2.93379 6.77529 2.39543 |
| Au | 7.33447 19.479 2.39543 |
| Au | 1.46689 14.3975 2.39543 |
| Au | 19.0696 11.8568 2.39543 |
| Au | 14.6689 11.8568 2.39543 |
| Au | 10.2683 19.479 2.39543 |
| Au | 0 6.77529 2.39543 |
| Au | -4.40068 14.3975 2.39543 |
| Au | -8.80136 22.0197 2.39543 |
| Au | 8.80136 6.77529 2.39543 |
| Au | 4.40068 14.3975 2.39543 |
| Au | 0 22.0197 2.39543 |
| Au | 17.6027 6.77529 2.39543 |
| Au | 13.202 14.3975 2.39543 |
### Bis(NHC) complexes on Au(111)

**Optimized structure of Au(NHC1)₂ in xyz format (Å)**

| Au     | 8.80136 | 22.0197 | 2.39543 |
|--------|---------|---------|---------|
| Au     | 0.169382| 2.39543 |
| Au     | -4.40068| 9.31602 | 2.39543 |
| Au     | -8.80136| 16.9382 | 2.39543 |
| Au     | 8.80136 | 1.69382 | 2.39543 |
| Au     | 4.40068 | 9.31602 | 2.39543 |
| Au     | 0.169382| 2.39543 |
| Au     | 17.6027 | 1.69382 | 2.39543 |
| Au     | 13.202  | 9.31602 | 2.39543 |
| Au     | 8.80136 | 16.9382 | 2.39543 |
| C      | 8.07363 | 13.4906 | 13.4025 |
| C      | 8.49718 | 14.867  | 15.1169 |
| C      | 9.45546 | 13.838  | 15.1292 |
| C      | 9.9259  | 11.8382 | 13.5769 |
| C      | 6.55491 | 15.4584 | 13.5351 |
| N      | 9.1619  | 13.014  | 14.0491 |
| C      | 7.66734 | 14.6182 | 14.0303 |
| H      | 11.9722 | 12.4599 | 14.0691 |
| H      | 11.3584 | 13.08   | 12.5254 |
| H      | 11.8203 | 11.3828 | 12.6784 |
| H      | 8.78004 | 10.431  | 14.7608 |
| H      | 10.294  | 9.79226 | 14.1069 |
| H      | 10.3289 | 10.8758 | 15.5006 |
| H      | 9.40488 | 11.5554 | 12.6541 |
| C      | 9.8249  | 10.6732 | 14.5521 |
| H      | 7.04808 | 16.8411 | 13.1295 |
| H      | 6.2474  | 17.3684 | 12.6028 |
| H      | 4.53908 | 15.9876 | 14.0445 |
| H      | 5.61691 | 15.9795 | 15.443 |
| H      | 5.06453 | 14.4486 | 14.7399 |
| H      | 7.89614 | 16.7647 | 12.4426 |
| H      | 7.34702 | 17.4554 | 13.9824 |
| C      | 5.38219 | 15.4677 | 14.5062 |
| H      | 6.23513 | 14.9396 | 12.6232 |
| C      | 8.50466 | 15.8711 | 16.0826 |
| C      | 10.4445 | 13.7862 | 16.109 |
| C      | 7.77121 | 16.6668 | 16.0867 |
| H      | 11.1849 | 12.9974 | 16.1337 |
| C      | 9.49399 | 15.8157 | 17.0522 |
| C      | 10.4478 | 14.79   | 17.0652 |
| H      | 9.52762 | 16.5829 | 17.818 |
| H      | 11.2055 | 14.7789 | 17.8411 |

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**Au-xyz format**

| Au     | -1.46588 | 4.23494 | 9.57377 |
|--------|----------|---------|---------|
| Au     | -5.86746 | 11.8569 | 9.57531 |
| Au     | -10.2689 | 19.4783 | 9.57464 |
| Au     | 7.33575  | 4.23691 | 9.57779 |
| Au     | 2.92942  | 11.8588 | 9.55403 |
| Au     | -1.46602 | 19.478  | 9.57773 |
| Au     | 16.1356  | 4.23362 | 9.57595 |
| Au     | 11.7375  | 11.8564 | 9.54446 |
| Au     | 7.33335  | 19.4752 | 9.58188 |
| Au     | -2.93228 | 6.77538 | 9.57431 |
|       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|
| Au-7.3353 | 14.3971 | 9.57553 |
| Au-11.7356 | 22.0191 | 9.57363 |
| Au-5.87037 | 6.77802 | 9.58156 |
| Au-1.46435 | 14.3921 | 9.55933 |
| Au-2.93382 | 22.0194 | 9.5749 |
| Au-14.6706 | 6.77343 | 9.58112 |
| Au-10.2641 | 14.4007 | 9.55495 |
| Au-5.8679 | 22.0169 | 9.5769 |
| Au-5.86788 | 1.69453 | 9.57469 |
| Au-1.46975 | 9.3182 | 9.58209 |
| Au-2.93298 | 16.9373 | 9.57768 |
| Au-14.6687 | 1.69321 | 9.57524 |
| Au-10.2699 | 9.31409 | 9.54393 |
| Au-5.86335 | 16.9405 | 9.55996 |
| Au-23.4703 | 1.69274 | 9.57385 |
| Au-19.0703 | 9.31612 | 9.57629 |
| Au-14.6674 | 16.9363 | 9.57774 |
| Au-4.40217 | 4.23662 | 9.57602 |
| Au-0.00120614 | 11.856 | 9.58516 |
| Au-4.40042 | 19.4785 | 9.57452 |
| Au-13.2022 | 4.23591 | 9.57863 |
| Au-8.80243 | 11.8558 | 9.58801 |
| Au-4.39987 | 19.4786 | 9.58529 |
| Au-22.0039 | 4.23415 | 9.57398 |
| Au-17.6015 | 11.8558 | 9.57881 |
| Au-13.2088 | 19.4768 | 9.57605 |
| Au-2.93689 | 6.77863 | 9.57802 |
| Au-1.46771 | 14.3969 | 9.58246 |
| Au-5.86766 | 22.0198 | 9.57458 |
| Au-11.735 | 6.77342 | 9.575 |
| Au-7.3371 | 14.393 | 9.591 |
| Au-2.93379 | 22.0177 | 9.57821 |
| Au-20.5371 | 6.77525 | 9.57434 |
| Au-16.1346 | 14.3965 | 9.57973 |
| Au-11.7344 | 22.0176 | 9.57441 |
| Au-2.93406 | 1.69445 | 9.57358 |
| Au-1.46451 | 9.31605 | 9.57731 |
| Au-5.86766 | 16.9383 | 9.57481 |
| Au-11.7351 | 1.69453 | 9.57555 |
| Au-7.32958 | 9.31926 | 9.55612 |
| Au-2.93712 | 16.9409 | 9.56202 |
| Au-20.5367 | 1.69226 | 9.57433 |
| Au-16.138 | 9.31502 | 9.5811 |
| Au-11.7337 | 16.935 | 9.58117 |
| Au-1.46846 | 4.23605 | 9.57424 |
| Au-2.93264 | 11.8569 | 9.5786 |
| Au-7.33485 | 19.4787 | 9.57446 |
| Au-10.2686 | 4.23626 | 9.57979 |
| Au-5.87241 | 11.857 | 9.59547 |
| Au-1.46694 | 19.4779 | 9.583 |
| Au-19.0696 | 4.23384 | 9.57412 |
| Au-14.6706 | 11.8578 | 9.57394 |
| Au-10.2664 | 19.4745 | 9.5779 |
| Au-0.00240544 | 6.77653 | 9.57557 |
| Au-4.4009 | 14.3976 | 9.5768 |
| Au-8.80164 | 22.0197 | 9.57429 |
| Au-8.80385 | 6.77676 | 9.57873 |
| Au-4.4046 | 14.3947 | 9.52843 |
| Au-0.00010499 | 22.019 | 9.57673 |
| Au-17.6024 | 6.77518 | 9.5767 |
| Au 13.2023 | 14.395 | 9.57902 |
| Au 8.80089 | 22.0169 | 9.57548 |
| Au -2.00189e-05 | 1.69378 | 9.57324 |
| Au -4.3993 | 9.31602 | 9.57489 |
| Au -8.80207 | 16.9376 | 9.57529 |
| Au 8.80162 | 1.69466 | 9.57541 |
| Au 4.40323 | 9.31985 | 9.58268 |
| Au -0.0181132 | 16.9387 | 9.56906 |
| Au 17.6029 | 1.69223 | 9.57474 |
| Au 13.2095 | 9.3114 | 9.55171 |
| Au 8.79742 | 16.934 | 9.58457 |
| Au 7.33446 | 2.54084 | 7.16582 |
| Au 2.93276 | 10.1569 | 7.168 |
| Au -1.47019 | 17.787 | 7.16328 |
| Au 16.1358 | 2.53977 | 7.16542 |
| Au 11.7394 | 10.1605 | 7.15608 |
| Au 7.33819 | 17.7886 | 7.16286 |
| Au 24.9373 | 2.54035 | 7.16471 |
| Au 20.5371 | 10.1631 | 7.1655 |
| Au 16.1355 | 17.7852 | 7.16571 |
| Au 5.86847 | 5.08171 | 7.16648 |
| Au 1.46235 | 12.7017 | 7.15798 |
| Au -2.93382 | 20.3264 | 7.16555 |
| Au 14.6692 | 5.07964 | 7.1655 |
| Au 10.2624 | 12.704 | 7.16013 |
| Au 5.86748 | 20.3255 | 7.16677 |
| Au 23.4707 | 5.08154 | 7.16477 |
| Au 19.0704 | 12.7036 | 7.16591 |
| Au 14.6683 | 20.3253 | 7.16526 |
| Au 1.46773 | 7.62167 | 7.16667 |
| Au -2.9345 | 15.2443 | 7.16584 |
| Au -7.3347 | 22.8668 | 7.16498 |
| Au 10.2674 | 7.61694 | 7.15956 |
| Au 5.87499 | 15.2449 | 7.15805 |
| Au 1.46703 | 22.8653 | 7.16595 |
| Au 19.0694 | 7.62255 | 7.16556 |
| Au 14.6714 | 15.2456 | 7.1654 |
| Au 10.2684 | 22.8656 | 7.16508 |
| Au 4.40101 | 2.54139 | 7.16528 |
| Au 0.0001115 | 10.1624 | 7.16661 |
| Au -4.40129 | 17.785 | 7.16548 |
| Au 13.2023 | 2.53954 | 7.16589 |
| Au 8.79791 | 10.1676 | 7.16015 |
| Au 4.40005 | 17.789 | 7.15916 |
| Au 22.0034 | 2.54006 | 7.16484 |
| Au 17.6045 | 10.1635 | 7.16568 |
| Au 13.2021 | 17.7845 | 7.16643 |
| Au 2.93503 | 5.08242 | 7.16571 |
| Au -1.46779 | 12.7032 | 7.16722 |
| Au -5.86778 | 20.326 | 7.16503 |
| Au 11.7354 | 5.07745 | 7.16447 |
| Au 7.33383 | 12.7037 | 7.16934 |
| Au 7.29133 | 12.65 | 12.9441 |
| Au 2.93339 | 20.3261 | 7.16729 |
| Au 20.5363 | 5.0815 | 7.16493 |
| Au 16.1395 | 12.7053 | 7.16435 |
| Au 11.7347 | 20.3243 | 7.16576 |
| Au -1.46583 | 7.62279 | 7.16553 |
| Au -5.86714 | 15.2441 | 7.16554 |
| Au -10.2686 | 22.8666 | 7.16482 |
| Au  | 7.33428 | 7.61971 | 7.1615 |
| Au  | 2.92837 | 15.2472 | 7.1581 |
| Au  | -1.46651 | 22.8659 | 7.16559 |
| Au  | 16.1366 | 7.6218 | 7.16603 |
| Au  | 11.7377 | 15.246 | 7.16128 |
| Au  | 7.33432 | 22.8651 | 7.16547 |
| Au  | 1.4672 | 2.54084 | 7.1647 |
| Au  | -2.93283 | 10.1635 | 7.1607 |
| Au  | -7.33469 | 17.7851 | 7.1651 |
| Au  | 10.2684 | 2.54007 | 7.16622 |
| Au  | 5.86421 | 10.1661 | 7.16415 |
| Au  | 1.46457 | 17.788 | 7.16504 |
| Au  | 19.0695 | 2.53989 | 7.16492 |
| Au  | 14.6747 | 10.164 | 7.16283 |
| Au  | 10.2689 | 17.7837 | 7.16678 |
| Au  | 0.000773241 | 5.08158 | 7.16502 |
| Au  | -4.39989 | 12.7036 | 7.16601 |
| Au  | -8.8018 | 20.3259 | 7.16489 |
| Au  | 8.80154 | 5.07879 | 7.16532 |
| Au  | 4.4051 | 12.6968 | 7.15798 |
| Au  | -0.000187925 | 20.326 | 7.16615 |
| Au  | 17.6024 | 5.08145 | 7.16547 |
| Au  | 13.206 | 12.7069 | 7.15968 |
| Au  | 8.80175 | 20.3252 | 7.16668 |
| Au  | 4.40272 | 7.62179 | 7.16636 |
| Au  | -0.00438822 | 15.2448 | 7.16479 |
| Au  | -4.40063 | 22.8666 | 7.16521 |
| Au  | 13.2038 | 7.61645 | 7.16289 |
| Au  | 8.79726 | 15.2462 | 7.16347 |
| Au  | 4.40037 | 22.865 | 7.16599 |
| Au  | 26.4038 | -0.000722357 | 7.16476 |
| Au  | 22.0039 | 7.62253 | 7.1649 |
| Au  | 17.6035 | 15.2445 | 7.16617 |
| Au  | -1.46689 | 5.92838 | 4.79085 |
| Au  | -5.86757 | 13.5506 | 4.79085 |
| Au  | -10.2683 | 21.1728 | 4.79085 |
| Au  | 7.33446 | 5.92838 | 4.79085 |
| Au  | 2.93379 | 13.5506 | 4.79085 |
| Au  | -1.46689 | 21.1728 | 4.79085 |
| Au  | 16.1358 | 5.92838 | 4.79085 |
| Au  | 11.7351 | 13.5506 | 4.79085 |
| Au  | 7.33446 | 21.1728 | 4.79085 |
| Au  | 7.33446 | 0.846911 | 4.79085 |
| Au  | 2.93379 | 8.46911 | 4.79085 |
| Au  | -1.46689 | 16.0913 | 4.79085 |
| Au  | 16.1358 | 0.846911 | 4.79085 |
| Au  | 11.7351 | 8.46911 | 4.79085 |
| Au  | 7.33446 | 16.0913 | 4.79085 |
| Au  | 24.9372 | 0.846911 | 4.79085 |
| Au  | 20.5365 | 8.46911 | 4.79085 |
| Au  | 16.1358 | 16.0913 | 4.79085 |
| Au  | 5.86757 | 3.38764 | 4.79085 |
| Au  | -1.46689 | 11.0098 | 4.79085 |
| Au  | -2.93379 | 18.632 | 4.79085 |
| Au  | 14.6689 | 3.38764 | 4.79085 |
| Au  | 10.2683 | 11.0098 | 4.79085 |
| Au  | 5.86757 | 18.632 | 4.79085 |
| Au  | 23.4703 | 3.38764 | 4.79085 |
| Au  | 19.0696 | 11.0098 | 4.79085 |
| Au  | 14.6689 | 18.632 | 4.79085 |
| Au   | 16.1358 | 4.23456 | 2.39543 |
|------|---------|---------|---------|
| Au   | 11.7351 | 11.8568 | 2.39543 |
| Au   | 7.33446 | 19.479  | 2.39543 |
| Au   | -2.93379| 6.77529 | 2.39543 |
| Au   | -7.33447| 14.3975 | 2.39543 |
| Au   | -11.7351| 22.0197 | 2.39543 |
| Au   | 5.86757 | 6.77529 | 2.39543 |
| Au   | 1.46689 | 14.3975 | 2.39543 |
| Au   | -2.93379| 22.0197 | 2.39543 |
| Au   | 14.6689 | 6.77529 | 2.39543 |
| Au   | 10.2683 | 14.3975 | 2.39543 |
| Au   | 5.86757 | 22.0197 | 2.39543 |
| Au   | 5.86757 | 1.69382 | 2.39543 |
| Au   | 1.46689 | 9.31602 | 2.39543 |
| Au   | -2.93379| 16.9382 | 2.39543 |
| Au   | 14.6689 | 1.69382 | 2.39543 |
| Au   | 10.2683 | 1.69382 | 2.39543 |
| Au   | 5.86757 | 1.69382 | 2.39543 |
| Au   | 1.46689 | 9.31602 | 2.39543 |
| Au   | -2.93379| 16.9382 | 2.39543 |
| Au   | 14.6689 | 1.69382 | 2.39543 |
| Au   | 10.2683 | 1.69382 | 2.39543 |
| Au   | 5.86757 | 1.69382 | 2.39543 |
| Au   | -4.40068| 19.479  | 2.39543 |
| Au   | 13.202 | 4.23456 | 2.39543 |
| Au   | 8.80136 | 11.8568 | 2.39543 |
| Au   | 4.40068 | 19.479  | 2.39543 |
| Au   | 22.0034 | 4.23456 | 2.39543 |
| Au   | 17.6027 | 11.8568 | 2.39543 |
| Au   | 13.202 | 19.479  | 2.39543 |
| Au   | 2.93379 | 6.77529 | 2.39543 |
| Au   | -1.46689| 14.3975 | 2.39543 |
| Au   | -5.86757| 22.0197 | 2.39543 |
| Au   | 11.7351 | 6.77529 | 2.39543 |
| Au   | 7.33447 | 14.3975 | 2.39543 |
| Au   | 2.93379 | 22.0197 | 2.39543 |
| Au   | 20.5365 | 6.77529 | 2.39543 |
| Au   | 16.1358 | 14.3975 | 2.39543 |
| Au   | 11.7351 | 22.0197 | 2.39543 |
| Au   | 2.93379 | 1.69382 | 2.39543 |
| Au   | -1.46689| 9.31602 | 2.39543 |
| Au   | -5.86757| 16.9382 | 2.39543 |
| Au   | 11.7351 | 6.77529 | 2.39543 |
| Au   | 7.33447 | 9.31602 | 2.39543 |
| Au   | 2.93379 | 16.9382 | 2.39543 |
| Au   | 20.5365 | 6.77529 | 2.39543 |
| Au   | 16.1358 | 14.3975 | 2.39543 |
| Au   | 11.7351 | 16.9382 | 2.39543 |
| Au   | 1.46689 | 4.23456 | 2.39543 |
| Au   | -2.93379| 11.8568 | 2.39543 |
| Au   | -7.33447| 19.479  | 2.39543 |
| Au   | 10.2683 | 4.23456 | 2.39543 |
| Au   | 5.86757 | 11.8568 | 2.39543 |
| Au   | 1.46689 | 19.479  | 2.39543 |
| Au   | 19.0696 | 4.23456 | 2.39543 |
| Au   | 14.6689 | 11.8568 | 2.39543 |
| Au   | 10.2683 | 19.479  | 2.39543 |
| Au   | 0.677529| 2.39543 |
| Au   | -4.40068| 14.3975 | 2.39543 |
| Au   | -8.80136| 22.0197 | 2.39543 |
Optimized structure of Au(NHC2)₂ in xyz format (Å)
Au -1.46662 4.23464 9.57464
Au -5.86902 11.8565 9.57627
Au -10.2695 19.4781 9.5753
Au 7.33541 4.23788 9.57872
Au 2.92407 11.8586 9.55249
Au -1.46678 19.4785 9.57828
Au 16.1348 4.23398 9.57696
Au 11.7371 11.8574 9.54017
Au 7.33221 19.4767 9.58405
Au -2.93353 6.77506 9.57451
Au -7.33682 14.3966 9.57626
Au -11.7359 22.0189 9.57478
Au 5.8687 6.7769 9.58336
Au 1.46028 14.3933 9.56021
Au -2.93449 22.0198 9.57514
Au 14.6697 6.7738 9.58313
Au 10.2591 14.4059 9.54269
Au 5.86718 22.0177 9.57763
Au 5.86734 1.69441 9.57519
Au 1.46738 9.31763 9.58422
Au -2.93422 16.9371 9.57825
Au 14.6677 1.69426 9.57617
Au 10.2701 9.31389 9.53953
Au 5.85927 16.945 9.55279
Au 23.4697 1.69263 9.57481
Au 19.0691 9.31601 9.57724
Au 14.6658 16.9353 9.57885
Au 4.40157 4.23574 9.57688
Au -0.00373229 11.8557 9.58666
Au -4.40122 19.4786 9.57432
Au 13.2011 4.23714 9.57978
Au 8.79939 11.8575 9.59008
Au 4.3982 19.4809 9.58652
Au 22.0029 4.23417 9.57372
Au 17.6 11.8554 9.58011
Au 13.2007 19.4767 9.57705
Au 2.93514 6.77721 9.57923
Au -1.46987 14.3966 9.5841
Au -5.86834 22.0198 9.57461
Au 11.7341 6.77556 9.58132
Au 7.33421 14.3958 9.57304
Au 2.93284 22.0191 9.57886
Au 20.5357 6.77518 9.57411
Au 16.1325 14.3959 9.58118
Au 11.7344 22.0178 9.57539
Au 2.93357 1.69388 9.57457
Au -1.46605 9.31554 9.57792
Au -5.86873 16.9379 9.57503
Au 11.7344 1.6955 9.57623
Au 7.32288 9.31852 9.54868
Au 2.93302 16.9433 9.56117
Au 20.5359 1.69254 9.57459
Au 16.1369 9.31508 9.58296
Au 11.7331 16.9358 9.58322
Au 1.46765 4.23505 9.57515
Au -2.93456 11.8562 9.57912
Au -7.33565 19.4786 9.57463
Au 10.2677 4.23794 9.58085
Au 5.86874 11.8563 9.5721
Au 1.46541 19.4796 9.58411
Au 19.0685 4.23412 9.57408
Au 14.6685 11.8572 9.57779
Au 10.2662 19.4755 9.57936
Au 0.00123279 6.77594 9.58155
Au 3.9994 14.397 9.51172
Au -0.000917987 22.0201 9.57729
Au 17.6013 6.77538 9.57742
Au 13.1985 14.3944 9.5813
Au 8.80052 22.0172 9.57628
Au -0.000642269 1.69527 9.57552
Au 17.6019 1.69291 9.57499
Au 13.2085 10.163 7.16525
Au 7.3342 10.1595 7.15528
Au 7.3342 5.08124 7.16507
Au 16.1352 10.163 7.16525
Au 13.1985 5.08124 7.16507
Au 8.79831 5.08124 7.16507
Au 4.39697 10.1621 7.16706
Au -4.40178 17.7848 7.1657
Au 13.2019 17.7851 7.16686
Au 2.93423 22.8666 7.16633
Au -1.46943 12.7033 7.16781
Au -5.86811 20.3259 7.16507
| Au  | 16.1358 16.0913 4.79085 |
|-----|------------------------|
| Au  | 5.86757 3.38764 4.79085 |
| Au  | 1.46689 11.0098 4.79085 |
| Au  | -2.93379 18.632 4.79085 |
| Au  | 14.6689 3.38764 4.79085 |
| Au  | 10.2683 11.0098 4.79085 |
| Au  | 5.86757 18.632 4.79085 |
| Au  | 23.4703 3.38764 4.79085 |
| Au  | 19.0696 11.0098 4.79085 |
| Au  | 14.6689 18.632 4.79085 |
| Au  | 4.40068 5.92838 4.79085 |
| Au  | -4.9788e-08 13.5506 4.79085 |
| Au  | -4.40068 21.1728 4.79085 |
| Au  | 13.202 5.92838 4.79085 |
| Au  | 8.80136 13.5506 4.79085 |
| Au  | 4.40068 21.1728 4.79085 |
| Au  | 22.0034 5.92838 4.79085 |
| Au  | 17.6027 13.5506 4.79085 |
| Au  | 13.202 21.1728 4.79085 |
| Au  | 4.40068 0.846911 4.79085 |
| Au  | -4.9788e-08 8.46911 4.79085 |
| Au  | -4.40068 16.0913 4.79085 |
| Au  | 13.202 0.846911 4.79085 |
| Au  | 8.80136 8.46911 4.79085 |
| Au  | 4.40068 16.0913 4.79085 |
| Au  | 22.0034 0.846911 4.79085 |
| Au  | 17.6027 8.46911 4.79085 |
| Au  | 13.202 16.0913 4.79085 |
| Au  | 2.93379 3.38764 4.79085 |
| Au  | -1.46689 11.0098 4.79085 |
| Au  | -5.86757 18.632 4.79085 |
| Au  | 11.7351 3.38764 4.79085 |
| Au  | 7.33447 11.0098 4.79085 |
| Au  | 2.93379 18.632 4.79085 |
| Au  | 20.5365 3.38764 4.79085 |
| Au  | 16.1358 11.0098 4.79085 |
| Au  | 11.7351 18.632 4.79085 |
| Au  | 1.46689 5.92838 4.79085 |
| Au  | -2.93379 13.5506 4.79085 |
| Au  | -7.33447 21.1728 4.79085 |
| Au  | 10.2683 5.92838 4.79085 |
| Au  | 5.86757 13.5506 4.79085 |
| Au  | 1.46689 21.1728 4.79085 |
| Au  | 19.0696 5.92838 4.79085 |
| Au  | 14.6689 3.38764 4.79085 |
| Au  | 4.40068 11.0098 4.79085 |
| Au  | -8.80136 18.632 4.79085 |
| Au  | 8.80136 3.38764 4.79085 |
| Au  | 4.40068 11.0098 4.79085 |
Optimized structure of Au(NHC3)$_2$ in xyz format (Å)

Au -1.46645 4.23414 9.5745
Au -5.86963 11.8567 9.57561
Au -10.2692 19.477 9.5753
Au 7.33473 4.23593 9.57689
Au 2.93475 11.8706 9.52223
Au -1.46644 19.4783 9.57892
Au 16.1338 4.23615 9.57666
Au 11.7269 11.857 9.55389
Au 7.3365 19.483 9.56138
Au -2.93388 6.77556 9.57422
Au -7.33599 14.3964 9.5761
Au -11.7353 22.0182 9.57461
Au 5.87139 6.77976 9.58184
Au 1.46163 14.3991 9.57376
Au -2.93365 22.0198 9.57519
Au 14.667 6.77735 9.5815
Au 10.2471 14.3963 9.55263
Au 5.86713 22.0196 9.57696
Au 5.86819 1.69438 9.57521
Au 1.46424 9.31196 9.56235
Au -2.93335 16.9378 9.57889
Au 14.668 1.69543 9.57541
Au 10.2647 9.32198 9.55479
Au 5.8566 16.9279 9.52353
Au 23.4709 1.69366 9.57455
Au 19.067 9.31667 9.57696
Au 14.6658 16.9359 9.57689
Au 4.40259 4.23749 9.57723
Au -0.0030359 11.8567 9.57715
Au -4.40057 19.4784 9.57534
Au 13.2009 4.2394 9.57975
Au 8.79407 11.8585 9.61042
Au 4.3991 19.4812 9.57593
Au 22.0032 4.23474 9.57375
Au 17.5981 11.855 9.58042
Au 13.2001 19.4752 9.57773
Au 2.93715 6.77906 9.57967
Au -1.4673 14.3978 9.58535
null
| Au   | X    | Y    | Z    |
|------|------|------|------|
| 14.6684 | 20.3248 | 7.16595 |
| 1.46709 | 7.61689 | 7.16279 |
| -2.93431 | 15.2452 | 7.1668 |
| -7.33477 | 22.8661 | 7.16522 |
| 10.2708 | 7.62312 | 7.15821 |
| 5.87309 | 15.2362 | 7.15839 |
| 1.46601 | 22.8672 | 7.16279 |
| 19.0676 | 7.62304 | 7.16577 |
| 14.6747 | 15.2474 | 7.15836 |
| 10.2695 | 22.8667 | 7.16547 |
| 4.40123 | 2.54109 | 7.16581 |
| -0.00272059 | 10.164 | 7.16328 |
| -4.40072 | 17.7849 | 7.16585 |
| 13.2019 | 2.54199 | 7.16634 |
| 8.79775 | 10.1712 | 7.16491 |
| 4.39359 | 17.7892 | 7.15681 |
| 22.0033 | 2.54062 | 7.1648 |
| 17.6014 | 10.163 | 7.16667 |
| 13.2014 | 17.7841 | 7.16601 |
| 2.93568 | 5.08104 | 7.16628 |
| -1.47142 | 12.7063 | 7.16579 |
| -5.8675 | 20.3256 | 7.16513 |
| 11.7359 | 5.08145 | 7.1662 |
| 7.33534 | 12.7038 | 7.17844 |
| 7.43724 | 12.7487 | 12.963 |
| 2.92895 | 20.3282 | 7.16551 |
| 20.5357 | 5.08197 | 7.16486 |
| 16.1367 | 12.7028 | 7.16554 |
| 11.7361 | 20.3241 | 7.16649 |
| -1.46693 | 7.62225 | 7.16521 |
| -5.86725 | 15.2437 | 7.16575 |
| -10.2685 | 22.8663 | 7.16507 |
| 7.33098 | 7.62539 | 7.15852 |
| 2.92782 | 15.2479 | 7.16319 |
| -1.46612 | 22.8663 | 7.16572 |
| 16.1346 | 7.62261 | 7.16763 |
| 11.7297 | 15.2458 | 7.1576 |
| 7.33424 | 22.8664 | 7.16534 |
| 1.46757 | 2.54021 | 7.16524 |
| -2.93468 | 10.164 | 7.166 |
| -7.33425 | 17.7848 | 7.1653 |
| 10.2697 | 2.53937 | 7.16609 |
| 5.86269 | 10.1714 | 7.16249 |
| 1.46233 | 17.7871 | 7.16821 |
| 19.0689 | 2.54078 | 7.16494 |
| 14.6712 | 10.1616 | 7.1672 |
| 10.2675 | 17.7848 | 7.16491 |
| 0.000331181 | 5.08017 | 7.16531 |
| -4.40194 | 12.7038 | 7.1663 |
| -8.80149 | 20.3259 | 7.16518 |
| 8.80168 | 5.07421 | 7.15826 |
| 4.40961 | 12.7029 | 7.15716 |
| -0.00102409 | 20.3257 | 7.16693 |
| 17.6012 | 5.08266 | 7.16572 |
| 13.2019 | 12.6999 | 7.15692 |
| 8.80603 | 20.3285 | 7.16271 |
| 4.40157 | 7.62117 | 7.16495 |
| -0.00410802 | 15.2475 | 7.16811 |
| -4.4003 | 22.8661 | 7.16532 |
| 13.2034 | 7.61976 | 7.16729 |
Au 8.7899 15.2443 7.16408
Au 4.39933 22.8666 7.16508
Au 26.4044 -0.000924468 7.16525
Au 22.0028 7.62282 7.16419
Au 17.6043 15.2436 7.16606
Au -1.46689 5.92838 4.79085
Au -5.86757 13.5506 4.79085
Au -10.2683 21.1728 4.79085
Au 7.33446 5.92838 4.79085
Au 2.93379 13.5506 4.79085
Au -1.46689 21.1728 4.79085
Au 16.1358 5.92838 4.79085
Au 11.7351 13.5506 4.79085
Au 7.33446 21.1728 4.79085
Au 7.33446 0.846911 4.79085
Au 2.93379 8.46911 4.79085
Au -1.46689 16.0913 4.79085
Au 16.1358 0.846911 4.79085
Au 11.7351 8.46911 4.79085
Au 7.33446 16.0913 4.79085
Au 24.9372 0.846911 4.79085
Au 20.5365 8.46911 4.79085
Au 16.1358 16.0913 4.79085
Au 5.86757 3.38764 4.79085
Au 1.46689 11.0098 4.79085
Au -2.93379 18.632 4.79085
Au 14.6689 3.38764 4.79085
Au 10.2683 11.0098 4.79085
Au 5.86757 18.632 4.79085
Au 23.4703 3.38764 4.79085
Au 19.0696 11.0098 4.79085
Au 14.6689 18.632 4.79085
Au 4.40068 5.92838 4.79085
Au -4.9788e-08 13.5506 4.79085
Au -4.40068 21.1728 4.79085
Au 13.202 5.92838 4.79085
Au 8.80136 13.5506 4.79085
Au 4.40068 21.1728 4.79085
Au 22.0034 5.92838 4.79085
Au 17.6027 13.5506 4.79085
Au 13.202 21.1728 4.79085
Au 4.40068 0.846911 4.79085
Au -4.9788e-08 8.46911 4.79085
Au -4.40068 16.0913 4.79085
Au 13.202 0.846911 4.79085
Au 8.80136 8.46911 4.79085
Au 4.40068 16.0913 4.79085
Au 22.0034 0.846911 4.79085
Au 17.6027 8.46911 4.79085
Au 13.202 16.0913 4.79085
Au 2.93379 3.38764 4.79085
Au -1.46689 11.0098 4.79085
Au -5.86757 18.632 4.79085
Au 11.7351 3.38764 4.79085
Au 7.33446 11.0098 4.79085
Au 2.93379 18.632 4.79085
Au 13.202 3.38764 4.79085
Au 8.80136 11.0098 4.79085
Au 4.40068 18.632 4.79085
Au 22.0034 11.0098 4.79085
Au 17.6027 18.632 4.79085
Au 13.202 18.632 4.79085
Au 2.93379 3.38764 4.79085
Au -4.9788e-08 13.5506 4.79085
Au -4.40068 21.1728 4.79085
Au 13.202 5.92838 4.79085
Au 8.80136 13.5506 4.79085
Au 4.40068 21.1728 4.79085
Au 22.0034 5.92838 4.79085
Au 17.6027 13.5506 4.79085
Au 13.202 21.1728 4.79085
Au 4.40068 0.846911 4.79085
Au -4.9788e-08 8.46911 4.79085
Au -4.40068 16.0913 4.79085
Au 13.202 0.846911 4.79085
Au 8.80136 8.46911 4.79085
Au 4.40068 16.0913 4.79085
Au 22.0034 0.846911 4.79085
Au 17.6027 8.46911 4.79085
Au 13.202 16.0913 4.79085
Au 2.93379 3.38764 4.79085
Au -1.46689 11.0098 4.79085
Au -5.86757 18.632 4.79085
Au 11.7351 3.38764 4.79085
Au 7.33446 11.0098 4.79085
Au 2.93379 18.632 4.79085
Au 20.5365 3.38764 4.79085
Au 16.1358 11.0098 4.79085
Au 11.7351 18.632 4.79085
Au 1.46689 5.92838 4.79085
Au -2.93379 13.5506 4.79085
Au -7.33447 21.1728 4.79085
Au 10.2683 5.92838 4.79085
Au 5.86757 13.5506 4.79085
Au 1.46689 21.1728 4.79085
Au 19.0696 5.92838 4.79085
Au 14.6689 13.5506 4.79085
Au 10.2683 21.1728 4.79085
Au 1.46689 0.846911 4.79085
Au 8.40668 8.46911 4.79085
Au 5.86757 13.5506 4.79085
Au 1.46689 21.1728 4.79085
Au 19.0696 5.92838 4.79085
Au 14.6689 8.46911 4.79085
Au 10.2683 16.0913 4.79085
Au 1.46689e-08 3.38764 4.79085
Au -4.40068 11.0098 4.79085
Au -8.80136 18.632 4.79085
Au 8.80136 3.38764 4.79085
Au 4.40068 11.0098 4.79085
Au 2.4894e-08 18.632 4.79085
Au 17.6027 3.38764 4.79085
Au 13.202 11.0098 4.79085
Au 8.80136 18.632 4.79085
Au -1.46689 4.23456 2.39543
Au -5.86757 11.8568 2.39543
Au -10.2683 19.479 2.39543
Au 7.33446 4.23456 2.39543
Au 2.93379 11.8568 2.39543
Au -1.46689 19.479 2.39543
Au 16.1358 4.23456 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
Au -7.33447 14.3975 2.39543
Au -11.7351 22.0197 2.39543
Au 5.86757 6.77529 2.39543
Au 1.46689 14.3975 2.39543
Au -2.93379 22.0197 2.39543
Au 14.6689 11.8568 2.39543
Au 10.2683 14.3975 2.39543
Au 5.86757 22.0197 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
Au -7.33447 14.3975 2.39543
Au -11.7351 22.0197 2.39543
Au 5.86757 6.77529 2.39543
Au 1.46689 14.3975 2.39543
Au -2.93379 22.0197 2.39543
Au 14.6689 11.8568 2.39543
Au 10.2683 14.3975 2.39543
Au 5.86757 22.0197 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
Au -7.33447 14.3975 2.39543
Au -11.7351 22.0197 2.39543
Au 5.86757 6.77529 2.39543
Au 1.46689 14.3975 2.39543
Au -2.93379 22.0197 2.39543
Au 14.6689 11.8568 2.39543
Au 10.2683 14.3975 2.39543
Au 5.86757 22.0197 2.39543
Au 11.7351 11.8568 2.39543
Au 7.33446 19.479 2.39543
Au -2.93379 6.77529 2.39543
| Element | X | Y | Z   |
|---------|---|---|-----|
| Au      | 17.6027 | 11.8568 | 2.39543 |
| Au      | 13.202 | 19.479 | 2.39543 |
| Au      | 2.93379 | 6.77529 | 2.39543 |
| Au      | -1.46689 | 14.3975 | 2.39543 |
| Au      | -5.86757 | 22.0197 | 2.39543 |
| Au      | 11.7351 | 6.77529 | 2.39543 |
| Au      | 7.33447 | 14.3975 | 2.39543 |
| Au      | 2.93379 | 22.0197 | 2.39543 |
| Au      | 20.5365 | 6.77529 | 2.39543 |
| Au      | 16.1358 | 14.3975 | 2.39543 |
| Au      | 11.7351 | 22.0197 | 2.39543 |
| Au      | 2.93379 | 1.69382 | 2.39543 |
| Au      | -1.46689 | 9.31602 | 2.39543 |
| Au      | -5.86757 | 16.9382 | 2.39543 |
| Au      | 11.7351 | 1.69382 | 2.39543 |
| Au      | 7.33447 | 9.31602 | 2.39543 |
| Au      | 2.93379 | 16.9382 | 2.39543 |
| Au      | 20.5365 | 1.69382 | 2.39543 |
| Au      | 16.1358 | 9.31602 | 2.39543 |
| Au      | 11.7351 | 16.9382 | 2.39543 |
| Au      | 1.46689 | 4.23456 | 2.39543 |
| Au      | -2.93379 | 11.8568 | 2.39543 |
| Au      | -7.33447 | 19.479 | 2.39543 |
| Au      | 10.2683 | 4.23456 | 2.39543 |
| Au      | 5.86757 | 11.8568 | 2.39543 |
| Au      | 1.46689 | 19.479 | 2.39543 |
| Au      | 19.0696 | 4.23456 | 2.39543 |
| Au      | 14.6689 | 11.8568 | 2.39543 |
| Au      | 10.2683 | 19.479 | 2.39543 |
| Au      | 0.677529 | 2.39543 |
| Au      | -4.40068 | 14.3975 | 2.39543 |
| Au      | -8.80136 | 22.0197 | 2.39543 |
| Au      | 8.80136 | 6.77529 | 2.39543 |
| Au      | 4.40068 | 14.3975 | 2.39543 |
| Au      | 0.220197 | 2.39543 |
| Au      | 17.6027 | 6.77529 | 2.39543 |
| Au      | 13.202 | 14.3975 | 2.39543 |
| Au      | 8.80136 | 22.0197 | 2.39543 |
| Au      | 0.169382 | 2.39543 |
| Au      | -4.40068 | 9.31602 | 2.39543 |
| Au      | -8.80136 | 16.9382 | 2.39543 |
| Au      | 8.80136 | 1.69382 | 2.39543 |
| Au      | 4.40068 | 9.31602 | 2.39543 |
| Au      | 0.169382 | 2.39543 |
| Au      | 17.6027 | 1.69382 | 2.39543 |
| Au      | 13.202 | 9.31602 | 2.39543 |
| Au      | 8.80136 | 16.9382 | 2.39543 |
| C       | 5.63984 | 13.7293 | 13.0709 |
| C       | 4.11622 | 15.3787 | 13.1048 |
| C       | 3.43289 | 14.1459 | 13.0968 |
| C       | 4.27279 | 11.6955 | 13.3371 |
| C       | 6.62968 | 15.9625 | 13.3937 |
| N       | 4.41124 | 13.1557 | 13.0992 |
| N       | 5.47358 | 15.0743 | 13.1115 |
| C       | 4.4738 | 11.404 | 14.8223 |
| H       | 3.68169 | 11.8702 | 15.4164 |
| H       | 5.43838 | 11.7762 | 15.1746 |
| H       | 4.4364 | 10.3252 | 14.9962 |
| H       | 2.70289 | 11.4726 | 11.8407 |
| H       | 3.1132 | 10.0101 | 12.7203 |
H 2.14122 11.2494 13.5163
H 5.10154 11.2636 12.7635
C 2.97763 11.0886 12.8314
C 6.89604 15.9779 14.8969
H 7.78347 16.5798 15.1102
H 7.49816 17.8082 12.7492
H 5.90663 18.0242 13.4804
H 6.06614 17.3727 11.8317
H 7.06362 14.9694 15.2821
H 6.0508 16.4201 15.4332
C 6.50162 17.3691 12.8391
H 7.46106 15.4644 12.8807
C 3.41966 16.5866 13.0395
C 2.03949 14.1016 13.025
H 3.92641 17.5401 13.0124
H 1.49545 13.1695 12.9875
C 2.03598 16.5304 12.9674
C 1.35696 15.307 12.9608
H 1.47368 17.4547 12.8867
H 0.275476 15.2963 12.8761
C 9.24046 11.7656 13.0161
C 10.762 10.1154 13.0695
C 11.4475 11.3487 13.0557
C 10.6012 13.8099 13.2337
C 8.23644 9.53481 13.3125
N 10.4693 12.3396 13.0462
N 9.40519 10.4206 13.0681
C 10.2401 14.1744 14.6723
H 10.9592 13.7364 15.3715
H 9.23944 13.8227 14.9334
H 10.2661 15.2607 14.7941
H 12.3242 14.0253 11.9025
H 11.8448 15.4726 12.7662
H 12.7091 14.2046 13.6354
H 9.85176 14.2271 12.5481
C 11.955 14.39 12.8662
C 7.84545 9.6074 14.7869
H 6.94341 9.01396 14.959
H 7.42879 7.63296 12.7866
H 8.98978 7.50556 13.5954
H 8.88745 8.00956 11.889
H 7.64433 10.6358 15.0954
H 8.64329 9.20236 15.417
C 8.41671 8.0922 12.8729
H 7.44436 9.98514 12.7013
C 11.458 8.90687 13.0185
C 12.8421 11.3886 12.9968
H 10.9512 7.9539 12.9942
H 13.3889 12.3183 12.9571
C 12.8414 8.95984 12.9497
C 13.5225 10.1823 12.9419
H 13.4023 8.03388 12.8793
H 14.6044 10.191 12.8633