Supporting Information

Dynamic Interconversions of Single Molecules Probed by Recognition Tunneling at Cucurbit[7]uril-Functionalized Supramolecular Junctions

B. Xiao, S. He, M. Sun, J. Zhou, Z. Wang, Y. Li, S. Liu*, W. M. Nau*, S. Chang*
Table of Contents

S1 Recognition tunneling method
S2 Conductance measurements in dependence on CPT concentration
S3 Typical tunneling traces recorded at different pH values
S4 Two-dimensional histograms of CB7---CPT---CB7 junctions at different pH values
S5 Conductance distribution of CB7---CPT---CB7 junctions at different pH values
S6 Binding of CB7 to camptothecin
S7 DFT calculations for CB7---CPT---CB7 junctions
S8 Binding of CB7 to sanguinarine
S9 Binding of CB7 to chelerythrine
S10 Repeated release and binding studies of CPT at the supramolecular junctions
S11 Summary of analyte affinities to CB7 and their molecular conductance values at the supramolecular junctions
S12 Cartesian coordinates of the isolated CPT structures and the CB7---CPT junctions obtained by the DFT calculations
S1. Recognition tunneling method

Preparation of test solutions. Cucurbit[7]uril (CB7) was prepared according to the reported procedure\textsuperscript{1}. Camptothecin (CPT), sanguinarine (SA), chelerythrine (CHE), and berberine (BE) were purchased from Sigma Aldrich and used without further purification. Owing to the moderate solubility of CPT, SA and CHE, stock solutions of 5 mM were prepared in DMSO in order to allow the titration experiments. 0.5 mL of the CPT stock solution was added to Milli-Q water at the desired pH (adjusted with HCl\textsubscript{aq} and NaOH\textsubscript{aq}) and the solution was subsequently sonicated for 10 min to ensure rapid mixing. Test solutions of the other analytes were prepared accordingly.

Figure S1. (a). Control current traces at $G_B = 50$ pS and 20 pS showing a clean background and low electronic noise. b-d. Negative control experiments (without current switching signals) carried out under different experimental conditions, namely (b) with both electrodes non-functionalized, (c) a single electrode functionalized, and (d) without target molecules. (e) Typical recognition tunneling measurement with both electrodes functionalized and the target molecules (CPT, as an example) added. Distinctive current spikes are frequently observed in the current-time traces.

Tunneling measurements. The preparation and chemical modification of the STM tip and the substrate has been described in our previous work.\textsuperscript{2} The conductance measurements were performed at ambient temperature on a Keysight 6500 instrument. Before the conductance experiment, the distance between STM tip and substrate was adjusted to maintain a gap of set-point = 4 pA and the instrument was warmed up for 2 hours to stabilize the tip. All tunneling traces were collected at a bias of 0.2 V with a sampling rate of 10 kHz. A blank control experiment (without CB7 reader molecules) was performed with the HDPE-coated tip for a leakage test. The low-noise level in the tunneling traces at $G_B = 50$ pS (Noise = 2 pA) and 20 pS (Noise = 1 pA) indicated that the insulation probe is capable of single-molecule electronic detection (Figure S1a). In addition, we carried out control experiments in the STM studies, as shown in Figure S1 b-d. No current switching signals are generated when the electrodes are not functionalized (b) or only one electrode is functionalized (c), or when no target molecules are present (d). The current jump signals only appear when both electrodes are functionalized with CB7 and the target molecule is present in solution. Statistical analysis of the current spikes was automated by using home-built Labview programs as described
previously\(^2\). The conductance histograms comprised current spikes extracted from thousands of individual \(I(t)\) traces and the error bars were calculated from the full width at half-maximum (FWHM) of the fitting peaks.

**S2. Conductance measurements in dependence on CPT concentration**

As shown in Figure S2, the conductance peaks at \(G_B = 50\) pS remain unchanged, while the proportion of molecular junction events in \(G_A\) (CB7---CPTH\(^+\)--CB7) and \(G_W\) (CB7---CB7) increases with increasing concentration of CPT. The area of signal counts of \(G_A\) and \(G_W\) are integrated respectively and compared, the ratios of the two areas are listed in Table S1.

![Graphs showing conductance distributions for different CPT concentrations](image)

**Figure S2.** Signal distributions of \(G_W\) and \(G_A\) measured at \(G_B = 50\) pS in acidic solution (pH 2) with concentration of CPT varied from 0.25 mM to 2 mM.

| C\(_{CPT}\) (mM) | Log(\(G/G_0\)) | Area ratio |
|-----------------|----------------|------------|
|                 | \(G_W\)        | \(G_A\) | \(G_W\) | \(G_A\) |
| 0.25            | \(-6.26 \pm 0.29\) | \(-5.77 \pm 0.07\) | 0.82 | 0.18 |
| 0.5             | \(-6.46 \pm 0.25\) | \(-5.80 \pm 0.15\) | 0.54 | 0.46 |
| 1               | \(-6.40 \pm 0.16\) | \(-5.81 \pm 0.08\) | 0.40 | 0.60 |
| 2               | \(-6.21 \pm 0.14\) | \(-5.81 \pm 0.10\) | 0.30 | 0.70 |
S3. Typical tunneling traces recorded at different pH values

![Typical tunneling traces at different pH values](image)

**Figure S3.** Typical current-time traces of CB7---CPT---CB7 junctions obtained from pH 2 to pH 12.

S4. Two-dimensional histograms of CB7---CPT---CB7 junctions at different pH values

The 2D histograms were constructed by overlaying the selected current spikes from hundreds of individual $I(t)$ traces in each experiment over a wide pH range, using bins of 5 ms along the time axis and $10^{0.05} \, G_0$ bins along the conductance axis. We plotted the 2D histogram by setting the origin of the time axis to the start point at which the current suddenly increased and the end until it came back to the set-point current. As can be seen in Figure S4, the counts of constructed histograms decrease with increasing pH value, indicating that the CB7---CPT---CB7 supramolecular junction depletes at high pH. As the solution became less acidic from pH 2 to pH 6, the initially dominant protonated lactone form of CPT gradually converted into the neutral lactone form which bound less strongly to the junction compared to the protonated form. Besides, the proportion of CPT carboxylate form (which interacted only to a negligible extent with CB7) increased concomitantly above pH 6, as observed from the UV-vis absorption and fluorescence spectra (see Section S6), which further minimized the formation probability of the supramolecular junctions. In contrast to the reduction of the events probability, the absolute conductance values increased gradually from pH 2.0 to 7.8, as marked by the blue lines in Figure S4 a-h.
Figure S4. Two-dimensional histograms of CB7--CPT--CB7 junction conductance in aqueous solution of pH 2.0 (a), 3.8 (b), 4.3 (c), 5.0 (d), 6.4 (e), 7.1 (f), 7.4 (g), 7.8 (h). The bin size was 5 ms for the time and $10^{0.05} G_0$ for the conductance.

S5. Conductance distribution of CB7--CPT--CB7 junctions at different pH values
The conductance values at different pH were extracted from the 2D histogram and further constructed 1D conductance histograms (logarithmic bin 200 bins along the conductance axis). Overlaid 1D conductance histograms for CB7--CPT--CB7 junction over pH range of 2.0-7.8 are shown in Figure S5. The conductance histograms suggest that the conductance increases slowly from pH 2.0 to 4.3 and rises up rapidly from pH 6.4 to 7.8.

Figure S5. pH-dependent conductance distribution histograms and the corresponding Gaussian fittings for the CB7--CPT--CB7 peaks at each pH value.
Table S2. CB7--CPT--CB7 junction conductance parameters at different pH values

| pH | Conductance ($\times 10^{-7} G_0$) | Peak width ($\times 10^{-7} G_0$) |
|----|----------------------------------|-------------------------------|
| 2.0| 3.56                             | 1.04                          |
| 3.8| 3.98                             | 1.25                          |
| 4.3| 3.93                             | 1.05                          |
| 5.0| 4.59                             | 1.29                          |
| 6.4| 6.35                             | 1.70                          |
| 7.1| 6.91                             | 1.72                          |
| 7.4| 7.79                             | 1.76                          |
| 7.8| 7.81                             | 1.75                          |

S6. Binding of CB7 to camptothecin

Previous studies on CPT revealed its structural changes with the pH of the solution, which largely increases the complexity of the CB7•CPT binding system. Douhal et al. reported a pKₐ value of 1.85 for the excited-state of CPT.³ Meanwhile, Hazra et al. obtained a pKₐ value of 1.18 for CPT in the ground-state; they also found that a large excess of CB7 in solution can shift the pKₐ of CPT to 6.8 and 6.2, respectively, at the excited and the ground state.⁴ It was assumed that by forming a 1:2 complex with CB7, the protonation of the quinoline nitrogen became easier, possibly because the electron density is enriched by trapping between the portals of two CB7 hosts.⁴ As the pH rises, the carboxylate form of CPT gradually takes over the lactone form, and, as a result, the pharmacological activity of CPT is diminished. Above pH 8, CPT exists mostly in its carboxylate form.⁵ Dong et al. studied the binding behavior of CPT and CB7 at pH 2,⁶ and confirmed the formation of a 1:2 complex, as had been observed by Hazra near neutral pH. However, experimental structural information on the 1:2 complex remains elusive. Nonetheless, the 1:1 complex prevails in solution if CB7 and CPT are employed in low concentrations. This allowed us to use a 1:1 binding model in the fitting, the obtained binding constant is $8.4 \times 10^5$ M⁻¹ and $7.9 \times 10^5$ M⁻¹, respectively, from UV-vis and fluorescence titration. The increasing absorption at 407 nm as well as emission at 515 nm refers to the growing fraction of the protonated form, which is induced by encapsulation within CB7 (Figure S6).¹¹ H NMR studies of CPT and CB7 in D₂O revealed an upfield shift of the quinoline ring protons, while the protons on the other rings shifted downfield, indicating a preferential immersion of the quinoline ring inside the CB7 cavity while the other part of the drug molecule remains positioned outside the cavity⁶. This ¹¹ H NMR shift pattern corresponds better to a partial 1:1 inclusion complex than to a 2:1 inclusion complex, such that the second CB7 macrocycle interacts likely very weakly, and more superficially with CPT. At basic pH
values, we found no shift of the $^1$H NMR peaks of CPT upon addition of 2 equiv. of CB7, suggesting the absence of detectable binding; this is in line with the spectroscopic titration results (see Figures S6 and S7). We were not able to measure the $^1$H NMR in acidic D$_2$O, because the solubility of CPT was too low in this medium.

Figure S6. UV-vis and fluorescence spectra of CPT at pH 2. a. UV-vis spectral changes caused by gradual addition of up to 12 μM CB7 into a 3 μM CPT solution at pH 2. b. The absorbance at 407 nm was plotted against the concentration of CB7 and a binding constant of $(8.4 \pm 0.4) \times 10^5$ M$^{-1}$ was obtained by fitting according to the 1:1 binding model. c. Fluorescence spectra of 3 μM CPT in acidic solution (pH 2) upon addition of up to 12 μM of CB7 (excited at 407 nm). d. The emission intensity at 515 nm was plotted against the concentration of CB7 and a binding constant of $(7.9 \pm 0.7) \times 10^5$ M$^{-1}$ was obtained by fitting according to the 1:1 binding model.

Figure S7. $^1$H NMR spectra of 0.5 mM CPT alone (bottom) and in the presence of 1 mM CB7 (top) dissolved in a solvent mixture of basic D$_2$O (pD 12, 90%) and DMSO-d$_6$ (10%). The chemical shifts of CPT remained the same upon addition of CB7, suggesting no obvious host-guest interaction.
Figure S8. UV-vis absorption and fluorescence spectra (excited at 370 nm) of 3 μM CPT in basic solution (pH 12) in the absence and presence of 23.4 μM CB7. Only minor changes in the absorption and emission spectra were observed in the presence of 8 equiv. of CB7, pointing to no significant interaction.

S7. DFT calculations for CB7—CPT—CB7 junctions

Molecular geometry optimizations were carried out with the Gaussian 09 program by using dispersion-corrected density functional theory (DFT-D3) and the B3LYP functional along with the 6-31G(d,p) basis set. Grimme's D3 empirical dispersion correction with Becke-Johnson damping (GD3BJ) was used. Vibrational frequency analyses were performed for all geometry-optimized structures, confirming the absence of imaginary frequencies, and therefore identifying them as energy minima.

The host-guest complex structures were optimized between two gold electrodes to form molecular devices in the Atomistix-Tool-Kit software. We applied DFT methods within the generalized gradient approximation (GGA) by using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation function to simulate the optimized structures. The single zeta polarized level was used for Au atoms and the double zeta polarized level was adopted for C, H, O, N and Cl atoms based on the linear combination of atomic orbitals (LCAO) basis set approach. The Au electrodes were settled to a 6×6×2 supercell. The isolated organic complexes were optimized and the complexes were inserted between the left and right Au electrodes, and the resulting supramolecular junctions were relaxed until the total free energy reached a minimum. During the relaxation, the force tolerance was set to 0.5 eV/Å. It is worth noting that we placed one adjacent chloride atom in the CB7—CPT—HCl—CB7 system to simulate the effect of protonation (HCl) while maintaining an overall neutral assembly.

First principles calculations were carried out to investigate electronic transport properties. In the series of calculations, the exchange-correlation potential was approximated within the GGA-PBE functional for exchange and correlation effects. A mesh cutoff energy of 75 Hartree and a (1,1,89) k-point mesh within the Monkhorst-Pack scheme were utilized. The single-ζ polarization basis set was used for the gold atoms and the double-ζ polarization functions was used for all other atoms. According to the Landauer formalism,

\[
G = \frac{2e^2}{h} \sum_n T_n,
\]
the conductance $G$ of a supramolecular junction can be calculated, where $e$ is the electron charge, $h$ is Planck’s constant, and $T_n$ is the transmission coefficient of the individual transport channels which describes how effective a molecule performed in scattering an incoming electron from the right lead into the left lead. In this way, the conductance values of the molecule under zero bias voltage were obtained.

As shown in Figure S9, the blue and red arrows show the forward and backward electron transport pathways in the molecular system with the thickness of the arrow representing the absolute transmission magnitudes. The main transmission pathways for both systems are along Au→left CB7→CPT→Au. There is almost no arrow pointing to or from the CB7 molecule that encapsulates the quinoline ring; instead, this macrocycle serves to facilitate direct CPT---Au transmission through the formation of inclusion complexes. Therefore, the computational modelling results account for the experimental observation that the recognition tunneling signals are “switched on” upon addition of CPT, because the CPT is (expectedly, due to its aromatic character) more conductive than the aliphatic macrocyclic host. Secondly, and again in agreement with the experiment, the electron transmission modelling predicts a higher conductance for the neutral junction than for the protonated one, as indicated by the arrows connecting the right Au surface to the junction. This effect is fully consistent with the deeper immersion of the neutral quinoline ring (see Figure 2c), which places it more closely to the Au surface (3.25 versus 4.41 Å, see Figure S9). Counterintuitively, even though the neutral quinoline ring is more deeply immersed into CB7, this does not increase the distance of the lactone group to the second Au surface, but rather decreases it (10.14 and 10.64 Å for the Au-O and Au-C distances for CPT, shorter than in the case of CPTH+ with 10.71 and 10.77 Å), as a consequence of different quinoline protonation-induced tilting angles (also see Figure 2c); this shorter bridging distance for the neutral form may be a second contributor to the increased conductivity.

![Figure S9](image)

**Figure S9.** Electron transmission pathways in the neutral CB7---CPT---CB7 (a) and protonated CB7---CPTH+---CB7 (b) junctions; blue and red arrows indicate the forward and reverse loop current, respectively, and the thickness of the arrows is proportional to local transmission contribution.
S8. Binding of CB7 to sanguinarine

**Figure S10.** $^1$H NMR spectra of 0.5 mM SA alone (bottom) and in the presence of 1 mM CB7 (top) in a solvent mixture of acidic D$_2$O (pD 2, 90%) and DMSO-$d_6$ (10%). The $^1$H NMR spectrum in basic solution could not be recorded due to a poor solubility of the guest.

**Figure S11.** UV-vis absorption spectra of 6 μM SA in the absence and presence of up to 23.4 μM of CB7 in HCl solution (pH 2).

**Figure S12.** Fluorescence spectra of 6 μM SA in the absence and presence of up to 23.4 μM CB7 in HCl solution (pH 2, left), excited at 470 nm. The intensity at 542 nm was plotted against the concentration of CB7 (right) and a binding constant of $(6.1 \pm 0.7) \times 10^5$ M$^{-1}$ was obtained by fitting according to the 1:1 binding model.
Figure S13. UV-vis absorption (left) and fluorescence spectra (right, excited at 326 nm) of 6 μM SA in basic solution (pH 12) in the absence and presence of 23.4 μM of CB7.

S9. Binding of CB7 to chelerythrine

Figure S14. ¹H NMR spectra of 0.5 mM CHE alone (bottom) and in the presence of 1 mM CB7 (top) in DCl (pD 2). The ¹H NMR spectrum in basic solution could not be recorded due to a poor solubility of the guest.

Figure S15. UV-vis absorption spectra of 3 μM CHE in the absence and presence of up to 23.4 μM of CB7 in HCl solution (pH 2).
Figure S16. Fluorescence spectra of 3 μM CHE in the absence and presence of up to 23.4 μM of CB7 in HCl (pH 2, left), excited at 430 nm. The intensity at 535 nm was plotted against the concentration of CB7 (right) and a binding constant of \((1.4 \pm 0.2) \times 10^6 \text{M}^{-1}\) was obtained by fitting according to the 1:1 binding model.

Figure S17. UV-vis absorption (left) and fluorescence spectra (excited at 319 nm, right) of 3 μM CHE in the absence and presence of 23.4 μM of CB7 in basic solution (pH 12).

S10. Repeated release and binding studies of CPT at the supramolecular junctions

We conducted repeated release/binding studies by alternatively adding CPT and salt in the STM measurement cell and monitoring the tunneling current changes, as shown in Fig. S18. The STM gap was set to an initial current of 4 pA \((G_B = 20 \text{ pS})\) and both electrodes were functionalized with CB7. In the first 10 minutes, no current switching signals were observed in the absence of analyte. Once 0.5 mM CPT was added to the system, dramatic jumps occurred in the current and signal frequency (red points) that saturated after ca. 10 minutes. Subsequently, 0.1 M Ca^{2+} was added to the solution and an immediate reduction of the signal frequency (blue points) is seen in the time-resolved signal frequency change, suggesting the effective release of CPT from the supramolecular junction by competitive CB7 portal binding. Subsequently, we rinsed the electrodes with DI water and repeated the measurements by adding CPT and salt alternatively for another two cycles. The repeated release-binding results demonstrate the reversibility of the processes and robustness of the supramolecular junctions.
Figure S18. Repeated release and binding studies of CPT at doubly CB7-functionalized electrodes. The current jump spikes were statistically analyzed every five minutes during the repeated cycles of adding first CPT and subsequently salt. The red points represent the current signal frequency after adding CPT to the STM solution and the blue points denote the signal frequency after adding 0.1 M Ca$^{2+}$ to the measurement solution.

S11. Summary of analyte affinities to CB7 and their molecular conductance values at the supramolecular junctions

The conductance values of all studied molecules at different pH are summarized in Table S3. The $G_A$ values of SA and CHE are the same, within error, as might be expected from their closely related structures, but both display a slightly lower conductance than BE. In contrast to CPT, SA and CHE do not exhibit a change in conductance upon changing from acidic to neutral pH.

Table S3. Summary of the $pK_a$ values of CPT, SA, CHE, and BE, the conductance values ($\log(G_A/G_0)$) at different pH values, and their binding constants with CB7.

| Analyte | Binding constant$^a$ | $pK_a$ | $\log(G_A/G_0)$ | $\log(G_A/G_0)$ | $\log(G_A/G_0)$ |
|---------|---------------------|--------|-----------------|-----------------|-----------------|
|         | $(\times 10^6$ M$^{-1}$) |        | pH 2.0          | pH 7.0          | pH 12           |
| CPT     | 0.84 ± 0.04         | 1.2, −7$^b$ | −6.45 ± 0.25   | −6.10 ± 0.19$^c$ | n.d.$^d$         |
| SA      | 0.61 ± 0.07         | 8.3$^e$ | −6.39 ± 0.25    | −6.40 ± 0.21    | n.d.$^d$         |
| CHE     | 1.4 ± 0.2           | 9.2$^e$ | −6.43 ± 0.30    | −6.42 ± 0.28    | n.d.$^d$         |
| BE      | 24 ± 2$^f$          | -      | −6.19 ± 0.14    | −6.19 ± 0.15    | −6.19 ± 0.14    |

$^a$ Measured by optical titrations, this work, see Supporting Information, Sections S6-S9.
$^b$ Two $pK_a$ values, from ref. 5, 6.
$^c$ Measured at pH 7.8, assigned to the neutral CPT form, see text.
$^d$ No detectable conductance signal.
$^e$ From ref. 7.
$^f$ From ref. 8.
S12. Cartesian coordinates of the isolated CPT structures and the CB7---CPT junctions obtained by the DFT calculations

|     |     |     |     |
|-----|-----|-----|-----|
|     |     |     |     |
| 0   | 9.99268 | 4.18995 | 0.27239 | N | 8.76305 | 5.02791 | 1.60487 |
| 0   | 10.05336 | 2.22144 | 3.5298 | N | 8.82648 | 5.47696 | 0.79179 |
| 0   | 10.06986 | 1.53407 | 3.99252 | N | 8.82012 | 4.67512 | 2.88115 |
| 0   | 10.03625 | 4.22537 | 1.30992 | N | 8.83268 | 2.96141 | 4.60215 |
| 0   | 9.96605 | 3.83645 | 2.48405 | N | 8.78029 | 0.83885 | 5.30286 |
| 0   | 9.91859 | 0.65918 | 4.55673 | N | 8.70775 | 1.53677 | 4.76996 |
| 0   | 9.93206 | 2.9175 | 3.32204 | N | 8.69937 | 3.42776 | 3.57762 |
| 0   | 3.78681 | 4.68441 | 0.53416 | N | 8.71056 | 4.70891 | 1.50711 |
| 0   | 3.80074 | 2.63663 | 3.43432 | N | 8.77992 | 4.95343 | 0.71257 |
| 0   | 3.90843 | 1.32227 | 3.29065 | N | 8.85043 | 4.26908 | 3.039 |
| 0   | 3.85015 | 4.52354 | 0.96128 | N | 8.8983 | 2.69915 | 4.63058 |
| 0   | 3.82732 | 4.3009 | 2.28076 | N | 8.81304 | 0.3325 | 5.19889 |
| 0   | 3.78577 | 0.96331 | 3.73308 | N | 8.79587 | 1.89125 | 4.93373 |
| 0   | 3.79176 | 2.92875 | 2.53916 | N | 6.32088 | 3.72149 | 3.36931 |
| N   | 8.16247 | 5.22997 | 0.6976 | N | 6.30653 | 5.0228 | 1.54936 |
| N   | 8.18947 | 4.95472 | 1.52176 | N | 6.37244 | 5.35652 | 0.85844 |
| N   | 8.20241 | 3.63959 | 3.55799 | N | 6.37579 | 4.89298 | 3.04803 |
| N   | 8.14611 | 1.76177 | 4.76377 | N | 6.38397 | 3.13119 | 4.74015 |
| N   | 8.10204 | 0.67194 | 4.89425 | N | 6.32497 | 0.95294 | 5.23789 |
| N   | 8.11397 | 2.78788 | 4.18008 | N | 6.25219 | 1.43259 | 4.77352 |
| N   | 8.16011 | 4.64925 | 2.60294 | N | 6.27713 | 3.10668 | 3.28203 |
| N   | 8.19957 | 5.40527 | 0.50039 | N | 6.27052 | 4.44644 | 1.26024 |
| N   | 8.15638 | 5.17989 | 1.91248 | N | 6.32816 | 5.12026 | 0.87372 |
| N   | 8.12923 | 4.09671 | 3.87228 | N | 6.39945 | 4.42293 | 3.20851 |
| N   | 7.96917 | 1.90003 | 4.92456 | N | 6.43993 | 2.74216 | 4.68143 |
| N   | 7.92527 | 0.31664 | 5.2421 | N | 6.3614 | 0.41535 | 5.39924 |
| N   | 7.95041 | 2.64194 | 4.50102 | N | 6.3507 | 1.72557 | 4.7491 |
| N   | 8.0229 | 4.19957 | 2.89693 | C | 9.54474 | 4.21878 | 2.42882 |
| N   | 5.70832 | 5.34681 | 0.59059 | C | 9.35225 | 5.77428 | 0.51685 |
| N   | 5.74935 | 5.2639 | 1.63932 | H | 9.22698 | 6.85035 | 0.70993 |
| N   | 5.75151 | 3.88257 | 3.64043 | H | 10.41372 | 5.51745 | 0.49641 |
| N   | 5.69634 | 1.8258 | 4.51078 | C | 9.56462 | 4.74336 | 1.7097 |
| N   | 5.66119 | 0.59137 | 4.63339 | C | 9.4176 | 4.17702 | 4.09793 |
| N   | 5.68139 | 2.69966 | 3.89244 | H | 9.35895 | 4.95556 | 4.87376 |
| N   | 5.71329 | 4.56776 | 2.35365 | H | 10.46233 | 3.95416 | 3.86829 |
| N   | 5.76387 | 5.7371 | 0.45195 | C | 9.54651 | 1.76909 | 4.61737 |
| N   | 5.73315 | 5.59798 | 1.98591 | C | 9.29186 | 0.48486 | 5.56391 |
| N   | 5.67784 | 4.14191 | 3.67934 | H | 10.35813 | 0.46379 | 5.32787 |

15
| Element | X  | Y  | Z  |
|---------|----|----|----|
| H       | 9.1451 | 0.71371 | 6.6304 |
| C       | 9.49495 | 2.34825 | 3.94829 |
| C       | 9.23033 | 4.54491 | 2.84211 |
| H       | 10.30543 | 4.37922 | 2.74617 |
| C       | 9.03861 | 5.46763 | 3.41016 |
| C       | 9.524 | 4.54082 | 0.39227 |
| C       | 5.11706 | 2.00601 |
| H       | 10.4664 | 4.84601 | 1.89347 |
| C       | 9.60233 | 3.22395 | 3.55556 |
| C       | 9.346 | 1.6195 | 5.41878 |
| H       | 10.48493 | 1.51459 | 5.13719 |
| C       | 9.35414 | 1.88302 | 6.4841 |
| C       | 9.57112 | 0.75166 | 4.7501 |
| C       | 9.32342 | 3.2085 | 4.67051 |
| H       | 10.3913 | 3.08841 | 4.47915 |
| C       | 9.17016 | 3.83019 | 5.56973 |
| C       | 7.4861 | 4.55708 | 3.53908 |
| H       | 7.38492 | 5.16435 | 4.45233 |
| C       | 7.51466 | 5.41117 | 2.22744 |
| C       | 7.50952 | 6.4965 | 2.41414 |
| C       | 7.58938 | 5.97394 | 1.33754 |
| H       | 7.53395 | 7.06618 | 1.21214 |
| C       | 7.65026 | 5.52606 | 2.83915 |
| C       | 7.77242 | 6.36644 | 3.59334 |
| C       | 7.63819 | 2.90733 | 5.41282 |
| H       | 7.73339 | 3.59385 | 6.26795 |
| H       | 7.51675 | 1.39754 | 5.8351 |
| C       | 7.52749 | 1.25282 | 6.92571 |
| C       | 7.44254 | 2.15798 | 5.11227 |
| H       | 7.43672 | 2.41974 | 6.1818 |
| H       | 7.3845 | 3.40207 | 4.16878 |
| H       | 7.196 | 4.34587 | 4.70318 |
| H       | 7.43689 | 5.30686 | 1.19281 |
| H       | 7.28014 | 6.19984 | 1.81727 |
| C       | 7.55633 | 5.63061 | 0.33121 |
| H       | 7.64342 | 6.7073 | 0.54397 |
| H       | 7.68623 | 4.56954 | 3.84035 |
| C       | 7.77844 | 5.57726 | 4.27271 |
| C       | 7.68865 | 3.42895 | 4.91955 |
| H       | 7.71669 | 3.80872 | 5.95217 |
| C       | 7.61297 | 0.08941 | 5.89369 |
| C       | 7.70845 | 0.12683 | 6.96883 |
| H       | 7.5346 | 1.61966 | 5.57429 |
| Element | CB7 | CPT (0) | CB7 |
|---------|-----|--------|-----|
| N | 10.01439 | 0.92895 | 4.3712 | N | 8.81468 | 0.25841 | 4.96345 |
| O | 10.02841 | 3.86758 | 1.94777 | O | 8.84394 | 1.94282 | 4.56814 |
| O | 10.10891 | 3.78499 | 1.83403 | O | 8.82231 | 3.84316 | 3.04378 |
| O | 10.20227 | 0.74267 | 4.10823 | O | 8.80716 | 4.81843 | 1.03234 |
| O | 10.22481 | 2.95617 | 3.17588 | O | 8.74727 | 4.85165 | 1.39585 |
| O | 10.16865 | 4.54956 | 0.27199 | O | 8.77564 | 4.02206 | 3.47908 |
| O | 10.076 | 2.81179 | 3.63221 | O | 6.35687 | 1.95063 | 4.81554 |
| O | 3.97504 | 1.06478 | 3.4895 | O | 6.35718 | 0.18482 | 5.48038 |
| O | 3.97484 | 3.95962 | 1.66568 | O | 6.3844 | 2.55808 | 4.91168 |
| O | 4.07248 | 3.73462 | 1.41356 | O | 6.373 | 4.24354 | 3.44055 |
| O | 4.07892 | 0.48151 | 3.4078 | O | 6.27443 | 5.3857 | 1.2925 |
| O | 4.11708 | 3.2955 | 2.8844 | O | 6.27938 | 5.27015 | 0.93921 |
| O | 4.06552 | 4.83299 | 0.05991 | O | 6.31366 | 4.24208 | 3.13671 |
| O | 3.97613 | 2.83735 | 2.81792 | O | 6.31334 | 2.66915 | 4.72576 |
| N | 8.04753 | 0.03041 | 5.21826 | N | 6.36491 | 0.27332 | 5.1866 |
| N | 8.09808 | 2.21082 | 4.72104 | N | 6.3868 | 1.83339 | 4.44037 |
| N | 8.12605 | 4.1499 | 3.24593 | N | 6.36675 | 3.73948 | 2.9377 |
| N | 8.25089 | 5.19498 | 1.26442 | N | 6.35255 | 4.88302 | 1.02316 |
| N | 8.2113 | 4.97398 | 1.16726 | N | 6.29202 | 5.01267 | 1.41071 |
|      |       |       |       |       |       |       |       |       |       |       |       |       |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C    | 5.16226 | 3.08123 | 3.9646 | C    | 6.52086 | 1.48219 | 1.0917 |
| H    | 5.12075 | 3.68079 | 4.88636 | C    | 5.43699 | 0.7138  | 0.62478 |
| H    | 4.15044 | 2.87222 | 3.61157 | C    | 5.53076 | 0.71047 | 0.58412 |
| C    | 5.11655 | 0.62567 | 4.03034 | N    | 4.2754  | 1.31996 | 0.19083 |
| C    | 5.24244 | 1.65589 | 4.93764 | C    | 3.28005 | 0.61482 | 0.34802 |
| H    | 5.2443  | 1.85094 | 6.02055 | C    | 3.36598 | 0.78944 | 0.4804  |
| H    | 4.21556 | 1.62822 | 4.56902 | C    | 4.45872 | 1.45905 | 0.00481 |
| C    | 5.2091  | 3.5351  | 3.36579 | C    | 2.00192 | 1.0726  | 0.85156 |
| C    | 5.47605 | 5.77914 | 2.36805 | N    | 1.34852 | 0.05262 | 1.31899 |
| H    | 5.75088 | 6.71786 | 2.8623  | C    | 2.13202 | 1.28666 | 1.1755  |
| H    | 4.3899  | 5.68338 | 2.32057 | C    | 1.41819 | 2.30886 | 0.90311 |
| C    | 5.18124 | 5.31062 | 0.03054 | C    | 0.10614 | 2.38072 | 1.4411  |
| C    | 5.25009 | 5.37996 | 2.4837  | C    | 0.54301 | 1.2694  | 1.91769 |
| H    | 5.37781 | 6.32219 | 3.03277 | C    | 0.08057 | 0.05139 | 1.90982 |
| H    | 4.19171 | 5.20026 | 2.28453 | O    | 0.40448 | 1.08656 | 2.35541 |
| C    | 5.00946 | 3.10791 | 3.39791 | C    | 0.63443 | 3.6989  | 1.471   |
| C    | 4.98726 | 1.20132 | 4.92504 | C    | 1.52295 | 3.771   | 2.72743 |
| H    | 4.01331 | 1.12453 | 4.43746 | O    | 2.10587 | 2.66406 | 3.17974 |
| H    | 4.85288 | 1.40761 | 5.99887 | C    | 1.92271 | 1.39779 | 2.48899 |
| O    | 10.69558 | 0.91734 | 4.3773  | O    | 1.66293 | 4.83217 | 3.30837 |
| O    | 10.68697 | 2.90127 | 3.36127 | O    | 0.30078 | 4.76218 | 1.55159 |
| O    | 10.6568 | 4.79457 | 0.01577 | C    | 1.5066  | 3.84123 | 0.18999 |
| O    | 10.65292 | 3.1674  | 3.22128 | C    | 2.06304 | 5.25061 | 0.01178 |
| O    | 10.72205 | 0.68784 | 4.01184 | H    | 6.78666 | 2.40608 | 1.02355 |
| O    | 10.72306 | 3.67674 | 1.71066 | H    | 8.67278 | 1.03484 | 1.87853 |
| O    | 10.67399 | 3.79181 | 2.15395 | H    | 8.51768 | 1.43518 | 1.86012 |
| O    | 4.4822  | 0.64048 | 4.38276 | H    | 6.4612  | 2.56269 | 1.07569 |
| O    | 4.45243 | 2.95084 | 3.68133 | H    | 4.50562 | 2.54196 | 0.03927 |
| O    | 4.45032 | 4.42239 | 0.22333 | H    | 1.57194 | 2.03093 | 0.60228 |
| O    | 4.45972 | 2.8481  | 3.3372  | H    | 2.36721 | 1.7175  | 2.15271 |
| O    | 4.49656 | 0.52908 | 4.06489 | H    | 1.93066 | 3.19799 | 0.56811 |
| O    | 4.52266 | 3.54458 | 1.53162 | H    | 2.1256  | 0.62533 | 3.22804 |
| O    | 4.44826 | 3.70881 | 1.96267 | H    | 2.70029 | 1.32741 | 1.7214  |
| N    | 8.80383 | 2.11131 | 4.9987  | H    | 0.11249 | 5.39196 | 2.16921 |
| N    | 8.80484 | 0.11293 | 5.26062 | H    | 2.32826 | 3.12109 | 0.20442 |
| N    | 8.83147 | 2.47736 | 4.70212 | H    | 0.86268 | 3.58413 | 0.65809 |
| N    | 8.82988 | 4.29817 | 3.40144 | H    | 1.25452 | 5.98208 | 0.06208 |
| N    | 8.73126 | 5.34148 | 1.204   | H    | 2.70096 | 5.52562 | 0.85611 |
| N    | 8.71988 | 5.53608 | 1.02779 | H    | 2.65779 | 5.28269 | 0.90373 |
| N    | 8.75535 | 4.51268 | 3.24723 | H    | 4.17007 | 2.33345 | 0.29681 |
| N    | 8.76094 | 2.63359 | 4.46476 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| Au | 1.44188 | 0.83247 | 1.17729 | N | 3.73294 | 7.69995 | 27.34021 |
| Au | 4.32564 | 0.83247 | 1.17729 | C | 4.62026 | 5.4745 | 27.59525 |
| Au | 7.2094 | 0.83247 | 1.17729 | H | 3.97145 | 9.78423 | 27.74 |
| Au | 10.0915 | 0.83247 | 1.17729 | H | 2.31403 | 9.14813 | 27.98245 |
| Au | 12.97691 | 0.83247 | 1.17729 | C | 3.39042 | 8.90869 | 28.09806 |
| Au | 15.86067 | 0.83247 | 1.17729 | C | 4.24822 | 6.69622 | 28.12401 |
| Au | 0 | 3.32988 | 1.17729 | H | 5.03518 | 4.68706 | 28.22906 |
| Au | 2.88376 | 3.32988 | 1.17729 | O | 1.53427 | 11.49827 | 28.865 |
| Au | 5.76752 | 3.32988 | 1.17729 | O | 0.34374 | 7.96252 | 28.85843 |
| Au | 8.65128 | 3.32988 | 1.17729 | O | 1.57586 | 3.99911 | 28.8751 |
| Au | 11.53503 | 3.32988 | 1.17729 | O | 7.3096 | 4.90161 | 28.90462 |
| Au | 14.41879 | 3.32988 | 1.17729 | O | 4.57338 | 2.5208 | 28.91812 |
| Au | -1.44188 | 5.82729 | 1.17729 | O | 4.70687 | 11.94982 | 28.92539 |
| Au | 1.44188 | 5.82729 | 1.17729 | H | -0.07789 | 5.65061 | 28.96711 |
| Au | 4.32564 | 5.82729 | 1.17729 | H | -0.42959 | 10.25618 | 28.97832 |
| Au | 7.2094 | 5.82729 | 1.17729 | O | 7.06193 | 8.90267 | 28.98117 |
| Au | 10.0915 | 5.82729 | 1.17729 | H | 8.38051 | 6.92181 | 29.09863 |
| Au | 12.97691 | 5.82729 | 1.17729 | H | 6.92047 | 11.28031 | 29.1103 |
| Au | -2.88376 | 8.32469 | 1.17729 | H | 2.39418 | 1.70314 | 29.19549 |
| Au | 0 | 8.32469 | 1.17729 | H | 2.87202 | 13.45739 | 29.24082 |
| Au | 2.88376 | 8.32469 | 1.17729 | H | 6.9162 | 2.57184 | 29.23888 |
| Au | 5.76752 | 8.32469 | 1.17729 | C | 4.30188 | 7.19092 | 29.4981 |
| Au | 8.65128 | 8.32469 | 1.17729 | C | 3.76101 | 8.51833 | 29.4974 |
| Au | 11.53503 | 8.32469 | 1.17729 | H | -1.66201 | 5.1296 | 29.71718 |
| Au | -4.32564 | 10.8221 | 1.17729 | C | -0.31904 | 7.92012 | 29.88584 |
| Au | -1.44188 | 10.8221 | 1.17729 | C | -0.62194 | 5.48977 | 29.92487 |
| Au | 1.44188 | 10.8221 | 1.17729 | C | 1.06738 | 3.72104 | 29.95141 |
| Au | 4.32564 | 10.8221 | 1.17729 | C | 1.16645 | 11.79729 | 29.99081 |
| Au | 7.2094 | 10.8221 | 1.17729 | C | -0.80228 | 10.34104 | 30.02288 |
| Au | 10.0915 | 10.8221 | 1.17729 | C | 7.65482 | 9.09679 | 30.03148 |
| Au | -5.76752 | 13.31951 | 1.17729 | C | 7.73087 | 4.78258 | 30.0441 |
| Au | -2.88376 | 13.31951 | 1.17729 | C | 4.94039 | 12.33737 | 30.05951 |
| Au | 0 | 13.31951 | 1.17729 | H | 9.96606 | 6.94693 | 30.01521 |
| Au | 2.88376 | 13.31951 | 1.17729 | H | -1.81932 | 10.80043 | 30.0325 |
| Au | 5.76752 | 13.31951 | 1.17729 | C | 4.63248 | 2.17583 | 30.08981 |
| Au | 8.65128 | 13.31951 | 1.17729 | C | 8.85075 | 6.94883 | 30.10734 |
| Au | 0 | 1.66494 | 3.53187 | C | 7.24762 | 11.5242 | 30.14645 |
| Au | 2.88376 | 1.66494 | 3.53187 | H | 8.07795 | 12.27223 | 30.12498 |
| Au | 5.76752 | 1.66494 | 3.53187 | C | 2.25796 | 1.57729 | 30.29153 |
| Au | 8.65128 | 1.66494 | 3.53187 | C | 7.07365 | 2.42267 | 30.33194 |
| Au | 11.53503 | 1.66494 | 3.53187 | C | 2.83071 | 13.58202 | 30.34499 |
| Au | 14.41879 | 1.66494 | 3.53187 | H | 7.76486 | 1.56514 | 30.51251 |
| Au | -1.44188 | 4.16235 | 3.53187 | H | 1.84771 | 0.56665 | 30.51811 |
| Au  | 1.44188 | 4.16235 | 3.53187 | N  | -0.89195 | 9.0053 | 30.54414 |
| Au  | 4.32564 | 4.16235 | 3.53187 | N  | 4.76659  | 6.52017| 30.53808 |
| Au  | 7.2094  | 4.16235 | 3.53187 | N  | -0.68803 | 6.77091| 30.58902 |
| Au  | 10.09315| 4.16235 | 3.53187 | N  | 0.10957  | 4.47393| 30.64326 |
| Au  | 12.97691| 4.16235 | 3.53187 | H  | 2.68173  | 14.65154| 30.61326 |
| Au  | -2.88376| 6.65975 | 3.53187 | N  | 0.12818  | 11.20836| 30.7104 |
| Au  | 0       | 6.65975 | 3.53187 | N  | 1.29394  | 2.56754| 30.70291 |
| Au  | 2.88376 | 6.65975 | 3.53187 | C  | 3.67743  | 9.18566| 30.70027 |
| Au  | 5.76752 | 6.65975 | 3.53187 | N  | 7.72852  | 10.30335| 30.72931 |
| Au  | 8.65128 | 6.65975 | 3.53187 | N  | 8.43355  | 8.17637| 30.7332 |
| Au  | 11.53503| 6.65975 | 3.53187 | N  | 1.68324  | 12.82265| 30.78217 |
| Au  | -4.32564| 9.15716 | 3.53187 | H  | 3.25697  | 10.19591| 30.78809 |
| Au  | -1.44188| 9.15716 | 3.53187 | N  | 8.41464  | 5.75111| 30.77987 |
| Au  | 1.44188 | 9.15716 | 3.53187 | N  | 6.09541  | 12.10038| 30.80025 |
| Au  | 4.32564 | 9.15716 | 3.53187 | N  | 4.11159  | 13.1413 | 30.84264 |
| Au  | 7.2094  | 9.15716 | 3.53187 | N  | 7.68497  | 3.63055| 30.82727 |
| Au  | 10.09315| 9.15716 | 3.53187 | N  | 3.57477  | 1.70422| 30.86226 |
| Au  | -5.76752| 11.65457| 3.53187 | N  | 5.77504  | 2.11675| 30.8828 |
| Au  | -2.88376| 11.65457| 3.53187 | H  | -2.63611| 6.61627| 31.39449 |
| Au  | 0       | 11.65457| 3.53187 | H  | -1.50284| 3.4123 | 31.51904 |
| Au  | 2.88376 | 11.65457| 3.53187 | C  | -1.64154| 7.05961| 31.64481 |
| Au  | 5.76752 | 11.65457| 3.53187 | H  | -2.68536| 9.06197| 31.63933 |
| Au  | 8.65128 | 11.65457| 3.53187 | C  | -1.65803| 8.62761| 31.70084 |
| Au  | -7.2094 | 14.15198| 3.53187 | H  | 10.22839| 8.69689| 31.70984 |
| Au  | -4.32564| 14.15198| 3.53187 | C  | 4.71015  | 7.19006| 31.726 |
| Au  | -1.44188| 14.15198| 3.53187 | C  | -0.45959| 3.73309| 31.75718 |
| Au  | 1.44188 | 14.15198| 3.53187 | H  | 10.17466| 5.16841| 31.8005 |
| Au  | 4.32564 | 14.15198| 3.53187 | H  | 9.39823  | 11.00683| 31.80075 |
| Au  | 7.2094  | 14.15198| 3.53187 | H  | -1.16157| 12.44798| 31.83781 |
| Au  | 0       | 0       | 5.88645  | C  | 4.1658   | 8.5231 | 31.86173 |
| Au  | 2.88376 | 0       | 5.88645  | C  | 9.12291  | 8.76444| 31.85691 |
| Au  | 5.76752 | 0       | 5.88645  | C  | 8.58928  | 10.24055| 31.88176 |
| Au  | 8.65128 | 0       | 5.88645  | C  | -0.17737| 11.92951| 31.93273 |
| Au  | 11.53503| 0       | 5.88645  | C  | 0.53629  | 2.53398| 31.92325 |
| Au  | 14.41879| 0       | 5.88645  | H  | 6.94299  | 13.67241| 31.9333 |
| Au  | -1.44188| 2.49741 | 5.88645  | C  | 9.0672   | 5.19252| 31.94525 |
| Au  | 1.44188 | 2.49741 | 5.88645  | C  | 6.15136  | 12.88831| 32.01659 |
| Au  | 4.32564 | 2.49741 | 5.88645  | H  | 0.02385  | 1.54636| 32.02923 |
| Au  | 7.2094  | 2.49741 | 5.88645  | C  | 1.03606  | 12.92113| 32.06597 |
| Au  | 10.09315| 2.49741 | 5.88645  | C  | 8.42465  | 3.75952| 32.05453 |
| Au  | 12.97691| 2.49741 | 5.88645  | C  | 4.69675  | 13.48361| 32.11474 |
| Au  | -2.88376| 4.99482 | 5.88645  | H  | 9.18135  | 2.94161| 32.1359 |
| Au  | 0       | 4.99482 | 5.88645  | C  | 3.9823   | 1.24332| 32.16802 |
| Au  | 2.88376 | 4.99482 | 5.88645  | C  | 5.53955  | 1.51593| 32.17519 |
| Au  | 5.76752 | 4.99482 | 5.88645 | H | 0.72085 | 13.97562 | 32.25662 |
| Au  | 8.65128 | 4.99482 | 5.88645 | H | 4.68304 | 14.58979 | 32.258  |
| Au  | 11.53503 | 4.99482 | 5.88645 | H | 3.72448 | 0.16484 | 32.2919 |
| Au  | −4.32564 | 7.49222 | 5.88645 | H | 6.14374 | 0.58508 | 32.2856 |
| Au  | −1.44188 | 7.49222 | 5.88645 | H | 5.55534 | 5.49448 | 32.7699 |
| Au  | 1.44188 | 7.49222 | 5.88645 | C | 5.19033 | 6.52524 | 32.8909 |
| Au  | 4.32564 | 7.49222 | 5.88645 | N | −1.25025 | 6.8132 | 32.9774 |
| Au  | 7.2094 | 7.49222 | 5.88645 | N | −1.07016 | 8.9227 | 32.9920 |
| Au  | 10.09315 | 7.49222 | 5.88645 | N | −0.42157 | 4.38007 | 33.0438 |
| Au  | −5.76752 | 9.98963 | 5.88645 | N | 1.23604 | 2.86835 | 33.1504 |
| Au  | −2.88376 | 9.98963 | 5.88645 | C | 4.13246 | 9.12741 | 33.1457 |
| Au  | 0 | 9.98963 | 5.88645 | N | −0.12893 | 11.17582 | 33.1596 |
| Au  | 2.88376 | 9.98963 | 5.88645 | N | 8.76738 | 8.25166 | 33.1584 |
| Au  | 5.76752 | 9.98963 | 5.88645 | N | 7.93935 | 10.34173 | 33.1687 |
| Au  | 8.65128 | 9.98963 | 5.88645 | N | 1.76031 | 12.39672 | 33.2075 |
| Au  | −7.2094 | 12.48704 | 5.88645 | N | 8.7521 | 5.80255 | 33.2109 |
| Au  | −4.32564 | 12.48704 | 5.88645 | H | 3.67686 | 10.12116 | 33.2590 |
| Au  | −1.44188 | 12.48704 | 5.88645 | N | 6.30334 | 12.16198 | 33.2537 |
| Au  | 1.44188 | 12.48704 | 5.88645 | N | 4.15638 | 12.82174 | 33.2848 |
| Au  | 4.32564 | 12.48704 | 5.88645 | H | −2.40736 | 4.96894 | 33.2927 |
| Au  | 7.2094 | 12.48704 | 5.88645 | N | 7.65781 | 3.84251 | 33.2816 |
| Au  | 1.44188 | 0.83247 | 8.24103 | N | 3.50759 | 1.99845 | 33.3054 |
| Au  | 4.32564 | 0.83247 | 8.24103 | N | 5.72108 | 2.36461 | 33.3290 |
| Au  | 7.2094 | 0.83247 | 8.24103 | H | −2.13477 | 10.67938 | 33.4409 |
| Au  | 10.09315 | 0.83247 | 8.24103 | C | −1.38271 | 5.34728 | 33.5187 |
| Au  | 12.97691 | 0.83247 | 8.24103 | H | 10.41391 | 7.01986 | 33.5691 |
| Au  | 15.86067 | 0.83247 | 8.24103 | C | −1.12745 | 10.23203 | 33.6096 |
| Au  | 0 | 3.32988 | 8.24103 | H | 8.34832 | 12.34711 | 33.6440 |
| Au  | 2.88376 | 3.32988 | 8.24103 | C | 9.31041 | 7.03556 | 33.7266 |
| Au  | 5.76752 | 3.32988 | 8.24103 | H | 1.77132 | 0.93509 | 33.7989 |
| Au  | 8.65128 | 3.32988 | 8.24103 | C | 7.53299 | 11.59521 | 33.7647 |
| Au  | 11.53503 | 3.32988 | 8.24103 | C | −0.91629 | 7.77472 | 33.7735 |
| Au  | 14.41879 | 3.32988 | 8.24103 | C | 2.16011 | 1.98038 | 33.8235 |
| Au  | −1.44188 | 5.82729 | 8.24103 | H | 2.66124 | 14.1801 | 33.8705 |
| Au  | 1.44188 | 5.82729 | 8.24103 | C | 2.85655 | 13.08249 | 33.8627 |
| Au  | 4.32564 | 5.82729 | 8.24103 | H | 7.66212 | 1.83335 | 33.9180 |
| Au  | 7.2094 | 5.82729 | 8.24103 | C | 0.59488 | 3.88523 | 33.8567 |
| Au  | 10.09315 | 5.82729 | 8.24103 | C | 6.99125 | 2.72451 | 33.9128 |
| Au  | 12.97691 | 5.82729 | 8.24103 | C | 1.02396 | 11.42688 | 33.9862 |
| Au  | −2.88376 | 8.32469 | 8.24103 | C | 8.09452 | 9.18876 | 33.9358 |
| Au  | 0 | 8.32469 | 8.24103 | C | 5.12657 | 12.11465 | 33.9881 |
| Au  | 2.88376 | 8.32469 | 8.24103 | C | 7.91956 | 5.00985 | 33.9834 |
| Au  | 5.76752 | 8.32469 | 8.24103 | C | 4.52696 | 2.65587 | 33.9808 |
| Au  | 8.65128 | 8.32469 | 8.24103 | C | 5.16417 | 7.15238 | 34.1260 |
| Au   | 11.53503 | 8.32469 | 8.24103 | C    | 4.64196 | 8.46748 | 34.25223 |
| Au   | -4.32564 | 10.8221 | 8.24103 | H    | -1.25992 | 5.42888 | 34.62232 |
| Au   | -1.44188 | 10.8221 | 8.24103 | H    | -0.97989 | 10.0831 | 34.70324 |
| Au   | 1.44188  | 10.8221 | 8.24103 | H    | 9.10446  | 7.06024 | 34.81702 |
| Au   | 4.32564  | 10.8221 | 8.24103 | H    | 7.37975  | 11.4008 | 34.85086 |
| Au   | 7.2094   | 10.8221 | 8.24103 | H    | 2.21483  | 2.31719 | 34.88405 |
| Au   | 10.09315 | 10.8221 | 8.24103 | H    | 2.89084  | 12.71352 | 34.91267 |
| Au   | -5.76752 | 13.31951| 8.24103 | H    | 6.79243  | 3.02828 | 34.96738 |
| Au   | -2.88376 | 13.31951| 8.24103 | O    | -0.57509 | 7.741   | 34.94397 |
| Au   | 0       | 13.31951| 8.24103 | H    | 5.54107  | 6.63075 | 35.02005 |
| Au   | 2.88376  | 13.31951| 8.24103 | O    | 0.8631   | 4.2569  | 34.99028 |
| Au   | 5.76752  | 13.31951| 8.24103 | O    | 1.32977  | 10.90869| 34.95836 |
| Au   | 8.65128  | 13.31951| 8.24103 | O    | 4.40472  | 3.34801 | 34.98348 |
| Au   | -0.00887 | 1.65962 | 10.69901| O    | 4.9741   | 11.55754| 35.06683 |
| Au   | 2.8814   | 1.65308 | 10.68594| O    | 7.73146  | 9.0461  | 35.09384 |
| Au   | 5.77274  | 1.65523 | 10.68851| O    | 7.50635  | 5.28488 | 35.10848 |
| Au   | 8.65768  | 1.6614  | 10.69684| H    | 4.63176  | 8.97036 | 35.2328 |
| Au   | 11.53708 | 1.66495 | 10.71352| H    | -0.00152 | 0.00253 | 37.48604 |
| Au   | 14.41524 | 1.66698 | 10.70757| O    | 2.88117  | -0.00679 | 37.47652 |
| Au   | -1.45121 | 4.15557 | 10.69293| Au   | 5.7698   | -0.01076 | 37.49353 |
| Au   | 1.44141  | 4.15546 | 10.68133| Au   | 8.65129  | -0.00376 | 37.4863 |
| Au   | 4.32845  | 4.15282 | 10.68364| Au   | 11.53394 | 0.00705  | 37.46636 |
| Au   | 7.21479  | 4.15755 | 10.69007| Au   | 14.41915 | 0.00796  | 37.50662 |
| Au   | 10.10065 | 4.1577  | 10.69795| Au   | -1.44981 | 2.49702 | 37.5006 |
| Au   | 12.97378 | 4.15975 | 10.71061| Au   | 1.43905  | 2.48371 | 37.55915 |
| Au   | -2.89208 | 6.65288 | 10.69701| Au   | 4.32158  | 2.47012 | 37.56724 |
| Au   | -0.00179 | 6.66029 | 10.67952| Au   | 7.21951  | 2.47831 | 37.56332 |
| Au   | 2.8877   | 6.65643 | 10.68154| Au   | 10.09968 | 2.48859 | 37.49745 |
| Au   | 5.77074  | 6.65741 | 10.68918| Au   | 12.97542 | 2.49633 | 37.51031 |
| Au   | 8.65846  | 6.65739 | 10.68817| Au   | -2.8937  | 4.98973 | 37.48868 |
| Au   | 11.5398  | 6.65635 | 10.69911| Au   | -0.02017 | 4.99885 | 37.56679 |
| Au   | -4.326   | 9.16027 | 10.71285| Au   | 2.87417  | 4.98818 | 37.54655 |
| Au   | -1.45333 | 9.16062 | 10.68215| Au   | 5.76009  | 4.97618 | 37.59728 |
| Au   | 1.4384   | 9.16101 | 10.68176| Au   | 8.68072  | 4.98056 | 37.56943 |
| Au   | 4.33043  | 9.15511 | 10.68318| Au   | 11.54272 | 4.99305 | 37.50024 |
| Au   | 7.22032  | 9.15917 | 10.68201| Au   | -4.33134 | 7.49457 | 37.5088 |
| Au   | 10.10316 | 9.15719 | 10.69154| Au   | -1.46702 | 7.49088 | 37.54842 |
| Au   | -5.76679 | 11.65774| 10.71555| Au   | 1.44011  | 7.493   | 37.54491 |
| Au   | -2.88707 | 11.65659| 10.709  | Au   | 4.31979  | 7.4796  | 37.58916 |
| Au   | -0.00564 | 11.66429| 10.68715| Au   | 7.21508  | 7.47758 | 37.59127 |
| Au   | 2.88366  | 11.65695| 10.68219| Au   | 10.10428 | 7.49448 | 37.53307 |
| Au   | 5.77329  | 11.65985| 10.6848 | Au   | -5.75956 | 9.99515 | 37.50538 |
| Au   | 8.65908  | 11.66095| 10.69036| Au   | -2.88751 | 9.99563 | 37.48434 |
| Au   | -7.20954 | 14.14966| 10.71674| Au   | -0.00729 | 9.98805 | 37.55916 |
| Au   | 4.3273 | 14.14835 | 10.71421 | Au   | 2.89025 | 9.99173 | 37.56469 |
| Au   | -1.44303 | 14.14958 | 10.71264 | Au   | 5.78084 | 9.98882 | 37.60946 |
| Au   | 1.4444 | 14.16185 | 10.69961 | Au   | 8.67567 | 10.0079 | 37.56242 |
| Au   | 4.32594 | 14.16254 | 10.69387 | Au   | -7.20475 | 12.49485 | 37.48408 |
| Au   | 7.20943 | 14.1598 | 10.70191 | Au   | -4.32521 | 12.48802 | 37.50642 |
| Au   | -0.00218 | 0.0006 | 13.29361 | Au   | -1.44459 | 12.48192 | 37.48379 |
| Au   | 2.87952 | -0.0135 | 13.29636 | Au   | 1.4362 | 12.50096 | 37.54538 |
| Au   | 5.77018 | -0.01453 | 13.27161 | Au   | 4.32063 | 12.51118 | 37.57877 |
| Au   | 8.64986 | 0.0001 | 13.2734 | Au   | 7.2175 | 12.50078 | 37.53381 |
| Au   | 11.53624 | 0.01038 | 13.30117 | Au   | -0.00604 | 1.66171 | 40.07935 |
| Au   | 14.41934 | 0.00831 | 13.26947 | Au   | 2.88075 | 1.65609 | 40.08114 |
| Au   | -1.44913 | 2.49647 | 13.27852 | Au   | 5.76874 | 1.65678 | 40.08233 |
| Au   | 1.43193 | 2.47746 | 13.19354 | Au   | 8.65869 | 1.6579 | 40.0779 |
| Au   | 4.3216 | 2.46034 | 13.17929 | Au   | 11.5375 | 1.66328 | 40.06127 |
| Au   | 7.21713 | 2.47972 | 13.22011 | Au   | 14.41692 | 1.66699 | 40.06998 |
| Au   | 10.10009 | 2.48944 | 13.27186 | Au   | -1.44762 | 4.15866 | 40.07434 |
| Au   | 12.97594 | 2.49726 | 13.26612 | Au   | 1.43706 | 4.15752 | 40.08011 |
| Au   | -2.8967 | 4.98852 | 13.28411 | Au   | 4.32076 | 4.15369 | 40.0888 |
| Au   | -0.01906 | 4.99657 | 13.16631 | Au   | 7.2158 | 4.15557 | 40.0895 |
| Au   | 2.89073 | 4.9879 | 13.19796 | Au   | 10.10186 | 4.15553 | 40.07588 |
| Au   | 5.77045 | 4.97975 | 13.19828 | Au   | 12.9735 | 4.16095 | 40.06671 |
| Au   | 8.68222 | 4.9767 | 13.20514 | Au   | -2.88713 | 6.6562 | 40.06956 |
| Au   | 11.54244 | 4.9935 | 13.28153 | Au   | -0.00559 | 6.66095 | 40.07614 |
| Au   | -4.3333 | 7.49439 | 13.27165 | Au   | 2.87571 | 6.65442 | 40.09307 |
| Au   | -1.47162 | 7.49105 | 13.17898 | Au   | 5.77014 | 6.6585 | 40.09965 |
| Au   | 1.46081 | 7.48858 | 13.19014 | Au   | 8.66057 | 6.65716 | 40.0895 |
| Au   | 4.33832 | 7.48166 | 13.24629 | Au   | 11.54097 | 6.65729 | 40.07523 |
| Au   | 7.21901 | 7.47437 | 13.19252 | Au   | -4.32388 | 9.16035 | 40.06598 |
| Au   | 10.10665 | 7.49533 | 13.23019 | Au   | -1.44892 | 9.15887 | 40.07564 |
| Au   | -5.75875 | 9.99523 | 13.27205 | Au   | 1.43548 | 9.15893 | 40.08154 |
| Au   | -2.88631 | 9.99577 | 13.29205 | Au   | 4.3228 | 9.16031 | 40.10073 |
| Au   | -0.00378 | 9.98927 | 13.16885 | Au   | 7.2205 | 9.16069 | 40.09573 |
| Au   | 2.90801 | 9.98411 | 13.18959 | Au   | 10.10225 | 9.15786 | 40.07811 |
| Au   | 5.78567 | 9.97707 | 13.18563 | Au   | -5.7659 | 11.65765 | 40.06288 |
| Au   | 8.67732 | 10.00693 | 13.19601 | Au   | -2.88481 | 11.65584 | 40.06595 |
| Au   | -7.20484 | 12.4923 | 13.30409 | Au   | -0.00469 | 11.65963 | 40.07659 |
| Au   | -4.32473 | 12.48595 | 13.26803 | Au   | 2.8802 | 11.65848 | 40.08374 |
| Au   | -4.44351 | 12.48215 | 13.289 | Au   | 5.77146 | 11.6654 | 40.08951 |
| Au   | 1.43789 | 12.51077 | 13.19667 | Au   | 8.65664 | 11.66103 | 40.07906 |
| Au   | 4.32244 | 12.5113 | 13.1782 | Au   | -7.20816 | 14.15105 | 40.06037 |
| Au   | 7.21929 | 12.50177 | 13.21343 | Au   | -4.32602 | 14.14957 | 40.06004 |
| 0    | 1.55028 | 10.9503 | 15.58732 | Au   | -1.44258 | 14.1494 | 40.05934 |
| 0    | -0.27434 | 7.74081 | 15.61101 | Au   | 1.44248 | 14.1571 | 40.06786 |
| 0    | 5.20133 | 11.50334 | 15.61754 | Au   | 4.32458 | 14.16161 | 40.07436 |

26
|  |  |  |  |  |  |
|---|---|---|---|---|---|
| N | 8.83414 | 5.97601 | 17.55141 | Au | 1.44188 | 2.49741 | 44.8897 |
| N | 7.7269 | 4.0246 | 17.56264 | Au | 4.32564 | 2.49741 | 44.8897 |
| H | -0.04097 | 1.47554 | 18.46371 | Au | 7.2094 | 2.49741 | 44.8897 |
| H | 7.138 | 13.8186 | 18.50265 | Au | 10.90315 | 2.49741 | 44.8897 |
| H | -3.03803 | 6.76188 | 18.57921 | Au | 12.97691 | 2.49741 | 44.8897 |
| H | 9.99283 | 11.22968 | 18.57094 | Au | -2.88376 | 4.99482 | 44.8897 |
| C | 0.35925 | 2.51377 | 18.56788 | Au | 0 | 4.99482 | 44.8897 |
| C | -0.7679 | 3.61299 | 18.57678 | Au | 2.88376 | 4.99482 | 44.8897 |
| H | -1.79901 | 3.18597 | 18.57968 | Au | 5.76752 | 4.99482 | 44.8897 |
| C | 6.45972 | 12.93477 | 18.5964 | Au | 8.65128 | 4.99482 | 44.8897 |
| H | 3.79461 | 0.48607 | 18.61553 | Au | 11.53503 | 4.99482 | 44.8897 |
| C | 9.17683 | 10.4693 | 18.61826 | Au | -4.32564 | 7.49222 | 44.8897 |
| C | -1.96366 | 7.06282 | 18.64169 | Au | -1.44188 | 7.49222 | 44.8897 |
| C | 4.93449 | 13.32685 | 18.63278 | Au | 1.44188 | 7.49222 | 44.8897 |
| H | 10.8263 | 8.9218 | 18.6537 | Au | 4.32564 | 7.49222 | 44.8897 |
| H | 1.12988 | 13.72067 | 18.68724 | Au | 7.2094 | 7.49222 | 44.8897 |
| C | 9.71116 | 8.98725 | 18.6681 | Au | 10.00315 | 7.49222 | 44.8897 |
| H | 4.76443 | 14.42976 | 18.6669 | Au | -5.76752 | 9.98963 | 44.8897 |
| C | 1.3729 | 12.63027 | 18.69334 | Au | -2.88376 | 9.98963 | 44.8897 |
| C | -1.75878 | 8.62262 | 18.69124 | Au | 0 | 9.98963 | 44.8897 |
| C | 3.93297 | 1.59018 | 18.70285 | Au | 2.88376 | 9.98963 | 44.8897 |
| C | 0.09694 | 11.71062 | 18.71607 | Au | 5.76752 | 9.98963 | 44.8897 |
| H | -2.71769 | 9.19144 | 18.76151 | Au | 8.65128 | 9.98963 | 44.8897 |
| H | 10.31986 | 5.13131 | 18.79045 | Au | -7.2094 | 12.48704 | 44.8897 |
| H | -0.85886 | 12.28426 | 18.78639 | Au | -4.32564 | 12.48704 | 44.8897 |
| C | 9.22739 | 5.3632 | 18.80726 | Au | -1.44188 | 12.48704 | 44.8897 |
| C | 5.43761 | 2.02131 | 18.82591 | Au | 1.44188 | 12.48704 | 44.8897 |
| C | 8.32112 | 4.08279 | 18.87544 | Au | 4.32564 | 12.48704 | 44.8897 |
| H | 6.12939 | 1.16439 | 19.01019 | Au | 7.2094 | 12.48704 | 44.8897 |
| H | 8.89464 | 3.14582 | 19.07672 | Au | 0 | 1.66494 | 47.24355 |
| N | -0.52215 | 4.33328 | 19.09334 | Au | 2.88376 | 1.66494 | 47.24355 |
| N | 4.46081 | 12.70748 | 19.85109 | Au | 5.76752 | 1.66494 | 47.24355 |
| N | 8.44236 | 10.60349 | 19.85404 | Au | 8.65128 | 1.66494 | 47.24355 |
| N | 0.987 | 2.67535 | 19.85467 | Au | 11.53503 | 1.66494 | 47.24355 |
| N | 6.66543 | 12.28116 | 19.86254 | Au | 14.41879 | 1.66494 | 47.24355 |
| N | -1.38875 | 6.61404 | 19.88274 | Au | -1.44188 | 4.16235 | 47.24355 |
| N | -0.96901 | 8.81787 | 19.88665 | Au | 1.44188 | 4.16235 | 47.24355 |
| N | 0.28721 | 10.90225 | 19.89718 | Au | 4.32564 | 4.16235 | 47.24355 |
| N | 2.06211 | 12.27671 | 19.90723 | Au | 7.2094 | 4.16235 | 47.24355 |
| N | 3.35763 | 2.07351 | 19.92572 | Au | 10.09315 | 4.16235 | 47.24355 |
| N | 9.19773 | 8.49262 | 19.9213 | Au | 12.97691 | 4.16235 | 47.24355 |
| N | 5.44097 | 2.92092 | 19.9681 | Au | -2.88376 | 6.65975 | 47.24355 |
| N | 7.41323 | 4.36053 | 19.97197 | Au | 0 | 6.65975 | 47.24355 |
| N | 8.87885 | 6.07165 | 20.00336 | Au | 2.88376 | 6.65975 | 47.24355 |
| H    | 1.7574 | 0.75882 | 20.19579 | Au | 5.76752 | 6.65975 | 47.24355 |
| H    | 8.6917 | 12.65094 | 20.23645 | Au | 8.65128 | 6.65975 | 47.24355 |
| H    | -2.49133 | 4.88367 | 20.28638 | Au | 11.53503 | 6.65975 | 47.24355 |
| H    | 2.98106 | 14.08922 | 20.41146 | Au | -4.32564 | 9.15716 | 47.24355 |
| H    | 10.65759 | 7.07469 | 20.43273 | Au | -1.44188 | 9.15716 | 47.24355 |
| C    | 7.9354 | 11.84464 | 20.38943 | Au | 1.44188 | 9.15716 | 47.24355 |
| C    | -1.45083 | 5.27137 | 20.39912 | Au | 4.32564 | 9.15716 | 47.24355 |
| C    | 2.01836 | 1.82326 | 20.39621 | Au | 7.2094 | 9.15716 | 47.24355 |
| C    | 3.18262 | 12.99198 | 20.46317 | Au | 10.90315 | 9.15716 | 47.24355 |
| C    | -1.70494 | 10.67948 | 20.51759 | Au | -5.76752 | 11.65457 | 47.24355 |
| C    | -0.74177 | 10.10304 | 20.50617 | Au | -2.88376 | 11.65457 | 47.24355 |
| C    | 9.55657 | 7.23006 | 20.5238 | Au | 0 | 11.65457 | 47.24355 |
| C    | 0.45207 | 3.72626 | 20.60478 | Au | 2.88376 | 11.65457 | 47.24355 |
| C    | -0.83814 | 7.64906 | 20.64063 | Au | 5.76752 | 11.65457 | 47.24355 |
| C    | 6.66909 | 3.30998 | 20.63589 | Au | 8.65128 | 11.65457 | 47.24355 |
| C    | 5.50087 | 12.18698 | 20.62789 | Au | -7.2094 | 14.15198 | 47.24355 |
| C    | 1.39051 | 11.3077 | 20.65573 | Au | -4.32564 | 14.15198 | 47.24355 |
| C    | 4.23963 | 2.85462 | 20.67653 | Au | -1.44188 | 14.15198 | 47.24355 |
| C    | 8.53042 | 9.4678 | 20.66365 | Au | 1.44188 | 14.15198 | 47.24355 |
| C    | 7.80818 | 5.4964 | 20.69964 | Au | 4.32564 | 14.15198 | 47.24355 |
| H    | 7.32589 | 2.40813 | 20.72438 | Au | 7.2094 | 14.15198 | 47.24355 |
| H    | -1.17403 | 5.34191 | 21.47485 | Au | 1.44188 | 0 | 83247 | 49.59813 |
| H    | 7.77025 | 11.66397 | 21.47535 | Au | 4.32564 | 0 | 83247 | 49.59813 |
| H    | 2.03133 | 2.02238 | 21.49011 | Au | 7.2094 | 0 | 83247 | 49.59813 |
| H    | 3.26894 | 12.66099 | 21.52272 | Au | 10.90315 | 0 | 83247 | 49.59813 |
| H    | -0.40772 | 9.89331 | 21.54559 | Au | 12.97691 | 0 | 83247 | 49.59813 |
| H    | 9.2584 | 7.31362 | 21.59259 | Au | 15.86067 | 0 | 83247 | 49.59813 |
| H    | 6.41848 | 3.66295 | 21.66421 | Au | 0 | 3.32988 | 49.59813 |
| O    | 7.34832 | 5.89743 | 21.74848 | Au | 2.88376 | 3.32988 | 49.59813 |
| O    | 3.98615 | 3.34563 | 21.7642 | Au | 5.76752 | 3.32988 | 49.59813 |
| O    | -0.3706 | 7.55423 | 21.76036 | Au | 8.65128 | 3.32988 | 49.59813 |
| O    | 1.68648 | 10.91717 | 21.76286 | Au | 11.53503 | 3.32988 | 49.59813 |
| O    | 0.74764 | 4.01975 | 21.75085 | Au | 14.41879 | 3.32988 | 49.59813 |
| O    | 5.41703 | 11.76926 | 21.7668 | Au | -1.44188 | 5.82729 | 49.59813 |
| O    | 8.13716 | 9.36454 | 21.81058 | Au | 1.44188 | 5.82729 | 49.59813 |
| O    | 5.01284 | 5.36017 | 23.41494 | Au | 4.32564 | 5.82729 | 49.59813 |
| H    | 3.99999 | 7.15088 | 23.42957 | Au | 7.2094 | 5.82729 | 49.59813 |
| H    | 2.96804 | 5.69178 | 23.54946 | Au | 10.09315 | 5.82729 | 49.59813 |
| H    | 4.225 | 1.86677 | 23.72414 | Au | 12.97691 | 5.82729 | 49.59813 |
| O    | 6.42078 | 3.66843 | 23.75366 | Au | -2.88376 | 8.32469 | 49.59813 |
| C    | 3.90829 | 6.16132 | 23.91737 | Au | 0 | 8.32469 | 49.59813 |
| C    | 5.46226 | 4.34957 | 24.1468 | Au | 2.88376 | 8.32469 | 49.59813 |
| H    | 2.89196 | 1.18242 | 24.71481 | Au | 5.76752 | 8.32469 | 49.59813 |
| H    | 2.80985 | 3.71392 | 24.70356 | Au | 8.65128 | 8.32469 | 49.59813 |
Au–CB7——CPT (H)——CB7—Au:

Au 1.44188 0.83247 1.17729 C 4.64289 8.52747 27.51571
Au 4.32564 0.83247 1.17729 C 4.82428 6.15678 27.57003
Au 7.2094 0.83247 1.17729 H 4.95772 4.00682 27.68485
Au 10.09315 0.83247 1.17729 H 5.50863 9.19655 27.69146
Au 12.97691 0.83247 1.17729 Cl 2.26326 5.17039 27.49616
Au 15.86067 0.83247 1.17729 C 4.17749 6.58527 27.47976
Au 0 3.32988 1.17729 C 4.07281 8.00527 28.80919
Au 2.88376 3.32988 1.17729 H 0.02317 4.32079 29.39986
Au 5.76752 3.32988 1.17729 O 2.01751 3.06243 29.34126
Au 8.65128 3.32988 1.17729 O 0.40025 6.72669 29.42834
Au 11.53503 3.32988 1.17729 O 1.00293 10.01809 29.4432
Au 14.41879 3.32988 1.17729 O 7.16223 6.13012 29.45675
Au −1.44188 5.82729 1.17729 H −0.59097 8.87586 29.47976
Au 1.44188 5.82729 1.17729 O 6.6512 10.01809 29.49036
Au 4.32564 5.82729 1.17729 O 3.89167 12.07687 29.5655
Au 7.2094 5.82729 1.17729 H 8.20688 8.23625 29.51505
Au 10.09315 5.82729 1.17729 O 5.06895 3.12583 29.54751
Au 12.97691 5.82729 1.17729 H 7.3645 3.70012 29.6215
Au −2.88376 8.32469 1.17729 H 6.20655 12.41582 29.67665
Au 0 8.32469 1.17729 H 3.45922 1.30836 29.75472
Au 2.88376 8.32469 1.17729 H 3.88168 4.32365 29.76974
Au 5.76752 8.32469 1.17729 N 3.89695 5.85993 29.89901
Au 8.65128 8.32469 1.17729 H 1.63927 12.90321 29.8907
Au 11.53503 8.32469 1.17729 C 3.54362 8.64373 29.90807
Au −4.32564 10.8221 1.17729 H 9.74113 29.90773
Au −1.44188 10.8221 1.17729 H −1.41385 3.57993 30.2752
Au 1.44188 10.8221 1.17729 H −2.16685 9.20809 30.355
| Au  | 4.32564 | 10.8221 | 1.17729 | H | 9.81199 | 8.43305 | 30.37447 |
| Au  | 7.2094  | 10.8221 | 1.17729 | C | -0.43894 | 4.11773 | 30.39677 |
| Au  | 10.09315| 10.8221 | 1.17729 | C | -0.32683 | 6.59279 | 30.39047 |
| Au  | -5.76752| 13.31951| 1.17729 | C | 1.61311 | 2.76629 | 30.44104 |
| Au  | -2.88376| 13.31951| 1.17729 | C | -1.08955 | 8.92886 | 30.47939 |
| Au  | 0       | 13.31951| 1.17729 | C | 7.80332  | 6.02178 | 30.48783 |
| Au  | 2.88376 | 13.31951| 1.17729 | C | 8.70844  | 8.29858 | 30.50648 |
| Au  | 5.76752 | 13.31951| 1.17729 | C | 7.27021  | 10.28274| 30.50722 |
| Au  | 8.65128 | 13.31951| 1.17729 | C | 0.5049   | 10.78485| 30.53773 |
| Au  | 0       | 1.66494 | 3.53187 | C | 5.37242  | 2.6751  | 30.6415  |
| Au  | 2.88376 | 1.66494 | 3.53187 | C | 3.96408  | 12.50826| 30.64239 |
| Au  | 5.76752 | 1.66494 | 3.53187 | C | 7.65976  | 3.56152 | 30.6862  |
| Au  | 8.65128 | 1.66494 | 3.53187 | C | 6.41288  | 12.58005| 30.75699 |
| Au  | 11.53503| 1.66494 | 3.53187 | H | 8.52728  | 2.86145 | 30.75641 |
| Au  | 14.41879| 1.66494 | 3.53187 | C | 3.41928  | 1.17478 | 30.85783 |
| Au  | -1.44188| 4.16235 | 3.53187 | C | 1.55759  | 12.98928| 30.91424 |
| Au  | 1.44188 | 4.16235 | 3.53187 | H | 6.96721  | 13.53631| 30.91141 |
| Au  | 4.32564 | 4.16235 | 3.53187 | C | 3.31845  | 6.43507 | 31.00603 |
| Au  | 7.2094  | 4.16235 | 3.53187 | C | 3.13839  | 7.86104 | 31.03954 |
| Au  | 10.09315| 4.16235 | 3.53187 | N | -0.69727 | 5.39526 | 31.01678 |
| Au  | 12.97691| 4.16235 | 3.53187 | N | -1.0062  | 7.62054 | 31.05594 |
| Au  | -2.88376| 6.65975 | 3.53187 | N | 0.49395  | 3.26658 | 31.11007 |
| Au  | 0       | 6.65975 | 3.53187 | H | 3.39546  | 0.09596 | 31.13002 |
| Au  | 2.88376 | 6.65975 | 3.53187 | N | 8.4592   | 7.0471  | 31.17176 |
| Au  | 5.76752 | 6.65975 | 3.53187 | N | 8.16891  | 9.4547  | 31.17683 |
| Au  | 8.65128 | 6.65975 | 3.53187 | N | 8.07438  | 4.84393 | 31.17911 |
| Au  | 11.53503| 6.65975 | 3.53187 | N | 7.25657  | 11.49736| 31.18585 |
| Au  | -4.32564| 9.15716 | 3.53187 | N | 2.18993  | 1.79632 | 31.26547 |
| Au  | -1.44188| 9.15716 | 3.53187 | N | -0.40733 | 9.97088 | 31.20705 |
| Au  | 1.44188 | 9.15716 | 3.53187 | H | 1.07119  | 13.9494 | 31.20179 |
| Au  | 4.32564 | 9.15716 | 3.53187 | N | 0.71257  | 11.90556| 31.34305 |
| Au  | 7.2094  | 9.15716 | 3.53187 | N | 6.52378  | 2.96874 | 31.35722 |
| Au  | 10.09315| 9.15716 | 3.53187 | N | 4.64518  | 1.74799 | 31.37165 |
| Au  | -5.76752| 11.65457| 3.53187 | N | 5.12405  | 12.66303| 31.3995  |
| Au  | -2.88376| 11.65457| 3.53187 | N | 2.91098  | 12.99396| 31.41915 |
| Au  | 0       | 11.65457| 3.53187 | H | -2.60847 | 5.04093 | 31.84915 |
| Au  | 2.88376 | 11.65457| 3.53187 | H | -2.90824 | 7.48007 | 31.94873 |
| Au  | 5.76752 | 11.65457| 3.53187 | H | 9.92699  | 10.2852 | 32.01655 |
| Au  | 8.65128 | 11.65457| 3.53187 | H | 3.0853   | 4.54677 | 32.06495 |
| Au  | -7.2094 | 14.15198| 3.53187 | H | 10.35781 | 6.68352 | 32.03747 |
| Au  | -4.32564| 14.15198| 3.53187 | H | -0.73035 | 1.82272 | 32.07499 |
| Au  | -1.44188| 14.15198| 3.53187 | C | 2.93478  | 5.63524 | 32.10823 |
| Au  | 1.44188 | 14.15198| 3.53187 | C | -1.66128 | 5.59122 | 32.07174 |
| Au  | 4.32564 | 14.15198| 3.53187 | C | -1.85186 | 7.15364 | 32.11699 |
| Element | X Coord | Y Coord | Z Coord | Atomic Number | Charge | Mass Number | Isotopic Abundance |
|---------|---------|---------|---------|---------------|--------|-------------|--------------------|
| Au      | 7.2094  | 14.15198 | 3.53187 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 0       | 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 2.88376 | 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 5.76752 | 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 8.65128 | 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 11.53503| 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 14.41879| 0       | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -1.44188| 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 1.44188 | 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 4.32564 | 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 7.2094  | 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 10.09315| 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 12.97691| 2.49741 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -2.88376| 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 0       | 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 2.88376 | 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 5.76752 | 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 8.65128 | 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 11.53503| 4.99482 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -4.32564| 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -1.44188| 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 1.44188 | 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 4.32564 | 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 7.2094  | 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 10.09315| 7.49222 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -5.76752| 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -2.88376| 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 0       | 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 2.88376 | 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 5.76752 | 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 8.65128 | 9.98963 | 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -7.2094 | 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -4.32564| 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | -1.44188| 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 1.44188 | 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 4.32564 | 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 7.2094  | 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 14.1888 | 12.48704| 5.88645 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 4.32564 | 0.83247 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 7.2094  | 0.83247 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 10.09315| 0.83247 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 12.97691| 0.83247 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 15.86067| 0.83247 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au      | 0       | 3.32988 | 8.24103 | 197           | 0      | 197.9648    | 0.0000             |
| Au  | 2.88376 | 3.32988 | 8.24103 | C  | -1.67408 | 8.79683 | 34.06495 |
| --- | ------ | ------ | ------ | --- | -------- | ------- | -------- |
| Au  | 5.76752 | 3.32988 | 8.24103 | H  | 2.13903  | 5.62355 | 34.12841 |
| Au  | 8.65128 | 3.32988 | 8.24103 | H  | 1.8602   | 8.09087 | 34.2457  |
| Au  | 11.53503 | 3.32988 | 8.24103 | H  | 7.18188  | 13.3059 | 34.25345 |
| Au  | 14.41879 | 3.32988 | 8.24103 | C  | -1.08454 | 6.3949  | 34.21098 |
| Au  | -1.44188 | 5.82729 | 8.24103 | H  | 8.61541  | 3.12105 | 34.33524 |
| Au  | 1.44188  | 5.82729 | 8.24103 | C  | 1.1641   | 3.09302 | 34.29811 |
| Au  | 4.32564  | 5.82729 | 8.24103 | C  | 6.60259  | 12.37956 | 34.30235 |
| Au  | 7.2094  | 5.82729 | 8.24103 | C  | 3.25852  | 1.77639 | 34.33691 |
| Au  | 10.09315 | 5.82729 | 8.24103 | C  | 7.73035  | 3.8022  | 34.31209 |
| Au  | 12.97691 | 5.82729 | 8.24103 | H  | 3.23738  | 0.66178 | 34.3934 |
| Au  | -2.88376 | 8.32469 | 8.24103 | C  | 8.2384   | 6.21312 | 34.33934 |
| Au  | 0      | 8.32469 | 8.24103 | C  | 7.77751  | 10.21023 | 34.34717 |
| Au  | 2.88376 | 8.32469 | 8.24103 | C  | 0.26829  | 10.31433 | 34.36345 |
| Au  | 5.76752 | 8.32469 | 8.24103 | C  | 1.71484  | 12.3185 | 34.42042 |
| Au  | 8.65128 | 8.32469 | 8.24103 | C  | 5.35264  | 3.09626 | 34.42843 |
| Au  | 11.53503 | 8.32469 | 8.24103 | H  | 1.25772  | 13.33005 | 34.5564 |
| Au  | -4.32564 | 10.8221 | 8.24103 | C  | 4.16105  | 12.0288 | 34.46116 |
| Au  | -4.44188 | 10.8221 | 8.24103 | H  | -1.0918  | 4.02314 | 35.05122 |
| Au  | 1.44188  | 10.8221 | 8.24103 | H  | -1.52563 | 8.67819 | 35.16283 |
| Au  | 4.32564  | 10.8221 | 8.24103 | H  | 9.32751  | 8.37523 | 35.16416 |
| Au  | 7.2094  | 10.8221 | 8.24103 | H  | 3.21651  | 2.17533 | 35.37618 |
| Au  | 10.09315 | 10.8221 | 8.24103 | H  | 7.49647  | 4.07454 | 35.36681 |
| Au  | -5.76752 | 13.31951 | 8.24103 | H  | 6.53897  | 12.10519 | 35.38469 |
| Au  | -2.88376 | 13.31951 | 8.24103 | O  | 1.33763  | 3.68149 | 35.35706 |
| Au  | 0      | 13.31951 | 8.24103 | O  | -0.74821 | 6.39772 | 35.38634 |
| Au  | 2.88376 | 13.31951 | 8.24103 | H  | 1.87942  | 11.89338 | 35.44112 |
| Au  | 5.76752 | 13.31951 | 8.24103 | O  | 5.04631  | 3.75861 | 35.40763 |
| Au  | 8.65128 | 13.31951 | 8.24103 | O  | 0.69789  | 9.79216 | 35.38342 |
| Au  | -0.0043 | 1.66517  | 10.6489 | O  | 7.83483  | 6.41605 | 35.47237 |
| Au  | 2.88243  | 1.66076  | 10.6464 | O  | 7.44295  | 9.89249 | 35.47753 |
| Au  | 5.76819  | 1.66056  | 10.6468 | O  | 4.20031  | 11.29824 | 35.44085 |
| Au  | 8.65555  | 1.66474  | 10.6482 | Au | -0.00324 | -0.00532 | 37.61555 |
| Au  | 11.53621 | 1.66571  | 10.65135 | Au | 2.8859  | -0.02111 | 37.6086 |
| Au  | 14.41846 | 1.66666  | 10.65192 | Au | 5.76699  | -0.00418 | 37.6117 |
| Au  | -1.44622 | 4.16021  | 10.6432 | Au | 8.64974  | 0.00081 | 37.61069 |
| Au  | 1.44258  | 4.16217  | 10.6461 | Au | 11.52981 | 0.01193 | 37.60865 |
| Au  | 4.3256   | 4.15838  | 10.6457 | Au | 14.42376 | 0.01232 | 37.61081 |
| Au  | 7.20865  | 4.16258  | 10.6468 | Au | -1.45202 | 2.49198 | 37.62411 |
| Au  | 10.09734 | 4.16023  | 10.64704 | Au | 1.44113  | 2.45708 | 37.71968 |
| Au  | 12.97711 | 4.16077  | 10.64983 | Au | 4.32406  | 2.46768 | 37.7316 |
| Au  | -2.88603 | 6.65759  | 10.64985 | Au | 7.2195  | 2.47957 | 37.65797 |
| Au  | -0.00385 | 6.66995  | 10.64533 | Au | 10.10006 | 2.48797 | 37.6043 |
| Au  | 2.88232  | 6.65948  | 10.64185 | Au | 12.97446 | 2.49552 | 37.62404 |
| Au  | 5.76882 | 6.65951 | 10.64136 | Au  | -2.89327 | 4.98448 | 37.62503 |
| Au  | 8.6545  | 6.66093 | 10.64563 | Au  | -0.00704 | 4.97703 | 37.70914 |
| Au  | 11.53854 | 6.65736 | 10.64804 | Au  | 2.89301  | 4.99794 | 37.67489 |
| Au  | -4.32553 | 9.15891 | 10.65446 | Au  | 5.78942  | 5.01444 | 37.72145 |
| Au  | -1.44603 | 9.15808 | 10.64502 | Au  | 8.6824   | 4.96968 | 37.70304 |
| Au  | 1.43747  | 9.161   | 10.64467 | Au  | 11.54329 | 4.98898 | 37.6262 |
| Au  | 4.32605  | 9.15719 | 10.6429  | Au  | -4.32782 | 7.48983 | 37.61819 |
| Au  | 7.21358  | 9.16019 | 10.64489 | Au  | -1.47307 | 7.5123  | 37.72181 |
| Au  | 10.09717 | 9.15853 | 10.64501 | Au  | 1.43822  | 7.47626 | 37.66159 |
| Au  | -5.76602 | 11.65374 | 10.65272 | Au  | 4.31582  | 7.49418 | 37.62668 |
| Au  | -2.88519 | 11.65332 | 10.65226 | Au  | 7.19919  | 7.52984 | 37.74823 |
| Au  | -0.00116 | 11.65693 | 10.64583 | Au  | 10.11391 | 7.48618 | 37.65846 |
| Au  | 2.88256  | 11.65609 | 10.64642 | Au  | -5.75397 | 9.89411 | 37.60831 |
| Au  | 5.76846  | 11.65638 | 10.64634 | Au  | -12.90075 | 10.00334 | 37.613 |
| Au  | 7.65474  | 11.65684 | 10.64497 | Au  | -0.04955 | 10.00628 | 37.77475 |
| Au  | -7.20751 | 14.15085 | 10.65225 | Au  | 2.86514  | 9.97678 | 37.71025 |
| Au  | -4.32596 | 14.15044 | 10.648  | Au  | 5.74699  | 10.00016 | 37.7277 |
| Au  | -1.44386 | 14.15067 | 10.65134 | Au  | 8.70969  | 10.00449 | 37.7398 |
| Au  | 1.44287  | 14.15544 | 10.64507 | Au  | -7.19691 | 12.49552 | 37.62 |
| Au  | 4.32573  | 14.15734 | 10.6469 | Au  | -4.32531 | 12.48954 | 37.6289 |
| Au  | 7.20883  | 14.15615 | 10.64437 | Au  | -1.45256 | 12.4926 | 37.61235 |
| Au  | 0.00067  | -0.0021 | 13.15332 | Au  | 1.42933  | 12.50663 | 37.79192 |
| Au  | 2.88706  | -0.00472 | 13.15663 | Au  | 4.32724  | 12.53438 | 37.74703 |
| Au  | 5.76401  | -0.00655 | 13.15511 | Au  | 7.22704  | 12.50091 | 37.69405 |
| Au  | 8.65123  | -0.0039 | 13.15143 | Au  | -0.0106  | 1.66272 | 40.13193 |
| Au  | 11.53087 | 0.00064 | 13.15547 | Au  | 2.88138  | 1.6534 | 40.15008 |
| Au  | 14.42288 | 0.00808 | 13.15143 | Au  | 5.7767   | 1.65648 | 40.14065 |
| Au  | -1.45014 | 2.49454 | 13.17086 | Au  | 8.65982  | 1.66295 | 40.12792 |
| Au  | 1.42409  | 2.48435 | 13.11161 | Au  | 11.53584 | 1.66972 | 40.11902 |
| Au  | 4.32625  | 2.49135 | 13.10564 | Au  | 14.41466 | 1.66725 | 40.12566 |
| Au  | 7.22981  | 2.48284 | 13.10543 | Au  | -1.44814 | 4.15897 | 40.134 |
| Au  | 10.10398 | 2.4927  | 13.16553 | Au  | 1.44281  | 4.16056 | 40.14102 |
| Au  | 12.97766 | 2.49727 | 13.1441 | Au  | 4.32263  | 4.15649 | 40.13488 |
| Au  | -2.88765 | 4.99342 | 13.1539 | Au  | 7.2116   | 4.15662 | 40.1425 |
| Au  | -0.017   | 4.98355 | 13.101  | Au  | 10.10338 | 4.15599 | 40.13742 |
| Au  | 2.88168  | 5.0013  | 13.12115 | Au  | 12.97689 | 4.15726 | 40.1275 |
| Au  | 5.76658  | 4.99739 | 13.12482 | Au  | -2.89271 | 6.64981 | 40.1325 |
| Au  | 8.66765  | 4.97957 | 13.0959 | Au  | -0.00113 | 6.65945 | 40.13849 |
| Au  | 11.54166 | 4.99238 | 13.15303 | Au  | 2.88291  | 6.65801 | 40.14075 |
| Au  | -4.32567 | 7.49226 | 13.15906 | Au  | 5.76197  | 6.6581 | 40.14805 |
| Au  | -1.45469 | 7.49388 | 13.13729 | Au  | 8.66127  | 6.65566 | 40.14019 |
| Au  | 1.44642  | 7.50723 | 13.1012 | Au  | 11.54122 | 6.65247 | 40.1303 |
| Au  | 4.32738  | 7.49436 | 13.14508 | Au  | -4.32827 | 9.15934 | 40.12374 |
| Au  | 7.20603  | 7.49671 | 13.10896 | Au  | -1.45872 | 9.15695 | 40.157 |
|   |   |   |   |   |
|---|---|---|---|---|
| Au | 10.1064 | 7.49244 | 13.12622 | Au | 1.43776 | 9.15131 | 40.15113 |
| Au | -5.76133 | 9.98996 | 13.16443 | Au | 4.32553 | 9.15273 | 40.14732 |
| Au | -2.88915 | 9.98999 | 13.16433 | Au | 7.2188 | 9.16282 | 40.15883 |
| Au | -0.02342 | 9.99457 | 13.11489 | Au | 10.10698 | 9.1536 | 40.14634 |
| Au | 2.89591 | 9.99808 | 13.10949 | Au | -5.76436 | 11.65473 | 40.12147 |
| Au | 5.76314 | 9.99752 | 13.11268 | Au | -2.8872 | 11.65767 | 40.12295 |
| Au | 8.67444 | 9.99609 | 13.11076 | Au | -0.00937 | 11.66879 | 40.1571 |
| Au | -7.20256 | 12.49035 | 13.15418 | Au | 2.87895 | 11.6536 | 40.15019 |
| Au | -4.32595 | 12.48515 | 13.14756 | Au | 5.77368 | 11.65893 | 40.15336 |
| Au | -1.44907 | 12.48936 | 13.15187 | Au | 8.66032 | 11.66691 | 40.14723 |
| Au | 1.43071 | 12.49534 | 13.12506 | Au | -7.20633 | 14.1521 | 40.12392 |
| Au | 4.3231 | 12.52076 | 13.10118 | Au | -4.32503 | 14.15071 | 40.12363 |
| Au | 7.22022 | 12.49738 | 13.12027 | Au | -1.44888 | 14.15457 | 40.12027 |
| O | 0.63464 | 6.2353 | 15.53738 | Au | 1.44381 | 14.16918 | 40.13776 |
| O | 8.21731 | 5.98805 | 15.56528 | Au | 4.32449 | 14.17043 | 40.14296 |
| O | 7.49154 | 9.82815 | 15.57155 | Au | 7.20734 | 14.16359 | 40.1345 |
| O | 1.36199 | 10.0625 | 15.56294 | Au | 1.44188 | 0.83247 | 42.5344 |
| O | 2.63677 | 3.08038 | 15.57159 | Au | 4.32564 | 0.83247 | 42.5344 |
| O | 4.44232 | 11.75796 | 15.58888 | Au | 7.2094 | 0.83247 | 42.5344 |
| O | 6.14566 | 2.91999 | 15.57902 | Au | 10.09315 | 0.83247 | 42.5344 |
| H | 9.17522 | 8.17143 | 15.63994 | Au | 12.97691 | 0.83247 | 42.5344 |
| H | 0.32653 | 8.43335 | 15.65215 | Au | 15.86067 | 0.83247 | 42.5344 |
| H | 0.38921 | 3.82482 | 15.65841 | Au | 0 | 3.32988 | 42.5344 |
| H | 8.46263 | 3.54118 | 15.78545 | Au | 2.88376 | 3.32988 | 42.5344 |
| H | 6.76893 | 12.17138 | 15.79406 | Au | 5.76752 | 3.32988 | 42.5344 |
| H | 2.14646 | 12.40601 | 15.89315 | Au | 8.65128 | 3.32988 | 42.5344 |
| H | 4.34335 | 1.35445 | 15.9064 | Au | 11.53503 | 3.32988 | 42.5344 |
| C | 0.30836 | 6.14002 | 16.57402 | Au | 14.41879 | 3.32988 | 42.5344 |
| H | 10.7114 | 8.45297 | 16.55073 | Au | -1.44188 | 5.82729 | 42.5344 |
| C | 8.8223 | 5.91662 | 16.62568 | Au | 1.44188 | 5.82729 | 42.5344 |
| C | 8.03047 | 10.12496 | 16.62876 | Au | 4.32564 | 5.82729 | 42.5344 |
| H | -1.82066 | 8.75772 | 16.61763 | Au | 7.2094 | 5.82729 | 42.5344 |
| C | 0.90469 | 10.3261 | 16.67313 | Au | 10.09015 | 5.82729 | 42.5344 |
| C | 9.61721 | 8.24936 | 16.65966 | Au | 12.97691 | 5.82729 | 42.5344 |
| C | 2.3267 | 2.68926 | 16.68744 | Au | -2.88376 | 8.32469 | 42.5344 |
| C | -0.73576 | 8.49271 | 16.68604 | Au | 0 | 8.32469 | 42.5344 |
| C | 0.07167 | 3.67238 | 16.71487 | Au | 2.88376 | 8.32469 | 42.5344 |
| C | 6.35046 | 2.60628 | 16.74202 | Au | 5.76752 | 8.32469 | 42.5344 |
| C | 4.48291 | 12.13579 | 16.75005 | Au | 8.65128 | 8.32469 | 42.5344 |
| H | -0.81799 | 2.99755 | 16.72325 | Au | 11.53503 | 8.32469 | 42.5344 |
| C | 8.67393 | 3.4524 | 16.87476 | Au | -4.32564 | 10.8221 | 42.5344 |
| C | 6.93439 | 12.32865 | 16.88663 | Au | -1.44188 | 10.8221 | 42.5344 |
| C | 2.05131 | 12.49956 | 17.00061 | Au | 1.44188 | 10.8221 | 42.5344 |
| C | 4.30552 | 1.23949 | 17.01379 | Au | 4.32564 | 10.8221 | 42.5344 |
| H     | 9.53427 | 2.75514 | 17.01303 | Au | 7.2094 | 10.8221 | 42.5344 |
|-------|---------|---------|---------|----|--------|---------|---------|
| H     | 7.41866 | 13.3228 | 17.03949 | Au | 10.09315 | 10.8221 | 42.5344 |
| N     | -0.30507 | 4.95964 | 17.242 | Au | -5.76752 | 13.31951 | 42.5344 |
| H     | 1.57557 | 13.47861 | 17.24361 | Au | -2.88376 | 13.31951 | 42.5344 |
| H     | 4.33003 | 0.15293 | 17.26141 | Au | 0 | 13.31951 | 42.5344 |
| N     | -0.59372 | 7.18458 | 17.28113 | Au | 2.88376 | 13.31951 | 42.5344 |
| N     | 9.41636 | 6.9738 | 17.30933 | Au | 5.76752 | 13.31951 | 42.5344 |
| N     | 8.96918 | 9.36228 | 17.31712 | Au | 8.65128 | 13.31951 | 42.5344 |
| N     | 7.83832 | 11.30155 | 17.34179 | Au | 0 | 0 | 44.8897 |
| N     | 9.0577 | 4.7578 | 17.35773 | Au | 2.88376 | 0 | 44.8897 |
| N     | -0.01151 | 9.54174 | 17.36831 | Au | 5.76752 | 0 | 44.8897 |
| N     | 1.17893 | 3.03536 | 17.39762 | Au | 8.65128 | 0 | 44.8897 |
| N     | 1.18212 | 11.44058 | 17.45583 | Au | 11.53503 | 0 | 44.8897 |
| N     | 3.04557 | 1.78675 | 17.46076 | Au | 14.41879 | 0 | 44.8897 |
| N     | 7.49306 | 2.88296 | 17.48525 | Au | -1.44188 | 2.49741 | 44.8897 |
| N     | 5.63029 | 12.32202 | 17.51205 | Au | 1.44188 | 2.49741 | 44.8897 |
| N     | 3.39264 | 12.48093 | 17.53619 | Au | 4.32564 | 2.49741 | 44.8897 |
| N     | 5.48801 | 1.87566 | 17.55273 | Au | 7.2094 | 2.49741 | 44.8897 |
| H     | 10.605 | 10.37813 | 18.18526 | Au | 10.09315 | 2.49741 | 44.8897 |
| H     | 11.30445 | 6.62909 | 18.19454 | Au | 12.97691 | 2.49741 | 44.8897 |
| H     | -2.46831 | 6.96565 | 18.21772 | Au | -2.88376 | 4.99482 | 44.8897 |
| H     | -2.04136 | 4.5506 | 18.35395 | Au | 0 | 4.99482 | 44.8897 |
| C     | -1.39248 | 6.71574 | 18.39345 | Au | 2.88376 | 4.99482 | 44.8897 |
| H     | -1.56619 | 10.53225 | 18.39957 | Au | 5.76752 | 4.99482 | 44.8897 |
| C     | -1.11212 | 5.16772 | 18.41697 | Au | 8.65128 | 4.99482 | 44.8897 |
| C     | 9.55138 | 10.09733 | 18.42572 | Au | 11.53503 | 4.99482 | 44.8897 |
| C     | 10.21793 | 6.51309 | 18.42799 | Au | -4.32564 | 7.49222 | 44.8897 |
| H     | 0.17419 | 1.52898 | 18.48423 | Au | -1.44188 | 7.49222 | 44.8897 |
| C     | -0.50748 | 10.21238 | 18.55637 | Au | 1.44188 | 7.49222 | 44.8897 |
| C     | 8.59405 | 11.33384 | 18.56545 | Au | 4.32564 | 7.49222 | 44.8897 |
| C     | 9.76926 | 5.01733 | 18.58219 | Au | 7.2094 | 7.49222 | 44.8897 |
| C     | 1.02662 | 2.24264 | 18.60293 | Au | 10.09315 | 7.49222 | 44.8897 |
| H     | 9.13991 | 12.30561 | 18.65195 | Au | -5.76752 | 9.8963 | 44.8897 |
| H     | 10.62441 | 4.30656 | 18.68659 | Au | -2.88376 | 9.8963 | 44.8897 |
| C     | 0.48903 | 11.4149 | 18.71686 | Au | 0 | 9.8963 | 44.8897 |
| C     | 2.41969 | 1.52736 | 18.73122 | Au | 2.88376 | 9.8963 | 44.8897 |
| C     | 5.3452 | 12.91807 | 18.80059 | Au | 5.76752 | 9.8963 | 44.8897 |
| C     | 7.4646 | 2.28505 | 18.79952 | Au | 8.65128 | 9.8963 | 44.8897 |
| C     | 6.06984 | 1.5569 | 18.83685 | Au | -7.2094 | 12.48704 | 44.8897 |
| H     | 5.79532 | 13.94039 | 18.85096 | Au | -4.32564 | 12.48704 | 44.8897 |
| C     | 3.77147 | 12.92982 | 18.85327 | Au | -1.44188 | 12.48704 | 44.8897 |
| H     | -0.02364 | 12.39328 | 18.88974 | Au | 1.44188 | 12.48704 | 44.8897 |
| H     | 2.33548 | 0.42523 | 18.89862 | Au | 4.32564 | 12.48704 | 44.8897 |
| H     | 8.3298 | 1.5884 | 18.92341 | Au | 7.2094 | 12.48704 | 44.8897 |
| X   | Y   | Z   | Atom | C   | N   | H   | Au |
|-----|-----|-----|------|-----|-----|-----|----|-----|
| 6.15042 | 0.44841 | 18.95348 | Au | 0 | 1.66494 | 47.24355 |
| 3.34485 | 13.94505 | 19.04466 | Au | 2.88376 | 1.66494 | 47.24355 |
| -0.4627 | 4.96594 | 19.6947 | Au | 5.76752 | 1.66494 | 47.24355 |
| -0.98831 | 7.14619 | 19.70626 | Au | 8.65128 | 1.66494 | 47.24355 |
| 9.91887 | 7.0766 | 19.71409 | Au | 11.53503 | 1.66494 | 47.24355 |
| 9.48042 | 9.48445 | 19.72214 | Au | 14.41879 | 1.66494 | 47.24355 |
| 7.87207 | 11.047 | 19.79116 | Au | -1.41888 | 4.16235 | 47.24355 |
| 8.97955 | 5.04214 | 19.80095 | Au | 1.41888 | 4.16235 | 47.24355 |
| -0.3772 | 9.50789 | 19.80197 | Au | 4.32564 | 4.16235 | 47.24355 |
| 0.90755 | 2.95642 | 19.8476 | Au | 7.2094 | 4.16235 | 47.24355 |
| 11.35556 | 8.57888 | 19.87275 | Au | 10.09315 | 4.16235 | 47.24355 |
| 1.26344 | 11.0354 | 19.8815 | Au | 12.97691 | 4.16235 | 47.24355 |
| 3.00436 | 2.16797 | 19.88881 | Au | -2.88376 | 6.65975 | 47.24355 |
| 7.40179 | 3.19857 | 19.91804 | Au | 0 | 6.65975 | 47.24355 |
| 3.47012 | 12.04362 | 19.9534 | Au | 2.88376 | 6.65975 | 47.24355 |
| 5.71048 | 12.15358 | 19.96235 | Au | 5.76752 | 6.65975 | 47.24355 |
| 5.43249 | 2.13345 | 19.99065 | Au | 8.65128 | 6.65975 | 47.24355 |
| -2.30182 | 8.74147 | 20.04798 | Au | 11.53503 | 6.65975 | 47.24355 |
| -1.16062 | 3.02838 | 20.1119 | Au | -4.32564 | 9.15716 | 47.24355 |
| 10.299 | 8.38899 | 20.17361 | Au | -1.41888 | 9.15716 | 47.24355 |
| -1.24412 | 8.4521 | 20.26054 | Au | 1.41888 | 9.15716 | 47.24355 |
| -0.26322 | 3.66808 | 20.29458 | Au | 4.32564 | 9.15716 | 47.24355 |
| 7.54734 | 13.02157 | 20.44435 | Au | 7.2094 | 9.15716 | 47.24355 |
| 7.04851 | 12.02046 | 20.47392 | Au | 10.09315 | 9.15716 | 47.24355 |
| 8.56193 | 3.84183 | 20.48963 | Au | -5.76752 | 11.65457 | 47.24355 |
| 9.40485 | 3.10612 | 20.49981 | Au | -2.88376 | 11.65457 | 47.24355 |
| -0.5017 | 6.10816 | 20.50219 | Au | 0 | 11.65457 | 47.24355 |
| 9.15921 | 6.22782 | 20.51857 | Au | 2.88376 | 11.65457 | 47.24355 |
| 8.48738 | 10.03258 | 20.53701 | Au | 5.76752 | 11.65457 | 47.24355 |
| 4.18369 | 0.56198 | 20.55952 | Au | 8.65128 | 11.65457 | 47.24355 |
| 4.18734 | 1.67953 | 20.55071 | Au | -7.2094 | 14.15198 | 47.24355 |
| 2.16678 | 11.93424 | 20.55953 | Au | -4.32564 | 14.15198 | 47.24355 |
| 0.66422 | 9.99155 | 20.5964 | Au | -1.41888 | 14.15198 | 47.24355 |
| 1.70398 | 12.95167 | 20.62653 | Au | 1.41888 | 14.15198 | 47.24355 |
| 2.07007 | 2.91325 | 20.61709 | Au | 4.32564 | 14.15198 | 47.24355 |
| 6.20831 | 3.09717 | 20.62699 | Au | 7.2094 | 14.15198 | 47.24355 |
| 4.61041 | 11.66603 | 20.67087 | Au | 1.41888 | 0.83247 | 49.59813 |
| 10.20511 | 8.37003 | 21.28156 | Au | 4.32564 | 0.83247 | 49.59813 |
| -1.07907 | 8.35684 | 21.35716 | Au | 7.2094 | 0.83247 | 49.59813 |
| -0.13126 | 3.84974 | 21.38504 | Au | 10.09315 | 0.83247 | 49.59813 |
| 6.9588 | 11.66405 | 21.52522 | Au | 12.97691 | 0.83247 | 49.59813 |
| 8.32097 | 4.13023 | 21.53784 | Au | 15.86067 | 0.83247 | 49.59813 |
| 2.31961 | 11.51403 | 21.57962 | Au | 0 | 3.32988 | 49.59813 |
| 4.1392 | 2.06244 | 21.59104 | Au | 2.88376 | 3.32988 | 49.59813 |
|   |     |      |       |   |     |      |       |   |     |      |       |
|---|-----|------|-------|---|-----|------|-------|---|-----|------|-------|
| O | 5.90735 | 3.70328 | 21.64146 | Au | 5.76752 | 3.32988 | 49.59813 |
| O | 8.77583 | 6.47063 | 21.64779 | Au | 8.65128 | 3.32988 | 49.59813 |
| O | -0.21101 | 6.17389 | 21.68186 | Au | 11.53503 | 3.32988 | 49.59813 |
| O | 8.24249 | 9.71983 | 21.68711 | Au | 14.41879 | 3.32988 | 49.59813 |
| O | 0.96068 | 9.60765 | 21.71221 | Au | -1.44188 | 5.82729 | 49.59813 |
| O | 4.63714 | 11.06858 | 21.7294 | Au | -1.44188 | 5.82729 | 49.59813 |
| O | 2.22594 | 3.389 | 21.72733 | Au | 4.32564 | 5.82729 | 49.59813 |
| H | 5.99553 | 5.74527 | 22.91965 | Au | 7.2094 | 5.82729 | 49.59813 |
| H | 7.32449 | 1.10579 | 23.58972 | Au | 10.09315 | 5.82729 | 49.59813 |
| H | 4.60221 | 3.59059 | 23.63109 | Au | 0 | 8.32469 | 49.59813 |
| H | 6.1752 | 4.72671 | 23.7656 | Au | 2.88376 | 8.32469 | 49.59813 |
| C | 5.0306 | 1.4931 | 24.03975 | Au | 8.65128 | 8.32469 | 49.59813 |
| C | 8.07405 | 2.61862 | 24.23017 | Au | 11.53503 | 8.32469 | 49.59813 |
| C | 7.32321 | 3.58527 | 24.33787 | Au | -4.32564 | 10.8221 | 49.59813 |
| C | 4.84771 | 2.94228 | 24.49396 | Au | -1.44188 | 10.8221 | 49.59813 |
| H | 5.28481 | 0.84356 | 24.90086 | Au | 1.44188 | 10.8221 | 49.59813 |
| O | 5.94602 | 8.398 | 25.0214 | Au | 4.32564 | 10.8221 | 49.59813 |
| C | 6.03079 | 5.98677 | 25.0909 | Au | 7.2094 | 10.8221 | 49.59813 |
| H | 4.00033 | 3.02046 | 25.20706 | Au | 10.09315 | 10.8221 | 49.59813 |
| C | 6.09234 | 3.48869 | 25.25614 | Au | -5.76752 | 13.31951 | 49.59813 |
| C | 5.70978 | 7.3227 | 25.58184 | Au | -2.88376 | 13.31951 | 49.59813 |
| C | 5.77839 | 4.8453 | 25.83913 | Au | 0 | 13.31951 | 49.59813 |
| H | 7.17524 | 2.0684 | 25.90496 | Au | 2.88376 | 13.31951 | 49.59813 |
| O | 6.43505 | 2.58124 | 26.30371 | Au | 5.76752 | 13.31951 | 49.59813 |
| N | 5.07633 | 7.29926 | 26.84294 | Au | 8.65128 | 13.31951 | 49.59813 |
| H | 3.90356 | 9.07575 | 26.8969 | Au | 0 | 13.31951 | 49.59813 |
| C | 5.18846 | 4.90749 | 27.11251 | Au | 0 | 13.31951 | 49.59813 |

References

[1] A. Day, A. P. Arnold, R. J. Blanch, B. Snushall, *J. Org. Chem.* 2001, 66, 8094-8100.
[2] B. Xiao, F. Liang, S. Liu, J. Im, Y. Li, J. Liu, B. Zhang, J. Zhou, J. He, S. Chang, *Nanotechnology* 2018, 29, 365501.
[3] M. R. di Nunzio, B. Cohen, A. Douhal, *J. Phys. Chem. A* 2011, 115, 5094-5104.
[4] K. Gavvala, A. Sengupta, P. Hazra, *ChemPhysChem* 2013, 14, 532-542.
[5] J. Fassberg, V. J. Stella, *J. Pharm. Sci.* 1992, 81, 676-684.
[6] N. Dong, S.-F. Xue, Q.-J. Zhu, Z. Tao, Y. Zhao, L.-X. Yang, *Supramol. Chem.* 2008, 20, 663-671.
[7] M. Vlčková, P. Barták, V. Kubáň, *J. Chromatogr. A* 2004, 1040, 141-145.
[8] M. A. Alnajjar, W. M. Nau, A. Hennig, *Org. Biomol. Chem.* 2021, 19, 8521-8529.