FINAL REPORT
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Density Functional Theory Calculations of Selected Au Nanocluster Systems: Addressing Questions on Chirality and Ligand Exchange Related to Experimental Work

Host University:

Department of Chemistry
Kansas State University
Supervisor: Prof. Christine M. Aikens

Home University:

Institute of Materials Chemistry
TU Wien
Supervisors: Prof. Günther Rupprechter & Dr. Noelia Barrabés

Marshall Plan Scholarship Recipient:

Vera Truttmann

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Abstract

Several properties of Au nanoclusters can be studied and easily understood through analysis of experimental data. However, in many cases, additional investigations by quantum mechanical methods such as density functional theory (DFT) have been shown to be essential in order to interpret, for example, the electronic and structural properties of these clusters. Thus, within the framework of this Marshall Plan Research stay at Kansas State University, based on preliminary experimental results, the aim was to address some open questions on nanocluster chirality and ligand exchange dynamics.

One example was the chiral cluster $Au_{38}(2\text{-MeBuS})_{24}$, which was previously synthesized at TU Wien and showed a strong chiral signal in circular dichroism (CD) spectroscopy. This is usually an indication for the cluster being present in its enantiomeric form and not as a racemate (or a pair of diastereomers). Thus, a comparison between experimental and theoretical circular dichroism spectra was obtained by optimizing several Au_{38} isomers and calculating their excitations. Indeed, good agreement between the simulated spectrum of the enantiomer with anti-clockwise rotatory staple arrangement and the measured CD spectrum was found. However, contrary to what could be expected, this specific isomer was not lowest in energy, which will have to be further investigated.

Furthermore, the most likely binding positions of bidentate C_2-symmetric phosphine ligands on a biicosahedral Au_{25} nanocluster with a mixed ligand shell were investigated. Therefore, up to two such ligands were introduced into the cluster structure and the energies of isomers featuring different binding sites compared. Thereby, a dependence on the exact structure of the bidentate ligand was noted: While the relatively small *(S)*-dpb ligand preferred neighboring-like gauche positions on the two different icosahedral cores of the cluster, its bulkier counterpart *(S)*-BINAS seems to take binding positions which put the hydrocarbon frameworks as opposite of each other as possible. Introducing chiral thiolates with an asymmetric carbon atom or a bidentate chiral phosphine ligands with axial chirality in the structure evokes chiral properties, indicated by their calculated CD spectra. The bidentate ligand had a stronger effect, presumably related to greater structural distortion.

Finally, also ligand exchange reactions on Au nanoclusters were investigated: When evaluating different possibilities for a single ligand substitution on a $Au_{11}(PPh_3)_7Br_3$ cluster, it was found that the transformation to its Au_{11} analog by replacing a halide ligand with triphenylphosphine should be the most favorable process in moderately polar to polar solvents. The reaction pathway is assumed to follow an associative mechanism instead of ligand dissociation. Furthermore, the importance of including solvation effects and dispersion correction in the calculations of such a system was addressed.

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Contents

Abbreviations

ADF Amsterdam Density Functional

BINAP 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl

BINAS 1,1'-binaphthyl-2,2'-dithiol

BP86 Becke Perdew exchange-correlation functional

CD circular dichroism

DCM dichloromethane

DFT density functional theory

DIPAMP (Ethane-1,2-diyl)bis[(2-methoxyphenyl)(phenyl)phosphane]

dpb 1,4-diphosphino-1,3-butadiene

DZP double zeta polarized basis set

$\mathbf{E_{elec}}$ electronic energy

fcc face-centered cubic

FIR far-infrared

FWHM full width half-maximum

GGA generalized gradient approximation

GSH L-glutathione

HPLC high-performance liquid chromatography

HOMO highest occupied molecular orbital

LEIST ligand-exchange-induced size/structure transformation

LUMO lowest unoccupied molecular orbital

2-MeBuS *(S)*-2-methylbutanethiolate

2-MeBuSH *(S)*-2-methylbutanethiol

MeOH methanol

MS mass spectrometry

NMR nuclear magnetic resonance

***p*-BBT** *para*-bromobenzene thiol

2-PET 2-phenylethanethiol

***p*-MBA** *para*-mercaptobenzoic acid

PPh_3 triphenylphosphine

2-PPT 2-phenylpropanethiol

SR thiolate

TD-DFT time dependent-density functional theory

TD-DFT+TB time dependent-density functional theory plus tight binding

THF tetrahydrofuran

TZP triple zeta basis set

UV-Vis Ultraviolet-visible

VCD vibrational circular dichroism

XAS X-ray absorption spectroscopy

ZORA zeroth-order regular approximation

ZPE zero-point vibrational energy

1. State of the Art and Research Context

Within this chapter, a brief overview on Au nanoclusters is provided and the necessary background to the research questions addressed in this report is outlined.[a] It should be noted that although the research conducted within the framework of the stay in the USA as a Marshall Plan Scholarship recipient (further discussed in Chapters 2, 3 an 4) was purely of theoretical nature, it was motivated by previous experimental results obtained in Austria, which left open questions best addressed by combining experiment and theory. Thus, also a short overview on experimental techniques for obtaining and characterizing Au nanoclusters will be given in the following. In addition, note that the theoretical research questions and studies mentioned in this introductory section are described from an experimentalists point of view. Certainly, people with a background in theoretical chemistry or physics will approach these topics differently. However, besides summarizing the findings of the research stay at Kansas State University, one aim of this report is to provide an overview on how experiments and theory complement each other and to motivate other experimental chemists working on similar problems to reach out to their theoretical colleagues for input and further insight.

1.1. Au Nanoclusters at a Glance

Within the last decades, interest in Au nanocluster research has grown tremendously, motivated by their special properties which make them interesting for a number of applications.[2–11] Upon reducing the size of gold particles, the properties of the clusters start to deviate significantly from bulk gold: new geometric structures can be observed apart from the face-centered cubic (fcc) pattern[3,5,12–14] and also changes in the electronic structure occur, making these clusters comparable to molecules (instead of bulk metals).[12–15] Furthermore, by the use of organic protecting ligands and precisely optimized synthesis conditions, it has become possible to selectively synthesize Au nanoclusters with defined compositions.[5,13] This has been considered an important advantage compared to the slightly bigger Au nanoparticles, since those usually show size distributions, which can complicate reproducibility of syntheses and applications.[2,5]
Considering the basic structure of such Au nanoclusters, they are generally composed of a Au core that is protected by a monolayer of organic ligands.[5,8] This prevents agglomeration and

[a] This introductory section has been adapted and shortened from a previous version.[1]

thereby formation of bigger particles,[8] thus allowing access to gold cluster sizes even below 1 nm.[14] Depending on the exact nature of these ligands, their binding motifs toward gold can be different.[16] The two most prominent classes of ligands are phosphines (PR_3)[15–17] and thiolates (SR^-)[4,5,8,16] and examples of how the cluster structures are formed with such ligands are illustrated in Figure 1.1. As can be seen, phosphine ligands form end-on bonds with the Au core,[15–17] whereas each thiolate ligand connects to two Au atoms each, thereby creating $-(S–Au–S)_x$ units, often referred to as 'staples'.[14,16,18–20] This 'divide-and-protect' concept was originally described by Häkkinen and coworkers,[21] who conducted theoretical investigations on Au nanoclusters and has later also been detected in the first resolved crystal structure of a thiolate-protected gold cluster.[20] Notably, because of it, two different kinds of Au sites are present in a thiolate-protected Au nanocluster, namely neutral Au(0) atoms in the core and (partially) positively charged Au(I) in the described staple units.[18,19,21]

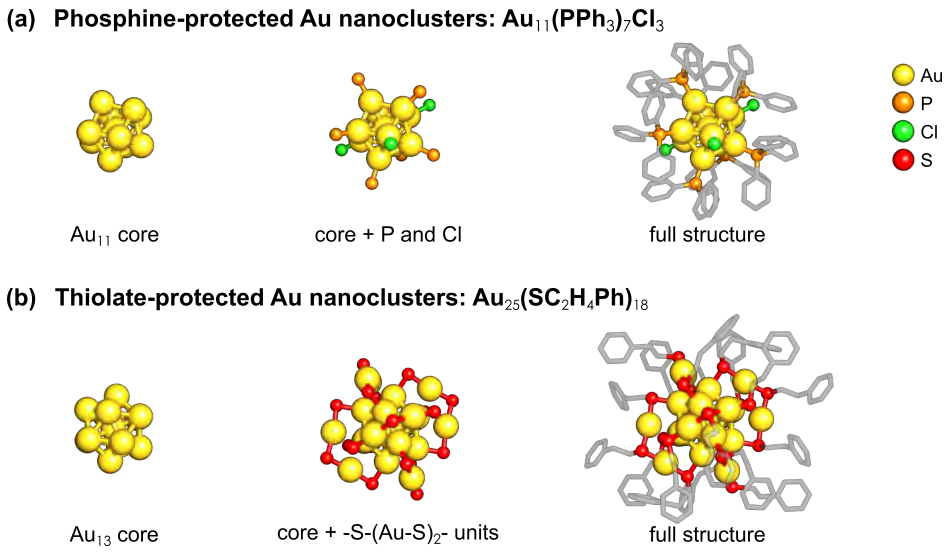

Figure 1.1.: Simplified representation of Au nanocluster structures: (a) $Au_{11}(PPh_3)_7Cl_3$ as an example for phosphine-protected Au nanoclusters and (b) $Au_{25}(SC_2H_4Ph)_{18}$ as an example for thiolate-protected Au nanoclusters. Reproduced with permission from reference[1].

1.2. Experimental Aspects of the Synthesis and Characterization of Au Nanoclusters

A number of detailed synthesis protocols toward different Au nanoclusters is available nowadays,[3,5,10,11,22] which are mostly based on a procedure originally reported by Brust and coworkers.[23] In the standard approach, a Au(III) salt is first dissolved and reacted with a suitable ligand, thereby forming Au(I) species. These are subsequently further reduced to form Au(0) clusters through addition of a reducing agent.[10] In the following, a size focusing

process takes place, which results in the reaction mixture slowly converting toward the most stable species under the present conditions.[5,24] To finally obtain only a single nanocluster size, different work-up protocols have been developed, often based on extraction and/or chromatographic separation procedures.[25] This synthesis process is schematically outlined also in Figure 1.2.
While the described Brust synthesis is a very simple and effective approach and requires no special requirement etc., care must be taken to conduct the procedure exactly as described. Already slight deviations in, for example, the chemicals[24,26–30] or reaction temperatures[24,26,31] can result in formation of different cluster compositions than anticipated.

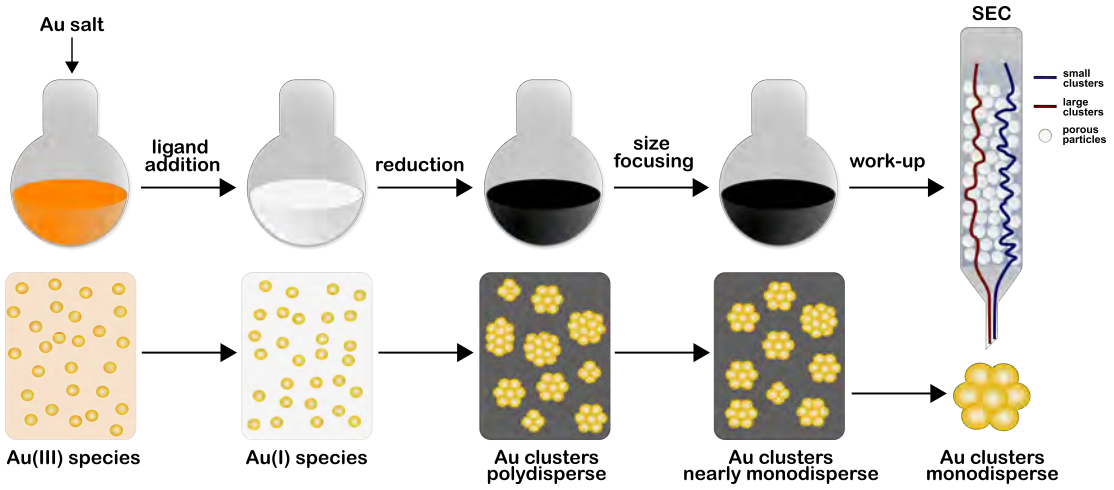

Figure 1.2.: Synthesis scheme of a classical Brust procedure followed by size-exclusion chromatography (SEC) and corresponding Au species present in each step. Note that the ligands are omitted in the illustration of the Au species for clarity. Reproduced with permission from reference[1].

To analyze and characterize the as-synthesized Au nanoclusters, usually a combination of different techniques is used. One of the most feasible ways for an initial assessment is measuring the optical absorption spectra using a Ultraviolet-visible (UV-Vis) spectrometer. Due to the clusters behaving similar to molecules, defined bands associated with their electronic transitions can be observed.[5,10,13,32] The positions of the maxima, as well as the features of the spectra are very characteristic for certain cluster structures and often allow for a first assignment.[17,33,34] The spectra are mainly influenced by the electronic structure of the Au core (i.e. more generally speaking the number of Au atoms in a cluster),[5,32] but also the charge state[35] or ligand sphere[36] can have an influence.
Another technique which is often applied is mass spectrometry (MS), since this allows the determination of the molecular mass of a certain Au nanocluster structure.[10,37–39] It should be noted that due to the high masses and the reduced stability of the metallic nanoclusters (compared to normal measurements of molecules), most measurements protocols applied

nowadays had to be specifically developed. Nevertheless, as of today, it often allows accurate determination of the cluster composition.
Another important aspect is the structure of the cluster (i.e. the core geometry and ligand arrangement), which can be investigated by a number of techniques. The most desired approach is often to resolve its crystal structure by X-ray crystallography,[5,10] however, growing a suitable crystal is often a complicated and time-consuming task, which does not always lead to a successful result.[10] As an alternative, some information on the structure can also be obtained by e.g. nuclear magnetic resonance (NMR)[10,36,40–43] or far-infrared (FIR)[44–46] spectroscopy.

1.3. Explaining Au Nanocluster Properties by Applying Theory – Examples

Obtaining a more thorough understanding of several properties of Au nanoclusters often requires theoretical approaches. Two illustrative examples, the nature of ligand bonding in thiolate-protected Au nanoclusters and a more in depth-understanding of their optical spectra will be briefly discussed in the following. However, also the following two sections explaining topics in Au nanocluster research that are highly relevant for the results presented in Chapters 2, 3 and 4 refer to theoretical studies and results.
To describe and understand the electronic properties of Au nanoclusters, Häkkinen and coworkers applied the superatom model in 2008.[18,19] Following it, several of the molecule-like cluster properties can be interpreted through the existence of superatomic orbitals, including e.g. stability, size-dependent properties and highest occupied molecular orbital (HOMO)–lowest unoccupied molecular orbital (LUMO) gaps.[18,19,47]
The same group also first proposed the so-called 'divide and protect' concept, which categorized the binding of ligands in thiolate-protected Au nanoclusters to be significantly different from the one known from phosphine ligands.[21] Indeed, the existence of the nowadays well-known $-(S–Au–S)_x$ staple structures, which were confirmed experimentally briefly afterwards,[20] were found to be consistent with this concept.[18–20]
Furthermore, theory and especially density functional theory (DFT) has been used to interpret the optical absorption spectra of Au nanoclusters. The bands therein can usually be attributed to discrete electronic transitions, which is related to the superatomic nature of the clusters.[10,13,32] By optimizing the structures of Au nanoclusters with DFT and then simulating their excitations e.g. with time dependent-density functional theory (TD-DFT), calculated spectra can be obtained and the specific transitions investigated. For one prominent example, $[Au_{25}(SH)_{18}]^-$, the bands building up the UV-Vis spectrum have been assigned by Zhu *et al.*[32] in 2008: The HOMO→LUMO transition, which is a sp→sp transition mostly based in the inner Au_{13} core, is responsible for the lowest-energy transition. The next two bands were assigned to a mixture of sp→sp and d→sp transitions and to a d→sp transition. It could be further noted that the ligand influence should be stronger in the HOMO orbital

series, since those are composed of up to 40 % S-based orbitals. Upon transitioning from SH-moieties to ligands typically used in cluster chemistry, such as 2-phenylethanethiol (2-PET), a shift of the bands to higher energies can be expected.[32]

1.4. Ligand Exchange as a Post-Synthetic Modification Tool

In some situations, modification of an as-synthesized gold nanocluster is required. Examples are certain cluster compositions that cannot be directly obtained through synthesis[8,48] or if a specific functionality is to be introduced.[49–55] In such cases, ligand exchange techniques can be applied for Au nanocluster fine-tuning.[49,56] Specifically, a part or even the complete ligand shell of a Au nanocluster is then replaced in a subsequent reaction due to exposure to a solution of a suitable exchange ligand.[49,56–60] Depending on the specific system used, also elevated temperatures might be applied.[48,49,56]

Different reaction outcomes are possible, which are summarized in Figure 1.3. In general, the harsher the conditions (i.e. the excess of exchange ligand, temperature etc.) and the more the original and the new ligand differ from each other, the more drastic the changes to the cluster structure are.[48] One example would be the size transformation from $Au_{11}(PPh_3)_7Cl_3$ to $[Au_{25}(SC_2H_4Ph)_5(PPh_3)_{10}Cl_2]^{2+}$ through exposure to a solution of exchange thiol,[61] a so-called ligand-exchange-induced size/structure transformation (LEIST) process.[48,56] However, reacting a cluster with an exchange ligand significantly similar to the one already present in the original cluster structure (e.g. $Au_{25}(SC_2H_5)_{18}$ with HSC_2H_4Ph, top example in Figure 1.3) will most likely not result in significant changes to the cluster size or geometry and solely the ligand sphere will be affected.[48,49]

The underlying mechanism of these ligand exchange processes is one of the best examples of how beneficial the combination of experiment and theory can be: Through analysis of single crystals of a $Au_{102}(p{-}MBA)_{40}(p{-}BBT)_4$ (with *para*-mercaptobenzoic acid = *p*-MBA and *para*-bromobenzene thiol = *p*-BBT) cluster and DFT studies, it could be attributed to a S_N2-like mechanism.[57]

Furthermore, within the same context of ligand exchange, computational chemistry has for example been applied to investigate preferential exchange positions: Aikens and coworkers showed in studies on $Au_{25}(SR)_{18}$ and $Au_{38}(SR)_{24}$ nanoclusters that the bond between a gold staple atom and the ligand in the middle of a dimeric staple was the least favorable position for ligand exchange reactions with monodentate thiols.[58,59] Moreover, they showed that the ligand exchange process is also highly dependent on the specific precursor cluster structure, since the preferential exchange sites of the Au_{25} cluster were the bonds between the Au atoms in the staple positions and a ligand in terminal position.[58] On the other hand, upon simulating a similar exchange with Au_{38}, replacement at the Au core atoms–ligand bond in the monomeric -S(R)–Au–(SR)- units was the most likely process.[59] Favorable positions for ligand replacement were also determined by Heineke *et al.*[57]

Furthermore, theoretical approaches toward ligand exchange are for example also useful to

predict binding sites and/or ligand conformations of bidentate ligands. This is of special interest since highly resolved NMR spectra or crystal structures would be required for an experimental confirmation, which, as already discussed above, are often not available. To that regard, optimization of different isomers can often provide a good estimate to which configuration would be preferentially formed. In the case of a monosubstituted $Au_{38}(BINAS)(SCH_3)_{22}$ cluster (with BINAS = 1,1'-binaphthyl-2,2'-dithiol), DFT proved that the bidentate exchange thiol replaces two monodentate ligands located in different -S(R)–[Au–S(R)]$_2$- units instead of within the same one.[62] Similarly, inter-staple bonding of 1,1'-binaphthyl-2,2'-dithiol (BINAS) has also been experimentally found in Pd and Pt doped $Au_{25}(BINAS)(SCH_3)_{16}$ clusters employing X-ray absorption spectroscopy (XAS).[63]

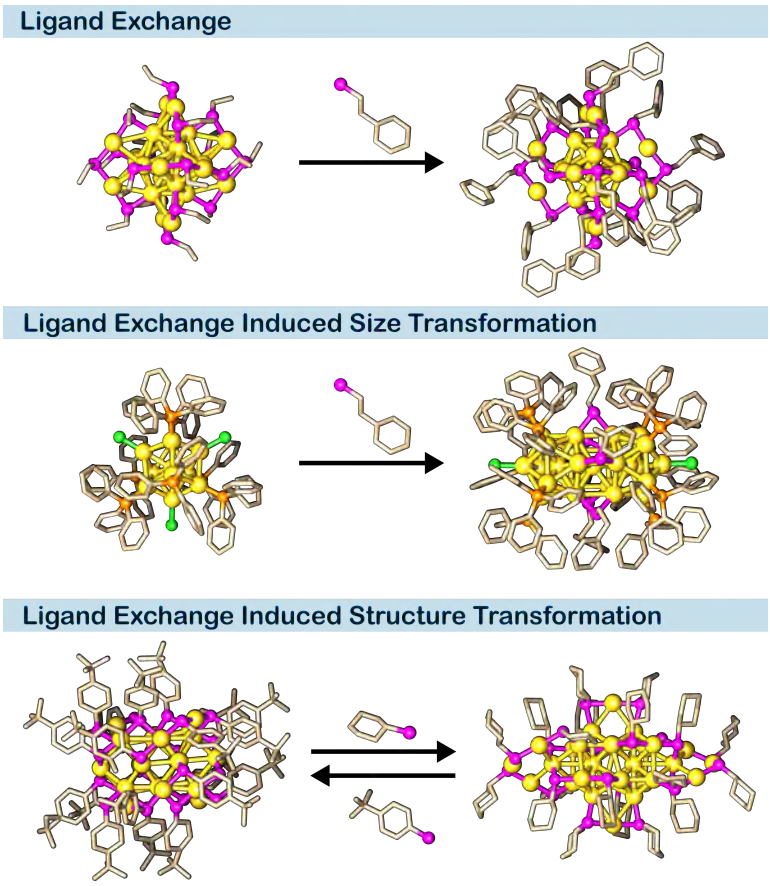

Figure 1.3.: Different ligand exchange processes on Au nanoclusters. Top: ligand exchange from $Au_{25}(SC_2H_5)_{18}$ to Au_{25}(2-PET)$_{18}$, middle: ligand exchange induced size transformation from $Au_{11}(PPh_3)_7Cl_3$ to $[Au_{25}(PPh_3)_{10}$(2-PET)$_5Cl_2]^{2+}$, bottom: reversible ligand exchange induced structure transformation between $Au_{28}(TBBT)_{20}$ and $Au_{28}(SC_8H_{11})_{20}$. Color code: Au = gold, S = magenta, P = orange, Cl = green, C = beige. Reproduced with permission from reference[1].

1.5. Au Nanocluster Chirality

Chirality in Au nanoclusters was first detected in the crystal structures of $Au_{102}(SR)_{44}$ [20] and $Au_{38}(SR)_{24}$.[64] For another famous chiral cluster, $Au_{144}(SR)_{60}$, the existence of a chiral structure has first been predicted by DFT [65] before being experimentally confirmed.[66] These thiolate-protected Au nanoclusters show chirality at the interface between Au core and the sulfur ligands, i.e. different rotatory arrangements of the staple structures.[67,68]
Notably, this structural chirality also influences the electronic structure, which can be probed by circular dichroism (CD) spectroscopy.[67,69] For clusters exhibiting this form of Au–S-interfacial chirality, strong CD signals can be observed in energy ranges typical for transitions dominated by the Au core, indicating the presence of chiral properties in the whole cluster (and not just the Au staple atoms).[67,69–72]
It was further shown that chirality might also be induced to the Au nanocluster structure if chiral ligands were used for protection.[51,73] This was experimentally confirmed by the resulting clusters showing significant CD signals, which could not be attributed to the ligand alone.[69,72–74]
For an increasing number of cluster structures, their chiral properties cannot be related to only a single origin. This has been recently termed as 'hierarchical chirality'.[67,73] Examples of different chiral origins are summarized in Figure 1.4.
Due to the importance of chiral structures in biology and chemistry, chiral Au nanocluster have received widespread attention in the community.[67] Obtaining them in their enantiomeric forms and measuring their chiral properties has become an important objective in the field.[68] However, intrinsically chiral clusters are usually obtained as racemic samples, which requires post-synthetic separation to isolate the individual enantiomers.[67–69] This task has been mostly undertaken by using chiral high-performance liquid chromatography (HPLC),[75–77] which is however only suitable for small amounts. A very effective and feasible approach that also allows for scale-up has recently been reported by Tang and coworkers,[78] who applied a chiral α-cyclodextrin solid phase for separation. Nevertheless, as for all racemate splitting processes, it also has the disadvantage of producing 50% waste if only one enantiomer is needed. The most elegant procedure is therefore a direct synthesis approach wherein the chirality can be directed in a way that one enantiomer of an intrinsically chiral cluster is formed preferentially – ideally even exclusively. This would require addition of a chiral reagent or auxiliary in the synthesis, such as a chiral ligand [79–82] or counter ion.[83] However, publications of such procedures are quite rare and mostly suffer from low yields.[68] To the knowledge of the author, the most 'obvious' pathway of using a monodentate chiral thiol ligand to direct the chirality in thiolate-protected Au nanoclusters has only been demonstrated for $Au_{38}(SR)_{24}$ so far.[79]
The chiral properties of Au nanoclusters have also been investigated by several theoretical groups, mainly applying DFT calculations, see e.g. references [70–72,74,84–86]. It allows, for example, to simulate the CD [70,71,74,84] or vibrational circular dichroism (VCD) [53] spectra of these chiral clusters and to elucidate which transitions/electronic effects are responsible for

the signals. Thus, the structural chirality can be related to the electronic structure, thereby allowing to obtain a more holistic understanding of this phenomenon.[69,87] Several chiral clusters have already been studied using DFT, including e.g. $Au_{25}(SR)_5(BINAP)_4Cl_4$,[88] $Au_{38}(SR)_{24}$,[70] or $Au_{144}(SR)_{60}$.[65,71,85,86] The example of $Au_{144}(SR)_{60}$ also further showcases the need for theoretical approaches in Au nanocluster chemistry: While it has already been possible to simulate its CD spectrum and evaluate the origin of chirality for this specific cluster,[71,85] up to now, the experimental separation of the racemic sample has not been successful.

Another important aspect that needs to be considered when working with intrinsically chiral Au nanoclusters is their stability. In solution at elevated temperatures, the clusters are known to undergo racemization processes and are then of no use anymore as chiral nanomaterials.[77,89] It is therefore important to investigate the 'boundaries' in between which chiral clusters can be handled without risking them undergoing structural dynamics leading to racemization. This can be investigated both experimentally – e.g. by measuring the cd intensity at at different temperatures[77,89,90] – and by applying theory. For example, Häkkinen and coworkers showed that the racemization barrier of the Au_{38} nanocluster can be expected to be around 1.0–1.5 eV by DFT, whereas the one of Au_{144} was expected to be around 2.5–2.8 eV.[86]

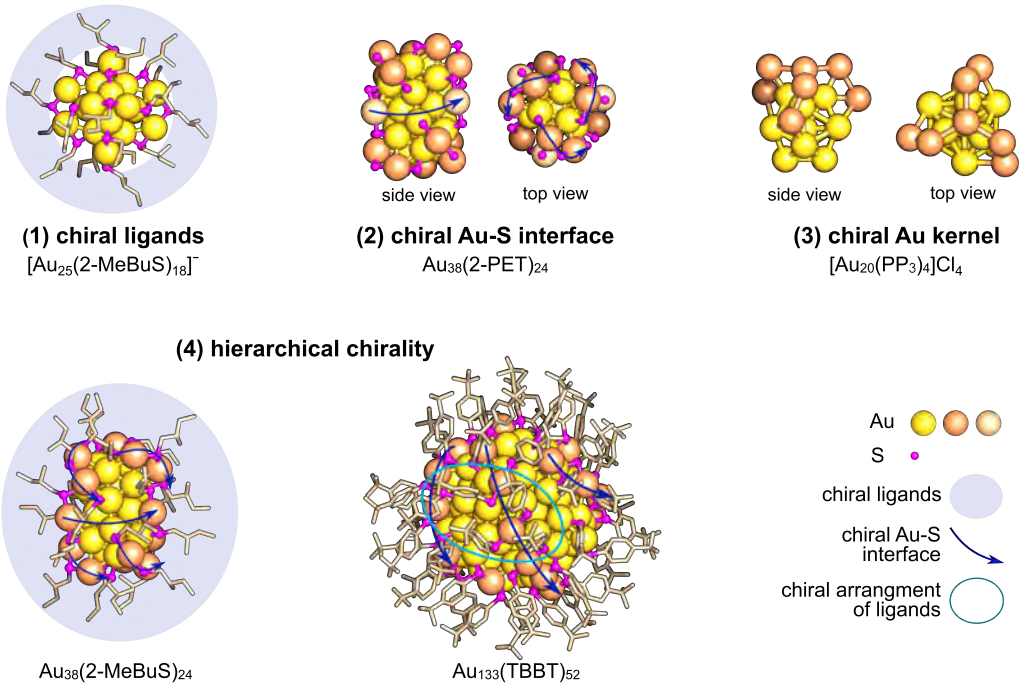

Figure 1.4.: Different forms of chirality in Au nanoclusters: (1) chiral ligands, (2) chiral Au–S interface, (3) chiral Au kernel and (4) hierarchical chirality by combining several different motifs. Note that for $Au_{38}(2\text{-PET})_{24}$, the hydrocarbon backbone of the ligands is omitted for clarity. Similarly, for $[Au(PP_3)_4]Cl_4$, only the chiral core itself is depicted. Reproduced with permission from reference[1].

1.6. Motivation for Theoretical Investigations of Au Nanoclusters within the Scholarship Project

As outlined in the sections above, understanding for example the geometries, optical properties and reactivity of Au nanoclusters often requires a joint effort between theory and experiment. It is common that the experimental results raise questions or lead to hypotheses, which are then further investigated by computations and/or simulations. On the other hand, theory has been able to predict, for example, bonding[21] or chirality[65] in Au nanoclusters quite accurately before being experimentally confirmed by the elucidation of cluster crystal structures.

In the project conducted within the framework of this Marshall Plan Scholarship, the density functional theory computations conducted at Kansas State University were motivated by previous experimental work on these systems at TU Vienna. Specifically, the work mostly focused on two main research questions: (1) investigating which enantiomer of an intrinsically chiral cluster had been formed during synthesis with a chiral ligand and comparing the experimental and theoretical circular dichroism spectra and (2) investigation of nanocluster ligand exchange products in terms of potential stability and binding sites.

2. Density Functional Theory Calculations of $Au_{38}(2\text{-MeBuS})_{24}$ and $[Au_{25}(2\text{-MeBuS})_{18}]^-$

Disclaimer: The content of this Chapter has already been published as a section of reference[1]. Since the results and observations to be reported have not changed since then, no rephrasing has been undertaken.

In experimental work carried out at TU Vienna previously to the research stay at Kansas State University, the chiral thiol ligand *(S)*-2-methylbutanethiol (2-MeBuSH) has been used in the synthesis of Au_{25}, Au_{38} and Au_{144} nanoclusters, resulting in suprisigly high yield of chiral clusters and presumably enantiopure samples after synthesis (instead of racemates). To be able to study the chiral properties of the synthesized clusters protected by 2-MeBuSH, density functional theory (DFT) calculations were carried out. The main objective thereby was to develop an adequate model of the clusters for use in future studies. However, another interest was to confirm which enantiomer of Au_{38} was present after synthesis (i.e. clockwise or counter-clockwise arrangement of the staple units). Due to its size, no DFT calculations were carried out for Au_{144}.

2.1. $Au_{38}(2\text{-MeBuS})_{24}$

Four different model structures of $Au_{38}(2\text{-MeBuS})_{24}$ were made, based on both the $Au_{38}(2\text{-PET})_{24}$ crystal structure[64] (isomer 1), as well as on the lowest energy structure of $Au_{38}(SCH_3)_{24}$ found by Lopez-Acevedo *et al.* (isomer 2), namely structure 1 in their work.[70] To avoid confusion, this structure 1 will be referenced to as *JACS2010* structure in the following. For both structures investigated in the framework of this thesis (isomer 1 and isomer 2), both an anti-clockwise (denoted by an appendix *a*) and a clockwise (denoted by an appendix *b*) conformer was created and optimized. Further refinements of each substructure produced the lowest energy isomers isomers 1a, 1b, 2a and 2b, the energy of which is compared in Table 2.1. The energies of all calculated isomers can also be found in Table A.1.

2.1.1. Comparison of the Crystal Structure and the JACS2010-based Structures of $Au_{38}(2\text{-MeBuS})_{24}$

As can already be seen from Table 2.1, the isomers based on the crystal structure (isomers 1a and 1b) tend to be higher in energy than the JACS2010 ones. This might by explained by the

Table 2.1.: Relative energies of the lowest energy structures of each subcategory. A = anti-clockwise and C = clockwise staple rotation. Isomers 1 are crystal structure [64] based and isomers 2 were obtained starting from the calculated structure by Lopez-Acevedo *et al.* [70] The energies of all calculated isomers can be found in Table A.1.

Enantiomer	**Structure**	**Relative Energy(kJ/mol)**	
		Enantiomer	Overall
A	isomer 1a	30.8	46.5
A	isomer 2a	0	15.7
C	isomer 1b	7.7	7.7
C	isomer 2b	0	0

slightly different arrangements of the ligands for the two structures. [64,70] Figure 2.1 shows a comparison of the two different anti-clockwise isomers 1a and 2a. For isomer 1a, the ligands in the monomeric staple units (see side view in (a)) are mostly facing outwards, whereas the ones of isomer 2a are also a slightly tilted up- and downwards, respectively. This is due to the different orientation of the -S(R)–Au–S(R)- units, which restricts the orientation of the hydrocarbon framework of the 2-MeBuSH ligand in isomer 1a. Furthermore, the top view of the nine ligands in the upper dimeric staple units show that isomer 2a has a very symmetric arrangement of these nine ligands, with each subset (i.e. the three top, middle and bottom ligands in line of sight) mostly following the idealized D_3 symmetry of the cluster. For isomer 1a, the same nine ligands are arranged in a much less symmetric fashion. Whereas the bottom three ligands still take symmetrical positions with respect to each other, the topmost ones as well as the ones in the middle of the staple units do not. This implies that the symmetry of isomer 1a is reduced as compared to 2a, which might be related with higher energy. However, besides symmetry, other structural factors (for example the different arrangement of the monomeric staples and its implication for the orientation of the surrounding ligands) will affect that as well.

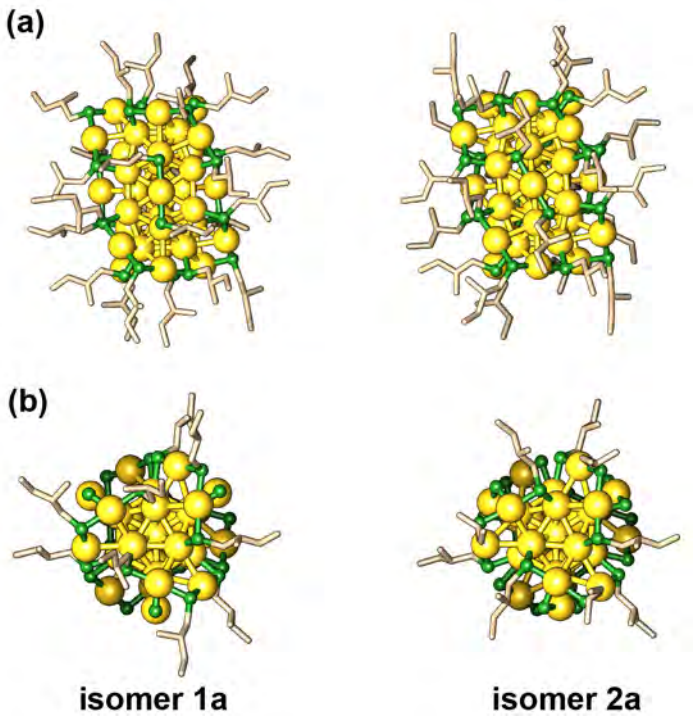

Figure 2.1.: Structures of isomer 1a and 2a: (a) side view and (b) top view. Note that in (b), the hydrocarbon framework of all but the 9 ligands in the dimeric staples on top is not shown to allow for better visualization.

For both isomers, the optical absorption as well as the CD spectrum were calculated using time dependent-density functional theory plus tight binding (TD-DFT+TB). Their comparison is shown in Figure 2.2. As is evident, besides small shifts in the positions of the UV-Vis and CD bands (especially at lower energy), the spectra are not affected much by these structural differences. This could be expected considering that these transitions are not usually sensitive to the ligand conformation.[67] Interestingly enough, isomer 2a shows a significant CD signal at 1295 nm, which is completely absent in isomer 1a.

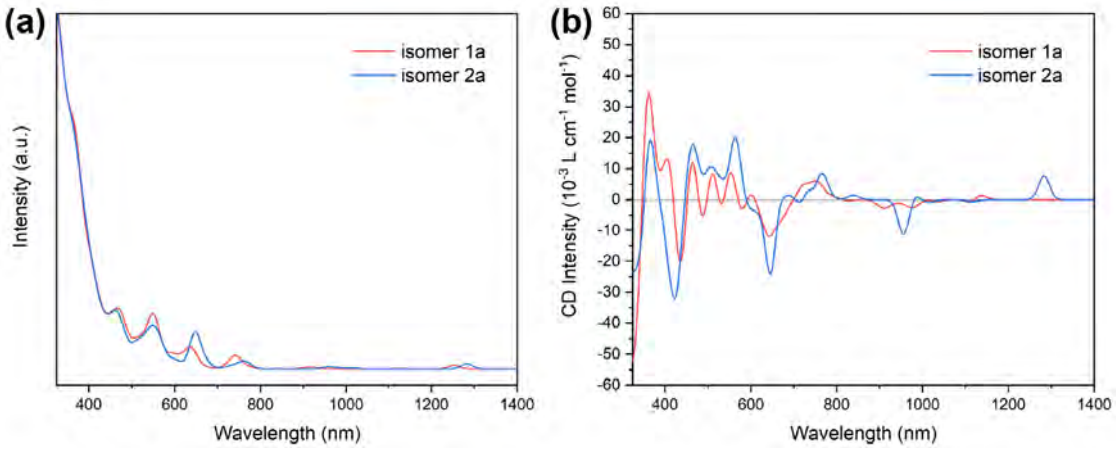

Figure 2.2.: Theoretical UV-Vis (a) and CD spectra (b) of isomers 1a (crystal structure) and 2a (JACS2010) in gas phase.

2.1.2. Comparison of the Different Staple Arrangements of Au_{38}(2-MeBuS)$_{24}$

As previously discussed, $Au_{38}(SR)_{24}$ can have two different orientations of its staple units, i.e. clockwise (C) or anti-clockwise (A) rotatory arrangement. The comparison of both structures is shown in Figure 2.3 and the comparison of the computed spectra in Figure 2.4. Since the differences between the isomers obtained starting from the crystal structure *vs.* the JACS2010 structure were deemed to be minor (especially compared to the deviations one usually observes between experiment and calculations), only the lowest energy anti-clockwise and clockwise isomers, namely 2a and 2b, were used for the following comparison.

As seen from Figure 2.4a, both clusters exhibit a very similar UV-Vis profile and only negligible differences are noted. Since the signal in the CD spectra of Au_{38}(2-MeBuS)$_{24}$ is expected to be mainly due to the chiral Au-S interface,[70] their CD spectra compare to mirror-images (see Figure 2.4b), even though these two clusters are diastereomers (as opposed to a pair of enantiomers). Note that above 800 nm (1.55 eV), the spectra appear to deviate more, which will have to be investigated further in the future. In this energy range, also the deviations between the TD-DFT and the TD-DFT+TB CD spectra of isomer 2b were most pronounced, as shown in Figure A.1.

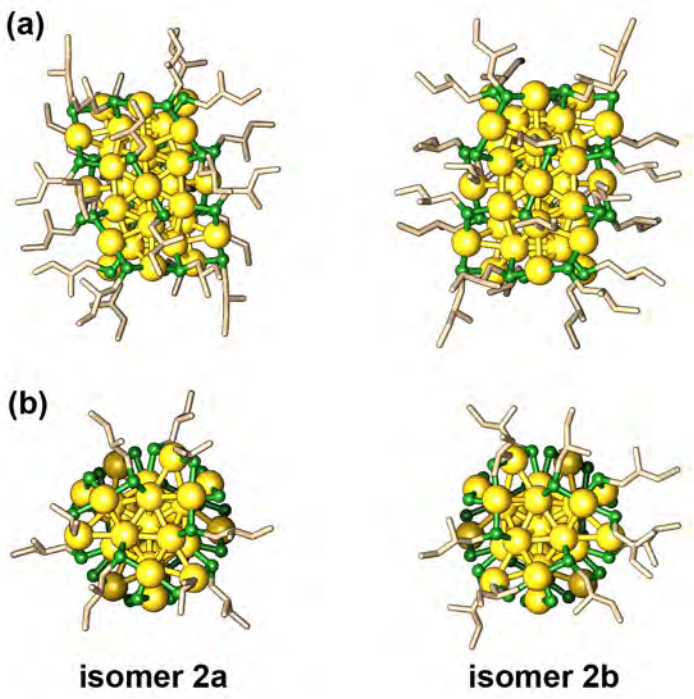

Figure 2.3.: Structures of isomer 2a and 2b: (a) side view and (b) top view. Note that in (b), the hydrocarbon framework of all but the 9 ligands in the dimeric staples on top is not shown to allow for better visualization.

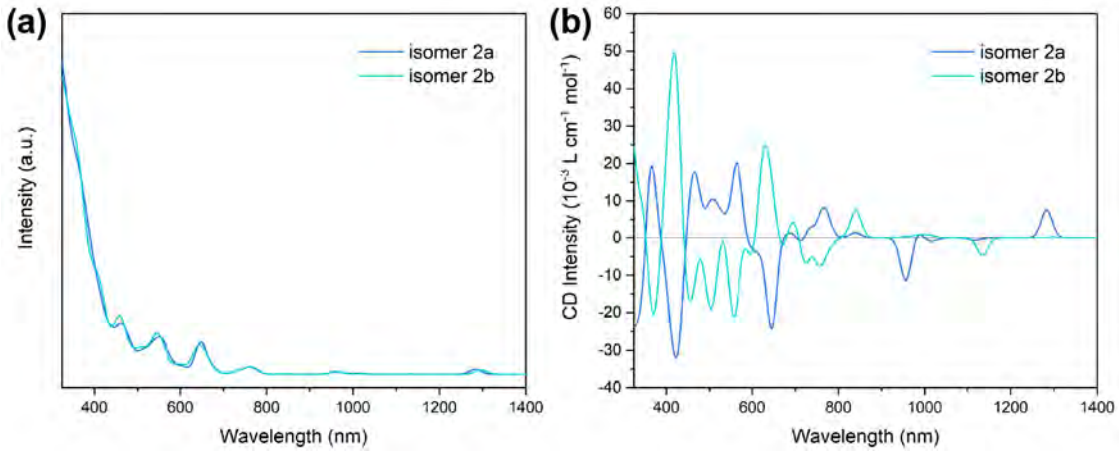

Figure 2.4.: Theoretical UV-Vis (a) and CD spectra (b) of isomers 2a and 2b in gas phase.

It is also worth comparing the spectra of isomer 2b to the JACS2010 structure studied by Lopez-Acevedo *et al.*[70] For both the UV-Vis and the CD spectrum, the shape and positions of the bands are found to be very similar. The lowest energy bands of isomer 2b are located at approximately 1295 nm/0.95 eV, 960 nm/1.29 eV, 765 nm/1.62 eV and 645 nm/1.92 eV and

thus compare well to those observed by Lopez-Acevedo *et al.*[70] The nature of the transitions causing the bands was also studied by them. Summarizing very briefly, the band at 1295 nm is due to the HOMO→LUMO transition, whereas the ones at 960 nm, 765 nm and 645 nm correspond to HOMO→LUMO+2, a mixture of mainly HOMO–1→LUMO and HOMO–2→LUMO and a mixture of several transitions, respectively.[70] Furthermore, also the CD bands of isomer 2b are very similar to the one of the JACS2010 structure (within the energy range that can be compared), except for said absent excitation at around 1295 nm/0.95 eV in isomer 2b. This indicates that the 2-MeBuSH ligand does not induce significant changes to the cluster kernel and staple geometry, which was expected owing to its small size.
To investigate which enantiomer is preferentially formed in a synthesis with *(S)*-2-MeBuSH, the experimental spectra of Au_{38}(2-MeBuS)$_{24}$ were compared to the calculated ones. This comparison is depicted in Figure 2.5. As can be seen in Figure 2.5a, the calculated optical absorption spectra are in good agreement with the experimental one. Note that no offset on the energy axis had to be applied in this case. Furthermore, the experimental CD spectrum mainly follows the same trend as the one of isomer 2b (see 2.5b), strongly indicating that this enantiomer has been formed during synthesis.

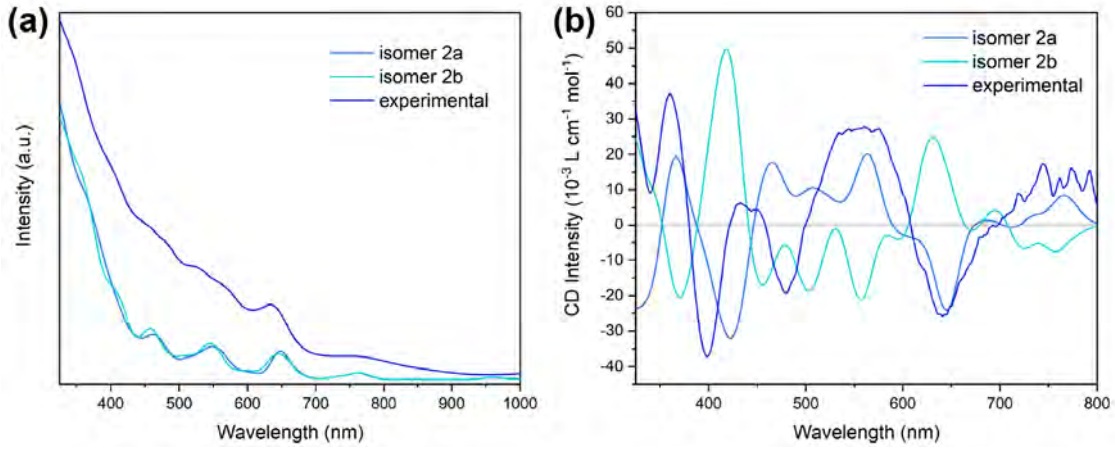

Figure 2.5.: Theoretical spectra of isomers 2a and 2b in gas phase and experimental spectrum of Au_{38}(2-MeBuS)$_{24}$: (a) UV-Vis and (b) CD spectra. Note that the experimental UV-Vis spectrum is offset on the intensity axis from the theoretical ones to allow for better visualization.

Interestingly, the isomers with the anti-clockwise staple unit arrangement (isomers 1a and 2a) are higher in energy than their clockwise counterparts at the level of theory used (see Table 2.1). Nevertheless, the comparison with experiment shows that this enantiomer is preferentially obtained when using *(S)*-2-MeBuSH as protecting ligand. As of yet, it is unclear if the same energy trend would also be observed at a different level of theory. Furthermore, it might also be possible that kinetic effects during the formation and size focusing of the clusters during the synthesis are responsible for the directed chirality observed in this case.

2.2. $[Au_{25}(2\text{-MeBuS})_{18}]^-$

The structure of $[Au_{25}(2\text{-MeBuS})_{18}]^-$ obtained after optimization at BP86/DZP level of theory is depicted in Figure 2.6. This cluster has an achiral arrangement of its dimeric staple units, thus, its chiral properties are solely due to induction by the chiral *(S)*-2-MeBuSH ligand. The theoretical optical absorption and the CD spectrum of $[Au_{25}(2\text{-MeBuS})_{18}]^-$ are presented in Figure 2.7 and compared to the experimental spectra. As can be seen, the energies of the optical absorption bands are significantly underestimated by TD-DFT+TB at this level of theory. This has been reported for Au_{25} calculated with the BP86 functional before.[32,91] For better visualization, the theoretical spectrum was shifted by +0.48 eV and then shows acceptable agreement with the experimental spectrum, especially considering the shape of the bands.

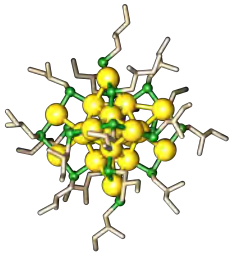

Figure 2.6.: Calculated structure of $[Au_{25}(2\text{-MeBuS})_{18}]^-$.

However, for the CD spectra, significant deviations are noticed as well, which cannot be corrected by a shift of the energy axis only. This shows that the current cluster model is not sufficient for comparison to the experiment. Further refinement, for example at a different level of theory, would be required.

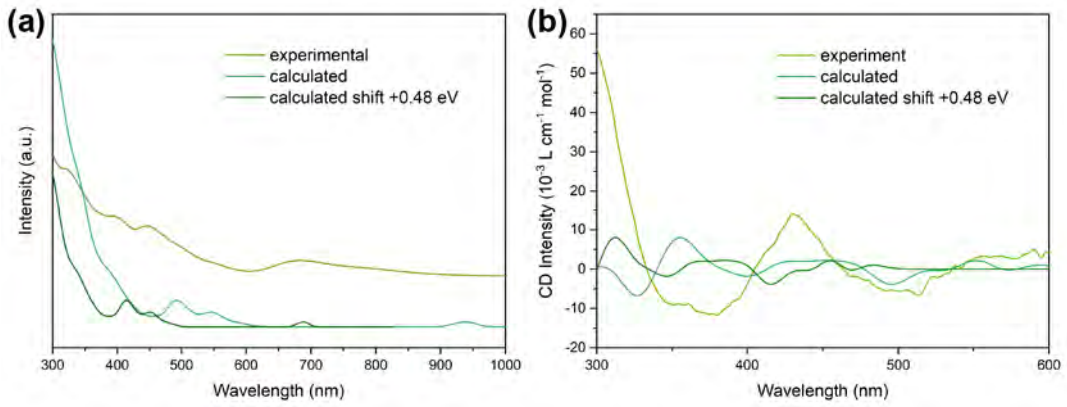

Figure 2.7.: Theoretical spectra of $[Au_{25}(2\text{-MeBuS})_{18}]^-$ in gas phase and experimental spectrum: (a) UV-Vis and (b) CD spectra. Note that the experimental UV-Vis spectrum is offset on the intensity axis from the theoretical ones to allow for better visualization.

2.3. Conclusions

Both $[Au_{25}(2\text{-MeBuS})_{18}]^-$ and $Au_{38}(2\text{-MeBuS})_{24}$ were optimized employing DFT at the BP86/DZP level of theory. For Au_{25}, the energies of the transitions were significantly red-shifted compared to the experiment, which has been reported for this cluster species before. The comparison of the theoretical and experimental CD spectra shows that the computational model structure still has to be improved. For Au_{38}, the simulated optical absorption spectrum is in good agreement with the experimental one. Four different substructures were generated based on the published crystal structure and a calculated one (JACS2010). The isomers obtained starting from the crystal structure coordinates were found to be higher in energy, which was attributed to structural differences and lowering of symmetry. Comparison of the experimental CD spectrum with the calculated ones using TD-DFT+TB indicated that the structure with anti-clockwise rotary arrangement of the staples is preferentially formed. However, these isomers (1a and 2a) were found to be higher in energy than the clockwise ones. Further calculations are required to determine if the same trend is also observed at a different level of theory.

3. Chiral Ligands on a Biicosahedral Au_{25} Cluster

As outlined already in the Introduction, ligand exchange can be a useful tool for introducing certain functionality after synthesis. However, while the number of exchanges ligands can be easily determined by mass spectrometry,[37–39] obtaining information about their conformation can be a more difficult task – especially in the case of bidentate ligands. Thus, the research presented in this Chapter followed mainly two objectives: (1) studying the influence of such chiral bidentate phosphine ligands on the optical absorption and circular dichroism spectra and (2) investigating different ligand conformations and finding a lowest energy isomer.

3.1. Testing the Model Accuracy with a Cluster with Chiral Thiolates

In a first step, the published crystal structure by Shichibu *et al.*[61] was adapted using MacMolPlt and the original thiolate ligands replaced by gas phase optimized structure of *(R)*-2-phenylpropanethiol (2-PPT). Three different isomers were created and subsequently optimized at the BP86/TZP level of theory (same also for all other DFT calculations in this Chapter). Figure 3.1 shows the lowest energy structure and their relative energies are summarized in Table 3.1. One can see that the energies are reasonably close to each other. Since this structure was not the main object of study in this project, no further isomers were optimized.

Table 3.1.: Relative energies of the $[Au_{25}(PPh_3)_{10}(SC_3H_6Ph)_5Cl_2]^{2+}$ isomers.

iso#	**Relative Energy (kJ/mol)**
1	0.0
2	8.8
3	31.2

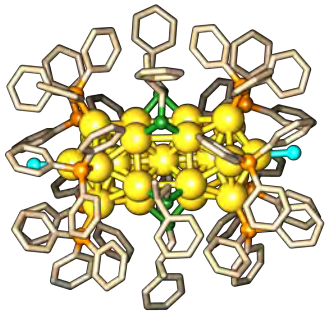

Figure 3.1.: Calculated structure of $[Au_{25}(PPh_3)_{10}(SC_3H_6Ph)_5Cl_2]^{2+}$. Color code: Au = yellow; P = orange; S = green; Cl = cyan; C = beige.

To obtain some comparison between experiment and theory, the optical absorption and circular dichroism spectrum of the cluster was simulated employing TD-DFT+TB. Refer to Chapter 5 for computational details. Figure 3.2 shows the calculated spectra. Comparison with the data published by Zhu *et al.*[92] shows that the bands in the simulated spectra appear significantly red-shifted (by roughly 0.5 eV) compared to the experimental optical absorption and CD spectra. Similar effects have already been observed for $[Au_{25}(2\text{-MeBuS})_{18}]^-$ (see Chapter 2 and are also reported in literature.[32,91] Aside from that, the qualitative agreement between the spectral features seems reasonable.

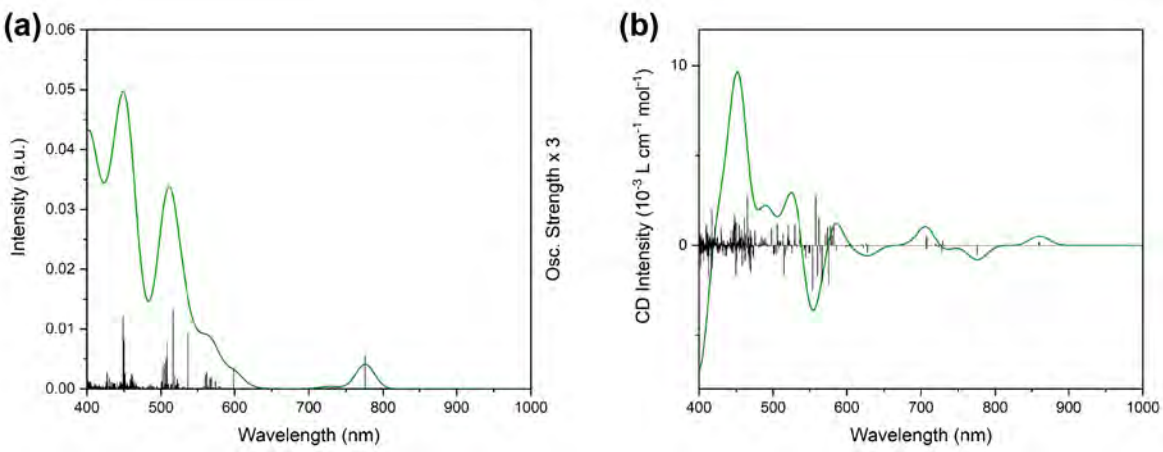

Figure 3.2.: Theoretical optical absorption (a) and circular dichroism spectra (b) of $[Au_{25}(PPh_3)_{10}(SC_3H_6Ph)_5Cl_2]^{2+}$ isomer #1.

3.2. Introducing BINAP Ligands to $[Au_{25}(PPh_3)_{10}(SC_2H_4Ph)_5Cl_2]^{2+}$

To study the binding motifs of biicosahedral C_2-symmetric phosphine ligands and their influence on the chiral properties of the Au nanocluster, exemplary clusters structures containing

one or two such ligands were created and optimized. The specific ligand investigated in this project was *(S)*-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) (see Figure 3.3a). To save on computational costs, first optimizations were performed not with the full ligand, but with the smaller model ligand 1,4-diphosphino-1,3-butadiene (dpb) (see Figure 3.3b).[74] Previous studies by Aikens and coworkers clarified that this substitution only alters the CD spectrum below 350 nm, at which energy range transitions from ligand based orbitals start to contribute significantly.[74] Thus, this exchange seems justified.
To achieve the most suitable comparison to the experimental work conducted by the author, replacement of ligands with *(S)*-BINAP started from a $[Au_{25}(PPh_3)_{10}(SC_2H_4Ph)_5Cl_2]^{2+}$ structure, which, in turn, was obtained by replacing the 2-PPT ligands on $[Au_{25}(PPh_3)_{10}(SC_3H_6Ph)_5Cl_2]^{2+}$ (Section 3.1) with 2-PET, followed by an optimization. Subsequently, dpb ligands were introduced and another optimization carried out. Note that all binding positions are symmetry equivalent for this first ligand substitution.
The relative energies of the cluster with one bidentate phosphine ligand are shown in Table 3.2. The dpb ligand on the lower energy isomer (isomer #2) was then replaced with BINAP (in two conformations, iso#2 and iso#2') and subjected to another optimization. Finally, the CD spectra of the lowest energy isomers (isomer #2 for both) were calculated, which are compared in Figure 3.4. The individual spectra of each isomer are shown in the Appendix in Figure A.8 (dpb) and Figure A.9 (BINAP). The inset of Figure A.9a also shows the structure of isomer #2 with the *(S)*-BINAP ligand.

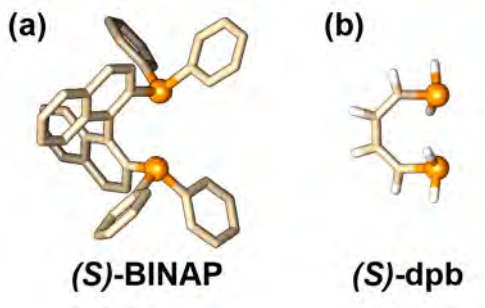

Figure 3.3.: Calculated structures of (a) *(S)*-BINAP and (b) *(S)*-dpb. Color code: P = orange; C = beige; H = white. The H atoms have been ommitted in (a) for clarity.

As can be seen from Figure 3.4, both the UV-Vis and CD spectra with the two ligands are very similar, which indicates that substituting the significantly larger BINAP ligand for the smaller dpb model is justified. However, the spectra are also quite comparable to the one obtained when using chiral thiolate ligands (see Figure 3.2) – even in the sign. This indicates that they affect the Au oritals in a similar way.
However, comparison with the experimental CD spectrum of a biicosahedral Au_{25} cluster fully protected by *(S)*-BINAP and chloride ligands[88] shows significant differences. This might be explained by more pronounced structural and electronic effects on the Au core if multiple bidentate C_2 ligands are used.

Table 3.2.: Relative energies of the $[Au_{25}(PPh_3)_8L(SC_2H_4Ph)_5Cl_2]^{2+}$ isomers, with L = *(S)*-dpb or *(S)*-BINAP. Note that both structures with *(S)*-BINAP originated from the *(S)*-dpb isomer #2 by replacing the bidentate ligand with two different conformations of *(S)*-BINAP (isomer #2 and #2').

	Relative Energy (kJ/mol)	
iso#	dpb	BINAP
1	20.1	-
2	0.0	0.0
2'	-	7.1

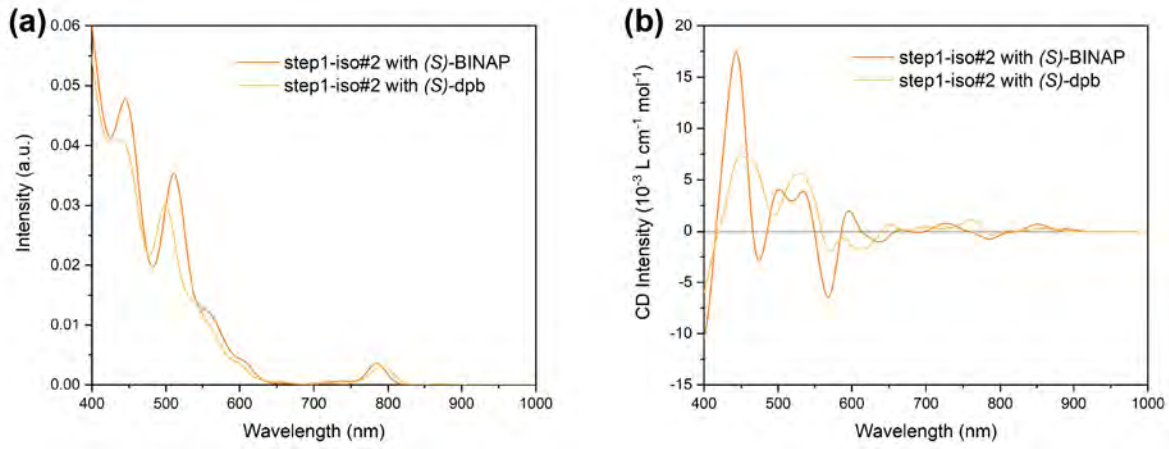

Figure 3.4.: Comparison of the theoretical optical absorption (a) and circular dichroism spectra (b) of $[Au_{25}(PPh_3)_8(\textit{(S)}-dpb)(SC_2H_4Ph)_5Cl_2]^{2+}$ isomer #2 and $[Au_{25}(PPh_3)_8(\textit{(S)}-BINAP)(SC_2H_4Ph)_5Cl_2]^{2+}$ isomer #2.

Next, starting from isomer #2 containing dpb, a second dpb ligand was introduced. In contrast to the first ligand, the positions are not equivalent anymore. To specify, four different positions for replacement are possible, which are depicted in Figure 3.5. Optimization of all four structures results in the energies displayed in Table 3.3. As can be seen, adding another ligand on the same icosahedron core is significantly less favorable than the three possibilities on the second core: eclipsed configuration (isomer #2), neighboring positions (isomer #3) and opposite positions (isomer #4); viewed from the front. Among those three, the two dpb ligands seem to prefer positions next to eachother (isomer #3). However, also the eclipsed position is only slightly higher in energy (isomer #2).

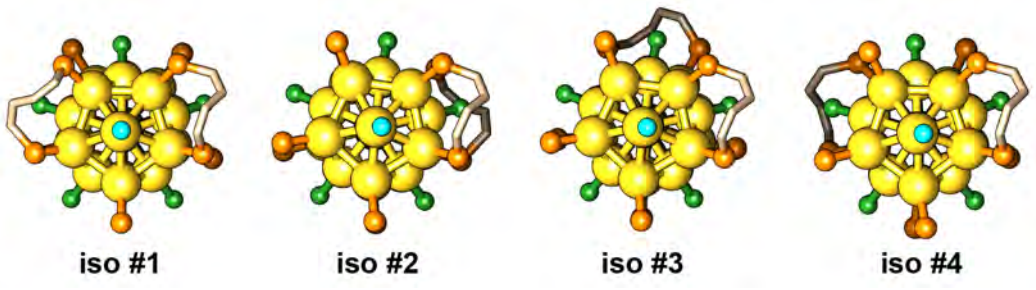

Figure 3.5.: Front view on the calculated structures of $[Au_{25}(PPh_3)_6(dpb)_2(SC_2H_4Ph)_5Cl_2]^{2+}$: both ligands on the same icosahedran (isomer #1), eclipsed configuration (isomer #2), neighboring positions (isomer #3) and opposite positions (isomer #4). Color code: Au = yellow; P = orange; S = green; Cl = cyan; C = beige. Note that all other ligand frameworks expect for the one of *(S)*-dpb have been ommitted for clarity.

The difference in energy of isomers #2–#4 is not too big, which is why all three options were also attempted with the full BINAP ligands in place. This was done since differences in the binding positions of dpb and BINAP seemed possible at this point due to the increased bulkiness of BINAP, as well as its ability to form π–π-stacking interactions of the phenyl rings. As can be seen from Table 3.3, the most favorable second binding site of dpb and BINAP is indeed different: Whereas the lowest energy isomer for dpb featured the two bidentate ligands on two different cores, but situated next to eachother (front view line of sight), the two BINAP ligands tend to take opposite positions. This might indeed be related to them being significantly bigger than the dpb model ligand.

Table 3.3.: Relative energies of the $[Au_{25}(PPh_3)_6L_2(SC_2H_4Ph)_5Cl_2]^{2+}$ isomers, with L = *(S)*-dpb or *(S)*-BINAP. Note that the structures with *(S)*-BINAP originated from the corresponding *(S)*-dpb isomer by replacing the bidentate ligand with *(S)*-BINAP.

	Relative Energy (kJ/mol)	
iso#	dpb	BINAP
1	34.0	-
2	4.2	4.6
3	0.0	8.1
4	16.9	0.0

It also indicates that isomer #1 indeed should not need to be considered with BINAP, since this would be the most sterically demanding configuration. Of note, the second best isomer found for this step does indeed feature an ecplised configuration, which might be related to favorable longer-range interactions. However, to confirm this, a more thorough isomer search would have to be conducted, especially considering that all three isomers are still quite

close in energy. The current lowest energy structure obtained with two BINAP ligands on a biicosahedral Au_{25} cluster (isomer #4) is presented in Figure 3.6.

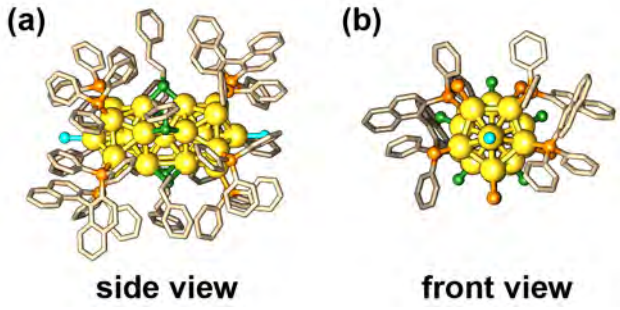

Figure 3.6.: Calculated structure of $[Au_{25}(PPh_3)_6(BINAP)_2(SC_2H_4Ph)_5Cl_2]^{2+}$ isomer #4 (lowest in energy): (a) side view and (b) front view. Color code: Au = yellow; P = orange; S = green; Cl = cyan; C = beige. In (b), all other ligand frameworks expect for the one of *(S)*-BINAP have been ommitted for clarity.

3.3. Conclusions

The introduction of chiral ligands into biicosahedral Au_{25} clusters was studied by DFT calculations. Both introduction of chiral thiolates with an achiral C atom (*(R)*-PPT) and a C_2-symmetric ligand (*(S)*-BINAP) resulted in circular dichroism activity of the clusters. Notably, the observed transition are mostly independent of the exact ligand used, as becomes evident through the very similar CD spectra of all isomers. Nevertheless, the signal intensity was higher when the bidentate phosphine ligand was used. Comparison to published experimental spectra showed that the bands appear shifted to lower energy, which is a known phenomenon when calculating excitation spectra of Au nanoclusters.
Regarding the substitution site of a second incoming bidentate phosphine ligand, this was first tested with the simpler model ligand *(S)*-dpb. Adding a second ligand on the same biicosahedron resulted in the highest energy, whereas the structure with the two ligands on two cores in neighboring gauche-like positions exhibited the lowest energy. When optimizing the structures with *(S)*-BINAP instead, the lowest energy isomer was the one with the two bulky ligands facing away from each other.
In the next steps, further CD spectra of the isomers with more than one bidentate ligand in the structure should be calculated and compared to the previous ones. Furthermore, also introducing even more bidentate phosphines (up to four) should be investigated and compared to experimental data.

4. Potential Structural Transformations in Ligand Exchange Reactions of $Au_{11}(PPh_3)_7Br_3$

One of the most common phosphine-protected clusters, $Au_{11}(PPh_3)_7Br_3$, is well known to undergo ligand exchange with different thiolates.[36,61,93–97] For example, exposure to organic exchange thiols leads to incomplete replacement of the ligand sphere and formation of biicosahedral $[Au_{25}(PPh_3)_{10}(SR)_5X_2]^{2+}$ clusters (with X = halide).[61,96] This exchange has already been reported by Hutchison and coworkers in the early 2000s,[94,95] however, the cluster was only later crystallized and its structure resolved in 2007 by Tsukuda and coworkers.[61] Notably, exposure to the polar thiol ligand L-glutathione (GSH) results in formation of $Au_{25}(SR)_{18}$ clusters instead.[36,93] Further investigation of this specific exchange reaction by McKenzie *et al.*[36] showed that in fact only one Au_{11} isomer, namely $Au_{11}(PPh_3)_7X_3$ does undergo this size/structure transformation, whereas its analogue $[Au_{11}(PPh_3)_8X_2]X$ does only produce decomposed cluster fragments in the water phase after exchange.
Nevertheless, experimental investigations by the author showed an indication that the ligand exchange pathway might indeed by different when the organic thiol 2-PET is used: Just a few minutes into the exchange, changes in the clusters' UV-Vis spectrum occur, which are potentially related to a structural transformation from $Au_{11}(PPh_3)_7X_3$ to $[Au_{11}(PPh_3)_8X_2]X$. This assumption is mainly based on a comparison with the spectra of both clusters reported by McKenzie *et al.*[36] and needs to be further addressed by different experiments and additional computations, which are currently in progress. In the following, only a brief summary of the results from the DFT calculations conducted up to now is provided. It needs to be noted that since not all data were available at the time this report was completed, the hypotheses made here require further confirmation.

4.1. Estimated Ligand Binding Energies

In an effort to reduce the amount of potential structures/transition states to investigate, the aim was to briefly evaluate different possible pathways first. In principle, different mechanisms are possible for ligand exchange reactions: (1) a concerted reaction in which binding of the new and dissociation of the old ligand happen simultaneously (S_N2 type) and (1) dissociation of the old ligand followed by binding of the new one in a second step (S_N1

type).[98] Previous studies on ligand exchange with Au nanoclusters have suggested the former to be more likely.[57,98,99] However, these studies were conducted for thiolate-for-thiolate exchanges, whereas the initial exchange site in $Au_{11}(PPh_3)_7Br_3$ will be a Au–P or Au–Br bond. Thus, also structures with dissociated ligands have been investigated to determine the binding energy at these specific positions.

Indeed, an extensive study by Hutchison and coworkers[100] on the mechanism of the ligand exchange reaction between phosphine-protected Au nanoclusters and non-polar thiolates has found no evidence of free triphenylphosphine (PPh_3) in the reaction solution. Their NMR experiments showed indication of the reaction progressing in three steps, which presumably occur to some extent simultaneously: (1) a rapid dissociation of $AuCl(PPh_3)$ units from the particle and simultaneous binding of the incoming thiolate; (2) dissociation of either free PPh_3 or direct binding to a $AuCl(PPh_3)$ compound located nearby (once no more halides are available for $AuCl(PPh_3)$ formation); and (3) reorganization of the thiolate ligand sphere on the exchanged particle.

This is significantly different to the suggested mechanism for a single thiolate-for-thiolate exchange on a $Au_{11}(PPh_3)_7(SR)_3$ cluster, for which DFT calculations suggested an associative mechanism,[101] comparable to the results from thiolate-protected Au nanoclusters.[57,98,99] Furthermore, it was found that longer organic frameworks of the exchange ligand increase the reaction energy, as well as a strong dependence on the overall ligand structure, indicated by a significant decrease in the reaction energy when cysteine was used as exchange ligand.[101]

The dynamic nature of the phosphine ligands has also been adressed by NMR studies by Petroski *et al.*,[102] which indicated that the phosphine ligands on PPh_3-protected Au nanoclusters exchange rapidly, leading to magnetic equivalence in the spectra.

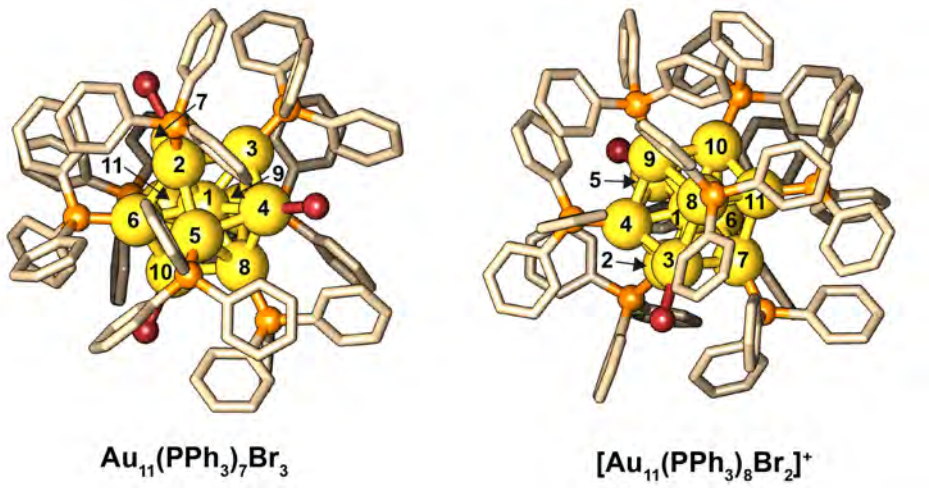

Figure 4.1.: The two forms of the Au_{11} nanocluster with the relevant Au–ligand positions marked with numbers. Color code: Au = yellow; P = orange; Br = red; C = beige.

The two different optimized Au_{11} isomers investigated in this project are shown in Figure 4.1. The different positions at which substitution can occur are marked with the number of the Au atom at this site (numbers 2–11; 10 exchange positions per cluster). The Au atom #1 is located in the core center. All structures studied were derived from the crystal structures of $Au_{11}(PPh_3)_7Cl_3$ and $[Au_{11}(PPh_3)_8Cl_2]Cl$ reported by McKenzie *et al.*[36] by replacing Cl with Br using the MacMolPlt software.[103] Table 4.1 shows the binding energy of the PPh_3 and bromide ligands at each position derived by Equations (4.1)–(4.4). The gas phase optimized structures of the clusters (BP86/TZP level of theory for all calculations in this Chapter) and the ligands were used for this estimation. The energies of the 'dissociated' forms of the clusters were obtained by removing one ligand per cluster (for each position) and performing a single point calculation without further optimization.

$$E_{BE,elec}(PPh_3) = E_{elec}(Au_{11}(PPh_3)_6Br_3) + E_{elec}(PPh_3) - E_{elec}(Au_{11}(PPh_3)_7Br_3) \quad (4.1)$$

$$E_{BE,elec}(Br^-) = E_{elec}([Au_{11}(PPh_3)_7Br_2]^+) + E_{elec}(Br^-) - E_{elec}(Au_{11}(PPh_3)_7Br_3) \quad (4.2)$$

$$E_{BE,elec}(PPh_3) = E_{elec}([Au_{11}(PPh_3)_7Br_2]^+) + E_{elec}(PPh_3) - E_{elec}([Au_{11}(PPh_3)_8Br_2]^+) \quad (4.3)$$

$$E_{BE,elec}(Br^-) = E_{elec}([Au_{11}(PPh_3)_8Br]^{2+}) + E_{elec}(Br^-) - E_{elec}([Au_{11}(PPh_3)_8Br_2]^+) \quad (4.4)$$

Table 4.1.: Estimated electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7') and $[Au_{11}(PPh_3)_8Br_2]^+$ ('Au11P8'). Gas phase optimized structures of Au11P7, Au11P8 and PPh_3 were used. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position and calculation of the single point energy. For better visibility, the position with halide atoms are marked in blue.

	Au11P7		**Au11P8**	
pos#	PPh_3/Br	Energy (kJ/mol)	PPh_3/Br	Energy (kJ/mol)
2	P	122.2	P	126.9
3	P	130.4	Br	531.5
4	Br	378.7	P	133.3
5	P	123.2	Br	540.9
6	P	123.0	P	109.6
7	Br	379.3	P	115.9
8	P	110.8	P	122.1
9	P	130.6	P	113.4
10	Br	378.6	P	113.6
11	P	131.2	P	102.9

As can be seen, the energy required for removal of a phosphine ligand is comparable between the two clusters, with slightly lower energies for $[Au_{11}(PPh_3)_8Br_2]^+$. These energies are in a

similar range as the ones determined by Ligare *et al.*[104] for triphenylphosphine-protected Au_8 nanoclusters. Slight differences can be noticed for the different positions: For $Au_{11}(PPh_3)_7Br_3$, the most favorable position for PPh_3 dissociation is pos#8, with all other being about 11–20 kJ/mol higher in energy. For $[Au_{11}(PPh_3)_8Br_2]^+$, the best position to remove a PPh_3 ligand is pos#11 (also being the most favorable exchange site overall). Note that when comparing the core structures of the two clusters, this specific pos#11 in $[Au_{11}(PPh_3)_8Br_2]^+$ would become pos#4 in $Au_{11}(PPh_3)_7Br_3$, which features a Au–Br bond. Thus, one should expect the phosphine at this position to be the most weakly bonded one.
Removing a halide, on the other hand, is significantly higher in energy in both cases. However, in this case, also a pronounced difference between the two cluster structures is found, with $[Au_{11}(PPh_3)_8Br_2]^+$ exhibiting even higher binding energies for Br than $Au_{11}(PPh_3)_7Br_3$. This is presumably related to the former already bearing a positive charge, which would increase even further upon removing a second halide atom. This strong charge separation can be considered an unfavorable reaction for these systems since being optimized in vacuum. It thus computes artificially high energies, even though one might expect the Au–Br bond to be weaker than Au–P.

4.2. Influence of Solvent and Dispersion

To improve the performance of these estimations, solvation was included in the calculations by employing the SM12 solvent model.[105,106] Four different solvents were investigated: toluene, dichloromethane (DCM), tetrahydrofuran (THF) and methanol (MeOH) – the choice of which was based on commonly used solvents with Au_{11} nanoclusters. The previously optimized structures of $Au_{11}(PPh_3)_7Br_3$ and $[Au_{11}(PPh_3)_8Br_2]^+$ without solvation were used and solvation was only applied for the calculation of the single point energies. The results of these calculations are presented in Table 4.2 for $Au_{11}(PPh_3)_7Br_3$. Refer to Table A.3 for energies of $[Au_{11}(PPh_3)_8Br_2]^+$.
Compared to a cluster in vacuum, ligand removal becomes more favorable in a solvent environment. For dissociation of a bromide ligand, a clear trend can be observed: the binding energy decreases with increasing polarity, which can be attributed to better stabilization of the charged compounds (cluster and free bromide ligand) after dissociation. Whereas a strong reduction in energy is observed when moving from gas phase to toluene and further to THF, the improvements are significantly smaller from THF to DCM. Especially for clusters in THF and DCM, similar values are observed. The trend is comparable for PPh_3, however, not nearly as pronounced. While using a toluene or THF environment instead of vacuum leads to a clear energy reduction, almost no change in energy is observed when further increasing the solvent polarity.
It should be noted that when considering solvation effects, the trend that a PPh_3 ligand is easier to remove than a halide one reverses upon transitioning from toluene to THF: While it seems more favorable to dissociate a PPh_3 ligand from a $Au_{11}(PPh_3)_7Br_3$ cluster in vacuum

or toluene, the removal of bromide is lower in energy when THF, DCM or MeOH are the solvents.
Furthermore, also addition of a dispersion correction (DFT-D3 by Grimme)[107] was attempted. Table 4.3 shows the difference between the binding energies derived from a $Au_{11}(PPh_3)_7Br_3$ optimized with and without dispersion correction. The full tables with all energies can be found in the Appendix in Tables A.3 and A.4.

Table 4.2.: Estimated electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7'). Gas phase optimized structures of Au11P7 and PPh_3 were used. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations in a solvent environment, solvation was included using the SM12 model. For better visibility, the position with halide atoms are marked in blue.

		Energy (kJ/mol)				
pos#	PPh3/Br	gas phase	toluene	THF	DCM	MeOH
2	P	122.2	107.7	97.4	97.1	95.5
3	P	130.4	116.4	106.6	107.2	107.2
4	Br	378.7	177.0	77.0	71.1	46.4
5	P	123.2	109.0	98.8	98.6	97.4
6	P	123.0	108.6	98.5	98.3	96.8
7	Br	379.3	177.5	77.6	72.0	46.7
8	P	110.8	101.4	93.1	91.9	92.6
9	P	130.6	116.8	107.0	107.3	107.6
10	Br	378.6	177.0	77.2	71.4	46.0
11	P	131.2	117.4	107.8	108.5	108.1

As is evident, including a dispersion correction in the optimization raises the energy necessary to remove any ligand from the cluster (energy differences 'd-nd' in Table 4.3). The effect is significantly more pronounced for the phosphine ligands, but also removal of Br^- becomes more endothermic. Nevertheless, as can be seen from Table A.3, halide dissociation is now already favored over the phosphine one even in a very non-polar solvent such as toluene. Moreover, the difference $\Delta_{\text{disp-nodisp}}$ is quite similar for all solvents and also for a cluster in vacuum. This indicates that dispersion and solvation effects can be treated independently.
To save computational costs, it would be favorable to include the dispersion correction only in the calculation of the single point energies instead of conducting the whole optimization process with it. Thus, also the energy difference between structures optimized with the Grimme3 model and those which were optimized without dispersion correction, but for which dispersion was then included in the single point energy calculations was analyzed (differences 'opt-sp' in Table 4.3). As can be seen, the values are reasonably close for the bromide ligands, but do diverge for the phosphines. Considering the overall differences between with and without

dispersion (d-nd values), the opt-sp energy differences are in a range of roughly 15–20 % of those and are therefore not to be neglected. Thus, when considering dispersion effects, one might opt to implement it already in the optimization, even though the costs will be higher.

Table 4.3.: Estimated energy differences (dispersion–w/o dispersion) of the electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7'). Gas phase optimized structures of Au11P7 and PPh_3 were used. The Grimme3 model was used in the optimization. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations in a solvent environment, solvation was included using the SM12 model. For better visibility, the position with halide atoms are marked in blue.

		Energy difference (kJ/mol)									
pos#	**PPh_3/ Br**	**gas phase**		**toluene**		**THF**		**DCM**		**MeOH**	
		d-nd	opt-sp	d-nd	opt-sp	d-nd	opt-sp	d-nd	opt-sp	d-nd	opt-sp
2	P	227.2	37.9	231.9	42.6	235.2	45.8	239.5	50.2	234.7	45.4
3	P	199.1	29.9	202.4	33.1	204.6	35.3	208.7	39.5	204.1	34.9
4	Br	41.9	-5.8	42.1	-5.6	42.8	-4.9	46.6	-1.0	41.3	-6.4
5	P	228.8	40.8	233.5	45.5	236.8	48.8	241.1	53.1	236.1	48.1
6	P	227.8	40.4	232.1	44.8	235.1	47.7	239.1	51.7	234.2	46.8
7	Br	41.0	-5.9	41.5	-5.5	41.9	-5.0	46.3	-0.7	40.9	-6.0
8	P	240.4	45.1	244.1	48.8	246.7	51.4	249.5	54.2	242.8	47.5
9	P	201.8	33.5	204.7	36.5	207.0	38.7	211.1	42.9	206.4	38.2
10	Br	41.8	-5.4	42.0	-5.1	42.5	-4.7	46.7	-0.5	41.6	-5.6
11	P	201.3	34.1	204.7	37.4	206.4	39.1	210.8	43.5	206.1	38.9

The energy difference (d-nd) denotes the difference in binding energy between structures optimized with dispersion correction (d) and those without (nd), whereas the difference (opt-sp) denotes the difference in binding energy obtained by including dispersion correction already in the cluster optimization (opt) *vs.* only in the single point calculation (sp).

Finally, for the two solvents the author most commonly exposed Au_{11} to, namely DCM and THF, optimizations of the nanocluster structures including solvation and dispersion effects were also carried out. The results are presented in Table 4.4 for $Au_{11}(PPh_3)_7Br_3$ and Table A.2 for $[Au_{11}(PPh_3)_8Br_2]^+$. As a comparison between the structures optimized with solvation and those with solvation only included when calculating the single point energies show, only minor differences in the energies are observed (a few kJ/mol). For $Au_{11}(PPh_3)_7Br_3$, the energies are slightly overestimated if solvation in DCM is not considered already in the optimization, whereas they are a bit underestimated for THF. However, as can be seen from Table A.2, this general trend cannot be confirmed for the $[Au_{11}(PPh_3)_8Br_2]^+$ cluster. Summarizing, for this type of project, considering solvation effects is quite important. However, a reasonably good estimation can be obtained if the effects are only considered in calculating the energies of a cluster structure previously optimized without solvation effects.

Table 4.4.: Estimated electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7'). Gas phase optimized structures of Au11P7 and PPh_3 with Grimme3 dispersion correction were used. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations, solvation was included using the SM12 model. For better visibility, the position with halide atoms are marked in blue.

		Energy (kJ/mol)					
		DCM			**THF**		
pos#	PPh_3/Br	no solv	solv	$\Delta_{s\text{-}ns}$	gas opt	no solv	$\Delta_{s\text{-}ns}$
2	P	336.6	334.4	-2.2	332.6	333.8	1.2
3	P	315.9	313.5	-2.4	311.1	311.8	0.6
4	Br	117.8	114.4	-3.4	119.7	120.3	0.6
5	P	339.7	337.6	-2.1	335.6	338.4	2.7
6	P	337.4	335.8	-1.5	333.6	336.4	2.8
7	Br	118.4	114.4	-4.0	119.5	120.1	0.5
8	P	341.4	341.0	-0.4	339.8	342.5	2.7
9	P	318.5	317.1	-1.4	314.0	316.8	2.8
10	Br	118.1	114.2	-3.9	119.7	120.2	0.5
11	P	319.3	316.5	-2.8	314.2	316	1.8

The energy difference (s-ns) denotes the difference in binding energy between structures optimized with solvation (solv) and those with solvation only considered for calculating the single point energies but not in the initial optimization (no solv).

4.3. Single Halide Ligand Exchanges on $Au_{11}(PPh_3)_7Br_3$: Replacement with Thiolate *vs.* Conversion to $[Au_{11}(PPh_3)_8Br_2]^+$

The reaction energy of a single ligand exchange on $Au_{11}(PPh_3)_7Br_3$ was investigated. Based on the results of the calculations in Section 4.2, only exchanges at the halide positions were considered, since those seemed to be the more likely exchange sites. Table 4.5 shows the reaction energies for the displacement of a single halide by a thiolate (2-PET). The energies were estimated based on Equations (4.5)–(4.6).

$$\begin{aligned}\Delta E_{elec,neutral} = E_{elec}(Au_{11}(PPh_3)_7(SC_2H_4Ph)Br_2) + E_{elec}(HBr) \\ -E_{elec}(Au_{11}(PPh_3)_7Br_3) - E_{elec}(PhC_2H_4SH)\end{aligned} \tag{4.5}$$

$$\begin{aligned}\Delta E_{elec,anionic} = E_{elec}(Au_{11}(PPh_3)_7(SC_2H_4Ph)Br_2) + E_{elec}(Br^-) \\ -E_{elec}(Au_{11}(PPh_3)_7Br_3) - E_{elec}(PhC_2H_4S^-)\end{aligned} \tag{4.6}$$

Table 4.5.: Reaction energies for replacing a single bromide ligand on $Au_{11}(PPh_3)_7Br_3$ by 2-PET. All structures were optimized in gas phase including disperison correction. Solvation effects were considered for calculating single point energies.

	ΔE_{elec} (kJ/mol)				
pos#	gas phase	toluene	THF	DCM	MeOH
neutral					
4	3.5	12.0	19.0	26.1	28.4
7	15.6	22.3	27.0	32.1	31.8
10	5.3	11.5	16.8	23.8	25.8
anionic					
4	-129.3	-135.7	-130.2	-123.1	-120.4
7	-117.3	-125.5	-122.2	-117.2	-117.0
10	-127.6	-136.2	-132.4	-125.5	-123.1

The replacement of a single halide ligand by a thiolate seems to an exothermic reaction when writing it as a reaction equation with anionic species (thiolate, bromide), whereas it appears to be slightly endothermic when neutral species are considered. The same trend has already been observed by Heinecke *et al.* for a single thiolate-for-thiolate exchange (although to a considerably lesser extent).[57] Note that only the electronic energies are considered here without correcting for the zero-point vibrational energy (ZPE).
The reaction seems to be more favorable in less polar solvents such as toluene compared to e.g.

MeOH. Furthermore, positions #4 and #10 appear to be better exchange sites than position #7. This is possible considering that the incoming thiolate is significantly more bulky than the bromide that has been bonded there before. However, it should be noted that only one isomer of each form has been studied so far. To further confirm this results, a proper isomer search would have to be conducted.
As mentioned earlier in this Chapter, when conducting such a ligand exchange of $Au_{11}(PPh_3)_7Br_3$ with 2-PET, a slight change in the optical absorption spectra was noticed experimentally, which might be explained by a transformation to the other Au_{11} isomer $[Au_{11}(PPh_3)_8Br_2]^+$. In a net reaction, this can be written as a replacement of one halide ligand by PPh_3 (as in Equation (4.7)):

$$\begin{aligned} \Delta E_{elec} = E_{elec}([Au_{11}(PPh_3)_8Br_2]^+) + E_{elec}(Br^-) \\ -E_{elec}(Au_{11}(PPh_3)_7Br_3) - E_{elec}(PPh_3) \end{aligned} \tag{4.7}$$

The reaction energies for such a transformation are summarized in Table 4.6. The exchange seems to become more exothermic with increasing solvent polarity. As one can see from comparison with the numbers in Table 4.5, replacing a halide ligand by PPh_3 is more exothermic than replacing it with 2-PET at the same position for solvents with a polarity like THF or even more polar, whereas the situation is not that clear for toluene. These results further affirm the theory that such kind of halide-for-phosphine exchanges might also take place during (early stages) of exposure to an exchange thiolate ligands as side reactions. Again, however, a proper isomer search would be needed to confirm the numbers in Table 4.6.

Table 4.6.: Reaction energies for replacing a single bromide ligand on $Au_{11}(PPh_3)_7Br_3$ by PPh_3. All structures were optimized in gas phase including disperison correction. Solvation effects were considered for calculating single point energies.

	ΔE_{elec} (kJ/mol)				
pos#	gas phase	toluene	THF	DCM	MeOH
4	87.6	-108.6	-204.4	-204.5	-231.4
7	149.3	-45.9	-140.7	-140.7	-167.3
10	142.9	-54.4	-151.1	-151.6	-179.5

Another observation is that exchange at position #4 is clearly more favorable than at the other two sites. This is especially interesting because upon studying the crystal structures of these two cluster forms, this is the exact position one would expect the ligand replacement to occur. Thus, the energies for this isomer were compared to the energy of $[Au_{11}(PPh_3)_8Br_2]^+$ (with the cluster isomer obtained by optimization of the crystal structures). The result is presented in Table 4.7; a comparison of the cluster transformations at different levels of theory can be found in the Appendix (Table A.5). As one can see, the same trend can be observed,

Table 4.7.: Difference in energy between a clusters structure obtained by replacing a single bromide ligand on $Au_{11}(PPh_3)_7Br_3$ with PPh_3 (Au11P7-posx-PPh_3) and $[Au_{11}(PPh_3)_8Br_2]^+$ ('Au11P8') from optimization of the crystal structure. All structures were optimized in gas phase including disperison correction. Solvation effects were considered for calculating single point energies.

	ΔE_{elec} (Au11P7-posx-PPh_3 – Au11P8) (kJ/mol)				
pos#	gas phase	toluene	THF	DCM	MeOH
4	-11.5	-13.1	-14.1	-13.9	-13.1
7	50.2	49.6	49.7	49.9	50.9
10	43.7	41.1	39.3	39.0	38.7

with the energy of the isomer obtained by exchange at position #4 being much closer to the energy of the cluster crystal structure. Furthermore, this difference in energy is also reasonably small and might be even further reduced if more isomers would be studied.

4.4. Conclusions

In summary, a preliminary investigation of potential structural dynamics in Au_{11} by DFT has been performed. Regarding the level of theory to be used, it was observed that including solvation effects in the calculation significantly changes trends and results and can be useful for a proper estimation. It is, however, not necessary to conduct the whole optimization with a simulated solvent environment, since including solvation effects only when calculating single point energies computes reasonably close energies and reduces computational costs. Dispersion corrections, however, should be implemented already in the optimization processes, since the deviation is much stronger in this case.
Regarding removal of a single ligand from $Au_{11}(PPh_3)_7Br_3$, bromide removal is essentially preferred in the more polar solvents studied in this project, whereas depending on the level of theory used, either phosphine or bromide removal is the better choice for a $Au_{11}(PPh_3)_7Br_3$ cluster in toluene. Both exchanges of a halide by 2-PET or PPh_3 are likely to occur for a $Au_{11}(PPh_3)_7Br_3$ in solution, of which exchange with PPh_3 is even more favorable. Moreover, Br-for-PPh_3 replacement is most likely to occur at position #4, which is structurally consistent with a transformation from $Au_{11}(PPh_3)_7Br_3$ to $[Au_{11}(PPh_3)_8Br_2]^+$. The isomer obtained after replacement and optimization also shows an energy very close to that of a $[Au_{11}(PPh_3)_8Br_2]^+$ isomer obtained by optimization of the crystal structure.
With these initial results, a proper isomer search for the exchange structures of interest can now be undertaken to affirm the trends in reactivity. In addition, for a comparison with experimental results, the reaction energies might be corrected for the ZPE. To further investigate the exchange mechanism, one might also want to conduct a search for transition states. At this point, an associative mechanism seems to be more likely; however, to rule

out ligand dissociation, it might be worth to perform a geometry optimization of the lowest energy isomers with a dissociated ligand.

5. Computational Details

The Amsterdam Density Functional (ADF) 2021.1 package[108] was used for all DFT calculations. Unles noted otherwise, all geometry optimizations were done in gas-phase, using a generalized gradient approximation (GGA) Becke Perdew exchange-correlation functional (BP86).[109,110] Depending on the cluster/ligand type, both double zeta polarized basis set (DZP) an triple zeta basis set (TZP) were used.[111] Scalar relativistic effects were considered using the zeroth-order regular approximation (ZORA).[112,113] For optimizations, a gradient convergence of 10^{-3} and an energy convergence of 10^{-4} were used. If dispersions corrections were to be considered, this was achieved using the DFT-D3 correction (Grimme3) by Grimme.[107] The SM12 solvent model has been used to consider solvation.[105,106] Alterations to the cluster structures have been done using the MacMolPlt software.[103]
Optical absorption and circular dichroism (CD) spectra were obtained after a linear response TD-DFT+TB[114] calculation and subsequent convolution of the excitation energies into a spectrum by applying a Gaussian fit with a full width half-maximum (FWHM) of 30 nm. The CD spectrum of the *(S)*-2-MeBuSH ligand was obtained by employing a Gaussian fit with a FWHM of 15 nm. Refer to the literature for details on the fitting procedure.[84,115] The energy axis was converted to wavelength units to be able to compare them to the experimental spectra. To confirm that TD-DFT+TB was applicable for the calculations of the nanoclusters in question, some spectra were also simulated employing time dependent-density functional theory (TD-DFT) (see Figure A.1).[116]
The molecular graphics were created using the UCSF Chimera software[117], developed by the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco, with support from NIH P41-GM103311.

5.1. Specifics of the Individual Systems

5.1.1. Au_{38}(2-MeBuS)$_{24}$ and [Au_{25}(2-MeBuS)$_{18}$]$^-$

The initial structures used for geometry optimization were reported crystal structures[64,70,118]. The structure of the desired 2-MeBuSH ligand was optimized first in gas phase and then used to replace the original ligands on the clusters. Optimizations were generally conducted at the BP86/DZP level of theory. To conduct a proper isomer search, after the first geometry optimization of the different Au_{38} structures, different isomers of each were calculated obtained by manually modifying the structures in MacMolPlt.

5.1.2. Biicosahedral Au_{25} Clusters

All calculations were conducted at the BP86/TZP level of theory. The initial cluster structure of the cluster was adapted from the crystal structure by Shichibu *et al.*[61] Publicly available structures of *S*-BINAP[119] and *S*-(Ethane-1,2-diyl)bis[(2-methoxyphenyl)(phenyl)phosphane] (DIPAMP)[120] were used for intial optimization of the ligand structure. All other ligand structures were directly created in MacMolPlt.

5.1.3. $Au_{11}(PPh_3)_7Br_3$, $[Au_{11}(PPh_3)_7Br_2]^+$ and Related Structures

All calculations were conducted at the BP86/TZP level of theory. Solvation and dispersion correction were considered in several cases, which is always specifically mentioned in Chapter 4. The initial strutures of the Au_{11} clusters were derived by optimization of the crystal structures publsihed by McKenzie *et al.*[36]

6. Conclusions and Outlook

In summary, different aspects related to Au nanocluster ligand effects were investigated by DFT calculations. Three different research questions were addressed: (1) influence of chiral thiolate ligands on the chiral properties of the overall Au nanocluster structure, (2) binding sites and influence of bidentate (chiral) ligands and (3) evaluation of potential structural dynamics at the beginning of a ligand exchange reaction.

As discussed in Chapter 2, using the chiral thiolate 2-MeBuSH as protecting ligand resulted in strong chiroptical signals of the synthesized clusters. Through comparison of experimental and theoretical spectra, it can be assumed that the intrinsically chiral Au_{38} cluster exists only in its anti-clockwise enantiomeric form. However, according to the calculations, this stereoisomer should be higher in energy. Thus, this should be further clarified by e.g. including dispersion correction in the calculations or using a different functional. Optimization of further isomers could also be beneficial.
Nevertheless, the simulated spectra of Au_{38} show good agreement with the experimental ones, which confirms that suitable model structures for further spectroscopic investigations have been found. In the case of $[Au_{25}(2\text{-MBT})_{18}]^-$, however, further improvements of the model structure still have to be performed since a significant discrepancy between the calculated and measured spectra was obvious. This might also be related with the ligands having more influence on the CD spectra of an achiral cluster species.

Further investigations on the introduction of chiral ligands into a cluster structure were also carried out for a biicosehdral Au_{25} clusters with a mixed ligand shell of phosphines, thiolates and halides. Thereby, replacing all 2-PET thiolate ligands with the structurally very similar chiral 2-PPT analogue resulted in inducement of chiral properties, evidenced by the cluster now showing CD bands. However, comparison with experimental data of other authors showed that the bands appear shifted to lower energies. Furthermore, the intensity is significantly lower compared to the intrinsically chiral Au_{38} clusters. Introducing a bidentate chiral phosphine ligand such as *(S)*-BINAP instead results in stronger signals, potentially because of increased distortion to the cluster structure. The overall profile of the CD spectrum is, however, comparable to the one with the 2-PPT ligands in place. This shows that the contribution of ligand orbital-based transitions should not be too pronounced, which agrees with literature. Indeed, the chiral ligands used only showed significant CD signals below 400 nm.
Potential binding sites of a second bidentate phosphine ligand were also investigated. First

optimizations with a simpler version (*(S)*-dpb) of the ligand showed that binding of both ligands on the same icosahedron is energetically unfavorable and a gauche-like geometry with the two ligands on separate cores is the most favorable geometry. Testing all three different possibilities with two BINAP ligands on two cores showed that the more bulky ligand preferred a position in which the ligands are positioned on opposite sites instead. Nevertheless, it should be pointed out that further isomers would need to be investigated for a definite assignment. Furthermore, the influence of more than one *(S)*-BINAP ligand on the chiroptical properties still needs to be evaluated.

Finally, also structural dynamics in ligand exchange reactions of Au nanoclusters were addressed using the example of an $Au_{11}(PPh_3)_7Br_3$ nanocluster and the thiolate exchange ligand 2-PET. For this system, an evaluation of different levels of theory showed that including both dispersion correction and solvation effects seems to increase the accuracy of the calculated relative energies.
Furthermore, it seemed that ligand removal is not generally a favorable process, even though significant differences between the halide ligands and the phosphines were detected, with the binding energies of the bromide ligands being lower for most investigated systems. Thus, ligand replacement can be assumed to follow an associative mechanism. Replacing the halide ligands with either another PPh_3 ligand (i.e. conversion from $Au_{11}(PPh_3)_7Br_3$ to $[Au_{11}(PPh_3)_8Br_2]^+$) or with 2-PET resulted in lower reaction energies of the former process. In addition, according to the calculations, a preferential exchange site exists in this case, which is the exact same position one would expect the replacment to occur upon comparing the cluster crystal structures. Next steps should involve optimization of further isomers to affirm these preliminar results. In addition, transition state structures could be investigated to obtain further information about the mechanistic aspects.

Appendix

A. Appendix

A.1. Additional Data for Chapter 2

This section contains a comparison of the UV-Vis and CD spectra obtained from the same structure by a TD-DFT *vs.* a TD-DFT+TB calculation (Figure A.1), as well as the individual representations of the UV-Vis and CD spectra of the Au_{38} isomers, of Au_{25}, and of the 2-MeBuSH ligand including the plots of the calculated linear response TD-DFT+TB oscillator/rotatory strength (Figures A.2, A.3, A.4, A.5, A.6 and A.7), and the relative energies of all calculated Au_{38} isomers (Table A.1). The coordinates of the Au_{25} structure as well as of the Au_{38} isomers 1a, 1b, 2a and 2b can be found in Chapter B.

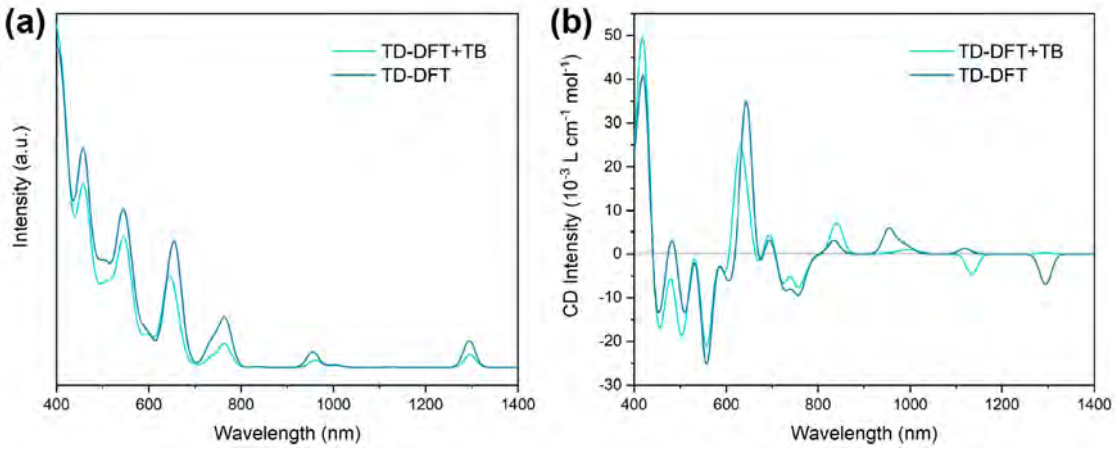

Figure A.1.: Comparison of the UV-Vis (a) and CD spectra (b) of $Au_{38}(2\text{-MeBuS})_{24}$ isomer 2b obtained by TD-DFT and TD-DFT+TB.

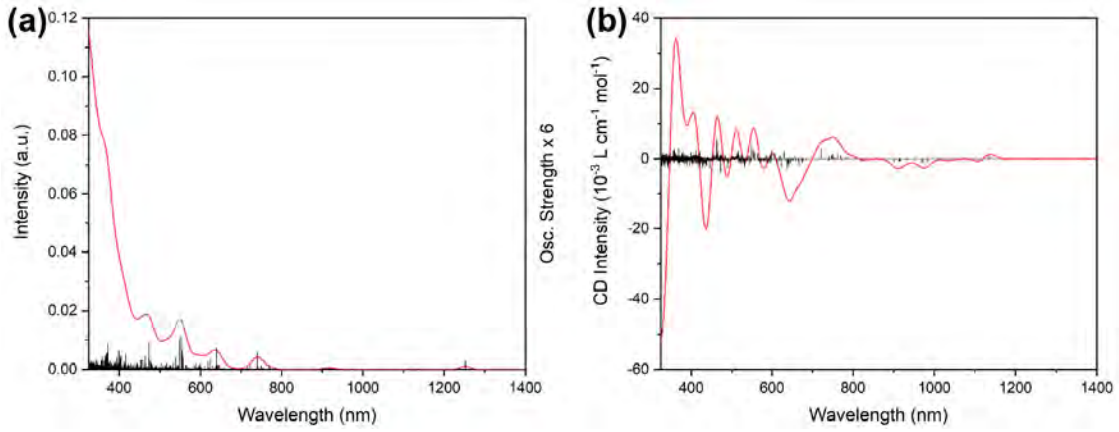

Figure A.2.: Calculated linear response TD-DFT+TB spectra of isomer 1a: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

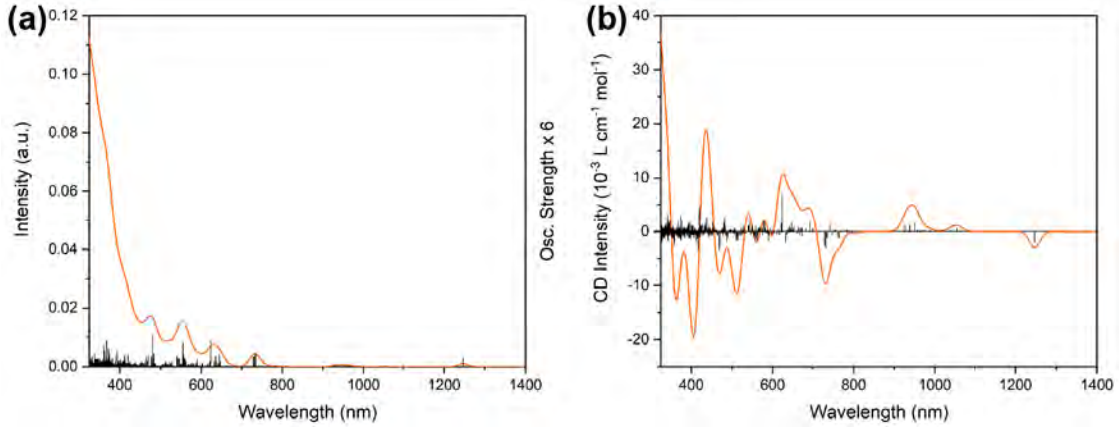

Figure A.3.: Calculated linear response TD-DFT+TB spectra of isomer 1b: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

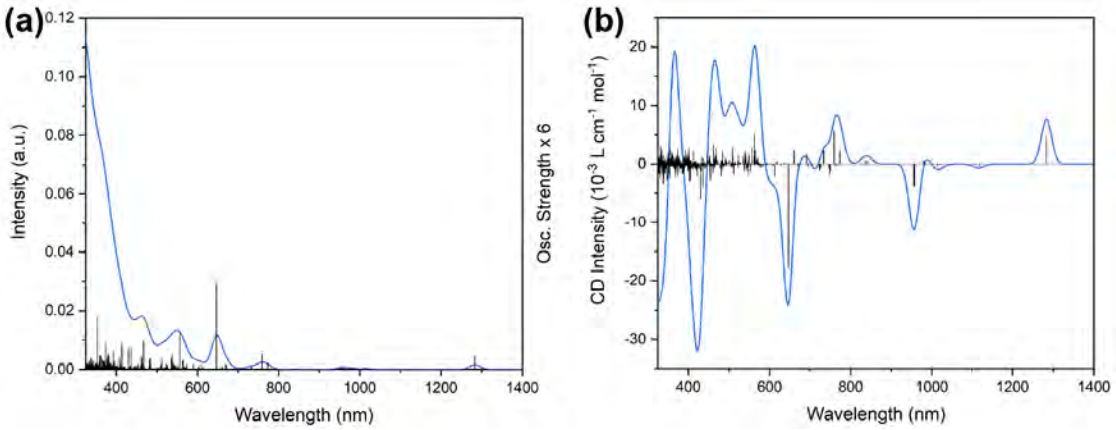

Figure A.4.: Calculated linear response TD-DFT+TB spectra of isomer 2a: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

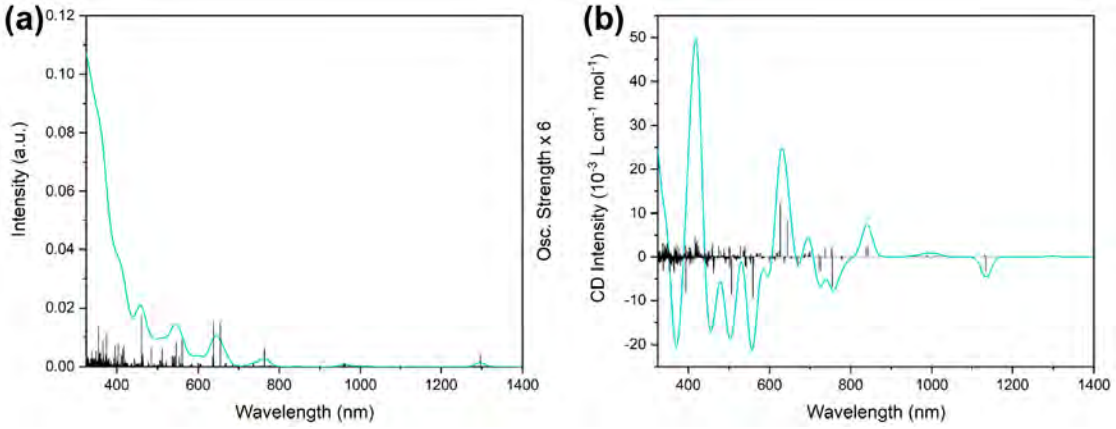

Figure A.5.: Calculated linear response TD-DFT+TB spectra of isomer 2b: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

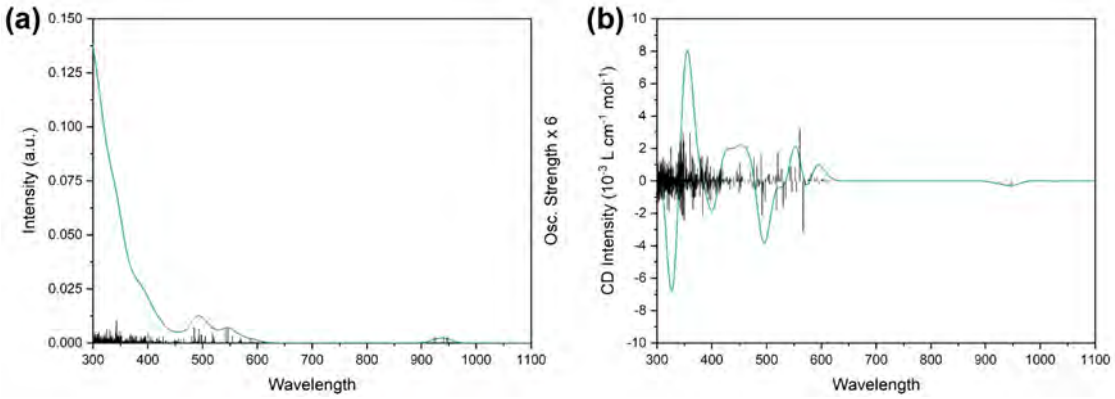

Figure A.6.: Calculated linear response TD-DFT+TB spectra of $[Au_{25}(2\text{-MeBuS})_{18}]^-$: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

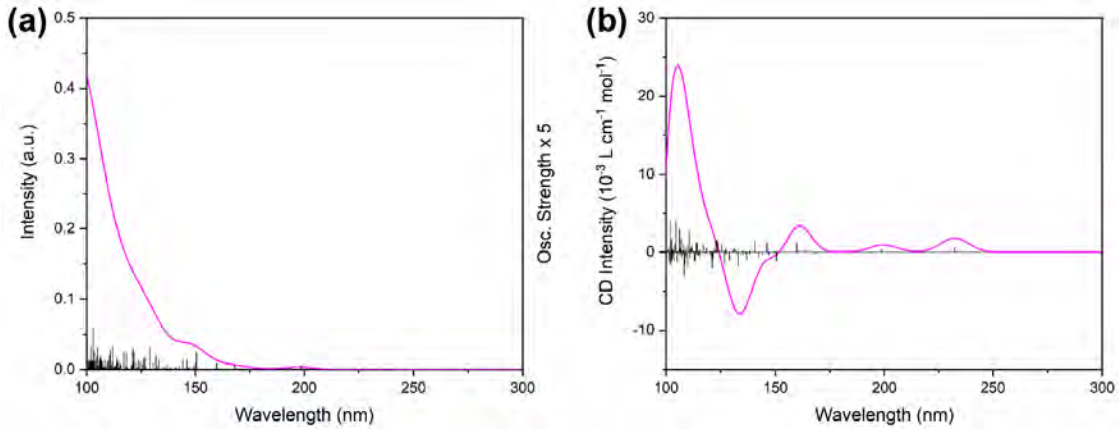

Figure A.7.: Calculated linear response TD-DFT+TB spectra of *(S)*-2-MeBuSH: (a) oscillator strength and optical absorption spectrum and (b) rotatory strength and CD spectrum.

Table A.1.: Relative energies of all calculated $Au_{38}(2\text{-MeBuS})_{24}$ isomers. A = anti-clockwise and C = clockwise staple rotation. Isomers 1 are crystal structure [64] based and isomers 2 were obtained starting from the calculated structure by Lopez-Acevedo *et al.* [70]

Cluster isomer	**Structure**	**Relative Energy (kJ/mol)**		
		group	enantiomer	overall
A	**isomer 1a**	**0.0**	30.8	46.5
A	isomer 1a-2	11.4		
A	isomer 1a-3	33.8		
A	isomer 1a-4	33.9		
A	**isomer 2a**	**0.0**	**0.0**	15.7
A	isomer 2a-2	0.1		
A	isomer 2a-3	0.5		
A	isomer 2a-4	1.1		
A	isomer 2a-5	2.1		
A	isomer 2a-6	4.0		
A	isomer 2a-7	5.7		
A	isomer 2a-8	5.9		
C	**isomer 1b**	**0.0**	7.7	7.7
C	isomer 1b-2	7.8		
C	isomer 1b-3	8.1		
C	isomer 1b-4	8.5		
C	isomer 1b-5	13.0		
C	**isomer 2b**	**0.0**	**0.0**	**0.0**
C	isomer 2b-2	0.2		
C	isomer 2b-3	5.0		
C	isomer 2b-4	25.1		
C	isomer 2b-5	45.1		

A.2. Additional Data for Chapter 3

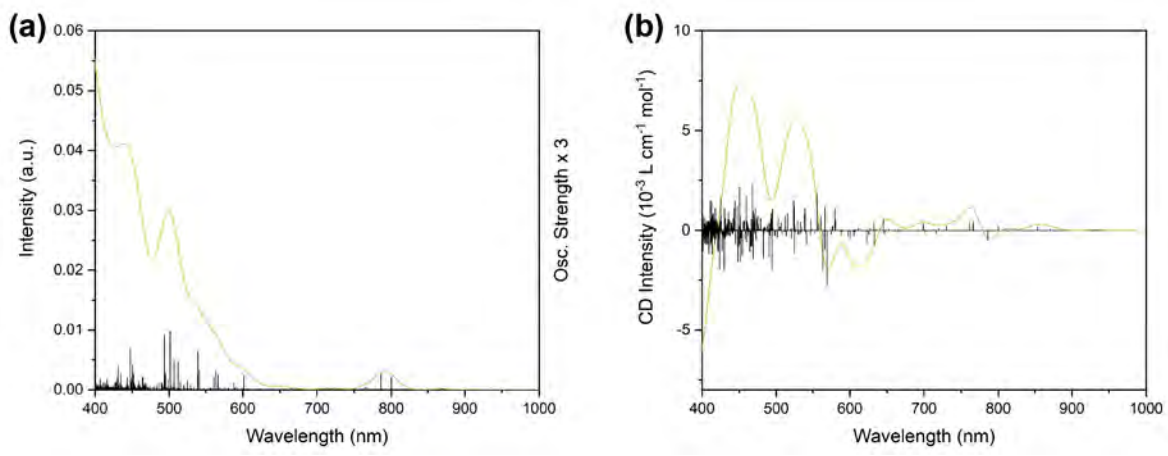

Figure A.8.: Theoretical optical absorption (a) and circular dichroism spectra (b) of $[Au_{25}(PPh_3)_8(\textit{(S)}-dpb)(SC_2H_4Ph)_5Cl_2]^{2+}$ isomer #2.

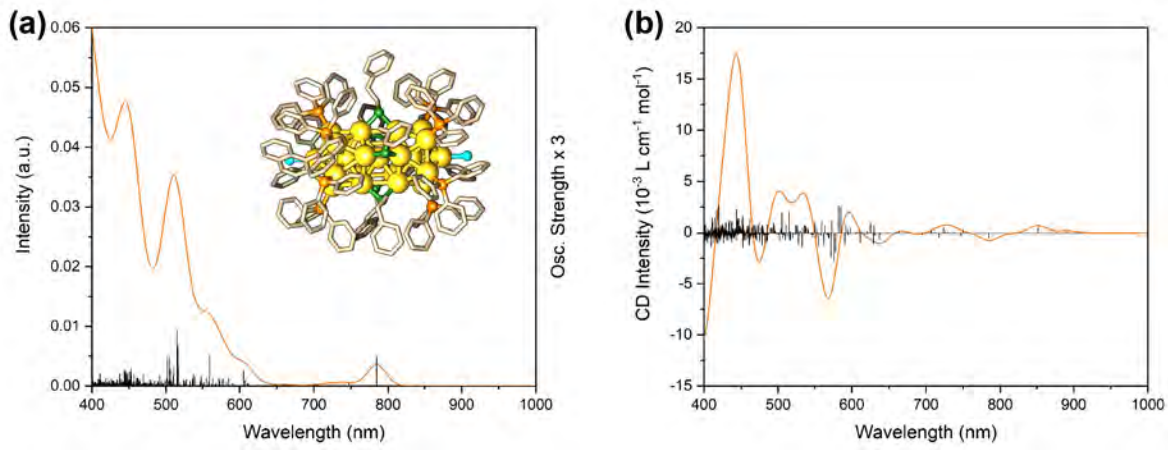

Figure A.9.: Theoretical optical absorption (a) and circular dichroism spectra (b) of $[Au_{25}(PPh_3)_8(\textit{(S)}-BINAP)(SC_2H_4Ph)_5Cl_2]^{2+}$ isomer #2. The inset shows the calculated structure of the isomer.

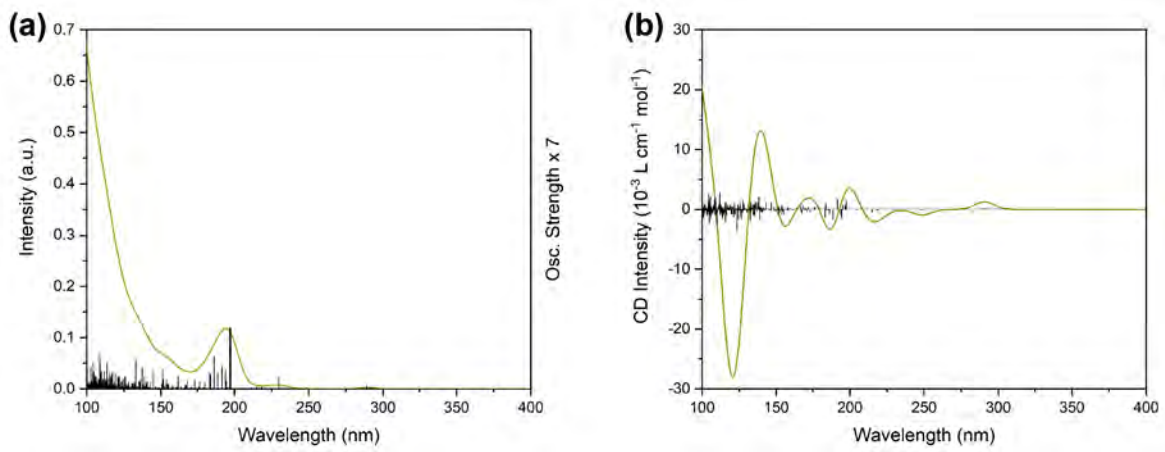

Figure A.10.: Theoretical optical absorption (a) and circular dichroism spectra (b) of the *(R)*-PPT ligand.

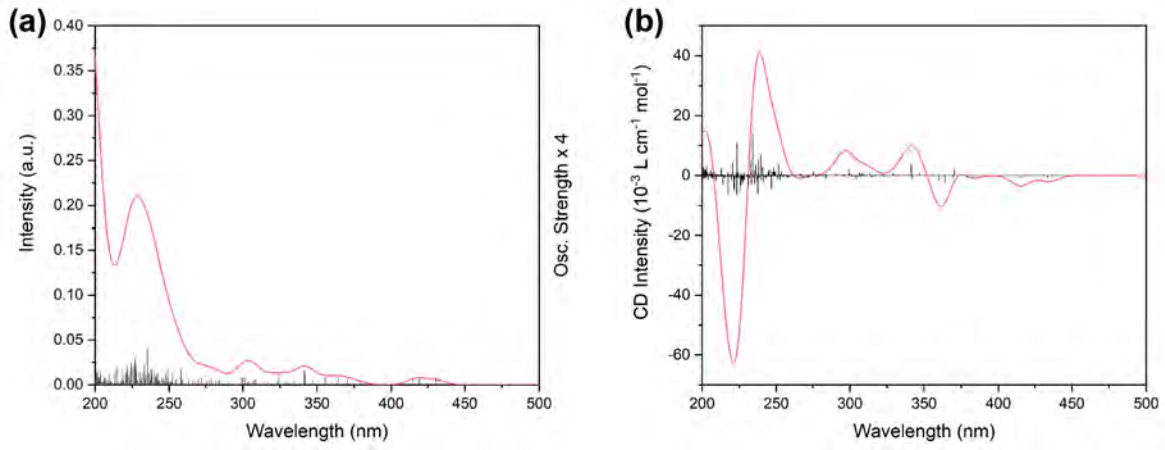

Figure A.11.: Theoretical optical absorption (a) and circular dichroism spectra (b) of the *(S)*-BINAP ligand.

A.3. Additional Data for Chapter 4

Table A.2.: Estimated electric binding energies for all ligands in $[Au_{11}(PPh_3)_8Br_2]^+$ ('Au11P8'). Gas phase optimized structures of Au11P8 and PPh_3 with Grimme3 dispersion correction were used. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations, solvation was included using the SM12 model.

		Energy (kJ/mol)					
		DCM			**THF**		
pos#	PPh_3/Br	no solv	solv	$\Delta_{s\text{-}ns}$	gas opt	no solv	$\Delta_{s\text{-}ns}$
2	P	353.2	354.7	1.5	354.2	355.7	1.5
3	P	142.2	146.1	3.9	152.2	156.1	3.9
4	Br	335.8	332.6	-3.2	336.6	333.5	-3.1
5	P	153.7	153.5	-0.2	164.0	163.4	-0.6
6	P	325.0	329.2	4.2	325.4	330.1	4.6
7	Br	335.6	344.6	9.0	336.2	345.1	8.9
8	P	316.4	316.4	-0.1	317.1	317.6	0.4
9	P	368.8	367.1	-1.7	369.6	367.4	-2.3
10	Br	360.2	364.9	4.8	361.1	365.2	4.1
11	P	339.6	346.0	6.4	339.5	345.8	6.3

The energy difference (s-ns) denotes the difference in binding energy between structures optimized with solvation (solv) and those with solvation only considered for calculating the single point energies but not in the initial optimization (no solv).

Table A.3.: Estimated electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7') and $[Au_{11}(PPh_3)_8Br_2]^+$ ('Au11P8'). Gas phase optimized structures of Au11P7, Au11P8 and PPh_3 were used. For the calculations including dispersion, all optimizations were carried out including the Grimme3 dispersion correction. The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations in a solvent environment, solvation was included using the SM12 model.

Energy (kJ/mol)																
		gas phase			**toluene**			**THF**			**DCM**			**MeOH**		
pos#	PPh_3/Br	w/o disp	disp	Δ_{disp}	w/o disp	disp	Δ_{disp}	w/o disp	disp	Δ_{disp}	w/o disp	disp	Δ_{disp}	w/o disp	disp	Δ_{disp}
Au11P7																
2	P	122.2	349.4	227.2	107.7	339.6	231.9	97.4	332.6	235.2	97.1	336.6	239.5	95.5	330.2	234.7
3	P	130.4	329.6	199.1	116.4	318.7	202.4	106.6	311.1	204.6	107.2	315.9	208.7	107.2	311.3	204.1
4	Br	378.7	420.6	41.9	177.0	219.0	42.1	77.0	119.7	42.8	71.1	117.8	46.6	46.4	87.7	41.3
5	P	123.2	352.1	228.8	109.0	342.5	233.5	98.8	335.6	236.8	98.6	339.7	241.1	97.4	333.4	236.1
6	P	123.0	350.8	227.8	108.6	340.8	232.1	98.5	333.6	235.1	98.3	337.4	239.1	96.8	331.0	234.2
7	Br	379.3	420.3	41.0	177.5	219.0	41.5	77.6	119.5	41.9	72.0	118.4	46.3	46.7	87.6	40.9
8	P	110.8	351.1	240.4	101.4	345.5	244.1	93.1	339.8	246.7	91.9	341.4	249.5	92.6	335.4	242.8
9	P	130.6	332.4	201.8	116.8	321.5	204.7	107.0	314.0	207.0	107.3	318.5	211.1	107.6	314.0	206.4
10	Br	378.6	420.4	41.8	177.0	219.1	42.0	77.2	119.7	42.5	71.4	118.1	46.7	46.0	87.6	41.6
11	P	131.2	332.5	201.3	117.4	322.0	204.7	107.8	314.2	206.4	108.5	319.3	210.8	108.1	314.2	206.1
Au11P8																
2	P	126.9	375.5	248.6	113.3	363.4	250.2	102.4	354.2	251.8	101.7	353.2	251.5	97.4	349.6	252.2
3	Br	531.5	588.1	56.5	245.0	297.2	52.3	101.8	152.2	50.4	92.4	142.2	49.8	52.0	101.4	49.3
4	P	133.3	355.5	222.2	118.9	344.7	225.9	107.9	336.6	228.6	107.2	335.8	228.5	103.7	332.9	229.2
5	Br	540.9	602.4	61.5	251.6	310.1	58.5	106.5	164.0	57.5	96.5	153.7	57.2	55.1	111.9	56.8
6	P	109.6	340.7	231.1	99.8	331.8	231.9	93.1	325.4	232.4	92.9	325.0	232.1	91.1	323.0	231.8
7	P	115.9	356.3	240.4	105.5	344.5	239.0	98.1	336.2	238.1	98.1	335.6	237.6	96.0	333.3	237.3
8	P	122.1	333.1	210.9	111.4	323.6	212.2	103.9	317.1	213.3	103.5	316.4	213.0	101.0	314.1	213.1
9	P	113.4	381.5	268.1	103.6	374.7	271.0	96.4	369.6	273.2	96.0	368.8	272.9	93.3	366.3	273.0
10	P	113.6	371.3	257.7	106.0	365.1	259.2	100.5	361.1	260.6	100.3	360.2	259.9	98.4	358.5	260.1
11	P	102.9	344.1	241.2	99.4	341.0	241.7	97.5	339.5	242.0	97.4	339.6	242.2	97.0	339.0	241.9

Table A.4.: Estimated electric binding energies for all ligands in $Au_{11}(PPh_3)_7Br_3$ ('Au11P7') and $[Au_{11}(PPh_3)_8Br_2]^+$ ('Au11P8'). Gas phase optimized structures of Au11P7, Au11P8 and PPh_3 were used. Dispersion was implemented by the Grimme3 correction either in the optimizations (disp) or only in the calculation of the single point energies (disp sp). The energies of the dissociated cluster structures were derived by removing the ligand at the specific position. For all single point energy calculations in a solvent environment, solvation was included using the SM12 model.

Energy (kJ/mol)															
		gas phase			**toluene**			**THF**			**DCM**			**MeOH**		
pos#	PPh_3/Br	disp sp	disp	Δ_{disp}	disp sp	disp	Δ_{disp}	disp sp	disp	Δ_{disp}	disp sp	disp	Δ_{disp}	disp sp	disp	Δ_{disp}
Au11P7															
2	P	311.5	349.4	37.9	297.0	339.6	42.6	286.7	332.6	45.8	286.4	336.6	50.2	284.8	330.2	45.4
3	P	299.7	329.6	29.9	285.6	318.7	33.1	275.8	311.1	35.3	276.4	315.9	39.5	276.4	311.3	34.9
4	Br	426.4	420.6	-5.8	224.6	219.0	-5.6	124.6	119.7	-4.9	118.8	117.8	-1.0	94.1	87.7	-6.4
5	P	311.2	352.1	40.8	297.0	342.5	45.5	286.8	335.6	48.8	286.6	339.7	53.1	285.4	333.4	48.1
6	P	310.4	350.8	40.4	296.0	340.8	44.8	285.8	333.6	47.7	285.7	337.4	51.7	284.2	331.0	46.8
7	Br	426.2	420.3	-5.9	224.5	219.0	-5.5	124.6	119.5	-5.0	119.0	118.4	-0.7	93.7	87.6	-6.0
8	P	306.1	351.1	45.1	296.7	345.5	48.8	288.4	339.8	51.4	287.2	341.4	54.2	287.9	335.4	47.5
9	P	298.9	332.4	33.5	285.0	321.5	36.5	275.3	314.0	38.7	275.6	318.5	42.9	275.8	314.0	38.2
10	Br	425.8	420.4	-5.4	224.2	219.1	-5.1	124.3	119.7	-4.7	118.6	118.1	-0.5	93.2	87.6	-5.6
11	P	298.4	332.5	34.1	284.6	322.0	37.4	275.0	314.2	39.1	275.7	319.3	43.5	275.3	314.2	38.9
Au11P8															
2	P	343.9	375.5	31.6	330.3	363.4	33.1	319.5	354.2	34.7	318.8	353.2	34.5	314.5	349.6	35.1
3	Br	583.3	588.1	4.8	296.7	297.2	0.5	153.6	152.2	-1.3	144.1	142.2	-1.9	103.8	101.4	-2.4
4	P	327.1	355.5	28.4	312.7	344.7	32.1	301.7	336.6	34.8	301.0	335.8	34.7	297.5	332.9	35.4
5	Br	598.1	602.4	4.3	308.8	310.1	1.4	163.7	164.0	0.3	153.7	153.7	0.0	112.3	111.9	-0.3
6	P	318.9	340.7	21.8	309.2	331.8	22.6	302.4	325.4	23.0	302.3	325.0	22.7	300.5	323.0	22.5
7	P	322.6	356.3	33.7	312.2	344.5	32.3	304.8	336.2	31.3	304.8	335.6	30.9	302.7	333.3	30.6
8	P	306.1	333.1	27.0	295.4	323.6	28.3	287.8	317.1	29.3	287.4	316.4	29.0	284.9	314.1	29.1
9	P	323.6	381.5	57.9	313.8	374.7	60.9	306.6	369.6	63.1	306.1	368.8	62.7	303.5	366.3	62.8
10	P	332.3	371.3	39.0	324.7	365.1	40.5	319.2	361.1	41.9	319.0	360.2	41.2	317.1	358.5	41.4
11	P	318.8	344.1	25.4	315.3	341.0	25.8	313.3	339.5	26.2	313.3	339.6	26.3	312.9	339.0	26.1

Table A.5.: Reaction energies for the transformation from $Au_{11}(PPh_3)_7Br_3$ to $[Au_{11}(PPh_3)_8Br_2]^+$. W/o dispersion = no dispersion correction, solvation in single point (sp) calculation; dispersion in sp = dispersion correction & solvation in sp calculation; dispersion = dispersion correction in optimization, solvation in sp calculation; dispersion & solvation = dispersion correction & solvation in optimization.

	ΔE_{elec} (kJ/mol)				
	gas phase	toluene	THF	DCM	MeOH
w/o dispersion	328.2	132.2	36.3	31.1	9.0
dispersion in sp	126.9	-69.1	-165.1	-170.3	-192.3
dispersion	99.1	-95.5	-190.3	-190.6	-218.3
dispersion & solvation	-	-	-184.5	-188.8	-

B. Coordinates of Relevant Structures

B.1. Coordinates of the Lowest Energy Isomers of $Au_{38}(2\text{-MeBuS})_{24}$ and $[Au_{25}(2\text{-MeBuS})_{18}]^-$

Isomer 1a

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	-2.25050449	9.13961124	21.40570641
2	Au	-1.62261558	10.68276215	19.04342270
3	Au	-2.78735828	13.30908108	19.72196007
4	Au	-0.47498831	12.95487690	17.75946426
5	Au	2.49938011	12.05049515	21.53145409
6	Au	-4.29084682	10.75326443	20.23686028
7	Au	-0.18833321	12.63096237	20.64192772
8	Au	-2.49080849	11.90609837	22.24284935
9	Au	-4.33987141	9.97326660	23.21131325
10	Au	-3.13672161	8.27631474	18.80020714
11	Au	1.26266420	10.76781464	19.04148483
12	Au	0.48251584	10.04690361	21.77543068
13	Au	0.15205055	12.39676476	23.44605827
14	Au	1.24284768	14.73297215	21.95830345
15	Au	-0.21995199	8.17002392	19.65839767
16	Au	-0.22292744	7.41700172	22.59944916
17	Au	-0.52561080	15.22060680	19.46110153
18	Au	-2.08292317	10.29452705	16.05222130
19	Au	-4.89307928	8.03634548	21.16094398
20	Au	2.06413698	13.64417744	19.18049812
21	Au	-1.40259457	9.85332584	24.02861404
22	Au	-4.78126287	5.53897381	18.78040695
23	Au	-1.58341360	14.60442543	22.26203156
24	Au	-2.58602047	15.54462814	17.10396957
25	Au	-2.90254784	7.35788774	23.54168510
26	Au	-1.29562151	5.46827841	17.93603134
27	Au	-7.33921766	9.95759201	21.55299950
28	Au	0.92431223	15.65415287	16.61462593
29	Au	-2.28484559	6.33032417	20.74123001
30	Au	-1.22514164	4.53809500	23.42140388
31	Au	-4.42339325	13.43409824	24.02822685
32	Au	-0.40993261	17.51630592	22.04165268
33	Au	0.31814504	15.49395084	24.85599709
34	Au	4.53028774	11.70686531	18.83138466
35	Au	-0.71865678	7.06035566	25.86891556
36	Au	-6.29546404	7.68493557	24.10104561
37	Au	4.56924343	14.43558216	21.09506226
38	Au	3.06055355	8.77224350	22.74677467
39	S	0.82292110	6.44658470	18.25320244
40	C	1.15046036	7.19223881	16.57147217
41	C	1.91979456	6.24220991	15.64137840
42	C	2.46709418	7.06353331	14.45645142
43	C	3.35606956	6.27320147	13.49319458
44	C	1.06442857	5.05980158	15.17898750
45	H	1.74137843	8.10042095	16.76455498
46	H	0.19239688	7.50301170	16.12925339
47	H	2.78676629	5.84776068	16.20667648
48	H	3.04060698	7.91614771	14.85933495
49	H	1.61457229	7.49851322	13.90317535
50	H	4.18797731	5.78930092	14.03046322
51	H	3.79161215	6.93679476	12.73104954
52	H	2.79456377	5.48846960	12.96521664
53	H	0.65491301	4.50789165	16.03796959
54	H	1.64885867	4.35028696	14.57407475
55	H	0.21378826	5.41278410	14.57231331
56	S	-3.32755041	4.51259184	17.23644638
57	C	-3.23400283	2.74391174	17.82098198
58	C	-4.55281258	1.98296750	17.64297104
59	C	-4.43073702	0.61360413	18.34121513
60	C	-5.72672081	-0.20046198	18.36547470
61	C	-4.93646765	1.85438931	16.16534233
62	H	-2.91108036	2.75337481	18.87184525
63	H	-2.43325424	2.28437424	17.21680069
64	H	-5.34171295	2.56073022	18.16347122
65	H	-4.09137392	0.78097689	19.37825966
66	H	-3.63324451	0.02823465	17.84567451
67	H	-6.54433537	0.37245581	18.83141708
68	H	-5.59534454	-1.12748444	18.94425011
69	H	-6.04988146	-0.48719195	17.35352898
70	H	-4.96154308	2.83994579	15.67655182
71	H	-5.92757130	1.39462471	16.04183578
72	H	-4.20056772	1.23044276	15.62997437
73	S	-1.01777995	9.33581161	26.40567017
74	C	0.72035104	9.85720348	26.85983086
75	C	0.93975252	9.91841412	28.37740326
76	C	2.28824973	10.61973000	28.64287758
77	C	2.56792903	10.91684532	30.11835480
78	C	0.86221892	8.53764820	29.03451538
79	H	0.85704386	10.85346889	26.41527557
80	H	1.42919707	9.16906643	26.37694740
81	H	0.14000133	10.55442524	28.80496216
82	H	2.30559063	11.56662655	28.07566071
83	H	3.10057878	9.99313927	28.23164558
84	H	1.75856876	11.52005577	30.55990028
85	H	3.50481391	11.48382473	30.23070908
86	H	2.66582584	9.99680519	30.71315765
87	H	-0.10434513	8.05576324	28.82697678
88	H	0.97611701	8.60354519	30.12692833
89	H	1.65698373	7.87996817	28.64390182
90	S	-3.18625689	8.23881435	16.36356926
91	C	-4.95592642	8.49098206	15.84396744
92	C	-5.13356590	8.67097569	14.33105183
93	C	-6.63074636	8.89535999	14.03636742
94	C	-6.93373489	9.29878998	12.59126759
95	C	-4.56460905	7.48857355	13.54100895
96	H	-5.36318684	9.34851742	16.39704514
97	H	-5.46861935	7.57576323	16.18669510
98	H	-4.58368921	9.58726215	14.03971100
99	H	-7.01066971	9.67807674	14.71482182
100	H	-7.18420267	7.97136164	14.28684902
101	H	-6.38031244	10.20946980	12.31189823
102	H	-8.00684166	9.50510788	12.45872974
103	H	-6.66171694	8.50654125	11.87810230
104	H	-3.50337720	7.32748127	13.78004360
105	H	-4.64463282	7.65361261	12.45676708
106	H	-5.10880232	6.56147194	13.78953838
107	S	0.46995991	13.29946709	25.69739914
108	C	-1.15238893	13.05450916	26.58617592
109	C	-1.09890294	13.50509071	28.05305290
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112	C	-1.07540083	15.02927017	28.19556427
113	H	-1.34475827	11.97292805	26.52611732
114	H	-1.94933748	13.56770420	26.02709961
115	H	-0.16885373	13.09627819	28.49477386
116	H	-2.27990437	11.78343010	28.60762787
117	H	-3.22811913	13.25694752	28.36200905
118	H	-1.34474862	12.76607704	30.76497078
119	H	-3.11040759	12.56217384	30.79583740
120	H	-2.41255951	14.17525005	30.56015205
121	H	-0.24635848	15.46665573	27.61805153
122	H	-0.95121342	15.33661652	29.24467278
123	H	-2.01588869	15.46385479	27.81635857
124	S	-4.35150957	14.49506474	18.25144005
125	C	-4.92503023	13.19296074	17.04208755
126	C	-5.96257496	13.70948505	16.03435707
127	C	-6.65638638	12.48980427	15.39217663
128	C	-7.80942202	12.83919621	14.44823933
129	C	-5.34810734	14.63787842	14.98350716
130	H	-5.36537075	12.40448284	17.67012215
131	H	-4.04691505	12.76379776	16.53675842
132	H	-6.72913408	14.27538967	16.59898567
133	H	-7.03538418	11.84105301	16.20162964
134	H	-5.89622068	11.89898968	14.84898949
135	H	-8.56320095	13.46028137	14.95842171
136	H	-8.31402588	11.92796230	14.09305477
137	H	-7.46346140	13.38986874	13.56135941
138	H	-4.82020998	15.47830486	15.46048832
139	H	-6.11494589	15.05939102	14.31645679
140	H	-4.61690617	14.08742809	14.36757278
141	S	-3.39930010	15.52146435	23.62501144
142	C	-4.51812553	16.33603096	22.37728882
143	C	-5.89884186	16.70127678	22.93379402
144	C	-6.76073027	17.24866676	21.77899742
145	C	-8.22073460	17.51338387	22.15358925
146	C	-5.80400944	17.68289185	24.10515594
147	H	-4.60497904	15.66616726	21.51157379
148	H	-3.97166419	17.23968887	22.05795097
149	H	-6.36711073	15.76535892	23.29613495
150	H	-6.72698784	16.52577400	20.94616127
151	H	-6.30039787	18.17974854	21.39776230
152	H	-8.69126892	16.60900879	22.57292557
153	H	-8.80195999	17.81489372	21.26904106
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155	H	-5.15602493	17.28448296	24.90037346
156	H	-6.79130554	17.88212967	24.54685020
157	H	-5.38095140	18.64419937	23.76725006
158	S	-0.96990710	12.28822327	15.46453190
159	C	0.69533318	11.76589298	14.80835819
160	C	0.64874256	11.07286167	13.44159698
161	C	2.09181237	10.68470001	13.05902672
162	C	2.21220827	9.87157726	11.76796818
163	C	-0.01819270	11.94357872	12.37347984
164	H	1.17479885	11.12472248	15.55972290
165	H	1.26992118	12.70577145	14.74515057
166	H	0.05899091	10.14252758	13.55672264
167	H	2.53033066	10.10915089	13.89183331
168	H	2.69554901	11.60778046	12.97142124
169	H	1.59791005	8.95842648	11.81438828
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171	H	1.89253867	10.44805145	10.88716888
172	H	-1.03098488	12.24199200	12.68333244
173	H	-0.10407333	11.41154480	11.41462708
174	H	0.57151055	12.86047840	12.20271778
175	S	3.03905249	14.89884281	17.33332443
176	C	3.84123302	16.40530968	18.09473228
177	C	4.80024242	17.12643242	17.13973236
178	C	5.59856415	18.16673470	17.95372391
179	C	6.72711372	18.84695625	17.17503357
180	C	4.07624388	17.75697708	15.94769859
181	H	4.38877869	16.01644516	18.97019577
182	H	3.05520511	17.07892609	18.46414757
183	H	5.51884127	16.37623024	16.75499344
184	H	6.02438116	17.66651535	18.84152603
185	H	4.89799452	18.93105698	18.33865929
186	H	7.42585707	18.10164833	16.76275826
187	H	7.30181742	19.51996040	17.83008003
188	H	6.34445286	19.44999695	16.33874321
189	H	3.50559330	17.00310326	15.38653088
190	H	4.78408146	18.22682190	15.24895573
191	H	3.36999750	18.53069878	16.29188919
192	S	-6.64490509	11.13396358	19.63679886
193	C	-7.16331911	12.89669323	19.97439003
194	C	-8.47055531	13.24792099	19.25071716
195	C	-8.66475677	14.77717304	19.28603935
196	C	-9.82690144	15.28242970	18.42719078
197	C	-9.67123604	12.49567223	19.83190346
198	H	-6.33887577	13.52483654	19.60627747
199	H	-7.24583054	13.04187202	21.06145096
200	H	-8.35138798	12.95036602	18.19044685
201	H	-7.73062181	15.25632858	18.94432449
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203	H	-9.71607113	14.95333481	17.38161278
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206	H	-9.50630569	11.40873623	19.80506134
207	H	-10.59303284	12.70948410	19.27020836
208	H	-9.83372784	12.78499031	20.88383675
209	S	6.10132217	13.04747009	19.96578217
210	C	6.88308382	14.17630672	18.69446945
211	C	8.22674465	13.64191437	18.18094254
212	C	8.90285969	14.75134373	17.34885216
213	C	10.33958054	14.43521595	16.92560768
214	C	8.06481266	12.33987713	17.39241028
215	H	7.03109598	15.13759327	19.20834160
216	H	6.16809654	14.32053089	17.87160301
217	H	8.86656094	13.44383240	19.06364250
218	H	8.90264130	15.68386078	17.94027519
219	H	8.28654289	14.94938374	16.45202446
220	H	10.96987247	14.21769333	17.80282402
221	H	10.78657150	15.29027176	16.39563942
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223	H	7.58725166	11.56198788	18.00451851
224	H	9.03698063	11.94790077	17.05876541
225	H	7.43442535	12.50302696	16.50193787
226	S	-8.20174122	8.93657303	23.48879814
227	C	-9.36247635	7.62529945	22.84297943
228	C	-9.86706161	6.67569065	23.93586349
229	C	-10.67347908	5.54430676	23.26726341
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231	C	-10.67315960	7.41315365	25.00912857
232	H	-8.83430386	7.06412888	22.05991554
233	H	-10.20041752	8.17778683	22.38470078
234	H	-8.97543144	6.22174120	24.41109467
235	H	-10.06209183	5.11018848	22.45725441
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238	H	-11.61153316	3.62025714	23.67166328
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240	H	-10.09192562	8.24096870	25.44184303
241	H	-10.96007442	6.74115372	25.83080101
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243	S	-6.41923428	6.36907339	20.25782394
244	C	-7.54098558	7.32865572	19.12025833
245	C	-8.34692764	6.43554258	18.16955566
246	C	-9.10586739	7.33647966	17.17479134
247	C	-9.81257534	6.57557106	16.04983521
248	C	-9.27966976	5.48783302	18.92993355
249	H	-6.92589045	8.04764652	18.56330490
250	H	-8.20628262	7.90607548	19.78581619
251	H	-7.62185144	5.82767725	17.59352112
252	H	-8.38870430	8.04825592	16.73025703
253	H	-9.84123802	7.94682980	17.73149300
254	H	-9.10258770	5.93823814	15.49849892
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256	H	-10.61765671	5.93015337	16.43155479
257	H	-8.71685410	4.88075686	19.65494537
258	H	-9.79923248	4.79784393	18.24916077
259	H	-10.04273319	6.06031227	19.48429680
260	S	-5.71901369	11.52701855	24.49564552
261	C	-5.47154760	11.09736443	26.28962898
262	C	-6.14062691	12.07621861	27.26359177
263	C	-5.88998652	11.57441998	28.70083427
264	C	-6.29886389	12.56283092	29.79608536
265	C	-7.63435650	12.25064373	26.97140694
266	H	-4.39370871	11.01430035	26.48721123
267	H	-5.92347527	10.09481430	26.38521767

268	H	-5.64151525	13.05786705	27.14618111
269	H	-4.81817722	11.33733940	28.81249046
270	H	-6.43473148	10.62196922	28.84062958
271	H	-5.76635790	13.52078533	29.68356323
272	H	-6.06100702	12.16220284	30.79339600
273	H	-7.37854719	12.77347660	29.77642059
274	H	-7.79910040	12.59544659	25.94052505
275	H	-8.09290123	12.98476887	27.64946365
276	H	-8.16554165	11.29118252	27.09250450
277	S	-4.59326124	6.26670599	24.88953972
278	C	-4.27109146	6.88954306	26.61689377
279	C	-5.39565277	6.55593348	27.60330009
280	C	-5.09748220	7.26239061	28.94114494
281	C	-6.22602749	7.16389227	29.97093582
282	C	-5.57927370	5.04449797	27.76777458
283	H	-4.10215139	7.97255230	26.55916405
284	H	-3.32006884	6.41901731	26.92054558
285	H	-6.33283138	6.98245907	27.19469452
286	H	-4.89124203	8.32740402	28.73593712
287	H	-4.16612673	6.84467125	29.36763382
288	H	-7.17053127	7.55558157	29.56006241
289	H	-5.98360538	7.74885511	30.87130356
290	H	-6.40251589	6.12617016	30.29036331
291	H	-5.75889158	4.56254482	26.79504967
292	H	-6.43282938	4.80820942	28.41980171
293	H	-4.67524672	4.59274578	28.21107674
294	S	0.25390804	17.78230476	24.28865814
295	C	-1.24062812	18.37937355	25.23921776
296	C	-1.43524134	19.90052795	25.17105293
297	C	-2.39631200	20.31600571	26.30554581
298	C	-2.58311296	21.82826614	26.45052719
299	C	-1.93605447	20.36036873	23.79954338
300	H	-1.03884912	18.07099724	26.27654457
301	H	-2.12540984	17.83165550	24.88131905
302	H	-0.45407423	20.37540436	25.37029457
303	H	-2.01090312	19.90943146	27.25765419
304	H	-3.37718439	19.83488846	26.13496780
305	H	-1.61424267	22.33331299	26.59370422
306	H	-3.21401572	22.06057358	27.32215500
307	H	-3.06718731	22.26889229	25.56655502
308	H	-1.27499604	20.00632477	22.99441147
309	H	-1.98478234	21.45719337	23.73231125
310	H	-2.94438386	19.95803833	23.60608864
311	S	-0.98899674	17.58471870	19.76134872
312	C	0.41433737	18.52458191	18.95482063
313	C	0.01203483	19.95380974	18.57356644
314	C	1.12699330	20.55179024	17.69050217
315	C	0.79349929	21.92150307	17.09439468
316	C	-0.28179389	20.81557655	19.80463982
317	H	0.66808939	17.94377899	18.05369568
318	H	1.27937520	18.51667213	19.63388252
319	H	-0.90646464	19.88825417	17.95827484
320	H	1.33323050	19.84603310	16.86754036
321	H	2.05593276	20.62205124	18.28698730
322	H	-0.14043605	21.87944031	16.51157761
323	H	1.59522033	22.25753784	16.41901398
324	H	0.67397064	22.69013405	17.87162209
325	H	-1.07791913	20.36909103	20.41764641
326	H	-0.60970998	21.82647514	19.52008820
327	H	0.61862445	20.91037560	20.43496895
328	S	-1.01984906	16.68394089	15.75751686
329	C	-1.32814384	15.94520664	14.06868267
330	C	-0.56819004	16.66094017	12.94376659
331	C	-1.16710877	16.20289612	11.59650326
332	C	-0.59396476	16.92045021	10.37172699
333	C	0.94165856	16.42097473	13.01199913
334	H	-2.41291904	16.05713844	13.91993237
335	H	-1.09649563	14.87019348	14.10802269
336	H	-0.76000077	17.74740028	13.04658985
337	H	-2.25957823	16.36316872	11.62707996
338	H	-1.01520061	15.11284733	11.49228764
339	H	-0.70349443	18.01295662	10.46598434
340	H	-1.12163091	16.60869026	9.45751953
341	H	0.47340056	16.69835472	10.22755718
342	H	1.34698427	16.70868492	13.99307537
343	H	1.47807384	17.00141525	12.24680424
344	H	1.16977191	15.35332870	12.85627270
345	S	-0.11098599	4.82544518	25.48133278
346	C	-1.13021934	3.80304050	26.66470337
347	C	-0.85293770	2.30113769	26.52457809
348	C	-1.88811624	1.52501190	27.36303902
349	C	-1.82013321	0.00490682	27.19638443
350	C	0.58970362	1.95492291	26.90652275
351	H	-2.19110298	4.02726936	26.48851967
352	H	-0.85630971	4.15728569	27.67289925
353	H	-1.01000583	2.03126454	25.46263885
354	H	-2.89766288	1.87117672	27.07948112
355	H	-1.75536501	1.78814542	28.42954445
356	H	-1.92636085	-0.27879634	26.13726234
357	H	-2.62938786	-0.48585203	27.75860214
358	H	-0.86808044	-0.40674472	27.56265640
359	H	1.30716443	2.55512595	26.32751274
360	H	0.81389725	0.89499778	26.71874809
361	H	0.76478183	2.15719581	27.97721863
362	S	4.35548401	10.70986843	22.38433456
363	C	4.69545078	11.36560535	24.09396553
364	C	5.57370090	10.44282722	24.94719696
365	C	5.70468569	11.05839443	26.35464859
366	C	6.39512396	10.15129948	27.37639427
367	C	6.93578005	10.18567371	24.29661560
368	H	3.73207760	11.55793762	24.58580589
369	H	5.20133305	12.33119488	23.92073059
370	H	5.04002810	9.47707081	25.04327393
371	H	4.69560528	11.31120110	26.72350502
372	H	6.25679922	12.01345634	26.27631760
373	H	5.87834644	9.18133640	27.45473099
374	H	6.39277077	10.61504173	28.37480736
375	H	7.44336987	9.95320797	27.10739326
376	H	6.81706381	9.78378296	23.27964783
377	H	7.52850771	9.46305466	24.87628365
378	H	7.51243401	11.12366104	24.22390747
379	S	-2.27739501	3.97579646	21.39199638
380	C	-4.05697346	3.62830687	21.82575226
381	C	-4.30027866	2.19921255	22.33409309
382	C	-5.79268837	1.86078966	22.13383484
383	C	-6.17486334	0.42907608	22.51754189
384	C	-3.86356020	2.02641916	23.79171753
385	H	-4.59310341	3.79733157	20.87623787
386	H	-4.40577078	4.37855387	22.55014229
387	H	-3.70915008	1.50660014	21.70268822
388	H	-6.04725122	2.02980447	21.07299232
389	H	-6.40056944	2.57890296	22.71499252
390	H	-5.55718040	-0.30381978	21.97424889
391	H	-7.22829247	0.22790743	22.26923752
392	H	-6.04901218	0.24388778	23.59447861
393	H	-2.81999445	2.34983206	23.93099594
394	H	-3.93815041	0.97859699	24.11715317
395	H	-4.49423695	2.64346385	24.45406342
396	S	2.01160765	6.74737883	23.31206512
397	C	2.53717041	5.46090221	22.07140541
398	C	3.97032094	4.95367193	22.27516747
399	C	4.26859999	3.90863490	21.18040466
400	C	5.72405291	3.43685722	21.13610077
401	C	4.18556261	4.38643694	23.68191719
402	H	2.39562893	5.86835527	21.06148911
403	H	1.81452954	4.63978052	22.21706390
404	H	4.65539932	5.81159782	22.12977600
405	H	3.99860644	4.33796883	20.20088387
406	H	3.60115695	3.03918433	21.33117294
407	H	6.41169024	4.28675079	20.99921989
408	H	5.88235235	2.73845387	20.29992104
409	H	6.01501799	2.91381383	22.05928612
410	H	3.93616915	5.13044405	24.45273209
411	H	5.23026419	4.07950640	23.83611298
412	H	3.54055834	3.50607586	23.84328270
413	S	3.23139691	10.04651737	17.77889633
414	C	3.87452793	8.49822140	18.60656548
415	C	4.97738743	7.80339956	17.79607010
416	C	5.19777679	6.39989901	18.39623642
417	C	6.19423676	5.52924633	17.62729645
418	C	6.26951694	8.62173748	17.74136353
419	H	3.00147843	7.83715582	18.70915604
420	H	4.21947241	8.75653553	19.61863708
421	H	4.60381651	7.67093229	16.76214218
422	H	4.22236109	5.88465452	18.43461037
423	H	5.53194952	6.51092863	19.44423294

424	H	5.90288973	5.43423796	16.56880760
425	H	6.23574448	4.51588583	18.05466652
426	H	7.21332121	5.94242668	17.66080093
427	H	6.08647585	9.62140179	17.32215691
428	H	7.03030539	8.13184071	17.11575890
429	H	6.68671417	8.75219727	18.75403786
430	S	3.29526925	15.99482346	22.30878448
431	C	3.78297639	15.62432384	24.07088661
432	C	5.23952150	15.97824287	24.39096451
433	C	5.55950451	15.48109055	25.81529617
434	C	7.02937031	15.62686825	26.21748161
435	C	5.51421356	17.47517776	24.21916389
436	H	3.58328891	14.56140995	24.25930595
437	H	3.08645797	16.21655273	24.68771553
438	H	5.88072014	15.41845703	23.68197250
439	H	5.27110815	14.41783810	25.88892746
440	H	4.92079449	16.02417946	26.53658485
441	H	7.68839693	15.11719513	25.49642754
442	H	7.20821810	15.18258858	27.20853615
443	H	7.33772087	16.68149948	26.26956749
444	H	5.23995161	17.81241989	23.20820427
445	H	6.57704592	17.71127892	24.37388039
446	H	4.92273808	18.06124878	24.94304276

Isomer 1b

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	2.29825670	9.15972786	21.28387360
2	Au	1.65888040	10.70996275	18.92198378
3	Au	2.81994083	13.29634509	19.55484038
4	Au	0.42239799	12.96435640	17.66041202
5	Au	-2.42087952	12.11388843	21.59853202
6	Au	4.34541910	10.74467396	20.10956735
7	Au	0.24844991	12.65154348	20.55776546
8	Au	2.57815152	11.91756615	22.12211029
9	Au	4.40612378	9.98633949	23.13077282
10	Au	3.23064634	8.33677660	18.65065150
11	Au	-1.25307872	10.77850930	19.04080281
12	Au	-0.41919922	10.07474524	21.72571605
13	Au	0.00201050	12.46664262	23.36348755
14	Au	-1.10125954	14.79264741	21.92128648
15	Au	0.26809298	8.22438919	19.54771151
16	Au	0.25823297	7.40381315	22.44825596
17	Au	0.56378188	15.24253936	19.34752836
18	Au	2.12822541	10.40432819	15.97981100
19	Au	4.93681876	8.05733684	21.09167642
20	Au	-2.07127694	13.61601192	19.18809715
21	Au	1.49083615	9.85154335	23.91064324
22	Au	4.86710935	5.62175832	18.67192973
23	Au	1.75035747	14.64730977	22.06548658
24	Au	2.59478221	15.50593520	16.95221322
25	Au	2.93580147	7.34963490	23.40702043
26	Au	1.45834280	5.72377465	17.60322015
27	Au	7.33735271	10.05564019	21.63438618
28	Au	-0.96275827	15.65361314	16.64850034
29	Au	2.35428365	6.37820675	20.53597651
30	Au	1.24688124	4.52675411	23.21111577
31	Au	4.48069103	13.45803635	23.86754336
32	Au	0.53578912	17.54753211	21.99731642
33	Au	-0.19359927	15.51015975	24.82353791
34	Au	-4.54368659	11.58955557	19.12302236
35	Au	0.75950108	7.02447995	25.68709356
36	Au	6.28782872	7.62552924	24.01918841
37	Au	-4.43656604	14.52070062	21.09213459
38	Au	-2.92694355	8.85107302	22.81301138
39	S	-0.67600932	6.67349626	17.90732585
40	C	-0.86645125	7.62126778	16.31203321
41	C	-0.95654363	6.71253642	15.07951458
42	C	-0.92379957	7.59391230	13.81531619
43	C	-0.87167469	6.80803678	12.50245863
44	H	-1.78588718	8.21887405	16.43028907
45	H	-0.01664541	8.31439545	16.22952147
46	H	-1.80850497	8.25671436	13.81764303
47	H	-0.03804157	8.24976504	13.87526678
48	H	-1.78111037	6.20911251	12.34577052
49	H	-0.77363090	7.48925243	11.64302594
50	H	-0.00771561	6.12448935	12.48778873
51	S	3.50291266	4.74696938	16.95540602
52	C	3.25071121	2.93607459	17.34479994
53	C	4.33178591	2.02810697	16.74409378
54	C	3.84125688	0.56791073	16.83737306
55	C	4.75286646	-0.45067334	16.14892877
56	H	3.16727295	2.81362778	18.43482456
57	H	2.27191330	2.69855333	16.90131926
58	H	3.72137581	0.29921172	17.90312999
59	H	2.83402002	0.50756517	16.38781664
60	H	5.73816210	-0.51463462	16.63340072
61	H	4.30445810	-1.45558602	16.17987819
62	H	4.91145490	-0.18659706	15.09093408
63	S	0.98983369	9.30759820	26.24888010
64	C	-0.80115061	9.73964706	26.54297474
65	C	-1.37346343	9.08935384	27.80939780
66	C	-2.89919370	9.30718720	27.83263301
67	C	-3.61800552	8.58935552	28.97845954
68	H	-0.83473092	10.83952545	26.61342457
69	H	-1.36743887	9.43602759	25.65155439
70	H	-3.10686383	10.39158155	27.88357203
71	H	-3.31371702	8.95320511	26.87266323
72	H	-3.31618873	8.97927588	29.96175432
73	H	-4.70847149	8.71504607	28.89458879
74	H	-3.40391555	7.50861225	28.96082519
75	S	3.48247058	8.49256453	16.22018325
76	C	5.19520240	9.11900672	15.82488589
77	C	6.16537447	7.98295491	15.47589236
78	C	7.57083801	8.59887097	15.30878867
79	C	8.66552516	7.60409735	14.91578081
80	H	5.08232123	9.79095542	14.96074349
81	H	5.55290268	9.70825325	16.68034522
82	H	7.51664668	9.39630058	14.54353475
83	H	7.84949770	9.09964183	16.25308504
84	H	8.50463200	7.19687114	13.90672516
85	H	9.65370249	8.08988428	14.92245283
86	H	8.70390974	6.75517105	15.61559070
87	S	-0.29807276	13.30262833	25.64448788
88	C	1.36531180	13.15438729	26.47381431
89	C	1.52246300	14.10372250	27.66967300
90	C	2.98178192	14.05028108	28.16137808
91	C	3.32124197	15.08283338	29.23944851
92	H	1.44029869	12.10062297	26.79130236
93	H	2.14046107	13.33892056	25.71574634
94	H	3.19369379	13.03379942	28.54000729
95	H	3.64581017	14.20880680	27.29367732
96	H	2.75332532	14.91293153	30.16627920
97	H	4.39109500	15.04172070	29.49591726
98	H	3.10137105	16.10374106	28.88864723
99	S	4.38165209	14.44598594	18.06439595
100	C	4.94478675	13.16910760	16.82965359
101	C	5.53595158	13.79066043	15.55740684
102	C	5.79152141	12.67063781	14.53058558
103	C	6.24631604	13.16766929	13.15577989
104	H	5.69744674	12.56338111	17.36188053
105	H	4.08829170	12.52029589	16.59404065
106	H	6.54493273	11.97379965	14.94147777
107	H	4.85856257	12.09186572	14.41265638
108	H	7.22758949	13.66284306	13.20119811
109	H	6.33174935	12.33057648	12.44576277
110	H	5.52460912	13.88718775	12.73752157
111	S	3.66995861	15.59166150	23.26182209
112	C	4.90349880	16.09200183	21.94846581
113	C	4.55930269	17.41179372	21.25296883
114	C	5.57927597	17.64717039	20.11996415
115	C	5.23596719	18.83029922	19.21080753
116	H	5.87114511	16.16896741	22.47117258
117	H	4.96151913	15.27505719	21.21749203
118	H	6.58207244	17.79358692	20.56403714
119	H	5.63492443	16.73319859	19.50462157
120	H	5.25469402	19.78753010	19.75328523
121	H	5.95576295	18.90663201	18.38117943

122	H	4.23271039	18.70400261	18.77558747
123	S	0.78569351	12.23772941	15.34918318
124	C	-0.79648458	11.39493916	14.82226023
125	C	-1.86641862	12.38582370	14.35081933
126	C	-3.19271526	11.62236172	14.15875431
127	C	-4.39242077	12.52372820	13.85530363
128	H	-0.51562774	10.70945252	14.00631407
129	H	-1.15877653	10.80149213	15.67183846
130	H	-3.06561047	10.88223855	13.34599791
131	H	-3.40158019	11.04839005	15.07806279
132	H	-4.28159494	13.05236017	12.89647355
133	H	-5.31965876	11.93298876	13.80149711
134	H	-4.51751022	13.27708846	14.64848633
135	S	-3.06424473	14.83920065	17.33620718
136	C	-3.88215806	16.35839007	18.03961989
137	C	-4.35453860	17.34433950	16.96421278
138	C	-4.89177883	18.60819986	17.66537650
139	C	-5.24012026	19.75747713	16.71632457
140	H	-4.73050346	15.98485448	18.63787758
141	H	-3.17800489	16.83731836	18.73149333
142	H	-5.78207671	18.33497819	18.26208979
143	H	-4.13213826	18.95788954	18.38494905
144	H	-6.06872532	19.49737783	16.04097454
145	H	-5.54477148	20.65061143	17.28255270
146	H	-4.37267056	20.03370435	16.09562079
147	S	6.70484090	11.32572148	19.74409466
148	C	6.94671611	13.04942726	20.41561784
149	C	8.41934730	13.38987017	20.67838224
150	C	8.49188302	14.72892148	21.43825636
151	C	9.90170062	15.12200001	21.88729847
152	H	6.51206418	13.72364998	19.65891919
153	H	6.35133911	13.13482801	21.33578622
154	H	8.06715671	15.52708403	20.80234824
155	H	7.84148760	14.65587005	22.32700063
156	H	10.56812432	15.31089004	21.03283022
157	H	9.87579615	16.04006312	22.49401744
158	H	10.35436203	14.32778586	22.50215594
159	S	-6.02452863	12.95694129	20.33817756
160	C	-6.97711018	13.85414584	19.00705975
161	C	-7.89355090	12.92092300	18.20625429
162	C	-8.48972552	13.71198503	17.02480864
163	C	-9.29363792	12.86026818	16.03892740
164	H	-7.56289686	14.62892600	19.53052026
165	H	-6.25360165	14.34285466	18.34211170
166	H	-9.12815968	14.52391020	17.42135242
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170	H	-8.68420324	12.02825156	15.65197068
171	S	8.10541593	9.06849496	23.63352199
172	C	9.50091575	7.92638825	23.16063198
173	C	10.75956467	8.68240030	22.71836102
174	C	11.79810665	7.65820626	22.21877953
175	C	13.04941342	8.28119071	21.59442870
176	H	9.70423828	7.32859280	24.06536320
177	H	9.14404924	7.24926892	22.37260735
178	H	12.08978572	7.00373260	23.06193924
179	H	11.31326315	7.00471375	21.47388700
180	H	13.63461093	8.85171592	22.33068357
181	H	13.70853012	7.50263125	21.18132918
182	H	12.78215819	8.96474207	20.77266349
183	S	6.40606050	6.27482491	20.33812439
184	C	7.80142964	7.11787555	19.42710254
185	C	9.01857920	6.20336761	19.23136924
186	C	10.16961215	7.05413248	18.65457594
187	C	11.49277104	6.30361313	18.47997672
188	H	7.42162819	7.49111415	18.46509466
189	H	8.06681322	7.99117581	20.04709112
190	H	9.85204576	7.46830217	17.68086710
191	H	10.32799943	7.92202708	19.31888143
192	H	11.41984297	5.51742989	17.71396781
193	H	12.29282059	6.99290928	18.16949718
194	H	11.80901072	5.82649016	19.42131230
195	S	5.59075685	11.52780506	24.62961356
196	C	4.89051956	11.25902407	26.33619777
197	C	5.69520815	10.23040945	27.14032287
198	C	4.91922883	9.93493315	28.44060617
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200	H	4.92409888	12.23801392	26.83845164
201	H	3.84069536	10.95328594	26.23193748
202	H	4.77065403	10.88540753	28.98713773
203	H	3.91150508	9.57245506	28.17157720
204	H	6.53644864	9.30880140	29.78384235
205	H	4.93611278	8.67227357	30.21662995
206	H	5.82167981	7.98804190	28.83483206
207	S	4.63981715	6.02925569	24.52753159
208	C	4.31597837	6.15153240	26.36286417
209	C	4.98907329	5.01256768	27.14119025
210	C	4.42939164	4.99470270	28.57870792
211	C	4.88627703	3.79976703	29.41903471
212	H	4.64868470	7.13733741	26.71717783
213	H	3.21927965	6.10789337	26.46641741
214	H	4.71350040	5.93392946	29.08605974
215	H	3.32668100	4.99543176	28.52462740
216	H	5.97183511	3.81185132	29.59619961
217	H	4.39189225	3.80399285	30.40258438
218	H	4.63495637	2.84872267	28.92292496
219	S	-0.09056924	17.79366460	24.25339380
220	C	1.42767100	18.38863286	25.15726048
221	C	1.79633178	19.83648572	24.81236149
222	C	3.11327759	20.18598168	25.53438251
223	C	3.71764988	21.53092263	25.12346692
224	H	1.17964565	18.29550151	26.22821625
225	H	2.25267674	17.70069913	24.92425387
226	H	2.93391561	20.17639369	26.62616294
227	H	3.84890552	19.38789252	25.33367143
228	H	3.06263135	22.37459418	25.38624551
229	H	4.68295330	21.69368432	25.62699506
230	H	3.89657257	21.56439784	24.03711200
231	S	0.96178129	17.61944862	19.68089955
232	C	-0.52647954	18.56254071	19.07371314
233	C	-0.39632319	20.06847629	19.34155924
234	C	-1.75271861	20.74644585	19.06612652
235	C	-1.79465891	22.23521827	19.42108510
236	H	-0.59319626	18.35437076	17.99280079
237	H	-1.41383807	18.14711646	19.57101627
238	H	-2.01249933	20.61181582	17.99985453
239	H	-2.52864176	20.21935902	19.64800035
240	H	-1.10616603	22.82492066	18.79806343
241	H	-2.80586651	22.64336048	19.27232593
242	H	-1.51934357	22.39611211	20.47579374
243	S	0.95058152	16.73837551	15.79168783
244	C	0.99800492	16.18400882	14.00683359
245	C	1.94321245	17.03096187	13.14424560
246	C	1.63814551	16.73328970	11.66088711
247	C	2.41761800	17.60179548	10.67027884
248	H	1.26285848	15.11692843	13.97927518
249	H	-0.03782635	16.29592609	13.65441704
250	H	1.84439794	15.66528239	11.46118797
251	H	0.55653214	16.87785549	11.48996004
252	H	3.49933369	17.40945100	10.71780146
253	H	2.09239329	17.40167582	9.63796997
254	H	2.25452481	18.67281157	10.87186122
255	S	0.17710490	4.77387372	25.30309313
256	C	1.16894245	3.77278073	26.53055638
257	C	0.66646884	2.32755433	26.65877889
258	C	1.28817306	1.70609418	27.92742609
259	C	0.76986502	0.30566980	28.26339738
260	H	2.23124594	3.80284483	26.24830002
261	H	1.04456929	4.30177986	27.48764091
262	H	2.38687428	1.67489992	27.80702278
263	H	1.08805614	2.37704206	28.78177627
264	H	1.03879660	-0.42857457	27.49002153
265	H	1.19404578	-0.04772114	29.21559010
266	H	-0.32729414	0.30527128	28.36412539
267	S	-4.13810277	10.87567495	22.83039173
268	C	-3.98079394	11.39694042	24.61430951
269	C	-4.65584996	12.73993322	24.91522375
270	C	-4.37055168	13.08786728	26.39168058
271	C	-4.86926970	14.46570023	26.83289937
272	H	-4.45555673	10.59230202	25.19967595
273	H	-2.91291159	11.43363952	24.86697209
274	H	-4.82844546	12.30947189	27.03061667
275	H	-3.28098731	13.03240169	26.55890378
276	H	-5.96449486	14.54905999	26.76804497
277	H	-4.58442162	14.66542592	27.87758733

278	H	-4.42920778	15.26010230	26.21200171
279	S	2.22587113	4.01995748	21.13027614
280	C	3.97319982	3.56605764	21.58679900
281	C	4.08848368	2.23332643	22.33558341
282	C	5.55867472	2.04741746	22.76180929
283	C	5.80855718	0.83042632	23.65578551
284	H	4.51950304	3.53177159	20.62820321
285	H	4.39220955	4.38294299	22.18850911
286	H	6.18734522	1.97603192	21.85460636
287	H	5.88312971	2.95855233	23.29317205
288	H	5.59095687	-0.11488517	23.13680036
289	H	6.86055313	0.79432760	23.97851279
290	H	5.18210746	0.87025842	24.56123954
291	S	-2.01632334	6.68970264	23.01416955
292	C	-2.63484130	5.77969554	21.50694382
293	C	-2.18560328	4.31388460	21.49370177
294	C	-2.51934402	3.71028492	20.11451345
295	C	-1.97787504	2.29393863	19.90248829
296	H	-3.73420042	5.84763883	21.54212294
297	H	-2.27590322	6.31229291	20.61656749
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300	H	-2.43955459	1.56815704	20.58827015
301	H	-2.17789046	1.95163192	18.87541070
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304	C	-3.83916549	8.42908124	18.78974587
305	C	-5.30110684	8.07418078	18.48760312
306	C	-5.72553734	6.90355661	19.39659167
307	C	-7.20344035	6.52090023	19.27958001
308	H	-3.15985494	7.63618994	18.43538510
309	H	-3.67661199	8.56286437	19.86915894
310	H	-5.09476456	6.02506984	19.16763932
311	H	-5.50945997	7.18274893	20.44252173
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315	S	-3.05064504	16.25817730	21.86445111
316	C	-3.61265092	16.61097783	23.61668576
317	C	-3.90470307	18.10213953	23.82215502
318	C	-4.08865881	18.35950581	25.33101352
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321	H	-2.80356708	16.27333262	24.28097155
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324	H	-5.16629958	20.27050712	25.27675661
325	H	-4.30493939	19.95726764	26.79560621
326	H	-3.39296191	20.42661945	25.34278272
327	H	-0.04896166	6.07846880	15.07235486
328	C	-2.18868611	5.80481191	15.12889061
329	H	-2.20190003	5.09435203	14.28938086
330	H	-3.11143577	6.40678828	15.08208741
331	H	-2.20927112	5.22037093	16.06094583
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333	C	5.69489327	2.22220799	17.41175227
334	H	5.65021059	1.92713997	18.47355026
335	H	6.01276224	3.27408552	17.37010050
336	H	6.47380410	1.61914857	16.92215819
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339	H	-0.90592490	10.68548722	29.21370642
340	H	-1.02901355	9.07675458	29.97242589
341	H	0.40417102	9.49251123	29.00862149
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343	C	5.71177751	7.21599967	14.23025814
344	H	6.36503913	6.35525738	14.02716020
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346	H	5.72607151	7.87442156	13.34440113
347	H	1.32930181	15.12981061	27.29923002
348	C	0.51958342	13.78976627	28.78325878
349	H	-0.51216815	13.81020923	28.40059069
350	H	0.58509038	14.51822362	29.60482819
351	H	0.70998383	12.78620747	29.19931388
352	H	4.76809888	14.46652818	15.13537283
353	C	6.79528115	14.61100279	15.85314211
354	H	7.16468094	15.12365573	14.95304616
355	H	7.60029876	13.95897963	16.23215155
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357	H	3.56376969	17.29819418	20.78745690
358	C	4.50636166	18.58200835	22.23715907
359	H	4.19530133	19.51101530	21.73858486
360	H	5.49630655	18.75066767	22.69591684
361	H	3.78737510	18.38165204	23.04378235
362	H	-2.01965256	13.12698325	15.15678247
363	C	-1.43485173	13.12670127	13.08181310
364	H	-1.34293506	12.42363823	12.23545941
365	H	-0.45975229	13.61498753	13.22192972
366	H	-2.16054433	13.90433966	12.80223022
367	H	-3.46746786	17.63493768	16.36850084
368	C	-5.38954513	16.71746424	16.02582646
369	H	-5.00173475	15.79416342	15.57041331
370	H	-5.66304462	17.40197555	15.20943756
371	H	-6.30912166	16.46517775	16.58054362
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373	C	9.23818485	13.40418817	19.38429212
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384	H	10.54611863	10.26664333	24.20805548
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388	C	8.69980378	4.98287667	18.36389575
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390	H	7.87945199	4.39386731	18.79800014
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398	C	6.51689965	5.12062908	27.11087684
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405	H	0.47721820	20.81673353	26.24408820
406	H	0.91931859	21.84070194	24.85262775
407	H	-0.17214668	20.19389543	20.41862029
408	C	0.74417764	20.68627510	18.52694090
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412	H	1.70419814	18.09660482	13.33065631
413	C	3.41382955	16.78937803	13.49139109
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416	H	3.69193976	15.74727828	13.26306158
417	H	-0.43085721	2.36807651	26.80532063
418	C	0.96371142	1.49908415	25.40621892
419	H	0.52744245	0.49163603	25.47571136
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422	H	-4.17299655	13.50681471	24.28020907
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428	C	3.56379435	1.05696951	21.50764044
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Isomer 2a

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6	Au	-2.83603001	-0.10838000	-1.69868004
7	Au	1.23901999	2.51215005	-1.61188996
8	Au	1.31098998	2.42580009	1.40204000
9	Au	1.26275003	-2.41926003	1.38627005
10	Au	-2.89197993	0.03047000	1.32422996
11	Au	1.44511998	-2.32467008	-1.63739002
12	Au	-1.31562996	-2.52151990	-2.94706988
13	Au	-1.59679997	2.42341995	-2.91427994
14	Au	2.73536992	-0.06120000	2.66488004
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16	Au	-1.51554000	2.54671001	2.58691001
17	Au	2.85762000	0.19101000	-2.83628011
18	Au	-1.80332005	-0.21036001	-4.46165991
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20	Au	0.93207002	1.48838997	4.16405010
21	Au	0.57656002	-1.65429997	4.15855980
22	Au	-1.95106006	0.22719000	4.11343002
23	Au	1.13133001	-1.36295998	-4.41556978
24	Au	-2.44385004	-4.29664993	-0.19866000
25	Au	-2.67102003	4.23720980	-0.25453001
26	Au	4.86793995	0.08085000	0.01074000
27	Au	-4.38853979	-2.02169991	-4.08450985
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38	Au	3.46984005	0.23683999	-5.87140989
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40	C	-3.01086998	-5.69723988	-3.13799000
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68	H	6.12857008	0.96688002	2.96620011
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84	H	-5.99747992	-7.23043013	5.72796011
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87	S	-1.82201004	4.87806988	1.84371996
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95	H	-4.84221983	6.15868998	4.74396992
96	H	-3.35332990	8.65653992	5.78996992
97	H	-4.89062023	8.00512028	6.38898993
98	H	-3.39070010	7.07473993	6.60692978
99	S	4.97664022	1.18454003	-2.06417990
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103	C	8.54747009	1.05403996	-6.10963011
104	H	7.24605989	0.34895000	-2.11033010
105	H	6.19646978	-0.62119001	-3.18168998
106	H	8.92440033	0.30181000	-4.11011982
107	H	7.68585014	-0.59086001	-5.01000023
108	H	9.02715969	2.03077006	-5.94568014
109	H	9.28283978	0.40561000	-6.61020994
110	H	7.70502996	1.20275998	-6.80364990
111	S	-5.13204002	-0.77829999	-2.22534990
112	C	-5.57722998	-2.02995992	-0.91668999
113	C	-7.00705004	-2.57258010	-1.04753995
114	C	-7.40748978	-3.19826007	0.30555001
115	C	-8.85832024	-3.68073010	0.37568000
116	H	-4.82810020	-2.83640003	-0.92493999
117	H	-5.46567011	-1.47878003	0.02916000
118	H	-6.72307014	-4.03819990	0.52144998
119	H	-7.23651981	-2.44905996	1.09792995
120	H	-9.05405998	-4.50380993	-0.32745001
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123	S	1.86924005	4.83095980	-2.10356998
124	C	1.00934994	5.84669018	-0.79636002
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126	C	0.96480000	7.99069023	0.47187999
127	C	1.30676997	9.47902012	0.57367003
128	H	-0.07014000	5.63918018	-0.83552003
129	H	1.39183998	5.44220018	0.15267999
130	H	-0.11129000	7.83949995	0.67238998
131	H	1.50577998	7.43949986	1.26063001
132	H	0.71319997	10.08708000	-0.12517001

133	H	1.10748005	9.85513973	1.58870995
134	H	2.37240005	9.65620995	0.35404000
135	S	2.92682004	4.18518019	1.95931995
136	C	4.26484013	4.06443024	0.66430002
137	C	5.34243011	5.14916992	0.79890001
138	C	6.10069990	5.24387980	-0.54233998
139	C	7.13750982	6.36878014	-0.60233003
140	H	4.69400978	3.05175996	0.68831003
141	H	3.73066998	4.17767000	-0.29091001
142	H	6.58978987	4.27331018	-0.74190003
143	H	5.36152983	5.38920021	-1.34894001
144	H	7.96089983	6.20919991	0.10933000
145	H	7.58013010	6.43702984	-1.60808003
146	H	6.67670012	7.34331989	-0.37323999
147	S	1.93954003	-4.71995020	1.89411998
148	C	1.14303994	-5.75074005	0.55931002
149	C	1.44295001	-7.25117016	0.67750001
150	C	1.13935995	-7.90756989	-0.68647999
151	C	1.49422002	-9.39435959	-0.76551998
152	H	0.06140000	-5.54803991	0.54900002
153	H	1.56660998	-5.35131979	-0.37458000
154	H	0.06814000	-7.76526022	-0.91727000
155	H	1.69772005	-7.36038017	-1.46589994
156	H	0.88595998	-10.00063992	-0.07779000
157	H	1.32516003	-9.78061008	-1.78222001
158	H	2.55469990	-9.56190014	-0.51556998
159	S	-5.23557997	0.59495002	1.76933002
160	C	-5.70225000	1.81306005	0.43549001
161	C	-7.16300011	2.27690005	0.51310003
162	C	-7.54023981	2.90052009	-0.84776002
163	C	-9.01369953	3.29643011	-0.97302997
164	H	-4.99949980	2.65962005	0.46454000
165	H	-5.52860022	1.26538002	-0.50294000
166	H	-6.89841986	3.78280997	-1.02338004
167	H	-7.29188013	2.17597008	-1.64251006
168	H	-9.28649044	4.09969997	-0.27246001
169	H	-9.23443031	3.65681005	-1.98934996
170	H	-9.67273998	2.43570995	-0.77395999
171	S	3.16476989	-4.00729990	-2.10877991
172	C	4.43212986	-3.78391004	-0.75860000
173	C	5.59734011	-4.77978992	-0.84021997
174	C	6.32085991	-4.78471994	0.52366000
175	C	7.43212986	-5.83101988	0.64216000
176	H	4.78131008	-2.74009991	-0.76686001
177	H	3.86557007	-3.93957996	0.17178001
178	H	6.73301983	-3.77658010	0.71016997
179	H	5.57138014	-4.96157980	1.31421006
180	H	8.25926018	-5.63601017	-0.05621000
181	H	7.85445976	-5.83725977	1.65910006
182	H	7.04606009	-6.84230995	0.43516999
183	S	0.76065999	-2.76556993	-6.37175989
184	C	1.35192001	-4.44302988	-5.80648994
185	C	0.98211998	-5.58349991	-6.76275015
186	C	1.46656001	-6.90890980	-6.14110994
187	C	1.04103005	-8.16036987	-6.91300011
188	H	2.44804001	-4.34658003	-5.71305990
189	H	0.94533002	-4.62381983	-4.80230999
190	H	2.56928992	-6.88242006	-6.05634022
191	H	1.07964003	-6.97241020	-5.10999012
192	H	1.51238000	-8.21187973	-7.90596008
193	H	1.32669997	-9.07143974	-6.36537981
194	H	-0.05082000	-8.18284035	-7.05831003
195	S	-2.94047999	0.93927002	-6.29249001
196	C	-4.61543989	1.29821002	-5.55236006
197	C	-5.41372013	2.36435008	-6.31252003
198	C	-6.68559980	2.68823004	-5.50265980
199	C	-7.49897003	3.86241007	-6.05329990
200	H	-5.14602995	0.33008000	-5.55037022
201	H	-4.46165991	1.59995997	-4.50746012
202	H	-7.32099009	1.78435004	-5.45557022
203	H	-6.38836002	2.91027999	-4.46294022
204	H	-7.90082979	3.65293002	-7.05569983
205	H	-8.35363007	4.08629990	-5.39673996
206	H	-6.88103008	4.77187014	-6.12099981
207	S	2.05995989	-2.00137997	6.06154013
208	C	3.25847006	-3.27934003	5.41855001
209	C	4.48120022	-3.48101997	6.32114983
210	C	5.47097015	-4.41675997	5.59813023
211	C	6.80921984	-4.59520006	6.32004976
212	H	2.67162991	-4.21096992	5.33221006
213	H	3.56035995	-2.97728992	4.40619993
214	H	4.99229002	-5.40319014	5.45300007
215	H	5.65660000	-4.01261997	4.58794022
216	H	6.68948984	-5.09929991	7.29051018
217	H	7.50030994	-5.20363998	5.71646976
218	H	7.29180002	-3.62159991	6.50252008
219	S	-3.02174997	-0.87645000	6.00480986
220	C	-4.73474979	-1.24775004	5.36745024
221	C	-5.54968023	-2.16120005	6.29079008
222	C	-6.88967991	-2.47852993	5.59715986
223	C	-7.75640011	-3.49853992	6.34034014
224	H	-5.22204018	-0.26284999	5.25554991
225	H	-4.63397980	-1.68701005	4.36550999
226	H	-7.45554018	-1.53723001	5.46409988
227	H	-6.67662001	-2.85654998	4.58323002
228	H	-8.10416031	-3.11437988	7.31106997
229	H	-8.64879990	-3.75602007	5.74947977
230	H	-7.19714022	-4.42926979	6.52845001
231	S	0.45980000	2.91312003	6.08432007
232	C	1.04489994	4.59472990	5.52608013
233	C	0.61983001	5.73894978	6.45436001
234	C	1.11452997	7.06448984	5.84049988
235	C	0.62459999	8.31846046	6.56900978
236	H	2.14532995	4.51566982	5.47606993
237	H	0.67575002	4.75927019	4.50496006
238	H	2.22047997	7.05692005	5.81713009
239	H	0.78473002	7.10677004	4.78855991
240	H	1.03639996	8.39151001	7.58683014
241	H	0.92629999	9.22723007	6.02618980
242	H	-0.47404000	8.32398987	6.65068007
243	S	2.16031003	2.14326000	-6.29967022
244	C	3.26770997	3.53004003	-5.72473001
245	C	4.45009995	3.80580997	-6.66142988
246	C	5.31190014	4.91976976	-6.03322983
247	C	6.61750984	5.20249987	-6.78067017
248	H	2.60868001	4.41325998	-5.65195990
249	H	3.61494994	3.28899002	-4.71090984
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256	C	-4.51929998	-2.41628003	-7.48028994
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260	H	-4.40326023	-1.33497000	-7.31642008
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265	H	-7.74435997	-2.33242011	-10.85116005
266	H	-7.71429014	-3.78595996	-9.82656002
267	S	-0.97551000	5.18435001	-5.83299017
268	C	0.14078000	5.26867008	-7.32296991
269	C	-0.64985001	5.32412004	-8.63669968
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271	C	-0.33392000	5.06377983	-11.18266010
272	H	0.74739999	6.18042994	-7.18912983
273	H	0.79973000	4.39019012	-7.30374002
274	H	1.00909996	6.07796001	-9.81474018
275	H	0.97920001	4.31698990	-9.64083004
276	H	-0.90705001	5.96330976	-11.45090961
277	H	0.41786000	4.90483999	-11.97068977
278	H	-1.02314997	4.20432997	-11.19859982
279	S	4.71234989	1.85304999	5.63595009
280	C	4.19417000	2.84457994	7.12645006
281	C	4.57193995	2.16395998	8.44775009
282	C	3.97211003	2.98433995	9.60708046
283	C	4.10981989	2.32326007	10.98087025
284	H	4.70377016	3.81787992	7.02433014
285	H	3.10798001	2.99829006	7.07123995
286	H	4.45118999	3.98140001	9.62570953
287	H	2.90231991	3.15550995	9.39760971
288	H	5.16202021	2.21237993	11.28090000

289	H	3.60803008	2.92529011	11.75364017
290	H	3.64842010	1.32272005	10.98326015
291	S	-0.98066998	-5.08420992	5.56618023
292	C	0.13750000	-5.12516022	7.05688000
293	C	-0.64528000	-5.13493013	8.37576962
294	C	0.35323000	-4.98131990	9.54069996
295	C	-0.30682999	-4.80007982	10.91009998
296	H	0.74089998	-6.04223013	6.94829988
297	H	0.79870999	-4.24931002	7.00641012
298	H	1.01835001	-5.86474991	9.56285954
299	H	0.99843001	-4.10988998	9.33528996
300	H	-0.88515002	-5.68636990	11.20919037
301	H	0.45247999	-4.62432003	11.68725967
302	H	-0.98885000	-3.93482995	10.90581036
303	S	-4.17745018	3.31803012	5.45620012
304	C	-4.84873009	2.38256001	6.92226982
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307	C	-4.67909002	2.71924996	10.79755974
308	H	-5.92983007	2.27390003	6.73297024
309	H	-4.38212013	1.38788998	6.92889977
310	H	-6.08749008	1.96570003	9.33187008
311	H	-4.49006987	1.20766997	9.26766014
312	H	-5.25359011	3.62837005	11.02869987
313	H	-4.91737986	1.97318995	11.57094955
314	H	-3.60810995	2.96247005	10.88547993
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316	C	4.52616978	-2.60590005	-7.22880983
317	C	4.93669987	-1.92972004	-8.54238033
318	C	4.40656996	-2.78186989	-9.71304989
319	C	4.58297014	-2.13615990	-11.08979034
320	H	5.05720997	-3.56378007	-7.09514999
321	H	3.44308996	-2.78811002	-7.21422005
322	H	4.91191006	-3.76584005	-9.69769955
323	H	3.33406997	-2.97904992	-9.54504013
324	H	5.64333010	-2.00622010	-11.35118961
325	H	4.12421989	-2.75935006	-11.87240982
326	H	4.10054016	-1.14628005	-11.12401009
327	C	-1.67332006	-7.69092989	-3.94938993
328	H	-1.31110001	-8.24551964	-4.82639980
329	H	-0.79622000	-7.32949018	-3.39326000
330	H	-2.21597004	-8.40003967	-3.29989004
331	H	-2.04310989	-5.86283016	-5.04784012
332	C	-4.83291006	6.87404013	-1.79075003
333	H	-3.99770999	7.58933020	-1.70025003
334	H	-4.72806978	6.13360977	-0.98330998
335	H	-5.77314997	7.42122984	-1.62511003
336	H	-5.69605017	5.54067993	-3.25082994
337	C	8.18929005	-0.03671000	1.46647000
338	H	7.48621988	-0.26719999	0.65047002
339	H	9.16586018	-0.46803999	1.20088005
340	H	8.29788971	1.06007004	1.51415002
341	H	7.66868019	-1.68763995	2.75597000
342	H	-4.13759995	-4.88108015	4.58984995
343	C	-5.82002020	-5.57025003	3.41704988
344	H	-5.97104979	-4.63963985	2.85071993
345	H	-6.51845980	-5.56474018	4.26577997
346	H	-6.09122992	-6.41447020	2.75911999
347	C	-1.97424996	7.68944979	3.48500991
348	H	-1.08574998	7.32427979	2.95015001
349	H	-2.50376010	8.39361954	2.81957006
350	H	-1.63028002	8.25020981	4.36538982
351	H	-2.36268997	5.86810017	4.58684015
352	C	7.44025993	2.61213994	-3.65197992
353	H	7.72217989	3.22881007	-4.51702976
354	H	6.65610981	3.14779997	-3.09740996
355	H	8.32231045	2.52754998	-2.99312997
356	H	6.11427021	1.33427000	-4.78780985
357	H	-7.67969990	-1.71196997	-1.23403001
358	C	-7.14707994	-3.56456995	-2.20526004
359	H	-6.78205013	-3.12628007	-3.14657998
360	H	-8.19386005	-3.86573005	-2.36040998
361	H	-6.55251980	-4.47245979	-2.00620008
362	C	0.56217998	8.01780033	-2.04706001
363	H	-0.52595001	7.98473978	-1.86882997
364	H	0.76190001	7.50148010	-2.99871993
365	H	0.85740000	9.07059956	-2.16932988
366	H	2.39779997	7.46863985	-1.05356002
367	H	4.82838011	6.11700010	0.96385002
368	C	6.28400993	4.88970995	1.97783005
369	H	6.98317003	5.72518015	2.13243008
370	H	6.87538004	3.97515011	1.80075002
371	H	5.72006989	4.74745989	2.91265011
372	C	0.66544998	-7.90862989	1.82053995
373	H	0.94586003	-8.96459961	1.95005000
374	H	-0.41874999	-7.86231995	1.62198997
375	H	0.85268998	-7.39329004	2.77537990
376	H	2.52761006	-7.36576986	0.87322003
377	C	-7.40637016	3.24006009	1.67797995
378	H	-8.47266960	3.49048996	1.78346002
379	H	-6.84602022	4.17793989	1.52393997
380	H	-7.79523993	1.37820995	0.65823001
381	H	-7.07002020	2.80241990	2.63013005
382	C	6.54852009	-4.46694994	-1.99812996
383	H	6.00622988	-4.41882992	-2.95468998
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385	H	7.03632021	-3.49020004	-1.84001994
386	H	5.16769981	-5.78911018	-0.99687999
387	C	1.53954995	-5.36431980	-8.17183971
388	H	2.64258003	-5.35910988	-8.15515041
389	H	1.21385002	-6.15709019	-8.86153984
390	H	-0.12304000	-5.61945009	-6.82419014
391	H	1.20033002	-4.40266991	-8.58535957
392	C	-5.72513008	1.93748999	-7.74966002
393	H	-4.80520010	1.66385996	-8.28857040
394	H	-6.21716976	2.74228001	-8.31540012
395	H	-6.39577007	1.06197000	-7.75294018
396	H	-4.79005003	3.27871990	-6.34608984
397	C	4.08846998	-3.99784994	7.70782995
398	H	3.62841010	-4.99779987	7.63136005
399	H	4.95983982	-4.07368994	8.37469006
400	H	3.36139011	-3.32485008	8.18599033
401	H	4.97152996	-2.49495006	6.43957996
402	C	-5.74490976	-1.55066001	7.68127012
403	H	-6.34114981	-0.62503999	7.61660004
404	H	-4.77726984	-1.30061996	8.14140034
405	H	-6.26591015	-2.24450994	8.35721970
406	H	-4.98902988	-3.11021996	6.39859009
407	H	-0.48732001	5.76141977	6.46782017
408	C	1.11898005	5.54124022	7.88823986
409	H	2.22168994	5.54768991	7.91827011
410	H	0.77278000	4.58057022	8.29819965
411	H	0.75616002	6.33814001	8.55414963
412	C	3.99608994	4.15621996	-8.08108044
413	H	3.36047006	3.36193991	-8.49995041
414	H	3.41466999	5.09328985	-8.08069038
415	H	4.85343981	4.28809977	-8.75732040
416	H	5.06207991	2.88446999	-6.70511007
417	H	-6.00985003	-3.90531993	-7.88813019
418	C	-6.97594023	-2.31002998	-6.80519009
419	H	-6.99806023	-1.20802999	-6.77700996
420	H	-6.72160006	-2.66506004	-5.79595995
421	H	-7.99116993	-2.66509008	-7.03620005
422	H	-1.31234002	4.43722010	-8.65721989
423	C	-1.51322997	6.58543015	-8.73246002
424	H	-0.87751001	7.48689985	-8.76453018
425	H	-2.13877010	6.57758999	-9.63632965
426	H	-2.18267012	6.67502022	-7.86394978
427	H	4.08765984	1.16802001	8.45203018
428	C	6.08543015	1.97525001	8.58518028
429	H	6.49409008	1.41268003	7.73277998
430	H	6.34092999	1.42402995	9.50152969
431	H	6.59561014	2.95323992	8.62100029
432	C	-1.51818001	-6.38541985	8.51531982
433	H	-0.89051998	-7.29193020	8.56348038
434	H	-2.13391995	-6.34842014	9.42525005
435	H	-2.19876003	-6.49127007	7.65782022
436	H	-1.30016005	-4.24217987	8.37362003
437	H	-3.50502992	3.28555989	8.32499981
438	C	-5.31549978	4.46136999	8.30422974
439	H	-6.40959978	4.31835985	8.28310966
440	H	-5.04007006	5.09147978	7.44611979
441	H	-5.06160021	5.01644993	9.21874046
442	H	4.42487001	-0.94849002	-8.57896996
443	C	6.44841003	-1.69994998	-8.62224007
444	H	6.80577993	-1.11430001	-7.76315022
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Isomer 2b

1	Au	0.06985700	0.00573600	1.99666202
2	Au	0.04473300	0.07141300	-2.14765096
3	Au	1.04370201	-1.70433497	-0.10872300
4	Au	1.07919300	1.75804996	-0.05670900
5	Au	-1.94535100	0.06101100	-0.06092700
6	Au	2.83780789	-0.00716300	-1.60182798
7	Au	-1.28130305	2.50680995	-1.53806698
8	Au	-1.33981705	2.42349195	1.47687495
9	Au	-1.30532598	-2.40594602	1.40900004
10	Au	2.85386705	0.02228700	1.41771495
11	Au	-1.40452695	-2.31310606	-1.60603404
12	Au	1.38693404	-2.42633200	-2.88514090
13	Au	1.52563298	2.52509689	-2.80583811
14	Au	-2.77386689	-0.01915500	2.70431995
15	Au	1.51117003	-2.47695708	2.64117408
16	Au	1.48606300	2.46136808	2.71257401
17	Au	-2.81322694	0.15092200	-2.81382489
18	Au	1.84163105	-0.07380700	-4.37297392
19	Au	-0.70762902	1.75000203	-4.33640814
20	Au	-0.94036102	1.46907902	4.24300003
21	Au	-0.68803799	-1.65227199	4.19835997
22	Au	1.88814604	0.10461800	4.20624924
23	Au	-1.01916301	-1.35508502	-4.38158894
24	Au	2.50257993	-4.31168079	-0.15611500
25	Au	2.61030889	4.32745790	-0.01335200
26	Au	-4.92813683	0.09621200	-0.04317700
27	Au	4.51777077	-1.79898095	-4.01897621
28	Au	-0.56703401	4.91510391	-3.87314200
29	Au	-3.74494290	3.01428199	3.86661291
30	Au	-0.62105203	-4.83361292	3.72561407
31	Au	4.62026691	1.73117495	3.80025101
32	Au	-3.85348701	-2.83158112	-3.94472694
33	Au	1.71828794	-2.79963899	-5.97138977
34	Au	1.72448206	3.11153889	-5.85702085
35	Au	-3.27602291	0.07655900	5.80136681
36	Au	1.70221305	-3.07820797	5.71217012
37	Au	1.90725601	2.84519601	5.78244019
38	Au	-3.38178802	0.06237500	-5.89448214
39	S	1.76994896	-4.79259777	-2.34738493
40	C	3.32407594	-5.34193516	-3.21440601
41	C	3.82829404	-6.71277905	-2.74661398
42	C	5.22122908	-6.96178007	-3.35972595
43	C	5.89827681	-8.24869347	-2.88103294
44	C	2.83214092	-7.82574320	-3.08653998
45	H	4.08835793	-4.56624222	-3.06895399
46	H	3.06595612	-5.36833906	-4.28639984
47	H	3.94638991	-6.66568804	-1.64627898
48	H	5.86798620	-6.10213280	-3.11238909
49	H	5.13109207	-6.97467899	-4.46202612
50	H	5.97540379	-8.26786900	-1.78217995
51	H	6.91752911	-8.32901764	-3.28908300
52	H	5.34604883	-9.14584064	-3.19697905
53	H	1.83564198	-7.59856701	-2.67991304
54	H	3.15032005	-8.79408646	-2.67390609
55	H	2.73814702	-7.93596697	-4.18060207
56	S	3.39186096	4.01056910	-2.21777797
57	C	3.08897996	5.65962410	-3.03008699
58	C	3.93975902	6.79505920	-2.44933295
59	C	3.46881604	8.12839222	-3.06377602
60	C	4.12368298	9.36953354	-2.45177507
61	C	5.43678188	6.54918003	-2.66044807
62	H	2.01696110	5.88719320	-2.94706702
63	H	3.32290196	5.50229502	-4.09658384
64	H	3.73795605	6.83341980	-1.36089599
65	H	2.37437105	8.20091248	-2.93889594
66	H	3.65392494	8.10715580	-4.15406322
67	H	3.96559501	9.40081406	-1.36209798
68	H	3.69367003	10.28893185	-2.87867904
69	H	5.20764399	9.39657688	-2.63775492
70	H	5.73715782	5.57521296	-2.24689507
71	H	6.04680300	7.32319784	-2.17250896
72	H	5.67908382	6.55240202	-3.73713803
73	S	-5.02712202	-0.80863899	2.13334489
74	C	-6.25430393	0.29084599	3.00078011
75	C	-7.68710279	0.15004601	2.47492194
76	C	-8.56368065	1.22246897	3.15255904
77	C	-9.98912811	1.31388104	2.60267591
78	C	-8.23209190	-1.26667297	2.68012691
79	H	-5.90235186	1.32799196	2.91235709
80	H	-6.19974995	0.00248700	4.06419802
81	H	-7.66342306	0.36658600	1.38884997
82	H	-8.06943512	2.20236611	3.03273797
83	H	-8.59477043	1.02364302	4.24023199
84	H	-9.98094559	1.50274503	1.51737702
85	H	-10.54009914	2.13795805	3.08149910
86	H	-10.55942059	0.38993701	2.78139997
87	H	-7.56977320	-2.01339889	2.21845198
88	H	-9.23155689	-1.38404202	2.23679590
89	H	-8.30744553	-1.49786794	3.75669599
90	S	3.33679700	-3.99996209	2.03044605
91	C	3.01681709	-5.63740921	2.85936809
92	C	3.84763694	-6.78935099	2.28242493
93	C	3.36178589	-8.11079025	2.91083694
94	C	3.99653196	-9.36619282	2.30674505
95	C	5.34925079	-6.56239891	2.48205805
96	H	1.94124699	-5.85109997	2.78686595
97	H	3.26099300	-5.47412109	3.92282701
98	H	3.63815594	-6.83349705	1.19561100
99	H	2.26583195	-8.16968727	2.79236293
100	H	3.55295396	-8.08242989	3.99991298
101	H	3.83110905	-9.40592194	1.21842694
102	H	3.55705690	-10.27568340	2.74505210
103	H	5.08112383	-9.40583611	2.48635292
104	H	5.66017008	-5.59580612	2.05925703
105	H	5.94562006	-7.34830904	1.99639595
106	H	5.59843683	-6.56045914	3.55729389
107	S	1.93136299	4.82026386	2.19171000
108	C	3.51603198	5.29077578	3.04914999
109	C	4.12323809	6.60597277	2.54748297
110	C	5.51171923	6.78139591	3.19517899
111	C	6.30001497	7.98701620	2.67851710
112	C	3.19841290	7.79768085	2.81403804
113	H	4.22466898	4.45895481	2.93249893
114	H	3.25294089	5.36625290	4.11766815
115	H	4.26869583	6.50813103	1.45387101
116	H	6.09799385	5.86344910	3.01354694
117	H	5.38887215	6.85626888	4.29192591
118	H	6.41482210	7.94269323	1.58371401
119	H	7.30833483	8.01194763	3.11993194
120	H	5.80805111	8.93852425	2.92926311
121	H	2.20051003	7.62440777	2.38480997
122	H	3.59625793	8.72457886	2.37549710
123	H	3.08011508	7.95822001	3.89939404
124	S	-5.03699493	1.00294602	-2.21891499
125	C	-6.30361700	-0.06313900	-3.07192707
126	C	-7.72633696	0.11743300	-2.53112102
127	C	-8.63814068	-0.93359101	-3.19555497
128	C	-10.06021595	-0.98396802	-2.63211393
129	C	-8.23565769	1.54753602	-2.73516512
130	H	-5.97943211	-1.10953605	-2.98697996
131	H	-6.25198078	0.22377500	-4.13596392
132	H	-7.69672203	-0.09638700	-1.44467795
133	H	-8.16938782	-1.92584705	-3.07548594
134	H	-8.67381763	-0.73940402	-4.28396702
135	H	-10.04700947	-1.16706002	-1.54585695
136	H	-10.63714600	-1.79570901	-3.10114908
137	H	-10.60738754	-0.04619300	-2.81093311
138	H	-7.54995584	2.27793598	-2.28137398
139	H	-9.22767544	1.69195497	-2.28320694
140	H	-8.31485462	1.77794397	-3.81162810
141	S	5.16203785	-0.61221701	-2.08725691
142	C	5.56562901	-1.98882496	-0.89854199
143	C	6.82275915	-2.77605891	-1.28686297
144	C	6.93483877	-4.00438499	-0.36175400
145	C	8.07425308	-4.96134186	-0.72018403
146	C	8.07616329	-1.89646494	-1.24846494
147	H	4.68682909	-2.64710593	-0.83250999
148	H	5.69555616	-1.49786997	0.08008700
149	H	6.68197107	-3.14224601	-2.32262993
150	H	5.97775316	-4.55207300	-0.39415601
151	H	7.05267620	-3.65683794	0.68108600
152	H	7.99647188	-5.29390192	-1.76793396

153	H	8.04646873	-5.85759306	-0.08197100
154	H	9.06162739	-4.49405718	-0.58830601
155	H	7.95440578	-1.01344204	-1.89406502
156	H	8.96617413	-2.44260001	-1.59367299
157	H	8.26607800	-1.54295897	-0.22130200
158	S	-1.92459095	4.83408403	-1.95158398
159	C	-0.94894803	5.83552790	-0.72058898
160	C	-0.85895097	7.32519579	-1.07290804
161	C	0.08719400	8.00267124	-0.06080900
162	C	0.38117000	9.47565842	-0.35526800
163	C	-2.23978710	7.98597002	-1.11987495
164	H	0.05157500	5.38654900	-0.63375199
165	H	-1.46947300	5.69157982	0.24079700
166	H	-0.39848101	7.40521908	-2.07744789
167	H	1.03581405	7.43985081	-0.04315900
168	H	-0.34571701	7.90343809	0.95183098
169	H	0.79289597	9.60314846	-1.36913502
170	H	1.11886501	9.87583733	0.35722199
171	H	-0.52177602	10.09952831	-0.27820599
172	H	-2.89862609	7.46739101	-1.83236206
173	H	-2.17384911	9.03913307	-1.43034005
174	H	-2.71846390	7.94967890	-0.12672000
175	S	-2.97784400	4.18037415	1.96876097
176	C	-4.36135101	3.90282702	0.75257897
177	C	-5.66427803	4.61321497	1.13824201
178	C	-6.76866388	4.16106606	0.16157800
179	C	-8.16672134	4.68367481	0.49995399
180	C	-5.49504185	6.13508701	1.17045295
181	H	-4.51348782	2.81774211	0.65511799
182	H	-3.97910309	4.27961302	-0.21078500
183	H	-5.94517612	4.26963711	2.15346408
184	H	-6.78793621	3.05785704	0.14787200
185	H	-6.49004412	4.47439384	-0.86175901
186	H	-8.45532894	4.40610409	1.52668703
187	H	-8.91703796	4.25891209	-0.18429901
188	H	-8.22877884	5.77920294	0.41754201
189	H	-4.67806196	6.42404413	1.84890199
190	H	-6.41038799	6.63769293	1.51594996
191	H	-5.25207281	6.51612902	0.16434400
192	S	-2.00843692	-4.71562099	1.82800901
193	C	-1.07983398	-5.74459124	0.58309102
194	C	-1.02180099	-7.23512602	0.93868500
195	C	-0.10670500	-7.93920803	-0.08366600
196	C	0.16161500	-9.41578865	0.21744899
197	C	-2.41760111	-7.86180782	1.00637400
198	H	-0.06986600	-5.32172394	0.47825900
199	H	-1.61238003	-5.58964014	-0.36998799
200	H	-0.54966098	-7.32312393	1.93710494
201	H	0.85313100	-7.39654398	-0.12102800
202	H	-0.55397898	-7.83833790	-1.08981705
203	H	0.58775002	-9.54385090	1.22535396
204	H	0.87865198	-9.83637428	-0.50406599
205	H	-0.75502503	-10.02144146	0.16058400
206	H	-3.05373406	-7.32612896	1.72690296
207	H	-2.37320089	-8.91579342	1.31809497
208	H	-2.90881205	-7.81572199	0.01982000
209	S	5.20643902	0.54655403	1.85141301
210	C	5.62750578	1.92034197	0.66537100
211	C	6.90331221	2.68134308	1.04469502
212	C	7.03592920	3.90443897	0.11521500
213	C	8.19723034	4.83863497	0.46338800
214	C	8.13766384	1.77549505	1.00297999
215	H	4.76153898	2.59638309	0.60947400
216	H	5.73880386	1.42995095	-0.31600299
217	H	6.77556801	3.05330300	2.08017707
218	H	6.09072590	4.47202015	0.15194499
219	H	7.14027214	3.55126595	-0.92724103
220	H	8.12983227	5.18043900	1.50876999
221	H	8.18709087	5.73075485	-0.18117000
222	H	9.17381287	4.34898376	0.33171600
223	H	8.00128460	0.89793003	1.65303802
224	H	9.04071999	2.30446410	1.34094405
225	H	8.31463242	1.41362405	-0.02355200
226	S	-3.09542298	-4.02470016	-2.06305099
227	C	-4.45687008	-3.71512604	-0.83011699
228	C	-5.78258896	-4.38729095	-1.20692503
229	C	-6.86542082	-3.91204500	-0.21715599
230	C	-8.27897739	-4.39986706	-0.54300201
231	C	-5.65504122	-5.91300106	-1.25013494
232	H	-4.57740402	-2.62675309	-0.72513902
233	H	-4.07502079	-4.10836506	0.12680900
234	H	-6.06375313	-4.03004599	-2.21738696
235	H	-6.85785294	-2.80877399	-0.19952001
236	H	-6.58400822	-4.23582888	0.80214101
237	H	-8.57108021	-4.11215401	-1.56596994
238	H	-9.01210022	-3.95981503	0.15006199
239	H	-8.36614895	-5.49389505	-0.46348101
240	H	-4.85104895	-6.21961880	-1.93636799
241	H	-6.58611298	-6.38817501	-1.59242404
242	H	-5.41554308	-6.30727386	-0.24831600
243	S	-0.60788101	-2.77786994	-6.32145500
244	C	-1.17158699	-4.44801188	-5.70397091
245	C	-1.12224400	-5.55600786	-6.76500511
246	C	-1.98656499	-6.73333216	-6.26409388
247	C	-2.13091397	-7.88443995	-7.26217079
248	C	0.31083900	-5.98928881	-7.08411884
249	H	-2.21235895	-4.27549314	-5.37949419
250	H	-0.58479798	-4.71265507	-4.81187296
251	H	-1.58835697	-5.16398811	-7.69041777
252	H	-2.98976707	-6.34795809	-6.01088381
253	H	-1.55560100	-7.11235523	-5.31875610
254	H	-2.53467989	-7.52663803	-8.22314739
255	H	-2.81902790	-8.65101147	-6.87355089
256	H	-1.16845000	-8.37733936	-7.46280622
257	H	0.92900401	-5.12867594	-7.38076591
258	H	0.34041601	-6.72156096	-7.90488005
259	H	0.77727002	-6.44801807	-6.19605398
260	S	2.93462992	1.12123895	-6.20031118
261	C	4.62559700	1.46756899	-5.49093485
262	C	5.54475784	2.27788305	-6.41793585
263	C	7.00829983	1.99250901	-6.01787615
264	C	8.05172920	2.67651892	-6.90394878
265	C	5.22377396	3.77438211	-6.38067579
266	H	5.04336119	0.46097499	-5.31694889
267	H	4.50882196	1.95309401	-4.51052380
268	H	5.39936304	1.91044605	-7.45246792
269	H	7.16946793	0.90093499	-6.04671383
270	H	7.15490723	2.29701591	-4.96490812
271	H	7.90277004	2.41501498	-7.96387196
272	H	9.06871223	2.36285496	-6.62165689
273	H	8.00955105	3.77228189	-6.81732702
274	H	4.15578222	3.95391703	-6.58278990
275	H	5.80415583	4.33534622	-7.12828302
276	H	5.45180178	4.18691683	-5.38383484
277	S	-2.12127495	-1.94433296	6.14731789
278	C	-3.33828998	-3.24475002	5.57928181
279	C	-4.24177122	-3.76964307	6.70268488
280	C	-4.94572115	-5.04588604	6.19462299
281	C	-5.76262093	-5.78211784	7.25953388
282	C	-5.24058723	-2.71742511	7.19199324
283	H	-2.70609808	-4.05913782	5.18602180
284	H	-3.92235303	-2.84092903	4.73925400
285	H	-3.59236693	-4.05942011	7.55159712
286	H	-4.18039322	-5.73146677	5.78988123
287	H	-5.59833002	-4.77754498	5.34347296
288	H	-5.13845682	-6.03431177	8.13182640
289	H	-6.17053223	-6.72186708	6.85620022
290	H	-6.61198187	-5.18067598	7.61475706
291	H	-4.72588682	-1.80234897	7.51977396
292	H	-5.83483410	-3.08868909	8.04011536
293	H	-5.93481588	-2.44063807	6.38090706
294	S	2.89683604	-1.08414805	6.08207083
295	C	4.62049818	-1.44552004	5.46204185
296	C	5.54857302	-2.03486896	6.53257799
297	C	7.00517607	-1.88403106	6.04366207
298	C	8.06249332	-2.30293012	7.06819010
299	C	5.20126200	-3.48810506	6.86557293
300	H	4.99789715	-0.46257699	5.13007116
301	H	4.55254698	-2.09268999	4.57493782
302	H	5.43731117	-1.42538905	7.45081806
303	H	7.17289019	-0.82916200	5.76399994
304	H	7.13153696	-2.47180009	5.11530018
305	H	7.94155693	-1.74566400	8.01137257
306	H	9.07496452	-2.10047603	6.68667698
307	H	8.00720787	-3.37650299	7.30109596
308	H	4.14463091	-3.58627105	7.15505219

309	H	5.81271076	-3.87137794	7.69594002
310	H	5.37039709	-4.13288879	5.98693895
311	S	-0.42435199	2.97387409	6.09795904
312	C	-0.90736097	4.62724018	5.37828302
313	C	-0.64429098	5.82471514	6.30336094
314	C	-1.57134199	6.98082876	5.87049198
315	C	-1.48505902	8.22628307	6.75487423
316	C	0.82861900	6.24279308	6.29766083
317	H	-1.98904705	4.51797009	5.18684483
318	H	-0.40862900	4.75124598	4.40537024
319	H	-0.92612302	5.53246021	7.33404398
320	H	-2.61143088	6.61026096	5.86909723
321	H	-1.33946800	7.24884987	4.82276106
322	H	-1.67543602	7.97485590	7.81067896
323	H	-2.23305702	8.97407818	6.44885588
324	H	-0.49680501	8.70585823	6.69491720
325	H	1.48344100	5.38578892	6.52150011
326	H	1.03411603	7.02473211	7.04391003
327	H	1.10830998	6.63001919	5.30390882
328	S	-2.19833112	2.06860900	-6.23793983
329	C	-3.37379098	3.38964605	-5.63227892
330	C	-4.29277611	3.94241309	-6.72951603
331	C	-4.96069479	5.22663784	-6.19307184
332	C	-5.78879118	5.98744822	-7.23184395
333	C	-5.32258701	2.91470003	-7.20634508
334	H	-2.71506596	4.18831778	-5.25015116
335	H	-3.94552112	2.99237394	-4.78058481
336	H	-3.65753698	4.22851515	-7.59031105
337	H	-4.17323780	5.89411116	-5.80092907
338	H	-5.59788799	4.96219397	-5.32911205
339	H	-5.18036699	6.23767710	-8.11582088
340	H	-6.17086411	6.92997503	-6.81029320
341	H	-6.65637207	5.40431404	-7.57318401
342	H	-4.83165789	1.99697495	-7.56076908
343	H	-5.93197203	3.30757403	-8.03376961
344	H	-6.00000191	2.63773608	-6.38128996
345	S	4.05446482	-3.10262609	-5.92525578
346	C	4.64528322	-2.11217690	-7.38883781
347	C	6.17390299	-2.07961607	-7.50695896
348	C	6.55192900	-1.12574399	-8.65859890
349	C	8.05652046	-0.90014303	-8.82644653
350	C	6.75930500	-3.48246288	-7.69696903
351	H	4.22053814	-1.10063696	-7.31385994
352	H	4.20028877	-2.60888290	-8.26793480
353	H	6.57522821	-1.65619195	-6.56535578
354	H	6.05875206	-0.15391700	-8.48278809
355	H	6.12872601	-1.52033997	-9.60191631
356	H	8.50863171	-0.53203499	-7.89182281
357	H	8.25278854	-0.15285100	-9.61026764
358	H	8.58061981	-1.82342696	-9.11425400
359	H	6.44459391	-4.15616608	-6.88613319
360	H	7.85862303	-3.46287894	-7.70599413
361	H	6.41630220	-3.91703105	-8.65162182
362	S	0.73316097	5.25681877	-5.81275511
363	C	-0.52785099	5.27005386	-7.19068813
364	C	0.06311100	5.63019514	-8.56122875
365	C	-1.10755599	5.99399614	-9.50035954
366	C	-0.67981702	6.48450613	-10.88586330
367	C	0.92562503	4.50225401	-9.13163471
368	H	-1.26058900	6.03176498	-6.88197422
369	H	-1.02446795	4.28849411	-7.21953201
370	H	0.69045299	6.53493977	-8.43650246
371	H	-1.71544898	6.77794123	-9.01492023
372	H	-1.76339698	5.10986900	-9.60698223
373	H	-0.00062800	7.34855413	-10.80645847
374	H	-1.55547905	6.79977894	-11.47331333
375	H	-0.16454600	5.69974709	-11.45827579
376	H	1.72625697	4.21901989	-8.43200970
377	H	1.40112197	4.79642200	-10.07880020
378	H	0.31226301	3.60428596	-9.31562996
379	S	-4.69186211	1.95927501	5.74826193
380	C	-4.14377403	2.96999598	7.21461201
381	C	-4.83523417	4.33752203	7.28109598
382	C	-4.20083094	5.14944792	8.42807293
383	C	-4.71136379	6.58799791	8.54270363
384	C	-6.35348320	4.20068502	7.43202305
385	H	-3.04947400	3.06965709	7.17410898
386	H	-4.40343904	2.36046910	8.09667206
387	H	-4.62331200	4.86527920	6.33069181
388	H	-3.10699701	5.16534281	8.27994442
389	H	-4.37510490	4.61700392	9.38242531
390	H	-4.57642412	7.13322401	7.59496880
391	H	-4.16217709	7.13485098	9.32423592
392	H	-5.77940321	6.62523890	8.80396557
393	H	-6.77738905	3.58210206	6.62718821
394	H	-6.85226822	5.17992687	7.39727402
395	H	-6.60392523	3.72301698	8.39468765
396	S	0.70065600	-5.21672201	5.64362383
397	C	-0.55341798	-5.23281479	7.02964878
398	C	0.02365600	-5.69089890	8.37594223
399	C	-1.16219199	-5.99828005	9.31592941
400	C	-0.76047802	-6.56295204	10.68059158
401	C	0.98156202	-4.65880489	8.97470093
402	H	-1.32896996	-5.93721914	6.69160795
403	H	-0.99547797	-4.22833920	7.11002922
404	H	0.57600403	-6.63660812	8.20726013
405	H	-1.82956600	-6.71949720	8.81201172
406	H	-1.75085104	-5.07279205	9.45772934
407	H	-0.14042901	-7.46689892	10.56782341
408	H	-1.65198505	-6.83904123	11.26405239
409	H	-0.19119000	-5.83340883	11.27454472
410	H	1.79941499	-4.42430401	8.27789783
411	H	1.43513203	-5.02338696	9.90820885
412	H	0.44883600	-3.71798611	9.19263077
413	S	4.26679707	3.00621510	5.75197792
414	C	4.89610100	1.91893303	7.13430786
415	C	4.98100281	2.65564203	8.47864914
416	C	5.89368916	1.84219301	9.42057610
417	C	6.17525005	2.52063704	10.76333046
418	C	3.59773397	2.90130806	9.08648682
419	H	5.90116978	1.61215699	6.80607796
420	H	4.25548077	1.02671599	7.20237303
421	H	5.47125101	3.63280892	8.29778957
422	H	6.85312414	1.65751505	8.90514755
423	H	5.43500805	0.85105997	9.59415913
424	H	6.60102510	3.52599502	10.61491585
425	H	6.89783478	1.93410802	11.35125065
426	H	5.26380396	2.62455201	11.36996746
427	H	2.94146895	3.43122101	8.38020706
428	H	3.65959191	3.50765800	10.00200653
429	H	3.11190605	1.94348598	9.33740234
430	S	-4.81394005	-1.81548202	-5.84438515
431	C	-4.27668619	-2.91331410	-7.25775480
432	C	-5.01690578	-2.60416198	-8.56626511
433	C	-4.77904987	-3.77571797	-9.54214382
434	C	-5.58065605	-3.68354702	-10.84294701
435	C	-4.59541607	-1.25990999	-9.16429710
436	H	-4.51369476	-3.93432093	-6.92202520
437	H	-3.18631601	-2.82341909	-7.37913895
438	H	-6.10110903	-2.56969404	-8.33979416
439	H	-5.03934383	-4.71791792	-9.02809334
440	H	-3.69927907	-3.83317590	-9.77377701
441	H	-6.65911102	-3.59475303	-10.63534355
442	H	-5.43083000	-4.58480787	-11.45705032
443	H	-5.28011322	-2.81765699	-11.45026207
444	H	-4.74768686	-0.44100100	-8.44669628
445	H	-5.17531204	-1.02087402	-10.06811810
446	H	-3.52577496	-1.27532101	-9.43252468

$[Au_{25}(2\text{-}MeBuS)_{18}]^-$

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	8.15674581	0.08811668	-0.03184430
2	Au	9.00983867	1.00179549	2.51920070
3	Au	7.90160416	2.90148753	0.38788774
4	Au	6.05078173	0.94397808	1.70123496
5	Au	10.63981700	1.47519761	0.22862969
6	Au	10.26836271	-1.40541707	1.19414552
7	Au	12.31351568	0.79303596	2.80192633
8	Au	6.60334259	0.22613335	4.82526126
9	Au	10.44744514	3.88018423	2.42944351
10	Au	4.14000672	-1.39165841	2.77038125
11	Au	7.37851507	-1.52714919	2.16025345
12	Au	7.05165667	4.56464211	-2.26961949
13	Au	4.78037086	3.90358060	0.46596329
14	Au	7.29513018	-0.81404225	-2.58513371
15	Au	8.38632964	-2.73049895	-0.46561765
16	Au	10.25596313	-0.78520697	-1.76665996
17	Au	5.68140671	-1.32338021	-0.31460418
18	Au	6.04486539	1.58957185	-1.28651267
19	Au	3.98704296	-0.75226399	-2.86386587
20	Au	9.69431265	-0.04043719	-4.85725475
21	Au	5.83234008	-3.78457043	-2.46704527
22	Au	12.20957124	1.52609097	-2.74683096
23	Au	8.94463684	1.70210274	-2.23117528
24	Au	9.20747408	-4.38963952	2.18363912
25	Au	11.42118796	-3.80061569	-0.60710742
26	S	4.34802064	-0.45890538	4.93440197
27	S	12.57466212	3.11950238	3.10461155
28	S	7.31517007	-3.64439639	3.38879918
29	S	12.28429891	-1.55865372	2.58842656
30	S	5.22901992	5.56286052	-1.15085682
31	S	12.66548198	2.54986772	-0.67260726
32	S	8.80868534	1.05680899	4.96129233
33	S	8.40021063	4.85934609	1.77900771
34	S	4.18680447	2.44258430	2.22083464
35	S	11.98455389	0.51848693	-4.86972299
36	S	3.67596221	-3.08504838	-3.11886116
37	S	8.98525519	3.84269769	-3.41297762
38	S	4.05609932	1.60583552	-2.73175840
39	S	10.99739913	-5.43276250	1.04821299
40	S	3.67635988	-2.35241041	0.66723579
41	S	7.46186521	-0.79991095	-5.03453651
42	S	7.93096761	-4.67789605	-1.88938035
43	S	11.99425300	-2.39200253	-2.41296769
44	C	4.37984481	-1.89673783	6.12992231
45	C	2.99192611	-2.24804674	6.68239888
46	H	5.03783632	-1.57160314	6.94963388
47	H	4.84210182	-2.76115951	5.63052335
48	C	3.17032432	-3.21000264	7.87558739
49	C	1.87993513	-3.51497177	8.64134033
50	C	2.07074372	-2.82982203	5.60688341
51	H	2.54101000	-1.31136340	7.06640479
52	H	3.90545727	-2.77203193	8.57420963
53	H	3.61428310	-4.15345304	7.50741034
54	H	1.40943927	-2.58651189	9.00342749
55	H	2.08545977	-4.15093512	9.51659258
56	H	1.14630738	-4.04275482	8.01441890
57	H	1.98619057	-2.15234565	4.74456484
58	H	1.05705857	-3.00932762	5.99551429
59	H	2.47173384	-3.78832355	5.23724964
60	C	12.56023848	3.31925452	4.95907388
61	C	13.87087286	2.86194662	5.61059389
62	H	11.71128205	2.74595607	5.35418855
63	H	12.38336525	4.39189713	5.14796218
64	C	13.68305101	2.83625895	7.14023793
65	C	14.86589848	2.24215534	7.90984023
66	C	15.05085140	3.73925374	5.18077754
67	H	14.06021010	1.82448704	5.27572197
68	H	12.77665872	2.25024839	7.37139384
69	H	13.48721581	3.86577384	7.49575832
70	H	15.09192516	1.22516717	7.55211824
71	H	14.63997421	2.17763213	8.98570074
72	H	15.77604369	2.85043720	7.79846280
73	H	15.13203288	3.77575917	4.08402981
74	H	16.00452164	3.35779510	5.57482851
75	H	14.91626111	4.77173130	5.54716337
76	C	7.89207301	-3.28839743	5.12619602
77	C	7.59451445	-4.43502132	6.10083434
78	H	7.34942441	-2.37496344	5.42112132
79	H	8.96352850	-3.04486846	5.10802843
80	C	7.82853542	-3.93275750	7.54018495
81	C	7.39724963	-4.91610251	8.63153634
82	C	8.41684290	-5.68798093	5.78374139
83	H	6.52052184	-4.68876626	6.00052249
84	H	7.27949046	-2.98381012	7.67309622
85	H	8.90007267	-3.68898244	7.66126802
86	H	6.33300452	-5.18060170	8.52327419
87	H	7.53309718	-4.47547685	9.63164032
88	H	7.98144841	-5.84777557	8.59908083
89	H	8.27093234	-5.99918936	4.73901641
90	H	8.13801449	-6.53309660	6.43139408
91	H	9.49136959	-5.48478934	5.92782815
92	C	11.61453157	-2.18055682	4.21450207
93	C	12.71182787	-2.51303546	5.23547036
94	H	11.05119799	-3.09094077	3.94671879
95	H	10.90183970	-1.44274667	4.61275184
96	C	12.09499149	-3.35281499	6.37211158
97	C	13.10744319	-3.88609158	7.38961408
98	C	13.40601701	-1.25342375	5.76193656
99	H	13.46639256	-3.14219170	4.72410016
100	H	11.55837117	-4.20608927	5.92211504
101	H	11.33181025	-2.74385964	6.89118709
102	H	13.89197248	-4.47704499	6.88986075
103	H	12.61516288	-4.53828222	8.12767903
104	H	13.59908019	-3.07304040	7.94420572
105	H	13.80159437	-0.65165370	4.93017422
106	H	14.24316707	-1.50048577	6.43234316
107	H	12.68847663	-0.62716108	6.31827596
108	C	3.80815837	5.39705035	-2.34530392
109	C	2.48763379	5.91640326	-1.76299537
110	H	3.71755420	4.33485065	-2.61168682
111	H	4.09623350	5.97406524	-3.24060631
112	C	1.34285678	5.53131266	-2.72088455
113	C	-0.05659082	5.86167599	-2.19457793
114	C	2.53885645	7.42215160	-1.48590659
115	H	2.32170622	5.38417868	-0.80619391
116	H	1.40546280	4.44763853	-2.91745212
117	H	1.50216406	6.03587244	-3.69307099
118	H	-0.22589404	5.39228594	-1.21214600
119	H	-0.83036457	5.48640636	-2.88245194
120	H	-0.20980039	6.94565422	-2.08353374
121	H	3.39566201	7.67349781	-0.84272079
122	H	1.62637766	7.77239525	-0.98146195
123	H	2.64578977	7.98481060	-2.42996040
124	C	12.11567573	4.32001632	-0.87047138
125	C	13.18029902	5.23264590	-1.49730670
126	H	11.89681461	4.64040179	0.16215211
127	H	11.17836550	4.34350921	-1.44524390
128	C	12.83404826	6.69762981	-1.15833772
129	C	13.87349040	7.72019052	-1.62692217
130	C	13.30472499	5.00945368	-3.00751915
131	H	14.15111423	4.99642141	-1.01871289
132	H	12.71750376	6.78115465	-0.06374980
133	H	11.84955940	6.94157508	-1.59883260
134	H	14.87110949	7.47884187	-1.22493063
135	H	13.60971350	8.73297120	-1.28353934
136	H	13.95045457	7.75306636	-2.72385764
137	H	13.48182650	3.94543405	-3.22902808
138	H	14.13314086	5.59059666	-3.44030160
139	H	12.36949623	5.30368666	-3.51287924
140	C	8.54379600	2.83609958	5.44596723
141	C	8.19308504	3.01780918	6.92812036
142	H	7.75807468	3.25215347	4.80197869
143	H	9.48468298	3.35409913	5.19356762
144	C	7.83432098	4.49580741	7.17748974
145	C	7.30871158	4.78952532	8.58543137
146	C	9.32189046	2.53278653	7.84329494
147	H	7.28985469	2.40885258	7.12952012
148	H	7.07105260	4.79812922	6.44077011
149	H	8.72508517	5.12001325	6.97498106
150	H	6.43220729	4.16240413	8.81657141
151	H	7.00052738	5.84269362	8.67633643

152	H	8.07054569	4.60070060	9.35652970
153	H	9.58948865	1.49077184	7.61075327
154	H	9.03460470	2.57802445	8.90466960
155	H	10.22196033	3.15659301	7.70685460
156	C	8.82926375	6.28700010	0.65650317
157	C	8.92629514	7.62924115	1.39442929
158	H	8.01144504	6.31665855	-0.07995269
159	H	9.75884684	6.05406299	0.11758575
160	C	8.93600818	8.76386908	0.34895027
161	C	8.86617034	10.17267504	0.94486165
162	C	10.14022933	7.69052487	2.32575316
163	H	8.00697621	7.73909820	2.00347407
164	H	8.07829701	8.61863909	-0.33109785
165	H	9.84596352	8.66810584	-0.27218567
166	H	7.97732841	10.28290540	1.58759361
167	H	8.80028209	10.93116869	0.14886636
168	H	9.75319535	10.40724658	1.55227847
169	H	10.13898384	6.84376732	3.02775035
170	H	10.15481371	8.61993668	2.91503211
171	H	11.07414745	7.63868996	1.74123603
172	C	4.72135119	3.42728699	3.70885825
173	C	3.77323763	4.59268366	4.02112187
174	H	5.74135294	3.79197560	3.52471495
175	H	4.74985707	2.70759062	4.54506423
176	C	4.40291396	5.47377819	5.11719439
177	C	3.62974210	6.76226385	5.41212287
178	C	2.37618320	4.09437386	4.40370797
179	H	3.69262173	5.20416519	3.10148895
180	H	5.42894707	5.73632103	4.80477798
181	H	4.49788703	4.87852614	6.04443512
182	H	3.50676672	7.36321327	4.49638822
183	H	4.16437264	7.38077691	6.15001871
184	H	2.62804129	6.55545015	5.81748196
185	H	1.97068031	3.43628584	3.62052839
186	H	1.67094427	4.92714711	4.54351929
187	H	2.41801698	3.51514118	5.34212826
188	C	12.15427311	1.94330867	-6.05964661
189	C	13.61305200	2.39108221	-6.21998371
190	H	11.53269194	2.77028541	-5.69221477
191	H	11.74514878	1.59058021	-7.02167004
192	C	13.64356095	3.71837841	-7.00273679
193	C	15.03288312	4.35123546	-7.12072039
194	C	14.46657397	1.30051434	-6.87503548
195	H	14.01085588	2.58822391	-5.20633386
196	H	12.96919106	4.43314407	-6.50047864
197	H	13.22525742	3.54908700	-8.01344475
198	H	15.47529923	4.51070955	-6.12439886
199	H	14.97513276	5.32946824	-7.62319904
200	H	15.72412352	3.72139150	-7.70079748
201	H	14.38502891	0.35504449	-6.31823777
202	H	15.52994397	1.58015571	-6.90482402
203	H	14.13050903	1.11720740	-7.91043924
204	C	3.67193162	-3.41182177	-4.96149575
205	C	2.25851186	-3.50759925	-5.55053146
206	H	4.19426039	-4.37217111	-5.08533708
207	H	4.26179064	-2.62872071	-5.46010490
208	C	2.37219244	-4.03029109	-6.99765103
209	C	1.03182127	-4.34072151	-7.66920414
210	C	1.50586667	-2.17722858	-5.47173962
211	H	1.70345768	-4.26222584	-4.95835530
212	H	2.99037879	-4.94558259	-6.99322557
213	H	2.92419516	-3.28552711	-7.60071906
214	H	0.45401450	-5.06821462	-7.07608826
215	H	1.18739717	-4.77176243	-8.67043347
216	H	0.41494529	-3.43794407	-7.78987883
217	H	1.46579496	-1.80400213	-4.43795110
218	H	0.47124343	-2.27674112	-5.83327063
219	H	2.01169430	-1.41193068	-6.08361350
220	C	8.43164964	3.54435809	-5.16381696
221	C	8.27329743	4.83380561	-5.98095890
222	H	7.49252115	2.97718748	-5.13893076
223	H	9.20211050	2.88924735	-5.60446108
224	C	7.71130439	4.47365225	-7.37050839
225	C	7.34082664	5.68057526	-8.23721614
226	C	9.58714485	5.61564251	-6.07884084
227	H	7.52681237	5.46524423	-5.46051193
228	H	6.81750777	3.84242748	-7.23479899
229	H	8.45230587	3.84783723	-7.90266338
230	H	6.61597203	6.32957667	-7.71929675
231	H	6.88298581	5.35575774	-9.18467044
232	H	8.22061591	6.29189501	-8.48827847
233	H	9.99443682	5.81869053	-5.07744124
234	H	9.44869397	6.58087325	-6.58876002
235	H	10.33764835	5.03617867	-6.64317435
236	C	4.73978642	2.03717837	-4.40833866
237	C	3.78553179	1.69958394	-5.56189467
238	H	5.69106893	1.50112486	-4.52967995
239	H	4.95151925	3.12090702	-4.37224453
240	C	4.51584041	1.92548842	-6.89902828
241	C	3.74138719	1.44935749	-8.13110413
242	C	2.47301310	2.48222042	-5.46819941
243	H	3.55667375	0.61935894	-5.47927355
244	H	5.48454796	1.39778217	-6.85868772
245	H	4.74490696	3.00202468	-7.00353638
246	H	3.48026825	0.38274673	-8.04107469
247	H	4.34558952	1.56887063	-9.04417473
248	H	2.80767329	2.01391006	-8.27474891
249	H	1.98945542	2.31103103	-4.49486645
250	H	1.76262424	2.18297780	-6.25366715
251	H	2.66103221	3.56502931	-5.56955342
252	C	12.40626833	-5.31726675	2.26853478
253	C	13.62894629	-6.15719428	1.87063633
254	H	11.98547216	-5.68996854	3.21514463
255	H	12.67582015	-4.25716261	2.38908658
256	C	14.52437110	-6.32259368	3.11690096
257	C	15.73831873	-7.23192627	2.90977501
258	C	14.39008039	-5.54122253	0.69397061
259	H	13.26832610	-7.16338063	1.57752029
260	H	13.90879264	-6.72776753	3.93988984
261	H	14.86394053	-5.32187587	3.44331936
262	H	15.42814118	-8.22897432	2.55633334
263	H	16.29107960	-7.36632661	3.85280850
264	H	16.43967688	-6.81493323	2.17215324
265	H	13.71900893	-5.36095114	-0.15898401
266	H	15.20554560	-6.19517419	0.34993990
267	H	14.82176616	-4.56824169	0.98263700
268	C	4.21987659	-4.11507975	0.91681077
269	C	3.34104663	-4.89951703	1.89851658
270	H	5.26312072	-4.10044955	1.26030416
271	H	4.19151320	-4.56900419	-0.08967865
272	C	3.99423538	-6.27091829	2.15749400
273	C	3.31430182	-7.09895084	3.25149972
274	C	1.89683688	-5.02091230	1.40257817
275	H	3.34148813	-4.33827735	2.85273241
276	H	5.04869111	-6.10458852	2.43868198
277	H	4.00343606	-6.84512595	1.21256619
278	H	3.27693467	-6.53894530	4.19961992
279	H	3.86771776	-8.03320702	3.43699501
280	H	2.28326227	-7.37245064	2.98040053
281	H	1.47454009	-4.02772899	1.18760538
282	H	1.25102978	-5.50907670	2.14755143
283	H	1.85846888	-5.61273645	0.47177954
284	C	7.58850646	-2.59032234	-5.55067297
285	C	7.31332037	-2.81537949	-7.04224911
286	H	6.84004794	-3.11558802	-4.93523431
287	H	8.57853188	-2.97250756	-5.26385133
288	C	7.21809546	-4.33410502	-7.29508356
289	C	6.74195392	-4.71650645	-8.69890556
290	C	8.36516291	-2.14594673	-7.93163783
291	H	6.32516111	-2.36926412	-7.27198147
292	H	6.52898595	-4.77097424	-6.55127452
293	H	8.20784455	-4.78720901	-7.10135254
294	H	5.75636478	-4.27292076	-8.91377966
295	H	6.64600390	-5.80946096	-8.79489255
296	H	7.44191639	-4.37719872	-9.47737071
297	H	8.43291079	-1.06982471	-7.71496190
298	H	8.12778501	-2.26301477	-9.00011182
299	H	9.35851939	-2.58818335	-7.74845312
300	C	7.55128689	-6.14964734	-0.81530044
301	C	6.87400275	-7.30354447	-1.56517681
302	H	6.93071771	-5.81202981	0.02529718
303	H	8.52805646	-6.46760024	-0.41295618
304	C	6.49813864	-8.39968221	-0.54859256
305	C	5.65230239	-9.53700263	-1.12754336
306	C	7.75240826	-7.83974148	-2.69952160
307	H	5.93727315	-6.90554960	-2.00276357

308	H	5.94464140	-7.92985295	0.28244420	320	C	11.73896768	-4.51241906	-6.02035291
309	H	7.42599334	-8.81226499	-0.10900325	321	C	12.72496482	-5.24610109	-6.93430368
310	H	4.72871596	-9.14660254	-1.58543264	322	C	12.70887337	-5.36712777	-3.81993865
311	H	5.36040013	-10.24836650	-0.33885032	323	H	13.21322213	-3.51445771	-4.80544728
312	H	6.19734447	-10.10337717	-1.89764129	324	H	11.40900745	-3.58624617	-6.52201908
313	H	8.03063553	-7.03069907	-3.39136769	325	H	10.83411233	-5.13191374	-5.87639866
314	H	7.23507543	-8.61796691	-3.28037369	326	H	13.64534039	-4.65519849	-7.07153441
315	H	8.68300390	-8.27314001	-2.29369475	327	H	12.28502685	-5.41841337	-7.92909896
316	C	11.28336548	-3.26407146	-3.90454714	328	H	13.01135970	-6.22641291	-6.52525819
317	C	12.31099592	-4.13555575	-4.63777976	329	H	13.09102995	-5.07174340	-2.83208214
318	H	10.94432788	-2.44717806	-4.56212730	330	H	13.49280949	-5.95428365	-4.32257285
319	H	10.40427525	-3.84722495	-3.59097277	331	H	11.83485886	-6.02077963	-3.65870471

B.2. Coordinates of the Relevant Lowest Energy Isomers of Biicosehedral Au_{25} with Different Ligands

$[Au_{25}(PPh_3)_{10}(R)\text{-}(PPT)_5Cl_2]^{2+}$, isomer #1

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)	54	C	20.21114849	-4.05304174	10.74899013
1	Au	15.46559670	-0.42066595	9.06870457	55	H	20.21810264	-5.00088452	11.28917210
2	Au	18.09701205	1.02117419	8.35889520	56	C	19.03251123	-3.58914527	10.15972454
3	Au	15.91714552	0.76229468	6.29367259	57	H	18.10456602	-4.15627858	10.23946799
4	Au	13.23532977	1.02174118	7.68766094	58	C	19.02685317	-2.38089839	9.46011661
5	Au	13.75297885	1.48236260	10.71405583	59	H	18.09630719	-2.03627663	9.00569353
6	Au	16.80862846	1.35898136	11.06814414	60	C	20.68928407	-0.80760995	6.61783789
7	Au	15.57565458	2.29860755	8.67708832	61	C	21.30673011	-2.06222227	6.49400856
8	Au	17.79309600	3.78027801	9.69591507	62	H	21.37818344	-2.72454880	7.35618408
9	Au	17.42935785	3.40845792	6.78183869	63	C	21.84593487	-2.46243803	5.26844245
10	Au	14.53951415	3.37058452	6.22618452	64	H	22.33646514	-3.43352193	5.18808464
11	Au	13.12437054	3.76649301	8.79409075	65	C	21.75928106	-1.62443742	4.15534356
12	Au	15.16064930	4.04006188	10.92499157	66	H	22.18531074	-1.93624172	3.20072570
13	Au	15.64014777	5.27747828	8.25259465	67	C	21.11046409	-0.39104726	4.26448609
14	Au	17.90625341	7.02042595	9.06488083	68	H	21.00525748	0.25180126	3.38994845
15	Au	17.37925087	6.64692817	6.23722273	69	C	20.57803390	0.01736333	5.48823243
16	Au	14.47817831	6.61447630	5.85224499	70	H	20.07378565	0.98228898	5.56871499
17	Au	13.21638945	7.01850433	8.44809227	71	C	17.32274077	0.20874785	3.09548714
18	Au	15.32431494	7.27724077	10.44112842	72	C	17.40310812	-0.31187160	1.79098480
19	Au	15.68344120	8.30481966	7.81205460	73	H	16.81915927	-1.18981372	1.51287303
20	Au	18.19430408	9.37193902	7.02178689	74	C	18.22174047	0.29920782	0.83900623
21	Au	15.87136297	9.09049187	5.09274339	75	H	18.28334730	-0.11802011	-0.16720556
22	Au	13.30456080	9.35364089	6.66512259	76	C	18.95125283	1.44477362	1.17198235
23	Au	14.02295353	9.79873434	9.56935320	77	H	19.58676646	1.92365900	0.42585415
24	Au	17.05926426	9.70237916	9.87467603	78	C	18.84556268	1.98842987	2.45455647
25	Au	15.73841377	11.02915104	7.44527395	79	H	19.39109112	2.89565594	2.71711430
26	Cl	15.34849534	-2.80289899	9.37418576	80	C	18.03559338	1.37302110	3.41235417
27	Cl	15.75663958	13.40766773	7.12168004	81	H	17.94482258	1.80991882	4.41020288
28	P	20.16042676	-0.14145258	8.25605549	82	C	17.18402655	-2.17888829	4.82270949
29	P	16.31313708	-0.61389420	4.40047095	83	C	16.78217454	-2.84581688	5.99094948
30	P	11.39238781	-0.19279446	6.82248803	84	H	16.05473330	-2.39614187	6.66878240
31	P	12.24224619	0.75806523	12.40294385	85	C	17.31509947	-4.09734086	6.30355397
32	P	17.75030227	0.46102968	13.05670075	86	H	16.99281722	-4.59496142	7.21862072
33	P	20.26000734	10.35796035	6.40660793	87	C	18.25349651	-4.69315943	5.45674927
34	P	16.11755623	9.81409189	2.85087221	88	H	18.66593344	-5.67366481	5.69890735
35	P	11.38369105	10.28023772	5.63086711	89	C	18.67266698	-4.02327219	4.30427617
36	P	12.59341508	11.15192132	10.88645354	90	H	19.41419331	-4.47712722	3.64567932
37	P	18.20910653	10.88411691	11.58053214	91	C	18.14603416	-2.76842805	3.98742986
38	C	21.61212000	0.89733709	8.72183180	92	H	18.48664131	-2.25339991	3.09014370
39	C	21.40384405	2.09518329	9.42030527	93	C	14.85327164	-1.19096473	3.43066448
40	H	20.38490655	2.42792630	9.63338449	94	C	14.80148152	-2.47644120	2.86777631
41	C	22.48983792	2.87422117	9.82879949	95	H	15.57902204	-3.20552388	3.09466954
42	H	22.31099000	3.80560782	10.36854314	96	C	13.75799656	-2.82369068	2.00564162
43	C	23.79363325	2.46201404	9.54212026	97	H	13.73408672	-3.82109936	1.56419708
44	H	24.64059355	3.06797439	9.86591483	98	C	12.75251858	-1.90060945	1.71098152
45	C	24.00930061	1.28320887	8.82137997	99	H	11.93958902	-2.17351746	1.03656785
46	H	25.02441234	0.96769991	8.57555300	100	C	12.78149109	-0.63204583	2.29667757
47	C	22.92567364	0.50825517	8.40316695	101	H	11.98343134	0.08356256	2.09831805
48	H	23.10448768	-0.39454210	7.81782973	102	C	13.82680695	-0.27703583	3.15095390
49	C	20.20345728	-1.62400730	9.34590634	103	H	13.84752782	0.71574597	3.60467992
50	C	21.37911326	-2.07898307	9.96458970	104	C	10.02215115	-0.53086066	8.00775917
51	H	22.29464462	-1.49119610	9.90902225	105	C	9.39599453	-1.78492673	8.09046510
52	C	21.38019915	-3.29258031	10.65639069	106	H	9.75867037	-2.61950279	7.49149101
53	H	22.30044646	-3.64257853	11.12589805	107	C	8.29941801	-1.96717578	8.93745054

108	H	7.81854140	-2.94474741	8.99296438
109	C	7.82029321	-0.90395954	9.70471995
110	H	6.96316482	-1.04777363	10.36386599
111	C	8.45039662	0.34218762	9.63603577
112	H	8.09567745	1.17011824	10.24939318
113	C	9.54976108	0.52796512	8.79824552
114	H	10.04918743	1.49832133	8.76336253
115	C	10.52729076	0.65034579	5.43185814
116	C	9.20832363	0.31211039	5.07985928
117	H	8.64751219	-0.40385592	5.68189725
118	C	8.61026446	0.89190628	3.95885947
119	H	7.58911148	0.61744618	3.68945115
120	C	9.31565351	1.82146362	3.18863905
121	H	8.84888014	2.27005377	2.31050933
122	C	10.61264020	2.19010897	3.55586845
123	H	11.16162762	2.92978509	2.97184283
124	C	11.21440983	1.61071061	4.67603630
125	H	12.22134508	1.91521539	4.97291936
126	C	11.81238247	-1.87295802	6.19774801
127	C	11.14510629	-2.46454461	5.11322300
128	H	10.42675398	-1.89087417	4.52872050
129	C	11.39422801	-3.79852430	4.78187585
130	H	10.86517758	-4.25141284	3.94212470
131	C	12.31158952	-4.54970680	5.52134820
132	H	12.49871268	-5.59270763	5.26176691
133	C	12.99452317	-3.95723254	6.58661244
134	H	13.72574797	-4.52188481	7.16601684
135	C	12.74929355	-2.62455383	6.92309004
136	H	13.29888608	-2.18331610	7.75673646
137	C	11.89937370	-1.04864436	12.36789758
138	C	11.46384867	-1.74907353	13.50770164
139	H	11.38420831	-1.24107154	14.46904437
140	C	11.15442650	-3.10708566	13.41881064
141	H	10.81844499	-3.64315295	14.30742792
142	C	11.28252720	-3.77844358	12.19830632
143	H	11.04549271	-4.84140547	12.13372460
144	C	11.72962098	-3.09087217	11.06823682
145	H	11.85759894	-3.61229500	10.11960161
146	C	12.03808656	-1.73185678	11.15143101
147	H	12.40807586	-1.20238723	10.27228729
148	C	12.71733506	1.07417030	14.16054296
149	C	12.05840171	2.04206248	14.93559715
150	H	11.26518692	2.64629240	14.49883968
151	C	12.39012950	2.21508050	16.28247499
152	H	11.85505603	2.95650184	16.87737308
153	C	13.38379785	1.42898226	16.86805579
154	H	13.63116616	1.55232094	17.92318029
155	C	14.05608388	0.47767952	16.09594141
156	H	14.83283030	-0.14157966	16.54319481
157	C	13.73251006	0.30224548	14.74996435
158	H	14.25591365	-0.45531579	14.16616633
159	C	10.59073259	1.57584110	12.31328648
160	C	9.49464420	1.08400811	13.04286548
161	H	9.57679561	0.14895908	13.59689403
162	C	8.29332360	1.79364649	13.06836558
163	H	7.45192825	1.41013874	13.64721473
164	C	8.16938559	2.99145892	12.35546636
165	H	7.23057421	3.54604740	12.37383643
166	C	9.24690850	3.46987522	11.60667624
167	H	9.15259512	4.38774603	11.02589978
168	C	10.45556235	2.76704231	11.58901900
169	H	11.29663362	3.14537028	11.00255970
170	C	17.70040744	1.65273094	14.46265974
171	C	18.58889664	1.54827193	15.54817119
172	H	19.36863476	0.78521978	15.54661939
173	C	18.48637359	2.42747197	16.62817777
174	H	19.17608609	2.33376807	17.46838503
175	C	17.51103502	3.42929283	16.62599849
176	H	17.43910239	4.12200840	17.46568980
177	C	16.64488285	3.55466772	15.53726401
178	H	15.90380997	4.35414881	15.51429028
179	C	16.73458607	2.66986913	14.46086342
180	H	16.06161079	2.78002632	13.60725950
181	C	16.89733729	-1.05239368	13.67207979
182	C	16.91051776	-1.41211448	15.03152827
183	H	17.38189431	-0.76125549	15.76818959
184	C	16.31718705	-2.60628170	15.44599384
185	H	16.33611061	-2.88041324	16.50210321
186	C	15.70080961	-3.44706704	14.51277031
187	H	15.23466565	-4.37682378	14.84157387
188	C	15.68079074	-3.09081155	13.16257418
189	H	15.19750656	-3.72714857	12.42069724
190	C	16.27780368	-1.89936640	12.74206724
191	H	16.24849988	-1.63939811	11.68260766
192	C	19.52954463	-0.02880568	13.04459778
193	C	19.97415837	-1.23522835	13.60770854
194	H	19.25563655	-1.97153027	13.96548685
195	C	21.34239518	-1.49255401	13.72976933
196	H	21.67423233	-2.42778558	14.18244137
197	C	22.27688161	-0.55773817	13.28054341
198	H	23.34447534	-0.75751203	13.38336731
199	C	21.83937262	0.62880172	12.68493927
200	H	22.55968497	1.35450255	12.30676593
201	C	20.47423247	0.89324290	12.56683119
202	H	20.14200315	1.82566625	12.10734372
203	C	20.60473104	10.57608177	4.60736862
204	C	20.43460197	9.47428713	3.75471533
205	H	20.00442569	8.54848566	4.14054148
206	C	20.81692861	9.55408058	2.41503349
207	H	20.67054539	8.69211490	1.76377098
208	C	21.37178754	10.73442807	1.91185179
209	H	21.67772401	10.79361197	0.86634401
210	C	21.51767784	11.84261268	2.74788069
211	H	21.93645368	12.77217837	2.35995677
212	C	21.13196003	11.76912513	4.08911248
213	H	21.25380939	12.63973939	4.73213741
214	C	20.51928975	12.04648781	7.09439234
215	C	19.39982730	12.86836776	7.29497187
216	H	18.39105582	12.49362028	7.11255313
217	C	19.56433060	14.18396150	7.73647284
218	H	18.67991167	14.80305604	7.89075428
219	C	20.84401490	14.68895992	7.97943081
220	H	20.97240655	15.71590732	8.32400001
221	C	21.96352385	13.87301050	7.78434306
222	H	22.96488697	14.26324266	7.97217527
223	C	21.80504459	12.55645053	7.34569870
224	H	22.68333963	11.92671827	7.19986937
225	C	21.71764538	9.36812291	6.95219706
226	C	21.59081295	8.51677361	8.06020461
227	H	20.62579271	8.41785574	8.56276108
228	C	22.68731059	7.77575545	8.50613248
229	H	22.57008270	7.10197434	9.35539334
230	C	23.91926193	7.88074758	7.85547321
231	H	24.77385742	7.29862137	8.20299998
232	C	24.05087426	8.71909913	6.74437741
233	H	25.00617069	8.79425391	6.22292968
234	C	22.95494498	9.45461378	6.28842358
235	H	23.06039500	10.08762886	5.40667778
236	C	17.00675667	8.59578362	1.78874880
237	C	16.91514165	8.63445625	0.38571754
238	H	16.26975097	9.36531731	-0.10260208
239	C	17.63788191	7.72586837	-0.39068355
240	H	17.56282205	7.76684675	-1.47833217
241	C	18.44572036	6.76304426	0.22291697
242	H	19.00708141	6.05342724	-0.38643325
243	C	18.51583748	6.69906617	1.61690224
244	H	19.12647198	5.93995577	2.10728912
245	C	17.79670842	7.60879470	2.39560066
246	H	17.83494874	7.54027186	3.48571160
247	C	14.56788926	10.08783534	1.88827140
248	C	14.42335382	11.16447232	0.99929597
249	H	15.19277601	11.93388752	0.94131200
250	C	13.29811831	11.24840949	0.17471020
251	H	13.20198488	12.08353615	-0.52049948
252	C	12.30394822	10.27025242	0.23980137
253	H	11.42823211	10.33572996	-0.40737139
254	C	12.42658049	9.21570285	1.14907694
255	H	11.63761459	8.46815907	1.23301216
256	C	13.55099181	9.12421888	1.97029553
257	H	13.64109017	8.30204274	2.68327635
258	C	17.00870402	11.41460592	2.68831667
259	C	16.79896611	12.37982883	3.68566443
260	H	16.21464534	12.14203010	4.57651190
261	C	17.34055088	13.65949427	3.54974465
262	H	17.16989958	14.39183097	4.33945776
263	C	18.09305892	13.98679386	2.41897755

264	H	18.50943433	14.98923738	2.30868818
265	C	18.32268577	13.02268167	1.43332380
266	H	18.92008940	13.26912395	0.55444613
267	C	17.78930825	11.73859524	1.56672547
268	H	17.98147184	10.99324051	0.79536950
269	C	10.46112595	9.06401201	4.59392316
270	C	9.13428771	9.29745227	4.18851871
271	H	8.60988163	10.19624960	4.51426894
272	C	8.47119545	8.36944859	3.38265208
273	H	7.44354354	8.56244345	3.07152158
274	C	9.11637160	7.19289232	2.98839863
275	H	8.59386590	6.46680588	2.36413658
276	C	10.42314065	6.94034143	3.41345133
277	H	10.92911157	6.01617469	3.13171065
278	C	11.09145675	7.87090646	4.21290007
279	H	12.10569961	7.65892137	4.56069096
280	C	11.77214457	11.71901618	4.55338240
281	C	12.79213579	12.58550396	4.97681021
282	H	13.38581475	12.35419714	5.86322344
283	C	13.06193813	13.75545345	4.26475467
284	H	13.86197067	14.41168050	4.60899509
285	C	12.31822181	14.07033028	3.12477871
286	H	12.52636102	14.98708810	2.57068711
287	C	11.31436103	13.20140745	2.68768804
288	H	10.73839204	13.43707721	1.79175794
289	C	11.04282291	12.02647686	3.39299847
290	H	10.26398438	11.35281984	3.03629654
291	C	10.03667607	10.90065812	6.72766659
292	C	9.64846210	10.11183604	7.82134099
293	H	10.22669599	9.22267088	8.08041532
294	C	8.52886371	10.46043432	8.57811595
295	H	8.24511007	9.84490495	9.43209756
296	C	7.78487049	11.59750217	8.24954993
297	H	6.90418190	11.86391999	8.83568176
298	C	8.18327074	12.40225411	7.18024402
299	H	7.61746097	13.29992665	6.92733920
300	C	9.30887536	12.06214633	6.42482009
301	H	9.61295806	12.69703232	5.59281216
302	C	11.86070272	12.57411033	9.97853222
303	C	12.67735067	13.24767210	9.05690693
304	H	13.66612680	12.86343710	8.79860763
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306	H	12.89008977	14.93947827	7.75127592
307	C	10.97620860	14.94686671	8.77246243
308	H	10.63372104	15.87416181	8.31088445
309	C	10.15043938	14.26699967	9.67233622
310	H	9.16139127	14.65965330	9.91195182
311	C	10.58664658	13.08399529	10.27400415
312	H	9.93477100	12.56591462	10.97681364
313	C	13.34467410	11.96134141	12.36131450
314	C	14.03189897	11.15688429	13.28402056
315	H	14.18028359	10.09443239	13.08306244
316	C	14.52888529	11.71006199	14.46380877
317	H	15.05802434	11.07318984	15.17185451
318	C	14.36070153	13.07285992	14.72808632
319	H	14.75161223	13.50385743	15.65088862
320	C	13.69895922	13.88250247	13.80328554
321	H	13.57047488	14.94785285	13.99938935
322	C	13.19091494	13.33204337	12.62324035
323	H	12.66714795	13.97036982	11.91301603
324	C	11.18390268	10.21683500	11.62072095
325	C	10.79033573	9.00373408	11.03713952
326	H	11.35896499	8.59727219	10.19702037
327	C	9.68993148	8.30298302	11.53687209
328	H	9.39492745	7.36360400	11.06793860
329	C	8.97892681	8.80394661	12.63089537
330	H	8.11842501	8.25811722	13.02035888
331	C	9.38246010	9.99853395	13.23664438
332	H	8.84168967	10.38358616	14.10220148
333	C	10.48207488	10.70178824	12.73916431
334	H	10.79931635	11.62446503	13.22655815
335	C	17.74149576	10.36450556	13.28813983
336	C	17.10817852	9.12927110	13.48082426
337	H	16.80503830	8.53220658	12.61725802
338	C	16.85298123	8.66064468	14.77360209
339	H	16.34504738	7.70480166	14.90703989
340	C	17.23985105	9.41852704	15.88106527
341	H	17.04585493	9.04891332	16.88850980
342	C	17.86043319	10.65892591	15.69498251
343	H	18.15494273	11.25978909	16.55657946
344	C	18.10431505	11.13491215	14.40612209
345	H	18.58006077	12.10663303	14.27493147
346	C	20.04590160	10.69760730	11.62124769
347	C	20.82727729	11.35577980	10.65687532
348	H	20.35242714	11.95287197	9.87787181
349	C	22.21952961	11.27775590	10.70986222
350	H	22.81255398	11.80953430	9.96628050
351	C	22.84951754	10.53536850	11.71250572
352	H	23.93846817	10.49045902	11.75809491
353	C	22.07844803	9.85856419	12.65919191
354	H	22.55860820	9.27668966	13.44638274
355	C	20.68346255	9.93649765	12.61437015
356	H	20.09456498	9.42645523	13.37567695
357	C	17.96295492	12.70588348	11.52062711
358	C	16.81029323	13.20593717	10.89868913
359	H	16.11827448	12.51985507	10.40827937
360	C	16.55940568	14.57949541	10.87992614
361	H	15.66859621	14.95383054	10.37565108
362	C	17.45645122	15.46356742	11.48262844
363	H	17.26102703	16.53694802	11.46621323
364	C	18.61640506	14.97370950	12.09223910
365	H	19.32763806	15.66148805	12.55185700
366	C	18.87497566	13.60251860	12.10757464
367	H	19.79637638	13.23528145	12.56010111
368	S	19.43875030	5.50640293	10.20293649
369	C	19.21215185	6.02663219	11.98014357
370	H	18.14371499	5.96309522	12.21496510
371	H	19.49256056	7.08906368	12.01012364
372	C	20.00824893	5.21693840	13.00877202
373	H	19.68577048	4.16494767	12.92963340
374	C	19.61747994	5.72040904	14.41794073
375	H	18.53443818	5.63893395	14.57655888
376	H	20.12347408	5.13129189	15.19284618
377	H	19.91178164	6.77163007	14.54763267
378	C	22.20933291	6.27917975	12.20571568
379	C	21.52448859	5.24976969	12.86599307
380	C	22.28655343	4.25402566	13.50095719
381	C	23.68194311	4.28380312	13.48007760
382	C	24.35164251	5.31695525	12.81647119
383	C	23.60833769	6.31335325	12.18054696
384	H	21.65397775	7.07581591	11.70999034
385	H	21.77478295	3.44513300	14.02747102
386	H	24.24988355	3.50285931	13.98843360
387	H	25.44208143	5.34768270	12.80364576
388	H	24.11763372	7.13001506	11.66572741
389	S	18.71206928	4.85035817	5.27413892
390	C	20.39372530	5.12334252	6.04459835
391	H	20.30578436	4.93537585	7.12045447
392	H	20.62034399	6.18919255	5.91440460
393	C	21.49484785	4.23907879	5.44175837
394	H	21.14923754	3.19332489	5.48703865
395	C	22.76281179	4.35244730	6.31686966
396	H	22.55732895	4.04591706	7.35052447
397	H	23.56009516	3.71180141	5.91720160
398	H	23.13422551	5.38679388	6.32761094
399	C	22.07880726	5.85109104	3.53930227
400	C	21.86082388	4.54124913	3.99491269
401	C	22.12510543	3.48482737	3.10966016
402	C	22.58467691	3.72149030	1.81086123
403	C	22.79380517	5.03093778	1.37091285
404	C	22.54004162	6.09396234	2.24253656
405	H	21.91299074	6.69850299	4.20726011
406	H	21.98847232	2.45777719	3.45426367
407	H	22.79320932	2.88131249	1.14623333
408	H	23.16408539	5.22122657	0.36273005
409	H	22.71630556	7.12017477	1.91739075
410	S	13.69498425	4.79613439	4.42739749
411	C	14.94890615	4.83206186	3.04372874
412	H	15.94099800	4.68061483	3.48340222
413	H	14.92340962	5.85506791	2.64443198
414	C	14.71024918	3.79854478	1.93642360
415	H	14.70914364	2.79992735	2.40423167
416	C	15.89972501	3.85531088	0.95110675
417	H	16.84955357	3.67422484	1.47020052
418	H	15.78325463	3.09536538	0.16775735
419	H	15.94965127	4.83883975	0.46312297

420	C	12.83912972	5.18185577	0.84298058
421	C	13.41483321	3.93956743	1.14737748
422	C	12.83297813	2.78968653	0.58883310
423	C	11.71366957	2.87197128	-0.24220683
424	C	11.14782035	4.11640168	-0.53282600
425	C	11.71670777	5.26966940	0.01306763
426	H	13.27493836	6.10060359	1.23828405
427	H	13.27634635	1.81386632	0.79836387
428	H	11.28731954	1.96310177	-0.67043372
429	H	10.27872261	4.18758809	-1.18822560
430	H	11.29162630	6.24734222	-0.21829355
431	S	11.38004496	5.48720014	8.90388077
432	C	10.43996043	5.44312067	7.29002861
433	H	11.10687185	5.02711498	6.52683933
434	H	10.24550547	6.48918265	7.01984369
435	C	9.14205457	4.62610203	7.35104032
436	H	9.39184163	3.62947405	7.75047318
437	C	8.60711152	4.43527003	5.91417857
438	H	9.35018401	3.93408055	5.28117990
439	H	7.69358806	3.82698688	5.92455747
440	H	8.36052612	5.40619338	5.46178932
441	C	7.14718778	4.32012521	8.86610350
442	C	8.02565003	5.20058437	8.21384174
443	C	7.74422839	6.57366297	8.27355140
444	C	6.62558219	7.04861525	8.96534701
445	C	5.76135029	6.16003972	9.61008388
446	C	6.02726737	4.78903609	9.55677720
447	H	7.33774974	3.24569378	8.81564264
448	H	8.38730260	7.28996355	7.75969160
449	H	6.41940251	8.11983727	8.98464103
450	H	4.88266249	6.53111974	10.13916256
451	H	5.35321679	4.08161100	10.04279801
452	S	14.95108761	5.94605397	12.44681342
453	C	13.13344228	6.22941833	12.78709065
454	H	12.56475340	5.72131638	12.00017726
455	H	12.96463842	7.30754764	12.67451720
456	C	12.68574363	5.73571631	14.17327816
457	H	13.06352892	4.70905464	14.30537117
458	C	11.14267311	5.68497786	14.21181229
459	H	10.74854425	5.01313983	13.43735785
460	H	10.79423393	5.33203206	15.19219445
461	H	10.71437974	6.68329074	14.04718279
462	C	13.74449929	5.93652416	16.47038572
463	C	13.18633424	6.56663681	15.34788941
464	C	12.98728081	7.95554464	15.40220158
465	C	13.33480672	8.68782090	16.53954943
466	C	13.89218868	8.04614343	17.64975175
467	C	14.09893300	6.66528487	17.61043582
468	H	13.87894177	4.85282390	16.45930909
469	H	12.53268107	8.47669907	14.55696842
470	H	13.15661324	9.76377004	16.56300416
471	H	14.15122263	8.61611877	18.54317154
472	H	14.52097091	6.15088730	18.47554537

$[Au_{25}(PPh_3)_8$*(S)*$-(dpb)(SC_2H_4Ph)_5Cl_2]^{2+}$, isomer #2

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	15.75657527	-0.25505613	9.03412406
2	Au	18.29792697	1.15519761	8.31856291
3	Au	16.09606017	0.92473755	6.27788907
4	Au	13.50250186	1.24209849	7.67854198
5	Au	14.02891467	1.65344465	10.57341134
6	Au	16.96757398	1.62490941	11.05164469
7	Au	15.84801510	2.50262224	8.59982828
8	Au	18.04332721	3.95809531	9.57263940
9	Au	17.61517063	3.55390988	6.65902075
10	Au	14.69125218	3.52094705	6.18450452
11	Au	13.34718956	3.93287327	8.78714120
12	Au	15.39181547	4.20674090	10.86227650
13	Au	15.84469580	5.44451149	8.17240676
14	Au	18.06392241	7.19402140	9.04159844
15	Au	17.57029853	6.79502515	6.17885306
16	Au	14.67368338	6.72343458	5.75030255
17	Au	13.35453216	7.11414700	8.33728569
18	Au	15.43925872	7.40726201	10.37933409
19	Au	15.81931557	8.41574337	7.74548979
20	Au	18.33184213	9.50214360	7.04776389
21	Au	16.07603763	9.20192910	5.03316133
22	Au	13.43827346	9.38649018	6.51572095
23	Au	14.05627300	9.85669771	9.45208587
24	Au	17.09352875	9.84378406	9.83985147
25	Au	15.80361672	11.13183800	7.37052376
26	Cl	15.42778622	-2.58320463	9.48989560
27	Cl	15.74867626	13.50087353	7.02607004
28	P	20.32630719	-0.02167662	8.06596461
29	P	16.03966817	-0.51247623	4.42027360
30	P	17.56491065	0.80105382	13.17744096
31	P	20.41490842	10.46456101	6.47570312
32	P	16.33359008	9.89676171	2.78761657
33	P	11.47260158	10.19487326	5.47910838
34	P	12.55799005	11.10873905	10.78836245
35	P	18.18074447	11.01976382	11.58392614
36	C	21.81064359	0.99817053	8.44876627
37	C	21.68157905	2.06944690	9.34688881
38	H	20.69770155	2.32238179	9.74941964
39	C	22.79625677	2.83217791	9.70298991
40	H	22.68248418	3.66077806	10.40350997
41	C	24.04736971	2.53701274	9.15366007
42	H	24.91884033	3.13115791	9.43180814
43	C	24.17976186	1.48701411	8.23999813
44	H	25.15191680	1.26366797	7.79831644
45	C	23.06746756	0.72017453	7.88417009
46	H	23.17731682	-0.08742370	7.15956307
47	C	20.44851851	-1.51624475	9.12823124
48	C	21.68051914	-2.00735999	9.59204880
49	H	22.60220859	-1.46005508	9.39125102
50	C	21.72934547	-3.20331442	10.31179942
51	H	22.69012291	-3.58267350	10.66294323
52	C	20.55411622	-3.91120136	10.58196347
53	H	20.59699381	-4.84416074	11.14561412
54	C	19.32549722	-3.41739048	10.13572805
55	H	18.39815341	-3.95081489	10.34878753
56	C	19.27056933	-2.22444662	9.41229150
57	H	18.30219574	-1.84937183	9.07457321
58	C	20.66675284	-0.64752649	6.36725146
59	C	21.20497926	-1.92360082	6.13913493
60	H	21.35997228	-2.60935465	6.97156187
61	C	21.55145351	-2.31774212	4.84380824
62	H	21.97625513	-3.30859853	4.67844734
63	C	21.35933936	-1.44749339	3.76936607
64	H	21.63698162	-1.75410053	2.75983627
65	C	20.79868925	-0.18569937	3.98866037
66	H	20.62562531	0.48566726	3.14743592
67	C	20.44889192	0.21307063	5.27925179
68	H	20.00332064	1.19606049	5.44809219
69	C	16.70991502	0.20165410	2.86348874
70	C	16.35794265	-0.32447430	1.60788381
71	H	15.65244257	-1.15359905	1.53917204
72	C	16.90050542	0.21898202	0.44200038
73	H	16.62377337	-0.19620658	-0.52789634
74	C	17.78856117	1.29667042	0.51825067
75	H	18.20624270	1.72194127	-0.39558663
76	C	18.12451090	1.83753521	1.76235665
77	H	18.79697074	2.69420191	1.82608836
78	C	17.58748786	1.29362887	2.93243205
79	H	17.83259358	1.72866289	3.90388720
80	C	16.87676180	-2.12674143	4.67071996
81	C	16.67673908	-2.77631409	5.90117235
82	H	16.09776762	-2.30282540	6.69715928
83	C	17.21706186	-4.04424484	6.11887772
84	H	17.04628068	-4.53547928	7.07728073
85	C	17.96911253	-4.66839697	5.11905962
86	H	18.38954856	-5.66035499	5.28984878
87	C	18.18635162	-4.01727819	3.90196583
88	H	18.77879644	-4.49725082	3.12196467
89	C	17.64443895	-2.74926216	3.67418334
90	H	17.82036471	-2.25077279	2.72128948
91	C	14.31047104	-0.96717045	3.95986709

92	C	13.92013265	-2.29429554	3.72486084
93	H	14.63612757	-3.10577326	3.85398388
94	C	12.61229952	-2.58093907	3.31965101
95	H	12.32025157	-3.61572844	3.13587201
96	C	11.68887668	-1.54878009	3.14033287
97	H	10.67347164	-1.77394714	2.81132367
98	C	12.07062734	-0.22477984	3.38538700
99	H	11.35148509	0.58460259	3.24967371
100	C	13.37037956	0.06644943	3.80309684
101	H	13.65730901	1.10001217	4.01008212
102	C	17.71979981	2.11170559	14.46276275
103	C	18.61336198	1.98636192	15.54024297
104	H	19.26108919	1.11307515	15.61666589
105	C	18.67672532	2.98163849	16.51863947
106	H	19.37354581	2.87537611	17.35118716
107	C	17.84907389	4.10490929	16.43334415
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112	H	16.22113285	3.36940640	13.52882972
113	C	16.30378012	-0.36370422	13.84358344
114	C	15.73244197	-0.19697479	15.11492919
115	H	16.01588891	0.65335535	15.73498711
116	C	14.80696624	-1.12879994	15.59613144
117	H	14.37261402	-0.99401791	16.58770777
118	C	14.45350678	-2.23461189	14.81814433
119	H	13.74379079	-2.96866031	15.20289017
120	C	15.01642791	-2.39970393	13.54751120
121	H	14.75111790	-3.26023792	12.93148376
122	C	15.92805779	-1.46470874	13.05334053
123	H	16.33828716	-1.60283255	12.05098532
124	C	19.15371479	-0.11046838	13.31376602
125	C	19.30249213	-1.21643096	14.16572132
126	H	18.43926504	-1.62246517	14.69318280
127	C	20.56215569	-1.79315849	14.34744291
128	H	20.67135705	-2.64950754	15.01426326
129	C	21.67645094	-1.27146470	13.68548400
130	H	22.65939154	-1.71957807	13.83631622
131	C	21.52890557	-0.18164050	12.82237039
132	H	22.39160217	0.22104315	12.29098196
133	C	20.27195927	0.39318454	12.63134948
134	H	20.15827468	1.23966503	11.95183466
135	C	20.80263678	10.60290087	4.67897649
136	C	20.80580764	9.42789109	3.90897530
137	H	20.49960885	8.48064313	4.35641939
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140	C	21.62855174	10.66655310	1.99945825
141	H	21.96152792	10.68957511	0.96078745
142	C	21.60048865	11.84206995	2.75196023
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144	C	21.18742615	11.81503237	4.08730630
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148	H	18.49407570	12.58022177	7.06133570
149	C	19.61562539	14.31630312	7.65808141
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151	C	20.87799508	14.85406574	7.92014476
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153	C	22.01800863	14.05472622	7.78365902
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163	H	24.87428082	7.39707190	8.39433485
164	C	24.20873450	8.87785704	6.96837429
165	H	25.18902934	8.98774098	6.50210446
166	C	23.12828226	9.62063633	6.48886168
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172	H	17.71531177	7.76181204	-1.51513703
173	C	18.61721223	6.78549058	0.19262060
174	H	19.16072899	6.05783111	-0.41183478
175	C	18.71975049	6.75714381	1.58572072
176	H	19.33543619	6.00511342	2.08164630
177	C	18.02647170	7.69381221	2.35701941
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179	C	14.78558601	10.15403723	1.81885251
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185	H	11.65531050	10.44622867	-0.48203208
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187	H	12.08309970	8.34232105	0.79024323
188	C	13.88713423	9.08074681	1.70252203
189	H	14.07081984	8.15286476	2.24757680
190	C	17.22007528	11.49796852	2.61245847
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197	C	18.50822154	13.10152563	1.32634587
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199	C	17.98028858	11.81724968	1.47561297
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201	C	10.63709615	8.95505477	4.39836618
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203	H	8.70023141	9.93710952	4.42155609
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207	H	8.91280790	6.30876622	2.11394110
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234	C	11.78220949	12.52201308	9.90275659
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236	H	13.53248166	12.82535479	8.64847340
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248	C	14.25225399	11.64622523	14.49265720
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250	C	14.21239167	13.03162915	14.68094752
251	H	14.56932793	13.46713293	15.61515832
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253	H	13.68666015	14.93673264	13.80664943
254	C	13.24268745	13.29841956	12.47766215
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259	C	9.78624029	8.12012133	11.39571404
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261	C	9.07455386	8.55716824	12.51592739
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263	C	9.42367465	9.76133377	13.13677664
264	H	8.87777168	10.10199106	14.01756133
265	C	10.47759934	10.52928551	12.63719445
266	H	10.75874261	11.45347648	13.14301941
267	C	17.65123237	10.50702232	13.27542275
268	C	17.04307607	9.25637837	13.44875552
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276	C	17.94631245	11.29144029	14.40324323
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286	H	22.44884513	9.25177458	13.49710594
287	C	20.60673164	9.99388825	12.65840567
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289	C	17.96909471	12.84379920	11.50026480
290	C	16.87032438	13.35895073	10.79765538
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293	H	15.80708076	15.12255883	10.17367558
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296	C	18.63531626	15.10503120	12.08270824
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299	H	19.74435496	13.34757077	12.64716582
300	S	19.64192917	5.68970496	10.13271458
301	C	19.37402813	6.04587245	11.94500708
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306	C	22.36274971	6.02543296	12.38339581
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309	C	23.58187726	3.93781071	13.77274223
310	C	24.37135227	4.95182885	13.22036523
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312	H	21.90601798	6.85527566	11.84259947
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317	S	18.93040810	5.01341088	5.22699373
318	C	20.55705646	5.24460001	6.11695259
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320	H	20.84617567	6.29035864	5.95159458
321	C	21.65084904	4.29262649	5.61487852
322	H	21.29138643	3.25485291	5.67401057
323	C	23.02012467	5.68041254	3.99932322
324	C	22.16207950	4.59100466	4.22245475
325	C	21.80938061	3.78976343	3.12720454
326	C	22.29702033	4.06418482	1.84552304
327	C	23.14990533	5.15119655	1.63834207
328	C	23.50991882	5.95971359	2.72139007
329	H	23.32149039	6.30916609	4.84045048
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331	H	22.02360997	3.41893095	1.00884380
332	H	23.54352690	5.35949476	0.64260862
333	H	24.18607903	6.80285939	2.57187864
334	S	13.87578400	4.89772132	4.35541133
335	C	15.16766565	4.78035019	3.01087376
336	H	16.12487873	4.52659723	3.47890187
337	H	15.25434597	5.78661539	2.58122753
338	C	14.79516530	3.75574172	1.93142466
339	H	14.60007986	2.78041786	2.40060394
340	C	13.76548868	5.19466094	0.11948624
341	C	13.63268858	4.14660356	1.04527344
342	C	12.41072185	3.46118219	1.10053824
343	C	11.34986436	3.80853913	0.25781093
344	C	11.49559573	4.85399405	-0.65718885
345	C	12.70915816	5.54654546	-0.72351964
346	H	14.71365854	5.73262744	0.04554757
347	H	12.29660154	2.63246427	1.80172788
348	H	10.41205649	3.25272836	0.30671394
349	H	10.67477901	5.11882710	-1.32515197
350	H	12.83793748	6.35464428	-1.44511166
351	S	11.54755456	5.56341418	8.83107001
352	C	10.67013663	5.32490803	7.20430980
353	H	11.42030878	5.35510193	6.40630441
354	H	10.00474581	6.19200202	7.09014121
355	C	9.87283989	4.01203983	7.13973702
356	H	10.55787259	3.18734118	7.39592491
357	C	8.70698448	3.60718559	9.36480391
358	C	8.63572721	3.96873779	8.00908453
359	C	7.38223304	4.30952680	7.47593958
360	C	6.23336888	4.29487639	8.27123011
361	C	6.31910010	3.93871336	9.62009854
362	C	7.55996887	3.59478004	10.16434125
363	H	9.67337758	3.33723421	9.79438009
364	H	7.30393351	4.58324243	6.42113821
365	H	5.26793302	4.55561733	7.83504292
366	H	5.42262156	3.92195937	10.24099953
367	H	7.63353429	3.31294970	11.21624913
368	S	14.96780002	6.07322581	12.36536836
369	C	13.10833986	6.18096540	12.45775528
370	H	12.70963372	5.97447148	11.45887444
371	H	12.88347623	7.22706553	12.70267695
372	C	12.49501353	5.22664631	13.48935197
373	H	12.87585619	4.20938600	13.31298544
374	C	13.34354960	4.75409167	15.83704802
375	C	12.69380819	5.61302233	14.94013284
376	C	12.18656487	6.82788983	15.43221228
377	C	12.33132379	7.17415920	16.77691478
378	C	12.98357035	6.30743821	17.66062647
379	C	13.48880587	5.09513988	17.18603105
380	H	13.73525101	3.80071306	15.47646017
381	H	11.65691297	7.50586450	14.75891202
382	H	11.92174300	8.11791010	17.14079798
383	H	13.08741987	6.57227966	18.71370304
384	H	13.99176605	4.40799682	17.86810469
385	H	15.69254638	3.61984169	1.30496161
386	H	22.48690074	4.37086605	6.32941049
387	H	19.65925335	5.22831505	13.88453043
388	H	11.41192377	5.19649837	13.27719541
389	H	9.57776210	3.87083848	6.08752501
390	P	11.60693945	-0.07015622	7.31185434
391	P	12.52295214	0.38297293	11.81194987
392	C	10.24031655	0.06830810	8.50650390
393	C	12.20636937	-1.24334385	11.07104316
394	C	10.22245601	-0.54256390	9.70378556
395	C	11.25111877	-1.50066589	10.16270277
396	H	9.45120097	0.77791669	8.24442312
397	H	9.38659455	-0.33067042	10.38098856
398	H	10.90852688	0.05856065	6.08074740
399	H	11.87478578	-1.46631509	7.28091818
400	H	12.96996290	-1.99562549	11.28283457
401	H	11.24296192	-2.49555197	9.70124617
402	H	12.85223744	0.04171757	13.15291734
403	H	11.21865145	0.91526087	12.01371900

$[Au_{25}(PPh_3)_6(S)^{-}(dpb)_2(SC_2H_4Ph)_5Cl_2]^{2+}$, isomer #3

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	15.86829392	-0.39113844	9.14827460
2	Au	18.37894854	1.01896893	8.43623233
3	Au	16.13313120	0.84509081	6.41648024
4	Au	13.58396092	1.09854335	7.86846821
5	Au	14.12471579	1.50465794	10.75204471
6	Au	17.08028362	1.47070857	11.19573106
7	Au	15.93621457	2.37356083	8.77774501
8	Au	18.15081858	3.81125465	9.76035224
9	Au	17.69777844	3.42781035	6.82285060
10	Au	14.74799013	3.42200168	6.38325127
11	Au	13.42326371	3.78155776	8.99654944
12	Au	15.48256498	4.05845995	11.05896741
13	Au	15.95773243	5.28345626	8.37811741
14	Au	18.17946021	7.03902685	9.24075390
15	Au	17.71690046	6.57825413	6.32344208
16	Au	14.84049517	6.51725959	5.87348486
17	Au	13.46498677	6.94640612	8.44760407
18	Au	15.50874883	7.26012902	10.53495271
19	Au	15.96876008	8.19882979	7.91886173
20	Au	18.48854460	9.29729531	7.32036171
21	Au	16.40181759	8.93547646	5.23673169
22	Au	13.72227847	9.14463407	6.50595000
23	Au	14.06444076	9.71307813	9.37784407
24	Au	17.08268870	9.74634905	9.97958454
25	Au	15.96654570	10.94402273	7.45438782
26	Cl	15.57897768	-2.72151810	9.59327590
27	Cl	15.90019650	13.21898637	6.74887998
28	P	20.40230859	-0.13381226	8.07102708
29	P	16.01219318	-0.46762271	4.47454592
30	P	17.70321892	0.63609108	13.30871841
31	P	20.47416583	10.26822798	6.52847924
32	P	12.34149069	11.05084765	10.26767014
33	P	18.03251748	11.00152886	11.73376935
34	C	21.89512223	0.89346143	8.39569453
35	C	21.80052634	1.95347367	9.31122785
36	H	20.83540098	2.19423806	9.76359557
37	C	22.92531474	2.72053342	9.62346511
38	H	22.83812376	3.53898626	10.33915068
39	C	24.15215893	2.43899522	9.01575813
40	H	25.03194594	3.03516793	9.26185846
41	C	24.24946374	1.39987610	8.08531026
42	H	25.20215683	1.18706840	7.59824665
43	C	23.12660125	0.63022821	7.77125544
44	H	23.20825621	-0.16837790	7.03292110
45	C	20.59204513	-1.64278667	9.10306083
46	C	21.85241223	-2.12804184	9.49043630
47	H	22.75638626	-1.57065310	9.24341536
48	C	21.95217838	-3.33069748	10.19360034
49	H	22.93453082	-3.70519695	10.48516429
50	C	20.80002478	-4.05149625	10.52215801
51	H	20.88204862	-4.99011448	11.07212366
52	C	19.54409410	-3.56456548	10.15093756
53	H	18.63609656	-4.11058263	10.40932584
54	C	19.43764091	-2.36433631	9.44509272
55	H	18.44843526	-1.99545984	9.16593503
56	C	20.65831182	-0.72658338	6.34637540
57	C	21.19636550	-1.99269444	6.06792977
58	H	21.40576127	-2.68933597	6.87915229
59	C	21.47041933	-2.36381551	4.74871575
60	H	21.89514815	-3.34731612	4.54391536
61	C	21.20385816	-1.48131115	3.70033071
62	H	21.42230815	-1.77159252	2.67175273
63	C	20.64352010	-0.22929976	3.97117705
64	H	20.40752842	0.45136783	3.15272120
65	C	20.36802160	0.14752853	5.28623744
66	H	19.92254106	1.12306330	5.49426609
67	C	16.66362839	0.35312566	2.96229633
68	C	16.30197498	-0.08637589	1.67618061
69	H	15.60753895	-0.91894012	1.55577431
70	C	16.81768457	0.55187768	0.54636394
71	H	16.53553479	0.20226024	-0.44783253
72	C	17.68616545	1.63947551	0.68856425
73	H	18.08277159	2.13825411	-0.19702346
74	C	18.03272922	2.09423021	1.96403547
75	H	18.69502408	2.95303260	2.08375565
76	C	17.52363539	1.45350176	3.09741033
77	H	17.77899576	1.82136086	4.09408892
78	C	16.82722216	-2.10489300	4.61987128
79	C	16.68988527	-2.78788933	5.84108140
80	H	16.16771231	-2.32731300	6.68302843
81	C	17.22454499	-4.06802850	5.99127397
82	H	17.10466834	-4.58519189	6.94383007
83	C	17.90962847	-4.67059182	4.93209097
84	H	18.32866010	-5.67071240	5.05111096
85	C	18.06306639	-3.98779352	3.72233077
86	H	18.60330267	-4.45209878	2.89612321
87	C	17.52504147	-2.70807070	3.56194350
88	H	17.65286610	-2.18355337	2.61513107
89	C	14.26879589	-0.85753683	4.01245023
90	C	13.82840634	-2.16911272	3.78011869
91	H	14.51505249	-3.00654811	3.90382783
92	C	12.50878051	-2.40618596	3.38029217
93	H	12.17763034	-3.42903626	3.19649348
94	C	11.62423650	-1.33987677	3.20453598
95	H	10.60024866	-1.52679687	2.87838792
96	C	12.05659687	-0.03047045	3.44655503
97	H	11.36911840	0.80596693	3.31135470
98	C	13.36799809	0.21134692	3.85826225
99	H	13.69429740	1.23371326	4.06136617
100	C	17.89725870	1.94956961	14.58572330
101	C	18.80279778	1.81480091	15.65180330
102	H	19.43545181	0.93026156	15.72587968
103	C	18.89975544	2.81705049	16.62030217
104	H	19.60602053	2.70373397	17.44388314
105	C	18.09540731	3.95726217	16.53556175
106	H	18.17316003	4.73719222	17.29446000
107	C	17.19779837	4.09926662	15.47328545
108	H	16.56825903	4.98605877	15.39387122
109	C	17.10078701	3.10229399	14.50003718
110	H	16.41258444	3.23011737	13.66039908
111	C	16.44747993	-0.52072931	13.99752703
112	C	15.88714211	-0.34227706	15.27193292
113	H	16.17599654	0.51390415	15.88148560
114	C	14.96721228	-1.27083714	15.77012474
115	H	14.54163742	-1.12766051	16.76426498
116	C	14.60870223	-2.38447589	15.00587200
117	H	13.90396841	-3.11605360	15.40399712
118	C	15.16042634	-2.56090294	13.73156275
119	H	14.89072706	-3.42850456	13.12752848
120	C	16.06623288	-1.62955856	13.22038126
121	H	16.46878015	-1.77585445	12.21588001
122	C	19.28219714	-0.29653648	13.40031722
123	C	19.44998567	-1.38316439	14.27377440
124	H	18.60605202	-1.75502809	14.85498147
125	C	20.70302382	-1.98713407	14.40429873
126	H	20.82733661	-2.82885789	15.08683687
127	C	21.79190692	-1.51243105	13.66864176
128	H	22.76982628	-1.98310694	13.77773280
129	C	21.62473623	-0.44181322	12.78550231
130	H	22.46685316	-0.07784156	12.19649560
131	C	20.37379172	0.16074259	12.64609694
132	H	20.24184407	0.98968931	11.94836787
133	C	20.48607082	10.42552878	4.69247110
134	C	20.37918021	9.25370672	3.92152029
135	H	20.28035898	8.28198928	4.40883253
136	C	20.40569734	9.32518867	2.52825553
137	H	20.34598991	8.40787302	1.94137306
138	C	20.51623593	10.56658650	1.88996459
139	H	20.54165431	10.62139715	0.80069333
140	C	20.59969016	11.73494544	2.65143239
141	H	20.68703327	12.70496400	2.16001522
142	C	20.58827300	11.66794307	4.04883610
143	H	20.66644269	12.58350405	4.63485654
144	C	20.79218444	11.96775016	7.15275206
145	C	19.69396115	12.82605124	7.33583561
146	H	18.67489717	12.47911342	7.15030778
147	C	19.89774492	14.14273138	7.75436368
148	H	19.03545720	14.79670057	7.88627869
149	C	21.19128035	14.60891399	8.00511634
150	H	21.34820849	15.63643015	8.33566037
151	C	22.28539435	13.75513139	7.83641241

152	H	23.29635377	14.11425559	8.03351437
153	C	22.09104198	12.43916748	7.40945246
154	H	22.95120327	11.78252572	7.27780860
155	C	21.99195038	9.30042471	6.90149957
156	C	21.99694166	8.45791766	8.02384054
157	H	21.09159415	8.34905149	8.62505686
158	C	23.15010513	7.74531924	8.36255438
159	H	23.13903672	7.08720874	9.23202778
160	C	24.30321386	7.86735888	7.58279273
161	H	25.20350718	7.31066354	7.84627657
162	C	24.30152494	8.69725501	6.45658279
163	H	25.19843673	8.78835868	5.84238986
164	C	23.15027554	9.40865223	6.11118695
165	H	23.15110019	10.04376426	5.22459415
166	C	11.49390830	11.99075872	8.92968480
167	C	12.28048879	12.74098616	8.03692569
168	H	13.37101788	12.72644691	8.09971613
169	C	11.66903002	13.52467969	7.05592229
170	H	12.29295604	14.11896970	6.38628282
171	C	10.27452614	13.54986908	6.94060904
172	H	9.79860617	14.16676167	6.17694784
173	C	9.49155535	12.78570572	7.81005762
174	H	8.40405425	12.80017453	7.72494546
175	C	10.09576041	12.01116753	8.80525840
176	H	9.47601882	11.43205757	9.48992946
177	C	12.83147878	12.33683941	11.48705362
178	C	13.60070365	11.94231877	12.59449103
179	H	13.93920854	10.90881233	12.68733573
180	C	13.93024767	12.86899989	13.58397914
181	H	14.52206149	12.55040233	14.44181414
182	C	13.51473037	14.19934534	13.46790303
183	H	13.77748088	14.92356206	14.24013877
184	C	12.76500470	14.60020937	12.36014310
185	H	12.43993059	15.63688595	12.26292504
186	C	12.41867992	13.67358972	11.37248930
187	H	11.82354424	13.99318666	10.51774027
188	C	11.00787182	10.11459394	11.12083399
189	C	10.73390405	8.80052924	10.71152748
190	H	11.34089755	8.33360371	9.93234500
191	C	9.69555989	8.07993707	11.30575355
192	H	9.49384010	7.06033258	10.97466984
193	C	8.92978680	8.66307698	12.31946418
194	H	8.12047667	8.09986588	12.78639307
195	C	9.20440235	9.96880565	12.73830110
196	H	8.61056580	10.42636007	13.53072782
197	C	10.23849118	10.69568124	12.14348601
198	H	10.44769586	11.71217912	12.47770848
199	C	17.26977033	10.69658591	13.38350538
200	C	16.60040314	9.48420013	13.60812866
201	H	16.48263617	8.76706104	12.79167105
202	C	16.07010377	9.19353924	14.86832065
203	H	15.54631785	8.24965471	15.02652243
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205	H	15.79469368	9.88367895	16.89766917
206	C	16.86926467	11.32334244	15.69463615
207	H	16.97615471	12.04366437	16.50713975
208	C	17.39566864	11.61986829	14.43544195
209	H	17.89764389	12.57393955	14.27298133
210	C	19.82070555	10.64677420	12.00082783
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212	H	20.36619399	11.39629080	10.03720202
213	C	22.08964496	10.72339615	11.14089977
214	H	22.78317177	10.98108545	10.34007323
215	C	22.56604175	10.16889180	12.33373094
216	H	23.63472216	9.99741162	12.46916383
217	C	21.67010618	9.84331543	13.35438742
218	H	22.03505395	9.41341370	14.28814523
219	C	20.30123545	10.08041339	13.19139286
220	H	19.61204334	9.83855001	14.00017381
221	C	17.97282190	12.81979042	11.48146940
222	C	16.93947593	13.36158387	10.70230464
223	H	16.22566543	12.70189475	10.20658466
224	C	16.83730868	14.74455768	10.53672837
225	H	16.03954851	15.15193900	9.91546396
226	C	17.76364497	15.59393959	11.14703011
227	H	17.68309616	16.67416767	11.01676077
228	C	18.80434454	15.05916126	11.91338689
229	H	19.53663413	15.71866589	12.38103291
230	C	18.91504409	13.67713410	12.07752199
231	H	19.74216933	13.26684833	12.65793894
232	S	19.77604377	5.53790181	10.28533471
233	C	19.57476856	5.90989276	12.10320935
234	H	18.50382202	5.91486651	12.33145697
235	H	19.95124910	6.93272359	12.23716181
236	C	20.29540783	4.90982998	13.00221929
237	H	19.89834205	3.90173177	12.80714311
238	C	22.59011085	5.96117489	12.53318145
239	C	21.81215750	4.87035757	12.94891124
240	C	22.47774057	3.71789000	13.39894969
241	C	23.87201455	3.65653677	13.44141105
242	C	24.63540672	4.75174011	13.02598008
243	C	23.98764902	5.90257523	12.57072625
244	H	22.11021060	6.87648588	12.18417098
245	H	21.89108433	2.85780034	13.72923094
246	H	24.36475435	2.75250565	13.80226340
247	H	25.72485072	4.70971375	13.06249894
248	H	24.57313241	6.76542209	12.24890744
249	S	19.06051805	4.80635340	5.35260513
250	C	20.70757928	5.00892689	6.21637952
251	H	20.56742742	4.78685756	7.27959265
252	H	20.96853016	6.07039223	6.12170309
253	C	21.80061814	4.12050322	5.61179284
254	H	21.48038572	3.06865174	5.63444321
255	C	22.82032362	5.74628339	3.95057404
256	C	22.23732034	4.49499584	4.21014015
257	C	22.10567477	3.59215291	3.14613113
258	C	22.53737477	3.92509890	1.85825633
259	C	23.10965203	5.17538755	1.61291892
260	C	23.25041576	6.08525100	2.66590364
261	H	22.95711521	6.46038504	4.76607461
262	H	21.67578730	2.60668977	3.33488146
263	H	22.43545154	3.20270939	1.04668235
264	H	23.45602796	5.43494843	0.61155215
265	H	23.70926631	7.05894634	2.48690017
266	S	13.76451490	4.75710262	4.59812508
267	C	14.81140574	4.49845718	3.06650021
268	H	15.55911906	3.73311472	3.29922965
269	H	15.32895814	5.44294040	2.86347746
270	C	13.95168521	4.07000831	1.86588682
271	H	13.30799087	3.22741125	2.15980583
272	C	13.67767366	6.03964935	0.30308316
273	C	13.11648926	5.17484704	1.25674268
274	C	11.77245392	5.36078994	1.61390915
275	C	11.00972333	6.38012290	1.03508566
276	C	11.58074696	7.23285888	0.08562057
277	C	12.92006797	7.05893359	-0.27913371
278	H	14.71596970	5.89634654	-0.00609532
279	H	11.31530719	4.69051337	2.34386801
280	H	9.96012296	6.49635075	1.31082296
281	H	10.97982768	8.01246096	-0.38459420
282	H	13.36807894	7.70272896	-1.03803088
283	S	11.64190437	5.43054372	8.96973673
284	C	10.75641604	5.16395610	7.35268398
285	H	11.50390370	5.14651122	6.55105203
286	H	10.11513575	6.04661910	7.22023220
287	C	9.92371760	3.87176722	7.33543544
288	H	10.58976299	3.03599891	7.60438881
289	C	8.77805333	3.52148611	9.57919028
290	C	8.70074403	3.88745895	8.22532973
291	C	7.45708160	4.29172815	7.71419931
292	C	6.32368327	4.33621955	8.52998360
293	C	6.41551447	3.97507851	9.87716567
294	C	7.64628139	3.56668161	10.39911011
295	H	9.73691503	3.20189872	9.99172187
296	H	7.37270353	4.56729978	6.66015707
297	H	5.36528836	4.64657528	8.11118510
298	H	5.53047573	4.00373503	10.51388176
299	H	7.72385389	3.27935334	11.44920126
300	S	15.05814047	5.95665372	12.53341092
301	C	13.19810466	6.05359786	12.64340507
302	H	12.78833729	5.82861604	11.65282901
303	H	12.97103846	7.10183530	12.87725510
304	C	12.60908078	5.10829129	13.69700658
305	H	12.98557207	4.08962304	13.51935039
306	C	13.52973293	4.65833599	16.02190366
307	C	12.84578604	5.50553597	15.13924737

308	C	12.34099516	6.71830369	15.63885327
309	C	12.51864398	7.07292433	16.97759217
310	C	13.20343088	6.21715138	17.84720594
311	C	13.70868735	5.00801081	17.36448015
312	H	13.92164571	3.70733105	15.65526757
313	H	11.78650769	7.38763120	14.97702317
314	H	12.10764946	8.01348117	17.34824455
315	H	13.33226714	6.48757744	18.89607155
316	H	14.23728280	4.32967363	18.03588482
317	H	14.64342144	3.68078950	1.10110875
318	H	22.66838653	4.18940970	6.29018280
319	H	19.99307388	5.14439159	14.03920430
320	H	11.52108404	5.07624537	13.51241778
321	H	9.60779217	3.70899649	6.29217946
322	P	11.69328113	-0.21473634	7.49213283
323	P	12.67250341	0.18226931	12.00634114
324	C	10.34319201	-0.09989035	8.70697399
325	C	12.35804653	-1.42988446	11.23466400
326	C	10.35433694	-0.71989743	9.89991221
327	C	11.39776621	-1.67541317	10.32800348
328	H	9.54368304	0.60492551	8.46485602
329	H	9.53151159	-0.51899682	10.59607285
330	H	10.98497483	-0.06887338	6.26828908
331	H	11.96856260	-1.60869154	7.43717864
332	H	13.12951984	-2.18050044	11.42216526
333	H	11.39697056	-2.65951753	9.84390965
334	H	13.04207956	-0.18482542	13.32974312
335	H	11.36834262	0.69493321	12.25494276
336	P	16.42528833	10.09196662	3.21347854
337	P	12.12943153	10.01560113	5.04636008
338	C	15.35270468	11.55752265	3.20884297
339	C	12.40578711	9.66314054	3.28338746
340	C	14.03380337	11.52762352	2.95478460
341	C	13.28213940	10.33453465	2.51592981
342	H	15.81339616	12.46867030	3.59906072
343	H	13.46307155	12.45212734	3.10339874
344	H	17.66160492	10.61814381	2.74834909
345	H	16.01689100	9.37747043	2.05230379
346	H	11.91228018	8.77003185	2.89109173
347	H	13.45199770	9.97136802	1.49551817
348	H	10.77269580	9.62113672	5.20775809
349	H	11.96732875	11.42752933	5.09609812

$[Au_{25}(PPh_3)_8(S)$–$(BINAP)(SC_2H_4Ph)_5Cl_2]^{2+}$, isomer #2

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	15.76467189	-0.44062063	8.98661522
2	Au	18.21746480	1.10625282	8.22431252
3	Au	15.81638026	0.72959051	6.28449523
4	Au	13.20935570	1.05411093	7.89720492
5	Au	13.97382315	1.31846750	10.67112492
6	Au	16.93273217	1.42994156	11.00846469
7	Au	15.66319044	2.30476929	8.61703235
8	Au	17.86136075	3.82546624	9.59410637
9	Au	17.45212804	3.44660785	6.69706790
10	Au	14.54035731	3.35367619	6.21701404
11	Au	13.20102727	3.83803203	8.75107369
12	Au	15.19157132	3.96602875	10.88423768
13	Au	15.69593059	5.30393771	8.19990066
14	Au	17.95003181	7.05143035	9.04785735
15	Au	17.45496236	6.67521875	6.20686288
16	Au	14.57076657	6.63811750	5.78445631
17	Au	13.27561734	7.05904838	8.36379751
18	Au	15.34774294	7.26014072	10.39917665
19	Au	15.74264755	8.32623523	7.77513989
20	Au	18.27639531	9.37496180	7.07996272
21	Au	16.00549523	9.09696416	5.06178220
22	Au	13.39265249	9.36525970	6.55311952
23	Au	14.01252852	9.76843990	9.49979929
24	Au	17.03787131	9.71302758	9.88419797
25	Au	15.79633856	11.04653847	7.42899159
26	Cl	15.93012986	-2.81932620	9.26459581
27	Cl	15.79602197	13.42149590	7.09478666
28	P	20.33668379	0.08743501	7.95475411
29	P	16.04318876	-0.59574885	4.34095625
30	P	17.89129856	0.61084244	13.00935580
31	P	20.36569388	10.33011136	6.50928787
32	P	16.30317585	9.79238441	2.82120187
33	P	11.49371970	10.27728132	5.47302503
34	P	12.53398957	11.04285249	10.83512639
35	P	18.13637124	10.85947335	11.64145927
36	C	21.74070245	1.23736919	8.28424544
37	C	21.52963641	2.35376387	9.10618579
38	H	20.52699714	2.56487379	9.48509017
39	C	22.58749531	3.20933565	9.42441752
40	H	22.40475787	4.07026710	10.06933626
41	C	23.86484761	2.96081362	8.91461851
42	H	24.69327012	3.62469671	9.16559138
43	C	24.07807027	1.86581757	8.07134202
44	H	25.06920018	1.67752720	7.65641674
45	C	23.02245554	1.00851572	7.75299570
46	H	23.19677726	0.16588421	7.08329748
47	C	20.61560827	-1.36914118	9.04248523
48	C	21.86546188	-1.65928551	9.61254048
49	H	22.69966021	-0.96869514	9.49075759
50	C	22.04525921	-2.83944192	10.33871005
51	H	23.02085784	-3.06006961	10.77370901
52	C	20.98283947	-3.73139873	10.50742174
53	H	21.12775754	-4.65254860	11.07419135
54	C	19.73263526	-3.43509530	9.95792155
55	H	18.88843086	-4.11163720	10.09558150
56	C	19.54593135	-2.25867681	9.22999480
57	H	18.55878500	-2.04256759	8.81762416
58	C	20.73518152	-0.54522720	6.27028985
59	C	21.48357504	-1.71832411	6.08095165
60	H	21.75127666	-2.34011459	6.93503633
61	C	21.89800382	-2.08714837	4.79844740
62	H	22.48833636	-2.99475802	4.66387660
63	C	21.56079457	-1.29774574	3.69695465
64	H	21.88978876	-1.58446463	2.69704848
65	C	20.78691397	-0.14794714	3.87701915
66	H	20.49204382	0.45265356	3.01615297
67	C	20.37353766	0.22732380	5.15623149
68	H	19.76570189	1.12409465	5.29484056
69	C	16.74637634	0.32866763	2.90907515
70	C	16.51729909	-0.07927950	1.58336518
71	H	15.86608432	-0.92975806	1.37767177
72	C	17.11283551	0.60874212	0.52353677
73	H	16.93085181	0.28336971	-0.50150276
74	C	17.93339239	1.71270392	0.77535551
75	H	18.39413213	2.24898936	-0.05554754
76	C	18.14323364	2.13925960	2.09009650
77	H	18.75807528	3.01674928	2.29661408
78	C	17.55039258	1.45215440	3.15220389
79	H	17.69490036	1.80377723	4.17675513
80	C	17.10572984	-2.08267919	4.54424669
81	C	17.02471569	-2.78805488	5.75519671
82	H	16.42641063	-2.40824324	6.58550779
83	C	17.71157932	-3.99369528	5.91082758
84	H	17.63517607	-4.52871977	6.85794716
85	C	18.48897378	-4.50023957	4.86617155
86	H	19.02245083	-5.44416577	4.98791646
87	C	18.58871120	-3.79047241	3.66634796
88	H	19.20112528	-4.17605141	2.85028060
89	C	17.90318407	-2.58435255	3.50319313
90	H	17.98776529	-2.03997615	2.56298108
91	C	14.47287190	-1.28264768	3.66609167
92	C	14.36195960	-2.61732612	3.24591979
93	H	15.20266028	-3.30024797	3.36337821
94	C	13.17278645	-3.07594908	2.67245571
95	H	13.09729986	-4.11453926	2.34753130
96	C	12.08824827	-2.21092495	2.51765401
97	H	11.16112573	-2.57045984	2.06931699
98	C	12.18841912	-0.88531919	2.95085576
99	H	11.33653334	-0.21165587	2.85500871
100	C	13.37170861	-0.42296018	3.52689589
101	H	13.44018315	0.60856356	3.87852813
102	C	17.78901985	1.82279181	14.39632946
103	C	18.64837797	1.74239680	15.50647407

104	H	19.41251565	0.96527914	15.55220675
105	C	18.53504434	2.66166864	16.55185120
106	H	19.20440002	2.58852066	17.41028790
107	C	17.57300386	3.67524466	16.49486305
108	H	17.49108887	4.39575834	17.30995594
109	C	16.72689566	3.77041871	15.38673467
110	H	15.98543932	4.56831146	15.32417513
111	C	16.83449324	2.84939596	14.34138625
112	H	16.18968620	2.94496929	13.46358968
113	C	17.09674205	-0.92729708	13.62850599
114	C	16.82473750	-1.14428723	14.98813543
115	H	17.01607602	-0.35919626	15.71900451
116	C	16.30929304	-2.37203981	15.41199652
117	H	16.10311205	-2.53240178	16.47111624
118	C	16.06270999	-3.38907637	14.48647090
119	H	15.66487704	-4.34794235	14.82205910
120	C	16.32123006	-3.17117124	13.12982626
121	H	16.12604107	-3.95013477	12.39192103
122	C	16.83067358	-1.94530580	12.69829862
123	H	17.01200158	-1.79311942	11.63281876
124	C	19.68467428	0.18555786	12.99134661
125	C	20.18355544	-0.93596471	13.67357251
126	H	19.49847771	-1.64140776	14.14290709
127	C	21.56213518	-1.14575488	13.76210393
128	H	21.93970731	-2.01580304	14.30094494
129	C	22.45004469	-0.24465330	13.17010446
130	H	23.52608771	-0.40634744	13.24835146
131	C	21.95738878	0.85854886	12.46741064
132	H	22.64291030	1.55830446	11.98981522
133	C	20.58112667	1.07065730	12.37358419
134	H	20.20094786	1.93210182	11.82184672
135	C	20.76326589	10.47430118	4.71482010
136	C	20.74024032	9.30685770	3.93421378
137	H	20.40690265	8.36390052	4.37107578
138	C	21.16395341	9.34005612	2.60567222
139	H	21.15096527	8.42470666	2.01456779
140	C	21.60672214	10.53975546	2.04020440
141	H	21.94604497	10.56307277	1.00353657
142	C	21.60586692	11.70878524	2.80326622
143	H	21.94101004	12.65006911	2.36601475
144	C	21.18335068	11.68101805	4.13550725
145	H	21.19610239	12.59709368	4.72423974
146	C	20.59531252	12.04199321	7.14788330
147	C	19.46025027	12.85096154	7.31085824
148	H	18.46074114	12.45373536	7.12435064
149	C	19.59603131	14.18052291	7.71923848
150	H	18.69864673	14.78793856	7.84240458
151	C	20.86344232	14.71190300	7.96931428
152	H	20.97041199	15.74951421	8.28855793
153	C	21.99852450	13.90875447	7.81407416
154	H	22.99045839	14.31909718	8.00896365
155	C	21.86846386	12.57932018	7.40650945
156	H	22.75993025	11.96207952	7.29212858
157	C	21.80545824	9.35278504	7.12398623
158	C	21.63038052	8.46717537	8.19697874
159	H	20.64280515	8.34751483	8.64853602
160	C	22.70805085	7.71506322	8.67146893
161	H	22.55166999	7.01516603	9.49276183
162	C	23.96960221	7.84738351	8.08657310
163	H	24.81074408	7.25945886	8.45645858
164	C	24.15157555	8.72640494	7.01413898
165	H	25.13267911	8.82776435	6.54771941
166	C	23.07422197	9.46862380	6.52681221
167	H	23.21750511	10.12612448	5.66858829
168	C	17.19400091	8.55412609	1.78402137
169	C	17.08869698	8.56126437	0.38089223
170	H	16.44552277	9.28765977	-0.11695653
171	C	17.79285664	7.62682617	-0.38120647
172	H	17.70814259	7.64382909	-1.46882052
173	C	18.59612133	6.66936759	0.24709755
174	H	19.14426669	5.94074160	-0.35189945
175	C	18.68609313	6.64202684	1.64097595
176	H	19.29735272	5.89055487	2.14319952
177	C	17.98732425	7.57979567	2.40571523
178	H	18.04391608	7.54148288	3.49608682
179	C	14.77566156	10.06649533	1.82346198
180	C	14.59210167	11.21312539	1.03592686
181	H	15.31412209	12.02778873	1.07705193
182	C	13.49012652	11.30773410	0.18111783
183	H	13.36363042	12.19887334	-0.43530722
184	C	12.56268979	10.26673097	0.11046795
185	H	11.70822188	10.33965215	-0.56390503
186	C	12.72551115	9.13503357	0.91557654
187	H	11.99578432	8.32581187	0.88206756
188	C	13.82360028	9.03566261	1.77015108
189	H	13.94645747	8.14805611	2.39381961
190	C	17.21376151	11.38157829	2.66111331
191	C	17.02489747	12.34800975	3.66153127
192	H	16.44236723	12.11667931	4.55556381
193	C	17.58046878	13.62162463	3.52127452
194	H	17.42232660	14.35745524	4.31036018
195	C	18.32760593	13.93973589	2.38437876
196	H	18.75425857	14.93744505	2.27015115
197	C	18.53727441	12.97335047	1.39604439
198	H	19.12961489	13.21373211	0.51198822
199	C	17.98826222	11.69653554	1.53251650
200	H	18.16204526	10.94980476	0.75807168
201	C	10.61269239	9.06368152	4.39756442
202	C	9.28806335	9.28547826	3.97750748
203	H	8.74750977	10.17088583	4.31361768
204	C	8.65141310	8.36387695	3.14355681
205	H	7.62711370	8.54916384	2.81691076
206	C	9.32012448	7.20409950	2.73652795
207	H	8.81874730	6.48426455	2.08814784
208	C	10.62614047	6.96529380	3.17137390
209	H	11.15300310	6.05750333	2.87402111
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211	H	12.28440168	7.69268297	4.34904860
212	C	11.90006189	11.72834719	4.41835711
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215	C	13.20412849	13.76003045	4.15895604
216	H	14.00986321	14.40400162	4.51302353
217	C	12.45475058	14.10205477	3.03081065
218	H	12.66476875	15.02831756	2.49346965
219	C	11.44052483	13.24924534	2.58481704
220	H	10.85925580	13.50647242	1.69830662
221	C	11.16395483	12.06418000	3.27015618
222	H	10.37467948	11.40604433	2.90774844
223	C	10.11333379	10.87996642	6.53783801
224	C	9.53678548	9.98328625	7.45240500
225	H	9.96283578	8.98734427	7.58501427
226	C	8.40403325	10.35061269	8.17879660
227	H	7.95875361	9.64090960	8.87581583
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229	H	6.94861093	11.90144393	8.56748092
230	C	8.42441885	12.52292117	7.11738459
231	H	7.99487685	13.51641839	6.98290451
232	C	9.55909004	12.15975634	6.38623312
233	H	10.00189707	12.86945348	5.68862354
234	C	11.84323536	12.51824313	9.98124155
235	C	12.66113332	13.18823912	9.05835092
236	H	13.62933566	12.77532377	8.76779524
237	C	12.24638441	14.40036592	8.50187567
238	H	12.89928963	14.90597225	7.78958105
239	C	11.01267050	14.94999644	8.85893249
240	H	10.69154651	15.90025900	8.42963774
241	C	10.18455644	14.27439717	9.76067466
242	H	9.21567221	14.69412048	10.03466659
243	C	10.59305770	13.06155697	10.31953415
244	H	9.93923934	12.54471022	11.02182207
245	C	13.23483630	11.75001772	12.38591382
246	C	13.81386780	10.87174926	13.31687092
247	H	13.90643933	9.80926948	13.08475158
248	C	14.26711446	11.35095699	14.54529103
249	H	14.70857780	10.65844765	15.26137697
250	C	14.16795582	12.71238958	14.84994377
251	H	14.52498522	13.08520478	15.81102780
252	C	13.61754940	13.59387023	13.91839073
253	H	13.54264375	14.65796785	14.14626514
254	C	13.14906298	13.11711879	12.69044781
255	H	12.70641704	13.81099819	11.97716568
256	C	11.09523314	10.07550695	11.46104831
257	C	10.68893207	8.92781767	10.76531254
258	H	11.25334683	8.59547686	9.89136721
259	C	9.58201454	8.19365751	11.19859132

260	H	9.28095738	7.30290764	10.64543909
261	C	8.87411855	8.59878247	12.33319978
262	H	8.00925986	8.02728654	12.67267712
263	C	9.28250891	9.73331930	13.04231250
264	H	8.73997633	10.04635143	13.93532947
265	C	10.39058561	10.46764473	12.61377930
266	H	10.71418653	11.33932720	13.18353755
267	C	17.64103571	10.29454484	13.32695974
268	C	17.04415215	9.03556138	13.47779984
269	H	16.77660425	8.45108789	12.59376919
270	C	16.77921751	8.52742923	14.75346498
271	H	16.30324456	7.55100623	14.85144287
272	C	17.11374438	9.27281476	15.88646985
273	H	16.91408717	8.87481261	16.88226321
274	C	17.69271984	10.53855745	15.74152469
275	H	17.94639027	11.12959411	16.62278975
276	C	17.95033772	11.05149414	14.46955500
277	H	18.39677296	12.04085996	14.37016406
278	C	19.97158091	10.67515226	11.70052101
279	C	20.75844357	11.34667601	10.74929552
280	H	20.28779962	11.95666725	9.97735355
281	C	22.14993612	11.26190501	10.80481163
282	H	22.74738173	11.80289169	10.07136309
283	C	22.77322065	10.49829783	11.79593360
284	H	23.86176591	10.44511644	11.84196010
285	C	21.99662401	9.80915764	12.72913041
286	H	22.47205193	9.20839656	13.50502018
287	C	20.60207807	9.89483657	12.68308429
288	H	20.00919960	9.37362558	13.43388006
289	C	17.88545345	12.68035357	11.60873792
290	C	16.75375885	13.18888403	10.95535413
291	H	16.07565802	12.50872322	10.43768950
292	C	16.50835398	14.56330986	10.93896306
293	H	15.63578025	14.94503249	10.40890362
294	C	17.38971657	15.43949361	11.57575501
295	H	17.19978752	16.51384944	11.56010641
296	C	18.52781219	14.94111358	12.21867583
297	H	19.22658634	15.62350741	12.70450194
298	C	18.78124301	13.56882247	12.23174410
299	H	19.68747368	13.19371367	12.70816101
300	S	19.45988274	5.55245313	10.22440345
301	C	19.12194185	5.98612858	12.00943171
302	H	18.03827437	5.94468710	12.16071176
303	H	19.43735464	7.03213310	12.12352682
304	C	19.82163425	5.07332340	13.01038507
305	H	19.53736876	4.02865715	12.80488811
306	C	22.10512093	6.11522064	12.44889111
307	C	21.33250288	5.16831240	13.13437063
308	C	21.99114313	4.28871577	14.01117310
309	C	23.37259501	4.35015543	14.19712354
310	C	24.13275884	5.29748793	13.50284340
311	C	23.49257395	6.17828541	12.62945972
312	H	21.62753099	6.82128616	11.76904780
313	H	21.40642669	3.54668895	14.55904948
314	H	23.85804409	3.65968285	14.88841271
315	H	25.21267995	5.35055971	13.64760862
316	H	24.07271391	6.92739964	12.08777033
317	S	18.78321736	4.88499626	5.23746136
318	C	20.41979028	5.07966482	6.12071146
319	H	20.25479977	4.87323666	7.18367173
320	H	20.69981869	6.13559783	6.01783866
321	C	21.51188454	4.16460575	5.55290292
322	H	21.14547001	3.12837023	5.51882136
323	C	22.82931094	5.72864931	4.05581584
324	C	22.05421207	4.56561415	4.19766143
325	C	21.83478999	3.77355585	3.06162512
326	C	22.37155857	4.12777700	1.81952846
327	C	23.14047779	5.28719615	1.69343423
328	C	23.36704171	6.08764827	2.81804029
329	H	23.03065798	6.35337051	4.92945239
330	H	21.25531262	2.85368249	3.15843666
331	H	22.20250766	3.48762406	0.95180085
332	H	23.57274778	5.55876124	0.72945984
333	H	23.97692977	6.98834371	2.73321391
334	S	13.75958711	4.79828296	4.41569816
335	C	15.03729295	4.68401486	3.05833680
336	H	16.00334907	4.45781414	3.52190712
337	H	15.10063623	5.68733396	2.61817870
338	C	14.68369790	3.63481963	1.99958909
339	H	14.49422778	2.66805979	2.48861573
340	C	13.55476976	5.14751670	0.29882828
341	C	13.53206720	3.97874195	1.07814552
342	C	12.44637714	3.10409646	0.92685475
343	C	11.40974947	3.38693792	0.03128139
344	C	11.44261274	4.55588387	-0.73256883
345	C	12.52169731	5.43524898	-0.59580374
346	H	14.39996344	5.83517323	0.37583596
347	H	12.42423622	2.17748095	1.50376324
348	H	10.58211612	2.68457628	-0.08097599
349	H	10.64201261	4.77352587	-1.44077808
350	H	12.56686868	6.34212448	-1.20063057
351	S	11.42843239	5.53143200	8.71653242
352	C	10.67055693	5.42714553	7.01224403
353	H	11.40271857	4.95337682	6.34956380
354	H	10.52178223	6.45919912	6.67163704
355	C	9.34648355	4.65010120	7.00935446
356	H	9.47577501	3.72371655	7.58741342
357	C	7.53411292	5.08914800	8.73910943
358	C	8.14266619	5.41345036	7.51807174
359	C	7.58494426	6.45056295	6.75184890
360	C	6.45362360	7.14039605	7.19255683
361	C	5.85591725	6.80589519	8.41194509
362	C	6.40064554	5.77776829	9.18479802
363	H	7.94439236	4.27552604	9.34025221
364	H	8.03312761	6.71306649	5.79061826
365	H	6.03027874	7.93547464	6.57722335
366	H	4.96530712	7.33627959	8.75126819
367	H	5.93473228	5.50326581	10.13280050
368	S	14.86986312	5.88561866	12.35617852
369	C	13.01649950	6.07944175	12.49330752
370	H	12.57348530	5.72716945	11.55548952
371	H	12.83384639	7.15876976	12.56758569
372	C	12.41806399	5.33146685	13.68883781
373	H	12.74334535	4.28071137	13.66709262
374	C	13.23595321	5.15326051	16.08512204
375	C	12.69666118	5.93197332	15.05137073
376	C	12.36504903	7.26786382	15.33330632
377	C	12.57686735	7.80896464	16.60293378
378	C	13.12180051	7.02155587	17.62259562
379	C	13.44838203	5.68937270	17.35956830
380	H	13.47646954	4.10563247	15.89301143
381	H	11.91705578	7.89184150	14.55684043
382	H	12.30310725	8.84648553	16.80117631
383	H	13.27771798	7.44035698	18.61762512
384	H	13.86017739	5.06134155	18.15131808
385	H	15.59138804	3.49034617	1.38880740
386	H	22.33809465	4.17253679	6.28395420
387	H	19.38445370	5.29500078	13.99997573
388	H	11.32617207	5.31115506	13.52813495
389	H	9.15853397	4.34490123	5.96669991
390	P	11.13305644	-0.06641445	7.53184332
391	P	12.25919254	0.23645762	11.86205600
392	C	9.75973523	0.03628964	8.80993889
393	C	11.82131623	-1.40585661	11.11214734
394	C	10.32146307	0.64537423	6.02130934
395	C	8.76046761	1.02013306	8.55002868
396	H	8.86453674	1.66792295	7.68344685
397	C	7.64594228	1.15661090	9.34168975
398	H	6.89311384	1.90818157	9.09695042
399	C	7.44669551	0.31455598	10.46113925
400	C	6.27311925	0.39337386	11.25729242
401	H	5.50663678	1.12281119	10.98884923
402	C	6.09783898	-0.44145229	12.34017416
403	H	5.18812491	-0.38327105	12.93887795
404	C	7.10217363	-1.38032866	12.67385394
405	H	6.95868952	-2.04223624	13.52900612
406	C	8.25774587	-1.47141272	11.92499463
407	H	9.01568913	-2.20577425	12.19273556
408	C	8.46769848	-0.63914967	10.78882542
409	C	9.64719954	-0.74876368	9.96874717
410	C	11.42489466	-1.83905168	7.11783442
411	C	12.67690032	-0.18696964	13.60945093
412	C	12.81951852	-2.39211574	11.37275104
413	H	13.75196903	-2.09853881	11.85581274
414	C	12.62336845	-3.70978248	11.04298537
415	H	13.39946816	-4.44603944	11.25463348

416	C	11.40855139	-4.13415652	10.44922148
417	C	11.13271128	-5.50729823	10.21547491
418	H	11.88739814	-6.24616376	10.49137659
419	C	9.93059030	-5.90382384	9.66802141
420	H	9.72036883	-6.96264103	9.51128748
421	C	8.96715042	-4.93343285	9.30817934
422	H	8.01704560	-5.25032081	8.87613500
423	C	9.21956043	-3.58927683	9.49414706
424	H	8.46662975	-2.85574765	9.20924104
425	C	10.43418208	-3.14364627	10.08616111
426	C	10.67960012	-1.75381472	10.38135320
427	C	10.80534806	1.34157982	12.13212114
428	C	11.01143270	1.63413993	5.30578718
429	H	11.98319188	1.98178994	5.66818469
430	C	10.46861726	2.18841412	4.14231329
431	H	11.02431376	2.96040954	3.60762101
432	C	9.22614207	1.75582352	3.67573383
433	H	8.79913971	2.18543740	2.76825654
434	C	8.52091788	0.77856550	4.38699795
435	H	7.54075655	0.44801275	4.03997872
436	C	9.05840333	0.23355640	5.55321929
437	H	8.46837218	-0.48882793	6.11562041
438	C	10.46135948	-2.64795621	6.49173457
439	H	9.47046155	-2.26291306	6.26203900
440	C	10.76601763	-3.96448757	6.14797257
441	H	10.01037788	-4.58123291	5.65977499
442	C	12.02801101	-4.49442744	6.43325398
443	H	12.25857540	-5.52678422	6.16599639
444	C	12.98678234	-3.70019627	7.06321481
445	H	13.97328495	-4.09448295	7.30807248
446	C	12.68903103	-2.37804973	7.39732909
447	H	13.45043443	-1.76903967	7.88819867
448	C	13.45685665	0.73743990	14.32047705
449	H	13.90185218	1.58366308	13.79279490
450	C	13.65988515	0.58174884	15.69260563
451	H	14.26874348	1.30696121	16.23384912
452	C	13.09631983	-0.50522736	16.36606823
453	H	13.25261028	-0.62591237	17.43891923
454	C	12.34004375	-1.44389536	15.65928161
455	H	11.90681387	-2.30039504	16.17782937
456	C	12.12738136	-1.28744571	14.28704177
457	H	11.53146007	-2.02294317	13.74699830
458	C	9.94156212	1.16523384	13.22770937
459	H	10.05590664	0.30675647	13.88789607
460	C	8.94514999	2.10392999	13.49558456
461	H	8.28289656	1.95659385	14.34940019
462	C	8.80735410	3.23462896	12.68493508
463	H	8.03792185	3.97472131	12.90934289
464	C	9.66697794	3.41922774	11.60014558
465	H	9.59059672	4.30657334	10.97026823
466	C	10.66025563	2.47764836	11.32351289
467	H	11.34563674	2.64635699	10.48902796

$[Au_{25}(PPh_3)_6$*(S)*$-(BINAP)_2(SC_2H_4Ph)_5Cl_2]^{2+}$, isomer #4

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	15.65708040	-0.48176313	9.16639632
2	Au	18.13046008	0.96293587	8.31202497
3	Au	15.70947105	0.61612781	6.40474626
4	Au	13.14372785	1.02459197	8.00349132
5	Au	13.90792237	1.35134366	10.76988150
6	Au	16.89259666	1.42889638	11.09982921
7	Au	15.62175930	2.25146730	8.69661153
8	Au	17.85072663	3.78111382	9.62278369
9	Au	17.43070080	3.30538795	6.76351793
10	Au	14.52937629	3.28319205	6.26895376
11	Au	13.18737873	3.82742239	8.77478625
12	Au	15.17992152	3.96192171	10.91554383
13	Au	15.71620043	5.25707148	8.22081263
14	Au	17.99620050	7.04030566	9.01680625
15	Au	17.48758263	6.61701147	6.23195947
16	Au	14.60990245	6.60867788	5.79230162
17	Au	13.29846017	7.01589837	8.36705860
18	Au	15.33957940	7.20604105	10.41977374
19	Au	15.76484174	8.28819530	7.81698617
20	Au	18.27280846	9.39424036	7.00444481
21	Au	16.09096859	9.07158659	5.12664365
22	Au	13.48064382	9.30743946	6.45606151
23	Au	13.94209753	9.69342995	9.49284858
24	Au	16.99878123	9.63663284	9.97095390
25	Au	15.78089823	11.02429981	7.59706382
26	Cl	15.78605831	-2.84904001	9.55341650
27	Cl	15.81448892	13.41026941	7.38231223
28	P	20.21599119	-0.13235170	8.07655544
29	P	15.88730732	-0.79627957	4.51649760
30	P	17.90531481	0.69189336	13.10660796
31	P	11.66797788	10.21433490	5.23145301
32	P	12.37146898	10.94763389	10.73630159
33	P	18.08073110	10.64318471	11.81767200
34	C	21.64349178	1.01214385	8.29967493
35	C	21.45825933	2.19886915	9.02443742
36	H	20.46241670	2.45993072	9.39056326
37	C	22.53383045	3.05796015	9.26255612
38	H	22.37228331	3.97379101	9.83385787
39	C	23.80216582	2.74302487	8.76819196
40	H	24.64328320	3.41216467	8.95391809
41	C	23.98959412	1.57703011	8.01996347
42	H	24.97234160	1.33970958	7.61123532
43	C	22.91695776	0.71560896	7.78182845
44	H	23.07087370	-0.18276439	7.18319776
45	C	20.48704965	-1.51991374	9.25230336
46	C	21.73812064	-1.78365789	9.83204793
47	H	22.57412101	-1.10401469	9.66857411
48	C	21.91642470	-2.92344323	10.62032089
49	H	22.89329571	-3.12469030	11.06184065
50	C	20.85151818	-3.80076365	10.84121118
51	H	20.99554269	-4.69083368	11.45578678
52	C	19.59966529	-3.52857982	10.28276369
53	H	18.75432412	-4.19432011	10.46009278
54	C	19.41420571	-2.39303736	9.49244232
55	H	18.42634903	-2.19606722	9.07200754
56	C	20.57500712	-0.89445093	6.43546456
57	C	21.31288197	-2.08398487	6.32166361
58	H	21.58959371	-2.64394780	7.21465796
59	C	21.70641831	-2.54898070	5.06411146
60	H	22.28779254	-3.46893104	4.98876182
61	C	21.36022922	-1.83923356	3.91223041
62	H	21.67295795	-2.20183910	2.93188917
63	C	20.59628941	-0.67359428	4.01827947
64	H	20.29384126	-0.13183664	3.12141943
65	C	20.20178850	-0.20484398	5.27247935
66	H	19.60282998	0.70371247	5.35205719
67	C	16.62783693	0.02535633	3.03981065
68	C	16.39560412	-0.45525916	1.73897653
69	H	15.72398872	-1.29971037	1.58013513
70	C	17.01301463	0.15157757	0.64268240
71	H	16.82767241	-0.23103306	-0.36174578
72	C	17.86000248	1.24774872	0.83202239
73	H	18.33949606	1.72090718	-0.02658610
74	C	18.07228835	1.74665519	2.12037463
75	H	18.70572951	2.62122808	2.27601632
76	C	17.45759220	1.14189885	3.21992607
77	H	17.60355982	1.55414252	4.22134611
78	C	16.88934136	-2.31170221	4.80202163
79	C	16.76744331	-2.94521191	6.04822944
80	H	16.17954277	-2.49377943	6.84921645
81	C	17.39943258	-4.16830901	6.27874780
82	H	17.29126414	-4.64328426	7.25440244
83	C	18.16281093	-4.76484275	5.27206557
84	H	18.65443355	-5.72215397	5.45149548
85	C	18.30284509	-4.12802723	4.03577480
86	H	18.90578219	-4.58458426	3.24984845
87	C	17.67234265	-2.90425505	3.79836721
88	H	17.78940863	-2.41731240	2.83046503
89	C	14.30100582	-1.46354295	3.85598986
90	C	14.15947054	-2.80823048	3.47865033
91	H	14.97835144	-3.50971276	3.63364506
92	C	12.96877599	-3.25297676	2.89771325
93	H	12.87098376	-4.29914207	2.60464769

94	C	11.91153383	-2.36445924	2.69430758
95	H	10.98329020	-2.71306633	2.23971235
96	C	12.04049585	-1.02909680	3.08784731
97	H	11.20944501	-0.33587605	2.95608137
98	C	13.22637552	-0.58023467	3.66984645
99	H	13.31732400	0.46008564	3.98844675
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102	H	19.50208627	1.14464374	15.58760635
103	C	18.64503302	2.87143512	16.55196088
104	H	19.33788519	2.82976029	17.39376096
105	C	17.67722072	3.87899994	16.48710208
106	H	17.61441998	4.62670093	17.27917689
107	C	16.80170269	3.93355997	15.39942969
108	H	16.05340639	4.72414074	15.32907644
109	C	16.88460561	2.97771957	14.38355126
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114	C	16.38064545	-2.19368220	15.66229208
115	H	16.21118436	-2.31875295	16.73255111
116	C	16.08580894	-3.23520953	14.77876655
117	H	15.68703210	-4.17690862	15.15905058
118	C	16.29660598	-3.06386300	13.40740158
119	H	16.06256057	-3.86220882	12.70212620
120	C	16.80697651	-1.85996013	12.91908702
121	H	16.94996581	-1.74310170	11.84343773
122	C	19.69775494	0.26761198	13.06069070
123	C	20.21761043	-0.81744365	13.78461243
124	H	19.54630897	-1.50736188	14.29525482
125	C	21.59958618	-1.00881139	13.86269118
126	H	21.99406202	-1.84975155	14.43469080
127	C	22.46960123	-0.12552579	13.21946948
128	H	23.54836559	-0.27133382	13.29143438
129	C	21.95567118	0.93797873	12.47203742
130	H	22.62700509	1.62181313	11.95303783
131	C	20.57593202	1.13070307	12.38773882
132	H	20.17824791	1.95999287	11.80014770
133	C	10.87230087	9.01139045	4.08129858
134	C	9.55293998	9.19957402	3.63021053
135	H	8.96628967	10.04454368	3.99148164
136	C	8.98615270	8.30266974	2.72212455
137	H	7.96441011	8.46100300	2.37399573
138	C	9.72456618	7.20714473	2.26279736
139	H	9.28015990	6.50648033	1.55460147
140	C	11.02975379	7.00570698	2.71941996
141	H	11.60550062	6.14486441	2.37790561
142	C	11.60156169	7.90334759	3.62536399
143	H	12.61346042	7.72757557	3.99808571
144	C	12.19214231	11.62261229	4.17231719
145	C	13.06985736	12.56987313	4.72516958
146	H	13.48603773	12.42808390	5.72448789
147	C	13.42618959	13.70337844	3.99321103
148	H	14.10846505	14.42787120	4.43728971
149	C	12.92694728	13.89310441	2.70159060
150	H	13.21201632	14.77667034	2.12923294
151	C	12.07163124	12.94209860	2.13860529
152	H	11.68627731	13.08139175	1.12769867
153	C	11.70013244	11.81086145	2.86990580
154	H	11.02479340	11.07948293	2.42609722
155	C	10.21622689	10.86303317	6.16220506
156	C	9.60839691	10.02861846	7.11403159
157	H	10.05565328	9.06374012	7.35912243
158	C	8.42187930	10.41900899	7.73537679
159	H	7.95366191	9.75767046	8.46444621
160	C	7.83718198	11.64936149	7.41949053
161	H	6.90547666	11.95078390	7.90019337
162	C	8.45214752	12.49494252	6.49368557
163	H	8.00562295	13.45988613	6.25017323
164	C	9.63927703	12.10727701	5.86602014
165	H	10.10693185	12.76778002	5.13643791
166	C	11.71348612	12.42141170	9.85534728
167	C	12.60570147	13.16612780	9.06817626
168	H	13.62396709	12.81528849	8.88970582
169	C	12.20031997	14.37700745	8.50353367
170	H	12.91167069	14.94257816	7.90037298
171	C	10.90197423	14.84951158	8.71299111
172	H	10.58731612	15.79845301	8.27616014
173	C	10.00299710	14.09849966	9.47577006
174	H	8.98527229	14.45742592	9.63393195
175	C	10.40263887	12.88721417	10.04565101
176	H	9.69449709	12.31187818	10.64179206
177	C	12.99754366	11.65177551	12.31832290
178	C	13.59801324	10.78069352	13.24195953
179	H	13.75925168	9.73280066	12.98208581
180	C	13.98634475	11.24849581	14.49666339
181	H	14.44331867	10.56082938	15.20715787
182	C	13.80229843	12.59331375	14.83414970
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184	C	13.23023045	13.46970597	13.91040038
185	H	13.08879223	14.52096273	14.16508077
186	C	12.82411758	13.00287770	12.65664797
187	H	12.36281573	13.68994383	11.94833192
188	C	10.90115301	9.98227439	11.28421925
189	C	10.50704393	8.85692268	10.54631687
190	H	11.10613363	8.52982885	9.69393228
191	C	9.36732457	8.13643637	10.91237491
192	H	9.07297467	7.26450529	10.32637546
193	C	8.61688347	8.53102698	12.02324312
194	H	7.72604940	7.97045189	12.30958759
195	C	9.01440856	9.64074824	12.77616585
196	H	8.43802433	9.94545874	13.65074595
197	C	10.15255967	10.36392902	12.41224425
198	H	10.46236993	11.22159542	13.01013633
199	C	17.45992585	10.14759275	13.48206597
200	C	16.92702187	8.86226742	13.65512708
201	H	16.77267911	8.21448134	12.78930574
202	C	16.57427502	8.41119870	14.92954002
203	H	16.14302604	7.41630841	15.04397098
204	C	16.76080536	9.23587812	16.04252990
205	H	16.49306268	8.87904137	17.03798007
206	C	17.27192541	10.52635386	15.87353799
207	H	17.40501342	11.18152902	16.73584968
208	C	17.60845699	10.98748025	14.59864377
209	H	17.99211501	12.00031806	14.47536855
210	C	19.88070033	10.25437573	11.92834999
211	C	20.62353609	10.18721929	10.73965223
212	H	20.12340108	10.31632124	9.77847550
213	C	22.00091128	9.96394104	10.78287172
214	H	22.56577347	9.91662366	9.85188321
215	C	22.64907199	9.79862467	12.00946585
216	H	23.72530589	9.62532049	12.04292378
217	C	21.91281931	9.84270152	13.19558137
218	H	22.40978616	9.69886001	14.15574665
219	C	20.53477200	10.06699580	13.15856039
220	H	19.97145945	10.09475941	14.09036114
221	C	17.99025232	12.47999987	11.83172054
222	C	16.83716669	13.09163787	11.31663043
223	H	16.05926831	12.48323944	10.85281169
224	C	16.69289362	14.47890102	11.37549325
225	H	15.79804906	14.94414736	10.96144436
226	C	17.69778628	15.26467971	11.94676442
227	H	17.58393308	16.34869440	11.99323853
228	C	18.85616392	14.66154147	12.44658532
229	H	19.64668582	15.27268140	12.88470850
230	C	19.00807183	13.27415145	12.38541091
231	H	19.92171833	12.81191127	12.76096714
232	S	19.49604435	5.50226676	10.13909834
233	C	19.31284808	5.98810680	11.93411498
234	H	18.24525156	5.95783056	12.17473160
235	H	19.64587391	7.03360559	11.99153844
236	C	20.08970287	5.09787401	12.89899925
237	H	19.79683342	4.04790506	12.73461590
238	C	22.33009235	6.02410908	12.03682737
239	C	21.60538254	5.19893377	12.90698553
240	C	22.32235934	4.44206855	13.85073897
241	C	23.71439122	4.50207120	13.92098282
242	C	24.42647590	5.32355935	13.04014823
243	C	23.72767299	6.08282511	12.10045535
244	H	21.80840927	6.63190237	11.29698093
245	H	21.77628298	3.79846765	14.54394502
246	H	24.24602364	3.90911633	14.66696034
247	H	25.51501211	5.37373663	13.09237871
248	H	24.27033907	6.73317939	11.41222823
249	S	18.48516289	4.71556614	5.10549894

250	C	20.32192423	4.80166186	5.39116006
251	H	20.50778391	5.03144914	6.44592569
252	H	20.65498338	5.65393473	4.78340252
253	C	20.99684351	3.50308823	4.94871246
254	H	20.51561195	3.14742724	4.02335980
255	C	23.10678663	2.59123574	3.91291471
256	C	22.49379785	3.58203602	4.69911328
257	C	23.29996550	4.59704253	5.23037121
258	C	24.67723898	4.61935048	4.98747750
259	C	25.27501597	3.62675551	4.20875342
260	C	24.48114411	2.60890409	3.67018460
261	H	22.49691658	1.78992029	3.49015095
262	H	22.85605935	5.38735865	5.83606928
263	H	25.28489575	5.42389956	5.40436448
264	H	26.34882366	3.64721655	4.01660323
265	H	24.93389233	1.82918002	3.05557869
266	S	13.77319955	4.73914635	4.47249029
267	C	15.01316404	4.61678391	3.08376703
268	H	16.00799061	4.48904340	3.52540633
269	H	14.98357246	5.59396234	2.58368476
270	C	14.70952105	3.47945220	2.10377851
271	H	14.59590103	2.53811287	2.66125556
272	C	13.41153500	4.81925300	0.37243423
273	C	13.52359665	3.67580162	1.18102520
274	C	12.54689991	2.67748649	1.05129147
275	C	11.48745313	2.81401650	0.14870474
276	C	11.38604933	3.95843364	-0.64556777
277	C	12.35385369	4.96121748	-0.52865844
278	H	14.16529457	5.60749155	0.43324540
279	H	12.62869881	1.76989550	1.65248071
280	H	10.74741011	2.01740600	0.05620718
281	H	10.56723307	4.06410908	-1.35856743
282	H	12.29110236	5.85361141	-1.15306935
283	S	11.41551054	5.52548797	8.65991553
284	C	10.71586626	5.42367911	6.93059754
285	H	11.46726606	4.94821424	6.29096521
286	H	10.58176953	6.45715345	6.58727185
287	C	9.38958623	4.65187027	6.87973441
288	H	9.50399236	3.71177475	7.43834984
289	C	7.57784149	5.09930012	8.60717653
290	C	8.17715122	5.40732464	7.37707591
291	C	7.60302599	6.42183405	6.59322830
292	C	6.46449426	7.10584366	7.02496890
293	C	5.87610866	6.78771359	8.25320179
294	C	6.43726182	5.78172714	9.04369311
295	H	8.00214380	4.30339522	9.22199423
296	H	8.04388847	6.66942850	5.62482139
297	H	6.02723526	7.88217970	6.39553725
298	H	4.97942946	7.31261253	8.58494698
299	H	5.97828043	5.51889212	9.99834525
300	S	14.85683922	5.86633869	12.40107033
301	C	13.00379779	6.06801850	12.52746698
302	H	12.56452536	5.71544246	11.58810511
303	H	12.82354099	7.14799323	12.60073718
304	C	12.39793746	5.32230600	13.72108655
305	H	12.72027464	4.27071868	13.70058022
306	C	13.25104395	5.15695618	16.10678587
307	C	12.67510393	5.92309652	15.08346686
308	C	12.30880654	7.24803187	15.37443863
309	C	12.51950189	7.79038311	16.64361825
310	C	13.10021177	7.01538331	17.65325195
311	C	13.46357671	5.69464321	17.38062919
312	H	13.52022398	4.11780971	15.90718175
313	H	11.83451159	7.86131391	14.60512770
314	H	12.21646823	8.81818178	16.84968227
315	H	13.25433264	7.43431859	18.64855127
316	H	13.90430418	5.07620036	18.16426502
317	H	15.61405497	3.35050516	1.48392676
318	H	20.79698076	2.72775516	5.70621560
319	H	19.72667503	5.33634223	13.91381885
320	H	11.30664061	5.30606879	13.55701697
321	H	9.22589086	4.37106551	5.82675539
322	P	11.05481299	-0.07449358	7.65993661
323	P	12.17653756	0.33014175	11.99079108
324	C	9.68192894	0.08194816	8.93367363
325	C	11.71146343	-1.32852150	11.29456723
326	C	10.25364047	0.60519038	6.13057989
327	C	8.69732531	1.07342354	8.64774166
328	H	8.81184812	1.69886108	7.76605395
329	C	7.58325420	1.24475298	9.43307987
330	H	6.84138987	2.00024495	9.16780132
331	C	7.36980751	0.43336256	10.57238406
332	C	6.19451190	0.54609607	11.36177567
333	H	5.43800455	1.27809908	11.07261975
334	C	6.00440930	-0.26055365	12.46334426
335	H	5.09287578	-0.17719967	13.05642831
336	C	6.99552844	-1.20365348	12.82332511
337	H	6.84002579	-1.84407408	13.69269191
338	C	8.15285310	-1.32669148	12.08181909
339	H	8.89970612	-2.06491056	12.36938990
340	C	8.37763548	-0.52467233	10.92686124
341	C	9.55787942	-0.67023977	10.11277639
342	C	11.32829305	-1.86229117	7.29896186
343	C	12.60733650	-0.05073171	13.74333978
344	C	12.68660243	-2.32541514	11.59983188
345	H	13.61818406	-2.03439013	12.08579980
346	C	12.46921059	-3.64888112	11.30938050
347	H	13.22815918	-4.39224104	11.55614345
348	C	11.25626071	-4.06854784	10.70853951
349	C	10.95784673	-5.44275640	10.51203761
350	H	11.69189033	-6.18717054	10.82653411
351	C	9.76002453	-5.83276209	9.95078471
352	H	9.53224279	-6.89158832	9.82131867
353	C	8.82434338	-4.85543761	9.53953370
354	H	7.87848401	-5.16727233	9.09482357
355	C	9.09861479	-3.51130719	9.69173822
356	H	8.36703199	-2.77236828	9.36742405
357	C	10.30866202	-3.07129122	10.29708277
358	C	10.57395460	-1.67795352	10.55780308
359	C	10.73816372	1.46238950	12.22993514
360	C	10.95612827	1.56364512	5.38627453
361	H	11.93381559	1.90680966	5.73692158
362	C	10.41782344	2.09423077	4.20956129
363	H	10.98305849	2.84136887	3.65027875
364	C	9.16645641	1.66931876	3.75982107
365	H	8.74302152	2.08183142	2.84275316
366	C	8.44886819	0.72252765	4.49936921
367	H	7.46197273	0.39864335	4.16523316
368	C	8.98232511	0.20054295	5.67801592
369	H	8.38308225	-0.49621990	6.26309159
370	C	10.38607656	-2.66481204	6.63345386
371	H	9.42402547	-2.26119941	6.32622967
372	C	10.67896167	-3.99685107	6.34281133
373	H	9.94008165	-4.60803985	5.82285163
374	C	11.90712971	-4.54830959	6.71938186
375	H	12.12869766	-5.59234198	6.49314192
376	C	12.84566781	-3.75886614	7.38499916
377	H	13.80730337	-4.16719839	7.69709377
378	C	12.56001576	-2.42230736	7.66751401
379	H	13.30696574	-1.81780734	8.18550012
380	C	13.47150780	0.83743700	14.40081626
381	H	13.96190888	1.62934204	13.83085421
382	C	13.70441152	0.71140477	15.77145957
383	H	14.38071211	1.40684177	16.26980762
384	C	13.08367377	-0.30846762	16.49709069
385	H	13.26231831	-0.40582587	17.56878342
386	C	12.24225028	-1.21314019	15.84357927
387	H	11.76487205	-2.01885783	16.40304632
388	C	12.00260647	-1.08758291	14.47307635
389	H	11.34493637	-1.79887288	13.97358241
390	C	9.87307601	1.33235458	13.33080657
391	H	9.97724559	0.49451020	14.01846338
392	C	8.88905264	2.29193861	13.56915445
393	H	8.22637024	2.18090458	14.42815068
394	C	8.76466533	3.39736554	12.72248663
395	H	8.00558260	4.15442497	12.92376086
396	C	9.62490650	3.53570323	11.63124224
397	H	9.55778588	4.40366248	10.97394154
398	C	10.60631528	2.57340834	11.38470814
399	H	11.29305814	2.70600173	10.54489624
400	P	20.22360469	10.57395623	6.25038601
401	P	17.02801102	9.79765378	3.10238010
402	C	20.38175150	11.52361903	4.62544244
403	C	18.68477280	8.97559866	2.93656748
404	C	20.52717103	11.91453953	7.48991782
405	C	20.71120868	12.90577598	4.75369573

406	H	20.83153985	13.33824339	5.74228927	442	C	20.89941500	14.10885331	9.20178718
407	C	20.89210589	13.72034959	3.66227090	443	H	21.04501920	14.96513493	9.86127021
408	H	21.15190378	14.77076282	3.80610358	444	C	21.99045335	13.32341978	8.82229469
409	C	20.75014670	13.21494715	2.35057426	445	H	22.99126863	13.56100204	9.18564235
410	C	20.94257030	14.03849429	1.20878892	446	C	21.80891003	12.23324942	7.96775344
411	H	21.19792971	15.08897869	1.35930210	447	H	22.67257420	11.64157515	7.66748059
412	C	20.81640056	13.52178101	-0.06229168	448	C	22.97428843	9.95734739	5.85374181
413	H	20.97129475	14.15931846	-0.93371321	449	H	23.02454863	10.84790060	5.22704432
414	C	20.49214989	12.15540985	-0.23598031	450	C	24.14065250	9.24436114	6.14028183
415	H	20.40135195	11.74722953	-1.24355117	451	H	25.09290654	9.57589725	5.72436601
416	C	20.29632201	11.33364609	0.85480146	452	C	24.08894057	8.11788160	6.96603809
417	H	20.05817614	10.28306584	0.69782774	453	H	25.00450481	7.57291096	7.20007958
418	C	20.41231126	11.82988876	2.18502443	454	C	22.86438386	7.69191149	7.48937739
419	C	20.21584300	10.98606048	3.33787188	455	H	22.81418630	6.81065002	8.13046187
420	C	21.74424622	9.54568215	6.39169875	456	C	21.69476630	8.39865821	7.19906774
421	C	16.12479780	9.23944887	1.59322075	457	H	20.73780104	8.06859801	7.61207155
422	C	18.54887671	7.57977727	2.66665590	458	C	14.72212950	9.24746160	1.64085059
423	H	17.55334483	7.13562653	2.65723988	459	H	14.21406815	9.50719872	2.57118806
424	C	19.63562092	6.79082035	2.38959718	460	C	13.97570783	8.93292105	0.50343737
425	H	19.49760466	5.73307863	2.16146816	461	H	12.88654201	8.94284352	0.55515863
426	C	20.94192554	7.34108054	2.37484683	462	C	14.62222184	8.60000978	-0.69015733
427	C	22.07018025	6.56572820	1.99806694	463	H	14.04023939	8.35592296	-1.57999251
428	H	21.92361908	5.51450866	1.74461413	464	C	16.01894236	8.58036450	-0.74261154
429	C	23.32662697	7.12979673	1.93698197	465	H	16.52886598	8.31944636	-1.67098823
430	H	24.18452526	6.52843686	1.63543534	466	C	16.76892161	8.90127992	0.39159585
431	C	23.49870428	8.49428982	2.26174846	467	H	17.85730423	8.88306775	0.33923356
432	H	24.49025704	8.94395039	2.19421918	468	C	17.05454183	12.20024423	1.59226249
433	C	22.42412139	9.26596407	2.65601681	469	H	17.02181501	11.57375728	0.70222226
434	H	22.57568786	10.31856650	2.88605478	470	C	17.04357487	13.58863646	1.45520646
435	C	21.11130750	8.72284198	2.72806224	471	H	17.01192765	14.03048968	0.45842837
436	C	19.96005792	9.53508021	3.05241560	472	C	17.06945645	14.40856218	2.58762726
437	C	17.09560259	11.62016092	2.87281508	473	H	17.05961256	15.49387410	2.47470500
438	C	19.43057428	12.69362665	7.89690657	474	C	17.09073685	13.83631322	3.86136125
439	H	18.42141091	12.46820907	7.54675514	475	H	17.08149625	14.45737903	4.75743372
440	C	19.61947659	13.78863170	8.74128127	476	C	17.09250477	12.44792150	4.00434215
441	H	18.75565093	14.38429160	9.03690069	477	H	17.06554775	12.01373367	5.00500034

B.3. Coordinates of $Au_{11}(PPh_3)_7Br_3$, $[Au_{11}(PPh_3)_8Br_2]^+$ and related structures

$Au_{11}(PPh_3)_7Br_3$ without dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)	31	C	8.87619035	8.47704878	22.37182965
1	Au	7.69976090	6.63013684	16.97304685	32	H	9.16786322	8.05267433	21.40834981
2	Au	7.14397564	8.22718518	19.16381446	33	C	5.15099260	10.07560019	21.45738644
3	Au	9.50547543	8.70294541	16.95221374	34	C	4.73451674	11.30253227	22.00050680
4	Au	9.73366647	6.46114044	18.83505486	35	H	5.42921641	12.14202291	22.04705618
5	Au	7.14999908	5.12982009	19.22979436	36	C	3.42689913	11.45780001	22.46757699
6	Au	4.99985085	6.65801997	17.59198977	37	H	3.11374172	12.41581588	22.88622586
7	Au	6.57845577	9.09639950	16.41607995	38	C	2.52205582	10.39500699	22.39264850
8	Au	9.32262267	6.58543009	14.81965052	39	H	1.50035257	10.52068800	22.75389725
9	Au	9.16996422	4.31345105	16.79674009	40	C	2.92257799	9.17955539	21.83144813
10	Au	6.28155210	4.34369863	16.32187964	41	H	2.21569249	8.35412865	21.74151239
11	Au	6.31941564	6.80092832	14.60160874	42	C	4.22782281	9.02467485	21.36027381
12	Br	11.67540329	6.44357338	20.52045188	43	H	4.53375841	8.09095050	20.88553190
13	Br	5.51107003	11.34200650	15.76123177	44	C	7.44883698	11.48988805	20.49308943
14	Br	5.09637942	2.14598499	15.70714137	45	C	7.01604565	12.03761812	19.27375602
15	P	6.88949429	9.78350785	20.90494093	46	H	6.44163450	11.43875228	18.56293534
16	P	11.09743734	10.42377517	16.99371644	47	C	7.32036817	13.36099165	18.95367279
17	P	6.89861189	3.68769140	21.06517060	48	H	6.97473287	13.76722877	18.00219632
18	P	2.66233096	6.64628333	17.84651473	49	C	8.06459144	14.14599169	19.83973111
19	P	10.72379116	6.51849650	12.94620942	50	H	8.30053672	15.18144366	19.58787006
20	P	10.36767642	2.30142408	16.63608048	51	C	8.51883355	13.59670305	21.04132014
21	P	5.12281484	7.03822150	12.59782412	52	H	9.11366460	14.19840953	21.73038946
22	C	7.77694685	9.34359655	22.46157541	53	C	8.21621279	12.27205618	21.36916010
23	C	7.40104875	9.85029619	23.71785236	54	H	8.57515783	11.85069525	22.30810373
24	H	6.53560110	10.50795524	23.80803891	55	C	12.78800324	9.94473255	16.41373867
25	C	8.12788775	9.50543810	24.85947255	56	C	13.82515590	9.67078034	17.31945283
26	H	7.82847502	9.90428482	25.83040924	57	H	13.65237492	9.75492986	18.39181414
27	C	9.23035894	8.64967326	24.76007066	58	C	15.08883963	9.29742721	16.85383377
28	H	9.79233295	8.37717166	25.65503121	59	H	15.88509670	9.09350147	17.57134859
29	C	9.60079911	8.13414360	23.51595432	60	C	15.33376011	9.19556340	15.48261738
30	H	10.44893624	7.45489203	23.41623636	61	H	16.32362905	8.91327463	15.12023186

62	C	14.30026881	9.45094724	14.57636336
63	H	14.47558310	9.36537831	13.50358022
64	C	13.03331116	9.81384779	15.03546814
65	H	12.23713406	10.00837981	14.31575613
66	C	10.67579873	11.87476619	15.93930868
67	C	11.65061891	12.76997895	15.46161298
68	H	12.70514339	12.59963814	15.68156465
69	C	11.27341778	13.87130057	14.69056348
70	H	12.03712059	14.55902009	14.32259515
71	C	9.92440376	14.09008457	14.38808411
72	H	9.63394407	14.95088107	13.78301295
73	C	8.95326363	13.20168676	14.85605141
74	H	7.89666207	13.34614586	14.62482174
75	C	9.32710795	12.09702322	15.62590642
76	H	8.55715642	11.40278869	15.97149460
77	C	11.43703858	11.11451966	18.67056732
78	C	11.76859332	12.46322261	18.87503906
79	H	11.74380828	13.16705214	18.04322085
80	C	12.12975612	12.91057079	20.14758845
81	H	12.38578452	13.96108841	20.29584698
82	C	12.16623401	12.01915505	21.22402374
83	H	12.45591058	12.37082461	22.21595702
84	C	11.82125949	10.67976226	21.02800048
85	H	11.83794211	9.97280295	21.85814726
86	C	11.44897430	10.22816643	19.75914957
87	H	11.19037294	9.17538591	19.62181878
88	C	8.37279890	2.63983812	21.41966928
89	C	9.62361021	3.27849010	21.46720379
90	H	9.72084113	4.33892120	21.22302485
91	C	10.76391434	2.55944368	21.82634239
92	H	11.72497346	3.07425258	21.85689513
93	C	10.67059184	1.19803764	22.13174044
94	H	11.56356450	0.63735376	22.41289838
95	C	9.43265862	0.55424748	22.06208325
96	H	9.35472878	-0.51111592	22.28427650
97	C	8.28549146	1.26890747	21.70452556
98	H	7.32401107	0.75833953	21.65149193
99	C	5.48581842	2.50835004	20.93327300
100	C	4.89136221	1.91053985	22.05839094
101	H	5.24266678	2.15664339	23.06117959
102	C	3.83970815	1.00572726	21.89843263
103	H	3.38438266	0.54656750	22.77806788
104	C	3.36788534	0.69406622	20.61871471
105	H	2.54131412	-0.00835594	20.49812246
106	C	3.94837611	1.29280194	19.49791134
107	H	3.58835649	1.07376931	18.49148645
108	C	5.00085302	2.19806936	19.65405004
109	H	5.43392879	2.67105769	18.76933385
110	C	6.62480394	4.52278316	22.68986467
111	C	7.03906753	3.94944275	23.90378320
112	H	7.59773864	3.01300051	23.90162508
113	C	6.75078818	4.58238602	25.11531372
114	H	7.07869396	4.12893611	26.05224076
115	C	6.05353815	5.79388822	25.12800573
116	H	5.83262747	6.28788235	26.07543397
117	C	5.66004179	6.38201399	23.92301387
118	H	5.14104293	7.34099101	23.92149672
119	C	5.95261685	5.75328267	22.71125089
120	H	5.68337865	6.22840392	21.76639997
121	C	1.73617903	5.94163344	16.41765827
122	C	0.56616775	6.52187993	15.90473725
123	H	0.20965897	7.47421422	16.29707777
124	C	-0.14881543	5.87654497	14.89150404
125	H	-1.05987213	6.33324931	14.50135718
126	C	0.30044400	4.65644969	14.38001771
127	H	-0.26195433	4.15413625	13.59094125
128	C	1.47897650	4.08802949	14.87268144
129	H	1.85406837	3.14507548	14.47266741
130	C	2.19822541	4.72729082	15.88313322
131	H	3.12032639	4.26930022	16.24890572
132	C	1.91718721	8.30854370	18.13746496
133	C	2.63503475	9.43733430	17.71558678
134	H	3.62108032	9.32481139	17.25854619
135	C	2.10383344	10.71765890	17.88990098
136	H	2.68590741	11.57802951	17.55637749
137	C	0.85340851	10.88101651	18.49057377
138	H	0.44060695	11.88113709	18.63302571
139	C	0.13539864	9.76032249	18.92238298
140	H	-0.83894049	9.88355388	19.39890486
141	C	0.66377329	8.47892427	18.75095575
142	H	0.10285923	7.61244454	19.10332291
143	C	2.02741936	5.62859672	19.25233181
144	C	2.81178689	5.52038226	20.40952283
145	H	3.80584221	5.97045891	20.42180759
146	C	2.34604889	4.81678841	21.52153391
147	H	2.97222715	4.73816307	22.41082692
148	C	1.09408061	4.19722652	21.48114198
149	H	0.73292557	3.63780663	22.34526082
150	C	0.31661297	4.27626568	20.32238187
151	H	-0.65310490	3.77747991	20.27830367
152	C	0.77878168	4.98625860	19.21119516
153	H	0.17258538	5.02933541	18.30596134
154	C	11.07713549	8.16957158	12.20473661
155	C	12.26302271	8.45644115	11.50819565
156	H	13.03642928	7.69381797	11.40739896
157	C	12.46580340	9.72555168	10.95932443
158	H	13.39047985	9.94039370	10.42036209
159	C	11.49403294	10.71981045	11.11045119
160	H	11.65996254	11.71342503	10.69163681
161	C	10.31699602	10.44307954	11.81112682
162	H	9.56178804	11.21716119	11.94715897
163	C	10.10841287	9.17493528	12.35800816
164	H	9.19702559	8.96572184	12.92191457
165	C	12.39066184	5.79989465	13.27433065
166	C	12.92007356	5.94847564	14.56686085
167	H	12.33063030	6.44654169	15.33903420
168	C	14.18605075	5.44358267	14.87149803
169	H	14.58038696	5.55840968	15.88112342
170	C	14.93284059	4.78374151	13.89168018
171	H	15.91824274	4.38242993	14.13280984
172	C	14.40825076	4.62404398	12.60525729
173	H	14.98475710	4.10071909	11.84027473
174	C	13.14090498	5.12567128	12.29638184
175	H	12.72910408	4.97777419	11.29724552
176	C	10.05273771	5.51671786	11.54984990
177	C	10.37102000	5.76823482	10.20491988
178	H	11.02109775	6.60434559	9.94350435
179	C	9.83970283	4.96205679	9.19467030
180	H	10.09138071	5.16434600	8.15202110
181	C	8.98052433	3.90671281	9.51675063
182	H	8.55775234	3.28568748	8.72564792
183	C	8.65195795	3.65842763	10.85200624
184	H	7.96971500	2.84822852	11.11001166
185	C	9.18337941	4.45930812	11.86515524
186	H	8.90974468	4.27619115	12.90611158
187	C	12.09738428	2.41522284	17.26294014
188	C	13.11218264	1.52525929	16.86632072
189	H	12.90320663	0.74913858	16.12930355
190	C	14.39568533	1.64195884	17.40483375
191	H	15.17779678	0.94809523	17.09094882
192	C	14.67935685	2.64491365	18.33911798
193	H	15.68481046	2.73424923	18.75490873
194	C	13.67638805	3.53437196	18.73190826
195	H	13.87450175	4.33106618	19.45074437
196	C	12.39213640	3.42176073	18.19406192
197	H	11.62226679	4.13498403	18.49840746
198	C	10.56705387	1.60544635	14.93325077
199	C	11.48595441	2.20059695	14.05123750
200	H	12.08222244	3.05488996	14.37456594
201	C	11.65593829	1.69196429	12.76285087
202	H	12.38156101	2.15803570	12.09587823
203	C	10.90077678	0.59797546	12.32951753
204	H	11.03728818	0.20237754	11.32192251
205	C	9.96821864	0.01845279	13.19250434
206	H	9.36854892	-0.83170497	12.86362895
207	C	9.80117484	0.51639576	14.48770893
208	H	9.07693232	0.04777090	15.15284695
209	C	9.60818919	0.88980480	17.54971040
210	C	10.38136216	-0.10551406	18.16809132
211	H	11.46677980	-0.01412182	18.20395993
212	C	9.76237986	-1.21887372	18.74048260
213	H	10.37237760	-1.98759783	19.21787453
214	C	8.37095877	-1.34942238	18.70053669
215	H	7.89088684	-2.22516014	19.14147710
216	C	7.59687628	-0.35205830	18.10270030
217	H	6.51006635	-0.43518177	18.06966319

218	C	8.20944943	0.76912891	17.53657135	236	C	4.24179249	2.99597522	10.47992061
219	H	7.58909547	1.53517519	17.06501688	237	H	4.02380030	2.04083645	9.99830640
220	C	3.46603388	7.82577737	12.79317307	238	C	4.25249732	4.17365871	9.72353648
221	C	3.34106047	8.88789919	13.70322996	239	H	4.04316544	4.13962790	8.65281994
222	H	4.18590573	9.18892371	14.32753137	240	C	4.53210724	5.39818463	10.33408610
223	C	2.13718114	9.59038502	13.80001575	241	H	4.54866510	6.30984684	9.73613172
224	H	2.06391244	10.42151177	14.50222796	242	C	5.92479378	8.09969732	11.31274065
225	C	1.04590673	9.22828013	13.00647661	243	C	7.00507835	7.58730515	10.57284320
226	H	0.10619636	9.77802178	13.08340070	244	H	7.35170233	6.56707243	10.74276585
227	C	1.15771841	8.15335018	12.11991332	245	C	7.63094430	8.37314763	9.60416571
228	H	0.30496426	7.85601093	11.50724820	246	H	8.45990743	7.95660057	9.03124618
229	C	2.36157829	7.45404234	12.01038646	247	C	7.20317980	9.68413342	9.37325505
230	H	2.43767045	6.61771050	11.31581288	248	H	7.69533720	10.29602223	8.61584956
231	C	4.80326317	5.45339985	11.71329803	249	C	6.14634432	10.20646328	10.12184291
232	C	4.79946076	4.26771647	12.46243634	250	H	5.80725421	11.22999873	9.95485889
233	H	5.02700118	4.28789349	13.53093187	251	C	5.50807909	9.42068938	11.08535840
234	C	4.51742415	3.04465632	11.84848963	252	H	4.67967107	9.83921309	11.65566905
235	H	4.52547169	2.13863893	12.45636302					

$Au_{11}(PPh_3)_7Br_3$ optimized with dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)	55	C	12.66478335	9.82511046	16.69802482
1	Au	7.76529163	6.64374574	16.87011118	56	C	13.79272243	10.19740999	17.44205345
2	Au	6.82920792	8.32400024	18.75897251	57	H	13.69007134	10.87646619	18.28902822
3	Au	9.44002305	8.74505189	16.82321982	58	C	15.04636464	9.67383946	17.11267303
4	Au	10.12757767	6.55573828	18.48853253	59	H	15.91974172	9.95550974	17.70271951
5	Au	7.52665381	5.56826441	19.33060369	60	C	15.18004773	8.78363834	16.04345029
6	Au	5.23652886	6.16004377	17.65750644	61	H	16.15928612	8.37048409	15.79686562
7	Au	6.77568284	9.15534938	15.97666526	62	C	14.05415991	8.40634645	15.30369499
8	Au	9.29968135	6.55867155	14.77633798	63	H	14.14258487	7.69631243	14.48078980
9	Au	9.25245333	4.40023578	16.89616488	64	C	12.80138892	8.91731335	15.63519412
10	Au	6.59051186	4.22981427	15.92125790	65	H	11.91689593	8.59897002	15.08270103
11	Au	6.32225215	6.71596687	14.59762488	66	C	10.67812402	11.84150344	15.96028172
12	Br	12.04675107	6.67485402	20.16531212	67	C	11.71804596	12.60153910	15.40456216
13	Br	5.59335105	11.32466222	15.34775580	68	H	12.75593919	12.35413716	15.63377521
14	Br	5.56796557	1.96006353	15.36719201	69	C	11.41983899	13.65535209	14.53614088
15	P	6.68680922	9.76717455	20.51636214	70	H	12.22955235	14.24392368	14.10157311
16	P	10.97075114	10.41971977	17.07833075	71	C	10.08932145	13.94693031	14.21304496
17	P	7.21097170	4.09224206	21.03870665	72	H	9.86350439	14.76161313	13.52306476
18	P	2.96543223	6.24880728	17.83639638	73	C	9.05187811	13.18314681	14.75972920
19	P	10.64775739	6.49894916	12.95112516	74	H	8.00863716	13.37276394	14.50109149
20	P	10.27242654	2.35601389	16.86296394	75	C	9.34539903	12.13476374	15.63109829
21	P	4.99358917	7.04715821	12.76844102	76	H	8.52982939	11.52802907	16.02966032
22	C	7.66853160	9.17502936	21.95020100	77	C	11.09816532	11.11520883	18.76902669
23	C	7.41070527	9.59396840	23.26488213	78	C	11.51073336	12.43555619	19.00645041
24	H	6.61126162	10.30927571	23.46460425	79	H	11.66257710	13.11937011	18.17027898
25	C	8.15610002	9.06789099	24.32230406	80	C	11.72996048	12.86926663	20.31575193
26	H	7.94548373	9.38829432	25.34387213	81	H	12.05377228	13.89527393	20.49733355
27	C	9.15460777	8.11825438	24.07762396	82	C	11.52923202	11.99533183	21.38906247
28	H	9.72272062	7.69944868	24.90943928	83	H	11.70233082	12.33831211	22.41034561
29	C	9.41778488	7.70112386	22.77020602	84	C	11.09028473	10.68950372	21.15556155
30	H	10.20155402	6.97428662	22.55094623	85	H	10.91364172	10.00256996	21.98358584
31	C	8.67718453	8.22792953	21.71282682	86	C	10.87220800	10.24958027	19.84988649
32	H	8.88354748	7.88418492	20.69733534	87	H	10.55370161	9.22225448	19.66927835
33	C	4.97993490	9.95442507	21.15828787	88	C	8.70233732	3.09629307	21.39055166
34	C	4.51744526	11.13245346	21.76154946	89	C	9.93261967	3.76727424	21.28387939
35	H	5.17571501	12.00007640	21.83522183	90	H	9.96890092	4.82122103	21.00048045
36	C	3.20739179	11.19755574	22.24499057	91	C	11.12635171	3.08181034	21.49780558
37	H	2.84682865	12.11831787	22.70652615	92	H	12.06799719	3.62129932	21.38748985
38	C	2.35841245	10.09197322	22.13125851	93	C	11.10034942	1.72028142	21.81606582
39	H	1.33481620	10.15152813	22.50400874	94	H	12.03430914	1.17619068	21.96566603
40	C	2.81211027	8.92052932	21.51637833	95	C	9.87800844	1.04937906	21.91628548
41	H	2.15103596	8.06235723	21.39206477	96	H	9.85663992	-0.01792888	22.13772745
42	C	4.11230576	8.85826011	21.01989321	97	C	8.67704634	1.72961843	21.69881023
43	H	4.45130287	7.96945535	20.48481454	98	H	7.72976703	1.19143601	21.73629963
44	C	7.26985642	11.44908556	20.10123388	99	C	5.82859759	2.94017369	20.66914422
45	C	6.98453011	11.90674308	18.80389293	100	C	5.15604297	2.21967133	21.66877168
46	H	6.43988573	11.27645359	18.09795798	101	H	5.45847401	2.31716062	22.71262167
47	C	7.42646880	13.16235025	18.39115239	102	C	4.07372024	1.40392774	21.33106697
48	H	7.20837328	13.48839809	17.37346103	103	H	3.54766516	0.85336582	22.11268011
49	C	8.15953528	13.96678272	19.26910828	104	C	3.64928251	1.30879003	20.00063101
50	H	8.52417244	14.94182548	18.94189542	105	H	2.79244468	0.68349891	19.74569060
51	C	8.44879850	13.51138633	20.55879331	106	C	4.31716819	2.02126698	19.00153508
52	H	9.04262051	14.12612515	21.23596985	107	H	4.01957322	1.94879352	17.95409306
53	C	8.01137152	12.25257602	20.97810824	108	C	5.40173731	2.83104616	19.33640815
54	H	8.27350242	11.88557108	21.97075484	109	H	5.91028978	3.39021763	18.54841756

110	C	6.73598124	4.88850955	22.62002643
111	C	7.01351252	4.32438760	23.87335250
112	H	7.58307045	3.39539971	23.93702067
113	C	6.57550470	4.96547582	25.03568317
114	H	6.79635781	4.52815339	26.01071017
115	C	5.86285613	6.16632053	24.95240599
116	H	5.52696044	6.66404093	25.86314344
117	C	5.60379078	6.74211321	23.70460863
118	H	5.07635156	7.69336261	23.62595975
119	C	6.05071766	6.11188987	22.54522427
120	H	5.90041612	6.58244132	21.57184656
121	C	2.13222998	5.53119247	16.37779099
122	C	1.02968666	6.11477250	15.73959694
123	H	0.60565961	7.04604433	16.11533760
124	C	0.50369912	5.51987324	14.58961666
125	H	-0.34016016	5.98808133	14.08243141
126	C	1.07429178	4.35368466	14.07196473
127	H	0.67273769	3.90866848	13.16023461
128	C	2.17734092	3.77338176	14.70645835
129	H	2.65640574	2.87848125	14.30708846
130	C	2.70700087	4.36101792	15.85265502
131	H	3.59481170	3.92275627	16.31330829
132	C	2.37062847	7.97346318	18.03623493
133	C	3.24272877	9.02087649	17.70009783
134	H	4.23372157	8.80556294	17.29539842
135	C	2.86235515	10.34885808	17.89254019
136	H	3.56023818	11.13996289	17.61313346
137	C	1.60261945	10.63975335	18.42234965
138	H	1.30538623	11.67644460	18.58663888
139	C	0.72322483	9.60132924	18.75114908
140	H	-0.25820659	9.82834907	19.17045858
141	C	1.10446532	8.27102792	18.56442997
142	H	0.42832815	7.46395352	18.85193554
143	C	2.31988346	5.35154748	19.29824064
144	C	3.15094275	5.28641565	20.42861019
145	H	4.15672077	5.70743782	20.37971342
146	C	2.71691874	4.64871733	21.58832982
147	H	3.38020750	4.60278848	22.45271272
148	C	1.45546005	4.04530856	21.61800543
149	H	1.11921364	3.52880736	22.51807032
150	C	0.63482753	4.08063857	20.48589535
151	H	-0.34060718	3.59172824	20.50322015
152	C	1.06224100	4.73262461	19.32534878
153	H	0.43035882	4.74678064	18.43558447
154	C	11.28150610	8.16393454	12.53117564
155	C	12.56212301	8.37538419	12.00006226
156	H	13.20169418	7.52278388	11.76468154
157	C	13.03085024	9.67897180	11.81336750
158	H	14.03465823	9.84162945	11.41858406
159	C	12.22558475	10.76952830	12.15543014
160	H	12.60143444	11.78621623	12.03475330
161	C	10.94519569	10.56264680	12.67854244
162	H	10.32525273	11.41055632	12.96978001
163	C	10.47330199	9.26572249	12.87156790
164	H	9.49373579	9.10642996	13.32868263
165	C	12.09754288	5.41806160	13.22584052
166	C	12.55708484	5.28567602	14.55012351
167	H	12.07961686	5.84986448	15.35504740
168	C	13.58730457	4.39513758	14.84505548
169	H	13.92163587	4.28060349	15.87601527
170	C	14.15568342	3.62318821	13.82689742
171	H	14.93983510	2.90440372	14.06825488
172	C	13.70437269	3.75267352	12.51004510
173	H	14.14005019	3.14057546	11.71914275
174	C	12.67550461	4.64874780	12.20608929
175	H	12.30020056	4.72851600	11.18439291
176	C	9.76679348	5.87064766	11.47562449
177	C	10.03173647	6.33780250	10.18005480
178	H	10.83409070	7.05873617	10.01457203
179	C	9.23902122	5.91105981	9.11106372
180	H	9.43387123	6.29167907	8.10749019
181	C	8.18533241	5.01920880	9.33170139
182	H	7.55025777	4.70623092	8.50202054
183	C	7.92418515	4.54372261	10.62060132
184	H	7.09002516	3.86562843	10.79943494
185	C	8.70549811	4.97120869	11.69227551
186	H	8.46384519	4.64107320	12.70567998
187	C	12.04616024	2.41608911	17.32388766
188	C	13.00934930	1.56746806	16.75733565
189	H	12.71430110	0.82834063	16.01081050
190	C	14.35063503	1.69284717	17.12898437
191	H	15.09854384	1.03512828	16.68297384
192	C	14.73701984	2.67001407	18.05437420
193	H	15.78826593	2.77594399	18.32707490
194	C	13.77815811	3.52108159	18.61487951
195	H	14.05672458	4.30968245	19.31619648
196	C	12.43737423	3.39228413	18.25331252
197	H	11.70246195	4.07861634	18.67809189
198	C	10.23458878	1.61778876	15.18349296
199	C	10.30113231	2.49542744	14.08983941
200	H	10.34262476	3.57144592	14.26576635
201	C	10.29287991	1.99783808	12.78835812
202	H	10.33991862	2.69214751	11.94882210
203	C	10.20113597	0.61985866	12.56803343
204	H	10.17889919	0.22957977	11.54917940
205	C	10.11652074	-0.25713221	13.65366946
206	H	10.02575989	-1.33109170	13.48367806
207	C	10.13344597	0.23721612	14.96074041
208	H	10.04896744	-0.44762501	15.80553745
209	C	9.51481599	1.08661648	17.94569289
210	C	10.26885522	0.07230536	18.55488095
211	H	11.35562163	0.06866656	18.46236350
212	C	9.62384188	-0.93073400	19.28191540
213	H	10.21304108	-1.71929421	19.75256380
214	C	8.23224763	-0.91718872	19.41684462
215	H	7.73252716	-1.69896053	19.99137548
216	C	7.48248658	0.10704208	18.83163157
217	H	6.39853695	0.13894585	18.94481194
218	C	8.11943738	1.10663479	18.09633701
219	H	7.52878318	1.88948552	17.61816845
220	C	3.32343849	7.71477378	13.11894458
221	C	3.17691314	8.57481340	14.21791994
222	H	4.02604005	8.77671789	14.87270500
223	C	1.95187051	9.19758912	14.45823336
224	H	1.85339911	9.86212273	15.31690327
225	C	0.86959584	8.96669784	13.60487672
226	H	-0.08701103	9.45743129	13.79200833
227	C	1.00690898	8.09500784	12.51988152
228	H	0.15868218	7.90090840	11.86133543
229	C	2.22823916	7.46246270	12.27849529
230	H	2.33090506	6.77347880	11.43915299
231	C	4.73586502	5.52714567	11.77529911
232	C	4.72692224	4.30296556	12.46125687
233	H	4.87286517	4.27370468	13.54274035
234	C	4.56987855	3.10616771	11.76259263
235	H	4.59602913	2.16818258	12.31974593
236	C	4.41654907	3.12547872	10.37186789
237	H	4.30415566	2.19012161	9.82090310
238	C	4.42771200	4.34449705	9.68301530
239	H	4.32044045	4.36000262	8.59707306
240	C	4.59288095	5.54488128	10.37934459
241	H	4.63324527	6.49193151	9.83893232
242	C	5.74320141	8.25738604	11.60972764
243	C	7.14044140	8.23170245	11.47297382
244	H	7.72478956	7.52118191	12.05913402
245	C	7.77931118	9.11991758	10.61048629
246	H	8.86561252	9.09109993	10.52071437
247	C	7.02906112	10.05498619	9.88978951
248	H	7.52876123	10.76216484	9.22609240
249	C	5.63919543	10.09529802	10.03501993
250	H	5.05311400	10.83534757	9.48791637
251	C	4.99332018	9.19984224	10.89239266
252	H	3.91099547	9.24760880	11.01690594

$[Au_{11}(PPh_3)_8Br_2]^+$ without dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	2.67977478	5.59487799	21.73463429
2	Au	1.20651643	3.63658355	20.27412427
3	Au	1.77216379	3.40613941	23.19444563
4	Au	-0.10959955	5.39701978	22.31611596
5	Au	0.93564837	6.72180897	19.91525147
6	Au	3.47463387	5.29804188	19.09565935
7	Au	4.09735147	3.24940414	21.40625455
8	Au	3.11543367	5.75402433	24.43163511
9	Au	1.47921726	7.87481608	22.73753559
10	Au	3.69117635	7.94631576	20.67692521
11	Au	5.34964483	5.91825090	22.13232173
12	Br	0.79869575	1.42188669	24.45869834
13	Br	-0.66895973	7.78285934	18.22544988
14	P	-0.13405270	2.11992132	19.03487603
15	P	-2.32225014	5.25036180	23.09071373
16	P	4.08141445	5.13995589	16.80326060
17	P	5.13252735	1.13059152	21.60910283
18	P	3.53341499	5.75440342	26.76628322
19	P	0.50257477	9.91749678	23.45096945
20	P	4.51306092	10.01886915	19.86393475
21	P	7.67103683	6.25971166	22.41844990
22	C	0.59211438	1.61050147	17.41803290
23	C	-0.16130611	1.54882689	16.23595484
24	H	-1.20434971	1.86540362	16.23540508
25	C	0.42087204	1.07772744	15.05573881
26	H	-0.17272078	1.03452566	14.14154392
27	C	1.75492918	0.66499952	15.04791907
28	H	2.20703199	0.29625767	14.12597684
29	C	2.51128364	0.73221762	16.22227860
30	H	3.55606898	0.42133739	16.22124544
31	C	1.93727970	1.20801178	17.40113177
32	H	2.53426435	1.26144448	18.31349431
33	C	-0.51797106	0.49075767	19.81100229
34	C	-0.86706550	-0.62546177	19.02851553
35	H	-0.84437307	-0.56148335	17.94012636
36	C	-1.23814326	-1.82384726	19.64121297
37	H	-1.51908053	-2.68028554	19.02606113
38	C	-1.24124615	-1.92781801	21.03694478
39	H	-1.52543017	-2.86749549	21.51364748
40	C	-0.86182769	-0.83148699	21.81497492
41	H	-0.82418251	-0.90151802	22.90314115
42	C	-0.50765886	0.37580759	21.20612386
43	H	-0.20517892	1.21644450	21.83254906
44	C	-1.78211921	2.81264097	18.58120789
45	C	-1.87721351	4.19084130	18.33467103
46	H	-1.02020126	4.84727967	18.50103025
47	C	-3.07633783	4.74732304	17.88414265
48	H	-3.11962741	5.82187764	17.70083503
49	C	-4.19445508	3.93373559	17.68367730
50	H	-5.13131628	4.36712583	17.32974996
51	C	-4.11431348	2.56463853	17.95388830
52	H	-4.98792945	1.92567148	17.81537475
53	C	-2.91707075	2.00388833	18.40481034
54	H	-2.87067471	0.93676355	18.61993602
55	C	-3.36438362	6.67331144	22.55813855
56	C	-3.06552954	7.26960413	21.32296622
57	H	-2.19106082	6.95107677	20.75149363
58	C	-3.88370336	8.27991503	20.81200408
59	H	-3.63235230	8.72789533	19.84985116
60	C	-5.00075627	8.70867821	21.53262703
61	H	-5.64043233	9.49776337	21.13401339
62	C	-5.29179054	8.13177349	22.77287470
63	H	-6.15655059	8.47040520	23.34534081
64	C	-4.47929931	7.11904408	23.28638376
65	H	-4.71462220	6.68184565	24.25629961
66	C	-2.42824171	5.14274424	24.92947630
67	C	-3.60389776	4.71568136	25.57225263
68	H	-4.47183365	5.41653563	24.98373838
69	C	-3.65585692	4.63744725	26.96496329
70	H	-4.57198962	4.30232895	27.45338100
71	C	-2.53235160	4.96898264	27.72928788
72	H	-2.57164427	4.89498294	28.81717991
73	C	-1.35383364	5.37092769	27.09621090
74	H	-0.46758328	5.60914828	27.68598515
75	C	-1.30080737	5.45421029	25.70213684
76	H	-0.37243007	5.73982785	25.20280522
77	C	-3.31337561	3.77727656	22.58934489
78	C	-4.47360898	3.88795264	21.80911722
79	H	-4.78723938	4.85875035	21.42674986
80	C	-5.24478816	2.75408531	21.53636731
81	H	-6.15130251	2.85175455	20.93736608
82	C	-4.86420344	1.50793774	22.03737966
83	H	-5.47461387	0.62641748	21.83464146
84	C	-3.69521413	1.39195624	22.79669750
85	H	-3.38692661	0.42011219	23.18275588
86	C	-2.91543747	2.51635651	23.06808609
87	H	-2.00504034	2.41135355	23.66405307
88	C	2.65683435	5.24991068	15.63898572
89	C	2.83822332	5.60408874	14.28830148
90	H	3.83408185	5.83601616	13.90975915
91	C	1.74018783	5.69202006	13.43263398
92	H	1.89041043	5.96863989	12.38797273
93	C	0.45121257	5.44687456	13.91824785
94	H	-0.40807606	5.53309068	13.25144259
95	C	0.26459721	5.11259236	15.25994199
96	H	-0.73844602	4.94845209	15.65303877
97	C	1.36245755	5.01202149	16.11788584
98	H	1.21343233	4.77491107	17.17227972
99	C	4.99297147	3.59487615	16.36479999
100	C	4.98489823	3.05613057	15.06812949
101	H	4.34658710	3.49119017	14.29944728
102	C	5.79189673	1.95976556	14.75633717
103	H	5.78040803	1.55135535	13.74448162
104	C	6.61499898	1.39031164	15.73312241
105	H	7.25291587	0.54110048	15.48306863
106	C	6.61206299	1.90830084	17.03091004
107	H	7.24650244	1.46946482	17.80199646
108	C	5.79628556	2.99853415	17.34839968
109	H	5.77383934	3.38863476	18.36877031
110	C	5.18287488	6.45436985	16.10869255
111	C	6.42549504	6.18073334	15.51715976
112	H	6.80851097	5.16041134	15.49455220
113	C	7.16048070	7.20655438	14.91282996
114	H	8.11927856	6.97804290	14.44454055
115	C	6.66025781	8.50973486	14.88864221
116	H	7.22891745	9.30552354	14.40579736
117	C	5.42780099	8.79046920	15.48702710
118	H	5.02925586	9.80538367	15.47972550
119	C	4.69662277	7.77327181	16.09996504
120	H	3.73062185	8.00324375	16.55169010
121	C	4.34707463	-0.22189306	20.64242952
122	C	4.92356518	-0.71199132	19.45937551
123	H	5.87457570	-0.31272114	19.10864614
124	C	4.29167745	-1.72543200	18.73475743
125	H	4.75418554	-2.10535942	17.82253873
126	C	3.07945842	-2.25550878	19.18191714
127	H	2.58869871	-3.05037063	18.61873536
128	C	2.49274330	-1.75839840	20.34924734
129	H	1.53957884	-2.15688705	20.69638259
130	C	3.11396598	-0.74111173	21.07492978
131	H	2.64164493	-0.35837324	21.98196386
132	C	5.10337724	0.51082094	23.34711720
133	C	5.04781873	1.44479985	24.39180407
134	H	4.90218630	2.50217930	24.16143872
135	C	5.14269307	1.02409403	25.72054543
136	H	5.08355488	1.75639929	26.52635518
137	C	5.28004282	-0.33340415	26.01684857
138	H	5.34780011	-0.66150402	27.05493331
139	C	5.30405085	-1.27354615	24.98217838
140	H	5.38582350	-2.33749641	25.20944465
141	C	5.21337112	-0.85645471	23.65336626
142	H	5.20907169	-1.60049840	22.85616482
143	C	6.92504060	1.00739289	21.16883368
144	C	7.63424469	-0.20101161	21.29685021
145	H	7.12699674	-1.10324362	21.63694220
146	C	8.99328374	-0.25647356	20.98934368
147	H	9.53225910	-1.19977648	21.09047811
148	C	9.66385592	0.89363866	20.55746741
149	H	10.72868148	0.84876920	20.32410143
150	C	8.96901330	2.09726680	20.43249534
151	H	9.48451648	2.99908480	20.10279641

152	C	7.60416188	2.15206789	20.73495166
153	H	7.05763604	3.09301488	20.64560019
154	C	2.38770569	6.79077184	27.77644840
155	C	1.93558077	8.00687014	27.24376649
156	H	2.20437193	8.28273206	26.22220084
157	C	1.15142331	8.86766380	28.01647147
158	H	0.81703608	9.81441515	27.59261933
159	C	0.79535405	8.51241060	29.31965562
160	H	0.18023722	9.18386473	29.92078944
161	C	1.22363767	7.29137934	29.84894782
162	H	0.94309768	7.00489469	30.86401650
163	C	2.01915123	6.43409326	29.08498220
164	H	2.35459211	5.48786687	29.50916394
165	C	5.19511553	6.36668145	27.28950069
166	C	5.36191788	7.46973850	28.14090791
167	H	4.49377736	8.02809297	28.48922287
168	C	6.64056399	7.84495789	28.56618377
169	H	6.75501406	8.69739761	29.23786729
170	C	7.76085740	7.11884784	28.15587453
171	H	8.75538395	7.40082243	28.50482773
172	C	7.60212914	6.02645466	27.29629200
173	H	8.46945398	5.45586669	26.96446438
174	C	6.32986897	5.66093664	26.85411663
175	H	6.21985293	4.80851488	26.18188783
176	C	3.42414534	4.11276057	27.59851505
177	C	2.40381596	3.23925235	27.19443357
178	H	1.77464441	3.47658041	26.33477367
179	C	2.19736352	2.03570129	27.87198251
180	H	1.40920269	1.36727330	27.52457030
181	C	3.01149048	1.69012859	28.95295036
182	H	2.84964289	0.74892763	29.48099782
183	C	4.04472027	2.54627486	29.34860683
184	H	4.68955704	2.27815967	30.18711310
185	C	4.25189427	3.75495720	28.67861840
186	H	5.05354543	4.41885084	29.00166574
187	C	1.52197793	10.84763737	24.68099637
188	C	0.95344523	11.80157004	25.54482106
189	H	-0.11771708	12.00393398	25.50505325
190	C	1.75049870	12.47814435	26.47078432
191	H	1.29912183	13.21685558	27.13479922
192	C	3.11806301	12.19778775	26.55593887
193	H	3.73629598	12.71552608	27.29081803
194	C	3.68630550	11.24666746	25.70582384
195	H	4.74985281	11.01662910	25.77332529
196	C	2.89540565	10.57768799	24.76800628
197	H	3.33890890	9.82852632	24.10867617
198	C	0.18429496	11.10313408	22.07776311
199	C	-0.24776698	10.57729007	20.85063503
200	H	-0.29545739	9.49784344	20.69232303
201	C	-0.61882532	11.43250854	19.81083003
202	H	-0.94853522	10.99872009	18.86631792
203	C	-0.55805119	12.81734494	19.98467140
204	H	-0.85067930	13.48487394	19.17267174
205	C	-0.11233858	13.34666622	21.19999704
206	H	-0.05867646	14.42769127	21.33999364
207	C	0.26031575	12.49568779	22.24373510
208	H	0.60951060	12.91912137	23.18540510
209	C	-1.13179689	9.84287713	24.31087633
210	C	-2.18369866	10.72293150	24.01004561
211	H	-2.09163398	11.42487835	23.18195827
212	C	-3.35092737	10.71046562	24.77885002
213	H	-4.15892888	11.40332218	24.53949281
214	C	-3.48227979	9.82043594	25.84704433
215	H	-4.39208320	9.81760049	26.44883180
216	C	-2.45011214	8.92214130	26.13205933
217	H	-2.55130990	8.20464137	26.94703003
218	C	-1.28464143	8.92937424	25.36483406
219	H	-0.48579884	8.22368311	25.59365250
220	C	4.50409227	11.42036590	21.06295757
221	C	3.63535774	12.51216083	20.92986533
222	H	2.89759405	12.53145718	20.12794108
223	C	3.72586055	13.59366232	21.81215280
224	H	3.05221292	14.44254367	21.68966536
225	C	4.67725611	13.59387607	22.83281190
226	H	4.75474909	14.44537010	23.51019436
227	C	5.52809927	12.49395593	22.98563864
228	H	6.27256993	12.48214308	23.78280569
229	C	5.43711266	11.40818470	22.11603952
230	H	6.11685895	10.56307756	22.23800351
231	C	3.59056057	10.66090895	18.39714302
232	C	4.05548818	11.75873416	17.64925044
233	H	4.98055728	12.26392207	17.92646417
234	C	3.34048975	12.20405395	16.53690847
235	H	3.70793539	13.05772283	15.96517188
236	C	2.16172126	11.55365328	16.15084765
237	H	1.61117108	11.89813344	15.27407624
238	C	1.69662223	10.46385987	16.88795518
239	H	0.78274406	9.93811901	16.60742942
240	C	2.40557617	10.02213032	18.00968257
241	H	2.02721549	9.16861792	18.57671526
242	C	6.27378081	10.05146729	19.29379205
243	C	7.02498105	11.24092604	19.28087267
244	H	6.60515694	12.15880210	19.69256006
245	C	8.31861054	11.25479744	18.75659609
246	H	8.88726822	12.18599933	18.74668207
247	C	8.88108009	10.07994652	18.24822816
248	H	9.89184746	10.09057064	17.83694292
249	C	8.14703644	8.89239118	18.27385028
250	H	8.58248949	7.97031905	17.89012819
251	C	6.85030736	8.87605279	18.79515380
252	H	6.27879622	7.94706529	18.81321793
253	C	8.65109644	5.96378379	20.87567247
254	C	10.05487720	6.04490195	20.85835950
255	H	10.60134399	6.32407918	21.75888324
256	C	10.76488538	5.75926285	19.69156202
257	H	11.85377435	5.82732499	19.69114041
258	C	10.08349837	5.37454951	18.53145842
259	H	10.64106640	5.13779967	17.62395125
260	C	8.68982044	5.28846070	18.54168276
261	H	8.15124604	4.98564029	17.64397356
262	C	7.97583725	5.58812681	19.70647165
263	H	6.88445984	5.52442443	19.71813351
264	C	8.52459369	5.15311232	23.62829978
265	C	7.97405356	3.88634644	23.87083361
266	H	7.02053478	3.61895244	23.41181280
267	C	8.63710825	2.97070310	24.69244389
268	H	8.19461074	1.99023222	24.87145589
269	C	9.85726961	3.31459096	25.27962898
270	H	10.37793767	2.59909688	25.91761674
271	C	10.40588855	4.58210232	25.05526957
272	H	11.35331354	4.85903731	25.52041590
273	C	9.74177246	5.50069828	24.23924279
274	H	10.16618789	6.49418360	24.09101647
275	C	8.16415628	7.94534842	22.97662626
276	C	7.86548770	8.31675488	24.30035907
277	H	7.36414408	7.61439988	24.96775731
278	C	8.23254567	9.57519831	24.77784002
279	H	8.01731431	9.83886326	25.81433889
280	C	8.88344941	10.48543901	23.93763324
281	H	9.18152778	11.46462539	24.31573338
282	C	9.14996272	10.13497526	22.61234619
283	H	9.64440260	10.84221312	21.94582686
284	C	8.79209202	8.87180062	22.13004132
285	H	9.00897204	8.61268602	21.09401803

$[Au_{11}(PPh_3)_8Br_2]^+$ optimized with dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	2.56898746	5.48935619	21.59336591
2	Au	1.56992930	3.24659721	20.29290826
3	Au	1.92583346	3.28433072	23.23850269
4	Au	-0.06298534	4.87532429	22.00067010
5	Au	1.08033870	6.74661529	19.58805337
6	Au	3.51481717	5.12812708	19.09136456
7	Au	4.31957235	3.42845289	21.34489974
8	Au	2.91590501	5.83665554	24.22466121
9	Au	0.97722121	7.51557012	22.45536993
10	Au	3.47763895	7.94588452	20.86510687
11	Au	5.13504656	6.08591018	22.26469401

12	Br	1.33728174	1.12047172	24.38761345
13	Br	-0.39519999	7.77738955	17.80683864
14	P	0.09700850	1.93797596	19.11744043
15	P	-2.21247074	5.05172664	22.75572730
16	P	4.04493593	5.03509986	16.85777607
17	P	5.31064855	1.41139306	21.82992425
18	P	3.35981354	6.00231582	26.48358266
19	P	0.33625456	9.57881017	23.23727690
20	P	4.38625473	9.94863154	20.20657342
21	P	7.43275506	6.34210083	22.25027594
22	C	0.75260472	1.49889437	17.46826904
23	C	-0.04933893	1.46886474	16.31970641
24	H	-1.11628996	1.68363256	16.39530415
25	C	0.52972354	1.20689807	15.07533217
26	H	-0.09092302	1.20727469	14.17883108
27	C	1.90289023	0.96686487	14.97836743
28	H	2.35497570	0.77836618	14.00376361
29	C	2.70223946	0.98199974	16.12626681
30	H	3.77463762	0.80244852	16.05349577
31	C	2.13368500	1.25598405	17.36828734
32	H	2.76239188	1.30172621	18.26070579
33	C	-0.38677948	0.36580479	19.91001530
34	C	-0.81672255	-0.74449677	19.16610359
35	H	-0.83772969	-0.69794939	18.07609399
36	C	-1.19371012	-1.91585900	19.82709119
37	H	-1.52369397	-2.78054997	19.24979620
38	C	-1.13338539	-1.98573385	21.22457331
39	H	-1.41506439	-2.90787644	21.73465526
40	C	-0.69139510	-0.88333611	21.96315801
41	H	-0.60236742	-0.92706735	23.04935371
42	C	-0.32124355	0.29066645	21.30694626
43	H	0.06178215	1.13051376	21.88903779
44	C	-1.48994872	2.81739102	18.84714770
45	C	-1.46795839	4.21131731	18.68134551
46	H	-0.52704583	4.76324106	18.72330187
47	C	-2.65329419	4.91742973	18.47971760
48	H	-2.60334231	5.99852175	18.34799725
49	C	-3.87377099	4.23857227	18.45451480
50	H	-4.80363808	4.79155967	18.31448428
51	C	-3.90425041	2.85217684	18.62717640
52	H	-4.85566693	2.32072417	18.63134125
53	C	-2.72005663	2.14084204	18.82663345
54	H	-2.75905502	1.06437101	18.99041608
55	C	-2.95046146	6.65589942	22.26522838
56	C	-2.44677959	7.26681040	21.10479375
57	H	-1.66120308	6.78260852	20.52363726
58	C	-2.92465252	8.51134137	20.69730681
59	H	-2.50789105	8.96421960	19.79648164
60	C	-3.90501441	9.16111161	21.45174763
61	H	-4.26583079	10.14490516	21.14817536
62	C	-4.41447769	8.55683379	22.60543937
63	H	-5.16538152	9.06972508	23.20654169
64	C	-3.94109735	7.30827862	23.01393341
65	H	-4.31829060	6.86204939	23.93401694
66	C	-2.22913665	4.99066843	24.59680542
67	C	-3.40486062	4.70381921	25.30863517
68	H	-4.32485799	4.47034764	24.76986620
69	C	-3.39307173	4.69021016	26.70549010
70	H	-4.30956971	4.46251909	27.25176069
71	C	-2.20873701	4.95649335	27.40099006
72	H	-2.20153880	4.94497911	28.49170742
73	C	-1.02970263	5.21817754	26.69733048
74	H	-0.10046579	5.41345554	27.23332506
75	C	-1.03562500	5.22387018	25.30198990
76	H	-0.10563426	5.40468135	24.75492458
77	C	-3.37576909	3.72663463	22.27577542
78	C	-4.70521741	3.96091366	21.90139721
79	H	-5.08081288	4.98270644	21.83114936
80	C	-5.54308087	2.87948347	21.61300264
81	H	-6.57919144	3.06116430	21.32381315
82	C	-5.05473283	1.57178618	21.68469807
83	H	-5.71192160	0.73209862	21.45400867
84	C	-3.72006452	1.33946728	22.03480712
85	H	-3.32146606	0.32442328	22.06572727
86	C	-2.88191303	2.41271782	22.33056237
87	H	-1.84015626	2.23787061	22.60720979
88	C	2.55588293	5.06453444	15.79210279
89	C	2.61148494	5.51134489	14.46064279
90	H	3.55456526	5.86155534	14.03767311
91	C	1.44803874	5.54809187	13.69214843
92	H	1.49286734	5.89817603	12.65982731
93	C	0.22409644	5.16289582	14.25210705
94	H	-0.68692278	5.21466001	13.65476455
95	C	0.16498049	4.73757118	15.57974955
96	H	-0.78724817	4.46671713	16.03500529
97	C	1.32771064	4.68305391	16.34669580
98	H	1.28237653	4.36610773	17.38874114
99	C	5.01253648	3.54457464	16.39710404
100	C	5.24942309	3.19046609	15.05927250
101	H	4.82303365	3.78723439	14.25256238
102	C	6.01985823	2.06589757	14.75917693
103	H	6.20081771	1.79502454	13.71815755
104	C	6.55626795	1.28594498	15.79062762
105	H	7.16099637	0.41002242	15.55193905
106	C	6.30636776	1.62343833	17.12332664
107	H	6.71088926	1.01783010	17.93297778
108	C	5.52938692	2.74260540	17.42711947
109	H	5.31171987	2.99479256	18.46913749
110	C	4.99573408	6.48550313	16.26313876
111	C	6.23268503	6.41608548	15.60901530
112	H	6.69950310	5.44988558	15.41600721
113	C	6.86231461	7.59130682	15.18495632
114	H	7.82576102	7.53311462	14.67638911
115	C	6.26179727	8.83231786	15.40710322
116	H	6.75950543	9.74573673	15.08058410
117	C	5.02993601	8.90510716	16.06609415
118	H	4.56316951	9.87103756	16.25905815
119	C	4.40299577	7.73960415	16.50018727
120	H	3.44613205	7.79410590	17.02353751
121	C	4.57381069	0.08466420	20.81689104
122	C	5.31549673	-0.57610969	19.82757314
123	H	6.38118292	-0.37071280	19.72139305
124	C	4.69351906	-1.50745536	18.99252955
125	H	5.27279417	-2.01132856	18.21763490
126	C	3.33983370	-1.80415262	19.16615117
127	H	2.85383699	-2.53858432	18.52317542
128	C	2.60555397	-1.16303078	20.16968085
129	H	1.55736405	-1.41251788	20.31782059
130	C	3.20507656	-0.20014856	20.98073350
131	H	2.62173515	0.31095542	21.75189235
132	C	5.04048927	0.93305741	23.57214097
133	C	4.96507634	1.94387179	24.54430911
134	H	4.96416001	2.99361612	24.24240980
135	C	4.83698147	1.60748759	25.88992639
136	H	4.77096172	2.39205647	26.64140263
137	C	4.74641669	0.26693915	26.27064812
138	H	4.61683540	0.01375256	27.32324731
139	C	4.78383229	-0.74139676	25.30388729
140	H	4.68383848	-1.78725100	25.59654537
141	C	4.93548786	-0.41191653	23.95563069
142	H	4.94942332	-1.19722423	23.19824283
143	C	7.12184035	1.30133310	21.57548660
144	C	7.92245207	0.36316665	22.24486869
145	H	7.46740562	-0.36285597	22.91953132
146	C	9.30739022	0.38203787	22.06956435
147	H	9.92915454	-0.34141549	22.59860841
148	C	9.89939763	1.33382810	21.23150105
149	H	10.98369876	1.35528197	21.11433443
150	C	9.10369980	2.26134975	20.55402993
151	H	9.55330863	3.01617960	19.90906252
152	C	7.71942277	2.24229332	20.72660574
153	H	7.09664497	2.98500949	20.22864915
154	C	2.32056380	7.13055091	27.48777738
155	C	1.32504315	7.88158004	26.85442257
156	H	1.21789317	7.81941957	25.77084638
157	C	0.48015353	8.69989425	27.60756950
158	H	-0.29369351	9.27801787	27.10590238
159	C	0.62492941	8.76860207	28.99319057
160	H	-0.03926757	9.40530389	29.57967848
161	C	1.61694557	8.01574501	29.63334089
162	H	1.72680017	8.06176801	30.71769466
163	C	2.45963625	7.19467881	28.88587543
164	H	3.21756180	6.59373074	29.38915207
165	C	5.09794221	6.48279173	26.80313498
166	C	5.45683700	7.68483671	27.42863672
167	H	4.68243513	8.38374817	27.74552172

168	C	6.80507625	7.97749797	27.65755752	227	C	5.51239923	12.05217613	23.53489712
169	H	7.07776196	8.91064739	28.15305010	228	H	6.31430836	11.99415678	24.27080490
170	C	7.79753097	7.07111181	27.27449897	229	C	5.48598037	11.14008830	22.48248449
171	H	8.84778910	7.29691492	27.46182358	230	H	6.26097392	10.37714079	22.40382226
172	C	7.44284602	5.87931455	26.63247683	231	C	3.51715373	10.74551196	18.79762653
173	H	8.21130657	5.17629964	26.31455665	232	C	3.92586530	11.99293599	18.29432674
174	C	6.10291676	5.59469828	26.37806718	233	H	4.71427353	12.55663757	18.79360667
175	H	5.83611306	4.67162802	25.86031175	234	C	3.32555888	12.51133637	17.14747493
176	C	3.17917205	4.41426004	27.38573005	235	H	3.64634718	13.47919461	16.75932232
177	C	2.14780206	3.55245347	26.98796822	236	C	2.32421602	11.78579814	16.48742392
178	H	1.54750560	3.77912263	26.10547523	237	H	1.87151291	12.18651933	15.57918459
179	C	1.90990611	2.37065948	27.69069091	238	C	1.90541246	10.55545132	16.99508450
180	H	1.12699071	1.69861898	27.34064186	239	H	1.11828582	9.97653105	16.50995885
181	C	2.70313479	2.04090719	28.79149753	240	C	2.49181724	10.04465610	18.15494834
182	H	2.52212105	1.11262566	29.33564356	241	H	2.14236848	9.09080381	18.55423732
183	C	3.74608647	2.88859566	29.18366149	242	C	6.11266811	9.82587124	19.58687374
184	H	4.37845485	2.62367450	30.03225938	243	C	6.96597967	10.94198022	19.56122654
185	C	3.98661693	4.07366495	28.48555674	244	H	6.65902300	11.87579819	20.03252978
186	H	4.81296614	4.72067755	28.78214776	245	C	8.21598610	10.85460742	18.94899583
187	C	1.61634912	10.18758586	24.41819709	246	H	8.87154715	11.72651644	18.93148195
188	C	1.31587833	11.07582583	25.46153739	247	C	8.62418679	9.65266431	18.35987222
189	H	0.30962516	11.48627336	25.55974742	248	H	9.59853118	9.58471774	17.87399716
190	C	2.28680266	11.38978755	26.41659715	249	C	7.78777847	8.53667807	18.40405665
191	H	2.03879568	12.06577324	27.23580239	250	H	8.10193305	7.59797803	17.95375046
192	C	3.55575207	10.81037133	26.34486380	251	C	6.53793004	8.61696069	19.02125723
193	H	4.30197560	11.03709998	27.10782454	252	H	5.88466854	7.74309523	19.05089259
194	C	3.86624492	9.94050496	25.29659646	253	C	8.19813518	5.95916648	20.61929885
195	H	4.85505197	9.48624791	25.22465434	254	C	9.57997967	6.09655376	20.40836901
196	C	2.90731190	9.63715030	24.33361425	255	H	10.21834218	6.48797730	21.20079755
197	H	3.15577437	8.93879399	23.53238679	256	C	10.14527664	5.72687313	19.18729633
198	C	0.17688675	10.84775334	21.93027285	257	H	11.21791610	5.84596735	19.02903032
199	C	-0.02342697	10.41707997	20.61186522	258	C	9.34064071	5.18625971	18.17751537
200	H	-0.03439801	9.35240579	20.37193416	259	H	9.78468219	4.88245870	17.22875351
201	C	-0.19675553	11.35054965	19.58943895	260	C	7.96854183	5.03263650	18.38940558
202	H	-0.34598752	10.99168926	18.57163633	261	H	7.33757234	4.60301241	17.61393828
203	C	-0.16002232	12.71722805	19.87506603	262	C	7.39584788	5.42696476	19.60015734
204	H	-0.28333683	13.44608523	19.07316308	263	H	6.31945454	5.31151719	19.75617292
205	C	0.04571184	13.15236536	21.19040150	264	C	8.34905983	5.20434835	23.36207568
206	H	0.08522278	14.21963680	21.41369794	265	C	7.75989375	3.96269775	23.63435123
207	C	0.21626781	12.22237699	22.21702214	266	H	6.77194451	3.74274267	23.22842010
208	H	0.41346712	12.56386434	23.23390312	267	C	8.42627377	3.01986856	24.41603581
209	C	-1.22793866	9.64879435	24.19626807	268	H	7.94679304	2.06327429	24.62400919
210	C	-2.07289862	10.76810422	24.25308148	269	C	9.69555480	3.31202254	24.92436559
211	H	-1.86473384	11.64700760	23.64263335	270	H	10.22144774	2.57729329	25.53517295
212	C	-3.19310953	10.75143613	25.08769889	271	C	10.28728625	4.55346778	24.66041227
213	H	-3.84570654	11.62460244	25.12884012	272	H	11.27208462	4.78608376	25.06795373
214	C	-3.48323819	9.62313658	25.86331030	273	C	9.61553539	5.50306162	23.88678224
215	H	-4.35920384	9.61951922	26.51319981	274	H	10.06570019	6.48075296	23.70844789
216	C	-2.66276141	8.49558979	25.78364717	275	C	7.98837964	8.01011662	22.75664541
217	H	-2.88521937	7.59460545	26.35712218	276	C	7.64574410	8.39494850	24.06673400
218	C	-1.54974005	8.50922047	24.94416822	277	H	7.08427982	7.71092202	24.70481278
219	H	-0.92410596	7.62183109	24.86701120	278	C	8.03404019	9.64064030	24.55377368
220	C	4.45994863	11.20726057	21.52547977	279	H	7.78005655	9.91545631	25.57843076
221	C	3.44814732	12.16779487	21.65267905	280	C	8.73743328	10.52877207	23.73039959
222	H	2.64150159	12.21456356	20.92123612	281	H	9.03744158	11.50663132	24.10922995
223	C	3.47310909	13.06531291	22.72212929	282	C	9.03188235	10.16872132	22.41357963
224	H	2.67913589	13.80625618	22.81773732	283	H	9.54632592	10.86745185	21.75378910
225	C	4.50644345	13.01568813	23.65961256	284	C	8.66231419	8.91196878	21.92353586
226	H	4.52151360	13.71686514	24.49460738	285	H	8.88632920	8.64934457	20.89055098

Lowest energy isomer of Br-for-2PET replacement on $Au_{11}(PPh_3)_7Br_3$ (pos#10), optimized with dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)	13	Br	5.28421379	10.83958233	14.93161459
1	Au	7.73308235	6.49735287	16.97514585	14	P	6.19525138	9.38864636	20.51170065
2	Au	6.31027958	7.77358291	18.89029295	15	P	10.60932608	10.51027448	17.03446696
3	Au	9.11368500	8.79513335	16.94143906	16	P	7.27698292	3.59882890	20.90909472
4	Au	9.98473933	6.69427146	18.65103017	17	P	2.94930729	5.83934649	17.57529005
5	Au	7.26257593	5.12586940	19.22194753	18	P	10.84828980	6.59853119	13.20919000
6	Au	5.17501839	5.69982891	17.09744967	19	P	10.75419726	2.54438786	16.85611013
7	Au	6.60390052	8.80536395	15.76788847	20	P	5.52844349	6.40060407	12.51448191
8	Au	9.48508446	6.52823613	15.01951330	21	C	7.31432423	8.98569822	21.91129783
9	Au	9.49565816	4.43981151	17.04845383	22	C	7.10832183	9.50947059	23.19838134
10	Au	6.96813454	3.78900801	15.88449688	23	H	6.26529398	10.17608752	23.38758101
11	Au	6.66551800	6.24167549	14.49244285	24	C	7.97026383	9.15898005	24.23998550
12	Br	11.92994669	6.80652723	20.32064191	25	H	7.80221906	9.56366684	25.23934678

26	C	9.03694233	8.28386587	24.00619348
27	H	9.70066159	8.00298394	24.82527721
28	C	9.24854142	7.76451533	22.72626802
29	H	10.08394970	7.09496808	22.51652984
30	C	8.39011844	8.11361320	21.68410244
31	H	8.55650807	7.68827935	20.68989421
32	C	4.58956872	9.69435656	21.33980490
33	C	4.08996635	10.97933722	21.59043561
34	H	4.64859486	11.85268526	21.25121819
35	C	2.87990750	11.13523389	22.27390137
36	H	2.49284659	12.13733183	22.46456762
37	C	2.17156374	10.01474474	22.71660296
38	H	1.22984375	10.14054108	23.25326302
39	C	2.66114433	8.73035782	22.45293568
40	H	2.10003933	7.85052235	22.76988656
41	C	3.85657751	8.57091833	21.75532564
42	H	4.21812984	7.56963957	21.51622568
43	C	6.75784670	10.99878262	19.85121735
44	C	6.39135225	11.31039047	18.53193098
45	H	5.79946493	10.60941082	17.94159113
46	C	6.81248111	12.50452743	17.95038708
47	H	6.51825247	12.71578525	16.92202486
48	C	7.62554616	13.38304171	18.67198664
49	H	7.98629558	14.29979353	18.20332396
50	C	7.99854982	13.07415760	19.98329607
51	H	8.65732738	13.74204166	20.53809758
52	C	7.56554971	11.88645442	20.57717711
53	H	7.88546009	11.63689853	21.58879396
54	C	12.25706702	9.83306329	16.59797503
55	C	12.93652694	9.08205381	17.57247426
56	H	12.53855282	8.98652161	18.58316435
57	C	14.11289235	8.41058972	17.24260875
58	H	14.61123390	7.81337901	18.00727857
59	C	14.62769246	8.48762565	15.94460710
60	H	15.54340872	7.95611173	15.68384911
61	C	13.94064972	9.21384467	14.96883544
62	H	14.31469083	9.25266244	13.94555928
63	C	12.75054275	9.87244418	15.28419676
64	H	12.20738313	10.40469451	14.50348680
65	C	10.26973147	11.89782160	15.88925865
66	C	11.25565051	12.79313728	15.44145825
67	H	12.29166418	12.66905834	15.75965200
68	C	10.91315491	13.82579860	14.56564716
69	H	11.68400267	14.51335746	14.21333596
70	C	9.58773459	13.97874542	14.14016864
71	H	9.32661333	14.78840822	13.45645040
72	C	8.60514442	13.08686058	14.58046164
73	H	7.56946896	13.17152212	14.24613409
74	C	8.94790151	12.04429870	15.44205145
75	H	8.18231033	11.32909705	15.74846447
76	C	10.81888467	11.21827908	18.71772101
77	C	11.30842983	12.51423189	18.94057712
78	H	11.52501236	13.17260565	18.09878554
79	C	11.50637288	12.96920325	20.24563287
80	H	11.88470716	13.97882788	20.41381016
81	C	11.22214375	12.13578985	21.33397452
82	H	11.38315675	12.49506496	22.35154518
83	C	10.72422361	10.84939937	21.11587617
84	H	10.48587665	10.19056919	21.95183199
85	C	10.51282051	10.39601566	19.81323975
86	H	10.11695507	9.39224348	19.64999821
87	C	8.90850929	2.79970390	21.12293923
88	C	10.02681357	3.64463665	21.03039031
89	H	9.90373266	4.71049351	20.82850351
90	C	11.31065384	3.12259941	21.17147570
91	H	12.16202578	3.79902045	21.09172094
92	C	11.48820265	1.75217509	21.38582549
93	H	12.49455035	1.33977568	21.47239648
94	C	10.37760876	0.90781706	21.46889042
95	H	10.51295729	-0.16463721	21.60999572
96	C	9.08656143	1.42703518	21.34085942
97	H	8.22588510	0.75996182	21.37856690
98	C	6.05401312	2.25714824	20.64985118
99	C	5.60459499	1.42576356	21.68716935
100	H	5.96468814	1.57822458	22.70554082
101	C	4.68083985	0.41314230	21.42035388
102	H	4.33209699	-0.22846805	22.23117778
103	C	4.19941428	0.22620575	20.11967884
104	H	3.47493852	-0.56310625	19.91428297
105	C	4.64203646	1.05605872	19.08672660
106	H	4.28974429	0.91468698	18.06610267
107	C	5.55893841	2.07339788	19.34817340
108	H	5.89030869	2.71936301	18.53082269
109	C	6.92271320	4.35134712	22.54625500
110	C	7.34743253	3.76642079	23.74905117
111	H	7.91899663	2.83680493	23.72921355
112	C	7.07166148	4.39475255	24.96582388
113	H	7.40948052	3.94018268	25.89844971
114	C	6.38166819	5.61174361	24.98871225
115	H	6.18072709	6.10609919	25.94025859
116	C	5.97574949	6.20877812	23.79216342
117	H	5.47477381	7.17704261	23.79791809
118	C	6.25416846	5.58626280	22.57629519
119	H	5.99414323	6.07479462	21.63423105
120	C	1.75017535	5.37739150	16.27845662
121	C	0.37789202	5.65180381	16.37957369
122	H	-0.01052406	6.18348642	17.24959486
123	C	-0.48420931	5.25173708	15.35795513
124	H	-1.55179022	5.46297941	15.43554274
125	C	0.01788259	4.58028323	14.23831313
126	H	-0.65967655	4.26172986	13.44562727
127	C	1.38537540	4.32401063	14.12690946
128	H	1.78248138	3.81528159	13.24915589
129	C	2.25122636	4.72957125	15.14044852
130	H	3.32662523	4.56810420	15.05140795
131	C	2.52263347	7.54562501	18.09907870
132	C	3.20905134	8.61451115	17.49871218
133	H	3.98953326	8.42650557	16.75977735
134	C	2.92618274	9.92998872	17.86237946
135	H	3.47390321	10.73777542	17.37396363
136	C	1.96166365	10.18783622	18.84081715
137	H	1.75512130	11.21334243	19.14883418
138	C	1.27568222	9.12902660	19.44332810
139	H	0.53943526	9.33005481	20.22156810
140	C	1.55466975	7.80940930	19.07895905
141	H	1.04200057	6.98359672	19.57586821
142	C	2.58764943	4.79069298	19.03120237
143	C	3.43466223	4.93232804	20.14626337
144	H	4.23385976	5.67757586	20.12032838
145	C	3.29145064	4.08898332	21.24501079
146	H	3.96514177	4.19421376	22.09574984
147	C	2.31733746	3.08359804	21.23471161
148	H	2.22999237	2.40336038	22.08215412
149	C	1.47898038	2.93606656	20.12732925
150	H	0.72693123	2.14502253	20.11067344
151	C	1.60761741	3.79011731	19.02784911
152	H	0.96329840	3.66802406	18.15764633
153	C	11.10365598	8.31188923	12.61135368
154	C	12.28359628	8.72776035	11.97665783
155	H	13.09000951	8.01324876	11.80373656
156	C	12.44407990	10.06637448	11.60941074
157	H	13.36975632	10.38976198	11.13077882
158	C	11.42943476	10.99255017	11.87645626
159	H	11.56346381	12.04266944	11.61360300
160	C	10.24914493	10.57745746	12.49891570
161	H	9.46144426	11.29563972	12.72092522
162	C	10.08251606	9.24326600	12.86881949
163	H	9.16755733	8.93246142	13.37981083
164	C	12.50102646	5.87901389	13.55051341
165	C	12.92566423	5.85834617	14.88970210
166	H	12.30681172	6.30972052	15.66885329
167	C	14.12206054	5.22981833	15.23345451
168	H	14.42645802	5.19582681	16.27859356
169	C	14.90235457	4.61850083	14.24933300
170	H	15.82285083	4.10434540	14.52851348
171	C	14.49185457	4.64857796	12.91168656
172	H	15.09576029	4.16561251	12.14190066
173	C	13.29287675	5.27413429	12.56176912
174	H	12.95428054	5.25755550	11.52460770
175	C	10.17469580	5.65223185	11.78936201
176	C	10.53240160	5.93750253	10.46191608
177	H	11.21189385	6.76384778	10.24668418
178	C	9.99046883	5.18893719	9.41510773
179	H	10.26504863	5.41935573	8.38439824
180	C	9.07949316	4.16136140	9.68783543
181	H	8.63751454	3.58931836	8.87105245

182	C	8.71632468	3.88156790	11.00687877
183	H	7.99636139	3.09418180	11.22395868
184	C	9.25962741	4.62106239	12.05808565
185	H	8.96217658	4.40204232	13.08678783
186	C	12.51136323	2.75970027	17.32830694
187	C	13.55357740	1.95919151	16.83204216
188	H	13.34218810	1.17809194	16.10053181
189	C	14.86539593	2.18205817	17.25722763
190	H	15.67305031	1.56201411	16.86492086
191	C	15.14482868	3.19796531	18.17983559
192	H	16.17204163	3.36781710	18.50679942
193	C	14.11021528	4.00170584	18.66806861
194	H	14.30228765	4.81379640	19.37152781
195	C	12.80055791	3.78795727	18.23742862
196	H	12.00608916	4.44008456	18.60407412
197	C	10.73098692	2.01236985	15.10002238
198	C	11.66384556	2.51732207	14.17896965
199	H	12.48628442	3.14738457	14.51553814
200	C	11.53550520	2.21703669	12.82245701
201	H	12.26234967	2.62131575	12.11775725
202	C	10.46895670	1.43621845	12.36923590
203	H	10.36237814	1.22414969	11.30502182
204	C	9.52098365	0.96064835	13.27938296
205	H	8.66463830	0.37807592	12.93825150
206	C	9.65047589	1.24273634	14.63934385
207	H	8.89927083	0.86969606	15.33565284
208	C	10.11863709	1.08287185	17.76838619
209	C	10.94454425	0.00491311	18.12264364
210	H	12.02092313	0.06107586	17.95861723
211	C	10.38731311	-1.14177421	18.68993495
212	H	11.03325384	-1.97662845	18.96675989
213	C	9.00576412	-1.22321577	18.89855881
214	H	8.57265622	-2.12680312	19.33097026
215	C	8.18472820	-0.14494507	18.56454954
216	H	7.10872734	-0.18857716	18.73296525
217	C	8.73988826	1.01333496	18.01730758
218	H	8.09324195	1.85417145	17.75934526
219	C	3.78262853	6.92158377	12.74185634
220	C	3.44121691	7.61973897	13.90886636
221	H	4.20924914	7.83427582	14.65264395
222	C	2.12810304	8.04062105	14.12044831
223	H	1.88111232	8.57699165	15.03684703
224	C	1.14422782	7.75326137	13.17372556
225	H	0.11252654	8.06075292	13.34773697
226	C	1.47784399	7.05334954	12.00856868
227	H	0.70717498	6.82045720	11.27224807
228	C	2.79150488	6.63903753	11.78843216
229	H	3.04098009	6.08161752	10.88489577
230	C	5.44046050	4.84297852	11.55588679
231	C	5.48156148	3.65446519	12.30157172
232	H	5.64046190	3.69161106	13.38191668
233	C	5.39039832	2.41567990	11.66783835
234	H	5.44954774	1.51219970	12.27828225
235	C	5.27420593	2.35557463	10.27511686
236	H	5.21770680	1.38969541	9.77017205
237	C	5.24724284	3.53720463	9.52378857
238	H	5.16704249	3.49069746	8.43645137
239	C	5.32357196	4.77995350	10.15847514
240	H	5.30953056	5.69734889	9.56865906
241	C	6.31476468	7.69025617	11.48586345
242	C	7.37040485	7.38445681	10.61219021
243	H	7.63813195	6.34768872	10.41235635
244	C	8.09878037	8.41415640	10.01482764
245	H	8.92163404	8.16513080	9.34415066
246	C	7.79908028	9.74877569	10.30088610
247	H	8.39058146	10.54797809	9.85295583
248	C	6.76367834	10.05340825	11.19002450
249	H	6.53892825	11.08839533	11.45102529
250	C	6.01966688	9.03215910	11.78000036
251	H	5.24163894	9.28741122	12.50045613
252	C	2.07134625	0.86923714	15.31620251
253	C	1.42396581	1.30636580	16.48342297
254	C	0.05680283	1.58415426	16.48230982
255	C	-0.69135899	1.43318661	15.31059470
256	C	-0.05879293	1.00499915	14.14154801
257	C	1.31177722	0.72984385	14.14648131
258	C	3.55967032	0.61328066	15.32071279
259	H	2.00124532	1.43813626	17.40154999
260	H	-0.43165504	1.91980382	17.39870626
261	H	-1.75943843	1.65442524	15.30910662
262	H	-0.63279219	0.88938103	13.22034526
263	H	1.80304593	0.40030492	13.22836233
264	C	4.34843630	1.92973700	15.37883632
265	S	6.17079546	1.61407727	15.41164943
266	H	4.05740560	2.51255284	16.26500124
267	H	4.09359233	2.53523159	14.49693700
268	H	3.83795927	-0.01534287	16.18168351
269	H	3.85430503	0.05354819	14.42040906

Lowest energy isomer of Br-for-PPh_3 replacement on $Au_{11}(PPh_3)_7Br_3$ (pos#4), optimized with dispersion correction

Index	Symbol	x (angstrom)	y (angstrom)	z (angstrom)
1	Au	7.93946090	6.63585005	17.28949118
2	Au	7.09465476	8.15785987	19.36841558
3	Au	9.91974255	8.52513791	17.02443157
4	Au	10.08381889	6.22948970	18.87369783
5	Au	7.39946526	5.31493450	19.60833496
6	Au	5.30429516	6.30912612	17.82150999
7	Au	7.10774263	9.17535529	16.55999618
8	Au	9.23890586	6.55653819	14.99378846
9	Au	9.37517818	4.36780850	16.86107713
10	Au	6.60229010	4.28050582	16.21602242
11	Au	6.35413900	6.83287505	15.06332132
12	Br	5.93431120	11.36907269	16.04764675
13	Br	5.57328172	2.05626374	15.56264874
14	P	6.56021575	9.58587507	21.08924661
15	P	11.57639971	10.14551003	16.86473445
16	P	6.97408590	3.66284029	21.14254658
17	P	3.02586396	6.47320497	17.88564038
18	P	10.44586842	6.39560804	13.07102062
19	P	10.35946370	2.33092549	16.47607099
20	P	5.22584461	7.26609887	13.12141858
21	C	7.13682275	9.01608715	22.73830366
22	C	6.58245886	9.52090900	23.92618511
23	H	5.75939595	10.23675749	23.88318418
24	C	7.06843828	9.09024767	25.16258203
25	H	6.63548381	9.48590234	26.08260198
26	C	8.09849552	8.14596451	25.22038672
27	H	8.47315036	7.80681700	26.18706954
28	C	8.63118872	7.62029965	24.04172041
29	H	9.42302888	6.87307930	24.08558489
30	C	8.14899651	8.04680484	22.80416502
31	H	8.54951534	7.62808104	21.87929991
32	C	4.75562850	9.77799310	21.31814759
33	C	4.14642023	11.00590022	21.60996672
34	H	4.74697459	11.91444475	21.67053783
35	C	2.76383999	11.06244420	21.80454878
36	H	2.28850040	12.02009469	22.02096278
37	C	1.98968580	9.90233736	21.71053972
38	H	0.90961239	9.95557732	21.84972003
39	C	2.59445412	8.67786177	21.41064848
40	H	1.99647167	7.77229273	21.30258501
41	C	3.97122910	8.61904673	21.20668776
42	H	4.43978465	7.67721874	20.91727166
43	C	7.23034594	11.27770311	20.85018334
44	C	7.44121767	11.69276752	19.52478192
45	H	7.16064140	11.04606540	18.69135397
46	C	8.02203461	12.93263688	19.25859193
47	H	8.17612274	13.23248584	18.22075005
48	C	8.40257902	13.76555227	20.31524777
49	H	8.86793635	14.73099452	20.11075213
50	C	8.18355265	13.36245193	21.63766632
51	H	8.47778167	14.01223391	22.46312488
52	C	7.59733378	12.12352100	21.90879522
53	H	7.46334502	11.80222326	22.94170873
54	C	13.11630696	9.59718551	16.02359502
55	C	14.35779202	10.22441928	16.22739090

56	H	14.45276768	11.02735586	16.95841038
57	C	15.47643021	9.81295645	15.50100334
58	H	16.43732452	10.30210508	15.66723104
59	C	15.36535918	8.78301164	14.56059691
60	H	16.24019085	8.46769175	13.99046203
61	C	14.13456520	8.15458263	14.35938722
62	H	14.04028314	7.34247824	13.63955583
63	C	13.01845962	8.55380628	15.09576788
64	H	12.05886710	8.05713282	14.95648974
65	C	11.00400185	11.58782240	15.87565715
66	C	11.90426247	12.42283382	15.19526602
67	H	12.97312886	12.20972256	15.20936277
68	C	11.42853996	13.51855308	14.47397613
69	H	12.13262408	14.16080942	13.94286908
70	C	10.05551771	13.78884876	14.42512361
71	H	9.68857874	14.64186832	13.85256251
72	C	9.15690702	12.95936376	15.10162535
73	H	8.08035419	13.13407825	15.06574813
74	C	9.63074521	11.86302392	15.82554744
75	H	8.91394158	11.21137044	16.32963522
76	C	12.18251864	10.90934804	18.41951609
77	C	11.66143895	12.13076589	18.87115102
78	H	10.89816969	12.64931300	18.29078157
79	C	12.12415283	12.68772682	20.06503096
80	H	11.70695120	13.63375039	20.41211824
81	C	13.10619170	12.03464457	20.81472718
82	H	13.46307339	12.47186692	21.74769667
83	C	13.61618250	10.80977450	20.37491786
84	H	14.36721200	10.27981281	20.96134939
85	C	13.15108267	10.24333189	19.18968505
86	H	13.55390362	9.28836236	18.85524943
87	C	8.30358056	2.41145940	21.28390775
88	C	9.51234127	2.64730651	20.61110157
89	H	9.64302708	3.56617571	20.03536959
90	C	10.53501550	1.70052601	20.64871587
91	H	11.46324769	1.88897875	20.10929060
92	C	10.35913788	0.51247195	21.35909176
93	H	11.15417498	-0.23400321	21.37912084
94	C	9.15277471	0.26441759	22.02257081
95	H	9.00526679	-0.67604702	22.55515768
96	C	8.12191414	1.20340154	21.97655915
97	H	7.16415870	0.97810931	22.44773852
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102	H	2.89967336	0.91328983	22.06008251
103	C	3.17690510	1.29139434	19.94905873
104	H	2.28198465	0.74252505	19.65431672
105	C	3.97132091	1.90699644	18.97798925
106	H	3.72752167	1.83305376	17.91740135
107	C	5.10664646	2.62181001	19.35816280
108	H	5.70631335	3.11544067	18.58990488
109	C	6.60987014	4.33780218	22.80974658
110	C	6.93325691	3.70235793	24.01723319
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112	C	6.54128107	4.27238691	25.23287316
113	H	6.80099897	3.77697425	26.16952700
114	C	5.81453666	5.46669219	25.25066020
115	H	5.51172786	5.90719742	26.20101264
116	C	5.49682324	6.10822297	24.05001674
117	H	4.96323878	7.05863353	24.05183441
118	C	5.90847593	5.55642330	22.83987867
119	H	5.71065446	6.08595457	21.90603590
120	C	2.28551559	5.73532812	16.38862329
121	C	1.40026366	6.40341535	15.53334979
122	H	1.08091457	7.42171618	15.75021277
123	C	0.96223525	5.77409761	14.36373707
124	H	0.29075986	6.30758167	13.69131004
125	C	1.40510978	4.48870970	14.04514893
126	H	1.08070502	4.01256100	13.11923585
127	C	2.29286629	3.82335210	14.89823543
128	H	2.68121864	2.83585957	14.64806535
129	C	2.73748169	4.44436370	16.06102918
130	H	3.47229025	3.94032182	16.69110945
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134	C	3.01658074	10.56011248	18.19725249
135	H	3.78168972	11.33651016	18.18432676
136	C	1.66612908	10.87740946	18.35489317
137	H	1.36178462	11.91586895	18.49104145
138	C	0.70166119	9.86306399	18.33998949
139	H	-0.35408693	10.10917513	18.46154777
140	C	1.08694387	8.53116168	18.18410892
141	H	0.32916870	7.74740571	18.19731252
142	C	2.27957778	5.58523104	19.30665708
143	C	3.10320572	5.29257001	20.40388078
144	H	4.17351749	5.49671926	20.33554222
145	C	2.56647407	4.72556816	21.55860655
146	H	3.22010666	4.51328583	22.40472126
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148	H	0.78105767	3.97139413	22.51317132
149	C	0.38677047	4.66063026	20.50321342
150	H	-0.67063374	4.39408781	20.53554909
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154	C	12.09886635	8.25296459	11.65879457
155	H	12.67905711	7.40428462	11.29610132
156	C	12.51128122	9.54932655	11.34496636
157	H	13.39190573	9.69970665	10.71897165
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159	H	12.15065673	11.66234337	11.63046677
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166	H	11.85356709	5.64290328	15.49470374
167	C	13.66979352	4.63193966	14.90857131
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169	C	14.42937729	4.13886116	13.84494627
170	H	15.36969644	3.62252304	14.04149323
171	C	13.96890149	4.28357602	12.53103196
172	H	14.54833714	3.87867807	11.70026778
173	C	12.75860282	4.93404784	12.28025486
174	H	12.38652005	5.01227244	11.25745025
175	C	9.55652584	5.56443163	11.70868269
176	C	9.81222057	5.84300245	10.35732615
177	H	10.58221853	6.56552472	10.08293610
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185	H	8.31221921	4.46497911	13.11035419
186	C	12.13793704	2.28540496	16.92264813
187	C	13.06524508	1.42464432	16.31481566
188	H	12.74370764	0.74842658	15.52183787
189	C	14.40640751	1.45179015	16.70480723
190	H	15.12312577	0.78705350	16.22082945
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192	H	15.88049468	2.35148075	18.00473352
193	C	13.90960992	3.18274935	18.32342843
194	H	14.23542685	3.88662565	19.08964455
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196	H	11.85865179	3.86129223	18.38176573
197	C	10.18618980	1.86667372	14.71477275
198	C	11.14411863	2.19575438	13.74324999
199	H	12.09594029	2.63780562	14.03147918
200	C	10.87402388	1.96289299	12.39338072
201	H	11.62508970	2.22317012	11.64716564
202	C	9.64726343	1.42232218	12.00119027
203	H	9.43447106	1.26215197	10.94379228
204	C	8.68418476	1.11337009	12.96669751
205	H	7.71296335	0.71248161	12.67456655
206	C	8.94891074	1.33034181	14.31788372
207	H	8.17714769	1.11027948	15.05596210
208	C	9.57228402	0.96150355	17.40723441
209	C	10.19611878	-0.28880311	17.54050537
210	H	11.18204870	-0.46273667	17.10828498
211	C	9.55810033	-1.31122771	18.24248291

212	H	10.04678469	-2.28055854	18.35055129
213	C	8.29506500	-1.09470989	18.80613146
214	H	7.80146819	-1.89577380	19.35803900
215	C	7.66981725	0.14510417	18.66868485
216	H	6.68702046	0.32627970	19.10403616
217	C	8.30907171	1.17390821	17.97647157
218	H	7.82404942	2.14571357	17.87690865
219	C	3.64540231	8.16489811	13.37367574
220	C	3.50642334	8.94363967	14.53232962
221	H	4.30539676	8.97530992	15.27496864
222	C	2.34891320	9.69640294	14.73585276
223	H	2.26101571	10.30298836	15.63651238
224	C	1.31378953	9.65566875	13.79948951
225	H	0.40552808	10.23786103	13.96318340
226	C	1.43896433	8.86176571	12.65399749
227	H	0.62826604	8.82034435	11.92471853
228	C	2.60125422	8.12008221	12.43724776
229	H	2.68374200	7.49597762	11.54772278
230	C	4.83129186	5.79250375	12.11172045
231	C	4.74510175	4.56277832	12.77995673
232	H	4.95494499	4.49940746	13.84863473
233	C	4.39994900	3.40405570	12.08392621
234	H	4.35561021	2.46014086	12.62945180
235	C	4.14130785	3.46414572	10.71215012
236	H	3.87425107	2.55935018	10.16395087
237	C	4.23290533	4.68767347	10.03687135
238	H	4.03674462	4.73722188	8.96484307
239	C	4.57562203	5.84968867	10.73036927
240	H	4.65552777	6.79731229	10.19621243
241	C	6.26310652	8.39053592	12.11122922
242	C	7.09819164	7.91680995	11.08816452
243	H	7.09353181	6.86240482	10.81261206
244	C	7.94911304	8.80095224	10.42089754
245	H	8.59223680	8.42352627	9.62567284
246	C	7.99118016	10.14872033	10.78246231
247	H	8.66838868	10.83064279	10.26795493
248	C	7.19322777	10.61186375	11.83401382
249	H	7.24577955	11.65452528	12.14987239
250	C	6.33233400	9.74074083	12.49990465
251	H	5.73527707	10.11187717	13.33479954
252	P	11.71497182	6.53660223	20.45987410
253	C	11.80226437	5.22521010	21.72633994
254	C	10.61968373	4.99232866	22.45305660
255	H	9.72155316	5.57161743	22.22679218
256	C	10.57806748	3.99936381	23.42740770
257	H	9.65502885	3.83560547	23.98321849
258	C	11.69930047	3.19486999	23.65589806
259	H	11.65920078	2.40101270	24.40235004
260	C	12.86293608	3.39498894	22.90890862
261	H	13.73427742	2.75983062	23.07376487
262	C	12.92187691	4.41387945	21.95219825
263	H	13.84043770	4.57778584	21.38792945
264	C	11.38402592	8.06019788	21.42656988
265	C	11.81963024	8.21857320	22.75100736
266	H	12.35814240	7.41120865	23.25028137
267	C	11.52894648	9.39636934	23.44458644
268	H	11.85387266	9.50779925	24.47975502
269	C	10.81072157	10.41880520	22.81933262
270	H	10.57571080	11.33564064	23.36116063
271	C	10.38503324	10.26629941	21.49914476
272	H	9.84195083	11.06430791	21.00027646
273	C	10.65996972	9.09113857	20.80662428
274	H	10.29883500	8.96983288	19.78376594
275	C	13.38675093	6.76243927	19.74295259
276	C	13.52925998	6.65762704	18.34928878
277	H	12.66452583	6.38886914	17.73831444
278	C	14.75579248	6.93923355	17.74536671
279	H	14.84683367	6.88591634	16.66062627
280	C	15.84569662	7.32559915	18.52824507
281	H	16.79795628	7.56401618	18.05330989
282	C	15.71319223	7.42426446	19.91913147
283	H	16.56366346	7.73215789	20.52894284
284	C	14.48696034	7.14958512	20.52613688
285	H	14.37628297	7.25983552	21.60584878

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Bibliography

[1] Vera Truttmann. *The Ligand Shapes the Cluster: Influences and Modification Possibilities of Protecting Ligands on Au Nanoclusters*. PhD thesis, TU Wien, 2022.

[2] Rongchao Jin, Gao Li, Sachil Sharma, Yingwei Li, and Xiangsha Du. Toward Active-Site Tailoring in Heterogeneous Catalysis by Atomically Precise Metal Nanoclusters with Crystallographic Structures. *Chemical Reviews*, 121(2):567–648, sep 2020.

[3] Jun Fang, Bin Zhang, Qiaofeng Yao, Yang Yang, Jianping Xie, and Ning Yan. Recent advances in the synthesis and catalytic applications of ligand-protected, atomically precise metal nanoclusters. *Coordination Chemistry Reviews*, 322:1–29, sep 2016.

[4] Zhihe Liu, Zhennan Wu, Qiaofeng Yao, Yitao Cao, Osburg Jin Huang Chai, and Jianping Xie. Correlations between the fundamentals and applications of ultrasmall metal nanoclusters: Recent advances in catalysis and biomedical applications. *Nano Today*, 36:101053, feb 2021.

[5] Rongchao Jin, Chenjie Zeng, Meng Zhou, and Yuxiang Chen. Atomically Precise Colloidal Metal Nanoclusters and Nanoparticles: Fundamentals and Opportunities. *Chemical Reviews*, 116(18):10346–10413, sep 2016.

[6] Jianbo Zhao and Rongchao Jin. Heterogeneous catalysis by gold and gold-based bimetal nanoclusters. *Nano Today*, 18:86–102, feb 2018.

[7] Xi Kang, Hanbao Chong, and Manzhou Zhu. $Au_{25}SR_{18}$: the captain of the great nanocluster ship. *Nanoscale*, 10(23):10758–10834, 2018.

[8] Ricca Rahman Nasaruddin, Tiankai Chen, Ning Yan, and Jianping Xie. Roles of thiolate ligands in the synthesis, properties and catalytic application of gold nanoclusters. *Coordination Chemistry Reviews*, 368:60–79, aug 2018.

[9] Xi Kang and Manzhou Zhu. Tailoring the photoluminescence of atomically precise nanoclusters. *Chemical Society Reviews*, 48(8):2422–2457, 2019.

[10] Indranath Chakraborty and Thalappil Pradeep. Atomically Precise Clusters of Noble Metals: Emerging Link between Atoms and Nanoparticles. *Chemical Reviews*, 117(12):8208–8271, jun 2017.

[11] Tokuhisa Kawawaki, Ayano Ebina, Yasunaga Hosokawa, Shuhei Ozaki, Daiki Suzuki, Sakiat Hossain, and Yuichi Negishi. Thiolate-Protected Metal Nanoclusters: Recent Development in Synthesis, Understanding of Reaction, and Application in Energy and Environmental Field. *Small*, 17(27):2005328, feb 2021.

[12] Yuichi Negishi, Tafu Nakazaki, Sami Malola, Shinjiro Takano, Yoshiki Niihori, Wataru Kurashige, Seiji Yamazoe, Tatsuya Tsukuda, and Hannu Häkkinen. A critical size for emergence of nonbulk electronic and geometric structures in dodecanethiolate-protected au clusters. *Journal of the American Chemical Society*, 137(3):1206–1212, jan 2015.

[13] Huifeng Qian, Manzhou Zhu, Zhikun Wu, and Rongchao Jin. Quantum sized gold nanoclusters with atomic precision. *Accounts of Chemical Research*, 45(9):1470–1479, jun 2012.

[14] Rongchao Jin, Yan Zhu, and Huifeng Qian. Quantum-Sized Gold Nanoclusters: Bridging the Gap between Organometallics and Nanocrystals. *Chemistry - A European Journal*, 17(24):6584–6593, may 2011.

[15] Rohul H. Adnan, Jenica Marie L. Madridejos, Abdulrahman S. Alotabi, Gregory F. Metha, and Gunther G. Andersson. A Review of State of the Art in Phosphine Ligated Gold Clusters and Application in Catalysis. *Advanced Science*, n/a(n/a):2105692, 2022.

[16] Yu Wang, Huayan Yang, and Nanfeng Zheng. Structural Engineering of Heterometallic Nanoclusters. In *Frontiers of Nanoscience*, pages 73–102. Elsevier, 2015.

[17] Katsuaki Konishi. Phosphine-Coordinated Pure-Gold Clusters: Diverse Geometrical Structures and Unique Optical Properties/Responses. In *Structure and Bonding*, pages 49–86. Springer International Publishing, 2014.

[18] Hannu Häkkinen. Atomic and electronic structure of gold clusters: understanding flakes, cages and superatoms from simple concepts. *Chemical Society Reviews*, 37(9):1847, 2008.

[19] Michael Walter, Jaakko Akola, Olga Lopez-Acevedo, Pablo D. Jadzinsky, Guillermo Calero, Christopher J. Ackerson, Robert L. Whetten, Henrik Gronbeck, and Hannu Häkkinen. A unified view of ligand-protected gold clusters as superatom complexes. *Proceedings of the National Academy of Sciences*, 105(27):9157–9162, jul 2008.

[20] Pablo D. Jadzinsky, Guillermo Calero, Christopher J. Ackerson, David A. Bushnell, and Roger D. Kornberg. Structure of a Thiol Monolayer-Protected Gold Nanoparticle at 1.1 Å Resolution. *Science*, 318(5849):430–433, oct 2007.

[21] Hannu Häkkinen, Michael Walter, and Henrik Grönbeck. Divide and Protect: Capping Gold Nanoclusters with Molecular Gold-Thiolate Rings. *The Journal of Physical Chemistry B*, 110(20):9927–9931, apr 2006.

[22] Esma Khatun and Thalappil Pradeep. New Routes for Multicomponent Atomically Precise Metal Nanoclusters. *ACS Omega*, 6(1):1–16, dec 2020.

[23] Mathias Brust, Merryl Walker, Donald Bethell, David J. Schiffrin, and Robin Whyman. Synthesis of thiol-derivatised gold nanoparticles in a two-phase Liquid–Liquid system. *J. Chem. Soc., Chem. Commun.*, 0(7):801–802, 1994.

[24] Rongchao Jin, Huifeng Qian, Zhikun Wu, Yan Zhu, Manzhou Zhu, Ashok Mohanty, and Niti Garg. Size Focusing: A Methodology for Synthesizing Atomically Precise Gold Nanoclusters. *The Journal of Physical Chemistry Letters*, 1(19):2903–2910, sep 2010.

[25] Yuichi Negishi, Sayaka Hashimoto, Ayano Ebina, Kota Hamada, Sakiat Hossain, and Tokuhisa Kawawaki. Atomic-level separation of thiolate-protected metal clusters. *Nanoscale*, 12(15):8017–8039, 2020.

[26] Huifeng Qian, Yan Zhu, and Rongchao Jin. Size-Focusing Synthesis, Optical and Electrochemical Properties of Monodisperse $Au_{38}(SC_2H_4Ph)_{24}$ Nanoclusters. *ACS Nano*, 3(11):3795–3803, oct 2009.

[27] Xun Yuan, Bin Zhang, Zhentao Luo, Qiaofeng Yao, David Tai Leong, Ning Yan, and Jianping Xie. Balancing the Rate of Cluster Growth and Etching for Gram-Scale Synthesis of Thiolate-Protected Au_{25} Nanoclusters with Atomic Precision. *Angewandte Chemie International Edition*, 53(18):4623–4627, mar 2014.

[28] Yong Yu, Xi Chen, Qiaofeng Yao, Yue Yu, Ning Yan, and Jianping Xie. Scalable and Precise Synthesis of Thiolated $Au_{10–12}$, Au_{15}, Au_{18}, and Au_{25} Nanoclusters via pH Controlled CO Reduction. *Chemistry of Materials*, 25(6):946–952, mar 2013.

[29] Qiaofeng Yao, Yong Yu, Xun Yuan, Yue Yu, Jianping Xie, and Jim Yang Lee. Two-Phase Synthesis of Small Thiolate-Protected Au_{15} and Au_{18} Nanoclusters. *Small*, 9(16):2696–2701, feb 2013.

[30] Yong Yu, Zhentao Luo, Yue Yu, Jim Yang Lee, and Jianping Xie. Observation of Cluster Size Growth in CO-Directed Synthesis of $Au_{25}(SR)_{18}$ Nanoclusters. *ACS Nano*, 6(9):7920–7927, aug 2012.

[31] Huifeng Qian and Rongchao Jin. Controlling Nanoparticles with Atomic Precision: The Case of $Au_{144}(SCH_2CH_2Ph)_{60}$. *Nano Letters*, 9(12):4083–4087, sep 2009.

[32] Manzhou Zhu, Christine M. Aikens, Frederick J. Hollander, George C. Schatz, and Rongchao Jin. Correlating the Crystal Structure of A Thiol-Protected Au_{25} Cluster and Optical Properties. *Journal of the American Chemical Society*, 130(18):5883–5885, apr 2008.

[33] Yuichi Negishi, Yoshimitsu Takasugi, Seiichi Sato, Hiroshi Yao, Keisaku Kimura, and Tatsuya Tsukuda. Magic-Numbered Au_n Clusters Protected by Glutathione Monolayers (n = 18, 21, 25, 28, 32, 39): Isolation and Spectroscopic Characterization. *Journal of the American Chemical Society*, 126(21):6518–6519, may 2004.

[34] Yuichi Negishi, Katsuyuki Nobusada, and Tatsuya Tsukuda. Glutathione-Protected Gold Clusters Revisited: Bridging the Gap between Gold(I)-Thiolate Complexes and Thiolate-Protected Gold Nanocrystals. *Journal of the American Chemical Society*, 127(14):5261–5270, mar 2005.

[35] Marcus A. Tofanelli, Kirsi Salorinne, Thomas W. Ni, Sami Malola, Brian Newell, Billy Phillips, Hannu Häkkinen, and Christopher J. Ackerson. Jahn-Teller effects in $Au_{25}(SR)_{18}$. *Chemical Science*, 7(3):1882–1890, 2016.

[36] Lallie C. McKenzie, Tatiana O. Zaikova, and James E. Hutchison. Structurally Similar Triphenylphosphine-Stabilized Undecagolds, $Au_{11}(PPh_3)_7Cl_3$ and $[Au_{11}(PPh_3)_8Cl_2]Cl$, Exhibit Distinct Ligand Exchange Pathways with Glutathione. *Journal of the American Chemical Society*, 136(38):13426–13435, sep 2014.

[37] Tiankai Chen, Qiaofeng Yao, Ricca Rahman Nasaruddin, and Jianping Xie. Electrospray Ionization Mass Spectrometry: A Powerful Platform for Noble-Metal Nanocluster Analysis. *Angewandte Chemie International Edition*, 58(35):11967–11977, aug 2019.

[38] Yizhong Lu and Wei Chen. Application of Mass Spectrometry in the Synthesis and Characterization of Metal Nanoclusters. *Analytical Chemistry*, 87(21):10659–10667, jul 2015.

[39] Amala Dass, Anthony Stevenson, George R. Dubay, Joseph B. Tracy, and Royce W. Murray. Nanoparticle MALDI-TOF Mass Spectrometry without Fragmentation: $Au_{25}(SCH_2CH_2Ph)_{18}$ and Mixed Monolayer $Au_{25}(SCH_2CH_2Ph)_{18\text{-}x}(L)_x$. *Journal of the American Chemical Society*, 130(18):5940–5946, apr 2008.

[40] Joseph F. Parker, Jai-Pil Choi, Wei Wang, and Royce W. Murray. Electron Self-exchange Dynamics of the Nanoparticle Couple $[Au_{25}(SC_2Ph)_{18}]^{0/1-}$ Nuclear Magnetic Resonance Line-Broadening. *The Journal of Physical Chemistry C*, 112(36):13976–13981, aug 2008.

[41] Giovanni Salassa, Annelies Sels, Fabrizio Mancin, and Thomas Bürgi. Dynamic Nature of Thiolate Monolayer in $Au_{25}(SR)_{18}$ Nanoclusters. *ACS Nano*, 11(12):12609–12614, nov 2017.

[42] Zhikun Wu and Rongchao Jin. Stability of the Two Au-S Binding Modes in $Au_{25}(SG)_{18}$ Nanoclusters Probed by NMR and Optical Spectroscopy. *ACS Nano*, 3(7):2036–2042, jun 2009.

[43] Zhikun Wu, Chakicherla Gayathri, Roberto R. Gil, and Rongchao Jin. Probing the Structure and Charge State of Glutathione-Capped $Au_{25}(SG)_{18}$ Clusters by NMR and Mass Spectrometry. *Journal of the American Chemical Society*, 131(18):6535–6542, apr 2009.

[44] Igor Dolamic, Birte Varnholt, and Thomas Bürgi. Far-infrared spectra of well-defined thiolate-protected gold clusters. *Physical Chemistry Chemical Physics*, 15(45):19561, 2013.

[45] Belén Nieto-Ortega and Thomas Bürgi. Vibrational Properties of Thiolate-Protected Gold Nanoclusters. *Accounts of Chemical Research*, 51(11):2811–2819, nov 2018.

[46] Alfredo Tlahuice-Flores, Robert L. Whetten, and Miguel Jose-Yacaman. Vibrational Normal Modes of Small Thiolate-Protected Gold Clusters. *The Journal of Physical Chemistry C*, 117(23):12191–12198, may 2013.

[47] Haru Hirai, Shun Ito, Shinjiro Takano, Kiichirou Koyasu, and Tatsuya Tsukuda. Ligand-protected gold/silver superatoms: current status and emerging trends. *Chemical Science*, 11(45):12233–12248, 2020.

[48] Chenjie Zeng, Yuxiang Chen, Anindita Das, and Rongchao Jin. Transformation Chemistry of Gold Nanoclusters: From One Stable Size to Another. *The Journal of Physical Chemistry Letters*, 6(15):2976–2986, jul 2015.

[49] Yanan Wang and Thomas Bürgi. Ligand exchange reactions on thiolate-protected gold nanoclusters. *Nanoscale Advances*, 3(10):2710–2727, 2021.

[50] Stefan Knoppe, Asantha C. Dharmaratne, Ella Schreiner, Amala Dass, and Thomas Bürgi. Ligand Exchange Reactions on Au_{38} and Au_{40} Clusters: A Combined Circular Dichroism and Mass Spectrometry Study. *Journal of the American Chemical Society*, 132(47):16783–16789, nov 2010.

[51] Satyabrata Si, Cyrille Gautier, Julien Boudon, Rossana Taras, Serafino Gladiali, and Thomas Bürgi. Ligand Exchange on Au_{25} Cluster with Chiral Thiols. *The Journal of Physical Chemistry C*, 113(30):12966–12969, jul 2009.

[52] Stefan Knoppe and Thomas Bürgi. The fate of $Au_{25}(SR)_{18}$ clusters upon ligand exchange with binaphthyl-dithiol: interstaple binding vs. decomposition. *Physical Chemistry Chemical Physics*, 15(38):15816, 2013.

[53] Annelies Sels, Raymond Azoulay, Wybren Jan Buma, Mark A. J. Koenis, Valentin Paul Nicu, and Thomas Bürgi. Vibrational Circular Dichroism of Thiolate-Protected Au_{25} Clusters: Accurate Prediction of Spectra and Chirality Transfer within the Mixed Ligand Shell. *The Journal of Physical Chemistry C*, 123(36):22586–22594, aug 2019.

[54] Xueqi Hu, Youkun Zheng, Junyu Zhou, Danjun Fang, Hui Jiang, and Xuemei Wang. Silver-Assisted Thiolate Ligand Exchange Induced Photoluminescent Boost of Gold Nanoclusters for Selective Imaging of Intracellular Glutathione. *Chemistry of Materials*, 30(6):1947–1955, mar 2018.

[55] Cheng-An J. Lin, Ting-Ya Yang, Chih-Hsien Lee, Sherry H. Huang, Ralph A. Sperling, Marco Zanella, Jimmy K. Li, Ji-Lin Shen, Hsueh-Hsiao Wang, Hung-I Yeh, Wolfgang J. Parak, and Walter H. Chang. Synthesis, Characterization, and Bioconjugation of Fluorescent Gold Nanoclusters toward Biological Labeling Applications. *ACS Nano*, 3(2):395–401, jan 2009.

[56] Xi Kang and Manzhou Zhu. Transformation of Atomically Precise Nanoclusters by Ligand-Exchange. *Chemistry of Materials*, 31(24):9939–9969, nov 2019.

[57] Christine L. Heinecke, Thomas W. Ni, Sami Malola, Ville Mäkinen, O. Andrea Wong, Hannu Häkkinen, and Christopher J. Ackerson. Structural and Theoretical Basis for Ligand Exchange on Thiolate Monolayer Protected Gold Nanoclusters. *Journal of the American Chemical Society*, 134(32):13316–13322, aug 2012.

[58] Amendra Fernando and Christine M. Aikens. Ligand Exchange Mechanism on Thiolate Monolayer Protected $Au_{25}(SR)_{18}$ Nanoclusters. *The Journal of Physical Chemistry C*, 119(34):20179–20187, aug 2015.

[59] Amendra Fernando and Christine M. Aikens. Deciphering the Ligand Exchange Process on Thiolate Monolayer Protected $Au_{38}(SR)_{24}$ Nanoclusters. *The Journal of Physical Chemistry C*, 120(27):14948–14961, jun 2016.

[60] Thomas W. Ni, Marcus A. Tofanelli, Billy D. Phillips, and Christopher J. Ackerson. Structural Basis for Ligand Exchange on $Au_{25}(SR)_{18}$. *Inorganic Chemistry*, 53(13):6500–6502, jun 2014.

[61] Yukatsu Shichibu, Yuichi Negishi, Takahito Watanabe, Nirmalya K. Chaki, Hiroyuki Kawaguchi, and Tatsuya Tsukuda. Biicosahedral Gold Clusters $[Au_{25}(PPh_3)_{10}(SC_nH)_{(2n+1)5}Cl_2]^{2+}$ (n = 2-18): A Stepping Stone to Cluster-Assembled Materials. *The Journal of Physical Chemistry C*, 111(22):7845–7847, may 2007.

[62] Bertha Molina, Ariadna Sánchez-Castillo, Stefan Knoppe, Ignacio L. Garzón, Thomas BÃ¼rgi, and Alfredo Tlahuice-Flores. Structures and chiroptical properties of the BINAS-monosubstituted au38(SCH3)24 cluster. *Nanoscale*, 5(22):10956, 2013.

[63] Annelies Sels, Giovanni Salassa, Stephan Pollitt, Clara Guglieri, Günther Rupprechter, Noelia Barrabés, and Thomas Bürgi. Structural Investigation of the Ligand Exchange Reaction with Rigid Dithiol on Doped (Pt, Pd) Au_{25} Clusters. *The Journal of Physical Chemistry C*, 121(20):10919–10926, feb 2017.

[64] Huifeng Qian, William T. Eckenhoff, Yan Zhu, Tomislav Pintauer, and Rongchao Jin. Total Structure Determination of Thiolate-Protected Au_{38} Nanoparticles. *Journal of the American Chemical Society*, 132(24):8280–8281, jun 2010.

[65] Olga Lopez-Acevedo, Jaakko Akola, Robert L. Whetten, Henrik Grönbeck, and Hannu Häkkinen. Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster $Au_{144}(SR)_{60}$. *The Journal of Physical Chemistry C*, 113(13):5035–5038, jan 2009.

[66] Nan Yan, Nan Xia, Lingwen Liao, Min Zhu, Fengming Jin, Rongchao Jin, and Zhikun Wu. Unraveling the long-pursued Au_{144} structure by X-ray crystallography. *Science Advances*, 4(10), oct 2018.

[67] Yanfei Zhu, Jun Guo, Xueying Qiu, Shenlong Zhao, and Zhiyong Tang. Optical Activity of Chiral Metal Nanoclusters. *Accounts of Materials Research*, 2(1):21–35, dec 2020.

[68] Yingwei Li, Tatsuya Higaki, Xiangsha Du, and Rongchao Jin. Chirality and Surface Bonding Correlation in Atomically Precise Metal Nanoclusters. *Advanced Materials*, 32(41):1905488, mar 2020.

[69] Hiroshi Yao. Chiral ligand-protected gold nanoclusters: Considering the optical activity from a viewpoint of ligand dissymmetric field. *Progress in Natural Science: Materials International*, 26(5):428–439, oct 2016.

[70] Olga Lopez-Acevedo, Hironori Tsunoyama, Tatsuya Tsukuda, Hannu Häkkinen, and Christine M. Aikens. Chirality and Electronic Structure of the Thiolate-Protected Au_{38} Nanocluster. *Journal of the American Chemical Society*, 132(23):8210–8218, may 2010.

[71] Sami Malola and Hannu Häkkinen. Chiral footprint of the ligand layer in the all-alkynyl-protected gold nanocluster $Au_{144}(CCPhF)_{60}$. *Chemical Communications*, 55(64):9460–9462, 2019.

[72] Michael-Rock Goldsmith, Christopher B. George, Gérard Zuber, Ron Naaman, David H. Waldeck, Peter Wipf, and David N. Beratan. The chiroptical signature of achiral metal clusters induced by dissymmetric adsorbates. *Phys. Chem. Chem. Phys.*, 8(1):63–67, 2006.

[73] Chenjie Zeng and Rongchao Jin. Chiral Gold Nanoclusters: Atomic Level Origins of Chirality. *Chemistry – An Asian Journal*, 12(15):1839–1850, jun 2017.

[74] Makenzie R. Provorse and Christine M. Aikens. Origin of Intense Chiroptical Effects in Undecagold Subnanometer Particles. *Journal of the American Chemical Society*, 132(4):1302–1310, feb 2010.

[75] Igor Dolamic, Stefan Knoppe, Amala Dass, and Thomas Bürgi. First enantioseparation and circular dichroism spectra of Au_{38} clusters protected by achiral ligands. *Nature Communications*, 3(1), jan 2012.

[76] Stefan Knoppe, Igor Dolamic, Amala Dass, and Thomas Bürgi. Separation of Enantiomers and CD Spectra of $Au_{40}(SCH_2CH_2Ph)_{24}$: Spectroscopic Evidence for Intrinsic Chirality. *Angewandte Chemie International Edition*, 51(30):7589–7591, jun 2012.

[77] Noelia Barrabés, Bei Zhang, and Thomas Bürgi. Racemization of Chiral $Pd_2Au_{36}(SC_2H_4Ph)_{24}$: Doping Increases the Flexibility of the Cluster Surface. *Journal of the American Chemical Society*, 136(41):14361–14364, sep 2014.

[78] Yanfei Zhu, Hui Wang, Kaiwei Wan, Jun Guo, Chunting He, Yue Yu, Luyang Zhao, Yin Zhang, Jiawei Lv, Lin Shi, Renxi Jin, Xinxiang Zhang, Xinghua Shi, and Zhiyong Tang. Enantioseparation of $Au_{20}(PP_3)_4Cl_4$ Clusters with Intrinsically Chiral Cores. *Angewandte Chemie*, 130(29):9197–9201, jun 2018.

[79] Qian Xu, Santosh Kumar, Shenshen Jin, Huifeng Qian, Manzhou Zhu, and Rongchao Jin. Chiral 38-Gold-Atom Nanoclusters: Synthesis and Chiroptical Properties. *Small*, 10(5):1008–1014, oct 2013.

[80] Mizuho Sugiuchi, Yukatsu Shichibu, and Katsuaki Konishi. An Inherently Chiral Au_{24} Framework with Double-Helical Hexagold Strands. *Angewandte Chemie International Edition*, 57(26):7855–7859, may 2018.

[81] Huayan Yang, Juanzhu Yan, Yu Wang, Guocheng Deng, Haifeng Su, Xiaojing Zhao, Chaofa Xu, Boon K. Teo, and Nanfeng Zheng. From Racemic Metal Nanoparticles to Optically Pure Enantiomers in One Pot. *Journal of the American Chemical Society*, 139(45):16113–16116, nov 2017.

[82] Guocheng Deng, Sami Malola, Juanzhu Yan, Yingzi Han, Peng Yuan, Chaowei Zhao, Xiting Yuan, Shuichao Lin, Zichao Tang, Boon K. Teo, Hannu HÃ¤kkinen, and Nanfeng Zheng. From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated $Au_{13}Cu_2$ Nanoclusters. *Angewandte Chemie*, 130(13):3479–3483, feb 2018.

[83] Juanzhu Yan, Haifeng Su, Huayan Yang, Chengyi Hu, Sami Malola, Shuichao Lin, Boon K. Teo, Hannu HÃ¤kkinen, and Nanfeng Zheng. Asymmetric Synthesis of Chiral Bimetallic $[Ag_{28}Cu_{12}(SR)_{24}]^{4-}$ Nanoclusters via Ion Pairing. *Journal of the American Chemical Society*, 138(39):12751–12754, sep 2016.

[84] Natalia V. Karimova and Christine M. Aikens. Chiroptical Activity in BINAP- and DIOP-Stabilized Octa- and Undecagold Clusters. *The Journal of Physical Chemistry C*, 122(20):11051–11065, apr 2018.

[85] Sami Malola, Sami Kaappa, and Hannu Häkkinen. Role of Nanocrystal Symmetry in the Crossover Region from Molecular to Metallic Gold Nanoparticles. *The Journal of Physical Chemistry C*, 123(33):20655–20663, jul 2019.

[86] Sami Malola and Hannu Häkkinen. Chiral Inversion of Thiolate-Protected Gold Nanoclusters via Core Reconstruction without Breaking a Au–S Bond. *Journal of the American Chemical Society*, 141(14):6006–6012, mar 2019.

[87] Cecilia Noguez and Ignacio L. Garzón. Optically active metal nanoparticles. *Chemical Society Reviews*, 38(3):757, 2009.

[88] Takumi Nashimoto and Hiroshi Yao. Strong chiroptical activity in Au_{25} clusters protected by mixed ligands of chiral phosphine and achiral thiolate. *Physical Chemistry Chemical Physics*, 22(27):15288–15294, 2020.

[89] Stefan Knoppe, Igor Dolamic, and Thomas Bürgi. Racemization of a Chiral Nanoparticle Evidences the Flexibility of the Gold–Thiolate Interface. *Journal of the American Chemical Society*, 134(31):13114–13120, jul 2012.

[90] Stefan Knoppe, Sophie Michalet, and Thomas Bürgi. Stabilization of Thiolate-Protected Gold Clusters Against Thermal Inversion: Diastereomeric $Au_{38}(SCH_2CH_2Ph)_{24\text{-}2x}$(*R*-BINAS)$_x$. *The Journal of Physical Chemistry C*, 117(29):15354–15361, jul 2013.

[91] Christine M. Aikens. Effects of core distances, solvent, ligand, and level of theory on the TDDFT optical absorption spectrum of the thiolate-protected Au_{25} nanoparticle. *The Journal of Physical Chemistry A*, 113(40):10811–10817, sep 2009.

[92] Manzhou Zhu, Huifeng Qian, Xiangming Meng, Shenshen Jin, Zhikun Wu, and Rongchao Jin. Chiral Au_{25} Nanospheres and Nanorods: Synthesis and Insight into the Origin of Chirality. *Nano Letters*, 11(9):3963–3969, aug 2011.

[93] Yukatsu Shichibu, Yuichi Negishi, Tatsuya Tsukuda, and Toshiharu Teranishi. Large-Scale Synthesis of Thiolated Au_{25} Clusters via Ligand Exchange Reactions of Phosphine-Stabilized Au_{11} Clusters. *Journal of the American Chemical Society*, 127(39):13464–13465, sep 2005.

[94] Gerd H. Woehrle, Marvin G. Warner, and James E. Hutchison. Ligand Exchange Reactions Yield Subnanometer, Thiol-Stabilized Gold Particles with Defined Optical Transitions. *The Journal of Physical Chemistry B*, 106(39):9979–9981, sep 2002.

[95] Gerd H. Woehrle and James E. Hutchison. Thiol-Functionalized Undecagold Clusters by Ligand Exchange: Synthesis, Mechanism, and Properties. *Inorganic Chemistry*, 44(18):6149–6158, jul 2005.

[96] Yiyun Yang and Shaowei Chen. Surface Manipulation of the Electronic Energy of Subnanometer-Sized Gold Clusters: An Electrochemical and Spectroscopic Investigation. *Nano Letters*, 3(1):75–79, nov 2002.

[97] Christian D. Grant, Adam M. Schwartzberg, Yiyun Yang, Shaowei Chen, and Jin Z. Zhang. Ultrafast study of electronic relaxation dynamics in Au_{11} nanoclusters. *Chemical Physics Letters*, 383(1-2):31–34, jan 2004.

[98] Michael J. Hostetler, Allen C. Templeton, and Royce W. Murray. Dynamics of Place-Exchange Reactions on Monolayer-Protected Gold Cluster Molecules. *Langmuir*, 15(11):3782–3789, apr 1999.

[99] Rui Guo, Yang Song, Gangli Wang, and Royce W. Murray. Does Core Size Matter in the Kinetics of Ligand Exchanges of Monolayer-Protected Au Clusters? *Journal of the American Chemical Society*, 127(8):2752–2757, feb 2005.

[100] Gerd H. Woehrle, Leif O. Brown, and James E. Hutchison. Thiol-Functionalized, 1.5-nm Gold Nanoparticles through Ligand Exchange Reactions: Scope and Mechanism of Ligand Exchange. *Journal of the American Chemical Society*, 127(7):2172–2183, jan 2005.

[101] Allison Hadley and Christine M. Aikens. Thiolate Ligand Exchange Mechanisms of Au_1 and Subnanometer Gold Particle Au_{11}. *The Journal of Physical Chemistry C*, 114(42):18134–18138, mar 2010.

[102] Janet Petroski, Mei H. Chou, and Carol Creutz. Rapid Phosphine Exchange on 1.5-nm Gold Nanoparticles. *Inorganic Chemistry*, 43(5):1597–1599, feb 2004.

[103] Brett M. Bode and Mark S. Gordon. MacMolPlt: a graphical user interface for GAMESS. *Journal of Molecular Graphics and Modelling*, 16(3):133–138, jun 1998.

[104] Marshall R. Ligare, J. Ulises Reveles, Niranjan Govind, Grant E. Johnson, and Julia Laskin. Influence of Interligand Interactions and Core-Charge Distribution on Gold Cluster Stability: Enthalpy Versus Entropy. *The Journal of Physical Chemistry C*, 123(40):24899–24911, sep 2019.

[105] Aleksandr V. Marenich, Christopher J. Cramer, and Donald G. Truhlar. Generalized Born Solvation Model SM12. *Journal of Chemical Theory and Computation*, 9(1):609–620, dec 2012.

[106] Craig A. Peeples and Georg Schreckenbach. Implementation of the SM12 Solvation Model into ADF and Comparison with COSMO. *Journal of Chemical Theory and Computation*, 12(8):4033–4041, jul 2016.

[107] Stefan Grimme, Jens Antony, Stephan Ehrlich, and Helge Krieg. A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *The Journal of Chemical Physics*, 132(15):154104, apr 2010.

[108] G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, and T. Ziegler. Chemistry with ADF. *Journal of Computational Chemistry*, 22(9):931–967, 2001.

[109] A. D. Becke. Density-functional exchange-energy approximation with correct asymptotic behavior. *Physical Review A*, 38(6):3098–3100, sep 1988.

[110] John P. Perdew. Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Physical Review B*, 33(12):8822–8824, jun 1986.

[111] E. Van Lenthe and E. J. Baerends. Optimized Slater-type basis sets for the elements 1-118. *Journal of Computational Chemistry*, 24(9):1142–1156, may 2003.

[112] E. van Lenthe, E. J. Baerends, and J. G. Snijders. Relativistic regular two-component Hamiltonians. *The Journal of Chemical Physics*, 99(6):4597–4610, sep 1993.

[113] Erik van Lenthe, Andreas Ehlers, and Evert-Jan Baerends. Geometry optimizations in the zero order regular approximation for relativistic effects. *The Journal of Chemical Physics*, 110(18):8943–8953, may 1999.

[114] Robert Rüger, Erik van Lenthe, Thomas Heine, and Lucas Visscher. Tight-binding approximations to time-dependent density functional theory – A fast approach for the calculation of electronically excited states. *The Journal of Chemical Physics*, 144(18):184103, may 2016.

[115] Jochen Autschbach. Computing chiroptical properties with first-principles theoretical methods: Background and illustrative examples. *Chirality*, 21(1E):E116–E152, 2009.

[116] S.J.A. van Gisbergen, J.G. Snijders, and E.J. Baerends. Implementation of time-dependent density functional response equations. *Computer Physics Communications*, 118(2-3):119–138, may 1999.

[117] Eric F. Pettersen, Thomas D. Goddard, Conrad C. Huang, Gregory S. Couch, Daniel M. Greenblatt, Elaine C. Meng, and Thomas E. Ferrin. UCSF Chimera – A visualization system for exploratory research and analysis. *Journal of Computational Chemistry*, 25(13):1605–1612, 2004.

[118] Michael W. Heaven, Amala Dass, Peter S. White, Kennedy M. Holt, and Royce W. Murray. Crystal Structure of the Gold Nanoparticle $[N(C_8H_{17})_4][Au_{25}(SCH_2CH_2Ph)_{18}]$. *Journal of the American Chemical Society*, 130(12):3754–3755, mar 2008.

[119] Github Repository. https://github.com/QChASM/AaronTools.py/tree/master/Ligands (last accessed Apr 2022), 2020.

[120] National Center for Biotechnology Information. PubChem Compound Summary for CID 11419748, (S,S)-Dipamp. https://pubchem.ncbi.nlm.nih.gov/compound/S_S_-Dipamp (last accessed April 2022), 2022.