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Jeevithra Dewi Subramaniam, Yohei Hattori, Fumio Asanoma, Toshio Nishino, Kazuma Yasuhara, et al.. Synthesis of Ce(IV) Heteroleptic Double-Decker Complex with a New Helical Naphthalocyanine as a Potential Gearing Subunit. *Chemistry - A European Journal*, In press, 10.1002/chem.202402470 . hal-04664141

**HAL Id: hal-04664141**

**<https://hal.science/hal-04664141v1>**

Submitted on 29 Jul 2024

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# Synthesis of Ce(IV) Heteroleptic Double-Decker Complex with a New Helical Naphthalocyanine as a Potential Gearing Subunit

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**Abstract:** This paper describes the synthesis of a cerium(IV)-based molecular gear composed of a thioether functionalized phthalocyanine anchoring ligand, and a helical naphthalocyanine rotating cogwheel functionalized with four carbazoles. The naphthalocyanine ligand **9** was obtained after eleven steps (overall yield of 0.2%) as a mixture of three geometrical isomers, two of which are chiral and exhibit high levels of steric hindrance, as shown by DFT calculations. Their attributions have been made using <sup>1</sup>H-NMR based on their different symmetry groups. The ratio of isomers was also determined and the prochiral C<sub>4h</sub> naphthalocyanine shown to be the major compound (55%). Its heteroleptic complexation with cerium (IV) and the anchoring phthalocyanine ligand **10** gave the targeted molecular gear in a 16% yield.

## Introduction

A wide variety of molecular machines having various structures and tasks, ranging from intracellular transport to energy storage, are found in the biological world.<sup>[1]</sup> The synthesis of miniaturized analogs of biological machines is an active field of research, boosted by the Nobel Prize awarded in 2016 to Profs J.-P. Sauvage<sup>[2]</sup> and Sir J. F. Stoddart<sup>[3]</sup> for their pioneering investigations into mechanically-interlocked molecular machines, and to Prof. B. L. Feringa<sup>[4]</sup> for the development of a very efficient family of light-fueled motors based on overcrowded alkenes.<sup>[5]</sup> Since these breakthroughs, many synthetic motors with a variety of designs adapted to different media have been reported, powered by light,<sup>[6]</sup> chemical energy sources<sup>[7]</sup> or electrons.<sup>[8]</sup> With the development of tools based on near-field microscopies for manipulating molecules at the single molecular level, a new field has arisen aiming to control molecular machines on an individual basis. For instance, it has become possible to rotate step by step a molecular motor<sup>[8b]</sup> or to fuel a nanocar.<sup>[9]</sup>

With some of these milestones achieved, it has become highly desirable to try and exploit these motors by performing more advanced tasks, either by inducing cooperative behavior within a network of molecules<sup>[10]</sup> or by developing complex nanomachineries at the single-molecule level. One possibility is to follow a technomimetic<sup>[11]</sup> approach (i.e. taking macroscopic machines as an inspiration), integrating these motors into more sophisticated intramolecular devices such as motorized nanovehicles<sup>[12]</sup> or winches.<sup>[13]</sup> With the further aim of building functional multimolecular machineries, exploitation of the work provided by a single motor now requires its interconnection with distinct mechanical devices. In the case of surface-bound rotary motors, one interesting strategy consists of the transfer of rotational motion through a train of gears assembled on a surface.<sup>[14]</sup>

Indeed, whereas gearing motions can only be performed in solution at the intramolecular level,<sup>[15]</sup> intermolecular gearing can be achieved in anisotropic media<sup>[16]</sup> where it has become possible to precisely control and maintain the distances between molecular cogwheels. In particular, the transfer of rotational motion has been successfully demonstrated between systems of meshed star-shaped molecules anchored on a surface. In such experiments, the tip of a Scanning Tunneling Microscope (STM) is used to build a train of gears by initially positioning the single-molecule cogwheels at appropriate interlocking distances, and then allowing the tip to act as a source of mechanical energy inducing rotation of the first cogwheel. Propagation of the motion through the gears is evidenced by comparing successive STM images.

Only a few star-shaped molecules have thus far been studied as gears, including penta(*p*-*tert*-butylphenyl)(*p*-*tert*-butylpyrimido) benzene which has been used as a six-teeth cogwheel by Moresco *et al.*<sup>[17]</sup> When this molecule was moved laterally with the STM tip along an island of the same molecules on Cu(111), evidence of its rotation was observed on successive STM images, operating like a rack and pinion. Unfortunately, when working with a pair of molecules, all attempts to transfer rotation between them proved unsuccessful as the molecules preferred to diffuse apart.<sup>[18]</sup> Using an anchoring group to pin individual gears at precise interlocking distances is the key to overcoming this problem. This concept has been applied to the same molecule mounted on a Cu adatom, which acts as an atomic scale axle allowing precise positioning of the cogwheels on a Pb(111) surface<sup>[19]</sup> resulting in the transfer of a rotational motion from one molecule to the next. However, the transfer of rotation to a third molecule proved unsuccessful due to the fragility of the supramolecular anchoring structure. This underlines the importance of integrating an anchoring subunit into the molecular design. In collaboration with the group of Moresco,<sup>[20]</sup> we recently reported an anchoring strategy which takes advantage of the strong interactions between the Au(111) surface and the radical state of pentaarylcyclopentadienyl cogwheels, generated by homolytic cleavage of a brominated precursor upon on-surface deposition by sublimation. We obtained for the first time the transfer of gearing motion through three interlocked molecules. Unfortunately, this strategy is not suitable for building trains of gears having controlled shapes and lengths, since the anchoring position is random and once anchored, the radical species cannot be repositioned by lateral manipulation.

One promising alternative strategy relies on the use of a metallo-organic rotational axle, in which an anchoring ligand provides tight binding to the surface through specific functional groups, with the metal ion acting as a ball bearing, and a second coordinated ligand acting as the cogwheel. In our previous work,<sup>[10]</sup> a lanthanide-based double-decker molecular motor (Figure 1a) was anchored on an Au(111) surface through a naphthalocyanine having eight sulfur atoms on its periphery. This anchoring ligand showed a very good capacity to immobilize the motor on the surface as well as offering the possibility of lateral repositioning using the apex of the STM tip. This ability to reposition a molecule, after its random deposition on the surface, is a unique feature of this anchoring unit which gives us the prospect of building a linear train of gears. Herein we report the design and synthesis of a molecular gear based on a Ce(IV) heteroleptic double-decker complex (Figure 1b) taking into account all that we have learned from our recent contributions to the field.<sup>[21]</sup>

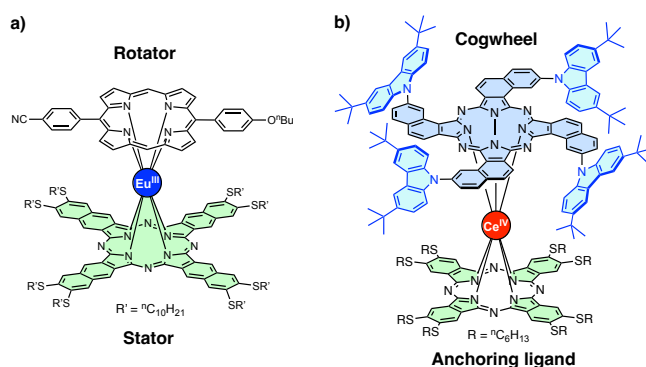


Figure 1. (a) Chemical structure of the lanthanide-based double-decker molecular motor and (b) the right-handed enantiomer of the newly designed molecular gear.

## Results and Discussion

### 1. Design of the Ce(IV) heteroleptic double-decker

Firstly, our target double-decker complex must be neutral, to allow for easy sublimation deposition under vacuum, while also avoiding undesirable counter ions. The latter could contaminate the surface, and at worst hinder or obstruct gearing motions through electrostatic interactions. Also, a diamagnetic complex will be easier to characterize, allowing standard NMR techniques to be used. To fulfill these requirements, Ce(IV) was selected as the metal for the ball bearing assembly, to be used in combination with two different dianionic phthalocyanine ligands.

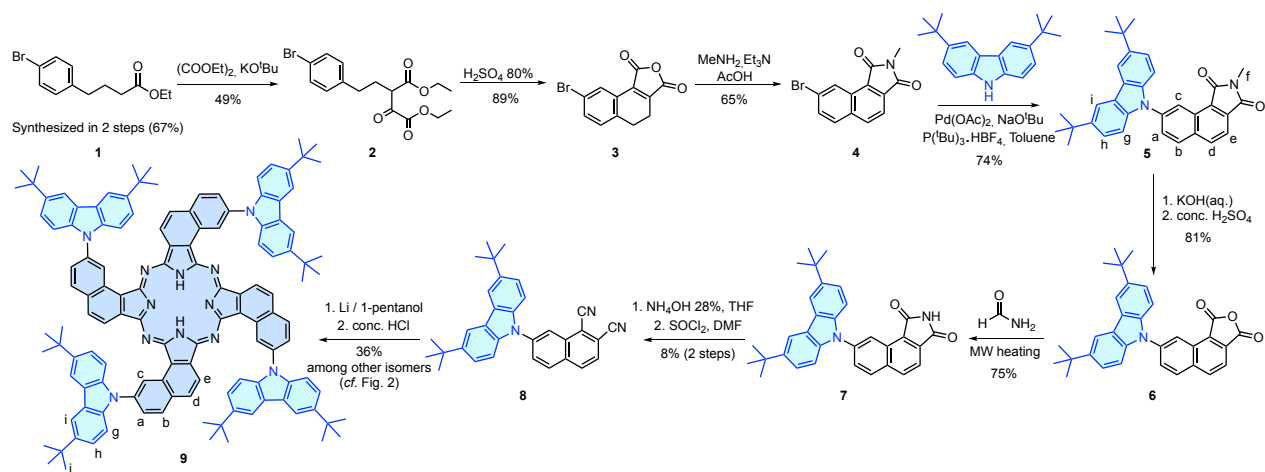
The anchoring ligand is the phthalocyanine analogue of the naphthalocyanine used in our previously reported motor (Figure 1a). For gearing applications, this is required as it is an anchoring ligand smaller than the rotating cogwheel.<sup>[21e]</sup> Also, one additional reason to have chosen this phthalocyanine is the fact it has only one proton in the aromatic region which makes its identification easy in a <sup>1</sup>H-NMR spectrum. Finally, the cogwheel that is the key part of our molecular gear was chosen. Instead of a linear 2,3-naphthalocyanine which would be easier to synthesize, we selected the functionalized angular 1,2-naphthalocyanine<sup>[22]</sup> represented in Figure 1b which is prochiral. It has been functionalized with 3,6-di-*tert*-butyl-9*H*-carbazole (Cbz) at the 7-position of the naphthalocyanine to make the cogwheel. Without these Cbz subunits, the interactions of two consecutive molecules will not be efficient, as the two naphthalocyanine ligands will be co-planar and parallel. In this conformation it will be easy for the cogwheel of the next molecule to escape rotation once the rotation of the first cogwheel occurs. We expect the Cbz fragments not only to extend the size of the cogwheel but also to act as 2D-paddles to prevent the next cogwheel escaping upon rotation.<sup>[21b]</sup>

Once complexed as a heteroleptic double-decker (Figure 1b), the target complex will present either left-handed or right-handed helicity, these two enantiomers differ depending on the direction of the coordination planes of the naphthalocyanine which can be clockwise or counterclockwise. As a consequence, two enantiomers (R and S) are predicted<sup>[23]</sup> to be observed on the surface in equal proportions, with each having a propensity to rotate more easily in one direction, as shown previously for other helical molecular motors.<sup>[21c]</sup> A left-handed helical molecule rotates preferentially in the opposite direction to its equivalent right-handed helical molecule. *Tert*-butyl groups have also been introduced to increase organic solubility of the target molecule and to allow for easier observation by STM techniques,<sup>[24]</sup> where they are known to induce good contrast in the imaging.

Since this metallo-organic anchoring subunit can be repositioned at will on the surface by pushing with the apex of a STM tip, it is envisioned to build a train of molecular gears with a tunable number of successive cogwheels, having precise control over their chirality. It is expected that the helical structure of these complexes on the surface will allow insight into the influence of cogwheel helicity on the efficiency of the rotation transfer from one molecule to the next at the molecular scale. Indeed, to allow for the disrotatory motions expected in a train of gears, it is envisioned to position a right-handed molecule (which rotates anticlockwise) next to a left-handed molecule (which rotates clockwise). Experimental on-surface studies and comparisons with homochiral trains of gears will thus allow verification of the assumption that chirality inversion in successive cogwheels will be helpful to transfer rotation in intermolecular gearing systems.

## 2. Synthesis of the pro-helical cogwheel

The angular 1,2-naphthalocyanine has been synthesized in eleven steps from commercially available 3-(4-bromo-benzoyl)propanoic acid (Scheme 1). The dihydronaphthalene anhydride **3** was prepared following a previously described strategy.<sup>[22]</sup> Wolff-Kishner reduction of the ketone group of 3-(4-bromobenzoyl)propanoic acid gave 4-(4-bromophenyl)butanoic acid in a 69% yield. This was subsequently esterified with ethanol using sulfuric acid. Ethyl 4-(4-bromophenyl)butanoate (**1**) was obtained in a 96% yield. Ester **1** was then reacted with diethyl oxalate to give the ketoester **2** which was subsequently cyclized by dehydration of the diacid in 80% sulfuric acid. The dihydronaphthalene anhydride **3** was formed in 89% yield. The corresponding benzo[*e*]isoindole-1,3-dione **4** was obtained in 65% yield by imidation and simultaneous aromatization in a one-pot reaction with



**Scheme 1.** Synthesis of the 2,3-naphthalocyanine **9** substituted with 3,6-di-*tert*-butyl-9H-carbazole at the four 7-positions. More details are given in the experimental part and the SI. The lettering in molecules **5** and **9** are used in attribution of the  $^1\text{H-NMR}$  signals.

methylamine in pure acetic acid.<sup>[25]</sup> The palladium-catalyzed Buchwald-Hartwig amination reaction<sup>[26]</sup> was attempted between **4** and 1.5 eq. of commercially-available 3,6-di-*tert*-butyl-9H-carbazole. While only 2% yield of aminated product was observed when using tris(dba)dipalladium(0) as catalyst, the use of palladium(II) acetate and (*tert*-Bu)<sub>3</sub>PHBF<sub>4</sub> as the catalytic system (Scheme 1) and sodium *tert*-butoxide as base, gave target compound **5** in 74% yield after 20 h in refluxing toluene.

To reach the desired 1,2-naphthalocyanine **9**, it is necessary to synthesize the appropriate starting 7-substituted-1,2-dicyanonaphthalene. Indeed, direct conversion of **5** or **6** to its corresponding dicyanonaphthalene **8** was not straightforward. Ring-opening of the methyl benzo[*e*]isoindole-1,3-dione derivative **5** failed as did the ring opening of the dihydronaphthalene anhydride **6**. Only the conversion to the cyclic benzo[*e*]isoindole-1,3-dione **7** (without *N*-methyl group) allowed preparation in three more steps of the naphthalocyanine precursor **8**. First, reaction of the dihydronaphthalene anhydride **6** with formamide acting as both nucleophile and solvent under microwave heating gave **7** with a yield of 75%. The opening of the dione to give two amides, precursors of the desired cyano groups, was conducted by reaction of **7** in tetrahydrofuran with an excess solution of 28% aqueous ammonium hydroxide. After evaporation of the solvent, the crude material appeared to be a mixture of the desired diamide and starting materials. Based on  $^1\text{H-NMR}$ ,

a maximum conversion of 50% was obtained after 24 h at room temperature. Increasing the temperature was counter-productive as the solubility of ammonia decreased, while going below room temperature inhibited the reaction. The mixture of the diamine and **7** appeared to be in equilibrium, which prevented purification. The mixture was then engaged in the next step, a von Braun amide dehydration reaction, performed using thionyl chloride.<sup>[27]</sup> After column chromatography, the 1,2-dicyanonaphthalene derivative **8** was obtained pure with an overall yield of 8% (for 2 steps) with 85% of pure starting material **7** also recovered. Unfortunately, direct conversion of the dihydronaphthalene anhydride **6** to the zinc(II) complex of naphthalocyanine **9** as described for similar substrates<sup>[28]</sup> without Cbz also failed.

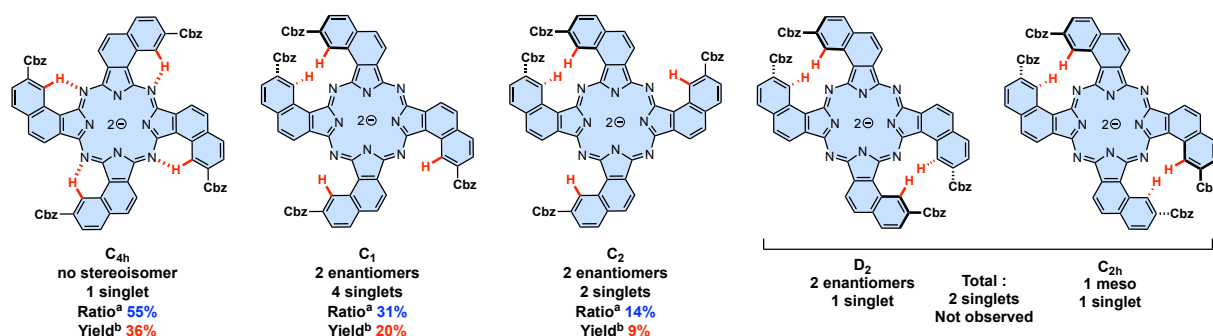
With the 1,2-dicyanonaphthalene derivative (**8**) in hand, the formation reaction of the naphthalocyanine ring was performed. Derivative **8** was added to a solution of lithium in *n*-pentanol, and the solution refluxed for 16 h and cooled to room temperature.<sup>[29]</sup> The dark green solution was neutralized with concentrated hydrochloric acid and purified using two successive column chromatography. The first one provided a green solid which appeared to be a mixture of geometrical isomers in an overall 65% yield. A second column chromatography was necessary to obtain pure the three geometrical isomers, including the targeted C<sub>4h</sub> pro-chiral naphthalocyanine (Figure 2) with an isolated yield of 36%. HR-MS confirmed the chemical formula of each compound and the <sup>1</sup>H-NMR in *o*-DCB-d<sub>4</sub> allowed attribution of their symmetries (Figure S1-S5).

Since phthalocyanine derivatives easily form aggregates in solution, the NMR spectra have been recorded at low concentration and high temperatures (60 to 95 °C) to prevent broadening of signals in the aromatic region and allow their assignation. Therefore, the internal NH signals tend to disappear due to exchange processes. Indeed, the signal around 11 ppm (Figure S1) corresponding to the proton at the 8-position of the naphthalene ring (*ortho* position of the Cbz, red in Figure 2) was found to be particularly helpful to assign the symmetries of the different isomers. This signal is strongly deshielded due to hydrogen-bonding between nitrogens on the naphthalocyanine ring and the considered proton, in addition to the strong ring current induced by the large naphthalocyanine ring. This interaction is shown in Figure 2 for the major C<sub>4h</sub> geometrical isomer using dotted red lines. This specific signal around 11 ppm acts as a probe of the different geometrical isomer symmetries. The C<sub>4h</sub> isomer gives only one singlet (Figure S1), whereas the other isomers give 2 or 4 singlets in the same ratio (Figure S4 for the C<sub>1</sub> isomer and Figure S5 for the C<sub>2</sub> isomer). Next to the major isomer,



the chiral geometrical isomers with  $C_1$  and  $C_2$  symmetry have been isolated with yields of 20% and 9% respectively.

Contrary to some examples in the literature<sup>[22,29]</sup> where steric control gave only one specific geometrical isomer, the tetramerization reaction of **8** is regioselective with the major isomer formed in a greater proportion compared to the other possible isomers depicted in Figure 2. Unsubstituted 1,2-naphthalocyanines have planar structures and present four different isomers of symmetries  $C_{4h}$ ,  $C_s$ ,  $C_{2v}$ , and  $D_{2h}$ . In our case, the steric hindrance between the Cbz subunits induces a twisting of the molecule, which leads to the loss of a plane of symmetry and therefore, these isomers become chiral with the resulting symmetry groups indicated in Figure 2. The ratio of isomers was determined as 55:31:14 for the  $C_{4h}$ ,  $C_1$  and  $C_2$  symmetries respectively. This distribution appears far from the calculated statistical mixture ratio (12.5:50:25), as well as the predicted 12.5% for the  $D_2$  and  $C_{2h}$  isomers that are not observed, which means the influence of thermodynamics, due to the high steric hindrance in some geometrical isomers, seems to be important.



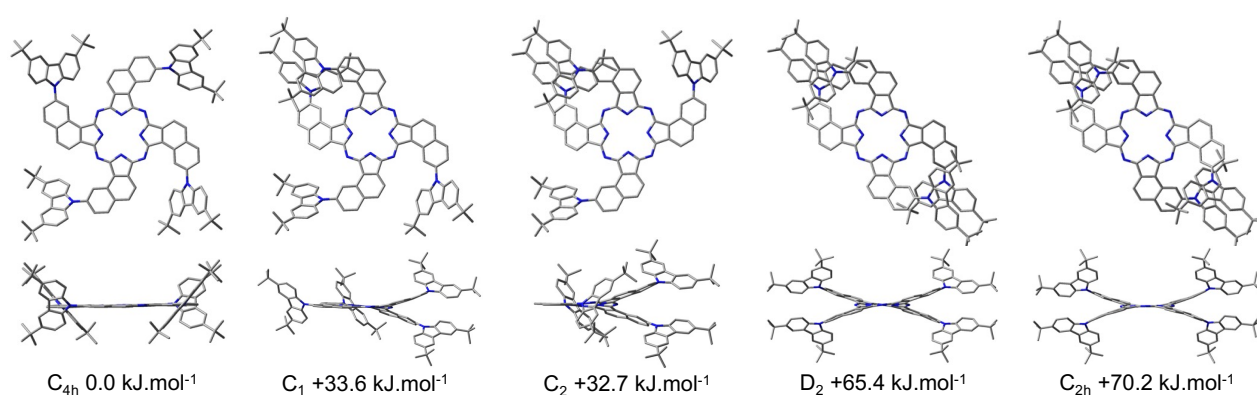
**Figure 2.** The four geometrical isomers of the dianion of the 1,2-naphthalocyanine ligand. The diastereoisomers with  $D_2$  and  $C_{2h}$  symmetries are stereoisomers of the each other. The symmetry groups are given without taking into account the conformation of the carbazoles (Cbz). When there is no steric hindrance between two consecutive benzo[*e*]isoindoles, they are coplanar with the naphthalocyanine ring but when there is some steric hindrance, they are twisted and the helicity of the two consecutive rings are linked, being left-handed (L) or right-handed (D). <sup>a</sup> from  $^1\text{H-NMR}$ ; <sup>b</sup> Isolated yield from  $^1\text{H-NMR}$  600 MHz, 60°C in *o*-DCB.

It must be noted that the major isomer is not chiral but instead prochiral in regards to the formation of the double-decker complex. However, the two minor isomers obtained are chiral and obtained as a racemic mixture. Since the isomer with two interacting angular 1,2-naphthalene

subunits was not observed, the constraint must be too high to allow its formation under these conditions. To clarify these observations, density functional theory (DFT) calculations have been performed.

### 3. DFT calculations of the geometrical isomers of naphthalocyanine **9**

As already mentioned, the naphthalocyanine substituted with four 3,6-di-*tert*-butyl-9*H*-carbazoles **9** was obtained as a mixture of three of the four possible geometrical isomers shown in Figure 2, in a ratio of 55:31:14:0. DFT calculations using the B3LYP functional and 6-31G(d) basis set were carried out (Gaussian16 suite of programs<sup>[30]</sup>) to compare the stability of the regioisomers and consequently explain the observed ratio. The results are given Figure 3.



**Figure 3.** Top and side views of the DFT optimized geometry of the four geometrical isomers of 1,2-naphthalocyanine ligand **9**. The  $C_{4h}$  isomer is the most stable and the relative energies of the other isomers are given. Colors: Carbon = grey; Nitrogen = blue; Hydrogens are not shown for clarity.

According to the DFT calculations, the chirality arises from the deformation of two adjacent angular 1,2-naphthalene subunits which point in the same direction. When there is no steric hindrance between two consecutive benzo[*e*]isoindoles, they remain coplanar with the naphthalocyanine ring, but when steric hindrance is present, it induces twisting of the ligand with the helicity of the two considered benzo[*e*]isoindoles rings linked, being left-handed (L) or right-handed (D).

Optimization of the geometrical isomers with symmetries  $C_{4h}$ ,  $C_1$ ,  $C_2$ ,  $D_2$  and  $C_{2h}$  confirms that due to the lack of steric hindrance the most stable isomer is the major product, the  $C_{4h}$  symmetric naphthalocyanine. Less stable by 32.7 and 33.6  $\text{kJ.mol}^{-1}$  are the two isolated minor isomers having  $C_2$  and  $C_1$  symmetries. These both present a similar distorted phthalocyanine ring due to twisting of two consecutive benzo[*e*]isoindole fragments. The fact that the  $C_2$  and  $C_1$  symmetric isomers have

similar energies, much higher than the  $C_{4h}$  isomer ( $K_{eq} = \exp(-\Delta G/RT) < 10^{-4}$ ) means that the regioisomer states are not in equilibrium and the ratio of isomers is kinetically controlled.

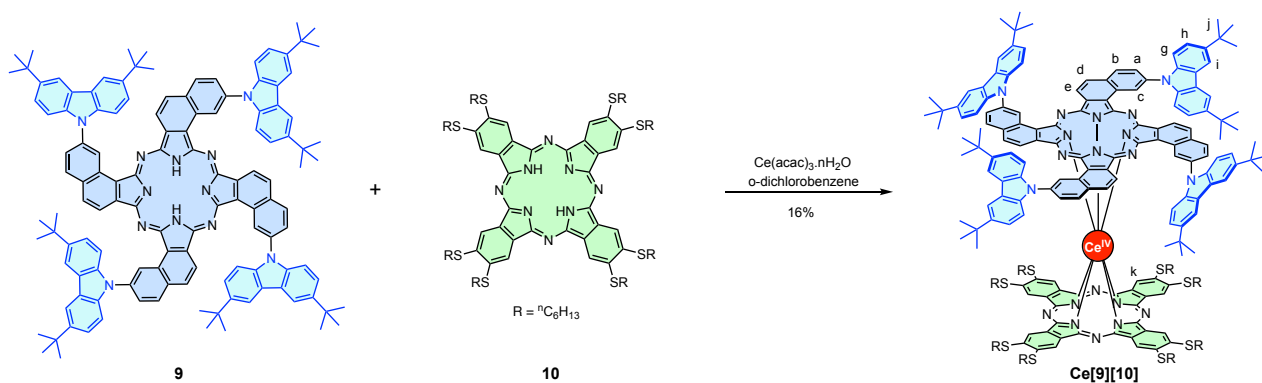
Even though we did not obtain them, we also calculated the energies of the DFT-optimized  $D_2$  and  $C_{2h}$  isomers (Figure 3). They both present the highest steric hindrance as they contain four twisted benzo[*e*]isoindole fragments. The  $D_2$  and  $C_{2h}$  isomers are higher in energy than the major  $C_{4h}$  isomer by 65.4 and 70.2  $\text{kJ}\cdot\text{mol}^{-1}$  respectively with the  $C_{2h}$  isomer the highest in energy and showing phthalocyanine rings with the most distortion.

It is interesting to note the absence of  $\pi$ -stacking between consecutive carbazoles. The distance measured for all the isomers is always more than 5 Å which too far to envision these interactions.

#### 4. Preparation of the Ce(IV) heteroleptic double-decker complex

After synthesis of the anchoring phthalocyanine **10** following a published procedure,<sup>[32]</sup> the complexation was achieved by reaction of Ce(III) acetylacetonate in *o*-dichlorobenzene at 270 °C (Scheme 2). In a first attempt, we followed the two-step strategy proposed by Pushkarev *et al.*<sup>[33]</sup> which is supposed to minimize formation of the undesired homoleptic complexes. First we mixed the naphthalocyanine **9** with the cerium salt and after one hour the anchoring phthalocyanine **10**, but as confirmed by MALDI-TOF MS, no desired compound was found. Then, we tried a microwave synthesis with a 1:1.5 ratio of the ligands **9** and **10**, but only traces of the desired heteroleptic double-decker complex were obtained, the main product being the homoleptic  $\text{Ce}^{\text{IV}}$  double-decker complex of ligand **10**. This illustrates the greater coordination ability of ligand **10** due to its electron-rich character thanks to the eight electron donating thioether groups. Surprisingly, we also observed by MALDI-TOF MS the formation of homoleptic  $\text{Ce}^{\text{IV}}$  double-decker complexes of ligand **9**. Perhaps stabilizing p-p interactions occur when the carbazole subunits of the two ligands coordinate to a cerium ion in an interlocked configuration. To minimize formation of this homoleptic complex, we proceeded the reaction with an excess of ligand **10**. The best yield of heteroleptic double-decker complex **Ce[9][10]** was obtained when the ratio of ligands **9** and **10** was 1:10.

According to the MS data, we confirmed the formation of by-products, including the expected homoleptic complex of ligand **9** **Ce[9]<sub>2</sub>** and an excess of the homoleptic complex of ligand **10** **Ce[10]<sub>2</sub>**. Due to co-elution between these different compounds incorporating multi hexyl chains, purification required three stages of chromatography. Initial column chromatography on silica followed by size exclusion chromatography allowed us to remove the triple deckers and free ligand **10**. Then, a final



**Scheme 2.** Formation of the Ce(IV) heteroleptic double-decker complex.

column of silica was needed to obtain the cerium (IV) heteroleptic double-decker complex **Ce[9][10]** as a dark green-blue solid in 16% yield. Along with this, **Ce[9]<sub>2</sub>** was also obtained with a yield of 14%. **Ce[9][10]** was characterized by <sup>1</sup>H-NMR (Fig. S6) and HR-MS (Fig. S8).

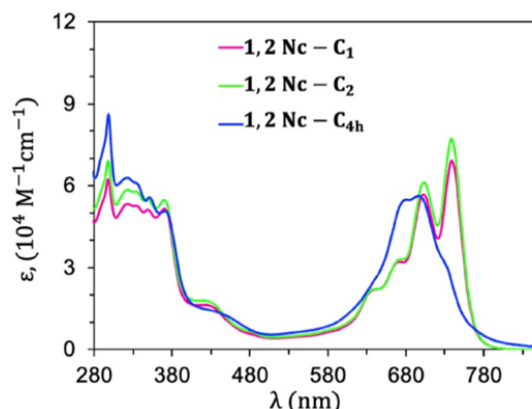
Once coordinated, all the proton signals are deshielded compared to the free ligand due to the +IV formal charge on the cerium ion. Four of the protons from the naphthyl fragment are strongly deshielded ( $H_a$ : +0.57 ppm,  $H_b$ : +0.49 ppm,  $H_d$ : +0.58 ppm and  $H_e$ : +0.69 ppm), while the other five protons are weakly deshielded. These correspond to the aromatic protons of the carbazole fragment as well as the remaining proton c on the naphthyl fragment ( $H_c$ : +0.17 ppm,  $H_g$ : +0.26 ppm,  $H_h$ : +0.28 ppm and  $H_i$ : +0.12 ppm).

As explained in the design section, the double-decker exists as a mixture of two enantiomers (R and S)<sup>[23]</sup> since the naphthalocyanine is prochiral. The S stereoisomer, exhibiting a right-handed helicity, is presented in Scheme 2. Interestingly, the transmission of rotation from one molecule to the next in a train of gears must necessarily follow a disrotatory motion. Since it has been shown that two enantiomeric complexes deposited on a surface rotate preferentially in opposite directions, to have both enantiomers of **Ce[9][10]** together is important in view of our goal to build a train of gears having successive opposite chiralities.

## 5. Absorption spectroscopy

The absorption spectra of the three isolated geometrical isomers of **9** have been measured in chloroform at 298 K (Figure 4 and Table 1). All of them show an intense band in the UV region with maxima at 299 nm and similar molar absorption coefficients, which can be assigned to the Soret band of the naphthalocyanine. In the visible region, the absorption spectra contain the four

expected Q bands in the 600-800 nm region.<sup>[31]</sup> In the case of the major C<sub>4h</sub> isomer, the bands are broadened with shoulders at 635 and 732 nm.



**Figure 4.** Absorption spectra of the three isolated geometrical isomers of the 1,2-naphthalocyanine ligands **9** (chloroform,  $c = 10 \cdot 10^{-6}$  M, 298 K).

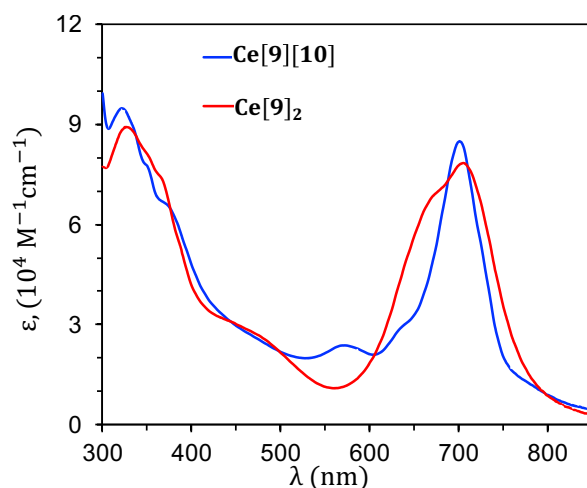
**Table 1.** Absorption parameters of the geometrical isomers of **9** (chloroform,  $c = 10 \cdot 10^{-6}$  M, 298 K).

	$\lambda_{\max}$ , nm ( $\epsilon_{\max}$ , $10^3 \text{ M}^{-1} \text{ cm}^{-1}$ )
<b>9-C<sub>4h</sub></b>	299 (86.0), 635 (23.1), 679 (54.7), 697 (56.3), 731 (31.1)
<b>9-C<sub>1</sub></b>	299 (62.5), 636 (21.7), 666 (31.2), 704 (56.9), 740 (69.2)
<b>9-C<sub>2</sub></b>	299 (69.2), 634 (21.5), 669 (32.4), 704 (61.3), 739 (77.3)

It is known that a broadening of the bands occurs when the molecules aggregate in solution which is very common for phthalocyanines.<sup>[34]</sup> In the visible region, the Q bands of the C<sub>1</sub> and C<sub>2</sub> isomers are sharper, with four well-defined Q bands. The highest energy band is similar for the three isomers (around 635 nm) but the others are more and more red-shifted with the last one being red shifted 9 nm compared to the C<sub>4h</sub> isomer (740 instead of 731 nm). This indicates that the HOMO-LUMO gap is similar for C<sub>1</sub> and C<sub>2</sub> but higher for the C<sub>4h</sub> isomer, as confirmed by the DFT calculations (See SI for details), which gave a gap of 1.951 eV for the C<sub>4h</sub> isomer compared to 1.917 eV and 1.918 eV for the C<sub>1</sub> and C<sub>2</sub> isomers respectively. The steric hindrance in the C<sub>1</sub> and C<sub>2</sub> isomers twists the naphthalocyanine rings which induces destabilization of the HOMO from -5.02 eV for the C<sub>4h</sub> isomer with its planar naphthalocyanine to -4.97 eV for the C<sub>1</sub> and C<sub>2</sub> isomers.

The UV-Vis spectrum (Figure 5 and Table 2) of the double-decker complexes **Ce[9][10]** and **Ce[9]<sub>2</sub>** further illustrates the increased symmetry with the number of Q bands decreasing from four in the naphthalocyanine ligand **9** to two upon metalation. It is noteworthy that the homoleptic and heteroleptic complexes differ significantly in the visible region with sharper bands observed for **Ce[9][10]** at 635 and 705 nm. While the spectrum of the homoleptic double-decker complex exhibits

similar molar absorption coefficient ( $\epsilon$ ) for both Q bands. For the heteroleptic double-decker complex, they have different values with the band at lower energy similar to those of the homoleptic complex (81400 vs. 75500  $\text{M}^{-1} \text{cm}^{-1}$ ) while the other is much weaker in intensity (28600 vs. 68000  $\text{M}^{-1} \text{cm}^{-1}$ ).



**Figure 5.** Absorption spectra of the double-decker complexes (chloroform,  $c = 10 \cdot 10^{-6} \text{ M}$ , 298 K).

**Table 2.** Absorption parameters of the double-decker complexes (chloroform,  $c = 10 \cdot 10^{-6} \text{ M}$ , 298 K).

	$\lambda_{\text{max}}$ , nm ( $\epsilon_{\text{max}}$ , $10^3 \text{ M}^{-1} \text{ cm}^{-1}$ )
<b>Ce[9][10]</b>	328 (92.7), 382sh (61.6), 577 (23.5), 635sh (28.6), 705 (81.4)
<b>Ce(9)<sub>2</sub></b>	336 (87.0), 370sh (67.3), 477 (26.5), 669sh (68.0), 714 (75.5)

## Conclusion

In this work, we designed and synthesized a cerium (IV) double-decker-based molecular gear composed of a thioether functionalized phthalocyanine anchoring ligand and a helical naphthalocyanine, functionalized with four carbazoles as a rotating cogwheel. Interestingly, the naphthalocyanine ligand **9** was obtained as a mixture of three geometrical isomers two of which are chiral and exhibit high steric hindrance as shown by DFT calculations. Their attributions were made by  $^1\text{H-NMR}$  spectroscopy thanks to their different symmetry groups. The ratio of isomers was also determined and the prochiral  $\text{C}_{4h}$  naphthalocyanine shown to be the major compound (61%).

This heteroleptic  $\text{Ce}^{\text{IV}}$  double-decker complex (**Ce[9][10]**) was difficult to separate from the homoleptic double-deckers complexes **Ce[9]<sub>2</sub>** and **Ce[10]<sub>2</sub>**. Three chromatographies were needed which could explain the yield of only 16%, but the quantity is enough for subsequent STM studies. Work is now underway to deposit these cogwheels on a Au(111) surface and study their rotational

motions. Building a train of gears with control over the chirality of consecutive cogwheels will allow us to verify the assumption that a chirality inversion in successive cogwheels will be helpful to transfer rotation in intermolecular gearing systems.

## Experimental Section

### General methods:

Synthetic procedures were carried out under dry nitrogen atmosphere, unless otherwise specified. All reagents and solvents were purchased at the highest commercial quality available and used without further purification, unless otherwise stated. Anhydrous tetrahydrofuran, chloroform, dichloromethane, isopropanol, Pd(OAc)<sub>2</sub> and P(*t*Bu)<sub>3</sub> were purchased from FUJIFILM Wako Pure Chemical Corporation. 3,6-di-*tert*-butyl-9*H*-carbazole from BLDpharm. Diethyloxalate, 40% methylamine and 3-(4-bromobenzoyl)propanoic acid were purchased from TCI. **1**<sup>[22]</sup> and **10**<sup>[32]</sup> were prepared according to literature procedures. Silica gel column chromatography and thin-layer (TLC) chromatography were performed using CHROMATOREX PSQ 100B and Merck silica gel 60 (F254) TLC plates, respectively. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a JEOL JNM-ECA600 (600 MHz for <sup>1</sup>H; 150 MHz for <sup>13</sup>C) spectrometer, a JEOL JNM-ECZ500 (500 MHz for <sup>1</sup>H; 126 MHz for <sup>13</sup>C) spectrometer, or a JEOL JNM-ECX400P (400 MHz for <sup>1</sup>H; 100 MHz for <sup>13</sup>C) spectrometer at a constant temperature of 293 K unless otherwise specified. Tetramethylsilane (TMS) was used as an internal reference for <sup>1</sup>H and <sup>13</sup>C-NMR measurements in CDCl<sub>3</sub>. A residual solvent peak was used as an internal reference for <sup>1</sup>H-NMR measurements in CD<sub>2</sub>Cl<sub>2</sub> and *o*-DCB-*d*<sup>4</sup>. Chemical shifts ( $\delta$ ) are reported in ppm. Attribution of the signals are given in Scheme 1 and 2. Coupling constants (*J*) are given in Hz and the following abbreviations have been used to describe the signals: singlet (s); broad singlet (br. s); doublet (d); triplet (t); quadruplet (q); quintuplet (qt); multiplet (m). The absorption spectra (UV-vis) were obtained using Hitachi U-3310 spectrometer in chloroform solutions (*c* = 10.10<sup>-6</sup> M for all samples) at room temperature in 1.0 cm quartz cells ( $\lambda$  in nm and  $\epsilon$  in mol<sup>-1</sup>dm<sup>3</sup>cm<sup>-1</sup>), sh for shoulder. EI mass spectrometry was performed using JEOL JMS-700. MALDI-TOF mass spectrometry was performed using JEOL JMS-S300 spectrometer. A CEM Discover SP setup was used for reactions involving microwave irradiation.

### 8-(3,6-di-*tert*-butyl-9*H*-carbazol-9-yl)-2-methyl-1*H*-benzo[*e*]isoindole-1,3(2*H*)-dione (5)

In a Schlenk tube, **4** (1.00 g, 1.0 eq., 3.45 mmol), 3,6-di-*tert*-butyl carbazole (1.45 g, 1.5 eq., 5.17 mmol), sodium *tert*-butoxide (0.40 g, 1.2 eq., 4.14 mmol), palladium(II) acetate (15.49 mg, 2%, 69 mmol), and (*tert*-Bu)<sub>3</sub>PHBF<sub>4</sub> (60 mg, 6%, 0.21 mmol) in 24 mL of dry toluene were stirred at reflux for 20 h. The reaction mixture was cooled down to room temperature and extracted with water and dichloromethane. The organic layer was dried over sodium sulfate removed under reduced pressure and then purified by column chromatography (SiO<sub>2</sub>, hexane:dichloromethane = 3:7) to afford **5** as an orange solid in a 66% yield (1.08 g, 228.4 mmol). Rf value: 0.34 (SiO<sub>2</sub>, hexane:dichloromethane = 3:7).

<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>): δ 9.18 (d, *J* = 2.4 Hz, H<sub>c</sub>, 1H), 8.25 (d, *J* = 8.4 Hz, H<sub>e</sub>, 1H), 8.16 (d, *J* = 1.2 Hz, H<sub>i</sub>, 2H), 8.15 (d, *J* = 9.0 Hz, H<sub>b</sub>, 1H), 7.93 (d, *J* = 8.0 Hz, H<sub>d</sub>, 1H), 7.92 (dd, *J* = 2.0, 8.8 Hz, H<sub>a</sub>, 1H), 7.53 (d, *J* = 7.7 Hz, H<sub>g</sub>, 2H), 7.49 (dd, *J* = 1.6, 8.0 Hz, H<sub>h</sub>, 2H), 3.23 (s, H<sub>f</sub>, 3H), 1.47 (s, H<sub>j</sub>, 18H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>): δ 169.7, 169.1, 143.7, 139.4, 138.7, 135.0, 134.9, 132.3, 130.5, 128.9, 127.6, 124.1, 124.0, 120.8, 118.6, 116.5, 109.3, 34.9, 32.1, 24.1. HR-MS (EI, positive) calcd. for [C<sub>33</sub>H<sub>32</sub>N<sub>2</sub>O<sub>2</sub>]<sup>+</sup>: 488.2464, found: 488.2460 [M]<sup>+</sup>.

#### **Tetra-(3,6-di-*tert*-butyl-9H-carbazol-9-yl)-1,2-naphthalocyanine (9)**

In a two-necked round bottom flask, lithium (3.2 mg, 2 eq., 0.45 mmol) was added to *n*-pentanol (2.0 mL) and the solution was heated at 130°C until total dissolution. The reaction mixture was then cooled to room temperature and **8** (103.4 mg, 1 eq., 0.23 mmol) was added. The solution was refluxed for 18 h to give a dark green solution which was neutralized with concentrated hydrochloric acid (1.5 mL). 8 mL of methanol was added to the solution while stirring and kept undisturbed for 1h. The fine green precipitate was filtered and washed with methanol. The green solid was dried under vacuum at 40°C for 2 h and purified by gradient column chromatography on silica (hexane:dichloromethane = 3:1 to chloroform). C<sub>4h</sub> isomer eluted first as a green band followed by C<sub>1</sub> and C<sub>2</sub> isomers respectively. Three fractions were isolated corresponding to the three geometrical isomers. All isomers were obtained as green solid. C<sub>4h</sub> isomer in a 36% yield (37.3 mg, 20.4 mmol), C<sub>1</sub> in a 20% yield (20.5 mg, 11.2 mmol), and the C<sub>2</sub> isomer in a 9% yield (9.2 mg, 5.04 mmol). Rf values are 0.66 for C<sub>4h</sub>, 0.53 for C<sub>1</sub> and 0.50 for C<sub>2</sub> (hexane:dichloromethane 2:3)

C<sub>4h</sub> isomer: <sup>1</sup>H-NMR (600 MHz, *o*-DCB-*d*<sup>4</sup>, 95 °C): δ 10.98 (s, H<sub>c</sub>, 4H), 8.62 (s, H<sub>e</sub>, 4H), 8.50 (s, H<sub>i</sub>, 8H), 8.12 (d, *J* = 6.0 Hz, H<sub>h</sub>, 8H), 8.04 (d, *J* = 7.2 Hz, H<sub>a</sub>, 4H), 7.98 (d, *J* = 6.6 Hz, H<sub>d</sub>, 4H), 7.86 (d, *J* = 6.6 Hz, H<sub>b</sub>, 4H), 7.58 (s, H<sub>g</sub>, 8H), 1.74 (s, H<sub>j</sub>, 72H); <sup>13</sup>C-NMR (150 MHz, *o*-DCB-*d*<sup>4</sup>, 25 °C): δ 137.9, 124.6, 124.5,



121.7, 120.8, 116.9, 109.5, 34.8, 32.4. (Quaternary carbons are not seen); HR-MS (MALDI-TOF, positive) calcd. for  $[C_{128}H_{118}N_{12}]^+$ : 1822.9597, found: 1822.9602  $[M]^+$ ; UV-vis (chloroform)  $\lambda_{\max}$  ( $\epsilon$ ): 299 (85990), 352, (55600), 373 (50300), 635 (23100, sh) 679 (54700, b), 697 (56300, b), 731 (31000, sh).

**C<sub>1</sub> isomer** : **C<sub>1</sub> isomer** :  $^1\text{H-NMR}$  (600 MHz, *o*-DCB- $d^4$ , 95 °C):  $\delta$  11.39 (s, H<sub>c</sub>, 1H), 11.34 (s, H<sub>c</sub>, 1H), 11.30 (bs, H<sub>c</sub>, 2H), 9.56 (d,  $J$  = 6.4 Hz, H<sub>e</sub>, 1H), 9.45 (d,  $J$  = 6.8 Hz, H<sub>e</sub>, 1H), 9.21 (d,  $J$  = 8.4 Hz, H<sub>e</sub>, 1H), 8.98 (s, H<sub>e</sub>, 1H), 8.58 – 7.33 (m, H<sub>a,b,d,f,g,h,i</sub>, 36H), 1.70 (s, H<sub>j</sub>, 18H), 1.62 (s, H<sub>j</sub>, 18H), 1.61 (s, H<sub>j</sub>, 18H), 1.54 (s, H<sub>j</sub>, 18H); HR-MS (MALDI-TOF, positive) calcd. for  $[C_{128}H_{118}N_{12}]^+$ : 1822.9597, found: 1822.9597  $[M]^+$ ; UV-vis (chloroform)  $\lambda_{\max}$  ( $\epsilon$ ): 299 (62500), 370 (51620), 636 (21730, sh), 666 (31220, sh), 704 (56850), 740 (69230).

**C<sub>2</sub> isomer** :  $^1\text{H-NMR}$  (600 MHz, *o*-DCB- $d^4$ , 95 °C):  $\delta$  11.72 (s, H<sub>c</sub>, 2H), 11.32 (s, H<sub>c</sub>, 2H), 9.68 (d,  $J$  = 8.8 Hz, H<sub>e</sub>, 2H), 9.31 (d,  $J$  = 8.0 Hz, H<sub>e</sub>, 2H), 8.67 – 7.60 (m, H<sub>a,b,d,f,g,h,i</sub>, 36H), 1.65 (s, H<sub>j</sub>, 36H), 1.52 (s, H<sub>j</sub>, 36H); HR-MS (MALDI-TOF, positive) calcd. for  $[C_{128}H_{118}N_{12}]^+$ : 1822.9597, found: 1822.9607  $[M]^+$ ; UV-vis (CHCl<sub>3</sub>)  $\lambda_{\max}$  ( $\epsilon$ ): 299 (69240), 371 (54840), 634 (21490, sh), 669 (32400, sh), 704 (61300), 739 (77300).

### **Heteroleptic Ce<sup>IV</sup> double-decker complex-Molecular gear Ce[9][10]**

In a 10 mL microwave vial, **9** (20.8 mg, 1.0 eq., 11.37  $\mu\text{mol}$ ), **10** (164 mg, 10.0 eq., 113.7  $\mu\text{mol}$ ) and Ce(acac)<sub>3</sub>.nH<sub>2</sub>O (27.3 mg, 5.5 eq., 62.6  $\mu\text{mol}$ ) were mixed in 4 mL of *o*-dichlorobenzene. The sample was then heated using microwave irradiation to 270 °C for 1 h. After the TLC in hexane:dichloromethane (1:1) showed the full consumption of **9** (confirmed by MALDI-TOF-MS), the reaction mixture was cooled down and concentrated under vacuum. The oily crude material was purified by column chromatography on silica eluted with chloroform This all green band was collected and subjected to size-exclusion column chromatography (Biobeads SX-1, 4x65 cm) with dichloromethane:toluene (2:1). The second green band was collected and subjected to a third column chromatography on silica eluting with a gradient eluent of hexane: dichloromethane (7:3, 1:1 and pure dichloromethane) + 1% triethylamine. The heteroleptic double-decker complex **Ce[9][10]** was collected in 16% yield (6.0 mg, 1.76  $\mu\text{mol}$ ) as a dark green-blue powder.

R<sub>f</sub> = 0.28 (SiO<sub>2</sub>, Hexane: dichloromethane 1:1 + 1% triethylamine).  $^1\text{H-NMR}$  (400 MHz, *o*-DCB- $d^4$ , 333 K):  $\delta$  11.15 (s, H<sub>c</sub>, 4H), 9.31 (d,  $J$  = 8.4Hz, H<sub>e</sub>, 1H), 9.16 (s broad, H<sub>k</sub>, 3H), 8.98 (s broad, H<sub>k</sub>, 1H), 8.62 (s, H<sub>i</sub>, 8H), 8.61 (d,  $J$  = 8.4 Hz, H<sub>a</sub>, 4H), 8.56 (d,  $J$  = 8.4 Hz, H<sub>c</sub>, 4H), 8.50 (s broad, H<sub>k</sub>, 4H), 8.40 (d,  $J$  =

8.8 Hz, H<sub>h</sub>, 8H), 8.35 (d, J = 8.4 Hz, H<sub>b</sub>, 4H), 7.84 (d, J = 7.6 Hz, H<sub>g</sub>, 8H), 3.02 (m, SCH<sub>2</sub>, 16H), 1.74 (s, H<sub>i</sub>, 72H), 0.8-1.6 (m, SCH<sub>2</sub>(CH<sub>2</sub>)<sub>4</sub>CH<sub>3</sub>, 88H); <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub> : δ 174.3, 167.9, 145.9, 143.8, 142.9, 140.8, 139.1, 138.7, 136.0, 133.3, 132.6, 132.0, 131.8, 131.0, 130.3, 130.0, 129.7, 128.9, 124.6, 124.4, 121.8, 120.8, 120.2, 116.5, 71.6, 68.3, 66.8, 38.9, 38.8, 35.2, 34.6, 34.3, 33.5, 32.5, 31.9, 31.6, 30.6, 30.5, 29.9, 29.3, 29.1, 28.7, 25.2, 23.9, 23.1, 22.9, 14.5, 14.4, 14.3, 14.2; UV-vis (chloroform) λ<sub>max</sub> (ε) : 328 (92700, Soret band), 382 (61600, sh), 577 (23500), 635 (28600, sh), 705 (81400, Q band); HR-MS (MALDI-TOF, positive): m/z calculated for [C<sub>208</sub>H<sub>228</sub>CeN<sub>20</sub>S<sub>8</sub>]<sup>+</sup> 3401.5271, found : 3401.5375.

Electronic supplementary information (ESI) are available with additional synthetic procedures for compounds **1**, **2**, **3**, **4**, **6**, **7** and **8** as well as the <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, HR-MS for **9**, and molecular gear **Ce[9][10]**. DFT calculations of all the optimized geometries for geometrical isomers of **9** are also given.

## Acknowledgements

This work has received funding from the JSPS KAKENHI Grant-in-Aid for Basic Research A (22H00325). The University Paul Sabatier (Toulouse) and NAIST are acknowledged for providing a crossed position to GR and the CNRS for their support through the International Research Project POEMES (2024-2028). Dr. Marine Louis is also warmly thanked for her contribution to the optimization of the Buchwald-Hartwig amination reaction (**5**) and Ms. Yoshiko Nishikawa for her contribution to the measurements of HR-MS spectra.

**Keywords:** Molecular Gear • Double-Decker Complex • Cerium • Helicity • Naphthalocyanine

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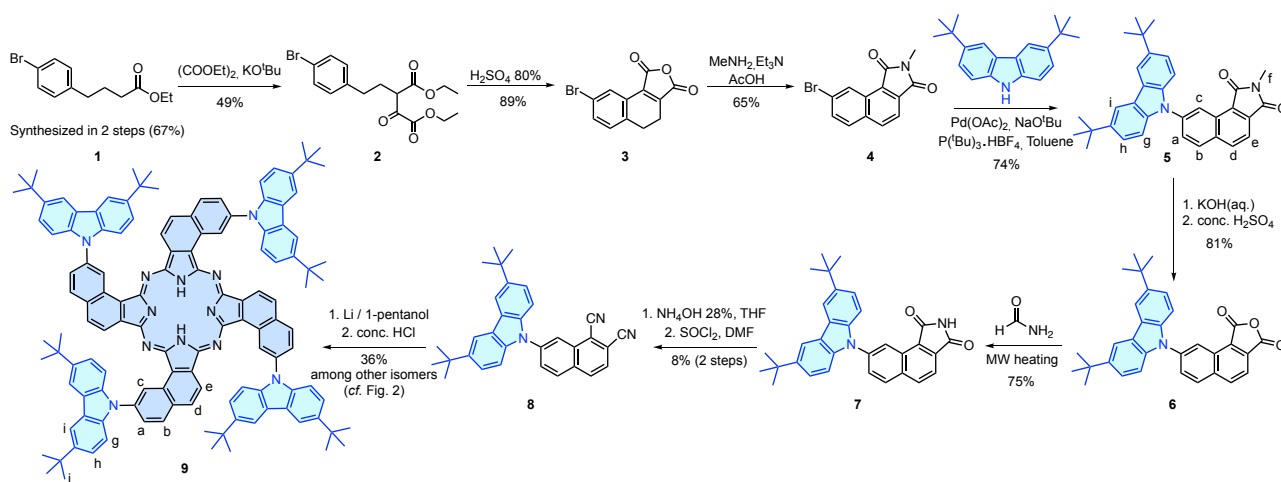
## Supporting Information

<b>1. Additional synthetic procedures</b>	page S2
a. Synthesis of <b>1</b>	page S2
b. Synthesis of <b>2</b>	page S3
c. Synthesis of <b>3</b>	page S3
d. Synthesis of <b>4</b>	page S3
e. Synthesis of <b>6</b>	page S4
f. Synthesis of <b>7</b>	page S4
g. Synthesis of <b>8</b>	page S5
<b>2. <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass spectra</b>	page S7
a. Naphthalocyanine ligand <b>9</b>	page S7
b. Molecular gear heteroleptic double-decker <b>Ce[9][10]</b>	page S11
<b>3. DFT calculations (B3LYP / 6-31G(d))</b>	page S15
<b>Cartesian coordinates of all the optimized geometries for geometrical isomers of <b>9</b></b>	page S15
a. C <sub>4h</sub> symmetry isomer	page S15
b. C <sub>1</sub> symmetry isomer	page S21
c. C <sub>2</sub> symmetry isomer	page S27
d. D <sub>2</sub> symmetry isomer	page S33
e. C <sub>2h</sub> symmetry isomer	page S39

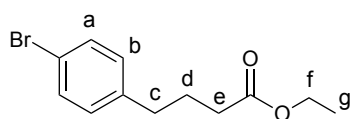
## 1. Additional synthetic procedures

Synthesis of the carbazole-functionalized benzo[e]isoindole-1,3(2H)-dione **5**, the naphthalocyanine ligand **9**, the phthalocyanine ligand **10** and the molecular gear double-decker **11** are given in the main part of the manuscript.

The numbering of the molecules is given in the following figure.



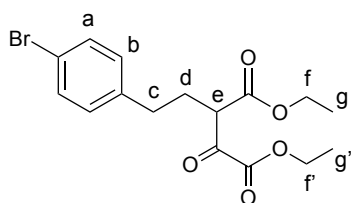
### a. Synthesis of **1**



Compound **1** was synthesized by following a modified reported procedure.<sup>[11]</sup> Ethyl 4-(4-bromophenyl)butanoate (2.94 g, 1 eq., 12 mmol) and ethanol (60.3 mL, 86 eq., 1.032 mol) were added in a round bottom-flask with a magnetic stir bar. Conc. H<sub>2</sub>SO<sub>4</sub> (0.90 mL, 1.4 eq., 0.017 mol) was then added dropwise and the reaction mixture refluxed for 5 h. The reaction was monitored by TLC using ethyl acetate/hexane (1:4) as eluant. The reaction mixture was concentrated using rotary evaporator and the resulting residue was extracted twice with ethyl acetate and washed with water. The organic layer was collected and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After filtration and evaporation of the solvent, the crude mixture was purified by column chromatography on silica gel with ethyl acetate/hexane (30:1) as eluant. With a R<sub>f</sub> value of 0.18, **1** was obtained as a colorless oil in a 96% yield (3.13 g). <sup>1</sup>H-NMR of compound **1** was in agreement with the literature.<sup>[11]</sup>

<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>): δ 7.40 (d, *J* = 8.4 Hz, H<sub>a</sub>, 2H), 7.05 (d, *J* = 8.0 Hz, H<sub>b</sub>, 2H), 4.12 (q, *J* = 7.2 Hz, H<sub>f</sub>, 2H), 2.61 (t, *J* = 7.2 Hz, H<sub>c</sub>, 2H), 2.30 (t, *J* = 7.6 Hz, H<sub>e</sub>, 2H), 1.92 (qt, *J* = 7.2 Hz, H<sub>d</sub>, 2H), 1.25 (t, *J* = 7.2 Hz, H<sub>g</sub>, 3H).

## b. Synthesis of **2**



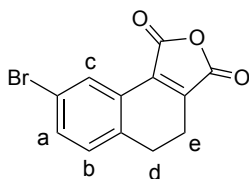
Potassium *tert*-butoxide (0.99 g, 1.2 eq., 8.86 mmol) in dry THF (4 mL) was cooled to 10 °C. Diethyl oxalate (1.5 mL, 11.07 mmol, 1.5 eq.) and **1** (2.00 g, 1 eq., 7.38 mmol) were dissolved in dry THF (4 mL) and added dropwise to the cold <sup>t</sup>BuOK solution to maintain the reaction temperature below 25°C. The ice bath was then removed and the reaction allowed to stir at room temperature for 19 h. The reaction was quenched with 100 g of ice and THF was removed under vacuum. The solution was then extracted twice with Et<sub>2</sub>O and the combined organic phase washed twice with 1 M NaOH. The aqueous layers were combined and acidified with concentrated HCl to pH 1 and extracted with Et<sub>2</sub>O. The Et<sub>2</sub>O phase was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated to yield 1.34 g (49%) of **1** with traces of diethyl oxalate, which was used in the next step without any more purification. R<sub>f</sub> value 0.31 in CH<sub>2</sub>Cl<sub>2</sub>/hexane (2:1).

<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>): δ 7.40 (AA'BB' system, H<sub>a</sub>, 2H), 7.06 (AA'BB' system, H<sub>b</sub>, 2H), 4.33 (q, *J* = 7.0 Hz, H<sub>f</sub>, 2H), 4.19 (dq, *J* = 7.0 Hz, H<sub>f'</sub>, 2H), 4.01 (t, *J* = 7 Hz, H<sub>e</sub>, 1H), 2.68-2.58 (m, H<sub>c</sub>, 2H), 2.28-2.15 (m, H<sub>d</sub>, 2H), 1.37 (t, *J* = 7.0 Hz, H<sub>g'</sub>, 3H), 1.25 (t, *J* = 7.5 Hz, H<sub>g</sub>, 3H).

<sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>): δ 189.0, 168.8, 160.4, 139.5, 131.7, 131.4, 130.5, 130.4, 120.2, 63.0, 61.9, 53.2, 32.53, 28.7, 14.1, 14.1.

HR-MS (EI, positive): *m/z* calculated for [C<sub>16</sub>H<sub>19</sub>BrO<sub>5</sub>]<sup>+</sup> 370.0416; 370.0425 (found).

## c. Synthesis of **3**



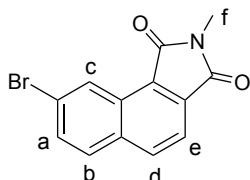
**3** (3.00 g, 1.0 eq., 8.08 mmol) was added to an ice-cold solution of 80% H<sub>2</sub>SO<sub>4</sub> (27.0 mL). The ice bath was removed and the reaction was stirred at room temperature for 6 h. The reaction was then poured onto 3 g of ice under vigorous stirring and the resulting yellow solid was collected by filtration, washed with water and dried. The product was recrystallized from a 1:1 mixture of EtOAc:MeCN to give **3** in a 89% yield (2.01 g).

<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>): δ 8.20 (d, *J* = 2.0 Hz H<sub>c</sub>, 1H), 7.54 (dd, *J* = 2.0, 8.0 Hz, H<sub>a</sub>, 1H), 7.17 (d, *J* = 8.0 Hz, H<sub>b</sub>, 1H), 3.06 (t, *J* = 8.4 Hz, H<sub>e</sub>, 2H), 2.81 (t, *J* = 8.4 Hz, H<sub>d</sub>, 2H).

**<sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>):** δ 163.9, 162.9, 141.6, 138.4, 135.7, 134.9, 129.2, 129.1, 126.8, 121.4, 26.6, 18.6.

**HR-MS (EI, positive):** m/z calculated for [C<sub>12</sub>H<sub>7</sub>BrO<sub>3</sub>]<sup>+</sup> 277.9579; 277.9578 (found).

#### d. Synthesis of **4**



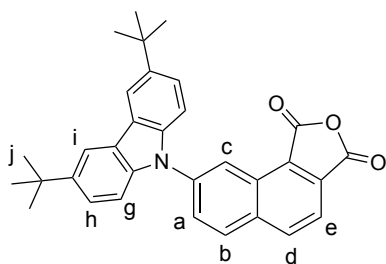
To a suspension of **3** (3.00 g, 1.0 eq., 10.75 mmol) in 250 mL pure acetic acid was added 40% methylamine (1.67 g, 2.0 eq., 21.50 mmol) at 0°C and triethylamine (34.5 mL, 23.0 eq., 10.75 mmol) was added dropwise under a vigorous stirring. The resulting mixture was refluxed at 120°C for 24 h. After cooling, the resulting precipitate was collected by filtration, washed with MeOH and dried in vacuo to give **4** as yellow powder in a 69% yield (2.17 g).

**<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>):** δ 9.11 (d, *J* = 2.0 Hz, H<sub>c</sub>, 1H), 8.13 (d, *J* = 8.0 Hz, H<sub>e</sub>, 1H), 7.87 (d, *J* = 8.4 Hz, H<sub>d</sub>, 1H), 7.82 (d, *J* = 8.8 Hz, H<sub>b</sub>, 1H) 7.72 (dd, *J* = 2.4, 9.2 Hz, H<sub>a</sub>, 1H), 3.23 (s, H<sub>f</sub>, 3H).

**<sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>):** δ 169.3, 168.7, 134.9, 132.4, 132.3, 130.8, 128.8, 127.2, 126.6, 124.5, 118.9, 24.1.

**HR-MS (EI, positive):** m/z calculated for [C<sub>16</sub>H<sub>19</sub>BrO<sub>5</sub>]<sup>+</sup> 288.9738; 288.9733 (found).

#### e. Synthesis of **6**



Potassium hydroxide (1.79 g, 12 eq., 31.93 mmol) was dissolved in 4.2 mL of water and heated to 60°C. Compound **5** (1.30 g, 1.0 eq., 2.66 mmol) was added while stirring vigorously and then refluxed for 24h. The resulting whitish-green suspension was cooled down to 0°C and conc. H<sub>2</sub>SO<sub>4</sub> was added dropwise while stirring until the pH reach a value of 1. After refluxing for 15 h, the orange suspension was cooled down, filtered and washed with water to remove the excess of acid. The solid was dried at 100°C under vacuum for 6 h and afford **6** as an orange solid in a 93% yield (1.18 g)

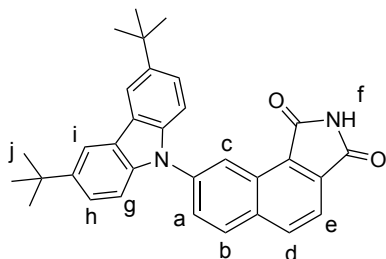
**<sup>1</sup>H-NMR (400. MHz, CDCl<sub>3</sub>):** δ 9.09 (d, *J* = 2.0 Hz, H<sub>c</sub>, 1H), 8.41 (d, *J* = 8.4 Hz, H<sub>e</sub>, 1H), 8.25 (d, *J* = 8.8 Hz, H<sub>b</sub>, 1H), 8.17 (d, *J* = 1.2 Hz, H<sub>i</sub>, 2H), 8.08 (dd, *J* = 2.4, 8.8 Hz, H<sub>a</sub>, 1H), 8.0 (d, *J* = 8.4 Hz, H<sub>d</sub>, 1H), 7.53 (d, *J* = 8.4 Hz, H<sub>g</sub>, 2H), 7.50 (dd, *J* = 1.6, 8.4 Hz, H<sub>n</sub>, 2H), 1.48 (s, H<sub>j</sub>, 18H).



**<sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>):** δ 163.3, 163.2, 144.2, 140.7, 138.6, 137.3, 135.4, 131.9, 130.9, 129.3, 129.0, 127.2, 124.2, 124.1, 120.6, 119.5, 116.7, 109.1, 34.9, 32.0

**HR-MS (EI, positive):** m/z calculated for [C<sub>32</sub>H<sub>29</sub>NO<sub>3</sub>]<sup>+</sup> 475.2147; 475.2146 (found).

#### f. Synthesis of **7**



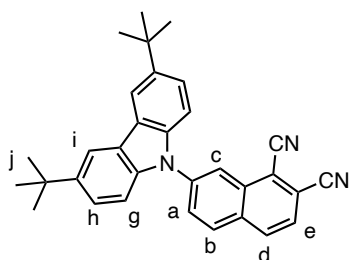
**6** (186 mg, 1.0 eq., 0.391 mmol) and formamide (1.6 mL, 100 eq., 39.11 mmol) were added in a 10 mL microwave vial and sealed with a cap. The mixture was stirred until the product was completely wetted and microwaved at 200°C for 3 cycles of 1 min with 15 s of pre-stirring. The mixture was cooled to 0°C and ice-cold water (1.6 mL) was added into the tube. The solid was filtrated, washed with water and cold hexane and dried under reduced pressure. The crude mixture was purified by column chromatography on silica with CH<sub>2</sub>Cl<sub>2</sub> as eluant to afford compound **7** in a 72% yield (133.9 mg).

**<sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>):** δ 11.41 (s, H<sub>f</sub>, 1H), 8.96 (d, *J* = 2.0 Hz, H<sub>c</sub>, 1H), 8.53 (d, *J* = 8.4 Hz, H<sub>e</sub>, 1H), 8.44 (d, *J* = 8.8 Hz, H<sub>b</sub>, 1H), 8.36 (d, *J* = 1.6 Hz, H<sub>i</sub>, 2H), 8.05 (dd, *J* = 2.0, 8.8 Hz, H<sub>a</sub>, 1H), 7.92 (d, *J* = 8.0 Hz, H<sub>d</sub>, 1H), 7.52 (dd, *J* = 2.0, 8.8 Hz, H<sub>h</sub>, 2H), 7.48 (d, *J* = 8.0 Hz, H<sub>g</sub>, 2H), 1.43 (s, H<sub>j</sub>, 18H)

**<sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>):** δ 171.2, 170.1, 143.8, 138.8, 138.6, 135.8, 135.1, 133.3, 131.8, 128.6, 127.7, 127.6, 124.5, 123.9, 119.9, 117.5, 109.5, 35.1, 32.3.

**HR-MS (EI, positive):** m/z calculated for [C<sub>32</sub>H<sub>30</sub>N<sub>2</sub>O<sub>2</sub>]<sup>+</sup> 474.2307; 474.2300 (found).

#### g. Synthesis of **8**



**7** (428 mg, 1.0 eq., 902 mmol,) was dissolved in 8 mL of THF in round-bottom flask. 28% ammonium hydroxide (4mL) was added at 0°C to the solution and capped with a rubber septum. The mixture was stirred at room temperature for 96 h and the precipitate formed was filtered, washed with water and dried at 60°C. The crude diamide was engaged in the dehydration step, performed in a two-necked round-bottom flask equipped with a stir bar and a nitrogen inlet. The solid was dissolved in dry DMF (5 mL) and SOCl<sub>2</sub> (0.3 mL, 5.0 eq., 4.5 mmol) was added dropwise with a syringe to the

stirred solution cooled to  $-15^{\circ}\text{C}$ . The reaction mixture was stirred for further 2 h at  $0^{\circ}\text{C}$ , at room temperature for overnight, and finally carefully poured onto ice. The suspension was filtered and the yellow solid obtained was washed with water and dissolved in  $\text{CHCl}_3$ . The organic solution was washed with 5% aqueous  $\text{NaHCO}_3$ , brine and dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the residue purified by gradient column chromatography (silica gel, 1:1 hexane: $\text{CHCl}_3$  to  $\text{CHCl}_3$ ) to afford compound **8** as a yellow solid in a 8% yield (33.3 mg).

**$^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ):**  $\delta$  8.53 (s,  $\text{H}_c$ , 1H), 8.28 (d,  $J = 9.0$  Hz,  $\text{H}_e$ , 1H), 8.21 (d,  $J = 9.0$  Hz,  $\text{H}_d$ , 1H), 8.17 (s,  $\text{H}_i$ , 1H), 8.08 (dd,  $J = 1.2, 8.4$  Hz,  $\text{H}_a$ , 1H), 7.93 (d,  $J = 8.0$  Hz,  $\text{H}_b$ , 1H), 7.81 (d,  $J = 8.4$  Hz,  $\text{H}_g$ , 1H), 7.52 (dd,  $J = 1.8, 8.4$  Hz,  $\text{H}_h$ , 2H), 7.50 (d,  $J = 8.4$  Hz,  $\text{H}_g$ , 2H), 1.47 (s,  $\text{H}_j$ , 18H)

**$^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ ):**  $\delta$  144.3, 140.5, 138.4, 133.6, 133.3, 132.3, 130.8, 129.2, 126.6, 124.2, 121.3, 116.6, 116.2, 115.9, 114.9, 114.4, 108.9, 34.8, 31.9.

**HR-MS (EI, positive):**  $m/z$  calculated for  $[\text{C}_{32}\text{H}_{29}\text{N}_3]^+$  455.2361; 455.2359 (found).

## 2. $^1\text{H-NMR}$ , $^{13}\text{C-NMR}$ and Mass spectra

### a. Naphthalocyanine ligand **9**

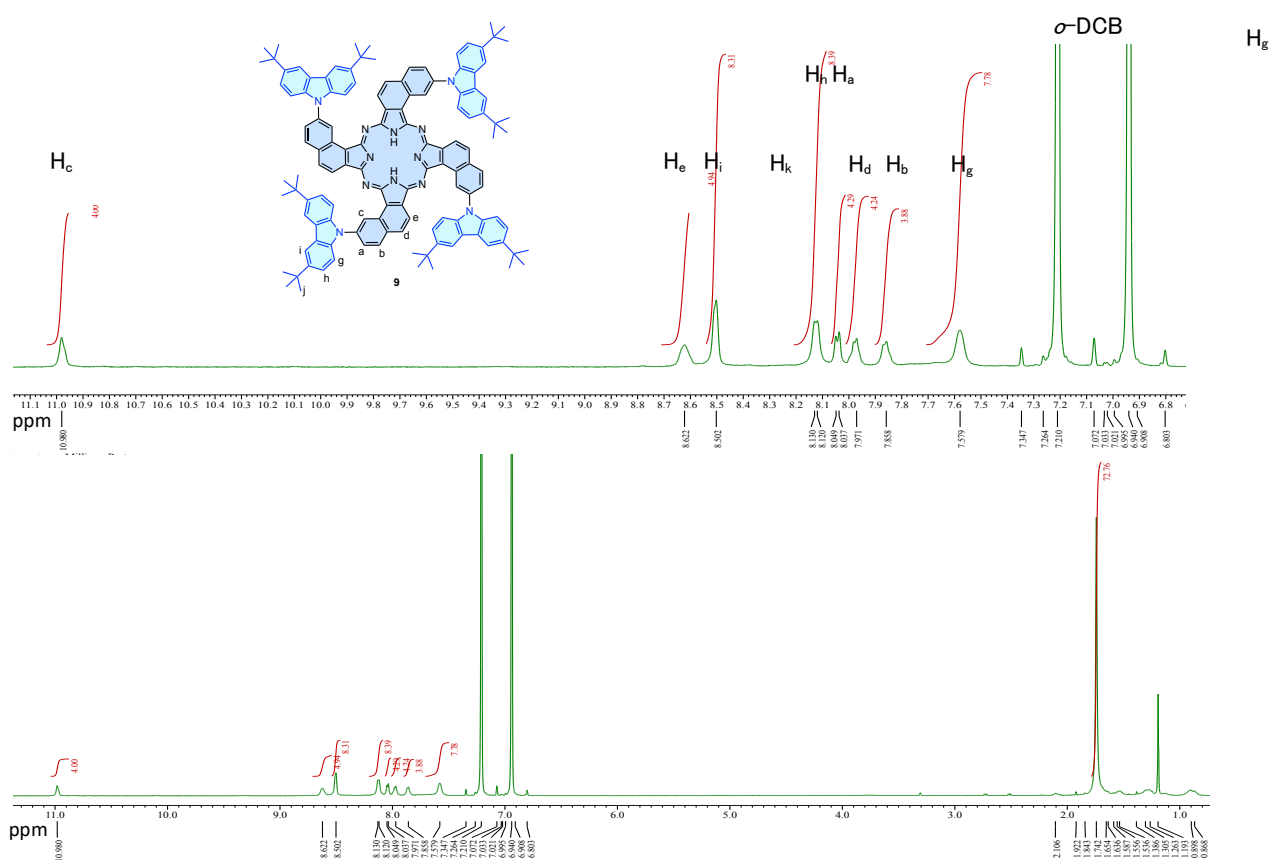


Figure S1.  $^1\text{H-NMR}$  spectrum of **9-C<sub>4h</sub>** (600 MHz,  $o\text{-DCB-}d^4$ , 368 K).

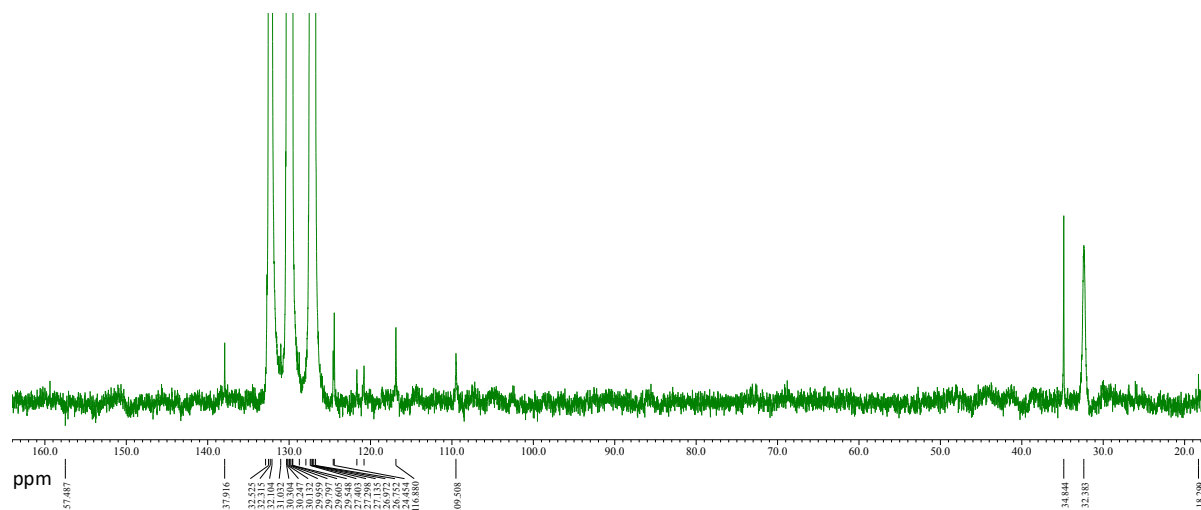
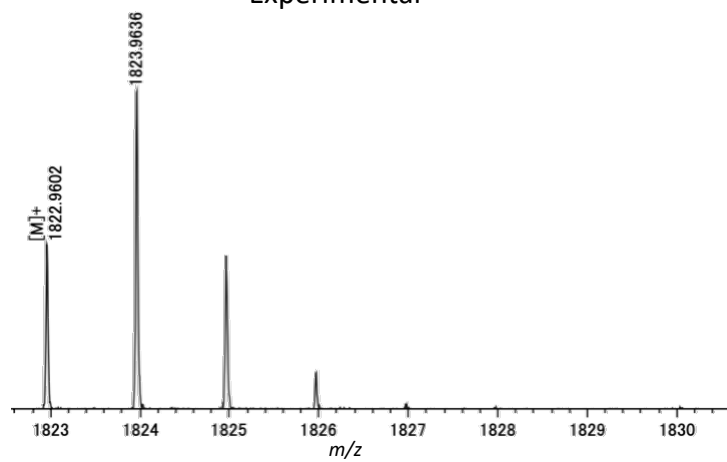


Figure S2.  $^{13}\text{C-NMR}$  spectrum of **9-C<sub>4h</sub>** (150 MHz,  $o\text{-DCB-}d^4$ , 298 K).

### Experimental



### Simulation

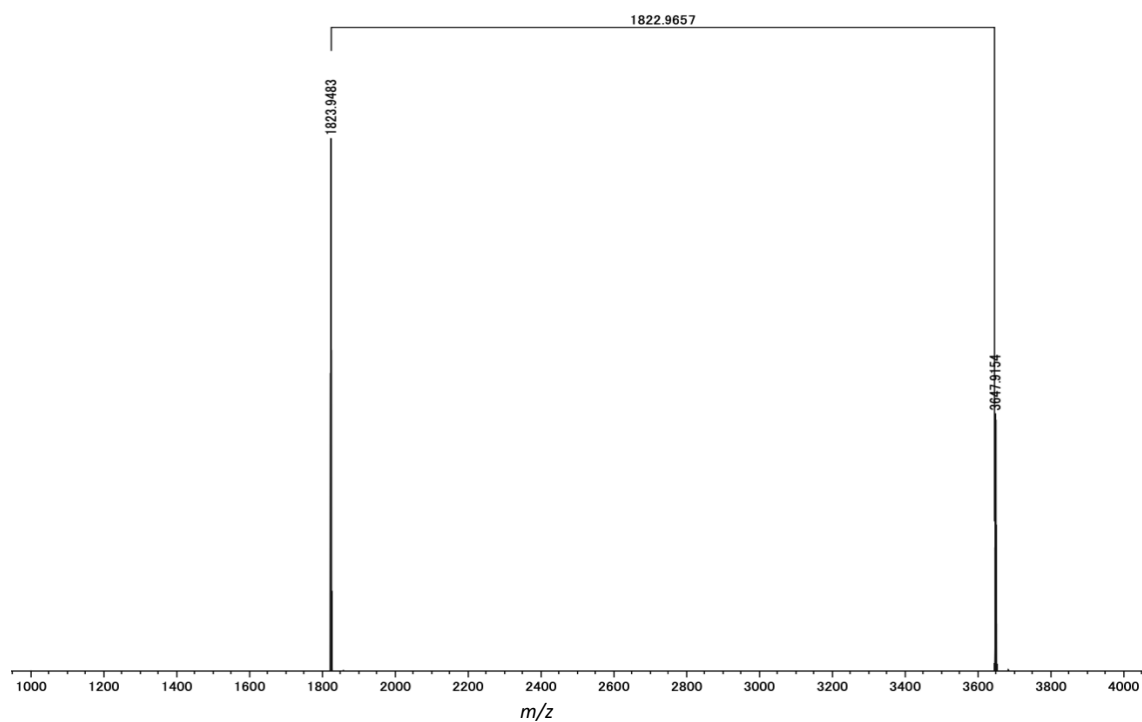
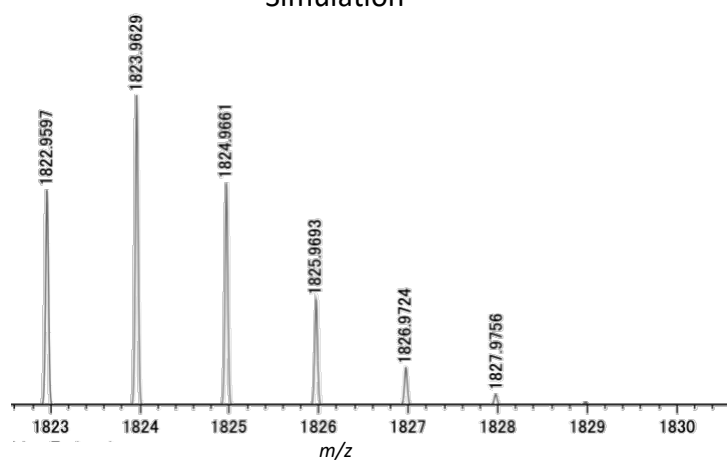


Figure S3. MALDI-TOF mass spectrum of **9-C<sub>4h</sub>** (positive mode).

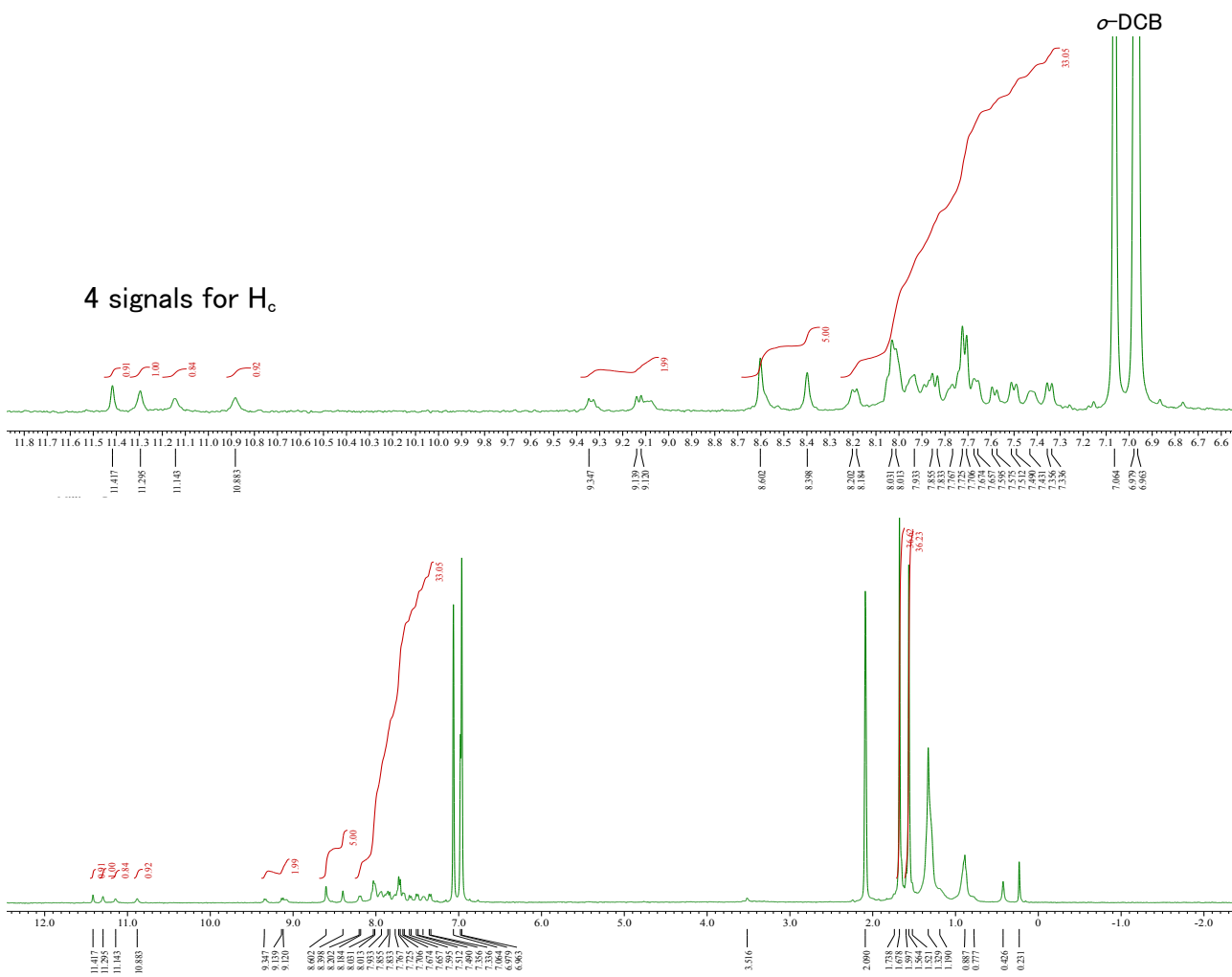


Figure S4. <sup>1</sup>H-NMR spectrum of **9-C<sub>1</sub>** (400 MHz, C<sub>6</sub>D<sub>6</sub>, 368 K).

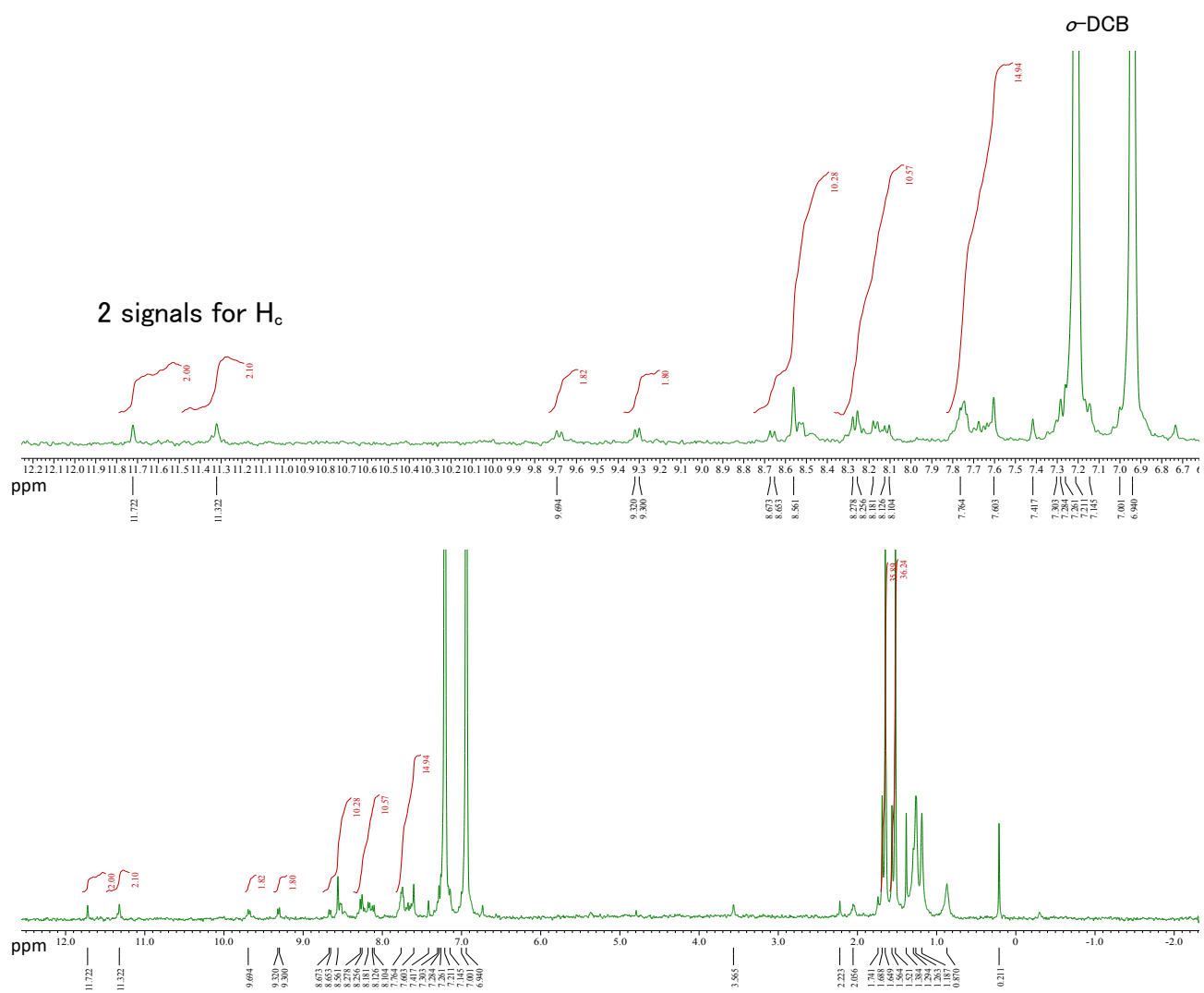


Figure S5. <sup>1</sup>H-NMR spectrum of **9-C<sub>2</sub>** (400 MHz, *o*-DCB-*d*<sup>6</sup>, 368 K).

**b. Molecular gear heteroleptic double-decker Ce[9][10]**

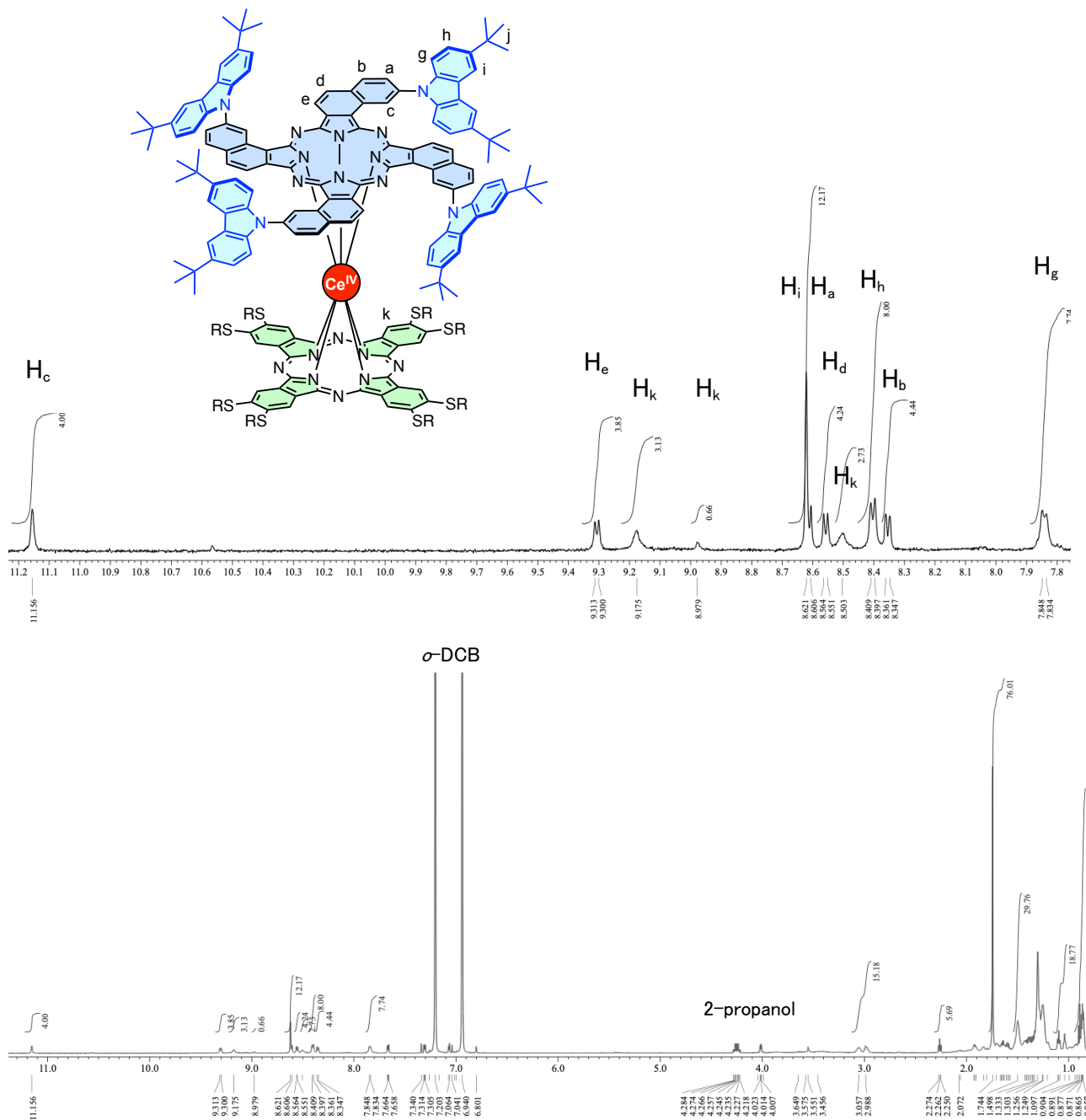


Figure S6. <sup>1</sup>H-NMR spectrum of the heteroleptic double-decker **Ce[9][10]** (400 MHz, *o*-DCB-*d*<sup>4</sup>, 333 K). Full spectrum (bottom) and zoom on the 7.8-11.2 ppm aromatic region.

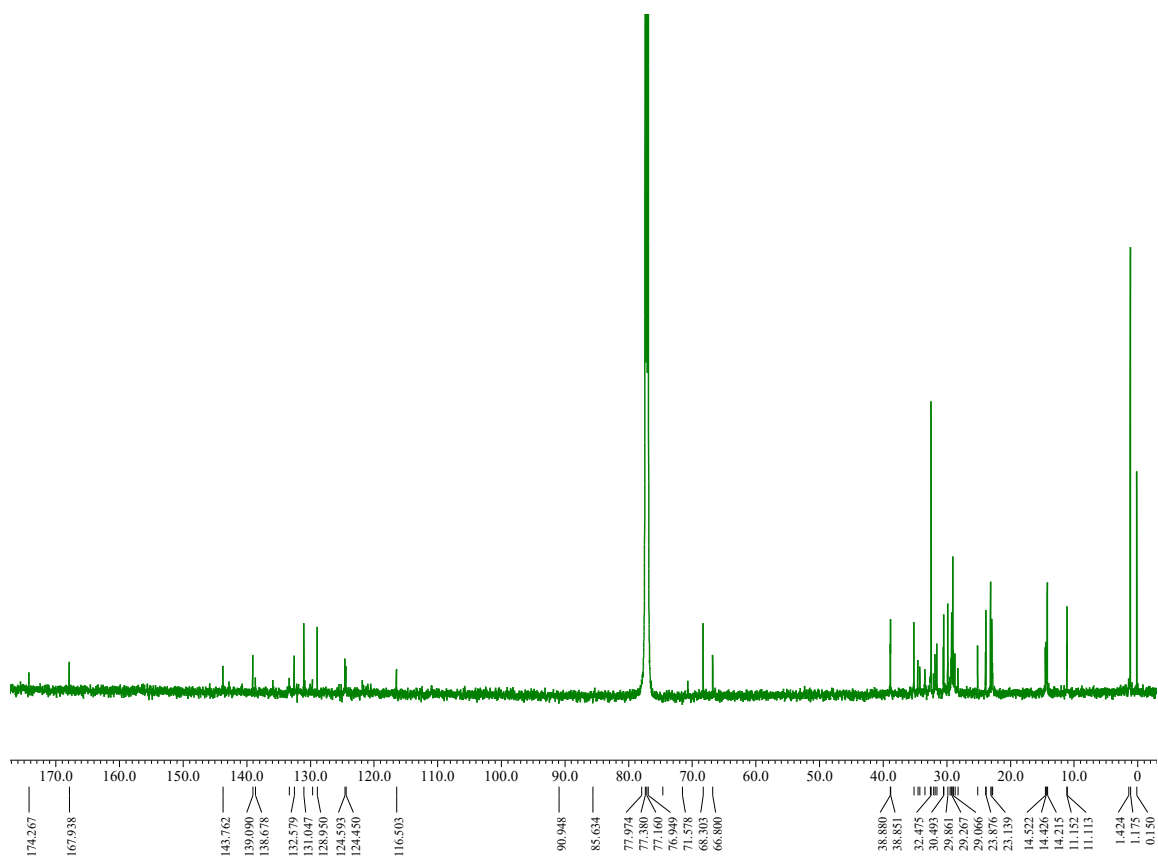


Figure S7.  $^{13}\text{C}$ -NMR spectrum of the heteroleptic double-decker double-decker  $\text{Ce}[\mathbf{9}][\mathbf{10}]$  (150 MHz,  $\text{CDCl}_3$ , 298K).



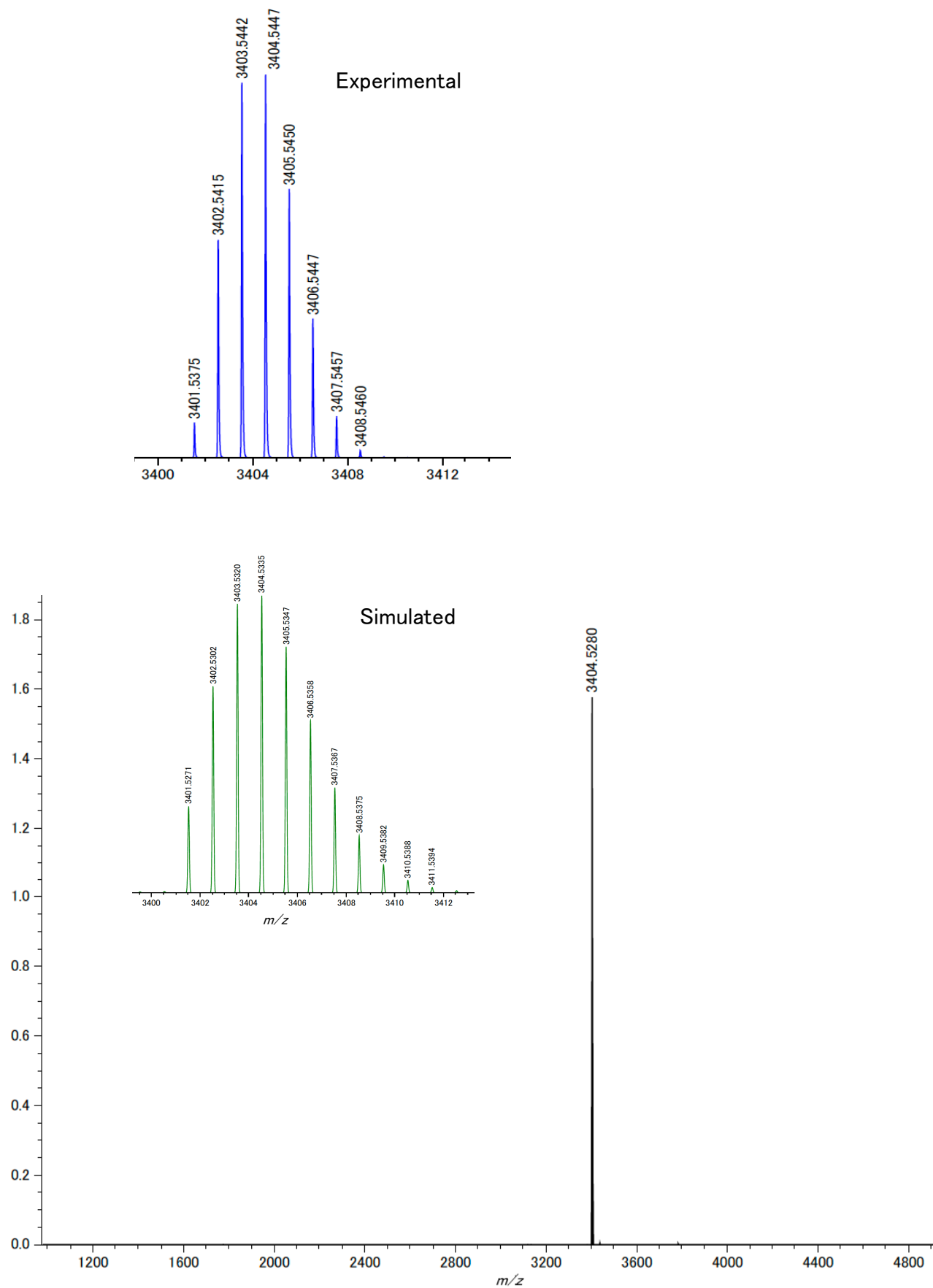


Figure S8. MALDI-TOF mass spectrum of heteroleptic double-decker **Ce[9][10]** (positive mode), full spectrum (bottom) and isotopic pattern of the molecular peak.

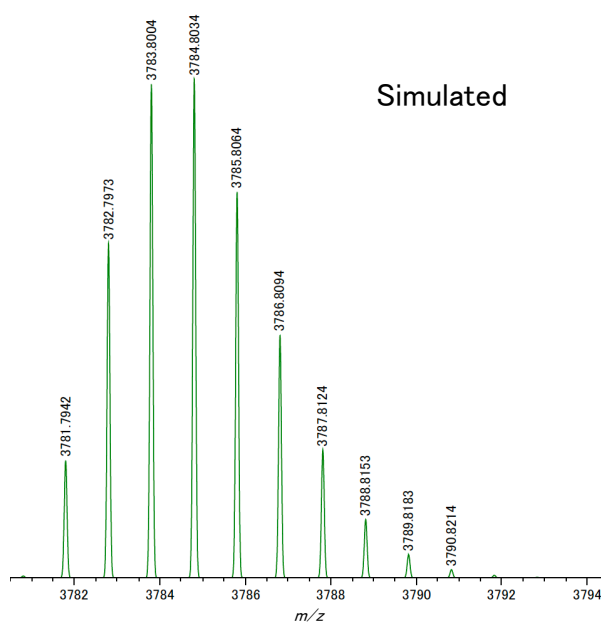
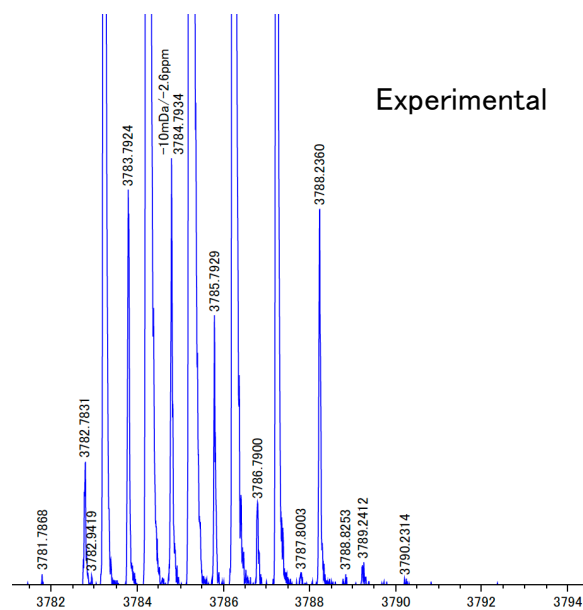


Figure S9. MALDI-TOF mass spectrum of homoleptic double-decker **Ce[9]<sub>2</sub>** (positive mode). The additional peaks in the measurements correspond to the polyethylene Glycol 3000 used for calibration.

### 3. DFT calculations

DFT calculations using the functional B3LYP with basis sets 6–31 G(d) were carried out with the suite of programs Gaussian16.

Reference : Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

#### Cartesian coordinates of all the optimized geometries for geometrical isomers of 9

##### a. C<sub>4h</sub> symmetry isomer

Standard orientation:

-----					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
-----					
1	7	0	-0.519067	1.874600	-0.129895
2	7	0	0.519064	-1.874618	-0.129889
3	6	0	-2.375631	-1.838861	-0.149191
4	6	0	-3.825662	-1.792549	-0.175286
5	6	0	-4.217408	-0.444998	-0.154912
6	6	0	-3.005801	0.355419	-0.137945
7	6	0	-1.789850	2.362531	-0.145802
8	6	0	-1.788831	3.829312	-0.160272
9	6	0	-0.451124	4.214212	-0.133975
10	6	0	0.313275	2.959428	-0.128813
11	6	0	2.375626	1.838843	-0.149189
12	6	0	3.825657	1.792531	-0.175275
13	6	0	4.217404	0.444981	-0.154904
14	6	0	3.005797	-0.355437	-0.137948
15	6	0	1.789848	-2.362550	-0.145807
16	6	0	1.788827	-3.829331	-0.160283
17	6	0	0.451120	-4.214230	-0.133977
18	6	0	-0.313278	-2.959445	-0.128811

19	7	0	-2.935730	1.673929	-0.147192
20	7	0	1.650334	2.940457	-0.142842
21	7	0	-1.650338	-2.940475	-0.142842
22	7	0	2.935727	-1.673947	-0.147197
23	1	0	0.976653	0.248219	-0.118946
24	1	0	-0.976657	-0.248236	-0.118936
25	7	0	1.949390	0.532664	-0.129894
26	7	0	-1.949394	-0.532682	-0.129887
27	6	0	-0.081841	5.589293	-0.124160
28	6	0	1.253985	6.054014	-0.047354
29	6	0	-1.158049	6.543024	-0.167798
30	6	0	1.531314	7.408683	-0.046228
31	1	0	2.051923	5.326693	0.027122
32	6	0	-0.832578	7.925053	-0.165821
33	6	0	0.472878	8.353926	-0.118299
34	1	0	-1.639494	8.651943	-0.217055
35	1	0	0.708847	9.412521	-0.148378
36	6	0	5.598632	0.082899	-0.160342
37	6	0	6.545427	1.160738	-0.211735
38	6	0	6.063156	-1.250959	-0.092350
39	6	0	7.926709	0.840427	-0.224513
40	6	0	7.420385	-1.526375	-0.105982
41	1	0	5.337810	-2.050429	-0.011877
42	6	0	8.359771	-0.465147	-0.184751
43	1	0	8.650833	1.649245	-0.281723
44	1	0	9.418757	-0.696863	-0.227196
45	6	0	0.081833	-5.589310	-0.124171
46	6	0	-1.253991	-6.054029	-0.047350
47	6	0	1.158038	-6.543044	-0.167840
48	6	0	-1.531324	-7.408697	-0.046251
49	1	0	-2.051927	-5.326709	0.027154
50	6	0	0.832563	-7.925071	-0.165889
51	6	0	-0.472895	-8.353942	-0.118362
52	1	0	1.639476	-8.651963	-0.217146
53	1	0	-0.708864	-9.412536	-0.148458
54	6	0	-5.598635	-0.082913	-0.160363
55	6	0	-6.063156	1.250945	-0.092364
56	6	0	-7.420384	1.526366	-0.106012
57	1	0	-5.337807	2.050410	-0.011870
58	6	0	-7.926712	-0.840435	-0.224574
59	6	0	-8.359771	0.465141	-0.184806
60	1	0	-8.650838	-1.649249	-0.281802
61	1	0	-9.418755	0.696859	-0.227267
62	6	0	-6.545431	-1.160750	-0.211777
63	6	0	-4.764292	-2.845381	-0.227694
64	6	0	-6.098638	-2.517483	-0.250131
65	6	0	-2.512830	6.101415	-0.212694
66	6	0	-2.841361	4.763144	-0.204241
67	6	0	4.764285	2.845365	-0.227665

68	6	0	6.098632	2.517469	-0.250084
69	6	0	2.512820	-6.101436	-0.212742
70	6	0	2.841354	-4.763166	-0.204272
71	1	0	-3.875198	4.436557	-0.242818
72	1	0	-3.298448	6.852299	-0.250289
73	1	0	6.847858	3.304017	-0.294961
74	1	0	4.434844	3.878155	-0.262804
75	1	0	3.875192	-4.436581	-0.242853
76	1	0	3.298435	-6.852322	-0.250354
77	1	0	-6.847865	-3.304029	-0.295029
78	1	0	-4.434851	-3.878171	-0.262837
79	6	0	3.366556	8.840599	0.895270
80	6	0	3.931799	7.431251	-0.791480
81	6	0	2.726635	9.536877	1.919710
82	6	0	4.747371	9.033796	0.646234
83	6	0	3.950108	6.503230	-1.832161
84	6	0	5.108213	8.135034	-0.433087
85	6	0	3.477166	10.445328	2.666842
86	1	0	1.677607	9.377359	2.145445
87	6	0	5.470524	9.949877	1.412338
88	6	0	5.159310	6.278434	-2.492859
89	1	0	3.054614	5.969749	-2.131990
90	6	0	6.301525	7.887048	-1.114033
91	6	0	4.848441	10.678916	2.434465
92	1	0	2.968165	10.982198	3.459123
93	1	0	6.529316	10.087597	1.209276
94	6	0	6.352445	6.950777	-2.155490
95	1	0	5.160129	5.554572	-3.299649
96	1	0	7.194827	8.436370	-0.828368
97	7	0	2.871184	7.868355	0.014408
98	6	0	7.683253	6.696889	-2.891187
99	6	0	5.669555	11.687552	3.262008
100	6	0	4.822228	12.396001	4.336266
101	1	0	3.995354	12.964165	3.894996
102	1	0	4.403320	11.687154	5.059604
103	1	0	5.448195	13.102949	4.892568
104	6	0	6.827727	10.950907	3.976249
105	1	0	7.498757	10.459612	3.263751
106	1	0	7.426339	11.656943	4.565332
107	1	0	6.442311	10.181938	4.655449
108	6	0	6.254904	12.770472	2.324584
109	1	0	6.905678	12.336810	1.557949
110	1	0	5.455647	13.317893	1.811939
111	1	0	6.849781	13.493057	2.897126
112	6	0	8.173190	8.011872	-3.543228
113	1	0	8.333041	8.800072	-2.799964
114	1	0	9.123313	7.850052	-4.067533
115	1	0	7.442092	8.383157	-4.270294
116	6	0	8.747749	6.202347	-1.883305

117	1	0	9.705690	6.028953	-2.389274
118	1	0	8.920324	6.928687	-1.082287
119	1	0	8.435897	5.260198	-1.416602
120	6	0	7.549795	5.635988	-4.000548
121	1	0	7.229998	4.666069	-3.602604
122	1	0	6.834868	5.940916	-4.773088
123	1	0	8.519702	5.488859	-4.489195
124	7	0	-7.883429	2.863334	-0.053780
125	6	0	-8.879771	3.354781	0.803660
126	6	0	-7.430271	3.927233	-0.848728
127	6	0	-9.597342	2.713064	1.811975
128	6	0	-9.071227	4.734748	0.550246
129	6	0	-6.478368	3.950257	-1.867156
130	6	0	-8.147560	5.099779	-0.506642
131	6	0	-10.525685	3.460730	2.537518
132	1	0	-9.439442	1.665058	2.043452
133	6	0	-10.007261	5.455065	1.294339
134	6	0	-6.242283	5.161291	-2.520488
135	1	0	-5.933098	3.058300	-2.155808
136	6	0	-7.888308	6.295008	-1.179809
137	6	0	-10.758361	4.830901	2.299190
138	1	0	-11.078951	2.950115	3.317351
139	1	0	-10.142985	6.513449	1.088120
140	6	0	-6.926795	6.351250	-2.197700
141	1	0	-5.498129	5.166168	-3.308455
142	1	0	-8.447971	7.185624	-0.906291
143	6	0	-11.788502	5.649083	3.102707
144	6	0	-6.658450	7.684485	-2.923655
145	6	0	-12.520244	4.799392	4.159328
146	6	0	-11.071725	6.808655	3.834681
147	6	0	-12.850113	6.232134	2.139831
148	6	0	-7.957658	8.170947	-3.609011
149	6	0	-6.194352	8.748055	-1.900395
150	6	0	-5.567935	7.557089	-4.004645
151	1	0	-13.075407	3.971155	3.704250
152	1	0	-11.827929	4.382233	4.899495
153	1	0	-13.242082	5.423229	4.698587
154	1	0	-10.565353	7.481299	3.134379
155	1	0	-11.793007	7.405184	4.407102
156	1	0	-10.318145	6.424804	4.531762
157	1	0	-12.399965	6.884468	1.384118
158	1	0	-13.383223	5.431824	1.613909
159	1	0	-13.587573	6.824879	2.695291
160	1	0	-8.765777	8.326404	-2.886461
161	1	0	-7.785460	9.122810	-4.126739
162	1	0	-8.306990	7.440275	-4.347332
163	1	0	-6.010123	9.707411	-2.399747
164	1	0	-6.942760	8.917193	-1.119165
165	1	0	-5.264452	8.437767	-1.409010

166	1	0	-4.607977	7.239599	-3.581648
167	1	0	-5.849859	6.843280	-4.786940
168	1	0	-5.411180	8.528741	-4.486735
169	7	0	-2.871199	-7.868359	0.014398
170	6	0	-3.366564	-8.840627	0.895235
171	6	0	-3.931821	-7.431221	-0.791461
172	6	0	-2.726631	-9.536949	1.919638
173	6	0	-4.747385	-9.033806	0.646214
174	6	0	-3.950139	-6.503162	-1.832108
175	6	0	-5.108237	-8.135001	-0.433068
176	6	0	-3.477154	-10.445428	2.666744
177	1	0	-1.677599	-9.377445	2.145362
178	6	0	-5.470530	-9.949915	1.412292
179	6	0	-5.159353	-6.278322	-2.492770
180	1	0	-3.054644	-5.969682	-2.131936
181	6	0	-6.301561	-7.886971	-1.113979
182	6	0	-4.848433	-10.679003	2.434375
183	1	0	-2.968145	-10.982331	3.458998
184	1	0	-6.529327	-10.087617	1.209245
185	6	0	-6.352491	-6.950655	-2.155394
186	1	0	-5.160177	-5.554432	-3.299534
187	1	0	-7.194866	-8.436290	-0.828315
188	6	0	-5.669538	-11.687674	3.261887
189	6	0	-7.683313	-6.696708	-2.891045
190	6	0	-4.822199	-12.396162	4.336109
191	6	0	-6.827706	-10.951065	3.976168
192	6	0	-6.254890	-12.770559	2.324423
193	6	0	-8.173341	-8.011667	-3.543063
194	6	0	-8.747744	-6.202106	-1.883122
195	6	0	-7.549842	-5.635820	-4.000418
196	1	0	-3.995347	-12.964334	3.894808
197	1	0	-4.403259	-11.687336	5.059450
198	1	0	-5.448167	-13.103108	4.892413
199	1	0	-7.498750	-10.459748	3.263697
200	1	0	-7.426305	-11.657127	4.565233
201	1	0	-6.442287	-10.182117	4.655390
202	1	0	-6.905679	-12.336868	1.557817
203	1	0	-5.455635	-13.317948	1.811742
204	1	0	-6.849751	-13.493177	2.896940
205	1	0	-8.333198	-8.799861	-2.799793
206	1	0	-9.123481	-7.849801	-4.067324
207	1	0	-7.442296	-8.382987	-4.270163
208	1	0	-9.705691	-6.028639	-2.389056
209	1	0	-8.920341	-6.928447	-1.082110
210	1	0	-8.435811	-5.259986	-1.416417
211	1	0	-7.229981	-4.665914	-3.602492
212	1	0	-6.834959	-5.940790	-4.772982
213	1	0	-8.519760	-5.488645	-4.489030
214	7	0	7.883436	-2.863342	-0.053759

215	6	0	8.879751	-3.354797	0.803707
216	6	0	7.430313	-3.927229	-0.848743
217	6	0	9.597288	-2.713090	1.812052
218	6	0	9.071227	-4.734759	0.550273
219	6	0	6.478442	-3.950240	-1.867201
220	6	0	8.147600	-5.099776	-0.506655
221	6	0	10.525614	-3.460762	2.537612
222	1	0	9.439374	-1.665089	2.043539
223	6	0	10.007243	-5.455080	1.294383
224	6	0	6.242391	-5.161261	-2.520568
225	1	0	5.933172	-3.058281	-2.155849
226	6	0	7.888381	-6.294993	-1.179856
227	6	0	10.758307	-4.830927	2.299268
228	1	0	11.078853	-2.950155	3.317470
229	1	0	10.142983	-6.513460	1.088150
230	6	0	6.926907	-6.351221	-2.197785
231	1	0	5.498265	-5.166129	-3.308561
232	1	0	8.448041	-7.185611	-0.906338
233	6	0	11.788427	-5.649116	3.102806
234	6	0	6.658594	-7.684446	-2.923771
235	6	0	12.520127	-4.799438	4.159467
236	6	0	11.071633	-6.808706	3.834733
237	6	0	12.850077	-6.232140	2.139956
238	6	0	7.957856	-8.170965	-3.608981
239	6	0	6.194336	-8.747992	-1.900556
240	6	0	5.568207	-7.557008	-4.004886
241	1	0	13.075292	-3.971183	3.704424
242	1	0	11.827785	-4.382304	4.899623
243	1	0	13.241957	-5.423277	4.698734
244	1	0	10.565291	-7.481341	3.134400
245	1	0	11.792900	-7.405241	4.407168
246	1	0	10.318026	-6.424874	4.531794
247	1	0	12.399960	-6.884466	1.384216
248	1	0	13.383198	-5.431817	1.614066
249	1	0	13.587523	-6.824889	2.695432
250	1	0	8.765892	-8.326450	-2.886345
251	1	0	7.785674	-9.122826	-4.126717
252	1	0	8.307297	-7.440315	-4.347273
253	1	0	6.010116	-9.707342	-2.399923
254	1	0	6.942653	-8.917157	-1.119246
255	1	0	5.264397	-8.437657	-1.409275
256	1	0	4.608219	-7.239455	-3.582003
257	1	0	5.850260	-6.843229	-4.787162
258	1	0	5.411450	-8.528660	-4.486976

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b. C<sub>1</sub> symmetry isomer

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.141116	-0.444439	-0.019318
2	7	0	-2.656321	-3.408818	0.070705
3	6	0	-4.262476	-1.012756	-0.065531
4	6	0	-5.039595	0.208105	-0.157363
5	6	0	-4.146848	1.291133	-0.181758
6	6	0	-2.803329	0.742308	-0.123374
7	6	0	-0.462174	0.860936	-0.228812
8	6	0	0.733697	1.651375	-0.537693
9	6	0	1.800941	0.755114	-0.540671
10	6	0	1.218019	-0.535509	-0.143521
11	6	0	1.461039	-2.815475	0.352910
12	6	0	2.189028	-4.000127	0.778816
13	6	0	1.288538	-5.076596	0.727408
14	6	0	-0.012923	-4.559461	0.356544
15	6	0	-2.335037	-4.728924	0.141840
16	6	0	-3.537575	-5.564794	0.102005
17	6	0	-4.615948	-4.687070	0.031939
18	6	0	-4.020636	-3.343783	0.015059
19	7	0	-1.674576	1.422619	-0.217289
20	7	0	1.964209	-1.613584	0.127601
21	7	0	-4.762924	-2.232870	-0.043690
22	7	0	-1.121153	-5.269088	0.290587
23	1	0	-0.596143	-2.569881	-0.078962
24	1	0	-2.165198	-1.271719	0.060603
25	7	0	0.153497	-3.209895	0.155454
26	7	0	-2.942773	-0.627579	-0.032065
27	6	0	3.091390	1.156711	-0.992305
28	6	0	4.181145	0.271596	-1.194422
29	6	0	3.239566	2.544736	-1.343405
30	6	0	5.354496	0.716231	-1.780138
31	1	0	4.067070	-0.768721	-0.918184
32	6	0	4.486037	2.977528	-1.866436
33	6	0	5.509072	2.092707	-2.103176
34	1	0	4.604347	4.024540	-2.134606
35	1	0	6.426518	2.427937	-2.573738
36	6	0	1.663481	-6.392335	1.067758
37	6	0	2.949021	-6.599060	1.505343
38	6	0	-5.954595	-5.170901	-0.000179
39	6	0	-7.099765	-4.338003	-0.018603
40	6	0	-6.121869	-6.599662	0.014664
41	6	0	-8.369755	-4.883865	-0.056681

42	1	0	-6.959549	-3.265405	0.015579
43	6	0	-7.441395	-7.121805	-0.028459
44	6	0	-8.538884	-6.294540	-0.075283
45	1	0	-7.576673	-8.200597	-0.038100
46	1	0	-9.540073	-6.707586	-0.139666
47	6	0	-4.626073	2.633638	-0.271900
48	6	0	-3.787473	3.772823	-0.269963
49	6	0	-4.327460	5.044811	-0.361550
50	1	0	-2.717451	3.632623	-0.182209
51	6	0	-6.566097	4.121992	-0.428533
52	6	0	-5.733306	5.217248	-0.447681
53	1	0	-7.642473	4.258771	-0.495788
54	1	0	-6.139042	6.218906	-0.543943
55	6	0	-6.049911	2.804230	-0.342867
56	6	0	-6.437411	0.385867	-0.240390
57	6	0	-6.918617	1.669473	-0.331185
58	6	0	2.139587	3.443245	-1.235136
59	6	0	0.885749	3.011573	-0.861220
60	6	0	3.508378	-4.180279	1.299029
61	6	0	3.872092	-5.520913	1.664590
62	6	0	-4.985854	-7.460032	0.074436
63	6	0	-3.702091	-6.962459	0.125781
64	1	0	0.039572	3.689845	-0.836747
65	1	0	2.297694	4.486177	-1.499180
66	1	0	-2.837118	-7.615523	0.180120
67	1	0	-5.156134	-8.533903	0.084444
68	1	0	-7.990006	1.842460	-0.396162
69	1	0	-7.103302	-0.470267	-0.242667
70	6	0	7.761083	0.047132	-2.043774
71	6	0	6.197646	-1.368337	-2.890476
72	6	0	8.458802	1.056920	-1.381805
73	6	0	8.459993	-0.968708	-2.738505
74	6	0	5.030139	-2.002533	-3.311939
75	6	0	7.463256	-1.876446	-3.270902
76	6	0	9.851519	1.065812	-1.472659
77	1	0	7.944986	1.817347	-0.803450
78	6	0	9.853132	-0.934804	-2.808867
79	6	0	5.147851	-3.156574	-4.087887
80	1	0	4.049304	-1.618969	-3.056499
81	6	0	7.548613	-3.035764	-4.043457
82	6	0	10.576891	0.093521	-2.191427
83	1	0	10.380734	1.861725	-0.961254
84	1	0	10.372091	-1.715336	-3.358891
85	6	0	6.391229	-3.703655	-4.463760
86	1	0	4.230657	-3.639847	-4.404535
87	1	0	8.529568	-3.411516	-4.322508
88	7	0	6.380567	-0.195406	-2.132385
89	6	0	6.512633	-4.985438	-5.311147
90	6	0	12.111536	0.134602	-2.329352

91	6	0	12.741180	1.309722	-1.557274
92	1	0	12.381613	2.277887	-1.923990
93	1	0	12.532361	1.252613	-0.482872
94	1	0	13.829742	1.293523	-1.683425
95	6	0	12.722726	-1.178753	-1.787108
96	1	0	12.359997	-2.054652	-2.335143
97	1	0	13.815930	-1.159380	-1.877510
98	1	0	12.469698	-1.319999	-0.730224
99	6	0	12.486138	0.289607	-3.823048
100	1	0	12.100264	-0.539263	-4.425937
101	1	0	12.076423	1.219262	-4.234339
102	1	0	13.576290	0.313931	-3.945822
103	6	0	7.267244	-4.669413	-6.624411
104	1	0	8.273858	-4.282981	-6.432937
105	1	0	7.368570	-5.574406	-7.236514
106	1	0	6.728838	-3.918409	-7.213744
107	6	0	7.297071	-6.057166	-4.517367
108	1	0	7.399222	-6.975512	-5.109168
109	1	0	8.304286	-5.714527	-4.257551
110	1	0	6.779906	-6.308904	-3.584389
111	6	0	5.139673	-5.578024	-5.682139
112	1	0	4.560509	-5.854067	-4.793596
113	1	0	4.540896	-4.879482	-6.277677
114	1	0	5.279019	-6.485698	-6.280433
115	7	0	-3.485751	6.184149	-0.384541
116	6	0	-3.628817	7.326315	0.416606
117	6	0	-2.389868	6.384566	-1.236636
118	6	0	-4.531891	7.597193	1.443322
119	6	0	-2.623448	8.263017	0.074348
120	6	0	-1.864330	5.566549	-2.235525
121	6	0	-1.834446	7.663179	-0.984602
122	6	0	-4.431816	8.823885	2.100768
123	1	0	-5.288820	6.878026	1.738357
124	6	0	-2.549313	9.481082	0.752372
125	6	0	-0.769374	6.037118	-2.963181
126	1	0	-2.289547	4.592814	-2.453998
127	6	0	-0.739770	8.104334	-1.730254
128	6	0	-3.455740	9.788520	1.775841
129	1	0	-5.140572	9.024236	2.896065
130	1	0	-1.772199	10.190075	0.479300
131	6	0	-0.182437	7.298720	-2.732371
132	1	0	-0.369783	5.391591	-3.736802
133	1	0	-0.326475	9.088804	-1.527286
134	6	0	-3.353693	11.142856	2.505074
135	6	0	1.023339	7.812968	-3.543759
136	6	0	-4.428158	11.305939	3.597257
137	6	0	-1.965939	11.265793	3.178218
138	6	0	-3.530237	12.293398	1.485687
139	6	0	0.625791	9.105920	-4.295388

140	6	0	2.199995	8.122720	-2.588156
141	6	0	1.512630	6.788186	-4.585075
142	1	0	-5.441918	11.258497	3.183333
143	1	0	-4.339571	10.539405	4.375571
144	1	0	-4.315591	12.282227	4.082284
145	1	0	-1.152009	11.203575	2.448226
146	1	0	-1.875131	12.228207	3.697143
147	1	0	-1.815626	10.467066	3.913465
148	1	0	-2.767611	12.262069	0.700393
149	1	0	-4.511117	12.238633	0.999721
150	1	0	-3.452490	13.266048	1.987369
151	1	0	0.307413	9.895254	-3.606265
152	1	0	1.474834	9.490490	-4.874205
153	1	0	-0.201026	8.916011	-4.989175
154	1	0	3.063450	8.498299	-3.151201
155	1	0	1.933347	8.880101	-1.843674
156	1	0	2.513621	7.222349	-2.046480
157	1	0	1.832052	5.849544	-4.117545
158	1	0	0.737683	6.554326	-5.323736
159	1	0	2.372588	7.195969	-5.128438
160	7	0	-9.512089	-4.045147	-0.089318
161	6	0	-10.637732	-4.158016	0.739745
162	6	0	-9.709195	-2.950144	-0.942883
163	6	0	-10.902338	-5.043425	1.783730
164	6	0	-11.563827	-3.139044	0.408055
165	6	0	-8.901172	-2.442620	-1.959807
166	6	0	-10.971618	-2.368516	-0.668254
167	6	0	-12.112327	-4.913858	2.466387
168	1	0	-10.190271	-5.808795	2.073488
169	6	0	-12.765807	-3.035971	1.110615
170	6	0	-9.363862	-1.340067	-2.680320
171	1	0	-7.940610	-2.887095	-2.196367
172	6	0	-11.405616	-1.266831	-1.407970
173	6	0	-13.067227	-3.925333	2.150540
174	1	0	-12.307111	-5.609441	3.274634
175	1	0	-13.466523	-2.249155	0.843828
176	6	0	-10.608473	-0.727143	-2.426306
177	1	0	-8.725584	-0.954502	-3.466968
178	1	0	-12.377102	-0.832944	-1.185944
179	6	0	-14.403890	-3.791856	2.906751
180	6	0	-11.110406	0.491779	-3.225581
181	6	0	-14.561495	-4.850313	4.015261
182	6	0	-14.489789	-2.394366	3.565338
183	6	0	-15.578584	-3.961257	1.914072
184	6	0	-12.438718	0.135196	-3.934594
185	6	0	-11.350619	1.679385	-2.263472
186	6	0	-10.103975	0.946547	-4.299923
187	1	0	-14.539624	-5.869546	3.612829
188	1	0	-13.777122	-4.765422	4.776024

189	1	0	-15.525237	-4.715610	4.519407
190	1	0	-14.429537	-1.590356	2.824254
191	1	0	-15.439426	-2.281202	4.103107
192	1	0	-13.673346	-2.248770	4.281861
193	1	0	-15.551134	-3.208834	1.118846
194	1	0	-15.550277	-4.948680	1.439244
195	1	0	-16.539040	-3.861162	2.434975
196	1	0	-13.216578	-0.154942	-3.220458
197	1	0	-12.812894	0.994959	-4.504330
198	1	0	-12.297931	-0.699298	-4.630856
199	1	0	-11.720666	2.552805	-2.814781
200	1	0	-12.087142	1.436152	-1.490525
201	1	0	-10.420496	1.966751	-1.758531
202	1	0	-9.143849	1.242190	-3.861677
203	1	0	-9.914473	0.161107	-5.040263
204	1	0	-10.503603	1.814888	-4.836033
205	6	0	5.986830	-4.686918	2.536068
206	6	0	5.617343	-3.357521	2.197163
207	1	0	6.921292	-4.862257	3.056762
208	7	0	6.450547	-2.285115	2.594018
209	6	0	7.856281	-2.298236	2.604593
210	6	0	6.025569	-1.153009	3.320120
211	6	0	8.755247	-3.178731	2.003828
212	6	0	8.328434	-1.180515	3.332253
213	6	0	4.744376	-0.714215	3.649453
214	6	0	7.161945	-0.445800	3.780479
215	6	0	10.120877	-2.958792	2.191603
216	1	0	8.416395	-4.012217	1.397849
217	6	0	9.699584	-0.985064	3.500472
218	6	0	4.619280	0.446733	4.414129
219	1	0	3.857184	-1.249108	3.331967
220	6	0	7.004775	0.714479	4.539920
221	6	0	10.624315	-1.881014	2.948200
222	1	0	10.808018	-3.656679	1.727040
223	1	0	10.042952	-0.129287	4.075520
224	6	0	5.728094	1.188521	4.867973
225	1	0	3.615932	0.777377	4.656680
226	1	0	7.890194	1.244464	4.881063
227	6	0	12.131061	-1.671245	3.196305
228	6	0	5.580872	2.476365	5.701819
229	6	0	12.998352	-2.723306	2.478997
230	6	0	12.557728	-0.272734	2.691917
231	6	0	12.416303	-1.771537	4.714292
232	6	0	6.280279	2.290803	7.069445
233	6	0	6.238252	3.657132	4.948396
234	6	0	4.107501	2.841190	5.966024
235	1	0	12.777188	-3.739292	2.825384
236	1	0	12.860812	-2.695321	1.392018
237	1	0	14.057603	-2.529561	2.682821

238	1	0	12.017776	0.529370	3.205850
239	1	0	13.629679	-0.114156	2.863091
240	1	0	12.364643	-0.168745	1.618251
241	1	0	11.857629	-1.019976	5.282141
242	1	0	12.134949	-2.757830	5.100766
243	1	0	13.483971	-1.618419	4.915920
244	1	0	7.347126	2.071373	6.955247
245	1	0	6.190474	3.202570	7.673152
246	1	0	5.828577	1.465030	7.630958
247	1	0	6.149039	4.582084	5.531835
248	1	0	7.303440	3.480243	4.765204
249	1	0	5.755499	3.818802	3.977860
250	1	0	3.556984	3.017171	5.034933
251	1	0	3.587274	2.057611	6.528659
252	1	0	4.056125	3.761664	6.558681
253	6	0	4.414497	-3.121280	1.547772
254	1	0	4.137386	-2.116458	1.256025
255	6	0	5.143801	-5.734721	2.252819
256	1	0	5.426142	-6.746037	2.534675
257	1	0	0.941747	-7.198844	0.995216
258	1	0	3.276807	-7.597382	1.784212

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c. C<sub>2</sub> symmetry isomer

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.368841	-1.958871	0.095517
2	7	0	-1.359408	-4.716789	-0.136696
3	6	0	1.184127	-6.103702	-0.007763
4	6	0	2.469997	-6.768210	0.054536
5	6	0	3.466822	-5.783677	0.136859
6	6	0	2.797748	-4.494670	0.136096
7	6	0	2.693148	-2.161255	0.335428
8	6	0	3.354042	-0.908128	0.713994
9	6	0	2.358682	0.067367	0.723612
10	6	0	1.143434	-0.620885	0.262032
11	6	0	-1.131877	-0.574819	-0.311558
12	6	0	-2.358393	0.053342	-0.775686
13	6	0	-3.351058	-0.940661	-0.790185
14	6	0	-2.734205	-2.198384	-0.415207
15	6	0	-2.710061	-4.534232	-0.227548
16	6	0	-3.421701	-5.819551	-0.206794
17	6	0	-2.424496	-6.788084	-0.127361
18	6	0	-1.152684	-6.061847	-0.094415
19	7	0	3.368968	-3.312819	0.291338
20	7	0	0.009252	0.029181	-0.027474
21	7	0	0.014371	-6.710718	-0.051421
22	7	0	-3.344421	-3.366258	-0.386274
23	1	0	-0.722733	-2.614783	0.089464
24	1	0	0.739333	-4.031625	-0.047432
25	7	0	-1.414737	-1.916218	-0.153841
26	7	0	1.447578	-4.754069	0.021827
27	6	0	2.618682	1.372622	1.232245
28	6	0	1.626337	2.365020	1.437210
29	6	0	3.973724	1.639596	1.637755
30	6	0	1.936053	3.553861	2.076192
31	1	0	0.611831	2.162846	1.118575
32	6	0	4.266407	2.901523	2.217824
33	6	0	3.279593	3.826405	2.455321
34	1	0	5.287559	3.109257	2.528060
35	1	0	3.508833	4.753911	2.967870
36	6	0	-4.677965	-0.675916	-1.186966
37	6	0	-4.977303	0.596730	-1.609525
38	6	0	-2.710583	-8.165967	-0.104792
39	6	0	-4.032771	-8.549287	-0.156515
40	6	0	4.846455	-6.144496	0.217135
41	6	0	5.904114	-5.207326	0.274782

42	6	0	7.219468	-5.633786	0.353957
43	1	0	5.667155	-4.151271	0.242890
44	6	0	6.503670	-7.947208	0.287090
45	6	0	7.518345	-7.020858	0.366206
46	1	0	6.737979	-9.008754	0.297706
47	1	0	8.551820	-7.339194	0.454176
48	6	0	5.145117	-7.548851	0.212440
49	6	0	2.773359	-8.146349	0.057696
50	6	0	4.094211	-8.515203	0.135747
51	6	0	4.977601	0.635573	1.523265
52	6	0	4.682231	-0.638594	1.089875
53	6	0	-2.631984	1.363949	-1.276405
54	6	0	-3.981719	1.616006	-1.698123
55	6	0	-4.797042	-6.184556	-0.255954
56	1	0	5.440279	-1.413992	1.058620
57	1	0	5.991289	0.883003	1.829387
58	1	0	4.366952	-9.567585	0.139003
59	1	0	1.974358	-8.877806	-0.000680
60	6	0	1.029981	5.875908	2.385755
61	6	0	-0.260427	4.157635	3.125940
62	6	0	1.992613	6.688014	1.787055
63	6	0	-0.075988	6.451564	3.055534
64	6	0	-0.795401	2.921800	3.485646
65	6	0	-0.903518	5.355859	3.519936
66	6	0	1.862238	8.071562	1.916552
67	1	0	2.821646	6.268348	1.227312
68	6	0	-0.180833	7.838606	3.165367
69	6	0	-1.986342	2.903463	4.212987
70	1	0	-0.308819	1.990842	3.219255
71	6	0	-2.096252	5.304938	4.243138
72	6	0	0.795837	8.677026	2.612376
73	1	0	2.622446	8.690669	1.454142
74	1	0	-1.029964	8.262479	3.694978
75	6	0	-2.666060	4.076002	4.599910
76	1	0	-2.391533	1.934526	4.481307
77	1	0	-2.576091	6.235937	4.533480
78	7	0	0.919042	4.476410	2.425046
79	6	0	-3.987932	4.046455	5.392102
80	6	0	0.679770	10.203581	2.790952
81	6	0	1.822082	10.967009	2.093980
82	1	0	2.802889	10.690741	2.497511
83	1	0	1.834839	10.787618	1.012857
84	1	0	1.694098	12.044493	2.248322
85	6	0	-0.660660	10.699738	2.199541
86	1	0	-1.521029	10.237947	2.695165
87	1	0	-0.753262	11.786647	2.316708
88	1	0	-0.726987	10.464224	1.131275
89	6	0	0.727174	10.547342	4.299226
90	1	0	-0.086799	10.065248	4.850900



91	1	0	1.672498	10.218211	4.745680
92	1	0	0.638096	11.630601	4.449842
93	6	0	-3.802248	4.785405	6.738761
94	1	0	-3.508805	5.830402	6.593195
95	1	0	-4.737612	4.778797	7.312299
96	1	0	-3.027399	4.303346	7.345762
97	6	0	-5.096654	4.749356	4.573142
98	1	0	-6.044399	4.744388	5.126074
99	1	0	-4.842774	5.792436	4.356447
100	1	0	-5.258101	4.240035	3.616198
101	6	0	-4.459109	2.611777	5.697814
102	1	0	-4.640608	2.037638	4.782136
103	1	0	-3.731071	2.063905	6.306917
104	1	0	-5.400130	2.644195	6.258743
105	7	0	8.276414	-4.694630	0.437583
106	6	0	9.435400	-4.690410	-0.352455
107	6	0	8.363343	-3.627364	1.343839
108	6	0	9.800976	-5.511863	-1.417676
109	6	0	10.269279	-3.619703	0.051873
110	6	0	7.489005	-3.229970	2.354211
111	6	0	9.586445	-2.943129	1.137969
112	6	0	11.019470	-5.264579	-2.051140
113	1	0	9.159530	-6.317114	-1.760126
114	6	0	11.481872	-3.398096	-0.603303
115	6	0	7.846657	-2.132486	3.140027
116	1	0	6.557559	-3.754653	2.537978
117	6	0	9.914546	-1.849356	1.941020
118	6	0	11.884135	-4.219733	-1.664726
119	1	0	11.294238	-5.910671	-2.877002
120	1	0	12.111414	-2.572320	-0.282620
121	6	0	9.049549	-1.419334	2.956192
122	1	0	7.158524	-1.833345	3.922242
123	1	0	10.857462	-1.335948	1.772244
124	6	0	13.229913	-3.954308	-2.368284
125	6	0	9.438467	-0.210507	3.830365
126	6	0	13.505837	-4.953897	-3.507794
127	6	0	13.226358	-2.529950	-2.972730
128	6	0	14.381720	-4.070219	-1.341641
129	6	0	10.758822	-0.516730	4.577030
130	6	0	9.638143	1.035593	2.935413
131	6	0	8.363930	0.125648	4.882222
132	1	0	13.550492	-5.986638	-3.143451
133	1	0	12.742607	-4.899920	-4.292488
134	1	0	14.472064	-4.726082	-3.972055
135	1	0	13.079540	-1.762200	-2.205744
136	1	0	14.180729	-2.323002	-3.472843
137	1	0	12.424144	-2.420430	-3.711381
138	1	0	14.269755	-3.353366	-0.521357
139	1	0	14.416256	-5.074454	-0.903902

140	1	0	15.347459	-3.875822	-1.824676
141	1	0	11.580306	-0.722977	3.882842
142	1	0	11.054648	0.336549	5.200053
143	1	0	10.645701	-1.390786	5.228386
144	1	0	9.923188	1.903411	3.543087
145	1	0	10.423288	0.880251	2.188136
146	1	0	8.715187	1.285423	2.398641
147	1	0	7.402146	0.376549	4.419949
148	1	0	8.200642	-0.703974	5.579331
149	1	0	8.683100	0.992658	5.471683
150	6	0	-3.303822	3.819291	-2.480954
151	6	0	-1.963807	3.562077	-2.084471
152	1	0	-3.538754	4.748046	-2.988255
153	7	0	-0.954996	4.500753	-2.406195
154	6	0	-1.096230	5.899080	-2.379511
155	6	0	0.246306	4.202595	-3.081840
156	6	0	-2.084847	6.695474	-1.802656
157	6	0	0.009007	6.492876	-3.033562
158	6	0	0.816342	2.977014	-3.421630
159	6	0	0.869276	5.411967	-3.472958
160	6	0	-1.982118	8.080556	-1.942092
161	1	0	-2.913232	6.263797	-1.251174
162	6	0	0.085870	7.880748	-3.154525
163	6	0	2.021407	2.980908	-4.125794
164	1	0	0.348931	2.035943	-3.157160
165	6	0	2.076398	5.383640	-4.172874
166	6	0	-0.918361	8.702841	-2.626712
167	1	0	-2.762787	8.686885	-1.497219
168	1	0	0.934562	8.317996	-3.673754
169	6	0	2.681220	4.165657	-4.508989
170	1	0	2.454142	2.019446	-4.377166
171	1	0	2.540051	6.323440	-4.461016
172	6	0	-0.836497	10.229350	-2.824083
173	6	0	4.018799	4.160708	-5.274788
174	6	0	-1.999792	10.974984	-2.142638
175	6	0	0.488561	10.766142	-2.233875
176	6	0	-0.884463	10.550576	-4.337404
177	6	0	3.843304	4.886958	-6.629684
178	6	0	5.094905	4.893356	-4.438574
179	6	0	4.527547	2.734972	-5.561418
180	1	0	-2.971873	10.672908	-2.548739
181	1	0	-2.014940	10.807669	-1.059582
182	1	0	-1.894657	12.053187	-2.308641
183	1	0	1.362693	10.315710	-2.715573
184	1	0	0.556860	11.852506	-2.370654
185	1	0	0.553205	10.552804	-1.160950
186	1	0	-0.056027	10.080518	-4.877886
187	1	0	-1.819122	10.192244	-4.783835
188	1	0	-0.820936	11.633439	-4.502908

189	1	0	3.524090	5.926117	-6.497043
190	1	0	4.789762	4.897550	-7.184608
191	1	0	3.091567	4.383942	-7.248638
192	1	0	6.053366	4.905927	-4.972554
193	1	0	4.813735	5.931922	-4.234172
194	1	0	5.248328	4.393815	-3.475215
195	1	0	4.703843	2.170947	-4.638522
196	1	0	3.823901	2.167103	-6.180788
197	1	0	5.478357	2.784917	-6.104244
198	6	0	-1.649189	2.367938	-1.452812
199	1	0	-0.638078	2.175050	-1.118149
200	6	0	-4.282559	2.878308	-2.268588
201	1	0	-5.301226	3.075827	-2.592868
202	6	0	-5.865422	-5.255711	-0.306181
203	6	0	-7.176742	-5.691271	-0.359025
204	6	0	-7.468715	-7.081521	-0.351588
205	7	0	-8.241844	-4.758139	-0.436239
206	1	0	-8.501860	-7.406095	-0.419587
207	6	0	-9.381061	-4.743265	0.380434
208	6	0	-8.350788	-3.704497	-1.354188
209	6	0	-9.720733	-5.550879	1.464838
210	6	0	-10.226354	-3.679455	-0.019334
211	6	0	-7.499151	-3.319616	-2.388949
212	6	0	-9.569639	-3.017601	-1.130075
213	6	0	-10.924685	-5.296757	2.122625
214	1	0	-9.070019	-6.350817	1.802174
215	6	0	-11.424200	-3.450995	0.660411
216	6	0	-7.875151	-2.232973	-3.181256
217	1	0	-6.572282	-3.847605	-2.586141
218	6	0	-9.916203	-1.934759	-1.940303
219	6	0	-11.800163	-4.258561	1.741969
220	1	0	-11.179363	-5.931988	2.963248
221	1	0	-12.062957	-2.631113	0.342669
222	6	0	-9.074476	-1.518017	-2.980237
223	1	0	-7.205778	-1.944980	-3.983817
224	1	0	-10.855527	-1.419489	-1.757478
225	6	0	-13.130314	-3.986296	2.472217
226	6	0	-9.484530	-0.321894	-3.862262
227	6	0	-13.376466	-4.968768	3.633287
228	6	0	-13.118200	-2.552744	3.054382
229	6	0	-14.305040	-4.121905	1.474381
230	6	0	-10.820622	-0.639871	-4.575298
231	6	0	-9.666437	0.936481	-2.980800
232	6	0	-8.434299	0.000979	-4.942411
233	1	0	-13.426604	-6.007153	3.286140
234	1	0	-12.595047	-4.900707	4.398750
235	1	0	-14.332189	-4.736278	4.116652
236	1	0	-12.991693	-1.796496	2.272491
237	1	0	-14.061647	-2.341101	3.572982

238	1	0	-12.299704	-2.429190	3.772693
239	1	0	-14.214248	-3.417598	0.640720
240	1	0	-14.345859	-5.132930	1.053136
241	1	0	-15.260236	-3.923158	1.976321
242	1	0	-11.626043	-0.837718	-3.860197
243	1	0	-11.131683	0.204309	-5.203346
244	1	0	-10.720495	-1.522755	-5.216770
245	1	0	-9.966392	1.795456	-3.593896
246	1	0	-10.434295	0.790516	-2.213967
247	1	0	-8.732146	1.195074	-2.468132
248	1	0	-7.462775	0.259462	-4.505204
249	1	0	-8.285080	-0.838195	-5.631133
250	1	0	-8.767714	0.859276	-5.536762
251	1	0	-4.296680	-9.603991	-0.141187
252	1	0	-1.905931	-8.891914	-0.048959
253	1	0	-5.635474	-4.197974	-0.290929
254	1	0	-5.426620	-1.460692	-1.175953
255	1	0	-5.988522	0.837120	-1.928511
256	6	0	-6.448053	-7.999973	-0.277678
257	1	0	-6.676074	-9.063053	-0.271931
258	6	0	-5.088805	-7.593212	-0.228820

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d. D<sub>2</sub> symmetry isomer

Standard orientation:

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Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
-----					
1	7	0	-1.382481	0.029504	1.355037
2	6	0	-1.162646	-0.083291	2.692071
3	6	0	-2.403884	-0.404185	3.400011
4	6	0	-3.394254	-0.503500	2.424109
5	6	0	-2.724807	-0.148644	1.162999
6	6	0	-2.786457	0.255848	-1.143918
7	6	0	-3.412476	0.591027	-2.412739
8	6	0	-2.412958	0.513705	-3.397250
9	6	0	-1.156056	0.210181	-2.743031
10	7	0	-0.007889	0.071762	3.346894
11	7	0	-3.388182	0.055977	0.017262
12	7	0	0.007869	0.071546	-3.346828
13	1	0	-0.752209	-0.046532	-0.675684
14	7	0	-1.441286	0.093879	-1.404794
15	6	0	-4.695502	-0.982038	2.751771
16	6	0	-5.703332	-1.275489	1.797937
17	6	0	-4.940873	-1.260517	4.142526
18	6	0	-6.887145	-1.881354	2.183843
19	1	0	-5.516443	-1.052101	0.755240
20	6	0	-6.198512	-1.808051	4.507003
21	6	0	-7.139061	-2.133461	3.560691
22	1	0	-6.390763	-2.022351	5.555484
23	1	0	-8.063505	-2.620185	3.850691
24	6	0	-2.676417	0.758068	-4.760563
25	6	0	-3.951495	1.130640	-5.110543
26	6	0	-3.921647	-1.054812	5.117140
27	6	0	-2.653074	-0.652347	4.761651
28	6	0	-4.727472	1.041025	-2.745255
29	6	0	-4.976981	1.313420	-4.133241
30	1	0	-1.859761	-0.541340	5.493657
31	1	0	-4.157201	-1.266190	6.157368
32	6	0	-9.222102	-2.273270	1.345625
33	6	0	-7.523026	-3.143094	0.112306
34	6	0	-10.019938	-1.578238	2.253887
35	6	0	-9.813885	-3.053659	0.323951
36	6	0	-6.294929	-3.556032	-0.401511
37	6	0	-8.730429	-3.601318	-0.468022
38	6	0	-11.405209	-1.719632	2.158768
39	1	0	-9.587845	-0.936867	3.014663
40	6	0	-11.202219	-3.173856	0.252997
41	6	0	-6.293651	-4.403178	-1.510603

42	1	0	-5.357166	-3.240373	0.040557
43	6	0	-8.696574	-4.444276	-1.580011
44	6	0	-12.026246	-2.522078	1.179678
45	1	0	-12.013096	-1.180794	2.876538
46	1	0	-11.638225	-3.789554	-0.529198
47	6	0	-7.475905	-4.858603	-2.128249
48	1	0	-5.330589	-4.712220	-1.900533
49	1	0	-9.634278	-4.782678	-2.013027
50	7	0	-7.824515	-2.323807	1.217683
51	6	0	-7.465557	-5.784397	-3.360561
52	6	0	-13.553889	-2.714934	1.109436
53	6	0	-14.301787	-1.886057	2.171126
54	1	0	-14.013100	-2.171067	3.189221
55	1	0	-14.121304	-0.811437	2.053162
56	1	0	-15.380942	-2.052283	2.076535
57	6	0	-14.074315	-2.290916	-0.284063
58	1	0	-13.626153	-2.886370	-1.086341
59	1	0	-15.162180	-2.420171	-0.342758
60	1	0	-13.844173	-1.238189	-0.483383
61	6	0	-13.890702	-4.207339	1.343606
62	1	0	-13.418524	-4.851337	0.594100
63	1	0	-13.544846	-4.536089	2.330311
64	1	0	-14.974571	-4.370257	1.290558
65	6	0	-8.197962	-7.104958	-3.023416
66	1	0	-9.238324	-6.930301	-2.729429
67	1	0	-8.205317	-7.772995	-3.893822
68	1	0	-7.701825	-7.627407	-2.197525
69	6	0	-8.188143	-5.086363	-4.537274
70	1	0	-8.196356	-5.734975	-5.422295
71	1	0	-9.227775	-4.845836	-4.290898
72	1	0	-7.684330	-4.150657	-4.805436
73	6	0	-6.037775	-6.136300	-3.820441
74	1	0	-5.469023	-5.243863	-4.105425
75	1	0	-5.476744	-6.665664	-3.041864
76	1	0	-6.083725	-6.792325	-4.697235
77	6	0	-7.193672	2.134657	-3.550766
78	6	0	-6.938204	1.887652	-2.175125
79	1	0	-8.127866	2.601259	-3.841970
80	7	0	-7.884520	2.305665	-1.209497
81	6	0	-9.281781	2.244817	-1.349468
82	6	0	-7.599085	3.119127	-0.093583
83	6	0	-10.067176	1.547815	-2.266861
84	6	0	-9.887657	3.013597	-0.327832
85	6	0	-6.379724	3.538135	0.435502
86	6	0	-8.815409	3.563516	0.477967
87	6	0	-11.454360	1.678570	-2.182516
88	1	0	-9.625220	0.911724	-3.026381
89	6	0	-11.277233	3.123635	-0.267583
90	6	0	-6.396423	4.376985	1.550904

91	1	0	-5.433978	3.233620	0.003124
92	6	0	-8.799812	4.398503	1.596169
93	6	0	-12.089129	2.471929	-1.205087
94	1	0	-12.052281	1.138554	-2.907710
95	1	0	-11.723838	3.731507	0.514682
96	6	0	-7.588128	4.818440	2.159860
97	1	0	-5.439649	4.689455	1.953167
98	1	0	-9.744613	4.725842	2.022098
99	6	0	-13.618349	2.656987	-1.149130
100	6	0	-7.597517	5.734346	3.399452
101	6	0	-14.351883	1.825722	-2.218963
102	6	0	-14.151065	2.229483	0.238568
103	6	0	-13.959084	4.148260	-1.385239
104	6	0	-8.338618	7.050927	3.065802
105	6	0	-8.324831	5.020130	4.563478
106	6	0	-6.177212	6.095041	3.875366
107	1	0	-14.055384	2.113710	-3.233971
108	1	0	-14.167085	0.751881	-2.100629
109	1	0	-15.432687	1.986274	-2.134184
110	1	0	-13.712111	2.824289	1.046362
111	1	0	-15.239646	2.356716	0.286721
112	1	0	-13.921638	1.176726	0.438259
113	1	0	-13.497340	4.793373	-0.630194
114	1	0	-13.604635	4.479624	-2.368020
115	1	0	-15.044110	4.306391	-1.343088
116	1	0	-9.374654	6.869511	2.760778
117	1	0	-8.360039	7.711728	3.941443
118	1	0	-7.839484	7.584544	2.248891
119	1	0	-8.346920	5.661361	5.453591
120	1	0	-9.360012	4.772661	4.305448
121	1	0	-7.815299	4.086723	4.828639
122	1	0	-5.603332	5.205485	4.158889
123	1	0	-5.613618	6.635362	3.106208
124	1	0	-6.237255	6.743824	4.756665
125	6	0	-5.738339	1.307948	-1.790455
126	1	0	-5.545899	1.085563	-0.748549
127	6	0	-6.244873	1.831680	-4.497900
128	1	0	-6.441674	2.042995	-5.546016
129	1	0	-1.881358	0.664908	-5.492671
130	1	0	-4.194103	1.336423	-6.150093
131	6	0	1.162627	-0.083455	-2.691994
132	7	0	1.382462	0.029422	-1.354970
133	6	0	2.403870	-0.404368	-3.399921
134	6	0	2.724796	-0.148688	-1.162924
135	6	0	3.394242	-0.503623	-2.424017
136	6	0	2.653053	-0.652600	-4.761548
137	7	0	3.388168	0.056004	-0.017201
138	6	0	4.695494	-0.982170	-2.751659
139	6	0	3.921625	-1.055082	-5.117021

140	1	0	1.859733	-0.541645	-5.493554
141	6	0	2.786431	0.255939	1.143971
142	6	0	5.703343	-1.275546	-1.797819
143	6	0	4.940856	-1.260728	-4.142400
144	1	0	4.157177	-1.266518	-6.157237
145	6	0	3.412446	0.591237	2.412765
146	7	0	1.441269	0.093970	1.404854
147	6	0	6.887156	-1.881425	-2.183702
148	1	0	5.516468	-1.052086	-0.755136
149	6	0	6.198493	-1.808281	-4.506857
150	6	0	2.412925	0.513971	3.397281
151	6	0	4.727429	1.041290	2.745255
152	6	0	1.156034	0.210368	2.743086
153	1	0	0.752191	-0.046513	0.675759
154	6	0	7.139055	-2.133626	-3.560536
155	7	0	7.824547	-2.323795	-1.217518
156	1	0	6.390732	-2.022645	-5.555326
157	6	0	2.676368	0.758454	4.760577
158	6	0	4.976923	1.313799	4.133222
159	6	0	5.738301	1.308155	1.790444
160	1	0	8.063496	-2.620366	-3.850515
161	6	0	9.222131	-2.273307	-1.345521
162	6	0	7.523083	-3.143056	-0.112112
163	6	0	3.951435	1.131081	5.110534
164	1	0	1.881302	0.665342	5.492683
165	6	0	6.244803	1.832112	4.497851
166	6	0	6.938155	1.887905	2.175079
167	1	0	5.545872	1.085689	0.748552
168	6	0	10.019949	-1.578319	-2.253833
169	6	0	9.813937	-3.053685	-0.323851
170	6	0	6.294996	-3.555945	0.401772
171	6	0	8.730499	-3.601297	0.468178
172	1	0	4.194035	1.336955	6.150067
173	6	0	7.193606	2.135028	3.550702
174	1	0	6.441587	2.043513	5.545953
175	7	0	7.884477	2.305851	1.209425
176	6	0	11.405220	-1.719756	-2.158775
177	1	0	9.587842	-0.936946	-3.014599
178	6	0	11.202270	-3.173926	-0.252959
179	6	0	6.293742	-4.403061	1.510887
180	1	0	5.357222	-3.240272	-0.040263
181	6	0	8.696668	-4.444221	1.580195
182	1	0	8.127789	2.601673	3.841876
183	6	0	9.281735	2.245004	1.349404
184	6	0	7.599049	3.119220	0.093443
185	6	0	12.026276	-2.522199	-1.179696
186	1	0	12.013091	-1.180945	-2.876579
187	1	0	11.638292	-3.789618	0.529231
188	6	0	7.476010	-4.858500	2.128495



189	1	0	5.330688	-4.712065	1.900868
190	1	0	9.634380	-4.782632	2.013184
191	6	0	10.067124	1.548072	2.266856
192	6	0	9.887621	3.013695	0.327704
193	6	0	6.379690	3.538190	-0.435678
194	6	0	8.815378	3.563554	-0.478142
195	6	0	13.553915	-2.715127	-1.109543
196	6	0	7.465689	-5.784261	3.360832
197	6	0	11.454309	1.678812	2.182506
198	1	0	9.625162	0.912038	3.026420
199	6	0	11.277198	3.123724	0.267456
200	6	0	6.396395	4.376944	-1.551152
201	1	0	5.433943	3.233714	-0.003274
202	6	0	8.799785	4.398443	-1.596417
203	6	0	14.301787	-1.886341	-2.171321
204	6	0	14.074466	-2.291075	0.283898
205	6	0	13.890624	-4.207564	-1.343665
206	6	0	8.198039	-7.104852	3.023685
207	6	0	8.188349	-5.086223	4.537497
208	6	0	6.037918	-6.136108	3.820785
209	6	0	12.089086	2.472092	1.205019
210	1	0	12.052223	1.138844	2.907741
211	1	0	11.723811	3.731527	-0.514858
212	6	0	7.588104	4.818339	-2.160146
213	1	0	5.439624	4.689385	-1.953444
214	1	0	9.744588	4.725739	-2.022376
215	1	0	14.013060	-2.171418	-3.189385
216	1	0	14.121327	-0.811710	-2.053426
217	1	0	15.380943	-2.052580	-2.076760
218	1	0	13.626327	-2.886460	1.086239
219	1	0	15.162327	-2.420401	0.342519
220	1	0	13.844414	-1.238322	0.483183
221	1	0	13.418452	-4.851495	-0.594097
222	1	0	13.544684	-4.536339	-2.330332
223	1	0	14.974487	-4.370548	-1.290679
224	1	0	9.238393	-6.930232	2.729646
225	1	0	8.205413	-7.772871	3.894104
226	1	0	7.701849	-7.627304	2.197827
227	1	0	8.196582	-5.734816	5.422532
228	1	0	9.227977	-4.845732	4.291071
229	1	0	7.684575	-4.150496	4.805661
230	1	0	5.469203	-5.243645	4.105762
231	1	0	5.476838	-6.665484	3.042251
232	1	0	6.083886	-6.792105	4.697601
233	6	0	13.618307	2.657141	1.149060
234	6	0	7.597498	5.734136	-3.399818
235	6	0	14.351834	1.825923	2.218935
236	6	0	14.151032	2.229568	-0.238613
237	6	0	13.959043	4.148425	1.385098

238	6	0	8.338610	7.050740	-3.066284
239	6	0	8.324804	5.019813	-4.563783
240	6	0	6.177194	6.094800	-3.875761
241	1	0	14.055346	2.113970	3.233930
242	1	0	14.167018	0.752079	2.100659
243	1	0	15.432640	1.986455	2.134143
244	1	0	13.712085	2.824336	-1.046439
245	1	0	15.239613	2.356800	-0.286764
246	1	0	13.921606	1.176802	-0.438255
247	1	0	13.497301	4.793499	0.630019
248	1	0	13.604589	4.479837	2.367861
249	1	0	15.044069	4.306554	1.342945
250	1	0	9.374646	6.869341	-2.761247
251	1	0	8.360034	7.711465	-3.941982
252	1	0	7.839482	7.584431	-2.249418
253	1	0	8.346896	5.660967	-5.453952
254	1	0	9.359983	4.772357	-4.305736
255	1	0	7.815262	4.086387	-4.828863
256	1	0	5.603304	5.205222	-4.159195
257	1	0	5.613610	6.635201	-3.106654
258	1	0	6.237242	6.743497	-4.757123

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e. C<sub>2h</sub> symmetry isomer

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.395536	-0.524382	-1.258053
2	6	0	-1.181773	-0.940488	-2.534628
3	6	0	-2.437028	-0.993148	-3.287177
4	6	0	-3.427547	-0.531485	-2.422887
5	6	0	-2.741318	-0.309274	-1.140511
6	6	0	-2.791033	0.322438	1.117366
7	6	0	-3.422641	0.539041	2.408638
8	6	0	-2.422729	0.992118	3.284043
9	6	0	-1.159187	0.971924	2.576342
10	7	0	-0.014960	-1.192090	-3.134426
11	7	0	-3.394915	0.000319	-0.013826
12	7	0	0.014748	1.192422	3.134156
13	1	0	-0.753488	0.449043	0.559027
14	7	0	-1.443267	0.573305	1.291816
15	6	0	-4.741056	-0.255174	-2.902727
16	6	0	-5.750350	0.392788	-2.145770
17	6	0	-4.997747	-0.581471	-4.280983
18	6	0	-6.946124	0.768102	-2.735060
19	1	0	-5.553670	0.628494	-1.107862
20	6	0	-6.268136	-0.257096	-4.824050
21	6	0	-7.210103	0.418927	-4.088119
22	1	0	-6.468927	-0.500945	-5.864446
23	1	0	-8.144180	0.727494	-4.543895
24	6	0	-2.683846	1.306371	4.633584
25	6	0	-3.961213	1.115132	5.099981
26	6	0	-3.975992	-1.145909	-5.098633
27	6	0	-2.694820	-1.330135	-4.627982
28	6	0	-4.738615	0.257966	2.893394
29	6	0	-4.988044	0.563023	4.274600
30	1	0	-1.898075	-1.704619	-5.262266
31	1	0	-4.219940	-1.386463	-6.130568
32	6	0	-9.280984	1.459105	-2.119178
33	6	0	-7.584075	2.773352	-1.371760
34	6	0	-10.077224	0.444364	-2.649224
35	6	0	-9.874910	2.592666	-1.514903
36	6	0	-6.357644	3.370201	-1.084441
37	6	0	-8.792927	3.426249	-1.029848
38	6	0	-11.463028	0.607353	-2.616642
39	1	0	-9.643596	-0.455277	-3.072765
40	6	0	-11.263657	2.726190	-1.494859
41	6	0	-6.359469	4.603356	-0.430849

42	1	0	-5.418594	2.904201	-1.358927
43	6	0	-8.762259	4.656948	-0.372141
44	6	0	-12.086168	1.743623	-2.060998
45	1	0	-12.069611	-0.184898	-3.040294
46	1	0	-11.701291	3.610813	-1.039871
47	6	0	-7.543162	5.268876	-0.053464
48	1	0	-5.397501	5.052100	-0.211062
49	1	0	-9.701328	5.140245	-0.115451
50	7	0	-7.883174	1.564916	-2.031468
51	6	0	-7.536090	6.624748	0.679586
52	6	0	-13.614623	1.942316	-2.071198
53	6	0	-14.360193	0.745156	-2.691196
54	1	0	-14.074238	0.583613	-3.736781
55	1	0	-14.174464	-0.183226	-2.139128
56	1	0	-15.439982	0.931628	-2.670452
57	6	0	-14.129356	2.131975	-0.624954
58	1	0	-13.682893	3.008787	-0.144353
59	1	0	-15.217890	2.268723	-0.619856
60	1	0	-13.891776	1.258054	-0.007894
61	6	0	-13.960058	3.201982	-2.901496
62	1	0	-13.490296	4.100860	-2.488288
63	1	0	-13.617803	3.093626	-3.937063
64	1	0	-15.044722	3.367479	-2.916602
65	6	0	-8.276596	7.680478	-0.175458
66	1	0	-9.316358	7.394154	-0.365743
67	1	0	-8.286535	8.650932	0.336461
68	1	0	-7.784671	7.812590	-1.145900
69	6	0	-8.252805	6.478609	2.043011
70	1	0	-8.263684	7.437565	2.576210
71	1	0	-9.291318	6.152125	1.923592
72	1	0	-7.742998	5.742937	2.675596
73	6	0	-6.109650	7.142968	0.945016
74	1	0	-5.535222	6.453333	1.573955
75	1	0	-5.553093	7.301843	0.014344
76	1	0	-6.157955	8.104728	1.468414
77	6	0	-7.201261	-0.431086	4.073847
78	6	0	-6.945089	-0.758377	2.715404
79	1	0	-8.132661	-0.746190	4.530152
80	7	0	-7.885172	-1.540386	2.002746
81	6	0	-9.283216	-1.453249	2.123093
82	6	0	-7.587276	-2.732717	1.310319
83	6	0	-10.080085	-0.457930	2.687670
84	6	0	-9.876647	-2.582079	1.510628
85	6	0	-6.361910	-3.309913	0.982085
86	6	0	-8.796307	-3.392471	0.983906
87	6	0	-11.464233	-0.638716	2.684670
88	1	0	-9.649360	0.441118	3.115390
89	6	0	-11.263507	-2.734215	1.520803
90	6	0	-6.366045	-4.529986	0.304148

91	1	0	-5.420537	-2.840108	1.240909
92	6	0	-8.768384	-4.609545	0.301485
93	6	0	-12.085383	-1.773943	2.125113
94	1	0	-12.070722	0.138178	3.135924
95	1	0	-11.699898	-3.616527	1.060299
96	6	0	-7.550762	-5.201443	-0.058076
97	1	0	-5.404635	-4.962203	0.051658
98	1	0	-9.708144	-5.097974	0.057540
99	6	0	-13.609626	-1.997600	2.175747
100	6	0	-7.546266	-6.542249	-0.818178
101	6	0	-14.356994	-0.817673	2.825996
102	6	0	-14.163531	-2.185544	0.743992
103	6	0	-13.909202	-3.269276	3.005764
104	6	0	-8.256164	-7.622583	0.032076
105	6	0	-8.295302	-6.376597	-2.161863
106	6	0	-6.120840	-7.039403	-1.125959
107	1	0	-14.046022	-0.660232	3.865030
108	1	0	-14.201041	0.118053	2.277058
109	1	0	-15.433823	-1.021387	2.832454
110	1	0	-13.714389	-3.048616	0.241613
111	1	0	-15.248585	-2.345051	0.770979
112	1	0	-13.964144	-1.301317	0.128269
113	1	0	-13.436302	-4.156622	2.571658
114	1	0	-13.538751	-3.162928	4.031797
115	1	0	-14.989975	-3.453516	3.050995
116	1	0	-9.294293	-7.351549	0.251497
117	1	0	-8.267669	-8.582618	-0.499020
118	1	0	-7.740882	-7.768820	0.988279
119	1	0	-8.307701	-7.324766	-2.713916
120	1	0	-9.334404	-6.064521	-2.012573
121	1	0	-7.807977	-5.622691	-2.790609
122	1	0	-5.568268	-6.331488	-1.754091
123	1	0	-5.541524	-7.210288	-0.211430
124	1	0	-6.171059	-7.991285	-1.666910
125	6	0	-5.748465	-0.373874	2.128106
126	1	0	-5.555991	-0.589298	1.085086
127	6	0	-6.254741	0.232291	4.817410
128	1	0	-6.451035	0.459090	5.862383
129	1	0	-1.884963	1.670583	5.270536
130	1	0	-4.204065	1.340124	6.135498
131	6	0	1.181570	0.940862	2.534330
132	7	0	1.395339	0.524831	1.257750
133	6	0	2.436814	0.993508	3.286892
134	6	0	2.741137	0.309712	1.140204
135	6	0	3.427351	0.531883	2.422598
136	6	0	2.694524	1.330418	4.627728
137	7	0	3.394721	0.000101	0.013528
138	6	0	4.740839	0.255542	2.902493
139	6	0	3.975663	1.146115	5.098441

140	1	0	1.897734	1.704859	5.261979
141	6	0	2.790826	-0.322010	-1.117673
142	6	0	5.750212	-0.392303	2.145533
143	6	0	4.997439	0.581711	4.280799
144	1	0	4.219569	1.386567	6.130409
145	6	0	3.422446	-0.538763	-2.408906
146	7	0	1.443046	-0.572763	-1.292149
147	6	0	6.945931	-0.767698	2.734877
148	1	0	5.553611	-0.627869	1.107579
149	6	0	6.267771	0.257231	4.823938
150	6	0	2.422531	-0.991888	-3.284290
151	6	0	4.738446	-0.257829	-2.893681
152	6	0	1.158983	-0.971548	-2.576628
153	1	0	0.753288	-0.448563	-0.559330
154	6	0	7.209782	-0.418732	4.088014
155	7	0	7.883068	-1.564401	2.031245
156	1	0	6.468475	0.500952	5.864381
157	6	0	2.683661	-1.306351	-4.633781
158	6	0	4.987907	-0.563142	-4.274824
159	6	0	5.748311	0.374072	-2.128467
160	1	0	8.143797	-0.727399	4.543844
161	6	0	9.280868	-1.458774	2.119424
162	6	0	7.584047	-2.772870	1.371537
163	6	0	3.961063	-1.115295	-5.100161
164	1	0	1.884761	-1.670583	-5.270700
165	6	0	6.254660	-0.232621	-4.817638
166	6	0	6.944998	0.758341	-2.715775
167	1	0	5.555790	0.589755	-1.085509
168	6	0	10.077063	-0.444088	2.649642
169	6	0	9.874860	-2.592450	1.515437
170	6	0	6.357642	-3.369578	1.083822
171	6	0	8.792934	-3.425940	1.030083
172	1	0	4.203942	-1.340474	-6.135630
173	6	0	7.201212	0.430786	-4.074144
174	1	0	6.450974	-0.459627	-5.862562
175	7	0	7.885144	1.540362	-2.003212
176	6	0	11.462856	-0.607278	2.617587
177	1	0	9.643414	0.455664	3.072926
178	6	0	11.263595	-2.726182	1.495919
179	6	0	6.359537	-4.602779	0.430315
180	1	0	5.418555	-2.903438	1.357936
181	6	0	8.762340	-4.656676	0.372441
182	1	0	8.132672	0.745719	-4.530446
183	6	0	9.283183	1.452838	-2.123265
184	6	0	7.587408	2.732854	-1.311017
185	6	0	12.086041	-1.743698	2.062302
186	1	0	12.069391	0.184936	3.041379
187	1	0	11.701259	-3.610908	1.041163
188	6	0	7.543276	-5.268472	0.053384

189	1	0	5.397590	-5.051418	0.210223
190	1	0	9.701437	-5.140103	0.116100
191	6	0	10.079894	0.457238	-2.687561
192	6	0	9.876780	2.581606	-1.510845
193	6	0	6.362112	3.310417	-0.983163
194	6	0	8.796540	3.392356	-0.984463
195	6	0	13.614454	-1.942672	2.073258
196	6	0	7.536285	-6.624386	-0.679591
197	6	0	11.464091	0.637637	-2.684264
198	1	0	9.649017	-0.441738	-3.115278
199	6	0	11.263685	2.733359	-1.520738
200	6	0	6.366406	4.530599	-0.305428
201	1	0	5.420688	2.840797	-1.242143
202	6	0	8.768771	4.609554	-0.302257
203	6	0	14.359954	-0.745523	2.693366
204	6	0	13.959215	-3.202239	2.903994
205	6	0	14.129901	-2.132749	0.627327
206	6	0	8.253463	-6.478405	-2.042790
207	6	0	8.276387	-7.680158	0.175750
208	6	0	6.109873	-7.142457	-0.945457
209	6	0	12.085430	1.772758	-2.124706
210	1	0	12.070462	-0.139488	-3.135275
211	1	0	11.700216	3.615616	-1.060262
212	6	0	7.551216	5.201816	0.056940
213	1	0	5.405052	4.963112	-0.053231
214	1	0	9.708596	5.097793	-0.058188
215	1	0	14.174585	0.182797	2.141069
216	1	0	14.073607	-0.583764	3.738809
217	1	0	15.439723	-0.932162	2.673087
218	1	0	13.489496	-4.101103	2.490705
219	1	0	15.043840	-3.367937	2.919709
220	1	0	13.616426	-3.093616	3.939357
221	1	0	13.683469	-3.009531	0.146646
222	1	0	13.892920	-1.258877	0.009968
223	1	0	15.218400	-2.269793	0.622848
224	1	0	9.291976	-6.152040	-1.923047
225	1	0	8.264399	-7.437389	-2.575938
226	1	0	7.743952	-5.742702	-2.675579
227	1	0	8.286377	-8.650640	-0.336116
228	1	0	9.316122	-7.393950	0.366359
229	1	0	7.784130	-7.812162	1.146039
230	1	0	5.552987	-7.301194	-0.014958
231	1	0	5.535736	-6.452804	-1.574642
232	1	0	6.158239	-8.104264	-1.468765
233	6	0	13.609756	1.995930	-2.174967
234	6	0	7.546898	6.542743	0.816834
235	6	0	14.356942	0.815599	-2.824695
236	6	0	13.909965	3.267309	-3.005204
237	6	0	14.163316	2.184044	-0.743098

238	6	0	8.295673	6.377130	2.160667
239	6	0	8.257182	7.622786	-0.033470
240	6	0	6.121535	7.040267	1.124306
241	1	0	14.200469	-0.119946	-2.275592
242	1	0	14.046278	0.658024	-3.863800
243	1	0	15.433843	1.018941	-2.830829
244	1	0	13.437216	4.154901	-2.571436
245	1	0	14.990808	3.451204	-3.050177
246	1	0	13.539767	3.160833	-4.031315
247	1	0	13.714351	3.047410	-0.241067
248	1	0	13.963418	1.300048	-0.127210
249	1	0	15.248435	2.343149	-0.769816
250	1	0	9.334726	6.064786	2.011602
251	1	0	8.308203	7.325385	2.712570
252	1	0	7.808068	5.623439	2.789454
253	1	0	8.268807	8.582902	0.497477
254	1	0	9.295289	7.351487	-0.252667
255	1	0	7.742096	7.768984	-0.989784
256	1	0	5.542403	7.211140	0.209657
257	1	0	5.568704	6.332575	1.752460
258	1	0	6.171880	7.992223	1.665115

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