

## Supporting Information

### Desymmetrised pentaporphyrinic gears mounted on metallo-organic anchors

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## I. Materials and methods

All chemicals and solvents were purchased from commercial suppliers and were used without further purification. Anhydrous dichloromethane, anhydrous tetrahydrofuran, anhydrous toluene, anhydrous *N,N*-dimethylformamide, methanol, anhydrous chloroform, anhydrous triethylamine, diisopropylamine, hydrochloric acid 37%, bis(triphenylphosphine)palladium(II) dichloride, tetrakis(triphenylphosphine)palladium(0), palladium(II) acetate, copper(I) thiophene-2-carboxylate (CuTC), copper(I) iodide, 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (SPhos), cesium carbonate, tetrabutylammonium fluoride, 3,5-bis-(*tert*-butyl)benzaldehyde, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), boron trifluoride diethyl etherate, nickel(II) acetylacetone and [1,1'-bis(diphenylphosphanyl)ferrocene]dichloropalladium(II) were purchased from Aldrich. 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-benzaldehyde was purchased from ABCR and trifluoroacetic acid from TCI. Compounds **1**,<sup>[S1]</sup> **2**,<sup>[S2]</sup> **3**,<sup>[S3]</sup> **4**,<sup>[S3]</sup> **8**,<sup>[S1]</sup> **9**<sup>[S1]</sup> and 4-(di(1*H*-pyrrol-2-yl)methyl)benzonitrile<sup>[S4]</sup> were synthesised according to previously reported procedures.

All reactions were carried out using standard Schlenk techniques under an argon atmosphere. Column chromatography was carried out on 230–400 mesh silica gel (Aldrich) unless otherwise stated. Thin layer chromatography (TLC) was performed on pre-coated aluminum-backed silica gel 60 UV254 plates (Macherey–Nagel) with visualisation effected using ultraviolet irradiation ( $\lambda = 254, 366$  nm). Melting points were measured on a Stuart SMP40 melting point apparatus reaching 400 °C. Up to that temperature, no melting of porphyrinic derivatives (porphyrin precursors, monoporphyrinic complexes and pentaporphyrinic cogwheels) was observed and no clear decomposition temperature could be established.

NMR and mass spectra were recorded by the appropriate services of the Toulouse Institute of Chemistry (ICT – FR2599).  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra were recorded on Bruker Avance III HD 500 MHz (cryoprobe Prodigy 5mm BBO, 1H ATMA) and Avance 500 MHz (cryoprobe 5mm  $^1\text{H}$ ,  $^{13}\text{C}$ ). Residual solvent signals were used as internal reference for  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra were referenced according to the solvent. Chemical shifts ( $\delta$ ) are reported in ppm. 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 (quint); multiplet (m). Full assignments of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were made with the assistance of COSY, HMBC, and HSQC spectra. The full width of  $^1\text{H}$  NMR spectra (at least -0.5 to 9.5 ppm, and mostly wider) and  $^{13}\text{C}$  NMR spectra (-10 to 210 ppm) is shown on purpose in section IV; in case some minor impurities such as grease or solvent traces are present, the corresponding peaks have been assigned. High-resolution mass spectra (HR-MS) were performed with a Waters Xevo G2 QTOF spectrometer for electrospray ionisation (ESI) and with a Waters MALDI micro MX spectrometer for matrix assisted laser desorption ionisation (MALDI) (matrix: *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile DTCB;  $\lambda = 337$  nm). UV/Vis spectra were recorded with a Shimadzu UV-26000 spectrometer (sh = shoulder,  $\epsilon$  [ $\text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ] is reported in parentheses). Cyclic voltammograms were obtained with an Autolab system (PGSTAT204) in  $\text{CH}_2\text{Cl}_2$  with 0.1 M tetrabutylammonium hexafluorophosphate  $n\text{Bu}_4\text{NPF}_6$  as the supporting electrolyte and a scan rate of 0.1 V s $^{-1}$  at 25 °C. A three electrode cell was used comprised of a 1 mm platinum disk working electrode, a platinum wire auxiliary electrode, and an aqueous SCE reference electrode.

## II. Synthesis of porphyrins 3-7

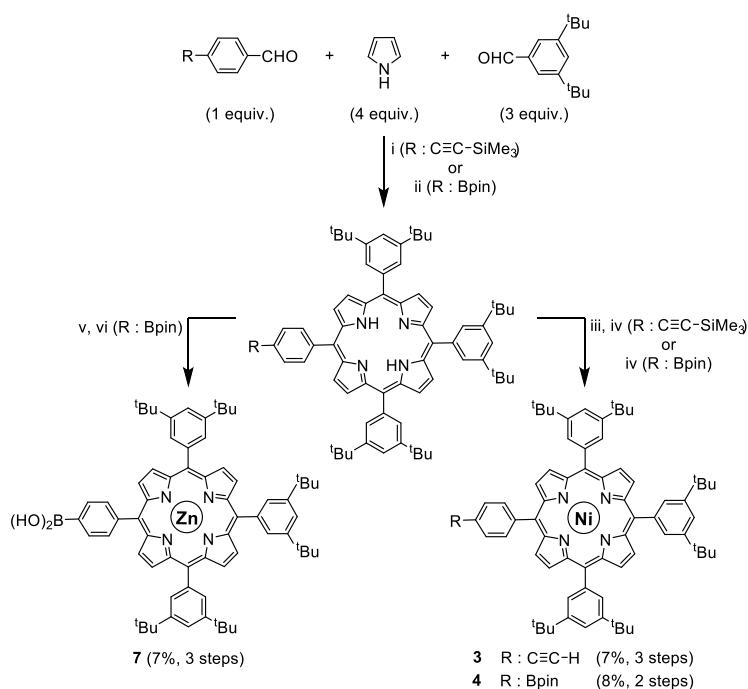
### 1. Synthetic route to A<sub>3</sub>B-type porphyrins 3, 4 and 7

A<sub>3</sub>B-type porphyrins **3**, **4** and **7** were synthesised under Lindsey statistical conditions.

For porphyrin **3** incorporating an ethynylphenyl substituent, pyrrole (4 equiv.) was reacted with stoichiometric amounts of 4-[(trimethylsilyl)ethynyl]benzaldehyde (1 equiv.) and 3,5-di-*tert*-butylbenzaldehyde (3 equiv.) in chloroform using BF<sub>3</sub>·OEt<sub>2</sub> as catalyst. After oxidation with DDQ, the target A<sub>3</sub>B-type porphyrin was isolated in 8% yield. Silyl deprotection of the alkyne was carried out under mild basic conditions and the resulting free-base porphyrin was finally metalated in the presence of nickel(II) acetylacetone in refluxing toluene to give porphyrin **3** in 7% overall yield (three steps).

In a similar way, porphyrin **4** was obtained in two steps, starting from 3,5-di-*tert*-butylbenzaldehyde and 4-(tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde. After condensation under Lindsey conditions and subsequent oxidation, the free base porphyrin carrying a boronic acid pinacol ester group was metalated in the presence of nickel(II) acetylacetone to afford nickel(II) porphyrin **4** (8% overall yield).

Alternatively, the intermediate free base porphyrin was submitted to acidic conditions and the resulting boronic acid derivative was then successfully metalated in the presence of zinc acetate dihydrate to give A<sub>3</sub>B-type zinc(II) porphyrin **7** in 7% yield over three steps.



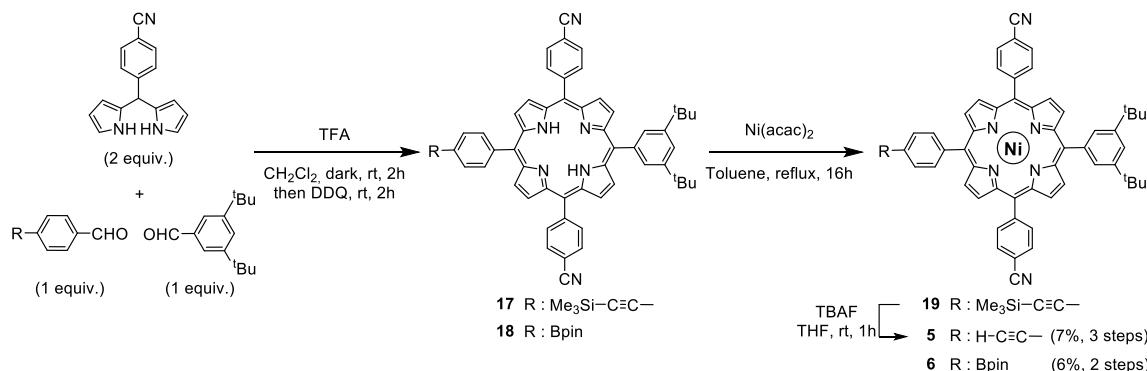
Reagents and conditions: i) BF<sub>3</sub>·OEt<sub>2</sub>, CHCl<sub>3</sub>, dark, rt, 1h then DDQ, rt, 1h; ii) BF<sub>3</sub>·OEt<sub>2</sub>, CHCl<sub>3</sub>, dark, rt, 1h then chloranil, reflux, 30 min; iii) K<sub>2</sub>CO<sub>3</sub>, MeOH / CH<sub>2</sub>Cl<sub>2</sub> 3:1, rt, 12h; iv) Ni(acac)<sub>2</sub>, toluene, reflux, 16h; v) HCl / H<sub>2</sub>O 4:1, rt, 12h; vi) Zn(OAc)<sub>2</sub>·2H<sub>2</sub>O, THF / MeOH 1:1, rt, 24h.

**Scheme S1.** Synthesis of A<sub>3</sub>B-type nickel(II) and zinc(II) *meso*-tetraarylporphyrins functionalised with a terminal alkyne (**3**), a boronic acid (**7**) or a boronic acid pinacol ester (**4**).

The detailed procedures for the synthesis of porphyrins **3** and **4** are reported elsewhere<sup>[S3]</sup> and the procedure for the synthesis of porphyrin **7** is available in section III (see below).

## 2. Synthetic route to *trans* A<sub>2</sub>BC-type porphyrins 5 and 6

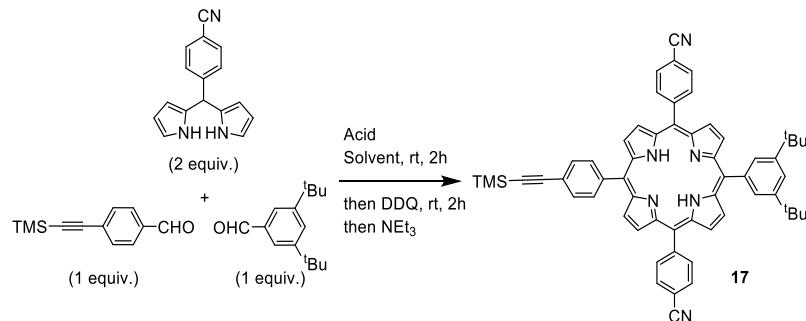
Nickel(II) porphyrin **5** was prepared in three steps, with the initial formation of A<sub>2</sub>BC-type free-base porphyrin **17** according to Lindsey conditions (Scheme S2).<sup>[55]</sup>



**Scheme S2.** Synthesis of *trans* A<sub>2</sub>BC-type nickel(II) *meso*-tetraarylporphyrins functionalised with a terminal alkyne (**5**) or a boronic acid pinacol ester (**6**).

4-[((Trimethylsilyl)ethynyl]benzaldehyde and 3,5-di-*tert*-butylbenzaldehyde were reacted with 4-(di(1*H*-pyrrol-2-yl)methyl)benzonitrile under stoichiometric conditions, and the nature and quantity of acid were carefully optimised (Table S1).

**Table S1.** Optimisation of the synthesis of *trans* A<sub>2</sub>BC-type free-base *meso*-tetraarylporphyrin **17**, incorporating two 4-cyanophenyl substituents.



Entry	Acid	Equiv.	Solvent	Yield <sup>a</sup>
1	TFA	2	CH <sub>2</sub> Cl <sub>2</sub>	<1
2	TFA	2	CHCl <sub>3</sub>	0
3	BF <sub>3</sub> ·OEt <sub>2</sub>	2	CHCl <sub>3</sub>	Traces
4 <sup>b</sup>	TFA	2	CH <sub>2</sub> Cl <sub>2</sub>	<1
5	TFA	6	CH <sub>2</sub> Cl <sub>2</sub>	8
6	TFA	20	CH <sub>2</sub> Cl <sub>2</sub>	3

<sup>a</sup> Isolated yield. <sup>b</sup> A saturated aqueous solution of sodium hydrogenocarbonate was used instead of triethylamine to neutralize the reaction medium.

Condensation was first attempted in dichloromethane using 2 equiv. of trifluoroacetic acid (TFA) as a Brønsted acid, followed by DDQ oxidation and subsequent basic treatment with triethylamine. In these conditions, the desired porphyrin was obtained in a very low yield (<1%) (entry 1) and extending the reaction time was not beneficial and led to scrambling. In an attempt to optimise the synthesis of the target porphyrin **17**, changing the solvent to chloroform (entry 2) or replacing the Brønsted acid by  $\text{BF}_3\cdot\text{OEt}_2$  as Lewis acid under similar conditions (entry 3) failed to improve the reaction efficiency. The same situation was encountered when sodium bicarbonate was used as a neutralizing agent instead of triethylamine (entry 4). Inspired by the conditions used for the preparation of *meso*-substituted *trans*-A<sub>2</sub>B<sub>2</sub>-porphyrins bearing pyridyl units,<sup>[56]</sup> the amount of TFA was gradually increased. This resulted in a higher yield of *trans*-A<sub>2</sub>BC porphyrin **17** with an optimal efficiency reached in the presence of 6 equiv. of TFA with dichloromethane as reaction solvent (entries 5 and 6). After DDQ oxidation and subsequent basic treatment with triethylamine, the *trans*-A<sub>2</sub>BC free-base porphyrin **17** was obtained in 8% yield. It was next metalated using nickel(II) acetylacetone and final deprotection of the alkyne with TBAF afforded *trans*-A<sub>2</sub>BC ethynylphenylporphyrin **5** in 7% overall yield over 3 steps.

The optimised procedure involving 5-(4-cyanophenyl)dipyrromethane was applied to the preparation of porphyrin **18** with 4-(tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde used as a precursor (Scheme S2). Subsequent metalation in the presence of nickel(II) acetylacetone gave the *trans*-A<sub>2</sub>BC nickel(II) porphyrin **6** in 6% yield over two steps.

The optimised procedure for the synthesis of free-base porphyrin **17** as well as detailed procedures for the synthesis of nickel(II) porphyrins **5** and **6** are available in section III (see below).

### III. Experimental procedures and characterisation

#### Nickel(II) 5-(4-ethynylphenyl)-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin (5):

In a Schlenk tube under argon, TBAF (1M in THF, 0.71 mL, 0.71 mmol, 1.2 equiv.) was added dropwise to a solution of porphyrin **19** (550 mg, 0.59 mmol, 1.0 equiv.) in dry THF (80 mL) and the mixture was stirred at room temperature for 1h. The reaction was then quenched with water and the solvents were evaporated. The precipitate was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and washed three times with water. The organic layer was dried over magnesium sulphate and filtered. After evaporation of the volatiles, the crude product was purified by column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/cyclohexane 2:1) to give porphyrin **5** as a red solid in 91% yield (462 mg, 0.54 mmol).

*R*<sub>f</sub> = 0.5 (CH<sub>2</sub>Cl<sub>2</sub>/cyclohexane 2:1).

<sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, 25 °C): δ = 8.84 (d, <sup>3</sup>J = 5.0 Hz, 2H, H<sub>β</sub>), 8.75 (d, <sup>3</sup>J = 5.0 Hz, 2H, H<sub>β</sub>), 8.64 (d, <sup>3</sup>J = 5.0, 2H, H<sub>β</sub>), 8.64 (d, <sup>3</sup>J = 5.0, 2H, H<sub>β</sub>), 8.14 (AA'BB' pattern, <sup>3</sup>J = 8.4 Hz, 4H, H<sub>k</sub>), 8.00 (AA'BB' pattern, <sup>3</sup>J = 8.4 Hz, 4H, H<sub>j</sub>), 7.97 (AA'BB' pattern, <sup>3</sup>J = 8.3 Hz, 2H, H<sub>q</sub>), 7.85 (d, <sup>4</sup>J = 1.8 Hz, 2H, H<sub>e</sub>), 7.83 (AA'BB' pattern, <sup>3</sup>J = 8.2 Hz, 2H, H<sub>r</sub>), 7.75 (t, <sup>4</sup>J = 1.8 Hz, 1H, H<sub>d</sub>), 3.29 (s, 1H, H<sub>u</sub>), 1.47 (s, 18H, H<sub>a</sub>) ppm.

<sup>13</sup>C{<sup>1</sup>H}-NMR (126 MHz, CDCl<sub>3</sub>, 25 °C): δ = 149.4 (C<sub>c</sub>), 145.9 (C<sub>h</sub>), 143.5 (C<sub>α</sub>), 142.7 (C<sub>α</sub>), 142.1 (C<sub>α</sub>), 142.0 (C<sub>α</sub>), 141.2 (C<sub>p</sub>), 139.5 (C<sub>f</sub>), 134.3 (C<sub>k</sub>), 133.7 (C<sub>q</sub>), 133.6 (C<sub>β</sub>), 132.7 (C<sub>β</sub>), 131.9 (C<sub>β</sub>), 131.7 (C<sub>β</sub>), 130.9 (C<sub>j</sub>), 130.9 (C<sub>r</sub>), 129.0 (C<sub>e</sub>), 122.1 (C<sub>s</sub>), 121.7 (C<sub>g</sub>), 121.6 (C<sub>d</sub>), 119.0 (C<sub>i</sub>), 118.7 (C<sub>o</sub>), 117.0 (C<sub>m</sub>), 112.2 (C<sub>i</sub>), 83.6 (C<sub>t</sub>), 78.6 (C<sub>u</sub>), 35.2 (C<sub>b</sub>), 31.8 (C<sub>a</sub>) ppm.

UV-Vis (CH<sub>2</sub>Cl<sub>2</sub>): λ<sub>max</sub> (ε) = 416 (241 000), 528 nm (18 000 mol<sup>-1</sup>dm<sup>3</sup>cm<sup>-1</sup>).

HR-MS (ESI<sup>+</sup>): calcd for C<sub>56</sub>H<sub>43</sub>N<sub>6</sub>Ni [M+H]<sup>+</sup>: 857.2903.3298, found: 857.2860.

#### Nickel(II) 5-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin (6):

In a three-neck round-bottom flask under argon and protected from light, 3,5-di-*tert*-butylbenzaldehyde (2 g, 9.16 mmol, 1.0 equiv.), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (2.13 g, 9.16 mmol, 1.0 equiv.) and 4-(di(1*H*-pyrrol-2-yl)methyl)benzonitrile<sup>[S4]</sup> (4.53 g, 18.32 mmol, 2.0 equiv.) were dissolved in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (1.3 L). The solution was degassed for 30 min and trifluoroacetic acid (4.08 mL, 54.96 mmol, 6.0 equiv.) was added dropwise. The solution was stirred in the dark for 2 h at room temperature and DDQ (6.24 g, 27.48 mmol, 3.0 equiv.) was added. The reaction mixture was stirred for another 2 h before triethylamine (7.64 mL, 54.96 mmol, 6.0 equiv.) was added to neutralize the acid. The mixture was stirred for a further 20 min and the solution was concentrated and filtered through a silica pad to give a purple mixture of porphyrins. Separation by column chromatography (SiO<sub>2</sub>, cyclohexane/CH<sub>2</sub>Cl<sub>2</sub> gradient from 3:1 to 0:1) afforded 825 mg of a mixture of free-base porphyrins, including *trans*-A<sub>2</sub>BC porphyrin **18**.

In a Schlenk tube under argon, a solution of this isolated mixture of free-base porphyrins and an excess of nickel(II) acetylacetone (938 mg, 3.65 mmol) in dry toluene (90 mL) was heated at 110 °C overnight. The mixture was cooled down to room temperature and volatiles were evaporated. The residue was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and washed with water (3x50 mL), dried over magnesium sulphate and filtered before the solvent was evaporated. The resulting crude product was purified by column chromatography (SiO<sub>2</sub>, cyclohexane/CH<sub>2</sub>Cl<sub>2</sub> 3:2) to give porphyrin **6** as a red solid in 6% yield over 2 steps (526 mg, 0.55 mmol).

*R*<sub>f</sub> = 0.4 (CH<sub>2</sub>Cl<sub>2</sub>/cyclohexane 2:1).

<sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, 25 °C): δ = 8.85 (d, <sup>3</sup>J = 5.0 Hz, 2H, H<sub>β</sub>), 8.77 (d, <sup>3</sup>J = 5.0 Hz, 2H, H<sub>β</sub>), 8.66–8.62 (m, 4H, H<sub>β</sub>), 8.14 (AA'BB' pattern, <sup>3</sup>J = 8.2 Hz, 6H, H<sub>k</sub> and H<sub>q</sub>), 8.02 (AA'BB' pattern, <sup>3</sup>J = 8.2 Hz, 2H, H<sub>r</sub>), 8.00 (AA'BB' pattern, <sup>3</sup>J = 8.4 Hz, 4H, H<sub>j</sub>), 7.86 (d, <sup>4</sup>J = 1.8 Hz, 2H, H<sub>e</sub>), 7.75 (t, <sup>4</sup>J = 1.8 Hz, 1H, H<sub>d</sub>), 1.48 (s, 30H, H<sub>a</sub> and H<sub>u</sub>) ppm.

<sup>13</sup>C{<sup>1</sup>H}-NMR (126 MHz, CDCl<sub>3</sub>, 25 °C): δ = 149.3 (C<sub>c</sub>), 146.0 (C<sub>h</sub>), 143.5 (C<sub>p</sub>), 143.4 (C<sub>a</sub>), 142.9 (C<sub>α</sub>), 142.1 (C<sub>a</sub>), 142.0 (C<sub>α</sub>), 139.6 (C<sub>f</sub>), 134.3 (C<sub>k</sub>), 133.5 (C<sub>β</sub>), 133.4 (C<sub>q</sub>), 133.4 (C<sub>r</sub>), 133.0 (C<sub>β</sub>), 131.7 (C<sub>β</sub>), 131.6 (C<sub>β</sub>), 130.9 (C<sub>j</sub>), 129.0 (C<sub>e</sub>), 121.6 (C<sub>d</sub>), 121.5 (C<sub>g</sub>), 119.7 (C<sub>o</sub>), 119.1 (C<sub>i</sub>), 116.9 (C<sub>m</sub>), 112.1 (C<sub>i</sub>), 84.3 (C<sub>t</sub>), 35.2 (C<sub>b</sub>), 31.8 (C<sub>a</sub>), 25.2 (C<sub>u</sub>) ppm.

UV-Vis (CH<sub>2</sub>Cl<sub>2</sub>): λ<sub>max</sub> (ε) = 416 (267 000), 528 nm (19 000 mol<sup>-1</sup>dm<sup>3</sup>cm<sup>-1</sup>).

HR-MS (ESI<sup>+</sup>): calcd for C<sub>60</sub>H<sub>54</sub>BN<sub>6</sub>NiO<sub>2</sub> [M+H]<sup>+</sup>: 959.3755, found: 959.3755.

### Zinc(II) 5,10,15-tris(3,5-di-tert-butylphenyl)-20-(4-boronophenyl)porphyrin (7):

In a Schlenk tube, 5,10,15-tris(3,5-di-tert-butylphenyl)-20-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]porphyrin<sup>[53]</sup> (200 mg, 0.19 mmol, 1.0 equiv.) was introduced in a mixture of THF and water (4:1, 20 mL). Then, a large excess of HCl (37% aqueous solution, 4 mL) was added and the green solution was stirred at room temperature for 12h. The solvents were evaporated, the residue was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and treated with a saturated solution of NaHCO<sub>3</sub>. The product was extracted with CH<sub>2</sub>Cl<sub>2</sub> and the organic layer was then washed with water and dried over magnesium sulphate. Volatiles were evaporated and the purple crude product was purified by column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/MeOH 99:1) to give 5,10,15-tris(3,5-di-tert-butylphenyl)-20-(4-boronophenyl)porphyrin in 90% yield (167 mg, 0.17 mmol). In a dry Schlenk tube under argon, to a mixture of this free-base porphyrin (150 mg, 0.15 mmol, 1.0 equiv.) and zinc acetate dihydrate (99 mg, 0.45 mmol, 3.0 equiv.) were added THF (20 mL) and methanol (20 mL). The solution was kept under stirring and progress of the reaction was monitored by TLC. After 24h at room temperature, solvents were evaporated and the crude residue was dissolved in CH<sub>2</sub>Cl<sub>2</sub>, washed with water and dried over magnesium sulphate. Volatiles were evaporated and subsequent purification by column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/ethyl acetate gradient from 20:1 to 4:1) gave zinc(II) porphyrin 7 as a greenish blue solid in 61% yield (98 mg, 93 μmol).

R<sub>f</sub> = 0.6 (CH<sub>2</sub>Cl<sub>2</sub>/AcOEt 4:1).

<sup>1</sup>H-NMR (500 MHz, DMSO-d<sub>6</sub>, 25 °C): δ = 8.82–8.78 (m, 8H, H<sub>β</sub>), 8.29 (s, 2H, H<sub>OH</sub>), 8.21 (AA'BB' pattern, <sup>3</sup>J = 8.0 Hz, 2H, H<sub>r</sub>), 8.16 (AA'BB' pattern, <sup>3</sup>J = 8.0 Hz, 2H, H<sub>q</sub>), 8.02 (d, <sup>4</sup>J = 1.8 Hz, 4H, H<sub>j</sub>), 8.01 (d, <sup>4</sup>J = 1.8 Hz, 2H, H<sub>e</sub>), 7.81 (t, <sup>4</sup>J = 1.8 Hz, 3H, H<sub>d</sub> and H<sub>k</sub>), 1.51 (s, 54H, H<sub>a</sub> and H<sub>h</sub>) ppm.

<sup>13</sup>C{<sup>1</sup>H}-NMR (126 MHz, DMSO-d<sub>6</sub>, 25 °C): δ = 149.4 (C<sub>a</sub>), 149.1 (C<sub>α</sub>), 148.1 (C<sub>c</sub> and C<sub>j</sub>), 144.5 (C<sub>p</sub>), 141.9 (C<sub>m</sub> and C<sub>f</sub>), 133.4 (C<sub>q</sub>), 132.2 (C<sub>r</sub>), 131.6 (C<sub>β</sub>), 131.4 (C<sub>β</sub>), 129.2 (C<sub>i</sub>), 129.1 (C<sub>e</sub>), 121.2 (C<sub>g</sub>), 121.2 (C<sub>n</sub>), 120.4 (C<sub>d</sub> and C<sub>k</sub>), 120.2 (C<sub>o</sub>), 34.6 (C<sub>b</sub> and C<sub>i</sub>), 31.4 (C<sub>a</sub> and C<sub>h</sub>) ppm.

UV-Vis (CH<sub>2</sub>Cl<sub>2</sub>): λ<sub>max</sub> (ε) = 422 (477 000), 549 (18 000), 588 nm (4 700 mol<sup>-1</sup>dm<sup>3</sup>cm<sup>-1</sup>).

HR-MS (ESI<sup>+</sup>): calcd for C<sub>68</sub>H<sub>78</sub>BN<sub>4</sub>O<sub>2</sub>Zn [M+H]<sup>+</sup>: 1056.5546, found: 1056.5520.

$\eta^5$ -**1,2,3,4-Tetra{p-[nickel(II) 10,15,20-tris(3,5-di-tert-butylphenyl)porphyrin-5-yl]phenylethynylphenyl}-5-{p-[nickel(II) 10,20-bis(4-cyanophenyl)-15-(3,5-di-tert-butylphenyl)porphyrin-5-yl]phenylethynylphenyl}cyclopentadienyl hydrotris{6-[(ethylsulfanyl)methyl]indazol-1-yl}borate ruthenium(II) (10):**

In a Schlenk tube under argon were placed complex **13** (20 mg, 8.7  $\mu\text{mol}$ , 1.0 equiv.), porphyrin **3** (54 mg, 52  $\mu\text{mol}$ , 6.0 equiv.),  $\text{Pd}(\text{OAc})_2$  (0.8 mg, 3.5  $\mu\text{mol}$ , 0.4 equiv.), SPhos (2.9 mg, 7.0  $\mu\text{mol}$ , 0.8 equiv.) and Cul (0.5 mg, 2.6  $\mu\text{mol}$ , 0.3 equiv.) followed by a mixture of anhydrous DMF (4 mL) and diisopropylamine (1 mL). The system was degassed for 10 min and heated for 48 h at 95 °C. After evaporation of the solvents, the residue was suspended in dichloromethane and filtered. The organic layer was then washed with water (3x10 mL), dried over magnesium sulphate, and the solvent was evaporated. The crude product was purified by column chromatography ( $\text{SiO}_2$ ,  $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  gradient from 4:1 to 1:1) to give complex **10** as a red solid in 49% yield (26 mg, 4.3  $\mu\text{mol}$ ).

$R_f = 0.5$  ( $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  1:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 8.84$  (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.82 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.80-8.75 (m, 32H,  $\text{H}_\beta$ ), 8.69 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.66 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.15 (AA'BB' pattern,  $^3J = 8.4$  Hz, 4H,  $\text{H}_k$ ), 8.13 (s, 3H,  $\text{H}_1$ ), 8.04 (AA'BB' pattern,  $^3J = 8.4$  Hz, 10H,  $\text{H}_{q,q',q''}$ ), 8.01 (br. s, 3H,  $\text{H}_6$ ), 7.99 (AA'BB' pattern,  $^3J = 8.4$  Hz, 4H,  $\text{H}_j$ ), 7.89-7.86 (m, 36H,  $\text{H}_{r,r',r''}$  and  $\text{H}_{e,e',e''}$  and  $\text{H}_{l,l',l''}$ ), 7.79 (t,  $^4J = 1.8$  Hz, 1H,  $\text{H}_d$ ), 8.78-8.76 (m, 4H,  $\text{H}_{d',d''}$ ), 7.73 (t,  $^4J = 1.6$  Hz, 8H,  $\text{H}_{k',k''}$ ), 7.63 (AA'BB' pattern,  $^3J = 8.4$  Hz, 10H,  $\text{H}_{13}$  and  $\text{H}_{18,18'}$ ), 7.54 (d,  $^3J = 8.6$  Hz, 3H,  $\text{H}_3$ ), 7.50 (AA'BB' pattern,  $^3J = 8.1$  Hz, 10H,  $\text{H}_{14}$  and  $\text{H}_{19,19'}$ ), 7.15 (d,  $^3J = 8.6$  Hz, 3H,  $\text{H}_4$ ), 3.98 (s, 6H,  $\text{H}_8$ ), 2.54 (q,  $^3J = 7.4$  Hz, 6H,  $\text{H}_9$ ), 1.48 (s, 90H,  $\text{H}_{a,a',a''}$ ), 1.44 (s, 144H,  $\text{H}_{h',h''}$ ), 1.33 (t,  $^3J = 7.4$  Hz, 9H,  $\text{H}_{10}$ ) ppm.

$^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 149.7$  ( $\text{C}_c$ ), 149.5 ( $\text{C}_{c',c''}$  and  $\text{C}_{j,j''}$ ), 146.0 ( $\text{C}_h$ ), 144.2 ( $\text{C}_2$ ), 143.8 ( $\text{C}_{\alpha 1}$ ), 143.4 ( $\text{C}_\alpha$ ), 143.3 ( $\text{C}_\alpha$ ), 143.2 ( $\text{C}_{\alpha 1}$ ), 142.8 ( $\text{C}_\alpha$ ), 142.6 ( $\text{C}_{\alpha 1}$ ), 142.4 ( $\text{C}_{\alpha 1}$ ), 141.7 ( $\text{C}_{p',p''}$ ), 141.1 ( $\text{C}_p$ ), 140.9 ( $\text{C}_1$ ), 140.3 ( $\text{C}_{f',f''}$  and  $\text{C}_{m',m''}$ ), 139.8 ( $\text{C}_f$ ), 138.2 ( $\text{C}_5$ ), 134.6 ( $\text{C}_{12}$  and  $\text{C}_{17,17'}$ ), 134.6 ( $\text{C}_k$ ), 134.2 ( $\text{C}_{13}$  and  $\text{C}_{18,18'}$  and  $\text{C}_{a,q',q''}$ ), 133.6 ( $\text{C}_\beta$ ), 132.8 ( $\text{C}_\beta$ ), 132.7 ( $\text{C}_\beta$ ), 132.6 ( $\text{C}_\beta$ ), 132.1 ( $\text{C}_{\beta 1}$ ), 131.9 ( $\text{C}_\beta$  and  $\text{C}_{\beta 1}$ ), 131.2 ( $\text{C}_{14}$  and  $\text{C}_{19,19'}$ ), 131.1 ( $\text{C}_j$ ), 130.6 ( $\text{C}_r$ ), 130.5 ( $\text{C}_{r',r''}$ ), 129.3 ( $\text{C}_e$ ), 129.1 ( $\text{C}_{r',r''}$ ), 129.1 ( $\text{C}_{e',e''}$ ), 123.3 ( $\text{C}_s$ ), 123.0 ( $\text{C}_{s',s''}$ ), 122.9 ( $\text{C}_{15}$  and  $\text{C}_{20,20'}$ ), 122.8 ( $\text{C}_4$ ), 122.7 ( $\text{C}_7$ ), 122.1 ( $\text{C}_d$ ), 121.8 ( $\text{C}_g$ ), 121.8 ( $\text{C}_{d',d''}$  and  $\text{C}_{k',k''}$ ), 120.9 ( $\text{C}_{g',g''}$ ), 120.8 ( $\text{C}_{n',n''}$ ), 120.6 ( $\text{C}_3$ ), 119.3 ( $\text{C}_l$ ), 119.2 ( $\text{C}_o$ ), 118.3 ( $\text{C}_{o',o''}$ ), 117.6 ( $\text{C}_m$ ), 112.4 ( $\text{C}_i$ ), 111.5 ( $\text{C}_6$ ), 90.7 ( $\text{C}_{u,u',u''}$ ), 90.5 ( $\text{C}_{t,t',t''}$ ), 88.3 ( $\text{C}_{11}$  and  $\text{C}_{16,16'}$ ), 37.0 ( $\text{C}_8$ ), 35.3 ( $\text{C}_{b,b',b''}$  and  $\text{C}_{l',l''}$ ), 31.8 ( $\text{C}_{a,a',a''}$  and  $\text{C}_{h',h''}$ ), 25.8 ( $\text{C}_9$ ), 14.8 ( $\text{C}_{10}$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\text{max}}$  ( $\varepsilon$ ) = 418 (1 365 000), 529 nm ( $101\ 000\ \text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (MALDI): calcd for  $\text{C}_{401}\text{H}_{395}\text{BN}_{28}\text{Ni}_5\text{RuS}_3[\text{M}]^+$ : 6107.6907, found 6107.7029.

$\eta^5$ -**1,2,3,4-Tetra{p-[nickel(II) 10,15,20-tris(3,5-di-tert-butylphenyl)porphyrin-5-yl]-4,4'-biphenyl}-5-{p-[ nickel(II) 10,20-bis(4-cyanophenyl)-15-(3,5-di-tert-butylphenyl)porphyrin-5-yl]-4,4'-biphenyl}cyclopentadienyl hydrotris{6-[(ethylsulfanyl)methyl]indazol-1-yl}borate ruthenium(II) (11):**

In a Schlenk tube, complex **14** (14 mg, 6.1  $\mu\text{mol}$ , 1.0 equiv.), porphyrin **4** (56 mg, 49.1  $\mu\text{mol}$ , 8.0 equiv.),  $\text{PdCl}_2(\text{dppf})$  (2.0 mg, 2.5  $\mu\text{mol}$ , 40 mol%) and  $\text{Cs}_2\text{CO}_3$  (24 mg, 74  $\mu\text{mol}$ , 12.0 equiv.) were successively introduced under an argon atmosphere in 2 mL of a degassed solution of DMF and water (99:1). The system was then degassed by three freeze-pump-thaw cycles and stirred at 100 °C for 48 h. After cooling to room temperature, the solvents were evaporated in vacuo. The residue was then dissolved in  $\text{CH}_2\text{Cl}_2$  and washed with water (3x10 mL). The organic layer was dried over magnesium sulphate,

filtered and the solvent was removed. The crude product was adsorbed onto silica and purified by column chromatography ( $\text{SiO}_2$ , cyclohexane/ $\text{CH}_2\text{Cl}_2$  gradient from 2:1 to 1:1) to give complex **11** as a red solid in 30% yield (11 mg, 1.8  $\mu\text{mol}$ ).

$R_f = 0.4$  ( $\text{CH}_2\text{Cl}_2$ /cyclohexane 1:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 8.87$  (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.83 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.82-8.74 (m, 32H,  $\text{H}_\beta$ ), 8.65 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.64 (d,  $^3J = 5.2$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.36 (s, 3H,  $\text{H}_1$ ), 8.13 (AA'BB' pattern,  $^3J = 8.4$  Hz, 4H,  $\text{H}_k$ ), 8.11 (AA'BB' pattern,  $^3J = 8.3$  Hz, 8H,  $\text{H}_{q',q''}$ ), 8.09 (AA'BB' pattern,  $^3J = 8.3$  Hz, 2H,  $\text{H}_q$ ), 8.06 (br. s, 3H,  $\text{H}_6$ ), 8.02 (AA'BB' pattern,  $^3J = 8.3$  Hz, 2H,  $\text{H}_r$ ), 8.02 (AA'BB' pattern,  $^3J = 8.3$  Hz, 8H,  $\text{H}_{r',r''}$ ), 7.96 (AA'BB' pattern,  $^3J = 8.4$  Hz, 4H,  $\text{H}_j$ ), 7.95 (AA'BB' pattern,  $^3J = 8.4$  Hz, 10H,  $\text{H}_{13}$  and  $\text{H}_{18,18'}$ ), 7.88 (d,  $^4J = 1.9$  Hz, 4H,  $\text{H}_{e'}$ ), 7.88 (d,  $^4J = 1.9$  Hz, 4H,  $\text{H}_{e''}$ ), 7.87 (d,  $^4J = 1.9$  Hz, 2H,  $\text{H}_e$ ), 7.85 (d,  $^4J = 1.9$  Hz, 16H,  $\text{H}_{l',l''}$ ), 7.83 (AA'BB' pattern,  $^3J = 8.4$  Hz, 8H,  $\text{H}_{19,19'}$ ), 7.82 (AA'BB' pattern,  $^3J = 8.3$  Hz, 2H,  $\text{H}_{14}$ ), 7.79 (t,  $^4J = 1.8$  Hz, 1H,  $\text{H}_d$ ), 7.77-7.76 (m, 4H,  $\text{H}_{d',d''}$ ), 7.70 (t,  $^4J = 1.9$  Hz, 8H,  $\text{H}_{k',k''}$ ), 7.57 (d,  $^3J = 8.5$  Hz, 3H,  $\text{H}_3$ ), 7.13 (d,  $^3J = 8.5$  Hz, 3H,  $\text{H}_4$ ), 3.99 (s, 6H,  $\text{H}_8$ ), 2.54 (q,  $^3J = 7.4$  Hz, 6H,  $\text{H}_9$ ), 1.48 (s, 18H,  $\text{H}_a$ ), 1.47 (s, 72H,  $\text{H}_{a',a''}$ ), 1.40 (s, 144H,  $\text{H}_{h',h''}$ ), 1.33 (t,  $^3J = 7.4$  Hz, 9H,  $\text{H}_{10}$ ) ppm.

$^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 149.7$  ( $\text{C}_c$ ), 149.5 ( $\text{C}_{c',c''}$ ), 149.4 ( $\text{C}_{j,j''}$ ), 146.1 ( $\text{C}_h$ ), 144.3 ( $\text{C}_2$ ), 143.7 ( $\text{C}_{\alpha 1}$ ), 143.5 ( $\text{C}_{\alpha 1}$ ), 143.3 ( $\text{C}_\alpha$ ), 143.0 ( $\text{C}_\alpha$ ), 142.5 ( $\text{C}_{\alpha 1}$ ), 142.4 ( $\text{C}_{\alpha 1}$ ), 141.1 ( $\text{C}_1$ ), 140.7 ( $\text{C}_{p',p''}$ ), 140.4 ( $\text{C}_p$ ), 140.4 ( $\text{C}_{p',p''}$ ), 140.3 ( $\text{C}_{m',m''}$ ), 140.1 ( $\text{C}_{s,s',s''}$ ), 140.0 ( $\text{C}_{20,20}$ ), 139.9 ( $\text{C}_{15}$ ), 139.8 ( $\text{C}_f$ ), 138.0 ( $\text{C}_5$ ), 135.1 ( $\text{C}_{18,18'}$ ), 134.7 ( $\text{C}_{13}$  and  $\text{C}_{q,q',q''}$ ), 134.6 ( $\text{C}_k$ ), 134.3 ( $\text{C}_{12}$ ), 134.1 ( $\text{C}_{17}$ ), 134.1 ( $\text{C}_{17'}$ ), 133.5 ( $\text{C}_{\beta 1}$ ), 133.1 ( $\text{C}_{\beta 1}$ ), 132.7 ( $\text{C}_\beta$ ), 132.5 ( $\text{C}_\beta$ ), 132.1 ( $\text{C}_\beta$ ), 132.0 ( $\text{C}_{\beta 1}$ ), 131.9 ( $\text{C}_{\beta 1}$ ), 131.1 ( $\text{C}_j$ ), 129.2 ( $\text{C}_e$ ), 129.2 ( $\text{C}_{l',l''}$ ), 129.2 ( $\text{C}_{e',e''}$ ), 126.6 ( $\text{C}_{14}$  and  $\text{C}_{19,19'}$ ), 125.9 ( $\text{C}_r$ ), 125.8 ( $\text{C}_{r',r''}$ ), 122.8 ( $\text{C}_7$ ), 122.6 ( $\text{C}_4$ ), 122.0 ( $\text{C}_d$ ), 121.8 ( $\text{C}_{d',d''}$ ), 121.7 ( $\text{C}_{k',k''}$ ), 120.8 ( $\text{C}_g$ ), 120.7 ( $\text{C}_{g',g''}$  and  $\text{C}_{n',n''}$ ), 120.6 ( $\text{C}_3$ ), 119.7 ( $\text{C}_o$ ), 119.2 ( $\text{C}_l$ ), 118.8 ( $\text{C}_{o',o''}$ ), 117.5 ( $\text{C}_m$ ), 112.4 ( $\text{C}_i$ ), 111.5 ( $\text{C}_6$ ), 88.7 ( $\text{C}_{11}$ ), 88.6 ( $\text{C}_{16}$ ), 88.5 ( $\text{C}_{16}$ ), 37.0 ( $\text{C}_8$ ), 35.3 ( $\text{C}_{b,b',b''}$ ), 35.2 ( $\text{C}_{l',l''}$ ), 31.8 ( $\text{C}_{a,a',a''}$ ), 31.8 ( $\text{C}_{h',h''}$ ), 25.8 ( $\text{C}_9$ ), 14.8 ( $\text{C}_{10}$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max} (\varepsilon) = 418$  (1 560 000), 529 nm ( $115\ 000\ \text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (MALDI): calcd. for  $\text{C}_{391}\text{H}_{395}\text{BN}_{28}\text{Ni}_5\text{RuS}_3$  [M] $^+$ : 5987.6904, found 5987.7018.

### $\eta^5\text{-1,2,3,4-Tetra}\{p\text{-[nickel(II) 10,15,20-tris(3,5-di-tert-butylphenyl)porphyrin-5-yl]-4,4'-biphenyl}\text{-5-p-[zinc(II) 10,15,20-tris(3,5-di-tert-butylphenyl)porphyrin-5-yl]-4,4'-biphenyl}\text{cyclopentadienyl hydrotris[6-[(ethylsulfanyl)methyl]indazol-1-yl]borate ruthenium(II)}$ (12):

In a Schlenk tube, complex **15** (20 mg, 8  $\mu\text{mol}$ , 1.0 equiv.), porphyrin **4** (74 mg, 65  $\mu\text{mol}$ , 8.0 equiv.),  $\text{PdCl}_2(\text{dpdpf})$  (2.7 mg, 3.25  $\mu\text{mol}$ , 40 mol%) and  $\text{Cs}_2\text{CO}_3$  (32 mg, 98  $\mu\text{mol}$ , 12.0 equiv.) were successively introduced under argon atmosphere in 3 mL of a degassed solution of DMF and water (99:1). The system was then degassed by three freeze-pump-thaw cycles and stirred at 100 °C for 48 h. After cooling to room temperature, the solvents were evaporated in vacuo. The residue was then dissolved in  $\text{CH}_2\text{Cl}_2$  and washed three times with water. The organic layer was dried over magnesium sulphate, filtered and the solvent was removed. The crude product was adsorbed onto silica and purified by column chromatography ( $\text{SiO}_2$ , heptane/ $\text{CH}_2\text{Cl}_2$  2:1) to give complex **12** as a red solid in 30% yield (15 mg, 2.4  $\mu\text{mol}$ ).

$R_f = 0.4$  ( $\text{CH}_2\text{Cl}_2$ /heptane 1:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 9.01$  (d,  $^3J = 4.6$  Hz, 2H,  $\text{H}_{\beta 1}$ ), 8.98-8.95 (m, 6H,  $\text{H}_{\beta 1}$ ), 8.84-8.81 (m, 8H,  $\text{H}_\beta$ ), 8.80-8.75 (m, 24H,  $\text{H}_\beta$ ), 8.38 (s, 3H,  $\text{H}_1$ ), 8.30 (AA'BB' pattern,  $^3J = 7.9$  Hz, 2H,  $\text{H}_q$ ), 8.14-8.09 (m, 10H,  $\text{H}_r$  and  $\text{H}_{q',q''}$ ), 8.09 (d,  $^4J = 1.7$  Hz, 2H,  $\text{H}_e$ ), 8.07 (s, 3H,  $\text{H}_6$ ), 8.06 (d,  $^4J = 1.7$  Hz, 4H,  $\text{H}_l$ ), 8.06-8.01 (m, 8H,  $\text{H}_{r',r''}$ ), 8.00-7.94 (m, 10H,  $\text{H}_{13}$  and  $\text{H}_{18,18'}$ ), 7.92-7.88 (m, 10H,  $\text{H}_{14}$  and  $\text{H}_{e',e''}$ ), 7.86 (br. s, 16H,

$H_{l,l''}$ ), 7.87-7.82 (m, 9H,  $H_d$  and  $H_{19,19'}$ ), 7.78-7.76 (m, 6H,  $H_k$  and  $H_{d',d''}$ ), 7.72-7.69 (m, 8H,  $H_{k,k'}$ ), 7.59 (d,  $^3J = 8.6$  Hz, 3H,  $H_3$ ), 7.14 (d,  $^3J = 8.6$  Hz, 3H,  $H_4$ ), 3.99 (s, 6H,  $H_8$ ), 2.54 (q,  $^3J = 7.4$  Hz, 6H,  $H_9$ ), 1.53 (s, 18H,  $H_a$ ), 1.48 (s, 72H,  $H_{a',a''}$ ), 1.46 (s, 36H,  $H_h$ ), 1.41 (s, 144H,  $H_{h',h''}$ ), 1.33 (t,  $^3J = 7.4$  Hz, 9H,  $H_{10}$ ) ppm.

$^{13}C\{^1H\}$ -NMR (126 MHz,  $CD_2Cl_2$ , 25 °C):  $\delta = 150.8$  ( $C_{\alpha 1}$ ), 150.4 ( $C_{\alpha 1}$ ), 149.5 ( $C_{c',c''}$ ), 149.5 ( $C_{j,j''}$ ), 149.1 ( $C_c$ ), 149.1 ( $C_j$ ), 144.3 ( $C_2$ ), 143.4 ( $C_\alpha$ ), 143.3 ( $C_\alpha$ ), 143.0 ( $C_\alpha$ ), 142.6 ( $C_p$ ), 142.3 ( $C_f$ ), 142.2 ( $C_m$ ), 141.2 ( $C_1$ ), 140.7 ( $C_{p',p''}$ ), 140.4 ( $C_{r',r''}$ ), 140.3 ( $C_{15}$  and  $C_{m',m''}$ ), 140.1 ( $C_{20,20'}$ ), 140.0 ( $C_{s',s''}$ ), 139.8 ( $C_s$ ), 138.0 ( $C_5$ ), 135.4 ( $C_o$ ), 135.1 ( $C_{13}$  and  $C_{18,18'}$ ), 134.7 ( $C_{q',q''}$ ), 134.2 ( $C_{17,17'}$ ), 134.1 ( $C_{12}$ ), 132.7 ( $C_\beta$ ), 132.7 ( $C_{\beta 1}$ ), 132.7 ( $C_\beta$ ), 132.5 ( $C_{\beta 1}$ ), 132.1 ( $C_\beta$ ), 132.0 ( $C_{\beta 1}$ ), 130.0 ( $C_l$ ), 130.0 ( $C_e$ ), 129.2 ( $C_{l',l''}$ ), 129.1 ( $C_{e',e''}$ ), 126.6 ( $C_{14}$  and  $C_{19,19'}$ ), 125.8 ( $C_{r',r''}$ ), 125.5 ( $C_r$ ), 122.8 ( $C_n$  and  $C_g$ ), 122.8 ( $C_7$ ), 122.6 ( $C_4$ ), 121.8 ( $C_{d',d''}$ ), 121.7 ( $C_{k,k'}$ ), 121.4 ( $C_d$ ), 121.4 ( $C_k$ ), 120.7 ( $C_{g',g''}$  and  $C_{n',n''}$ ), 120.7 ( $C_0$ ), 120.6 ( $C_3$ ), 118.8 ( $C_{o',o''}$ ), 111.6 ( $C_6$ ), 88.6 ( $C_{16,16'}$ ), 88.6 ( $C_{11}$ ), 37.0 ( $C_8$ ), 35.3 ( $C_{b,b',b''}$  and  $C_{i,i',i''}$ ), 31.8 ( $C_{a,a',a''}$  and  $C_{h,h',h''}$ ), 25.8 ( $C_9$ ), 14.8 ( $C_{10}$ ) ppm.

UV-Vis ( $CH_2Cl_2$ ):  $\lambda_{max}$  ( $\varepsilon$ ) = 421 (1 860 000), 529 (97 000), 548 (sh, 62 000), 586 nm (12 500  $mol^{-1}dm^3cm^{-1}$ ).

HR-MS (MALDI): calcd for  $C_{405}H_{429}BN_{26}Ni_4RuS_3Zn$  [M] $^+$ : 6168.9443, found 6168.9525.

### $\eta^5$ -1,2,3,4-Tetra(*p*-bromophenyl)-5-{*p*-[nickel(II) 10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin-5-yl]phenylethynylphenyl}cyclopentadienyl hydrotris{6-[{(ethylsulfanyl)methyl]indazol-1-yl}borate ruthenium(II) (13):

In a Schlenk tube under argon were placed complex **1** (59 mg, 37  $\mu$ mol, 1.0 equiv.), porphyrin **5** (64 mg, 75  $\mu$ mol, 2.0 equiv.),  $PdCl_2(PPh_3)_2$  (2.6 mg, 3.7  $\mu$ mol, 10 mol%) and  $CuI$  (0.43 mg, 2.2  $\mu$ mol, 6 mol%). Then, anhydrous THF (8 mL) and anhydrous triethylamine (2 mL) were added. The system was degassed for 10 min by bubbling argon and stirred for 24 h at 45 °C. The volatiles were then removed in vacuo and the resulting mixture was suspended in dichloromethane and filtered. The organic layer was washed with water (3x15 mL), dried over magnesium sulphate, filtered and the solvent was evaporated. Purification by column chromatography ( $SiO_2$ ,  $CH_2Cl_2$ /cyclohexane 2:1) gave complex **13** as a red solid in 62% yield (53 mg, 23  $\mu$ mol).

$R_f = 0.4$  ( $CH_2Cl_2$ /cyclohexane 2:1).

$^1H$ -NMR (500 MHz,  $CD_2Cl_2$ , 25 °C):  $\delta = 8.84$  (d,  $^3J = 5.0$  Hz, 2H,  $H_\beta$ ), 8.80 (d,  $^3J = 5.0$  Hz, 2H,  $H_\beta$ ), 8.68 (d,  $^3J = 5.0$  Hz, 2H,  $H_\beta$ ), 8.67 (d,  $^3J = 5.2$  Hz, 2H,  $H_\beta$ ), 8.16 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $H_k$ ), 8.02 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $H_j$ ), 8.01 (AA'BB' pattern,  $^3J = 8.5$  Hz, 2H,  $H_q$ ), 7.91 (br. s, 3H,  $H_6$ ), 7.87 (d,  $^4J = 1.8$  Hz, 2H,  $H_e$ ), 7.87 (s, 3H,  $H_1$ ), 7.82 (AA'BB' pattern,  $^3J = 8.4$  Hz, 2H,  $H_r$ ), 7.79 (t,  $^4J = 1.9$  Hz, 1H,  $H_d$ ), 7.41 (AA'BB' pattern,  $^3J = 8.6$  Hz, 2H,  $H_{13}$ ), 7.39 (d,  $^3J = 8.4$  Hz, 3H,  $H_3$ ), 7.35 (AA'BB' pattern,  $^3J = 8.6$  Hz, 2H,  $H_{14}$ ), 7.30 (AA'BB' pattern,  $^3J = 8.8$  Hz, 4H,  $H_{18}$  or  $H_{18'}$ ), 7.27 (AA'BB' pattern,  $^3J = 8.8$  Hz, 4H,  $H_{18}$  or  $H_{18'}$ ), 7.24 (AA'BB' pattern,  $^3J = 8.8$  Hz, 4H,  $H_{19}$  or  $H_{19'}$ ), 7.22 (AA'BB' pattern,  $^3J = 8.8$  Hz, 4H,  $H_{19}$  or  $H_{19'}$ ), 7.06 (d,  $^3J = 8.4$  Hz, 3H,  $H_4$ ), 3.92 (s, 6H,  $H_8$ ), 2.48 (q,  $^3J = 7.4$  Hz, 6H,  $H_9$ ), 1.48 (s, 18H,  $H_a$ ), 1.29 (t,  $^3J = 7.4$  Hz, 9H,  $H_{10}$ ) ppm.

$^{13}C\{^1H\}$ -NMR (126 MHz,  $CD_2Cl_2$ , 25 °C):  $\delta = 149.7$  ( $C_c$ ), 146.1 ( $C_h$ ), 144.1 ( $C_2$ ), 143.8 ( $C_\alpha$ ), 143.2 ( $C_\alpha$ ), 142.6 ( $C_\alpha$ ), 142.5 ( $C_\alpha$ ), 141.2 ( $C_p$ ), 140.7 ( $C_1$ ), 139.8 ( $C_f$ ), 138.2 ( $C_5$ ), 135.6 ( $C_{18,18'}$ ), 134.6 ( $C_k$ ), 134.2 ( $C_q$ ), 134.1 ( $C_{12}$ ), 134.0 ( $C_{13}$ ), 133.6 ( $C_\beta$ ), 132.8 ( $C_\beta$ ), 132.8 ( $C_{17}$ ), 132.6 ( $C_{17'}$ ), 132.1 ( $C_\beta$ ), 131.9 ( $C_\beta$ ), 131.2 ( $C_j$ ), 131.1 ( $C_{14}$ ), 131.1 ( $C_{19,19'}$ ), 130.5 ( $C_r$ ), 129.3 ( $C_e$ ), 123.2 ( $C_s$ ), 122.8 ( $C_{15}$ ), 122.8 ( $C_4$ ), 122.5 ( $C_7$ ), 122.3 ( $C_{20,20'}$ ), 122.1 ( $C_d$ ), 121.9 ( $C_g$ ), 120.4 ( $C_3$ ), 119.3 ( $C_l$ ), 119.2 ( $C_o$ ), 117.6 ( $C_m$ ), 112.4 ( $C_i$ ), 111.4 ( $C_6$ ), 90.5 ( $C_t$ ), 90.5 ( $C_u$ ), 88.3 ( $C_{11}$ ), 87.6 ( $C_{16}$  or  $C_{16'}$ ), 87.3 ( $C_{16}$  or  $C_{16'}$ ), 36.9 ( $C_8$ ), 35.3 ( $C_b$ ), 31.8 ( $C_a$ ), 25.8 ( $C_9$ ), 14.8 ( $C_{10}$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max} (\varepsilon) = 418$  (270 000), 529 nm ( $20\ 000\ \text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (ESI $^+$ ): calcd for  $\text{C}_{121}\text{H}_{96}\text{BBr}_4\text{N}_{12}\text{NiRuS}_3$  [M+H] $^+$ : 2303.2266, found: 2303.2292.

**$\eta^5\text{-1,2,3,4-Tetra}(p\text{-bromophenyl})\text{-5-}\{p\text{-[nickel(II) 10,20-bis(4-cyanophenyl)}\text{-15-(3,5-di-tert-butylphenyl)porphyrin-5-yl]-4,4'-biphenyl}\text{cyclopentadienyl hydrotris{6-[(ethylsulfanyl)methyl]indazol-1-yl}borate ruthenium(II)}$  (14):**

In a Schlenk tube, complex **1** (190 mg, 0.12 mmol, 1.0 equiv.), porphyrin **6** (116 mg, 0.12 mmol, 1.0 equiv.),  $\text{PdCl}_2(\text{dppf})$  (10 mg, 12  $\mu\text{mol}$ , 10 mol%) and  $\text{Cs}_2\text{CO}_3$  (79 mg, 0.24 mmol, 2.0 equiv.) were successively introduced under an argon atmosphere in 20 mL of a degassed solution of DMF and water (99:1). The system was then degassed by three freeze-pump-thaw cycles and stirred at 100 °C for 40 h. The reaction medium was cooled to room temperature and the solvents were evaporated in vacuo. The reddish residue was dissolved in  $\text{CH}_2\text{Cl}_2$  and washed with water (3x20 mL). The organic layer was dried over magnesium sulphate, filtered and the solvent was removed. The crude mixture of mono-, bis-, tris-, tetra- and penta-substituted ruthenium complexes was purified by column chromatography ( $\text{SiO}_2$ ,  $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  gradient from 1:1 to 2:1) to give complex **14** as a red solid in 8% yield (22 mg, 9.7  $\mu\text{mol}$ ).

$R_f = 0.4$  ( $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  2:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 8.84$  (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_\beta$ ), 8.83 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_\beta$ ), 8.68 (d,  $^3J = 5.0$  Hz, 2H,  $\text{H}_\beta$ ), 8.67 (d,  $^3J = 5.2$  Hz, 2H,  $\text{H}_\beta$ ), 8.16 (AA'BB' pattern,  $^3J = 8.0$  Hz, 4H,  $\text{H}_k$ ), 8.05 (AA'BB' pattern,  $^3J = 8.1$  Hz, 2H,  $\text{H}_q$ ), 8.01 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $\text{H}_j$ ), 7.94-7.91 (m, 6H,  $\text{H}_1$  and  $\text{H}_6$ ), 7.89 (AA'BB' pattern,  $^3J = 8.1$  Hz, 2H,  $\text{H}_r$ ), 7.88 (d,  $^4J = 1.8$  Hz, 2H,  $\text{H}_e$ ), 7.79 (t,  $^4J = 1.8$  Hz, 1H,  $\text{H}_d$ ), 7.62 (AA'BB' pattern,  $^3J = 8.3$  Hz, 2H,  $\text{H}_{14}$ ), 7.55 (AA'BB' pattern,  $^3J = 8.3$  Hz, 2H,  $\text{H}_{13}$ ), 7.40 (AA'BB' pattern,  $^3J = 8.4$  Hz, 3H,  $\text{H}_3$ ), 7.37 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $\text{H}_{18}$ ), 7.29 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $\text{H}_{18'}$ ), 7.26 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $\text{H}_{19}$ ), 7.23 (AA'BB' pattern,  $^3J = 8.5$  Hz, 4H,  $\text{H}_{19'}$ ), 7.06 (d,  $^3J = 8.3$  Hz, 3H,  $\text{H}_4$ ), 3.92 (s, 6H,  $\text{H}_8$ ), 2.48 (q,  $^3J = 7.4$  Hz, 6H,  $\text{H}_9$ ), 1.48 (s, 18H,  $\text{H}_a$ ), 1.29 (t,  $^3J = 7.4$  Hz, 9H,  $\text{H}_{10}$ ) ppm.

$^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta = 149.7$  ( $\text{C}_c$ ), 146.1 ( $\text{C}_h$ ), 144.1 ( $\text{C}_2$ ), 143.8 ( $\text{C}_\alpha$ ), 143.4 ( $\text{C}_\alpha$ ), 142.5 ( $\text{C}_\alpha$ ), 142.4 ( $\text{C}_\alpha$ ), 140.7 ( $\text{C}_1$ ), 140.2 ( $\text{C}_p$ ), 140.0 ( $\text{C}_{15}$ ), 140.0 ( $\text{C}_s$ ), 139.9 ( $\text{C}_f$ ), 138.2 ( $\text{C}_5$ ), 135.7 ( $\text{C}_{18}$ ), 135.6 ( $\text{C}_{18'}$ ), 134.6 ( $\text{C}_k$  and  $\text{C}_q$ ), 134.6 ( $\text{C}_{13}$ ), 133.5 ( $\text{C}_\beta$ ), 133.0 ( $\text{C}_{17}$ ), 133.0 ( $\text{C}_\beta$ ), 132.9 ( $\text{C}_{12}$ ), 132.8 ( $\text{C}_{17'}$ ), 132.0 ( $\text{C}_\beta$ ), 131.9 ( $\text{C}_\beta$ ), 131.2 ( $\text{C}_j$ ), 131.1 ( $\text{C}_{19,19'}$ ), 129.3 ( $\text{C}_e$ ), 126.5 ( $\text{C}_{14}$ ), 125.8 ( $\text{C}_r$ ), 122.7 ( $\text{C}_4$ ), 122.7 ( $\text{C}_7$ ), 122.3 ( $\text{C}_{20}$ ), 122.2 ( $\text{C}_{20'}$ ), 122.1 ( $\text{C}_d$ ), 121.9 ( $\text{C}_g$ ), 120.4 ( $\text{C}_3$ ), 119.6 ( $\text{C}_o$ ), 119.3 ( $\text{C}_l$ ), 117.5 ( $\text{C}_m$ ), 112.4 ( $\text{C}_i$ ), 111.4 ( $\text{C}_6$ ), 88.6 ( $\text{C}_{11}$ ), 87.7 ( $\text{C}_{16'}$ ), 87.3 ( $\text{C}_{16}$ ), 36.9 ( $\text{C}_8$ ), 35.3 ( $\text{C}_b$ ), 31.8 ( $\text{C}_a$ ), 25.8 ( $\text{C}_9$ ), 14.8 ( $\text{C}_{10}$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max} (\varepsilon) = 418$  (278 000), 529 nm ( $21\ 500\ \text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (MALDI): calcd for  $\text{C}_{119}\text{H}_{95}\text{BBr}_4\text{N}_{12}\text{NiRuS}_3$  [M] $^+$ : 2280.2178, found: 2280.2126.

**$\eta^5\text{-1,2,3,4-Tetra}(p\text{-bromophenyl})\text{-5-}\{p\text{-[zinc(II) 10,15,20-tris(3,5-di-tert-butylphenyl) porphyrin-5-yl]-4,4'-biphenyl}\text{cyclopentadienyl hydrotris{6-[(ethylsulfanyl)methyl]indazol-1-yl}borate ruthenium(II)}$  (15):**

In a Schlenk tube, complex **1** (52 mg, 33  $\mu\text{mol}$ , 1.0 equiv.), porphyrin **7** (52 mg, 50  $\mu\text{mol}$ , 1.5 equiv.),  $\text{Pd}(\text{PPh}_3)_4$  (2 mg, 1.7  $\mu\text{mol}$ , 5 mol%) and thiophene-2-carboxylate (CuTC) (10 mg, 50  $\mu\text{mol}$ , 1.5 equiv.) were successively introduced under argon atmosphere in 5 mL of degassed anhydrous THF. The system was then degassed by bubbling argon for 10 min and stirred at 45 °C for 24 h. The mixture was

cooled to room temperature and the solvents were evaporated. The residue was dissolved in  $\text{CH}_2\text{Cl}_2$  and washed with water (3x25 mL). The organic layer was dried over magnesium sulphate, filtered and the solvent was removed. The crude mixture was purified by column chromatography ( $\text{SiO}_2$ , cyclohexane/ $\text{CH}_2\text{Cl}_2$  3:2) to give complex **15** as a greenish blue solid in 47% yield (38 mg, 15  $\mu\text{mol}$ ).  
 $R_f = 0.4$  ( $\text{CH}_2\text{Cl}_2$ /cyclohexane 1:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta$  = 9.00-8.95 (m, 8H,  $\text{H}_\beta$ ), 8.25 (AA'BB' pattern,  $^3J$  = 7.9 Hz, 2H,  $\text{H}_q$ ), 8.29 (s, 6H,  $\text{H}_e$  and  $\text{H}_l$ ), 7.96 (s, 3H,  $\text{H}_6$ ), 7.96-7.92 (m, 5H,  $\text{H}_1$  and  $\text{H}_r$ ), 7.83 (s, 3H,  $\text{H}_d$  and  $\text{H}_k$ ), 7.68 (AA'BB' pattern,  $^3J$  = 7.9 Hz, 2H,  $\text{H}_{14}$ ), 7.57 (AA'BB' pattern,  $^3J$  = 7.9 Hz, 2H,  $\text{H}_{13}$ ), 7.42-7.37 (m, 7H,  $\text{H}_3$  and  $\text{H}_{18}$ ), 7.32-7.22 (m, 12H,  $\text{H}_{18'}$  and  $\text{H}_{19,19'}$ ), 7.04 (d,  $^3J$  = 8.6 Hz, 3H,  $\text{H}_4$ ), 3.89 (s, 6H,  $\text{H}_8$ ), 2.46 (q,  $^3J$  = 7.4 Hz, 6H,  $\text{H}_9$ ), 1.52 (s, 54H,  $\text{H}_a$  and  $\text{H}_h$ ), 1.27 (t,  $^3J$  = 7.4 Hz, 9H,  $\text{H}_{10}$ ) ppm.

$^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25 °C):  $\delta$  = 150.8 ( $\text{C}_\alpha$ ), 150.3 ( $\text{C}_\alpha$ ), 149.1 ( $\text{C}_c$  and  $\text{C}_j$ ), 144.2 ( $\text{C}_2$ ), 142.8 ( $\text{C}_p$ ), 142.3 ( $\text{C}_m$  and  $\text{C}_f$ ), 140.8 ( $\text{C}_1$ ), 140.3 ( $\text{C}_{15}$ ), 139.4 ( $\text{C}_s$ ), 138.0 ( $\text{C}_5$ ), 135.8 ( $\text{C}_{18}$ ), 135.6 ( $\text{C}_{18'}$  and  $\text{C}_q$ ), 134.6 ( $\text{C}_{13}$ ), 133.1 ( $\text{C}_{17}$ ), 132.8 ( $\text{C}_{17'}$  and  $\text{C}_{12}$ ), 132.6 ( $\text{C}_\beta$ ), 132.5 ( $\text{C}_\beta$ ), 131.9 ( $\text{C}_\beta$ ), 131.1 ( $\text{C}_{19,19'}$ ), 130.1 ( $\text{C}_l$  and  $\text{C}_e$ ), 126.6 ( $\text{C}_{14}$ ), 125.3 ( $\text{C}_r$ ), 122.7 ( $\text{C}_4$ ), 122.5 ( $\text{C}_7$  and  $\text{C}_o$ ), 122.4 ( $\text{C}_n$  and  $\text{C}_g$ ), 122.3 ( $\text{C}_{20,20'}$ ), 121.4 ( $\text{C}_d$  and  $\text{C}_k$ ), 120.5 ( $\text{C}_3$ ), 111.5 ( $\text{C}_6$ ), 87.7 ( $\text{C}_{11}$ ), 87.3 ( $\text{C}_{16,16'}$ ), 37.0 ( $\text{C}_8$ ), 35.3 ( $\text{C}_b$  and  $\text{C}_i$ ), 31.9 ( $\text{C}_a$  and  $\text{C}_h$ ), 25.9 ( $\text{C}_9$ ), 14.7 ( $\text{C}_{10}$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\text{max}}$  ( $\varepsilon$ ) = 423 (485 000), 550 (18 500), 589 nm ( $5 \cdot 700 \text{ mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (MALDI): calcd for  $\text{C}_{133}\text{H}_{129}\text{BBr}_4\text{N}_{10}\text{RuS}_3\text{Zn}$  [M] $^+$ : 2460.4716, found: 2460.4448.

### 5-[4-(Trimethylsilylethynyl)phenyl]-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin (**17**):

According to the optimised conditions reported in section II, 4-[(trimethylsilyl)ethynyl]benzaldehyde (1.88 g, 9.27 mmol, 1.0 equiv.), 3,5-di-*tert*-butylbenzaldehyde (2.02 g, 9.27 mmol, 1.0 equiv.) and 4-(di(*1H*-pyrrol-2-yl)methyl)benzonitrile<sup>[54]</sup> (4.58 g, 18.53 mmol, 2.0 equiv.) were dissolved in anhydrous  $\text{CH}_2\text{Cl}_2$  (1.3 L) in a three-neck round-bottom flask protected from light with aluminum foil. The solution was degassed for 30 min and an excess of trifluoroacetic acid (4.13 mL, 55.60 mmol, 6.0 equiv.) was then added dropwise. After stirring for 2 h at room temperature, DDQ (6.31 g, 27.8 mmol, 3.0 equiv.) was added and the reaction mixture was stirred for another 2 h. In order to neutralize the acid, triethylamine (7.73 mL, 55.60 mmol, 6.0 equiv.) was slowly added and the medium was stirred for a further 20 min. Finally, the dark solution was concentrated and filtered through a silica pad to give a purple mixture of porphyrins, which was separated by column chromatography ( $\text{SiO}_2$ , cyclohexane/ $\text{CH}_2\text{Cl}_2$  gradient from 4:1 to 3:2). Isolation of the second fraction gave pure 5-[4-(trimethylsilylethynyl)phenyl]-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin (**17**) as a purple solid in 8% yield (650 mg, 0.74 mmol).

$R_f = 0.6$  ( $\text{CH}_2\text{Cl}_2$ /cyclohexane 2:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 8.94 (d,  $^3J$  = 5.0 Hz, 2H,  $\text{H}_\beta$ ), 8.86 (d,  $^3J$  = 5.0 Hz, 2H,  $\text{H}_\beta$ ), 8.78 – 8.72 (m, 4H,  $\text{H}_\beta$ ), 8.34 (AA'BB' pattern,  $^3J$  = 8.4 Hz, 4H,  $\text{H}_k$ ), 8.15 (AA'BB' pattern,  $^3J$  = 8.3 Hz, 2H,  $\text{H}_q$ ), 8.08 (AA'BB' pattern,  $^3J$  = 8.4 Hz, 4H,  $\text{H}_j$ ), 8.05 (d,  $^4J$  = 1.8 Hz, 2H,  $\text{H}_e$ ), 7.89 (AA'BB' pattern,  $^3J$  = 8.3 Hz, 2H,  $\text{H}_r$ ), 7.83 (t,  $^4J$  = 1.8 Hz, 1H,  $\text{H}_d$ ), 1.53 (s, 18H,  $\text{H}_a$ ), 0.38 (s, 9H,  $\text{H}_v$ ), -2.81 (s, 2H,  $\text{H}_{\text{NH}}$ ) ppm.

$^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 149.2 ( $\text{C}_c$ ), 147.2 ( $\text{C}_h$ ), 142.1 ( $\text{C}_p$ ), 140.7 ( $\text{C}_f$ ), 135.1 ( $\text{C}_k$ ), 134.5 ( $\text{C}_q$ ), 130.7 ( $\text{C}_j$ ), 130.6 ( $\text{C}_r$ ), 130.1 ( $\text{C}_e$ ), 123.1 ( $\text{C}_g$  and  $\text{C}_o$ ), 121.6 ( $\text{C}_d$ ), 119.9 ( $\text{C}_s$ ), 119.1 ( $\text{C}_l$ ), 118.0 ( $\text{C}_m$ ), 112.2 ( $\text{C}_i$ ), 104.9 ( $\text{C}_t$ ), 96.0 ( $\text{C}_u$ ), 35.2 ( $\text{C}_b$ ), 31.9 ( $\text{C}_a$ ), 0.2 ( $\text{C}_v$ ) ppm.

UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  ( $\varepsilon$ ) = 421 (448 000), 517 (18 000), 551 (9 000), 591 (5 000), 647 nm (4 000  $\text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (ESI $^+$ ): calcd for  $\text{C}_{59}\text{H}_{53}\text{N}_6\text{Si} [\text{M}+\text{H}]^+$ : 873.4112, found: 873.4101.

**Nickel(II) 5-[4-(trimethylsilylethynyl)phenyl]-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl)porphyrin (19):**

In a Schlenk tube under argon, nickel(II) acetylacetone (706 mg, 2.75 mmol, 4.0 equiv.) was added to a solution of free base porphyrin **17** (600 mg, 0.69 mmol, 1.0 equiv.) in dry toluene (80 mL). The reaction mixture was then heated at 110 °C and monitored by TLC until total disappearance of the red fluorescent spot. After cooling to room temperature, solvents were evaporated and the crude product was dissolved in  $\text{CH}_2\text{Cl}_2$  (50 mL) and washed with water. The organic layer was dried over magnesium sulphate and filtered. The solvent was evaporated and the resulting solid was purified by column chromatography ( $\text{SiO}_2$ ,  $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  2:1) affording nickel(II) porphyrin **19** as a red solid in 95% yield (607 mg, 0.65 mmol).

$R_f$  = 0.5 ( $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$  2:1).

$^1\text{H-NMR}$  (500 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 8.84 (d,  $^3J$  = 5.0 Hz, 2H,  $\text{H}_\beta$ ), 8.74 (d,  $^3J$  = 5.0 Hz, 2H,  $\text{H}_\beta$ ), 8.65 – 8.62 (m, 4H,  $\text{H}_\beta$ ), 8.14 (AA'BB' pattern,  $^3J$  = 8.4 Hz, 4H,  $\text{H}_k$ ), 8.00 (AA'BB' pattern,  $^3J$  = 8.4 Hz, 4H,  $\text{H}_j$ ), 7.94 (AA'BB' pattern,  $^3J$  = 8.3 Hz, 2H,  $\text{H}_q$ ), 7.85 (d,  $^4J$  = 1.8 Hz, 2H,  $\text{H}_e$ ), 7.80 (AA'BB' pattern,  $^3J$  = 8.3 Hz, 2H,  $\text{H}_r$ ), 7.75 (t,  $^4J$  = 1.8 Hz, 1H,  $\text{H}_d$ ), 1.47 (s, 18H,  $\text{H}_a$ ), 0.36 (s, 9H,  $\text{H}_v$ ) ppm.

$^{13}\text{C}\{\text{H}\}$ -NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 149.4 ( $\text{C}_c$ ), 145.9 ( $\text{C}_h$ ), 143.5 ( $\text{C}_\alpha$ ), 142.8 ( $\text{C}_\alpha$ ), 142.1 ( $\text{C}_\alpha$ ), 142.0 ( $\text{C}_\alpha$ ), 140.9 ( $\text{C}_p$ ), 139.5 ( $\text{C}_f$ ), 134.3 ( $\text{C}_k$ ), 133.7 ( $\text{C}_q$ ), 133.6 ( $\text{C}_\beta$ ), 132.7 ( $\text{C}_\beta$ ), 131.9 ( $\text{C}_\beta$ ), 131.7 ( $\text{C}_\beta$ ), 130.9 ( $\text{C}_j$ ), 130.8 ( $\text{C}_r$ ), 129.0 ( $\text{C}_e$ ), 123.1 ( $\text{C}_s$ ), 123.1 ( $\text{C}_g$ ), 121.6 ( $\text{C}_d$ ), 119.0 ( $\text{C}_l$ ), 118.9 ( $\text{C}_o$ ), 117.0 ( $\text{C}_m$ ), 112.2 ( $\text{C}_i$ ), 104.9 ( $\text{C}_t$ ), 95.9 ( $\text{C}_u$ ), 35.2 ( $\text{C}_b$ ), 31.8 ( $\text{C}_a$ ), 0.2 ( $\text{C}_v$ ) ppm.

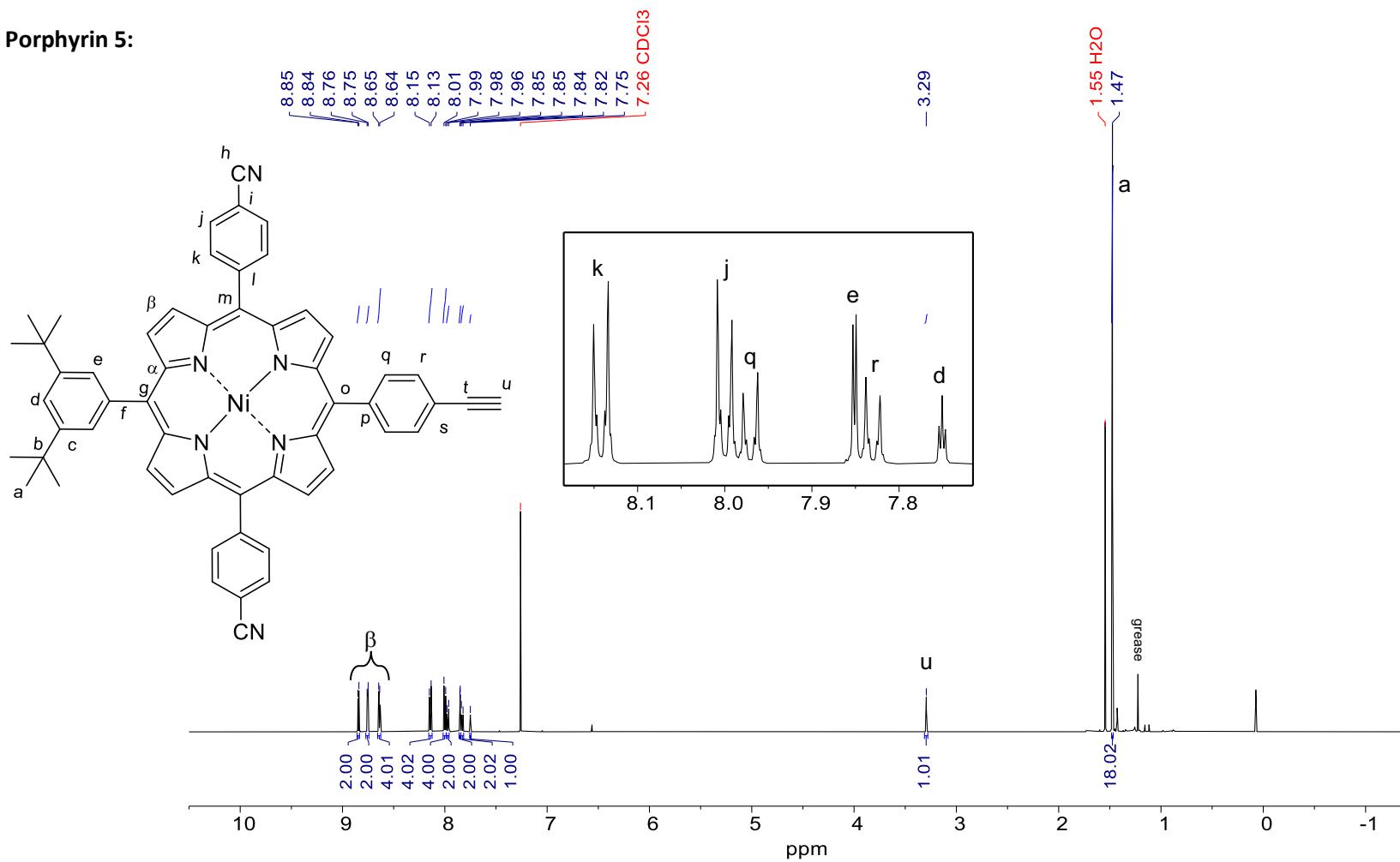
UV-Vis ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  ( $\varepsilon$ ) = 417 (266 000), 528 nm (19 000  $\text{mol}^{-1}\text{dm}^3\text{cm}^{-1}$ ).

HR-MS (ESI $^+$ ): calcd for  $\text{C}_{59}\text{H}_{51}\text{N}_6\text{SiNi} [\text{M}+\text{H}]^+$ : 929.3298, found: 929.3292.

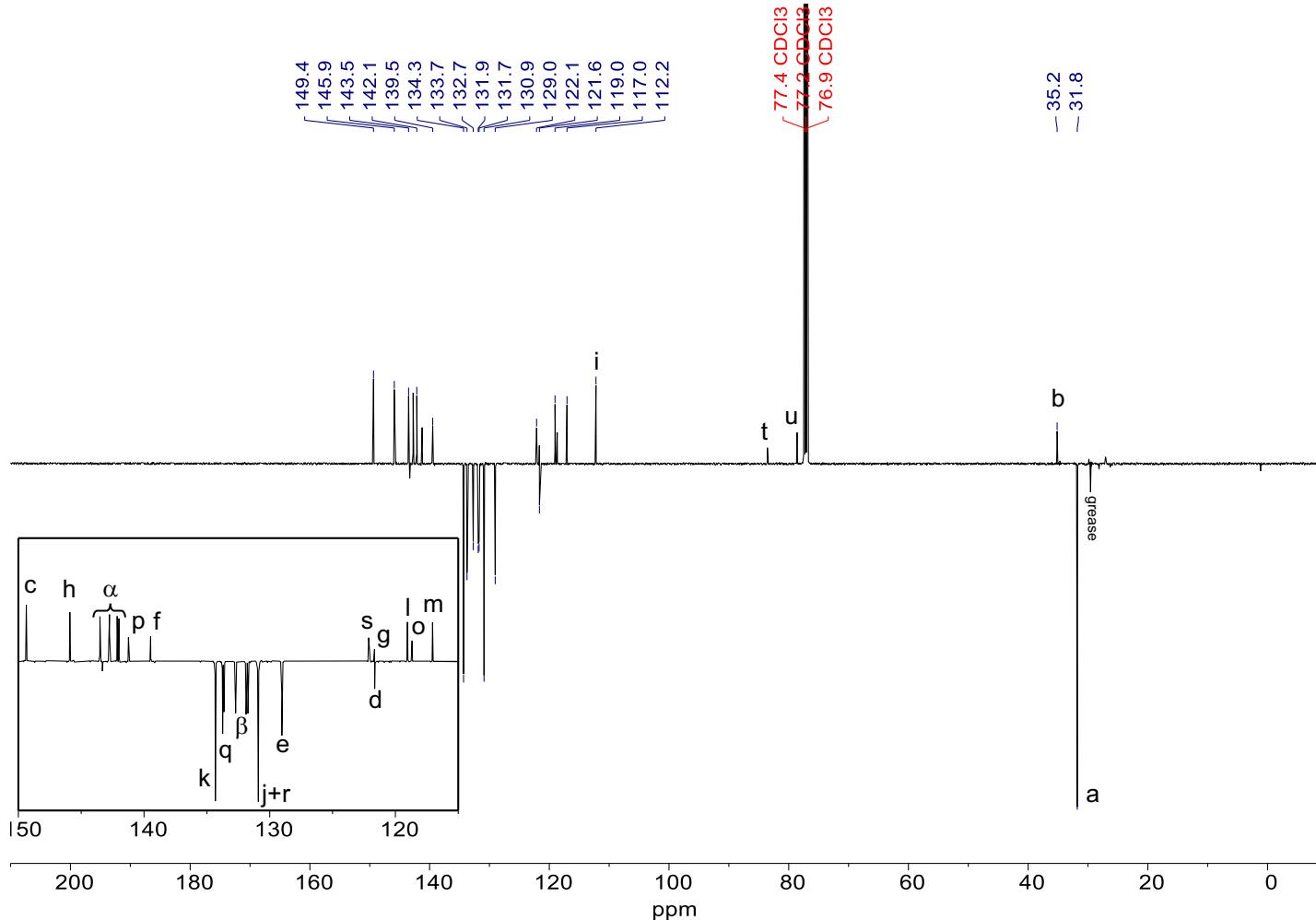
## IV. NMR spectroscopy

### 1. NMR Spectra of new compounds

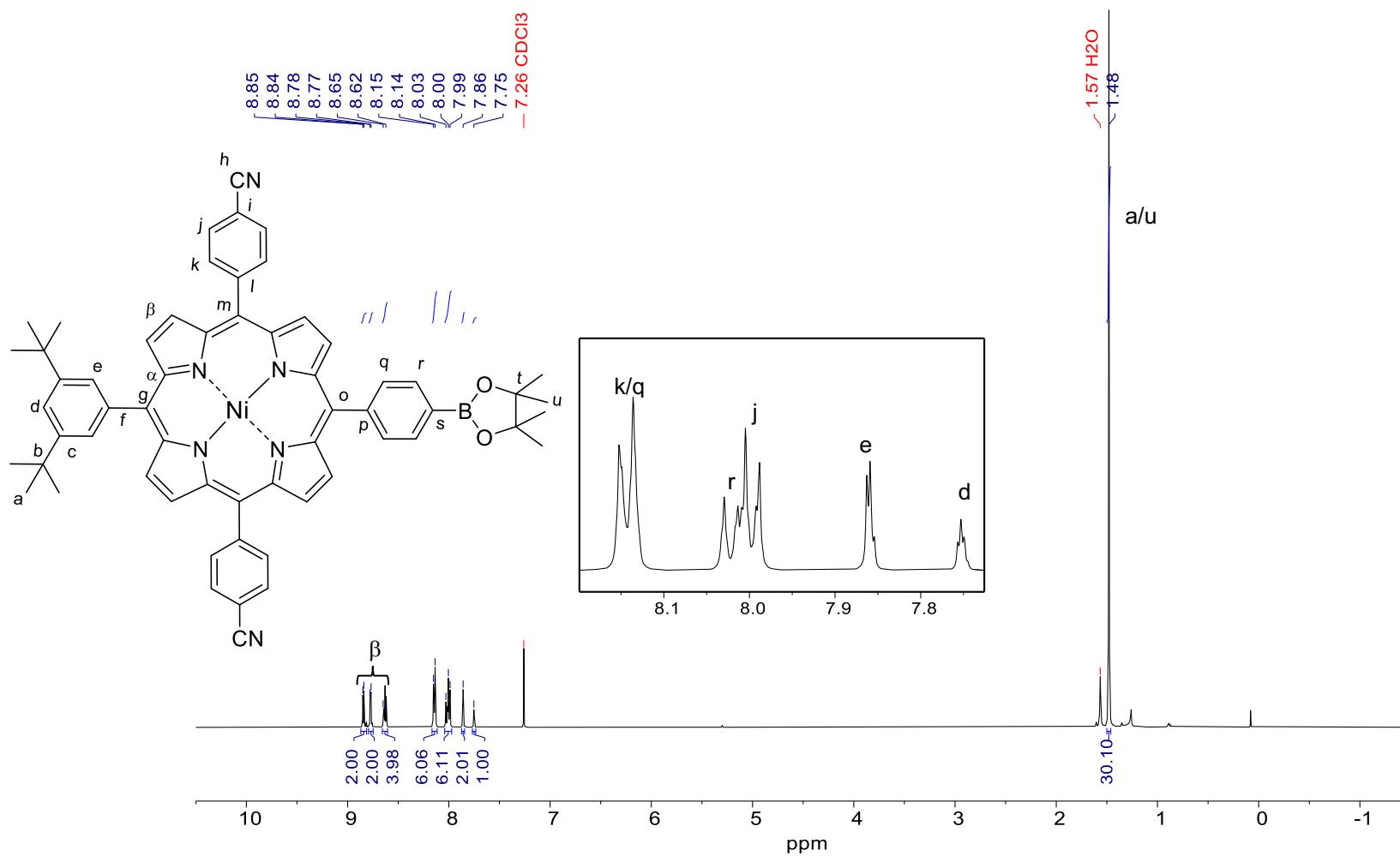
Porphyrin 5:



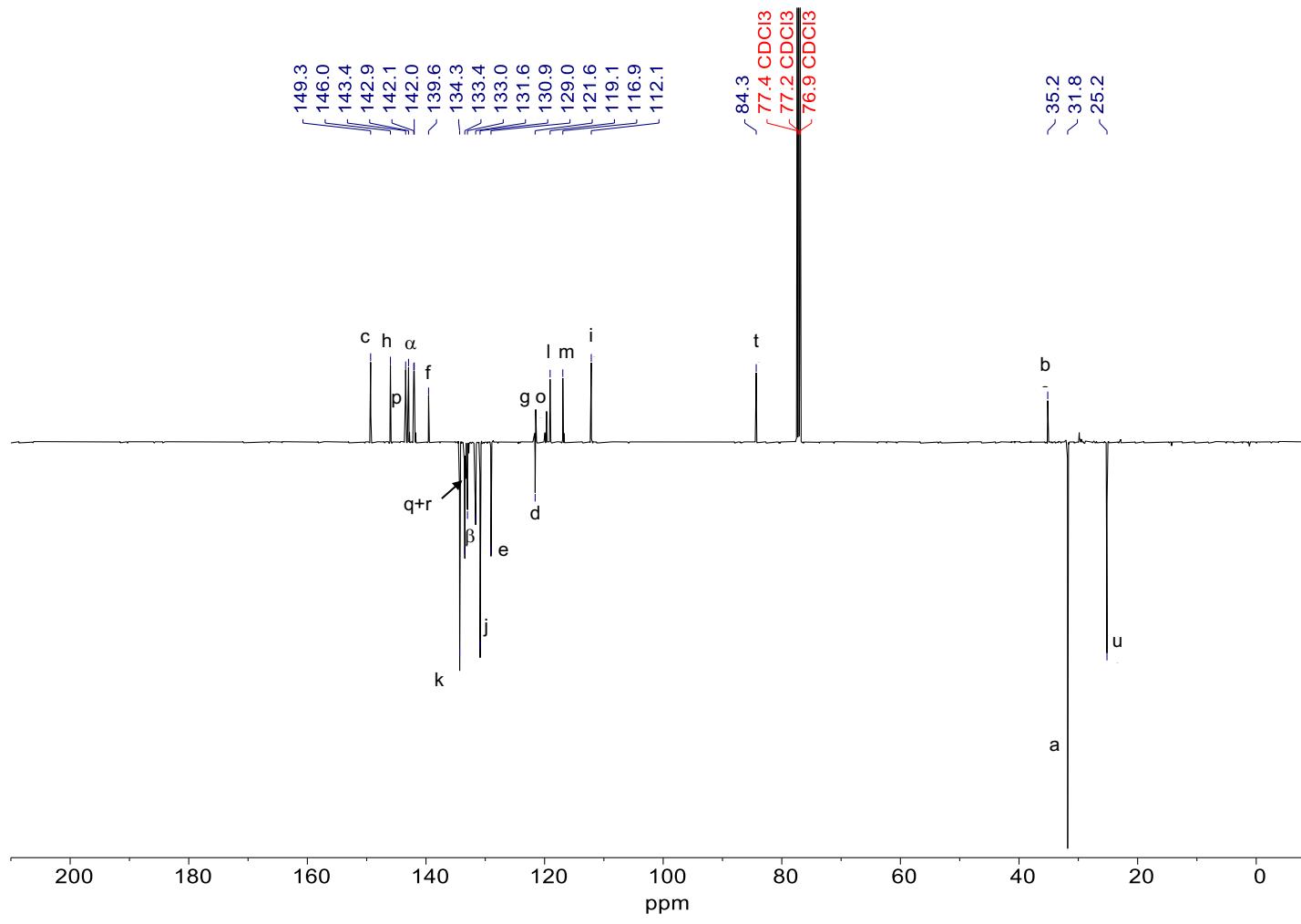
$^1\text{H}$ -NMR of porphyrin 5 (500 MHz,  $\text{CDCl}_3$ , 25°C).



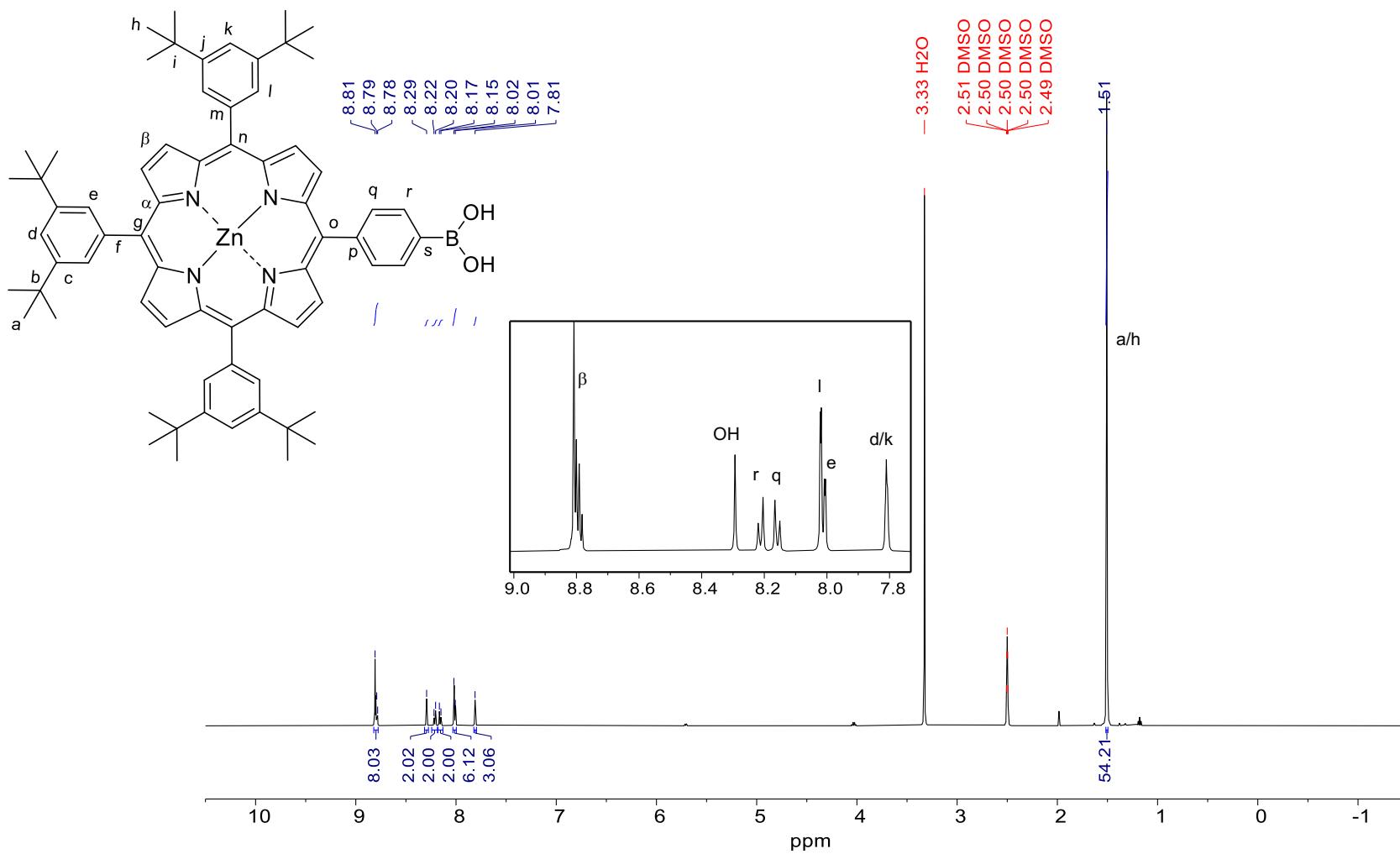
**Porphyrin 6:**



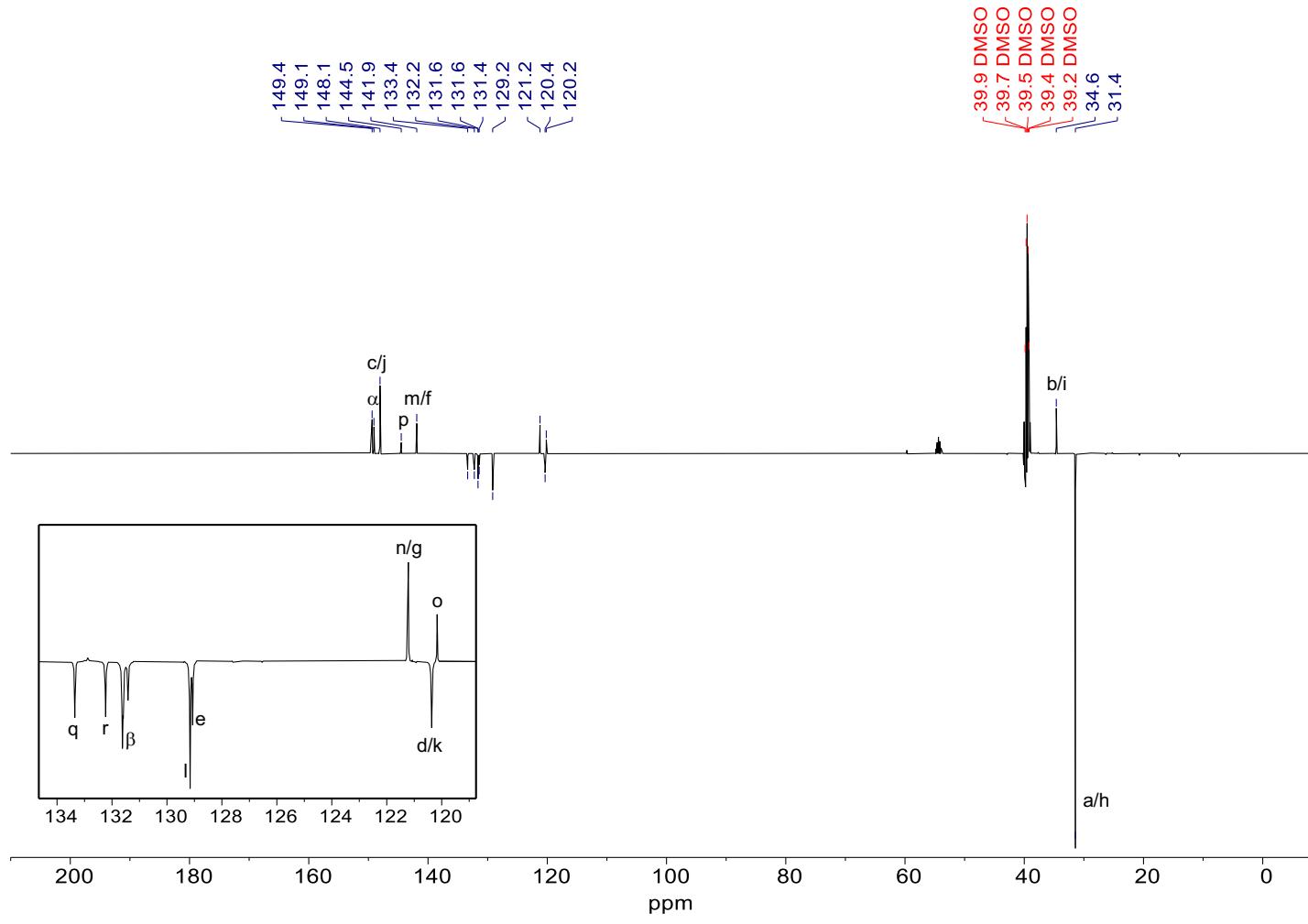
<sup>1</sup>H-NMR of porphyrin 6 (500 MHz, CDCl<sub>3</sub>, 25°C).



**Porphyrin 7:**

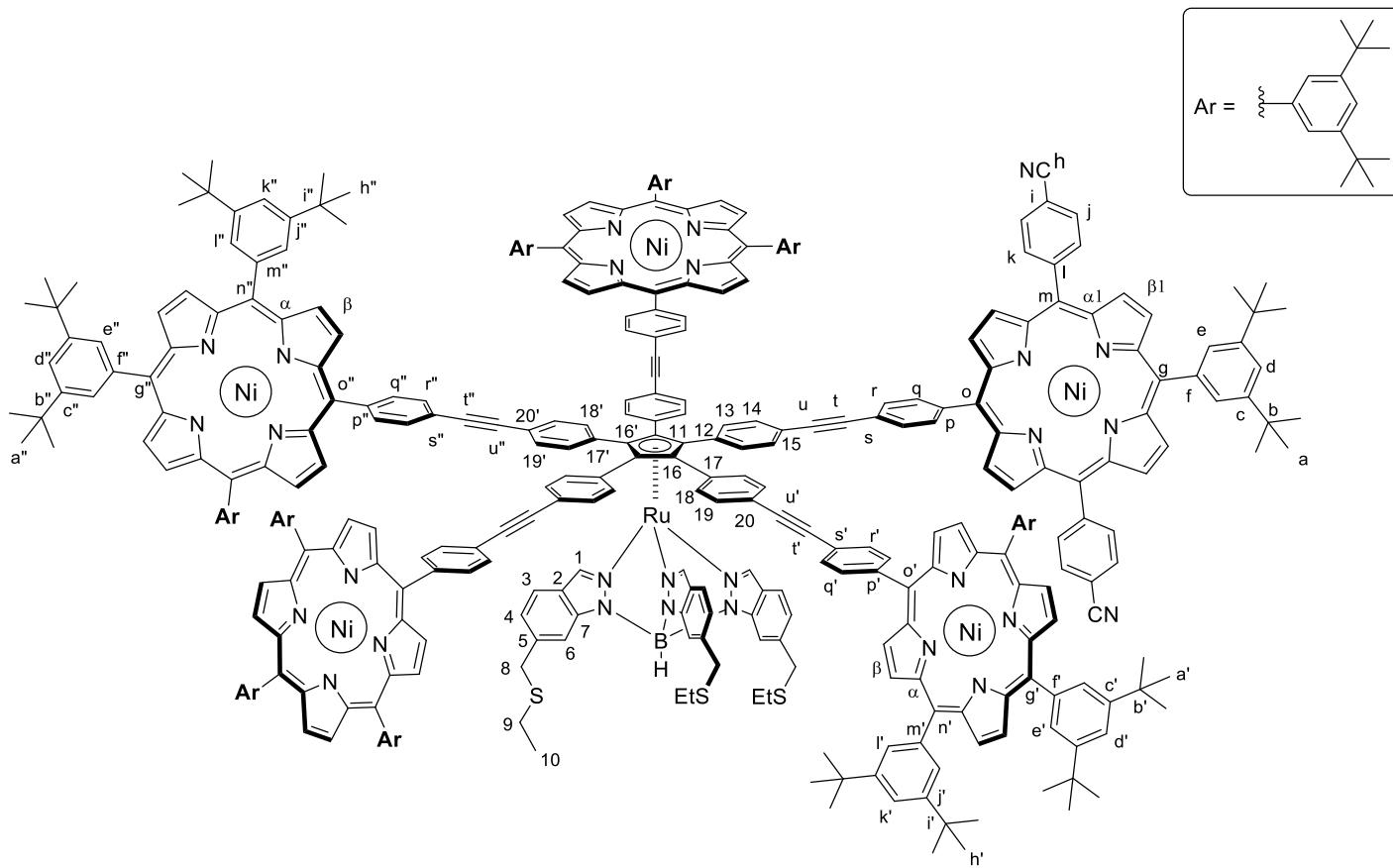


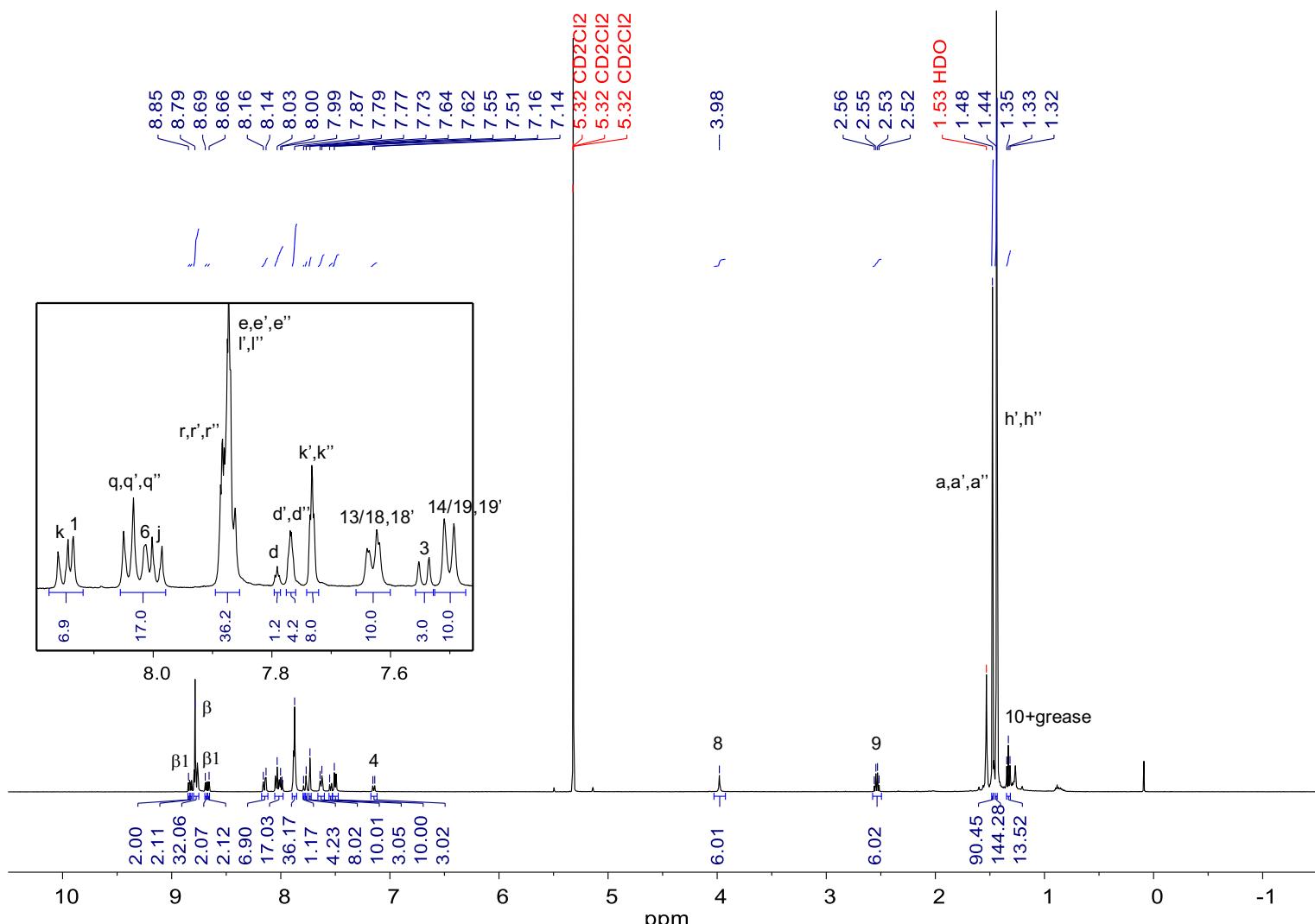
$^1\text{H}$ -NMR of porphyrin 7 (500 MHz,  $\text{d}_6\text{-DMSO}$ , 25°C).

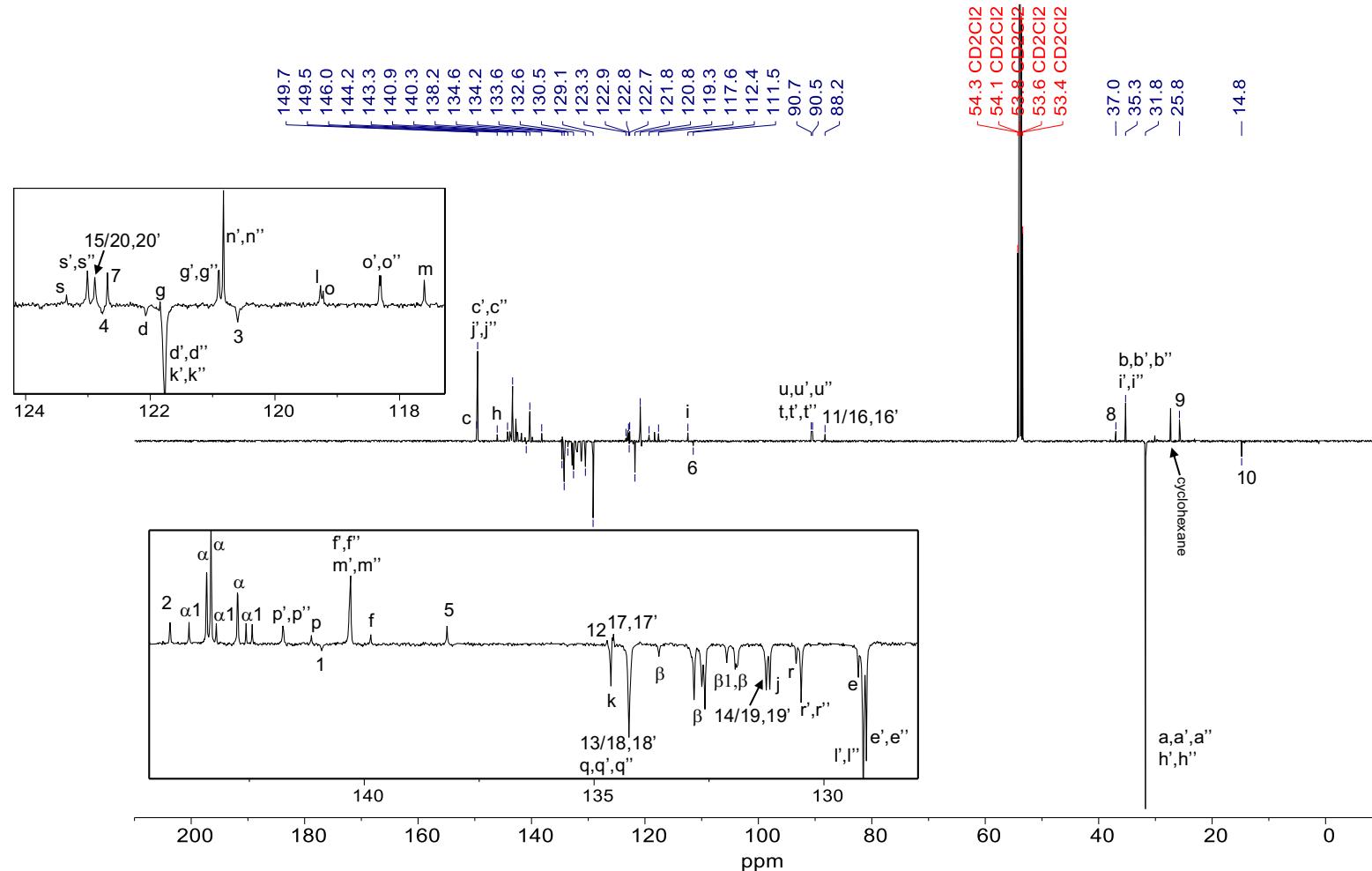


$^{13}\text{C}$ -Jmod-NMR of porphyrin 7 (126 MHz,  $\text{d}_6\text{-DMSO}$ , 25°C).

**Cogwheel 10:**

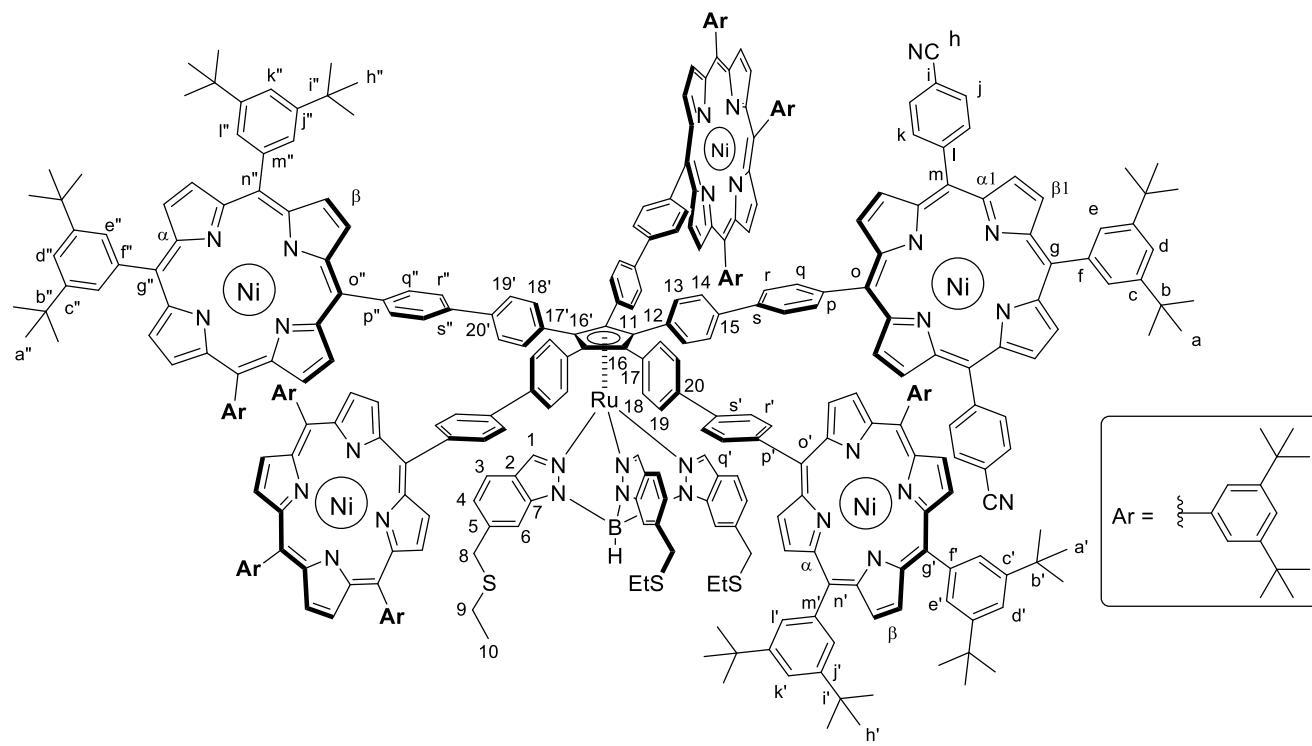


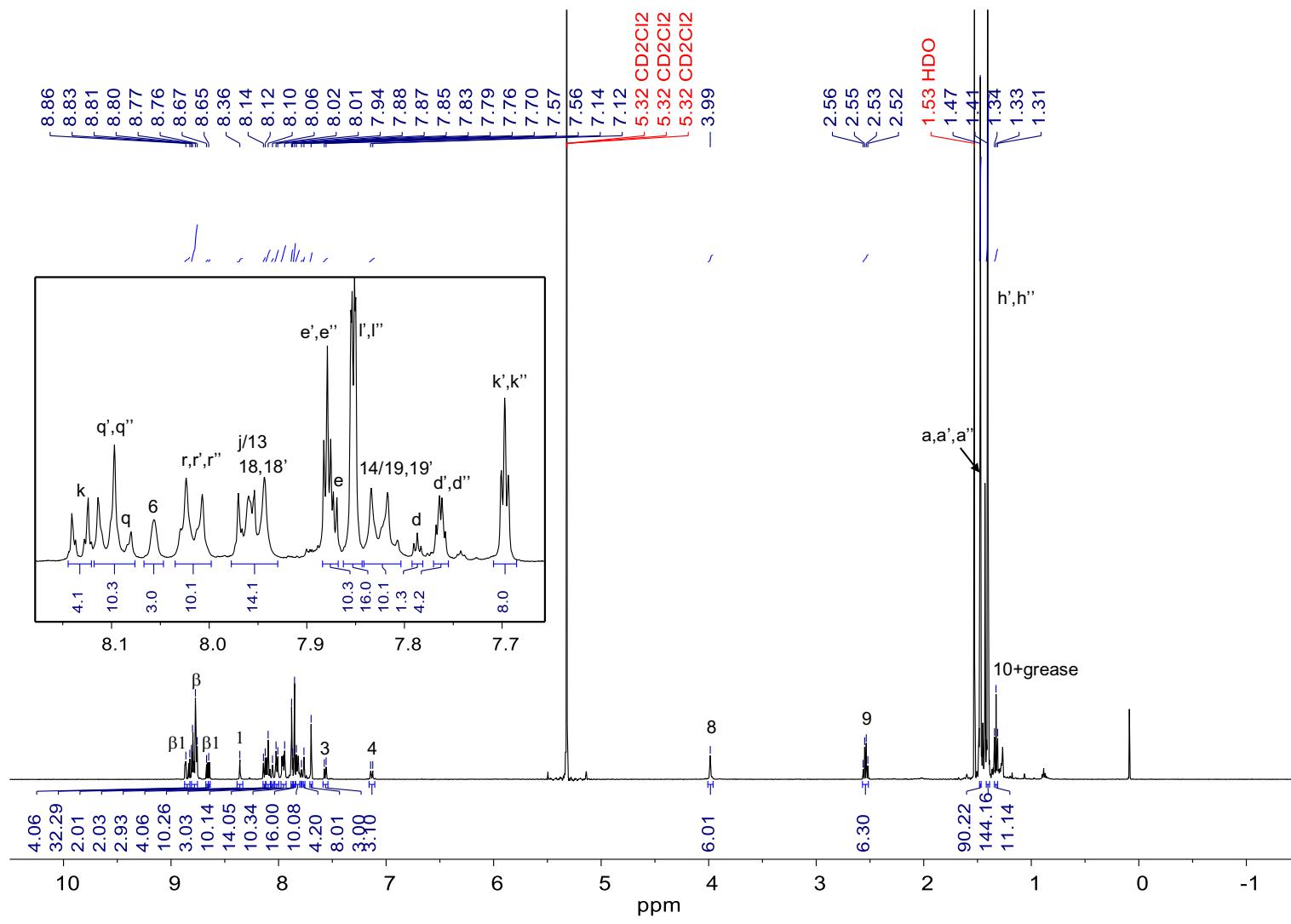


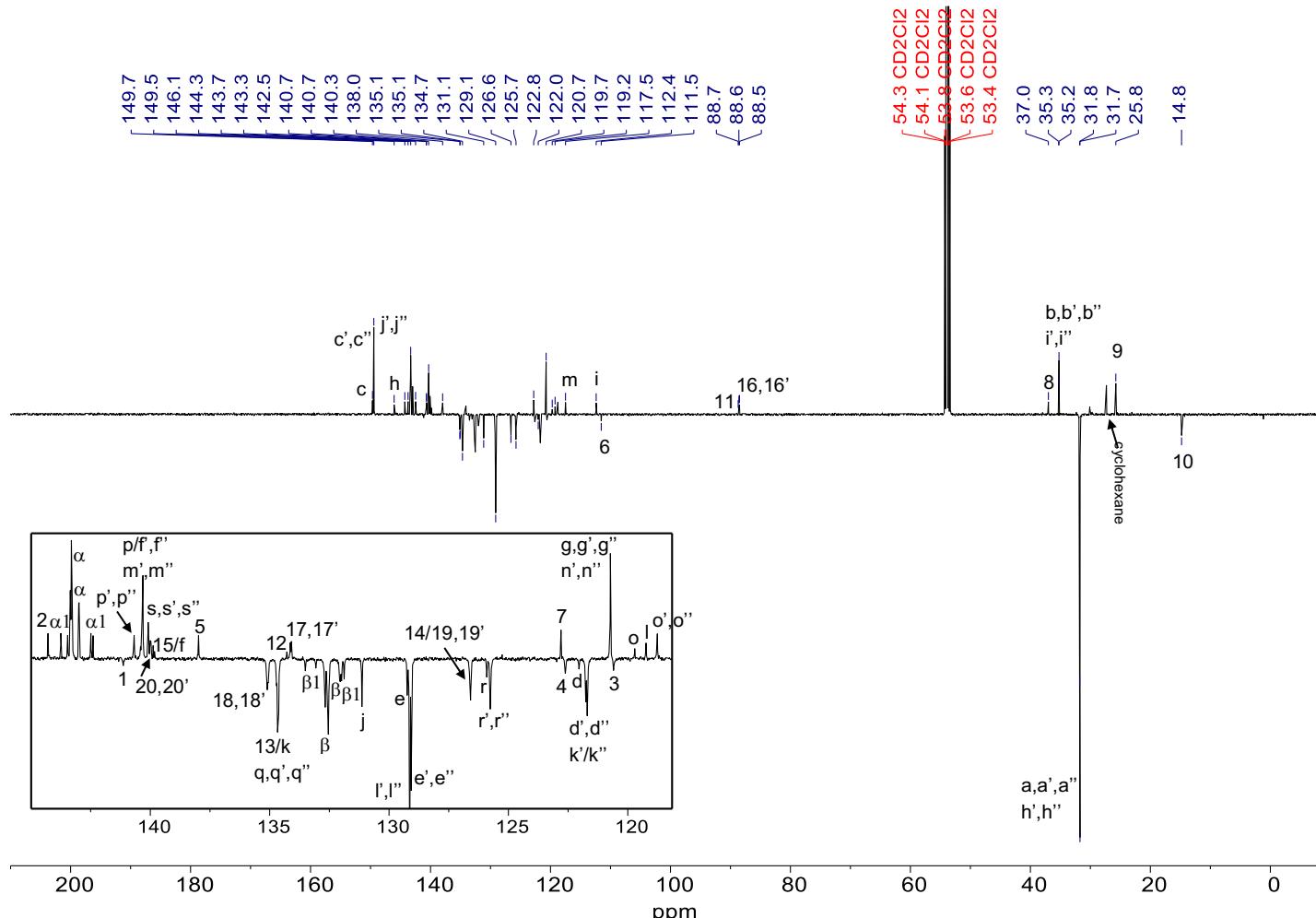


$^{13}\text{C}$ -Jmod-NMR of cogwheel **10** (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25°C).

**Cogwheel 11:**

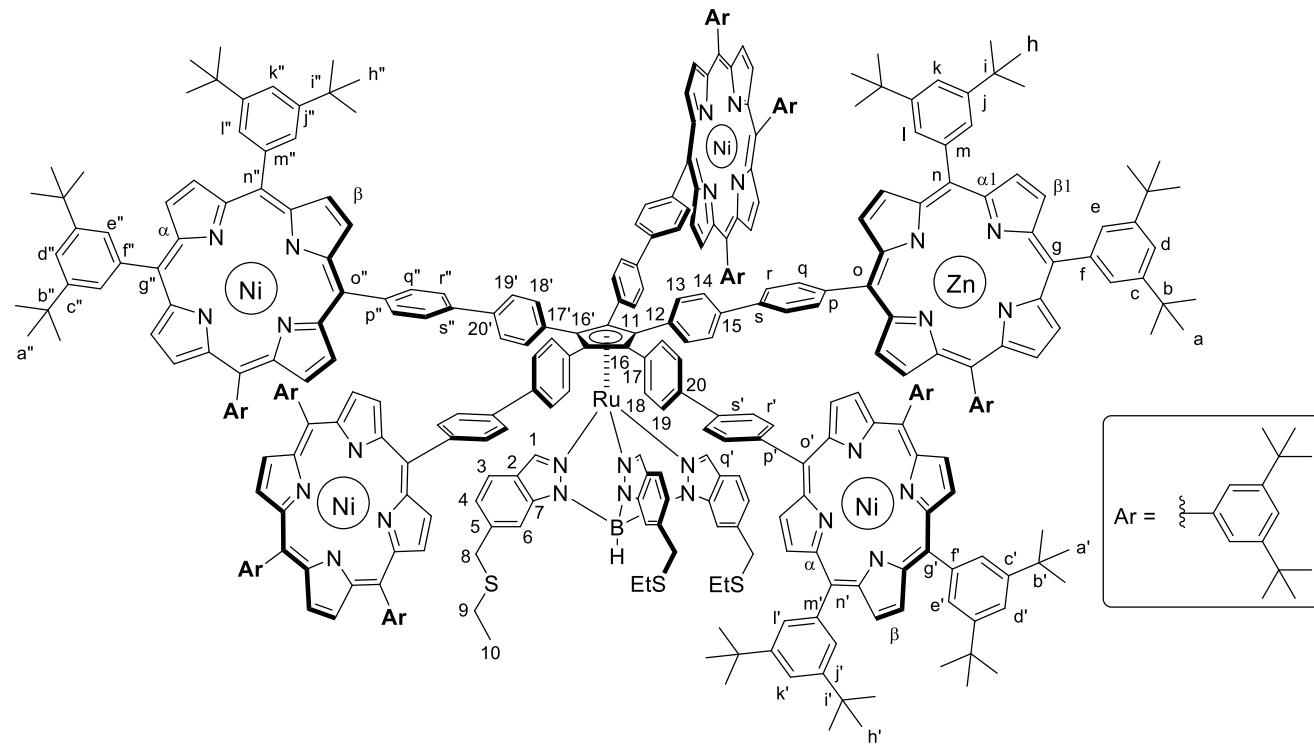


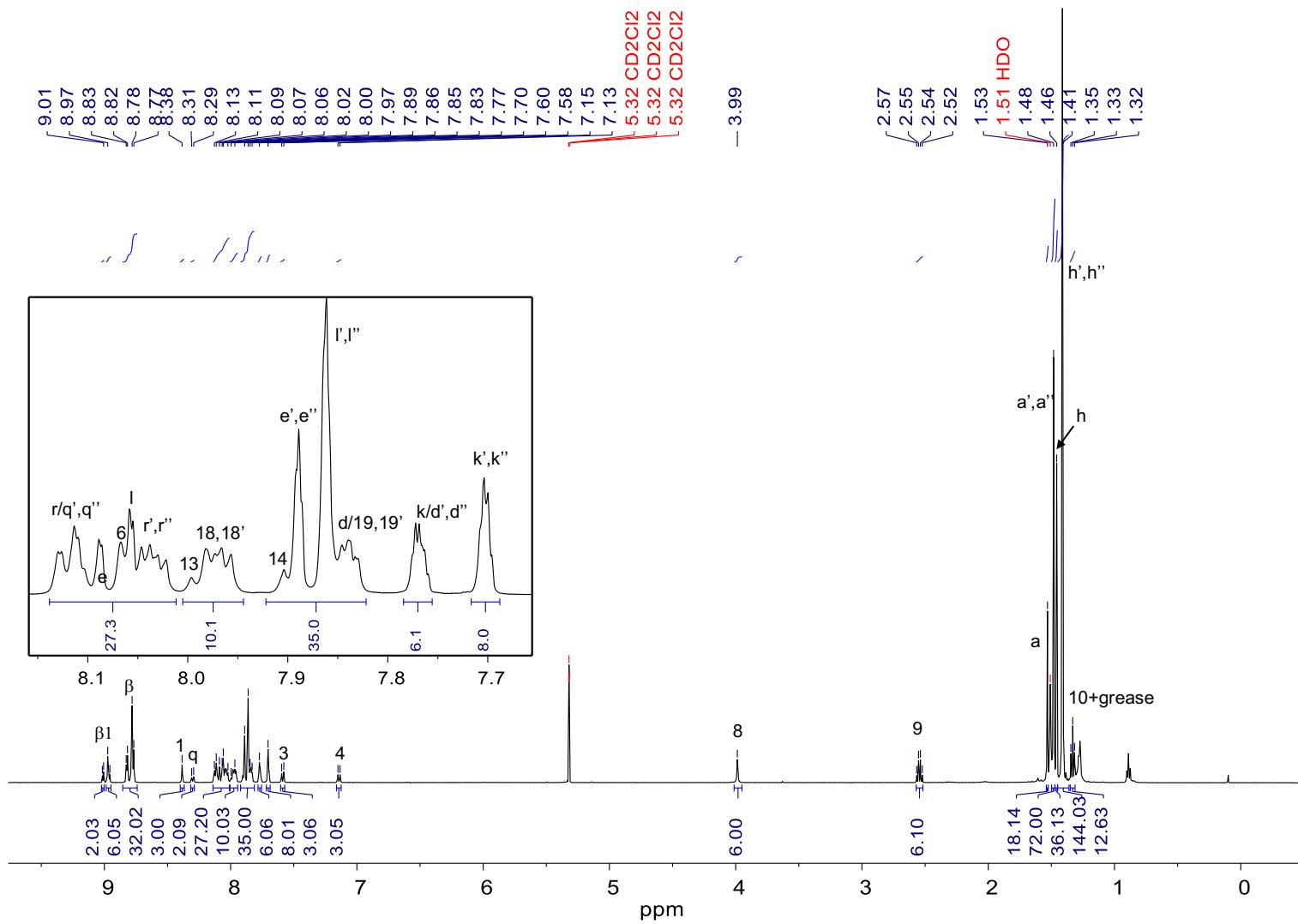


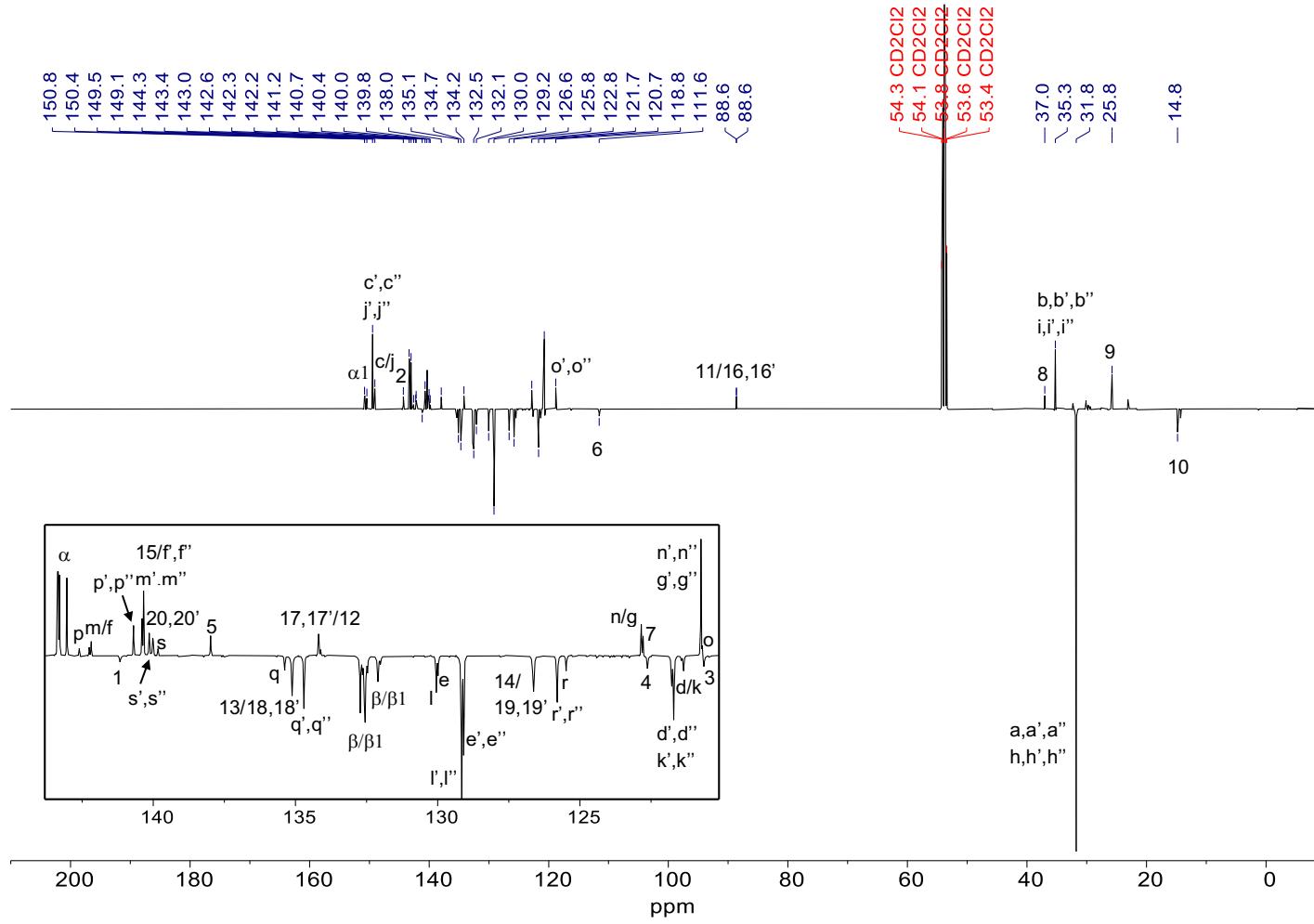


$^{13}\text{C}$ -Jmod-NMR of cogwheel **11** (126 MHz,  $\text{CD}_2\text{Cl}_2$ , 25°C).

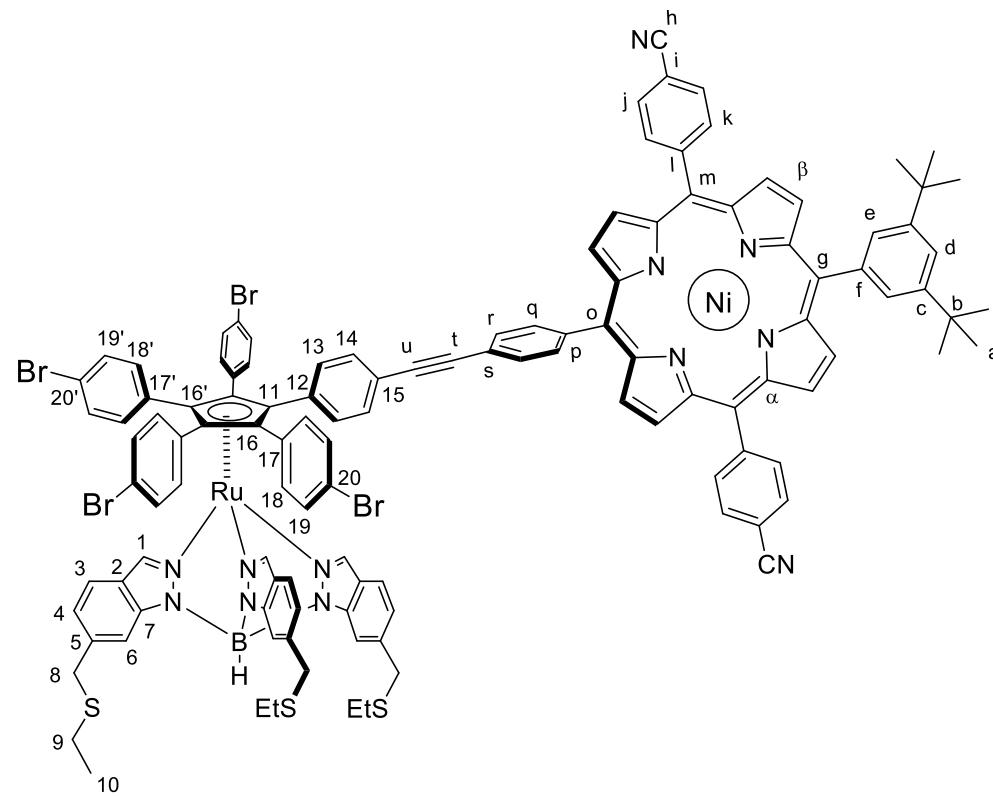
**Cogwheel 12:**

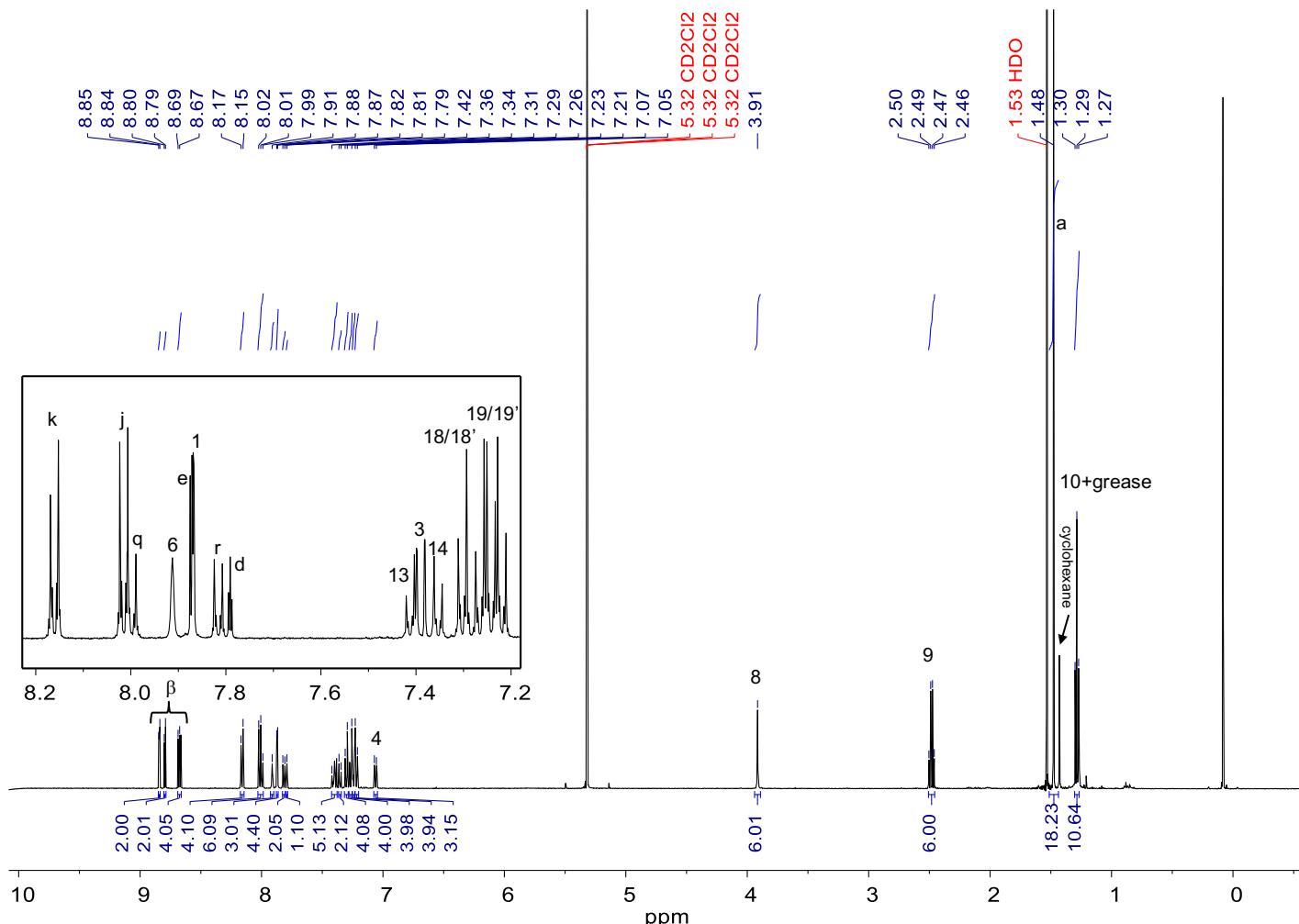




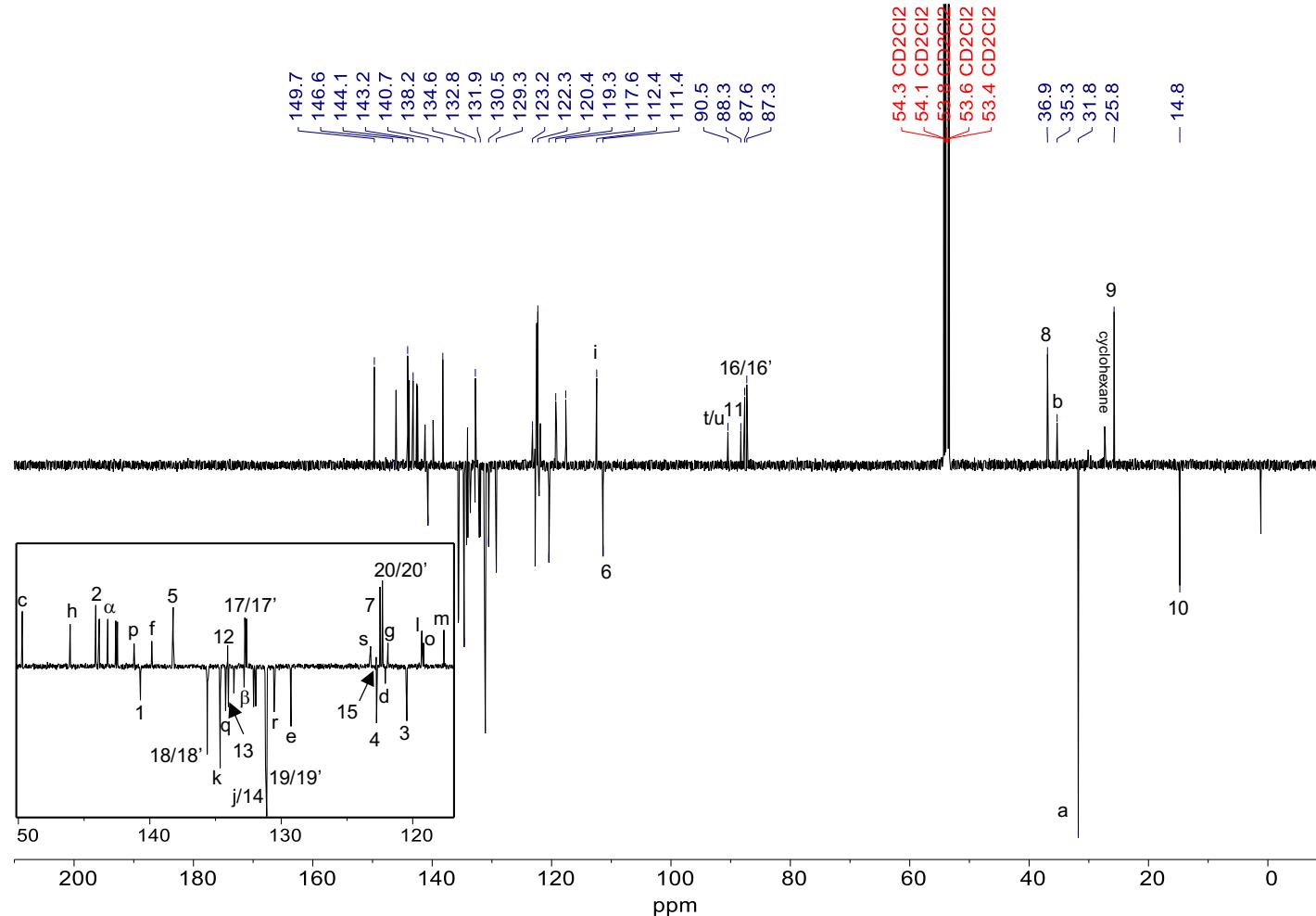


**Complex 13:**

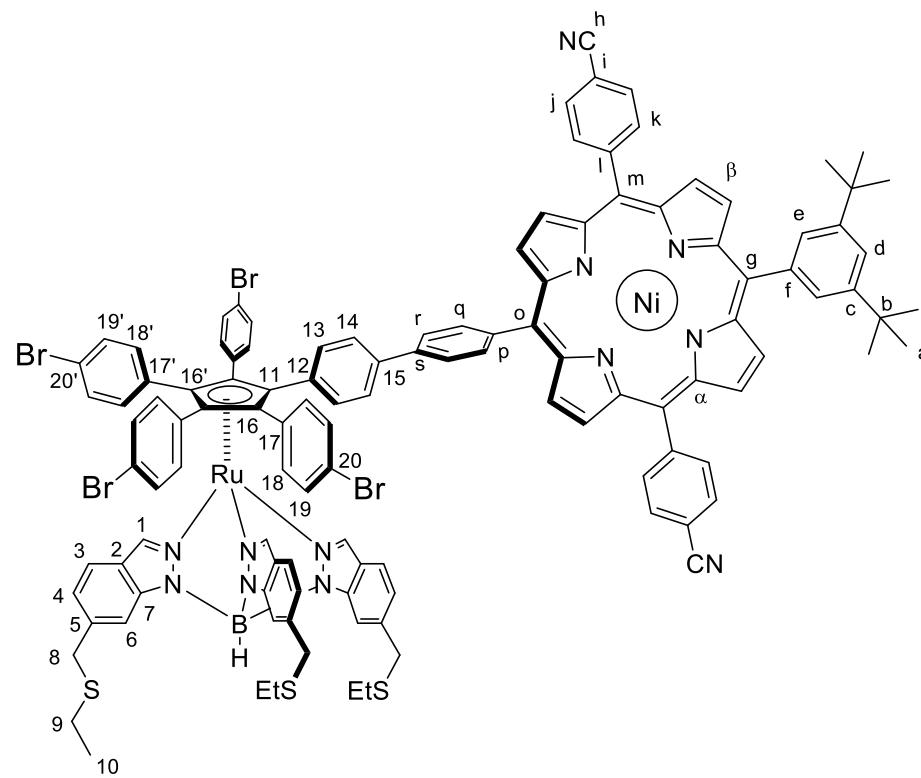


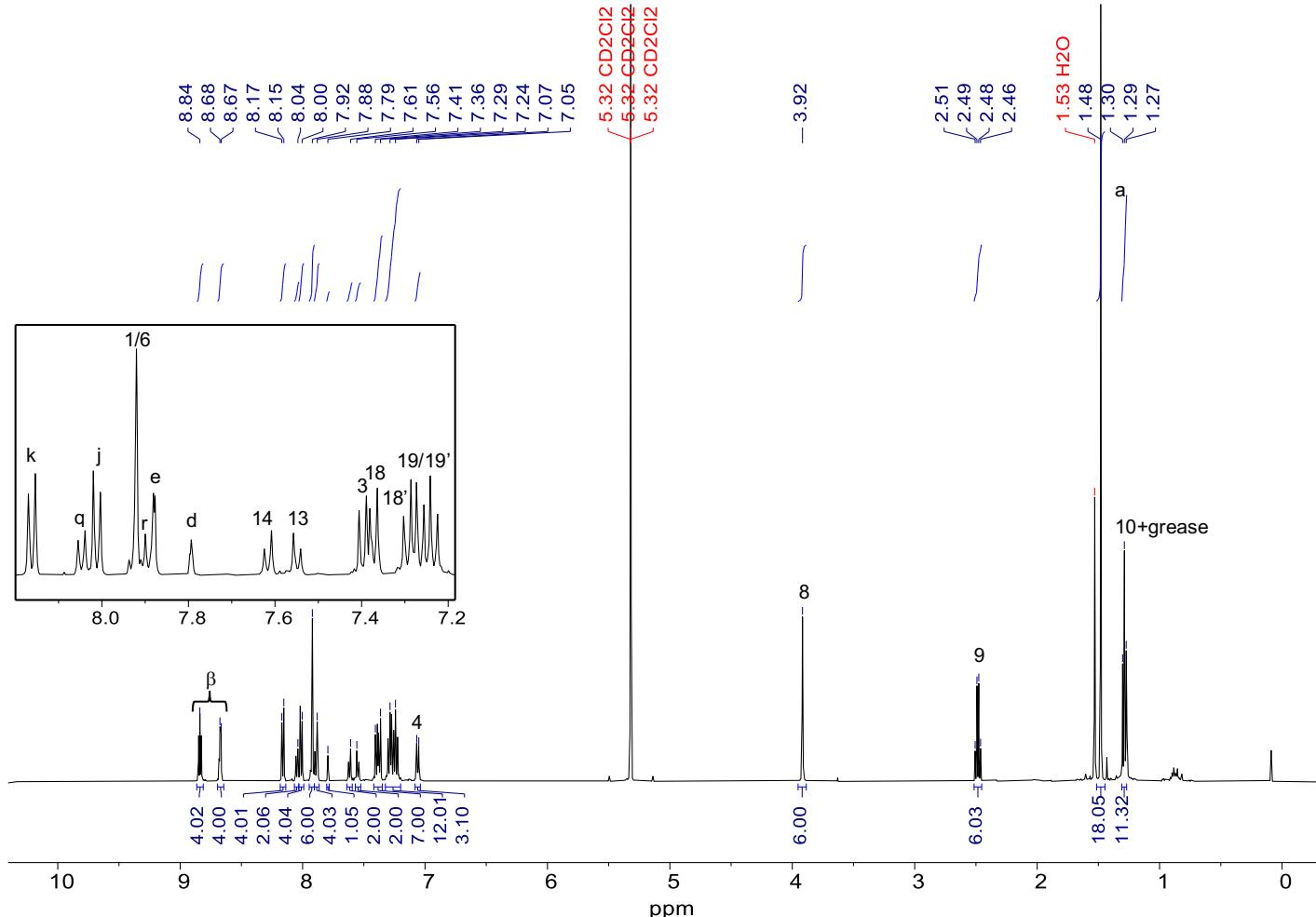


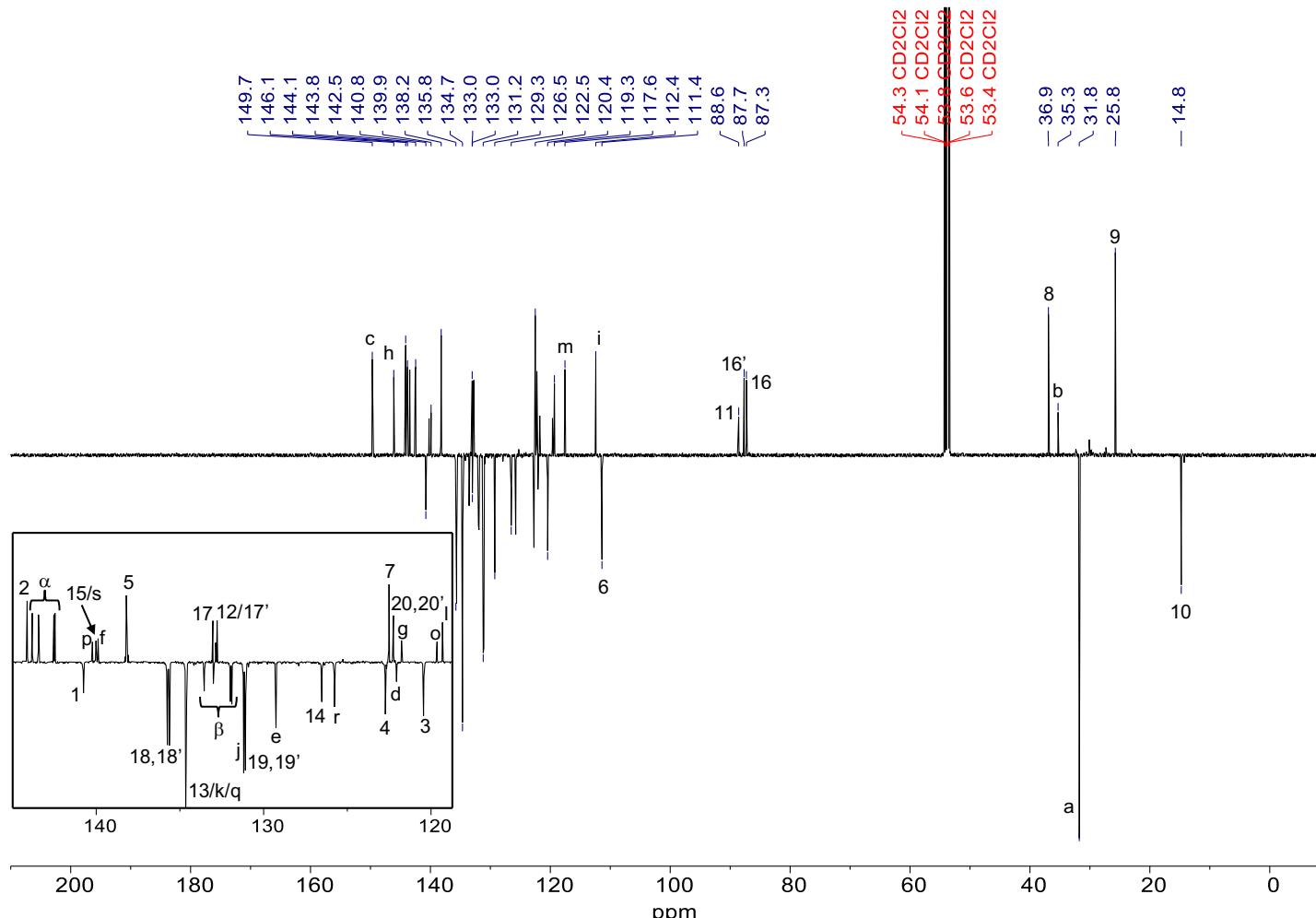
<sup>1</sup>H-NMR of complex **13** (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 25°C).



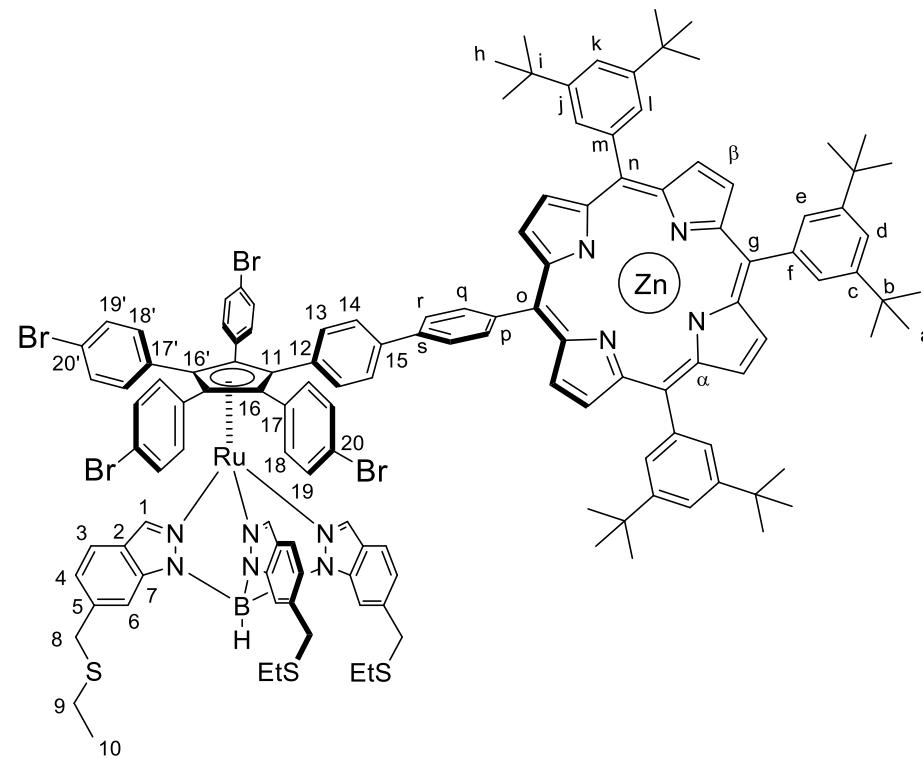
**Complex 14:**

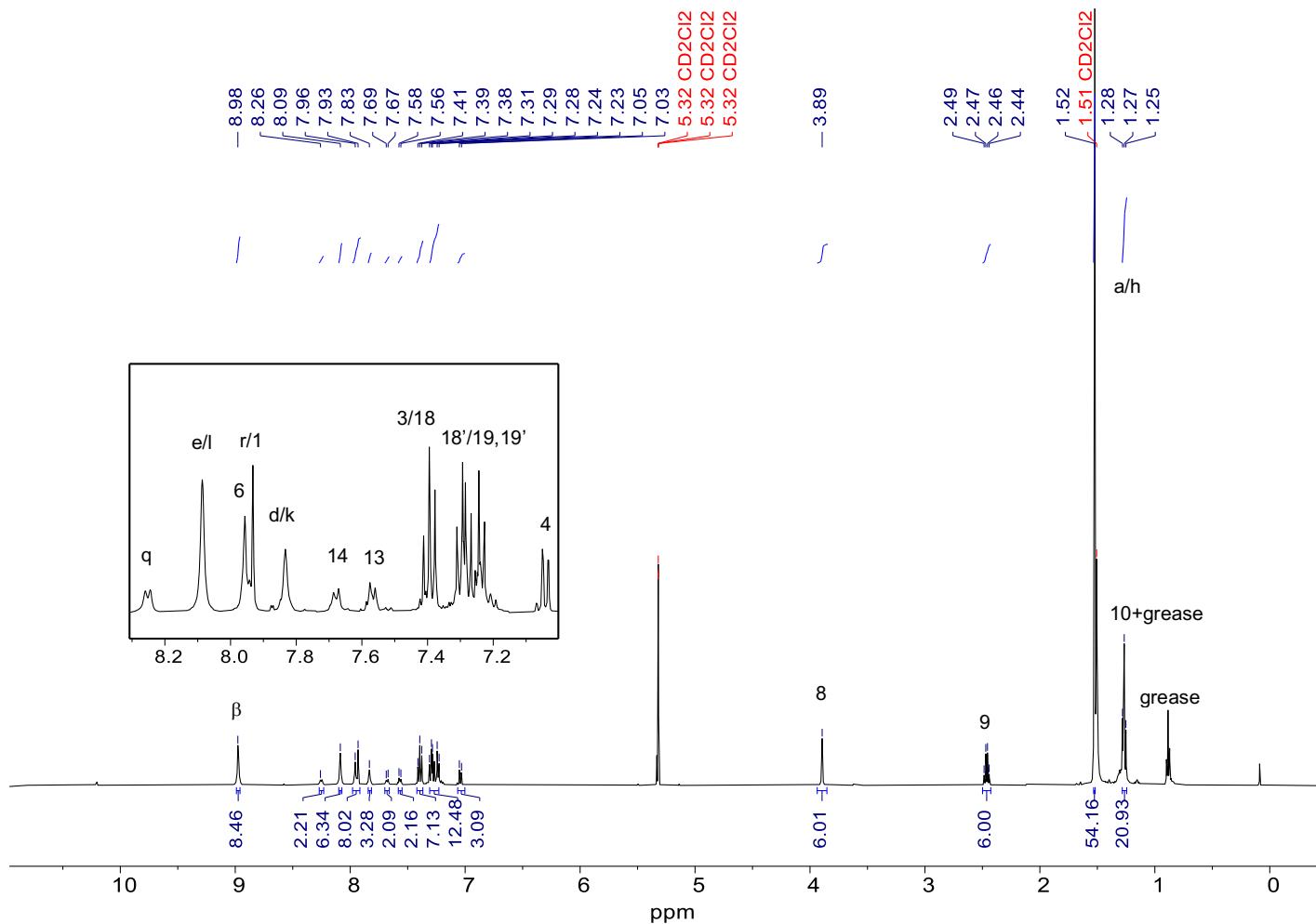


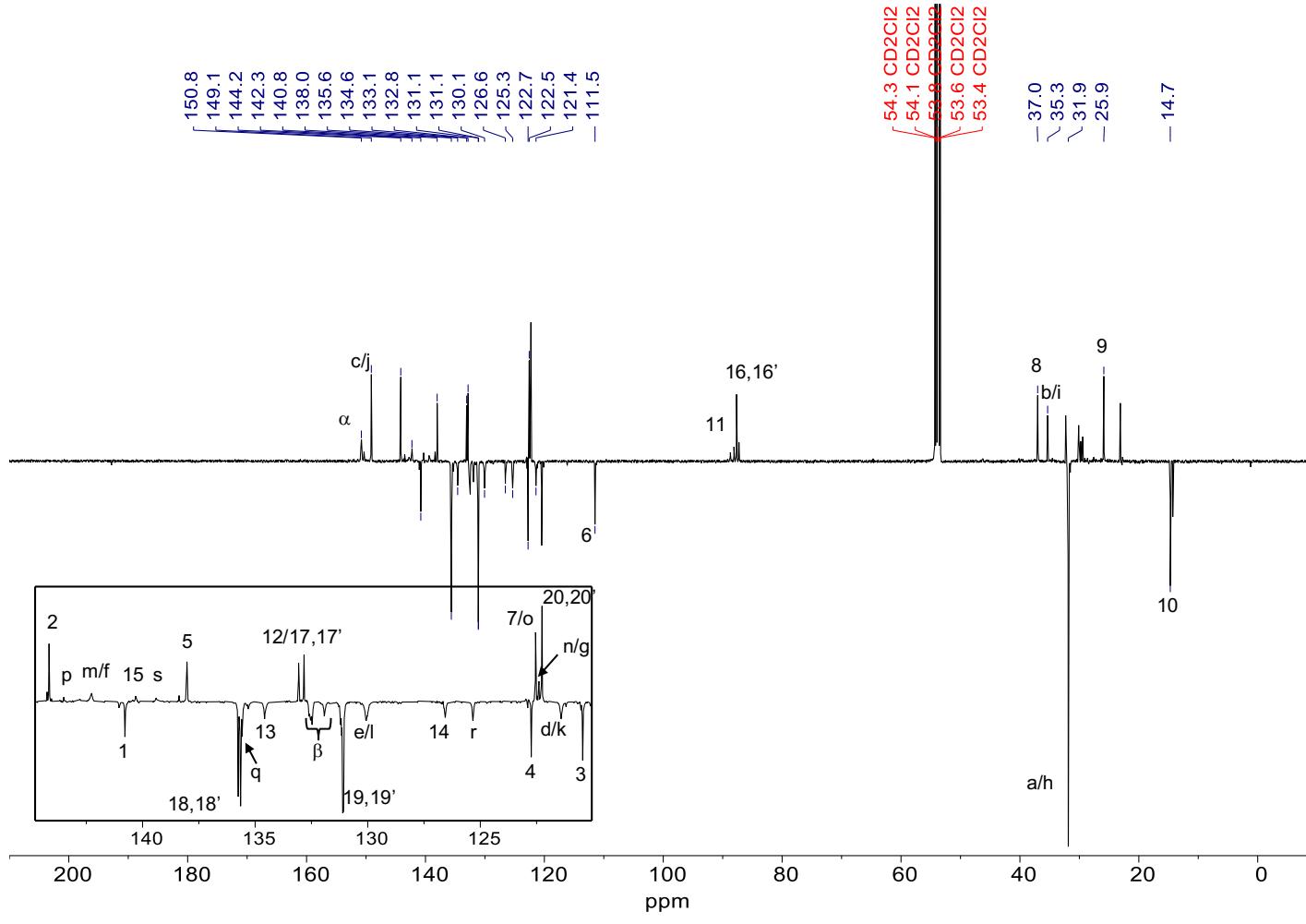




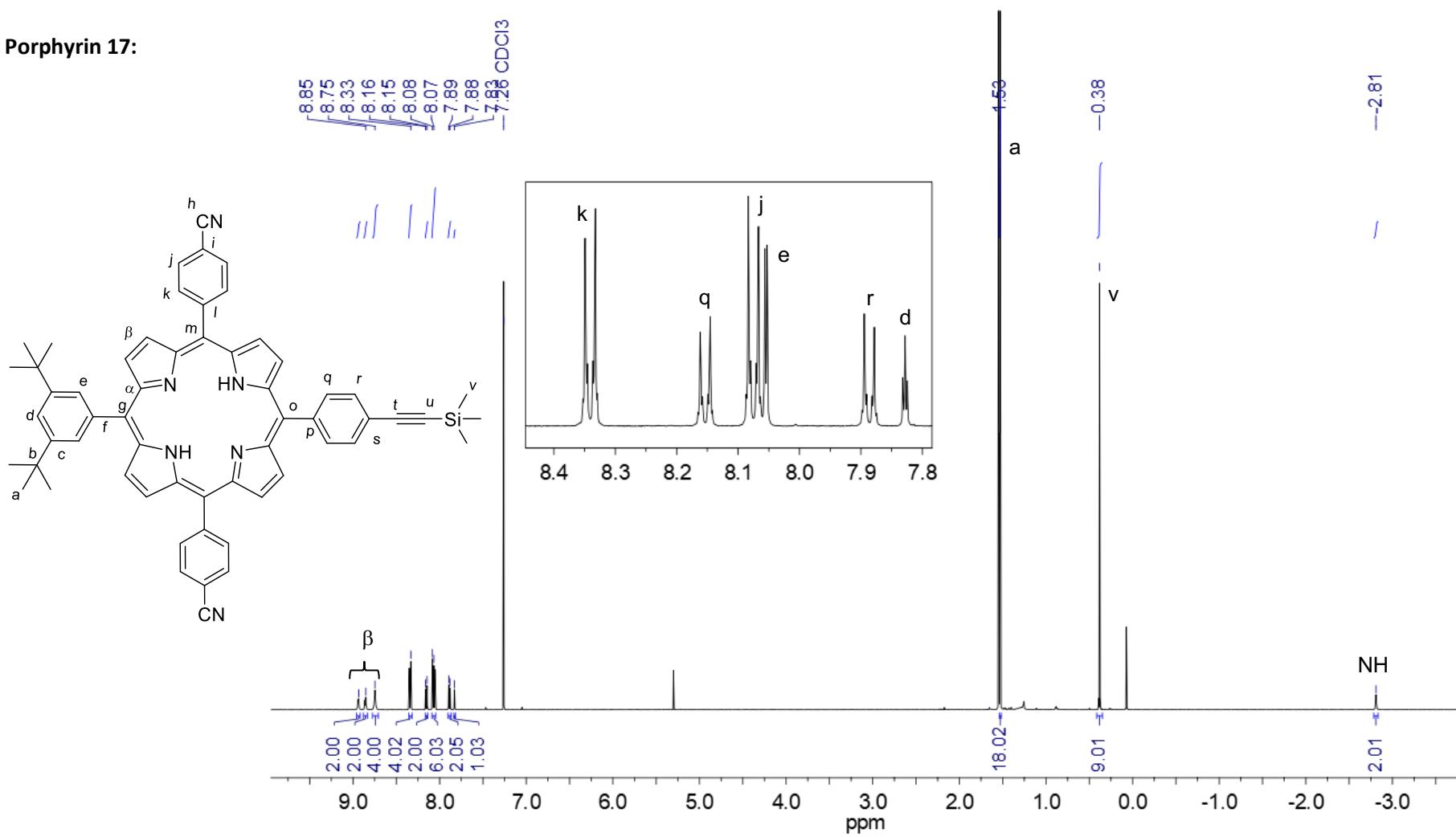
**Complex 15:**



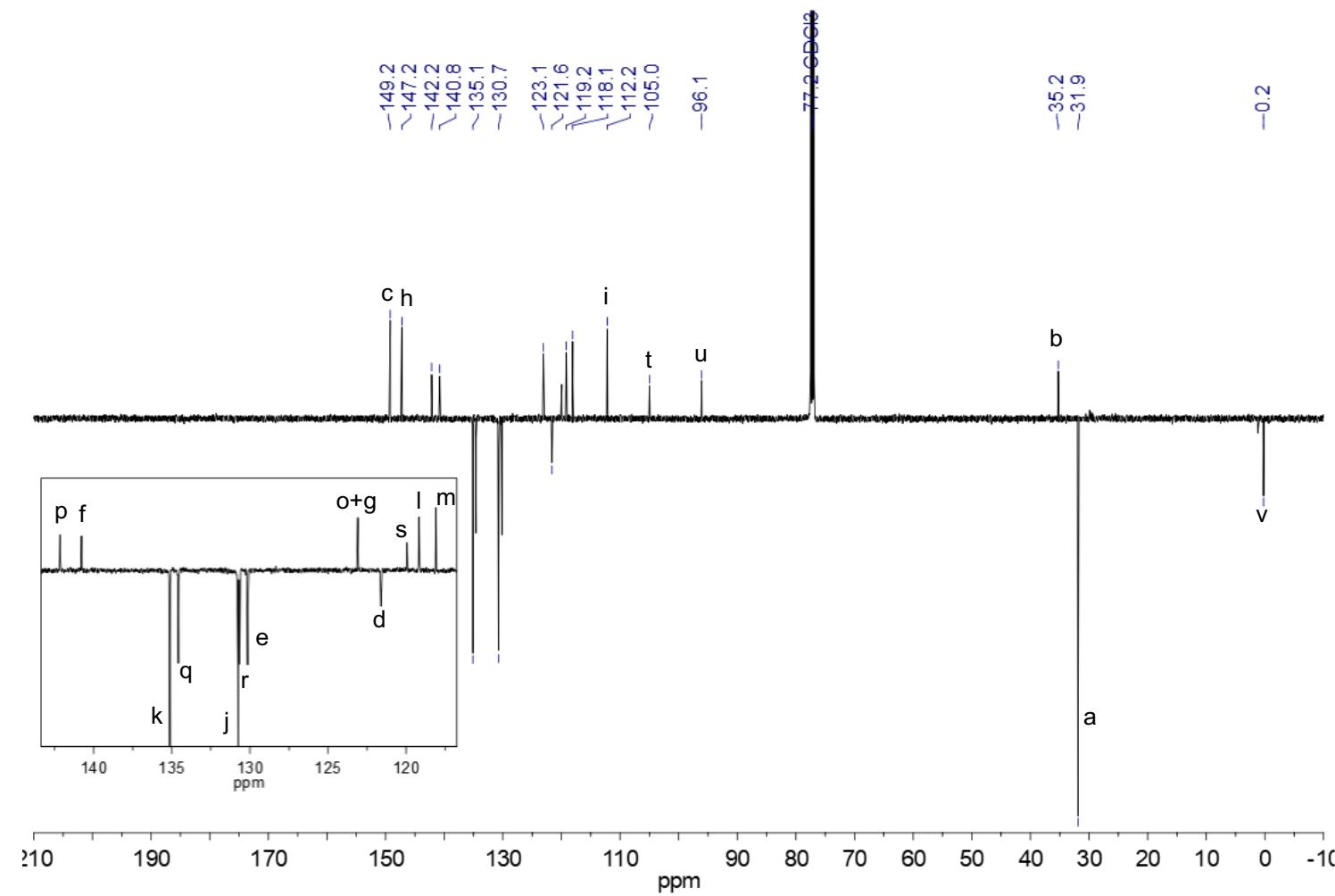




**Porphyrin 17:**

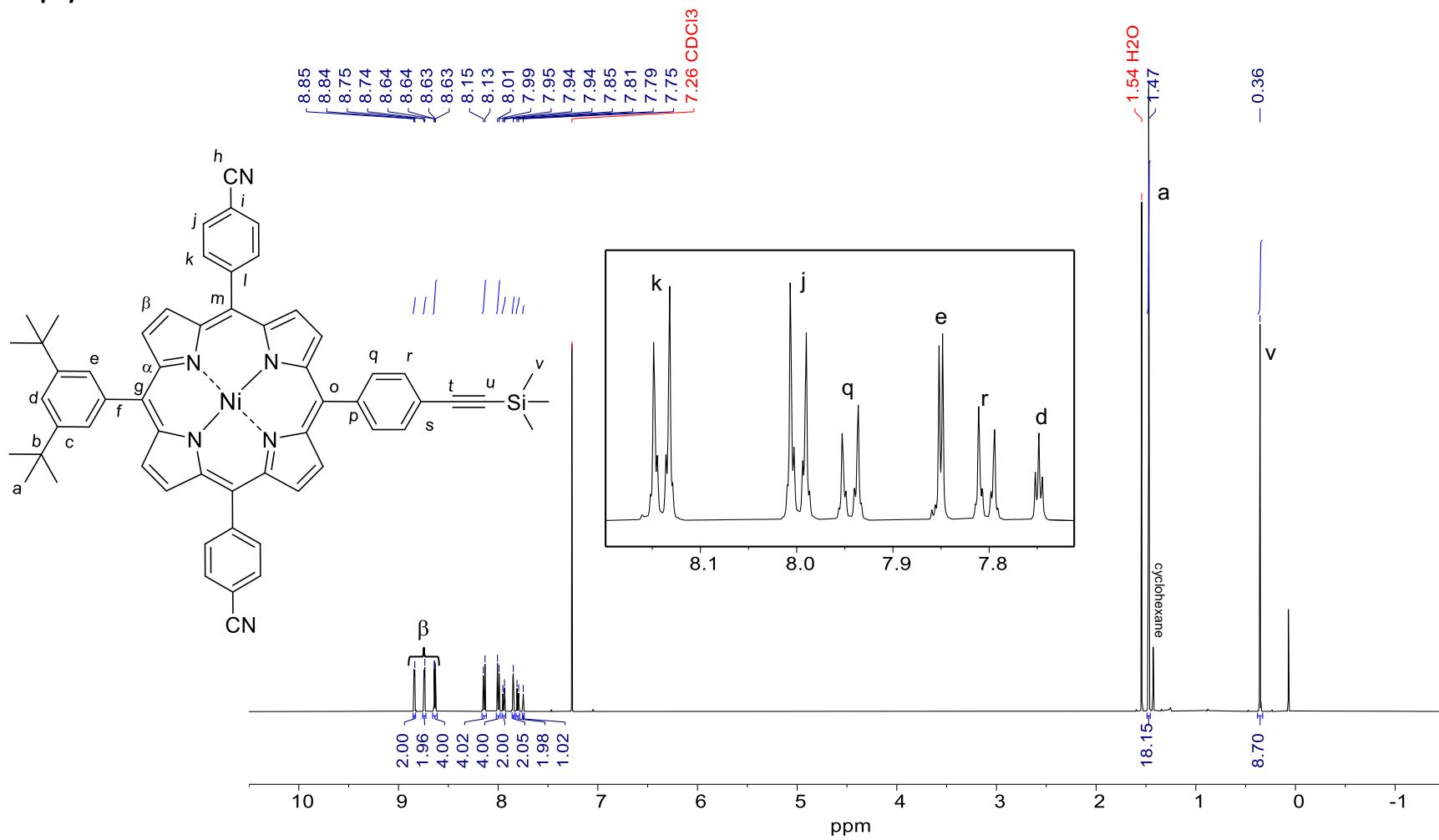


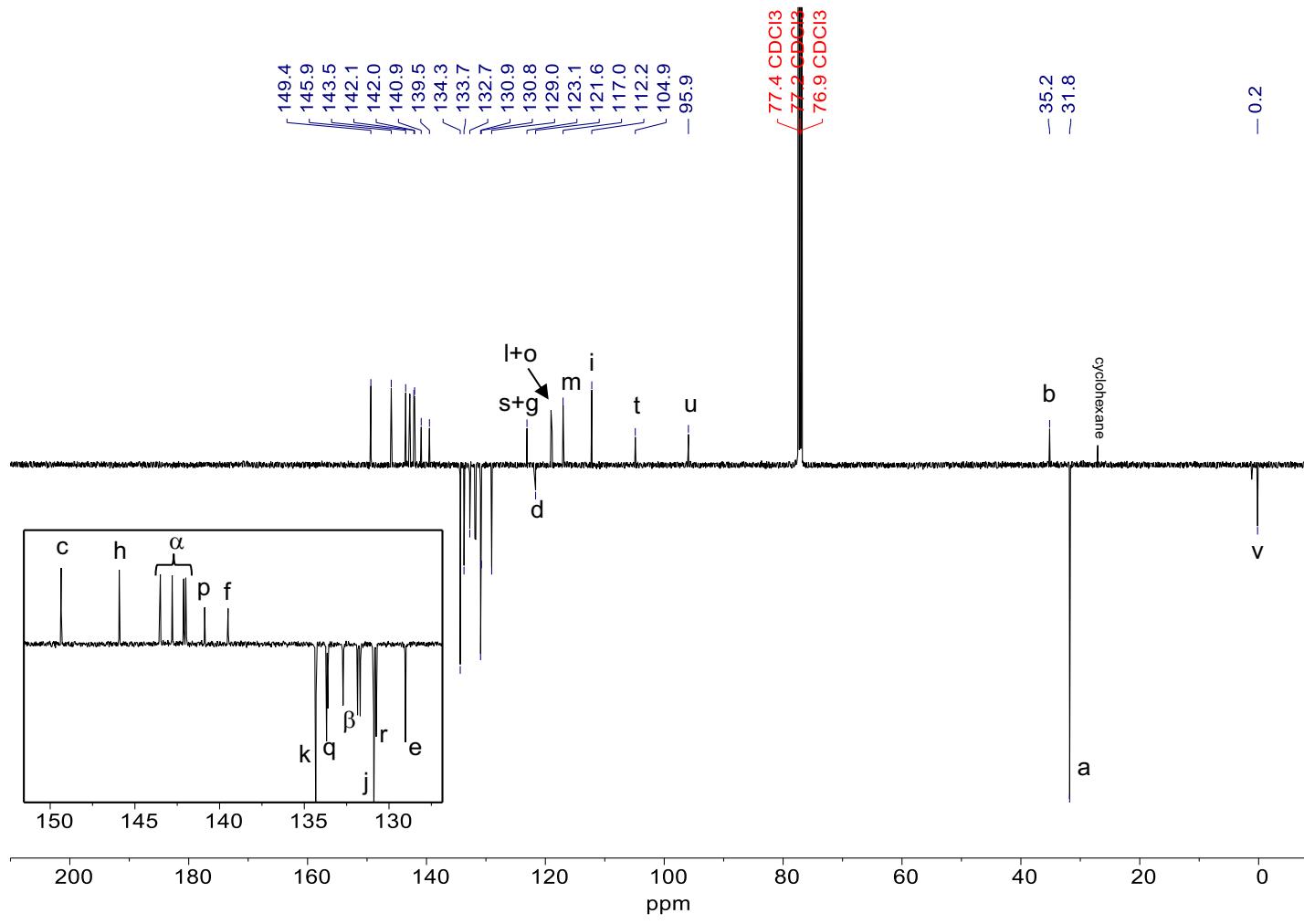
$^1\text{H}$ -NMR of porphyrin 17 (500 MHz,  $\text{CDCl}_3$ , 25°C).



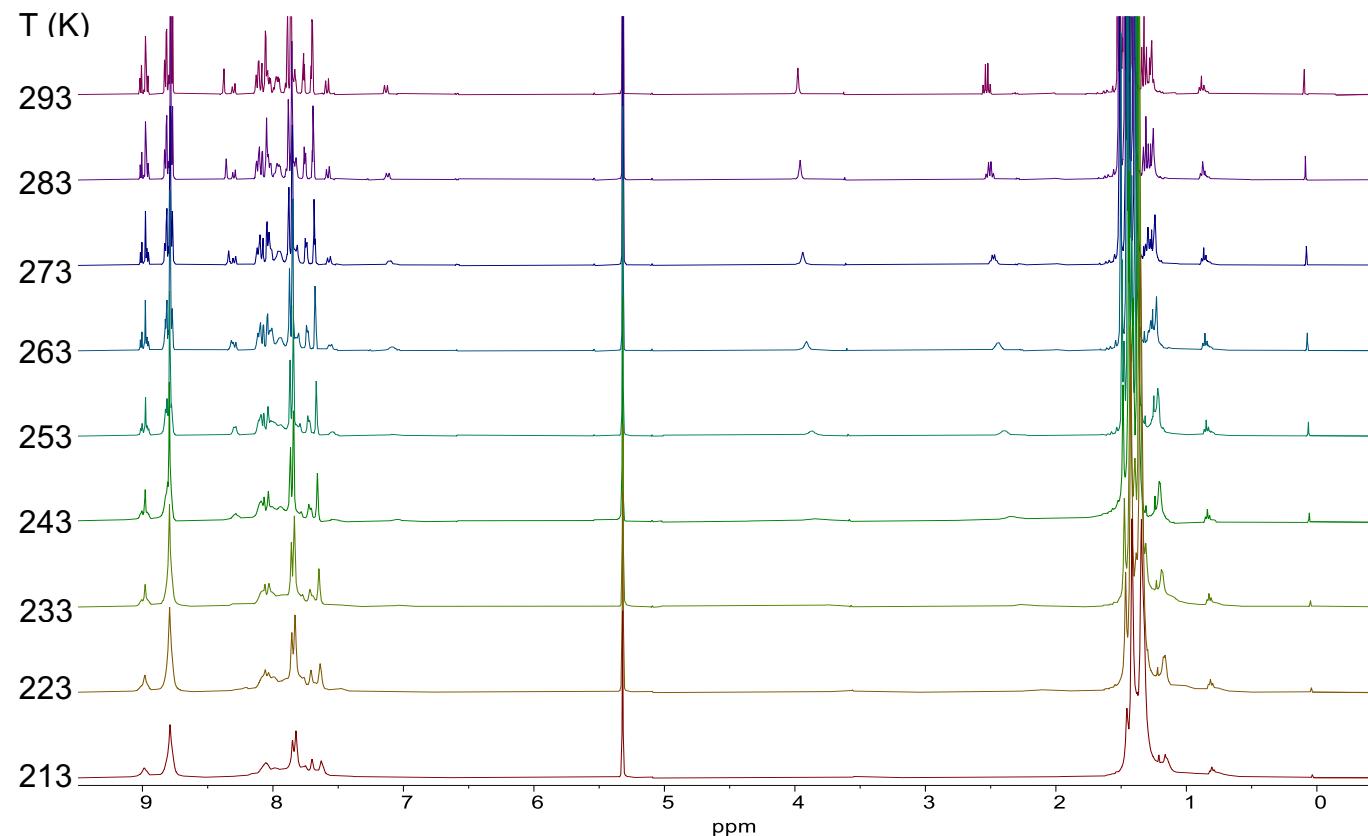
$^{13}\text{C}$ -Jmod-NMR of porphyrin **17** (126 MHz,  $\text{CDCl}_3$ , 25°C).

**Porphyrin 19:**



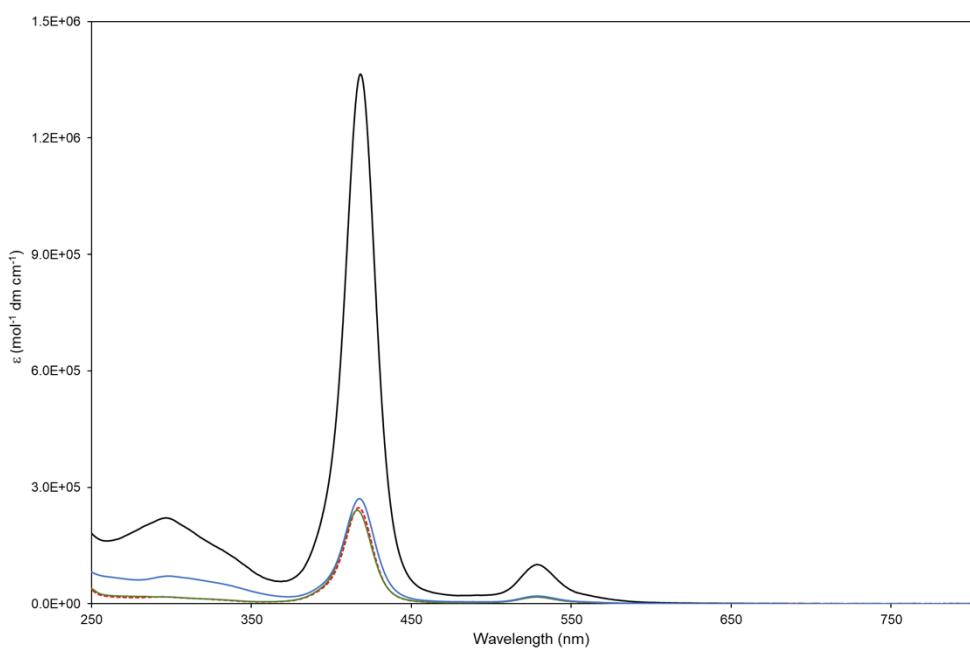


## 2. VT NMR of cogwheel 12

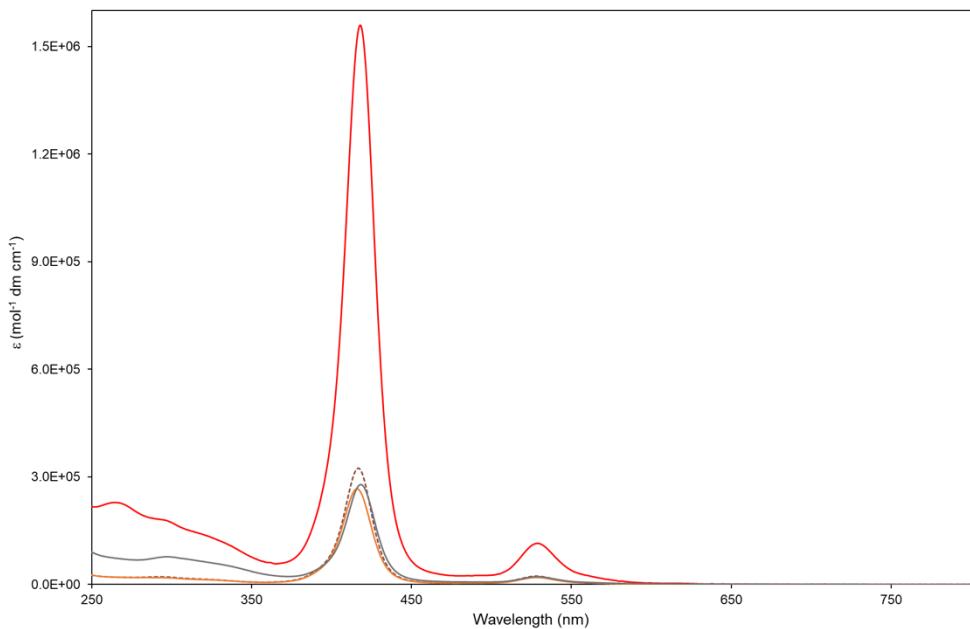


**Figure S1.** Variable Temperature  $^1\text{H}$ -NMR spectra of cogwheel **12** (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 293 K  $\rightarrow$  213 K by 10 K steps).

## V. UV-visible spectroscopy

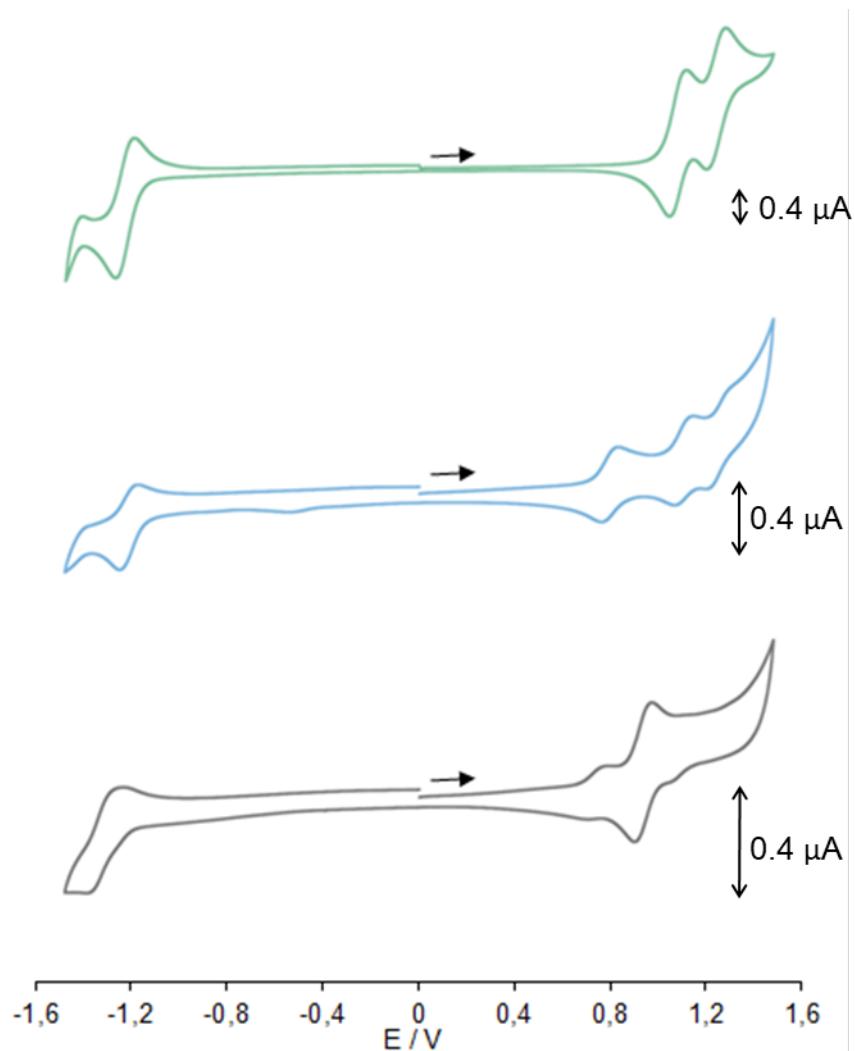


**Figure S2.** UV-Vis absorption spectra of porphyrins **3** (red dashed) and **5** (green), complex **13** (blue) and cogwheel **10** (black) in  $\text{CH}_2\text{Cl}_2$ .

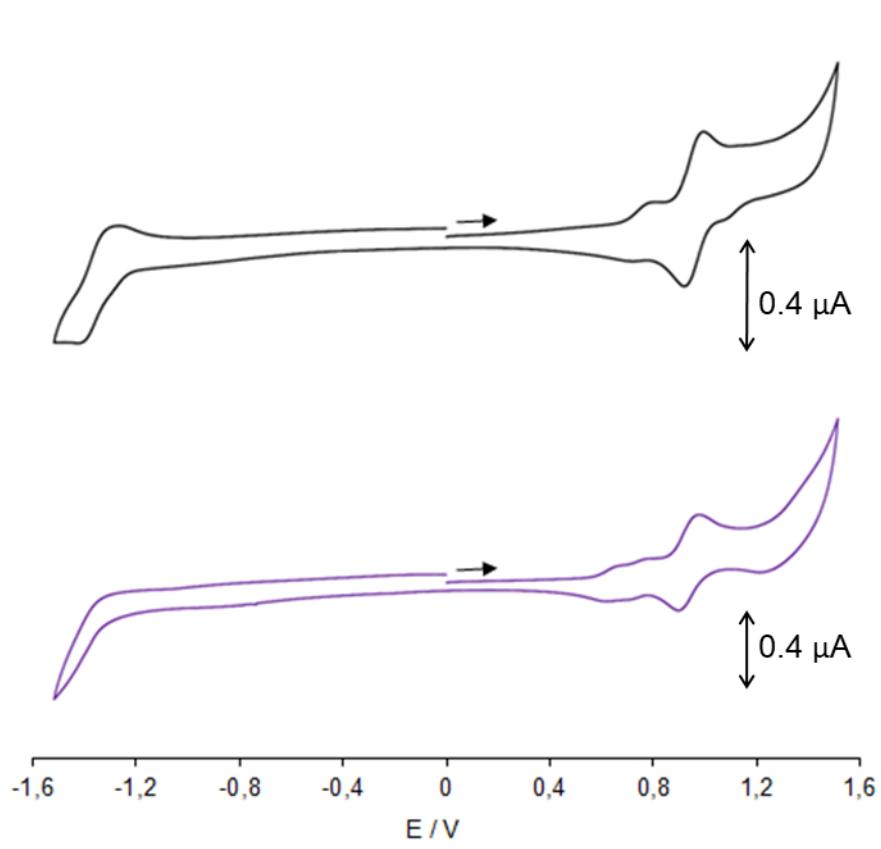


**Figure S3.** UV-Vis absorption spectra of porphyrins **4** (brown dashed) and **6** (orange), complex **14** (grey) and cogwheel **11** (red) in  $\text{CH}_2\text{Cl}_2$ .

## VI. Cyclic voltammetry



**Figure S4.** Cyclic voltammograms of porphyrin 5 (green), complex 13 (blue) and cogwheel 10 (black) in  $\text{CH}_2\text{Cl}_2$  ( $0.1 \text{ M } n\text{Bu}_4\text{NPF}_6$ ,  $25^\circ\text{C}$ ) versus SCE at a scan rate of  $0.1 \text{ V s}^{-1}$ .  
Concentrations:  $[10]=7.10^{-5} \text{ M}$ ,  $[5]=6.10^{-4} \text{ M}$ ,  $[13]=2.10^{-4} \text{ M}$



**Figure S5.** Cyclic voltammograms of cogwheels **10** (black) and **12** (purple) in  $\text{CH}_2\text{Cl}_2$  ( $0.1 \text{ M } n\text{Bu}_4\text{NPF}_6$ ,  $25^\circ\text{C}$ ) versus SCE at a scan rate of  $0.1 \text{ V s}^{-1}$ .  
Concentrations:  $[\mathbf{10}] = 7.10^{-5} \text{ M}$ ,  $[\mathbf{12}] = 5.10^{-5} \text{ M}$

## VII. Crystallographic data for compounds 5 and 13

Crystallographic data for compounds **5** and **13** were collected at 193(2) K, respectively on a Bruker-AXS APEX II CCD Quazar diffractometer equipped with a 30 W air-cooled microfocus source using Mo K $\alpha$  radiation ( $\lambda=0.71073 \text{ \AA}$ ) and on a Bruker-AXS D8-Venture diffractometer equipped with a Photon III detector and a 30W air-cooled microfocus source using Cu K $\alpha$  radiation ( $\lambda=1.54178 \text{ \AA}$ ). Phi- and omega-scans were used. Space group were determined on the basis of systematic absences and intensity statistics. Semi-empirical absorption correction was employed.<sup>[57]</sup> The structure were solved using an intrinsic phasing method (SHELXT),<sup>[58]</sup> and refined using the least-squares method on  $F^2$ .<sup>[59]</sup> All non-H atoms were refined with anisotropic displacement parameters. Hydrogen atoms were refined isotropically at calculated positions using a riding model with their isotropic displacement parameters constrained to be equal to 1.5 times the equivalent isotropic displacement parameters of their pivot atoms for terminal sp<sup>3</sup> carbon and 1.2 times for all other carbon atoms. Hydrogen on Boron atom (**13**) was located by difference Fourier map and was freely refined.

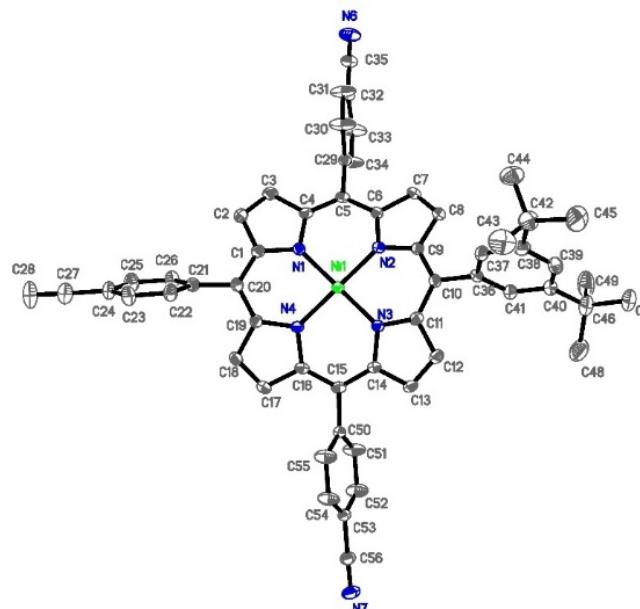
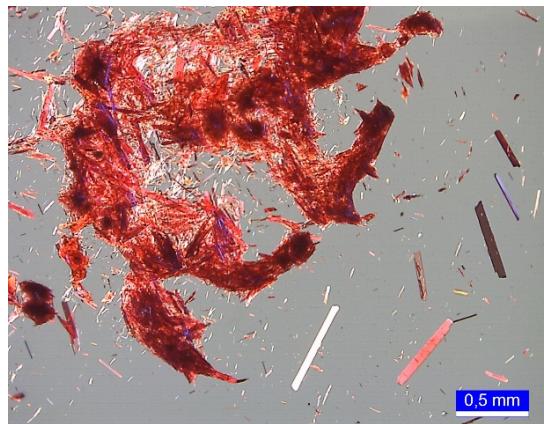
Both structures were disordered: <sup>t</sup>Bu groups and solvent in **5** and two thioether groups, <sup>t</sup>Bu groups and benzene in **13**. Several restraints (SAME, SIMU, DELU, ISOR) and constraints (EXYZ, EADP, DANG and DFIX) were applied to refine these disorders and to avoid the collapse of the structures during the least-squares refinement by the large anisotropic displacement parameters.

Some residual electron density were difficult to modelize (**13**) and therefore, the SQUEEZE function of PLATON<sup>[510]</sup> was used to eliminate the contribution of the electron density in the solvent region from the intensity data, and the solvent-free model was employed for the final refinement.

CCDC-2039772 (**5**) and CCDC-2039773 (**13**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/structures>.

### Porphyrin **5**:

Crystals of nickel(II) 5-(4-ethynylphenyl)-10,20-bis(4-cyanophenyl)-15-(3,5-di-*tert*-butylphenyl) porphyrin (**5**) suitable for X-ray diffraction were grown from a mixture of chloroform and methanol.



**Figure S6.** Picture of the crystals (left) and molecular structure of porphyrin **5** (right). Thermal ellipsoids drawn at 30% probability, hydrogen atoms, solvent molecule are omitted for clarity.

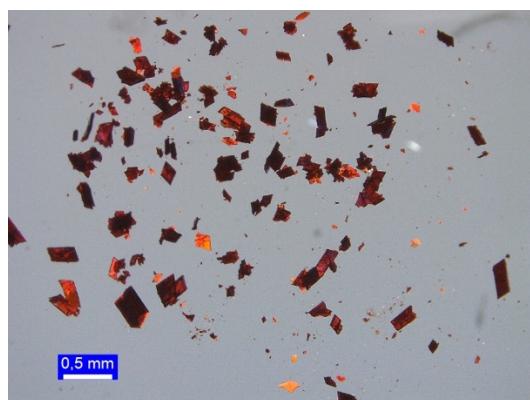
**Selected data for 5:** C<sub>56</sub>H<sub>42</sub>N<sub>6</sub>Ni, CHCl<sub>3</sub>  $M = 977.03$ , monoclinic, space group P2<sub>1</sub>/c,  $a = 9.4132(9)$  Å,  $b = 16.3463(12)$  Å,  $c = 31.800(3)$  Å,  $\beta = 91.407(3)^\circ$ ,  $V = 4891.6(7)$  Å<sup>3</sup>,  $Z = 4$ , crystal size 0.40 x 0.06 x 0.04 mm<sup>3</sup>, 78257 reflections collected (8617 independent, R<sub>int</sub> = 0.1447), 697 parameters, 246 restraints, R<sub>1</sub> [ $|I| > 2\sigma(I)$ ] = 0.0667, wR<sub>2</sub> [all data] = 0.1852, largest diff. peak and hole: 1.053 and -0.531 eÅ<sup>-3</sup>.

**Table S2.** Crystal data and structure refinement for porphyrin 5

Empirical formula	C <sub>57</sub> H <sub>43</sub> Cl <sub>3</sub> N <sub>6</sub> Ni	
Formula weight	977.03	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /c	
Unit cell dimensions	$a = 9.4132(9)$ Å	$\alpha = 90^\circ$ .
	$b = 16.3463(12)$ Å	$\beta = 91.407(3)^\circ$ .
	$c = 31.800(3)$ Å	$\gamma = 90^\circ$ .
Volume	4891.6(7) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.327 Mg/m <sup>3</sup>	
Absorption coefficient	0.605 mm <sup>-1</sup>	
F(000)	2024	
Crystal size	0.400 x 0.060 x 0.040 mm <sup>3</sup>	
Theta range for data collection	2.492 to 25.027°.	
Index ranges	-11≤h≤11, -19≤k≤19, -37≤l≤37	
Reflections collected	78257	
Independent reflections	8617 [R(int) = 0.1447]	
Completeness to theta = 25.027°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7365 and 0.6389	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	8617 / 246 / 697	
Goodness-of-fit on F <sup>2</sup>	1.030	
Final R indices [ $ I  > 2\sigma(I)$ ]	R <sub>1</sub> = 0.0667, wR <sub>2</sub> = 0.1487	
R indices (all data)	R <sub>1</sub> = 0.1321, wR <sub>2</sub> = 0.1852	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.053 and -0.531 e.Å <sup>-3</sup>	

**Complex 13:**

Single crystals of complex **13** suitable for X-ray diffraction were grown by slow evaporation of a solution of **13** in a mixture of benzene and methanol.



**Figure S7.** Picture of the crystals of complex **13**.

**Selected data for 13:**  $C_{121}H_{95}BBr_4N_{12}NiRuS_3$ ,  $C_6H_6$  (+solvent)  $M = 2381.60$ , triclinic, space group  $P\bar{1}$ ,  $a = 16.1291(6)$  Å,  $b = 19.1492(7)$  Å,  $c = 24.8626(10)$  Å,  $\alpha = 75.720(3)^\circ$ ,  $\beta = 89.677(3)^\circ$ ,  $\gamma = 66.509(3)^\circ$ ,  $V = 6787.8(5)$  Å<sup>3</sup>,  $Z = 2$ , crystal size  $0.20 \times 0.08 \times 0.05$  mm<sup>3</sup>, 125825 reflections collected (23204 independent,  $R_{int} = 0.1281$ ), 1511 parameters, 757 restraints,  $R1 [I > 2\sigma(I)] = 0.0587$ ,  $wR2$  [all data] = 0.1733, largest diff. peak and hole: 0.990 and -0.673 eÅ<sup>-3</sup>.

**Table S3.** Crystal data and structure refinement for complex **13**

Empirical formula	$C_{127}H_{101}BBr_4N_{12}NiRuS_3$	
Formula weight	2381.60	
Temperature	193(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 16.1291(6)$ Å	$\alpha = 75.720(3)^\circ$
	$b = 19.1492(7)$ Å	$\beta = 89.677(3)^\circ$
	$c = 24.8626(10)$ Å	$\gamma = 66.509(3)^\circ$
Volume	6787.8(5) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.165 Mg/m <sup>3</sup>	
Absorption coefficient	3.240 mm <sup>-1</sup>	
F(000)	2424	
Crystal size	$0.200 \times 0.080 \times 0.050$ mm <sup>3</sup>	
Theta range for data collection	2.610 to 65.541°	
Index ranges	$-18 \leq h \leq 19$ , $-22 \leq k \leq 22$ , $-29 \leq l \leq 29$	
Reflections collected	125825	
Independent reflections	23204 [ $R(\text{int}) = 0.1281$ ]	
Completeness to theta = 65.541°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7516 and 0.5902	
Refinement method	Full-matrix least-squares on $F^2$	

Data / restraints / parameters	23204 / 757 / 1511
Goodness-of-fit on F <sup>2</sup>	0.976
Final R indices [I>2sigma(I)]	R1 = 0.0587, wR2 = 0.1477
R indices (all data)	R1 = 0.1019, wR2 = 0.1733
Extinction coefficient	0.00054(4)
Largest diff. peak and hole	0.990 and -0.673 e. $\text{\AA}^{-3}$

## VIII. DFT and semi-empirical calculations

### Computational details:

DFT calculations allowing for a better understanding of the geometries of the molecular cogwheels were performed using the Gaussian 09 software.<sup>[S11]</sup> The common B3LYP functional was used in conjunction with the 6-31G(d,p) basis set<sup>[S12]</sup> for all atoms except metallic centres for which the LANL2DZ basis set<sup>[S13]</sup> was used. In order to simplify the system, effective core potentials were considered for the metallic atoms.

The input geometry was found to have a great influence on the ability of the geometry optimisation to reach convergence. To have a realistic geometry input and validate the calculation method, it was decided to run the above mentioned calculation on the structure obtained by single crystal X-ray diffraction for compound **13** until convergence. The resulting optimised geometry showed great similarities with the one obtained by single crystal X-ray diffraction, with only slightly distorted bonds and angles due to a calculation run on an isolated molecule in vacuum. This process thus allowed us to confirm the coherence of the calculation method employed. For this system, a frequency calculation was also performed using the same conditions on the optimised geometry, displaying no negative frequency and confirming that the obtained structure corresponds to a minimum on the potential energy map.

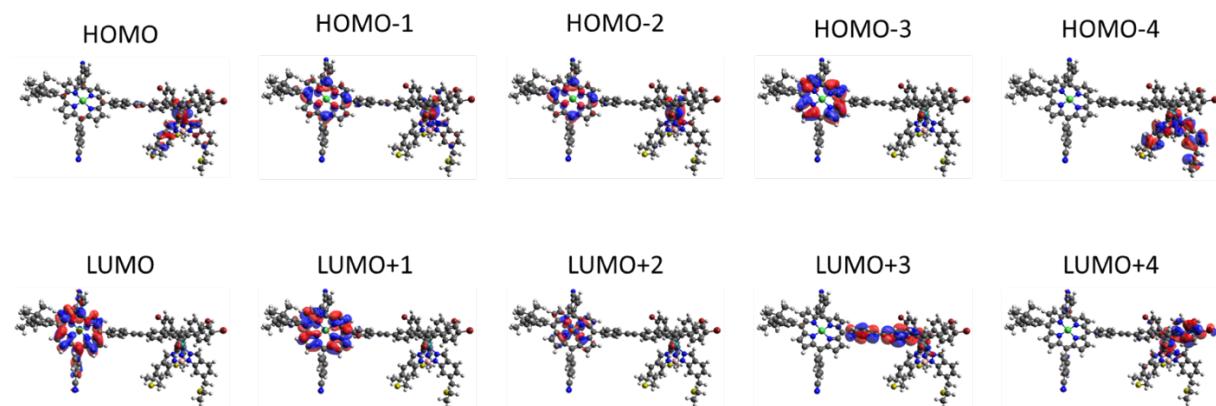
The geometry of the more complicated pentaporphyrinic systems **10**, **11** and **12** was then calculated using the same functional and basis sets, and the optimisation was run until Gaussian 09 convergence criterion were met, to give the optimised geometries displayed below. Once again, the input geometry had a great influence on the ability of the calculation to converge. All input geometries were built using the one obtained after optimising the X-ray crystal structure of compound **13** and replicating the porphyrin fragment to reach five-fold functionalisation. The resulting structure was then modified to take into account the chemical or steric tags, and used as the input geometry.

In order to assess the ability of the pentaporphyrinic cogwheel design to form a train of gears, we performed further calculations on a system consisting of two intertwined complexes **11**. Due to the large number of atoms in this system, DFT calculations were hardly achievable. Consequently, we used the GFN2-xTB semi-empirical tight-binding potential developed by Bannwarth, Ehlert and Grimme<sup>[S14]</sup> and implemented in the xTB code v. 6.2. The initial structures were constructed by hand using the following procedure: one complex **11** optimised at the DFT level was duplicated, then the two complexes were kept on the same plane with Ru atoms placed at the same position along the Ru-B axis. Three initial structures were generated with increasing initial Ru-Ru distances of 35.3, 37.5 and 41.2 Å and first roughly optimised using lax optimisation parameters and an accuracy of the SCC convergence criterion of 2.0. A subsequent optimisation was performed using tight optimisation parameters and an accuracy of the SCC convergence criterion of 0.5. All optimisations were performed constraining the Ru-Ru distance, which was thus kept constant along the optimisation. The coordinates of the three optimised structures are provided below.

An animation movie of the optimised geometry of intertwined complexes **11** with a Ru-Ru distance of 41.2 Å is provided as supplementary file: *SI\_3D\_intertwined\_11.mpg*.

**Complex 13:**

Calculation Type = FREQ. Calculation Method = RB3LYP. Basis Set = 6-31G(d,p). Charge = 0. Spin = Singlet. Electronic Energy = -17093.606 Hartree. RMS Gradient Norm = 7.7058922e-07 Hartree/Bohr. Imaginary Freq = None. Dipole Moment = 5.4143863 Debye.



**Figure S8.** Frontier orbitals of complex **13**.

Cartesian coordinates:

Ru	0.59217	0.74209	-0.27962	C	-0.26393	4.80442	-4.53668
Br	0.74709	2.07166	7.47614	C	-13.6091	18.51723	7.12597
Br	7.17573	2.07965	-4.60563	N	-13.1108	15.58958	-6.38442
Br	-0.81768	5.70966	-6.12506	C	-14.9703	17.95816	7.60472
Ni	-12.8949	11.59928	3.11583	C	0.30194	4.85936	-2.20001
Br	7.24884	-0.51899	3.67426	C	0.3736	2.77687	-3.41011
S	-7.00008	-2.40156	-2.01951	C	-18.7994	18.70813	3.83678
S	-0.11335	-5.63172	-6.93482	C	1.00078	2.13464	2.7704
N	-13.6405	13.22351	2.31471	C	-18.8821	17.25664	4.36708
N	-1.03887	-0.2568	0.34529	B	-0.81566	-2.46965	-0.82066
N	-11.7987	11.30537	1.5141	C	1.64688	-1.9289	-3.51156
C	-2.29943	-2.00041	1.18766	C	2.29966	-2.33832	-4.69176
S	-5.41595	-4.88226	4.37519	C	1.01926	2.80376	-0.96832
C	-10.7513	10.41927	1.37	C	1.15347	2.19025	1.28763
C	2.30463	2.17964	-0.76288	C	-13.5092	13.64432	1.01026
C	0.55201	3.47665	-2.20721	C	-14.8154	14.17635	4.26747
C	-0.96027	3.5596	0.56343	C	-2.74867	-5.64361	-5.87652
N	-13.9902	11.88658	4.71492	C	-19.905	17.1918	5.52641
N	-1.39497	-3.81988	-0.99474	C	-6.83624	-4.60712	3.24025
C	0.32791	1.03529	4.83675	C	-8.15277	-4.73456	4.00485
C	-14.7078	13.0174	5.03986	H	-0.13779	0.19828	5.34453
C	-13.0499	15.15323	-5.30769	H	-15.6374	11.003	7.48992
C	0.85753	2.09401	5.56913	H	-9.9717	7.46933	4.28808
C	-15.2216	11.5257	6.64209	H	-15.1021	16.23209	2.31383
C	-3.69065	-3.26359	2.72384	H	-9.36661	9.92852	-0.32396
N	0.89885	-0.84793	-1.66833	H	1.8984	3.98035	5.5104

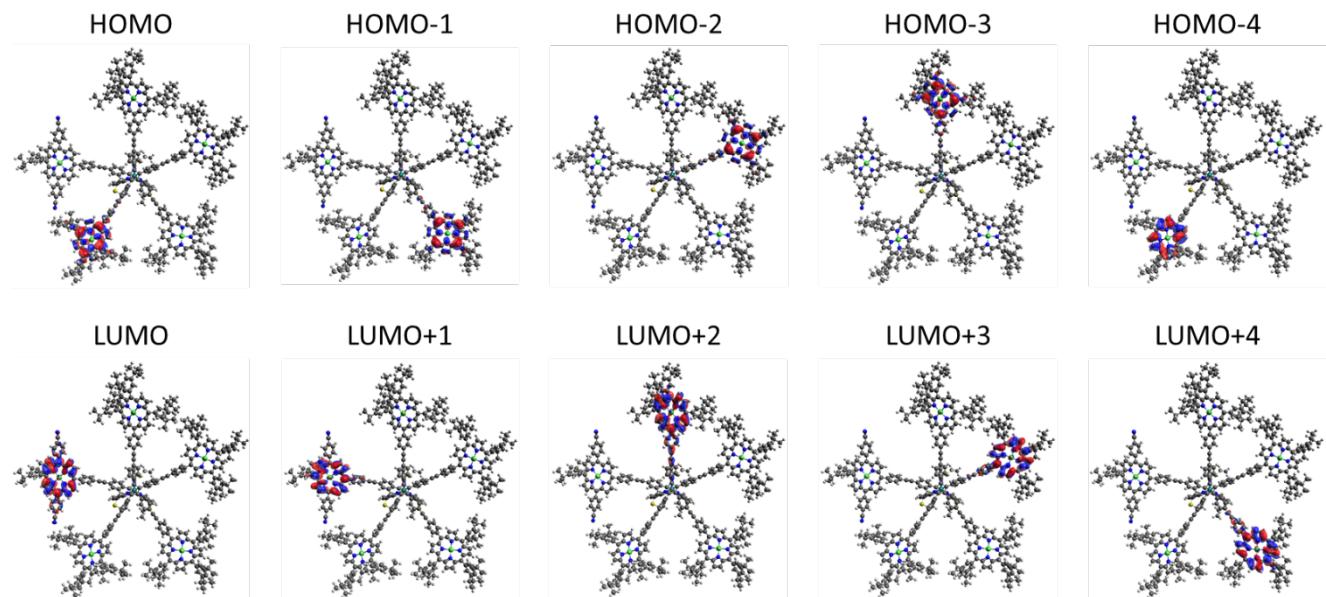
C	-10.7863	8.16991	4.39214	H	-15.6122	5.80103	7.47178
C	-15.5466	15.35105	4.83805	H	-16.1099	13.53451	6.70642
N	0.2082	-2.05977	-1.76634	H	4.9909	4.03457	-4.09457
C	-14.6014	15.31367	2.04852	H	-14.0082	15.77003	6.26241
C	-10.2045	10.50331	0.03949	H	-13.371	10.09797	8.54449
C	1.47483	3.16851	4.93011	H	-0.24701	4.65029	2.2844
C	-15.1226	6.74132	7.70239	H	-10.9355	15.24902	-3.66604
C	2.35831	1.73385	0.609	H	-14.1482	15.49007	-0.09185
C	-14.8968	7.09704	9.04253	H	-0.00901	-6.30088	-4.58952
C	-17.4962	16.8181	4.87916	H	1.54885	-6.30728	-5.41101
C	0.32284	2.85246	0.32111	H	-10.8106	14.32462	-1.37005
C	-15.4586	12.80431	6.25068	H	-0.29415	6.59327	-3.33687
C	-15.3071	6.22021	10.10037	H	-4.09905	3.91238	-0.74347
C	-14.0953	8.82153	6.9663	H	4.75182	2.91675	1.0152
C	-12.7708	13.00403	0.01196	H	-15.0009	13.87158	-3.99228
C	4.80468	3.19266	-3.43745	H	-0.41293	-4.63375	-3.02212
C	-10.3179	9.50513	2.3326	H	-0.16521	2.87832	-5.49634
C	-12.6153	9.31136	5.03257	H	-18.7318	16.38223	2.35555
C	-14.9807	16.07559	5.88902	H	-20.3801	16.71009	2.89641
C	-13.8697	9.16301	8.31038	H	-19.5082	15.31745	3.54336
C	-1.08491	4.47942	1.61942	H	3.05332	4.06512	-2.57927
C	-14.3357	14.22819	2.95816	H	-14.0811	8.58589	10.37544
C	-12.9749	14.616	-3.98029	H	2.36611	0.08449	-2.81651
C	-11.7905	14.73923	-3.23465	H	-10.868	11.69656	-1.67611
C	-14.1269	14.93505	0.83398	H	-6.53455	-3.99347	-3.78962
C	0.63908	-5.71966	-5.25042	H	-5.52434	-2.55	-3.85061
N	-0.69752	-4.92428	-0.55709	H	-4.75943	-0.27056	2.3677
C	3.43961	2.12139	-1.71644	H	-3.58782	-0.11814	3.6492
C	-11.7234	14.21641	-1.947	H	-17.414	18.37785	6.3484
C	-0.10374	5.5263	-3.35533	H	-17.2368	15.14377	3.53868
C	-2.62033	-4.19043	-1.5105	H	-2.0037	2.65881	-1.09511
N	-1.32342	-1.64614	0.20867	H	-9.97501	7.4987	0.49393
C	-3.25395	4.07352	-0.0822	H	2.42901	-3.89439	-6.15509
C	4.70158	1.92724	1.45961	H	4.17023	0.18991	-1.07853
C	-14.0863	13.9675	-3.41662	H	-14.9012	7.32129	5.64669
C	0.31866	-3.9802	-3.47161	H	-7.93687	9.64631	3.60543
C	-0.0294	3.43072	-4.57345	H	-2.34017	5.88999	2.64713
C	-19.3966	16.3592	3.22531	H	-2.30981	-4.14929	1.26128
C	-2.70094	-5.60052	-1.40052	H	-7.93974	6.15396	0.08392
C	-13.6697	9.72133	5.85169	H	0.00658	0.22943	2.8739
C	0.66561	-2.74142	-2.90387	H	-1.96747	1.26699	1.47885
C	3.70506	3.19965	-2.58042	H	6.70455	2.03295	2.25512
C	-14.2644	8.3157	9.34084	H	-4.92137	-2.22361	4.08141
C	1.73326	-0.77916	-2.69645	H	-11.9276	7.48539	6.13781
C	-5.59302	6.36852	1.3774	H	-14.8659	12.94712	-1.69537
C	-10.9639	11.39796	-0.64342	H	-1.11334	-6.96275	-0.51944

C	-5.90956	-3.32859	-3.1855	H	2.59899	-0.7151	1.79759
C	5.66659	2.09839	-3.4358	H	-6.99797	-4.36812	-0.60298
C	-3.85925	-0.74959	2.79005	H	-8.28473	-4.44339	-1.8217
C	-16.8872	17.5289	5.93017	H	-3.152	-5.07923	3.74614
C	-16.8065	15.7281	4.34298	H	-4.18297	-5.32385	2.35227
N	-15.6402	5.50909	10.95875	H	-3.93386	-7.34672	-1.79855
C	-2.07132	3.37277	-0.28138	H	-3.58121	-2.34506	-2.14472
C	-9.08035	7.68215	1.0813	H	2.04138	4.00666	3.04031
C	-11.9242	11.93011	0.29073	H	6.11821	0.17142	-2.58419
C	1.95349	-3.55448	-5.24022	H	-8.28762	-2.58853	0.64309
C	4.33739	1.03638	-1.73443	H	-9.2494	-4.06499	0.46136
C	-14.7224	7.59709	6.68114	H	-9.57238	-2.66536	-0.57432
C	-7.93803	8.88139	2.83462	H	-2.06091	-4.4684	-7.56835
C	-2.26588	5.18355	1.82679	H	-1.48894	-3.87047	-6.01407
C	-2.71738	-3.22039	1.63389	H	-14.261	17.54022	9.62859
C	-7.93817	6.9223	0.85024	H	-14.0967	16.16132	8.53431
C	0.40736	1.05936	3.44283	H	-15.6898	16.59832	9.16633
C	-1.96479	0.21092	1.25626	H	-15.3124	19.65649	8.90953
C	5.80516	1.43616	2.15532	H	-16.7998	18.81059	8.47549
C	-4.21132	-2.14185	3.264	H	-16.0031	19.8743	7.2994
C	3.532	1.16296	1.32041	H	-5.75028	-6.00861	-2.81551
C	-11.7799	8.17178	5.31771	H	-5.89981	8.29997	3.2043
C	-14.0066	13.44994	-2.12764	H	4.55197	-1.60246	3.05076
C	-15.6382	17.18176	6.4532	H	-13.1185	19.06947	7.93537
C	-1.46267	-5.9745	-0.78992	H	-13.742	19.20052	6.28069
C	3.49461	-0.11135	1.90384	H	-12.9295	17.72138	6.80734
C	-3.37344	4.99661	0.97713	H	0.42644	5.42227	-1.2803
C	-14.2737	10.97191	5.70791	H	0.53948	1.70516	-3.43031
C	-2.75078	-0.76933	1.77425	H	-18.4774	19.40946	4.61214
C	-7.78032	-3.78879	-1.10236	H	-19.7801	19.03819	3.47613
C	-4.01809	-4.66615	3.21456	H	-18.0907	18.78152	3.0051
C	-3.84713	-6.2666	-1.87087	H	3.05577	-1.70887	-5.15053
C	-4.77554	-4.09719	-2.54768	H	-2.98024	-6.53806	-6.46175
C	-3.64902	-3.42708	-2.07919	H	-3.67449	-5.07483	-5.73282
C	-9.09961	8.67869	2.07123	H	-2.41089	-5.96415	-4.8867
C	-11.0352	9.28189	3.50979	H	-19.6249	17.84733	6.35627
C	0.97063	-4.38174	-4.63504	H	-19.9878	16.17292	5.9189
C	1.54581	3.17777	3.53852	H	-20.8962	17.5024	5.17739
C	5.44089	1.01782	-2.58506	H	-6.78433	-5.34749	2.43418
C	-8.78026	-3.24007	-0.08497	H	-6.73777	-3.6128	2.79497
C	-1.70379	-4.78119	-6.5822	H	-8.25951	-5.72783	4.45168
C	-14.7405	17.00455	8.80153	H	-8.99875	-4.57548	3.32787
N	-12.1501	9.98068	3.9216	H	-8.21938	-3.99338	4.80713
C	-15.8281	19.14059	8.09322				
C	-4.86211	-5.51119	-2.43555				
C	-6.79193	8.1265	2.61136				

C	-6.77041	7.13397	1.61058
C	-4.57638	5.72768	1.18681
C	5.73888	0.1649	2.72329
C	4.59035	-0.6151	2.605
C	-12.8259	13.56013	-1.37456

**Cogwheel 10:**

Calculation Type = FOPT. Calculation Method = RB3LYP. Basis Set = 6-31G(d,p). Charge = 0. Spin = Singlet. Electronic Energy = -19212.437 Hartree. RMS Gradient Norm = 9.1612302e-07 Hartree/Bohr. Dipole Moment = 4.3862226 Debye.



**Figure S9.** Frontier orbitals of cogwheel **10**.

Cartesian coordinates:

Ru	0.25605	0.78722	3.52121	H	-20.6307	-6.01092	1.65865
Ni	3.21941	-16.1961	-0.76392	N	-17.3802	-5.95475	0.87258
S	-3.09096	2.65291	11.44968	H	-12.5652	-2.40536	0.36967
S	6.58804	2.38131	10.04169	N	-14.8697	-4.82811	0.48514
N	4.66943	-17.2431	-1.56692	C	-12.5523	-6.63438	0.62556
N	0.1286	-0.80277	4.99196	C	-10.3272	-4.77436	1.93809
N	4.38385	-14.6151	-0.70932	H	-10.7549	-5.31423	2.77756
C	0.19482	-1.70059	7.0322	C	-9.05735	-4.21886	2.05091
S	1.54335	-4.71661	10.80008	H	-8.49533	-4.32316	2.97341
C	4.011	-13.3102	-0.45979	C	6.78917	-0.51005	0.01813
C	0.67278	1.79627	1.55653	C	7.94775	-0.66942	-0.31775
C	2.77061	0.22087	1.23329	C	9.30805	-0.83889	-0.70338
C	0.60214	-1.97573	1.52747	C	9.69524	-0.73243	-2.0544
N	2.05507	-17.7693	-0.82883	H	8.94202	-0.52013	-2.80635
N	-0.59149	1.76221	6.3437	C	11.02815	-0.88204	-2.42228
C	-4.1343	-1.82775	2.56829	H	11.31223	-0.78019	-3.46516
C	2.26644	-18.9351	-1.53456	C	12.02088	-1.14783	-1.4638
H	11.85401	-15.0286	-1.75241	C	13.45913	-1.29572	-1.84158
C	-4.81562	-1.80567	1.33541	C	13.8574	-2.36569	-2.64606
C	0.29526	-19.2362	-0.49554	C	12.9406	-3.27688	-3.28403

C	0.08268	-3.242	8.86636	C	13.67733	-4.06551	-4.10815
N	1.88312	1.59341	4.7343	H	13.33202	-4.84674	-4.76763
C	0.5231	-13.4301	0.95385	C	15.05765	-3.70081	-3.91373
C	3.46487	-20.5675	-2.98296	C	16.12967	-4.39987	-4.47059
N	1.86507	1.45692	6.09536	C	15.86978	-5.49137	-5.4624
C	5.8528	-18.8778	-2.70288	C	16.26725	-5.32242	-6.79917
C	5.152	-12.4355	-0.5653	H	16.74431	-4.38928	-7.07388
C	-4.2073	-1.14747	0.24678	C	16.05186	-6.32182	-7.75099
C	-0.74712	1.54905	1.60076	C	16.47515	-6.1695	-9.22505
C	4.22867	-22.877	-3.17696	C	17.48817	-7.28209	-9.58675
C	0.33763	-0.52266	1.67899	H	18.38495	-7.21209	-8.96222
C	1.16154	-19.8409	-1.34905	H	17.06353	-8.28112	-9.45041
C	6.54418	-15.6488	-1.32202	H	17.79658	-7.19147	-10.6346
C	2.87241	4.6012	0.23264	C	15.23095	-6.29354	-10.1367
C	2.74197	-12.8883	-0.05752	H	15.51833	-6.19022	-11.1893
C	0.6093	-15.6519	0.61825	H	14.73446	-7.26155	-10.0219
C	2.76054	-20.7015	-4.18063	H	14.49816	-5.51309	-9.90663
C	-0.14997	-2.73676	0.61391	C	17.13983	-4.80839	-9.50635
C	4.57173	-18.4759	-2.17962	H	18.04978	-4.66866	-8.91377
C	10.78028	-15.1488	-1.67415	H	17.42145	-4.74808	-10.5627
C	9.95776	-14.5258	-2.61747	H	16.46412	-3.97282	-9.29686
C	6.74065	-17.91	-2.35817	C	15.42247	-7.50721	-7.32777
C	4.98459	3.20462	9.6282	H	15.25002	-8.28762	-8.05909
N	-0.87938	1.91806	5.01435	H	21.33807	5.07151	-2.1896
C	1.32946	3.12143	1.4047	C	18.45521	5.34434	0.02935
C	8.56923	-14.6979	-2.48741	C	17.8966	4.47498	0.98533
C	4.41123	-0.15742	-0.53194	C	17.65302	4.98085	2.42057
C	-1.37346	2.61129	7.07705	C	18.99143	5.44942	3.03972
N	0.36056	-0.54975	6.31429	H	19.44554	6.26021	2.46327
C	1.91749	-3.96886	2.0147	H	19.71112	4.62518	3.08553
C	-1.61753	3.53727	0.35066	H	18.83038	5.81643	4.05986
C	10.27106	-15.933	-0.62258	C	16.66338	6.1703	2.38315
C	3.35539	2.26884	7.96498	H	16.4804	6.54161	3.39862
C	5.10217	-0.20448	1.78507	H	17.04628	7.00276	1.78637
C	5.72137	-23.8235	-1.32416	H	15.70208	5.86292	1.9569
C	-2.19518	3.33359	6.17162	C	17.06013	3.89036	3.33323
C	0.17175	-16.9755	0.56249	H	17.72664	3.02622	3.42331
C	2.94282	2.1087	6.62664	H	16.90779	4.29523	4.33918
C	2.25162	3.36412	0.37093	H	16.0895	3.53644	2.97031
C	2.95131	2.31364	4.39663	H	18.69387	6.35738	0.33032
C	1.66395	-7.29264	0.72751	C	17.58437	3.17344	0.58395
C	6.23163	-13.2228	-0.8058	H	17.16316	2.46344	1.28571
C	-2.46215	4.04735	10.41701	C	15.04477	1.7456	-0.80649
C	2.58936	5.65255	1.12547	H	15.1206	2.76711	-0.46635
C	-0.38134	-4.04085	6.59707	C	13.93441	0.96918	-0.89945
C	3.51338	-22.9689	-4.38544	H	12.91418	1.23347	-0.66521

C	4.19255	-21.6625	-2.48784	C	18.54149	0.45467	-1.3836
C	1.64249	-2.62295	2.21974	C	19.91284	0.74453	-1.04938
C	3.12749	-10.7022	1.15972	H	20.26583	1.69333	-0.67475
C	5.74534	-14.573	-0.93265	C	20.62066	-0.39403	-1.2667
C	5.25966	3.55118	7.13066	H	21.67703	-0.56452	-1.12417
C	1.03788	4.18168	2.285	C	21.49928	-3.06294	-2.04739
C	1.54508	-10.7602	-0.65826	C	22.40678	-3.09656	-3.11943
C	0.11925	-4.08422	0.40266	H	22.05162	-2.79856	-4.09857
C	0.31518	-1.9511	8.4138	C	23.73354	-3.49117	-2.93131
C	2.86674	-9.34966	1.35009	C	24.75973	-3.53015	-4.08091
C	-2.895	-1.20973	2.70745	C	24.14554	-3.10746	-5.42915
C	-0.1777	-2.09319	4.85967	H	24.90981	-3.15192	-6.21199
C	-2.63747	4.40297	-0.02377	H	23.7635	-2.0819	-5.39961
C	-0.2604	-4.27905	7.94984	H	23.32602	-3.76834	-5.73014
C	-1.82449	2.5295	1.31286	C	25.92751	-2.56624	-3.76229
C	-0.14792	-14.5814	1.21498	H	26.66931	-2.58684	-4.56879
C	8.88487	-16.0793	-0.53034	H	25.5679	-1.53726	-3.65829
C	2.77355	-21.904	-4.90762	H	26.43825	-2.83668	-2.8333
C	-1.82139	2.84934	4.8944	C	25.31023	-4.96819	-4.23428
C	-3.11344	2.42051	1.87123	H	25.8027	-5.31713	-3.32185
C	1.1587	-4.7286	1.10138	H	26.04556	-5.01015	-5.04588
C	0.84566	-17.94	-0.18959	H	24.50519	-5.67239	-4.46926
C	-0.15196	-2.73111	6.12213	C	24.13309	-3.85621	-1.63223
C	-4.77315	2.43825	10.74195	H	25.16005	-4.16414	-1.47779
C	0.18666	-3.55165	10.34053	C	23.26109	-3.83366	-0.54003
C	-3.11453	4.28153	6.66118	C	23.69475	-4.23403	0.88341
C	-2.35259	3.7651	8.93494	C	23.49183	-3.03396	1.83897
C	-1.44597	2.82361	8.46455	H	24.09803	-2.17758	1.52519
C	2.47737	-11.4324	0.15003	H	22.44767	-2.70983	1.87106
C	1.72473	-13.7969	0.24717	H	23.78838	-3.30426	2.8589
C	4.51277	2.99465	8.21039	C	25.17504	-4.65524	0.95263
C	-2.968	-0.53644	0.39515	H	25.84585	-3.84334	0.65258
C	1.64844	5.42162	2.15046	H	25.38275	-5.52364	0.31871
C	-5.48943	1.28177	11.43836	H	25.43084	-4.92976	1.98116
C	6.15305	0.60944	9.83083	C	22.83339	-5.42535	1.36663
C	0.48733	-21.7398	-5.95669	H	22.96289	-6.29306	0.71125
N	1.76762	-15.1597	0.04952	H	21.7682	-5.17753	1.38468
C	2.11803	-23.3878	-6.89089	H	23.12438	-5.71958	2.3815
C	-3.182	4.48233	8.02739	C	21.93635	-3.4268	-0.77237
C	1.27634	-9.4081	-0.47494	H	21.223	-3.39379	0.04536
C	1.9355	-8.67662	0.53351	H	20.60194	-5.06385	-3.63268
C	1.43152	-6.11025	0.89715	N	17.87317	-3.17656	-3.21234
C	-3.92022	4.29759	0.54949	H	11.87153	-3.28633	-3.137
C	-4.137	3.2866	1.50693	N	15.1532	-2.64699	-3.02719
C	8.02469	-15.4623	-1.45348	C	14.35373	-0.29782	-1.4449
C	5.44093	-0.29473	0.42155	C	11.6319	-1.25093	-0.1175

C	2.51959	-20.9431	-7.22441	H	12.3862	-1.4548	0.63648
C	1.98768	-22.0026	-6.22962	C	10.30213	-1.10136	0.26063
C	3.10529	0.09089	-0.12742	H	10.018	-1.18759	1.30447
C	3.79002	0.04415	2.17866	C	3.2674	6.89828	1.00817
C	6.08178	-24.5054	-3.702	C	3.89044	7.93866	0.90738
C	-2.28621	-0.5561	1.62591	C	4.66863	9.12502	0.79422
C	5.00937	-24.1019	-2.66159	C	5.54103	9.30462	-0.29879
B	0.60556	0.89037	6.78046	H	5.58228	8.54544	-1.07307
C	3.6816	2.67139	5.55476	C	6.34482	10.43559	-0.38435
C	4.86029	3.40209	5.81955	H	7.01126	10.5578	-1.23282
C	1.34503	0.49479	1.58378	C	6.31204	11.42504	0.61273
C	-0.9645	0.12209	1.74391	C	7.20575	12.62166	0.54864
C	5.99503	-16.8825	-1.67617	C	8.58556	12.44849	0.67067
C	3.42701	-19.2716	-2.23302	C	9.2261	11.15856	0.72346
C	5.29674	0.02406	10.95294	C	10.56396	11.38106	0.68368
C	4.03338	-25.2836	-2.44838	H	11.35704	10.64937	0.6775
C	3.01376	-3.75124	10.27013	C	10.75051	12.81006	0.68894
C	4.28461	-4.56789	10.50219	C	11.99699	13.42835	0.79332
H	-4.59306	-2.32356	3.41773	C	13.23237	12.58652	0.7593
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H	6.0362	-19.7915	-3.24754	C	15.27052	11.89585	-0.37721
H	5.12547	-11.3637	-0.44307	C	15.54948	10.99286	0.66211
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H	-0.95014	-2.26802	0.05406	C	12.13097	14.79991	1.01555
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H	5.19072	4.26293	9.81836	C	13.08703	16.71452	1.70388
H	7.8927	-14.2395	-3.20204	C	11.68494	16.90668	1.43405
H	4.64874	-0.24833	-1.58689	C	11.04589	18.14442	1.50859
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H	7.26247	-12.9249	-0.9206	C	4.62608	19.73393	-2.51665
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H	-0.41815	-5.28037	8.33933	C	12.83685	19.89975	1.23076
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H	-4.94647	0.34134	11.30451	H	15.89271	22.17413	2.62944
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H	12.91662	-17.9936	0.31427	C	-15.3468	7.68471	-4.50306
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C	-11.0771	-4.63975	0.75767	H	-10.9405	19.60077	2.08465
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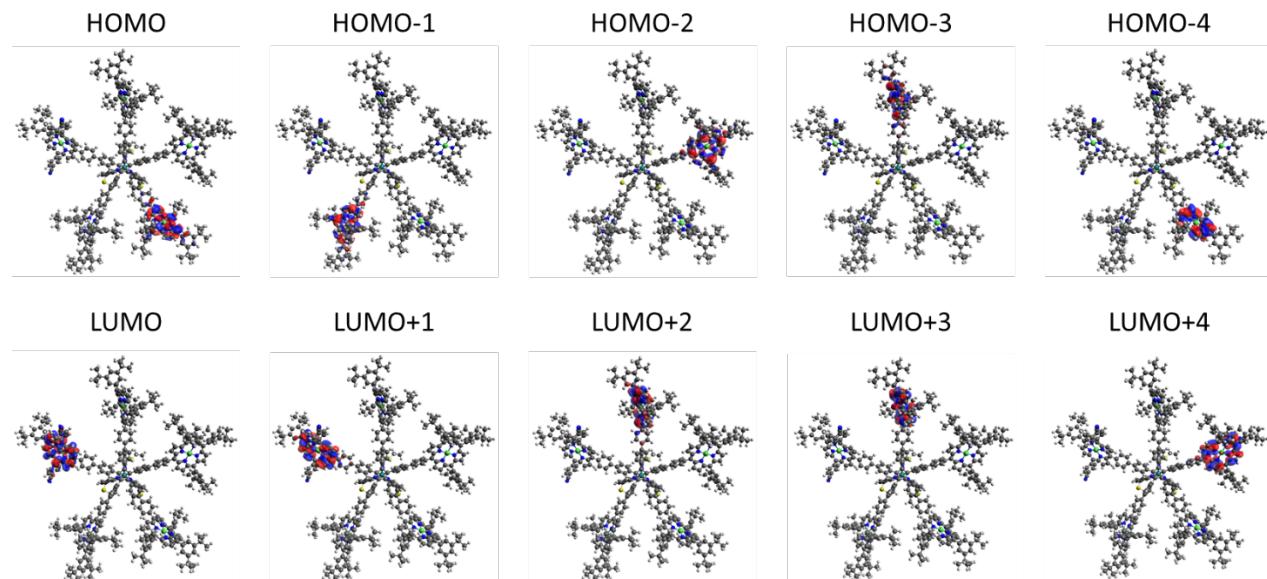
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C	-18.9894	2.39091	0.91106	C	-16.4061	14.83102	-5.87211
H	-18.5197	2.79079	0.00619	H	-16.9185	14.38266	-5.0295
H	-20.0438	2.19327	0.69088	C	-17.0754	15.70363	-6.73342
C	-18.9737	0.67188	2.72473	C	-18.5599	16.07532	-6.55069
H	-18.4804	-0.19549	3.17308	C	-19.1921	15.38252	-5.32846
H	-18.9708	1.47756	3.46766	H	-20.2428	15.67785	-5.24067
H	-20.0149	0.39772	2.52516	H	-18.692	15.66324	-4.39583
C	-17.6584	-1.23765	0.72537	H	-19.1629	14.29154	-5.41662
H	-17.1769	-1.36822	1.68956	C	-18.6902	17.60499	-6.35562
C	-17.8099	-4.68388	0.55653	H	-19.7422	17.88455	-6.22802
C	-19.2229	-4.5543	0.80806	H	-18.1415	17.93434	-5.46703
H	-19.7956	-3.65363	0.64549	H	-18.3007	18.16112	-7.21347
C	-19.6413	-5.73877	1.32378	C	-19.3558	15.65084	-7.80816
C	-18.4999	-6.61852	1.33109	H	-18.9838	16.14202	-8.71219
C	-18.5597	-7.9661	1.68751	H	-20.4136	15.91542	-7.69711
C	-17.4812	-8.82807	1.4808	H	-19.2914	14.56905	-7.96547
N	-16.2279	-8.4653	1.034	C	-16.3476	16.25869	-7.80244
Ni	-15.5509	-6.6503	0.75406	H	-16.8596	16.93584	-8.4752
N	-13.7261	-7.35556	0.62684	C	-14.9977	15.9726	-8.02599
C	-13.3507	-8.67182	0.44251	C	-14.1996	16.57538	-9.19859
C	-14.2024	-9.77618	0.48967	C	-12.9901	17.36702	-8.64647
C	-13.6531	-11.1471	0.24473	H	-13.3204	18.1848	-7.99733
C	-14.0448	-11.8611	-0.88946	H	-12.3163	16.7309	-8.06531

H	-14.7374	-11.3906	-1.58036	H	-12.4105	17.80011	-9.46964
C	-13.558	-13.1536	-1.14707	C	-15.0464	17.53401	-10.0569
C	-14.0147	-13.8967	-2.41762	H	-15.4195	18.38251	-9.47377
C	-13.6048	-13.0777	-3.66511	H	-15.9038	17.02666	-10.5113
H	-14.0555	-12.081	-3.66417	H	-14.4339	17.93683	-10.87
H	-12.518	-12.9523	-3.71088	C	-13.6908	15.43436	-10.1117
H	-13.9272	-13.5884	-4.57969	H	-14.5278	14.86312	-10.5267
C	-13.3887	-15.299	-2.53844	H	-13.046	14.73608	-9.57032
H	-12.296	-15.2552	-2.5951	H	-13.1117	15.84432	-10.9472
H	-13.7463	-15.7834	-3.45278	C	-14.3622	15.09103	-7.13494
H	-13.6628	-15.9427	-1.696	H	-13.3153	14.83748	-7.26978
C	-15.5535	-14.0579	-2.39427	H	-16.329	12.20668	-6.62515
H	-16.0649	-13.0919	-2.34966	N	-14.0613	11.25808	-4.35673
H	-15.8961	-14.5744	-3.29816	H	-10.8159	6.61247	-2.3707
H	-15.8727	-14.6453	-1.52685	N	-12.3315	9.5151	-3.05758
C	-12.6662	-13.7067	-0.22362	C	-10.0749	10.70971	-1.59314
C	-12.2498	-13.0221	0.93351	C	-7.7757	8.55073	-2.0221
C	-11.2692	-13.704	1.90796	H	-7.60803	9.27939	-2.80953
C	-11.9047	-15.0058	2.452	C	-6.73353	7.72629	-1.6124
H	-12.1426	-15.7106	1.64968	H	-5.7563	7.80906	-2.07709
H	-12.832	-14.7915	2.99344	H	15.94722	11.969	-1.22203
H	-11.2166	-15.5068	3.14237	H	14.89447	10.20681	2.5632
C	-9.95728	-14.0474	1.16232	N	17.65889	9.48105	0.56657
H	-9.25003	-14.5364	1.84219	N	1.54786	21.4326	-2.69954
H	-10.1308	-14.7236	0.32006	H	2.3663	19.38425	0.0141
H	-9.48091	-13.1424	0.77102	H	4.748	20.24069	-3.46811
C	-10.915	-12.8057	3.10838	H	13.65776	-10.9304	-6.29793
H	-11.7986	-12.5499	3.70208	H	12.39531	-12.9918	-4.61024
H	-10.2159	-13.3307	3.76747	H	-18.9541	3.1753	1.67403
H	-10.4342	-11.8741	2.7927	H	-16.0761	2.80274	-7.79234
H	-12.2779	-14.7026	-0.40004				
C	-12.7573	-11.739	1.15121				
H	-12.4754	-11.1751	2.03201				
C	-11.922	-8.76541	0.28166				
H	-11.3813	-9.67978	0.09147				
C	-11.4246	-7.51095	0.43365				
H	-10.3954	-7.1894	0.37994				
C	-15.5485	-9.6492	0.84079				
C	-16.3931	-10.7704	1.16637				
H	-16.0935	-11.8053	1.09951				
C	-17.5798	-10.2615	1.58723				
H	-18.4586	-10.7942	1.91762				
C	-19.8366	-8.53108	2.22881				
C	-20.9596	-8.69832	1.40128				
H	-20.875	-8.40761	0.36103				
C	-22.151	-9.23152	1.89886				

C	-23.4027	-9.42916	1.02122
C	-23.1779	-8.97003	-0.43207
H	-24.0931	-9.12558	-1.0125
H	-22.3776	-9.53587	-0.91996
H	-22.9275	-7.90572	-0.48912
C	-23.7857	-10.9282	0.99749
H	-24.6797	-11.0837	0.38283
H	-22.9751	-11.5319	0.57605
H	-24.0003	-11.3108	1.9997
C	-24.5773	-8.60958	1.60706
H	-24.8194	-8.91554	2.62908
H	-25.4778	-8.74399	0.99701
H	-24.3374	-7.54126	1.6269
C	-22.1907	-9.599	3.25693
H	-23.1109	-10.0134	3.65087
C	-21.094	-9.45097	4.11091
C	-21.1339	-9.84616	5.59991
C	-20.0533	-10.9187	5.87665
H	-20.2364	-11.8205	5.28285
H	-19.0491	-10.5585	5.63525
H	-20.0598	-11.2026	6.93517
C	-22.4989	-10.4229	6.0207
H	-22.7488	-11.3315	5.46275
H	-23.309	-9.69985	5.87911
H	-22.4753	-10.686	7.08324
C	-20.8509	-8.59753	6.46909
H	-21.6057	-7.82285	6.29822
H	-19.8713	-8.1624	6.25074
H	-20.8689	-8.86147	7.53264
C	-19.9149	-8.91162	3.56964
H	-19.0386	-8.77596	4.19595

**Cogwheel 11:**

Calculation Type = FOPT. Calculation Method = RB3LYP. Basis Set = 6-31G(d,p). Charge = 0. Spin = Singlet. Electronic Energy = -18831.664 Hartree. RMS Gradient Norm = 5.3695219e-07 Hartree/Bohr. Dipole Moment = 5.8497631 Debye.



**Figure S10.** Frontier orbitals of cogwheel 11.

Cartesian coordinates:

Ru	0.37119	-0.85672	3.24783	C	1.83988	7.02041	1.72382
Ni	-12.8688	5.52428	-0.61634	H	2.16881	6.56492	2.65315
S	3.95158	0.92858	11.12307	C	-4.69293	-5.3497	-0.21428
S	-2.08947	-6.74132	9.87993	C	-4.56121	-6.14847	-1.36281
N	-14.077	5.69259	-2.14879	H	-3.63926	-6.11288	-1.9358
N	-0.83856	0.20617	4.70463	C	-5.5781	-7.01375	-1.75973
N	-11.8918	4.09224	-1.53812	H	-5.44414	-7.6337	-2.64113
C	-1.56837	0.74098	6.74312	C	-6.76981	-7.11396	-1.02455
S	-4.71272	1.67098	10.56944	C	-7.87679	-8.03228	-1.43172
C	-10.672	3.55283	-1.18547	C	-8.57201	-7.79456	-2.61938
C	0.94621	-1.81901	1.30139	C	-8.18427	-6.80682	-3.59494
C	-1.56038	-2.61419	0.99753	C	-8.97897	-6.99132	-4.68067
C	-2.09091	0.42018	1.25121	H	-8.96426	-6.45539	-5.6172
N	-13.8481	6.94525	0.30618	C	-9.91583	-8.03245	-4.34209
N	1.674	-0.69285	6.06563	C	-10.9987	-8.39377	-5.14561
C	0.7485	4.22802	2.16123	C	-11.1239	-7.82303	-6.52451
C	-14.7679	7.81556	-0.23933	C	-10.9705	-8.66645	-7.63732
H	-14.645	0.629	-7.6716	H	-10.7552	-9.71281	-7.45675
C	1.10658	4.75414	0.90939	C	-11.0841	-8.17503	-8.9399
C	-14.6657	8.36882	1.93803	C	-10.9134	-9.07078	-10.1825

C	-2.69996	1.80694	8.56991	C	-12.213	-9.04231	-11.0222
N	0.07586	-2.61771	4.49154	H	-13.0612	-9.42189	-10.4429
C	-9.89685	4.76677	2.29124	H	-12.4623	-8.03057	-11.3555
C	-16.2093	8.84608	-1.98689	H	-12.1036	-9.66929	-11.9144
N	-0.02429	-2.49874	5.85065	C	-9.73795	-8.54439	-11.0403
C	-15.5825	6.53338	-3.69372	H	-9.6091	-9.16731	-11.9328
C	-10.2882	2.52857	-2.1236	H	-9.90433	-7.51584	-11.374
C	1.2867	3.84756	-0.15007	H	-8.80099	-8.56448	-10.474
C	1.5658	-0.51577	1.3154	C	-10.6159	-10.536	-9.81164
C	-18.4697	9.55477	-2.57483	H	-11.4265	-10.9814	-9.22571
C	-0.74975	-0.20111	1.402	H	-10.5022	-11.1313	-10.7236
C	-15.2633	8.71748	0.76926	H	-9.68797	-10.6311	-9.23848
C	-13.4021	3.70161	-3.45458	C	-11.3622	-6.80525	-9.10339
C	2.02139	-5.23828	0.01912	H	-11.4509	-6.41503	-10.1102
C	-9.94271	3.86662	-0.03699	C	-11.5289	-5.93514	-8.02184
C	-11.8441	5.88673	2.18319	C	-11.8451	-4.43662	-8.19631
C	-15.7481	10.14591	-2.20348	C	-10.7364	-3.59443	-7.52092
C	-2.29277	1.44613	0.31177	H	-9.76111	-3.79229	-7.97818
C	-14.9499	6.72876	-2.41397	H	-10.6548	-3.80872	-6.45138
C	-14.3848	1.25163	-6.82406	H	-10.9504	-2.52485	-7.62926
C	-13.2059	2.00144	-6.86999	C	-11.9262	-4.01971	-9.67694
C	-15.1381	5.3441	-4.17578	H	-10.9827	-4.19762	-10.2036
C	-0.45889	-5.98353	9.446	H	-12.7214	-4.55234	-10.2089
N	1.96255	-0.56349	4.73362	C	-13.2057	-4.11984	-7.53074
C	1.65322	-3.12078	1.17083	H	-13.202	-4.35779	-6.46319
C	-12.8966	2.79972	-5.75587	H	-13.4425	-3.05446	-7.63278
C	-2.85898	-3.71207	-0.75156	H	-14.0127	-4.69379	-7.99804
C	2.82309	-0.54822	6.79251	C	-11.4062	-6.47068	-6.72847
N	-0.75393	-0.09658	6.03432	H	-11.5382	-5.83381	-5.85939
C	-4.47219	0.51843	1.76012	C	-12.0261	-9.21071	-4.66803
C	3.70342	-0.98372	0.09294	C	-13.299	-9.34567	-5.33001
C	-15.2559	1.27362	-5.71891	H	-13.5423	-8.91231	-6.28842
C	-0.24782	-4.14743	7.74926	C	-14.1051	-10.0512	-4.49495
C	-3.32835	-4.19022	1.55517	C	-13.309	-10.4091	-3.34816
C	-20.347	7.81516	-2.49895	C	-13.7487	-11.2509	-2.32552
C	3.88577	-0.31429	5.8798	C	-12.8733	-11.7443	-1.35559
C	-12.8725	6.7468	2.56965	N	-11.5532	-11.3797	-1.19663
C	-0.13325	-3.74399	6.40374	Ni	-10.6002	-9.9576	-2.13927
C	1.33046	-4.03512	0.15392	N	-9.15976	-10.0556	-0.81808
C	0.02964	-3.91076	4.17633	C	-8.92396	-11.0716	0.08677
C	-11.3094	2.40247	-3.00973	C	-9.77894	-12.1439	0.34686
C	4.63615	-0.46579	10.12474	C	-9.37208	-13.1966	1.32996
C	3.06826	-5.57977	0.8894	C	-9.1242	-14.4981	0.88873
C	-3.10992	2.58713	6.28391	H	-9.22437	-14.7096	-0.17134
C	-17.9645	10.851	-2.7874	C	-8.74651	-15.5158	1.7807
C	-17.573	8.5625	-2.17194	C	-8.47682	-16.9352	1.24399

C	-3.21142	-0.03005	1.97136	C	-7.3136	-16.8854	0.22462
C	-8.43775	1.88172	0.42984	H	-7.53779	-16.2254	-0.61837
C	-12.2851	3.40753	-2.67056	H	-6.395	-16.5223	0.69734
C	-0.33482	-6.45602	6.95699	H	-7.11572	-17.8854	-0.17787
C	2.69739	-3.46795	2.04805	C	-8.09257	-17.9246	2.36018
C	-7.44326	4.05373	0.14417	H	-7.17691	-17.6206	2.87795
C	-3.55531	1.99483	0.10297	H	-7.91264	-18.9143	1.92808
C	-1.81481	0.83428	8.1275	H	-8.88873	-18.0298	3.10465
C	-7.17476	1.33142	0.63591	C	-9.74875	-17.4714	0.54462
C	0.57134	2.85799	2.34758	H	-10.0552	-16.8362	-0.29159
C	-1.69748	1.21466	4.55845	H	-9.57081	-18.4781	0.14957
C	5.01233	-0.66944	-0.25826	H	-10.5873	-17.5265	1.24696
C	-3.34499	2.67411	7.63994	C	-8.62774	-15.1814	3.13272
C	2.99045	-0.21021	1.02754	C	-8.87354	-13.8836	3.61861
C	-10.7673	5.48089	3.05053	C	-8.72368	-13.5967	5.12544
C	-14.909	2.07801	-4.63099	C	-9.69165	-14.5019	5.92416
C	-16.6161	11.1737	-2.60946	H	-9.49388	-15.5639	5.75137
C	3.26821	-0.3456	4.60553	H	-10.7319	-14.3059	5.64391
C	3.64583	0.91245	1.56724	H	-9.5885	-14.315	6.99912
C	-4.67455	1.54366	0.8208	C	-7.26858	-13.8925	5.56122
C	-13.7694	7.28023	1.64135	H	-7.14394	-13.6992	6.63271
C	-2.2053	1.60773	5.81927	H	-6.99058	-14.9344	5.37686
C	4.85678	2.3487	10.38813	H	-6.56115	-13.2574	5.0177
C	-2.9668	1.96238	10.04836	C	-9.0395	-12.1307	5.47795
C	5.19482	-0.12157	6.36201	H	-10.0688	-11.8611	5.21971
C	4.33991	-0.41168	8.64294	H	-8.91893	-11.9776	6.55525
C	3.04387	-0.59915	8.17962	H	-8.36581	-11.4337	4.96887
C	-8.5954	3.25302	0.17577	H	-8.3368	-15.9488	3.83996
C	-10.4697	4.67626	0.97164	C	-9.24862	-12.9018	2.69837
C	-0.34485	-5.50544	8.01974	H	-9.46026	-11.8906	3.02453
C	1.10399	2.48017	0.03467	C	-7.70178	-10.8218	0.80825
C	3.38993	-4.66504	1.9082	H	-7.27653	-11.4809	1.54958
C	4.41004	3.65196	11.0496	C	-7.23348	-9.61851	0.38678
C	-3.22455	-5.31599	9.64986	H	-6.34044	-9.10112	0.70372
C	-15.405	13.11099	-1.54212	C	-11.0505	-12.2209	-0.22721
N	-11.659	5.36948	0.91671	C	-12.0714	-13.1343	0.22019
C	-17.1505	13.59259	-3.26431	H	-11.9298	-13.8928	0.97504
C	5.4035	-0.17187	7.72787	C	-13.2062	-12.8207	-0.45752
C	-6.18038	3.50337	0.34973	H	-14.1792	-13.2827	-0.38619
C	-6.01915	2.13009	0.59945	C	-15.1724	-11.7141	-2.30866
C	5.67512	0.4346	0.30294	C	-15.6522	-12.6125	-3.27629
C	4.9575	1.2215	1.21891	H	-14.9624	-12.9626	-4.03475
C	-13.7301	2.84243	-4.63595	C	-16.9781	-13.0523	-3.2599
C	-3.61644	-4.41643	0.20049	C	-17.5393	-14.0365	-4.30476
C	-14.9938	12.54244	-3.96735	C	-16.4795	-14.4604	-5.33959
C	-16.058	12.5908	-2.84504	H	-16.9259	-15.1528	-6.06085

C	-1.85657	-2.8304	-0.36001	H	-15.6328	-14.9728	-4.87123
C	-2.32616	-3.303	1.94648	H	-16.0922	-13.6041	-5.90134
C	-20.3475	9.59249	-4.25635	C	-18.0517	-15.311	-3.59237
C	0.73434	1.95765	1.28628	H	-18.457	-16.0198	-4.32346
C	-19.9714	9.28108	-2.78794	H	-17.2407	-15.8088	-3.05056
B	0.26509	-1.13726	6.5136	H	-18.8444	-15.0854	-2.87309
C	-0.11308	-4.69135	5.34844	C	-18.7101	-13.3679	-5.06441
C	-0.21804	-6.069	5.63866	H	-19.5198	-13.0742	-4.39006
C	-0.50303	-1.61356	1.33102	H	-19.1278	-14.0586	-5.80583
C	0.52964	0.48932	1.44114	H	-18.3718	-12.4693	-5.59095
C	-14.1846	4.83562	-3.22231	C	-17.8193	-12.5686	-2.24028
C	-15.2572	7.7778	-1.54648	H	-18.8491	-12.9045	-2.22086
C	-3.14688	-4.2532	10.74538	C	-17.3781	-11.6781	-1.25731
C	-20.8016	10.18411	-1.84471	C	-18.2958	-11.1424	-0.1415
C	-4.91524	-0.09625	10.10922	C	-17.7057	-11.522	1.23764
C	-6.346	-0.5493	10.39814	H	-17.636	-12.6094	1.34814
H	0.58558	4.9008	2.99797	H	-16.7039	-11.1072	1.38208
H	-14.7903	8.81389	2.91353	H	-18.343	-11.1396	2.04304
H	-8.97153	4.3008	2.59491	C	-19.723	-11.716	-0.22491
H	-16.284	7.21796	-4.14564	H	-19.7315	-12.8067	-0.12701
H	-9.36938	1.96396	-2.08157	H	-20.2151	-11.4522	-1.1669
H	1.59832	4.21583	-1.12305	H	-20.3312	-11.308	0.58891
H	-15.9923	9.49417	0.5947	C	-18.3899	-9.60158	-0.25163
H	1.76252	-5.90677	-0.7967	H	-18.8163	-9.3042	-1.21542
H	-14.6918	10.34855	-2.05575	H	-17.4094	-9.12541	-0.1599
H	-1.45817	1.80914	-0.27573	H	-19.031	-9.20067	0.54176
H	-15.3916	4.8625	-5.10803	C	-16.0373	-11.2614	-1.31042
H	-0.23837	-5.1741	10.14699	H	-15.6507	-10.5686	-0.56949
H	0.25357	-6.79011	9.64667	H	-15.1396	-10.3243	-4.63673
H	-11.9982	3.40901	-5.75423	N	-12.0433	-9.86994	-3.45832
H	-3.08226	-3.82944	-1.80783	H	-7.38676	-6.0909	-3.46837
H	-5.30789	0.16727	2.35797	N	-9.64608	-8.52646	-3.08209
H	3.22237	-1.8304	-0.38134	C	-8.12978	-9.15808	-0.64369
H	-0.2467	-3.41711	8.55152	C	-6.89792	-6.32678	0.13057
H	-3.88391	-4.72816	2.31763	H	-7.81358	-6.38507	0.71152
H	-19.8155	7.11992	-3.15697	C	-5.88187	-5.46066	0.52619
H	-21.4196	7.67056	-2.66413	H	-6.02553	-4.83832	1.40443
H	-20.1327	7.53535	-1.46233	C	3.80855	-6.85679	0.74112
H	0.54173	-3.8009	-0.55064	C	3.15766	-8.03343	0.33203
H	0.10162	-4.22821	3.14862	H	2.08881	-8.01515	0.14115
H	-11.3917	1.71649	-3.83857	C	3.85443	-9.23111	0.18977
H	5.71474	-0.52444	10.29952	H	3.32789	-10.1251	-0.13131
H	4.18488	-1.35242	10.58088	C	5.23092	-9.30097	0.45474
H	-18.6534	11.62656	-3.0999	C	5.9988	-10.5744	0.29564
H	-17.9134	7.55095	-1.98617	C	5.75384	-11.6425	1.16013
H	-3.08649	-0.79637	2.72618	C	4.68276	-11.661	2.12395

H	-9.31559	1.24341	0.46619	C	4.65256	-12.9097	2.65573
H	-0.42879	-7.50904	7.20541	H	3.9658	-13.3013	3.39046
H	2.94819	-2.79538	2.8612	C	5.75751	-13.6357	2.08113
H	-7.54389	5.11941	-0.03972	C	6.14715	-14.9122	2.48928
H	-3.67833	2.76569	-0.65193	C	5.29815	-15.6662	3.46209
H	-1.31469	0.17492	8.82888	C	4.63284	-16.8341	3.05447
H	-7.0816	0.26324	0.80834	H	4.73415	-17.1707	2.02751
H	0.30834	2.47706	3.32797	C	3.84394	-17.5574	3.94344
H	-1.91956	1.60918	3.581	C	3.70795	-17.1221	5.27215
H	5.5186	-1.27541	-1.00369	C	2.89731	-17.8632	6.19407
H	-4.04431	3.41179	8.02195	C	4.37348	-15.9589	5.69394
H	-10.6922	5.72919	4.09823	C	5.15905	-15.2443	4.79488
H	-15.5436	2.12726	-3.75426	H	5.68084	-14.3527	5.12757
H	3.7112	-0.2219	3.63136	C	7.3563	-15.4833	2.08665
H	3.12824	1.545	2.27813	C	7.93314	-16.6429	2.71985
H	4.65748	2.37126	9.31272	H	7.4576	-17.2279	3.49273
H	5.93157	2.19278	10.5324	C	9.17789	-16.7966	2.1999
H	-2.77216	2.99043	10.37195	C	9.34368	-15.7715	1.20113
H	-2.30942	1.30891	10.62966	C	10.45058	-15.6833	0.35627
H	6.0194	0.06096	5.67921	C	10.47452	-14.8044	-0.72832
H	2.22615	-0.76565	8.87212	N	9.5192	-13.8544	-1.02366
H	1.26241	1.80194	-0.79939	Ni	7.9696	-13.3549	0.06307
H	4.16975	-4.91136	2.62269	N	7.71843	-11.752	-1.03757
H	3.33987	3.82482	10.90136	C	8.28637	-11.4851	-2.26638
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H	4.60693	3.64122	12.12605	C	9.76873	-11.857	-4.24062
H	-4.22072	-5.76819	9.62021	C	9.53516	-12.6951	-5.34362
H	-3.03568	-4.88418	8.66211	H	8.98586	-13.6201	-5.19942
H	-14.9964	14.11622	-1.69594	C	9.9889	-12.3525	-6.6134
H	-14.5856	12.4672	-1.20956	C	10.69551	-11.1534	-6.8042
H	-16.1388	13.16382	-0.73087	C	10.94095	-10.3094	-5.7081
H	-16.704	14.58023	-3.41872	C	11.16652	-10.7942	-8.1101
H	-17.9251	13.69754	-2.49728	C	10.48135	-10.6633	-4.4435
H	-17.6343	13.30028	-4.20218	H	10.68244	-10.0141	-3.59737
H	6.40631	-0.03205	8.12264	C	7.76801	-10.2503	-2.79963
H	-5.30897	4.15156	0.33988	H	8.02328	-9.83202	-3.76133
H	5.43919	2.07617	1.68444	C	6.93069	-9.7373	-1.86213
H	-14.5762	13.54082	-4.14071	H	6.35847	-8.82307	-1.90637
H	-15.4323	12.19021	-4.90692	C	9.8871	-13.3295	-2.24327
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H	-1.30697	-2.27724	-1.1172	H	11.58069	-13.737	-3.65531
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H	-19.7826	8.95831	-4.94767	C	11.60852	-16.6119	0.55366
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H	-3.87451	-3.45551	10.55266	C	12.56247	-18.8555	0.45588
H	-2.15601	-3.79016	10.78913	C	12.46565	-20.3665	0.16894
H	-20.6142	11.24643	-2.02682	C	11.06551	-20.7815	-0.32217
H	-20.5636	9.97802	-0.79595	H	11.04699	-21.8595	-0.51219
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H	-4.19803	-0.69371	10.68312	H	10.29047	-20.5651	0.42046
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H	-6.59317	-0.44081	11.45868	H	13.43359	-21.825	-1.13853
H	-6.46794	-1.60395	10.12942	H	13.29395	-20.2093	-1.85448
H	-7.06936	0.03263	9.81916	H	14.51767	-20.5292	-0.61869
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C	-16.5403	0.42269	-5.74653	H	12.71302	-22.2337	1.27675
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H	-15.6062	-1.26369	-6.81319	C	13.78006	-18.3119	0.90629
H	-15.5504	-1.4052	-5.05151	H	14.62098	-18.9807	1.04278
H	-17.0703	-1.69083	-5.91884	C	13.94531	-16.9511	1.17961
C	-17.3772	0.58319	-4.46289	C	15.27795	-16.352	1.66989
H	-18.2803	-0.03196	-4.53273	C	15.75776	-15.2773	0.66504
H	-16.8267	0.2604	-3.57329	H	15.92659	-15.7143	-0.32487
H	-17.6952	1.61972	-4.31046	H	15.03057	-14.4677	0.55336
C	-17.4173	0.85121	-6.94737	H	16.70023	-14.8329	1.00432
H	-18.3306	0.24677	-6.98668	C	16.3882	-17.4115	1.80231
H	-16.8951	0.72608	-7.90052	H	16.60653	-17.8961	0.84492
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H	-20.1437	10.63508	-4.51821	H	17.31116	-16.9347	2.14775
C	-12.1243	3.41869	-8.65336	C	15.06702	-15.6985	3.05661
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H	-13.0959	3.79312	-8.99241	H	16.0032	-15.2565	3.41584
C	-12.2526	1.98663	-8.08077	C	12.83469	-16.1103	0.9941
C	-10.8583	1.48963	-7.63011	H	12.9144	-15.047	1.19802
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C	-12.7482	1.06377	-9.21043	H	4.02689	-10.8306	2.33547
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H	-13.7235	1.37797	-9.59659	C	6.8837	-10.6865	-0.77889
H	-10.9162	0.47209	-7.22837	C	5.88534	-8.12714	0.85838
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H	-11.2026	8.38364	3.93057	H	5.72505	-6.03347	1.29479
C	-12.1158	8.46853	5.88786	C	7.07716	0.75533	-0.05928
C	-11.0879	9.4167	6.53615	C	7.51089	2.0855	-0.19135
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H	-12.2535	11.23163	6.14772	C	8.82963	2.38235	-0.52833
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H	-9.92707	7.80388	7.46195	C	11.1654	3.30828	-4.27678
C	-9.96052	9.81157	5.56325	H	10.75421	3.79873	-5.14575
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H	-13.2901	8.32597	7.67763	H	14.09647	6.11572	-5.439
C	-14.1801	7.1489	6.12296	C	13.26074	6.37253	-7.41675
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C	-15.3677	7.1763	8.39307	C	12.338	8.6899	-7.78446
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C	-16.6954	7.07758	6.27768	C	14.3775	8.42194	-6.36451
H	-16.7848	6.68919	5.25896	H	15.31873	7.89295	-6.18257
H	-17.5555	6.71214	6.85016	H	14.61932	9.47622	-6.53436
H	-16.7621	8.16948	6.22587	H	13.77277	8.36503	-5.45354
C	-14.0442	6.74992	4.78262	C	12.5798	5.70246	-8.45011
H	-14.7752	6.08485	4.33344	H	12.33388	6.25715	-9.34755
C	1.29028	6.21366	0.71301	C	12.21399	4.3559	-8.36405
C	0.91197	6.83857	-0.48761	C	11.48154	3.61355	-9.49875
H	0.45221	6.24962	-1.27582	C	10.12882	3.07655	-8.97296
C	1.07588	8.20986	-0.66966	H	9.48827	3.89672	-8.63158
H	0.75612	8.67175	-1.59906	H	10.26172	2.3856	-8.13517
C	1.62536	9.01267	0.34197	H	9.59743	2.53889	-9.76637
C	1.78946	10.48956	0.17265	C	11.19849	4.52083	-10.7112
C	2.72169	10.98053	-0.74313	H	10.55885	5.36962	-10.4473
C	3.44769	10.15042	-1.67103	H	12.12132	4.91138	-11.1526
C	4.12826	10.98521	-2.49809	C	12.35074	2.42702	-9.97949
H	4.76258	10.72827	-3.33258	H	12.55266	1.71619	-9.17302
C	3.88811	12.32651	-2.02919	H	11.84255	1.88307	-10.7838
C	4.54436	13.45144	-2.53039	H	13.31423	2.77827	-10.3634
C	5.43187	13.32138	-3.72969	C	12.54519	3.66489	-7.18637
C	5.05032	13.92189	-4.94092	H	12.28893	2.61568	-7.07799
H	4.1072	14.45443	-4.96952	C	14.90974	3.17583	-4.69938
C	5.85698	13.83526	-6.07796	C	15.91458	3.29282	-5.72575
C	5.46894	14.48119	-7.42236	H	15.75619	3.74962	-6.691
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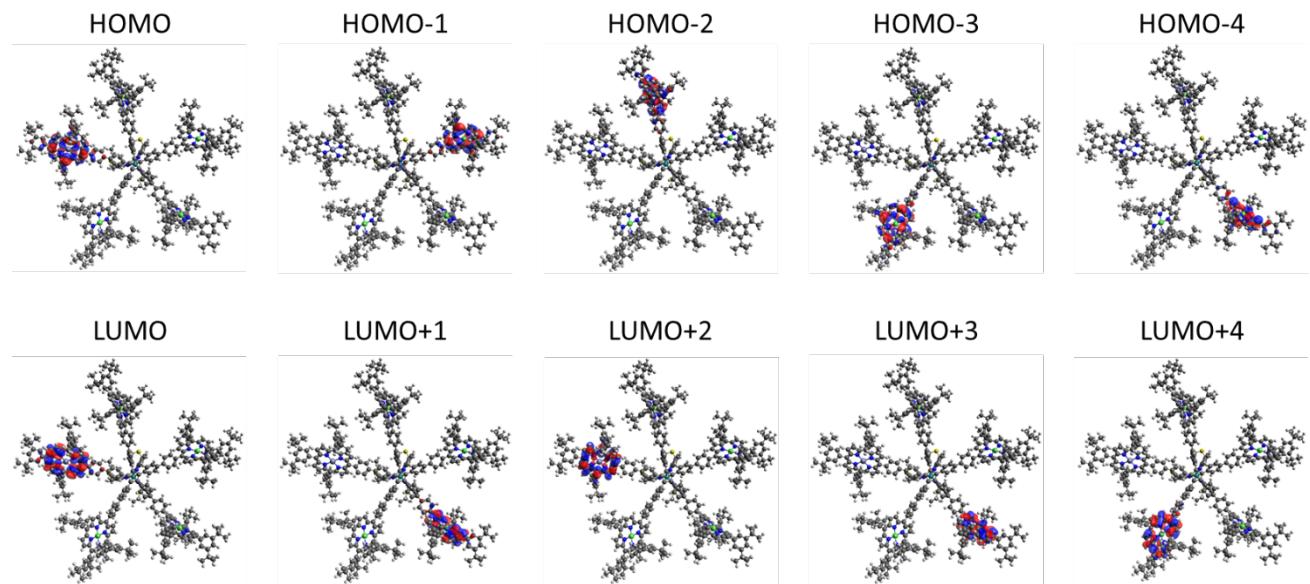
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H	6.33224	12.86787	-8.65044	N	13.52932	1.59366	-0.29206
H	4.6221	12.64207	-8.26079	C	14.07928	1.41084	0.96121
C	4.10886	15.20175	-7.35532	C	15.44279	1.37098	1.25573
H	4.11205	16.01131	-6.61832	C	15.88789	1.1975	2.67459
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C	7.06935	13.12875	-5.97056	C	16.98499	2.10973	4.65875
H	7.70292	13.05675	-6.84652	C	17.71175	3.28616	5.33894
C	7.48677	12.52216	-4.78205	C	16.7951	4.53282	5.3336
C	8.81942	11.75811	-4.65744	H	16.52176	4.83453	4.31843
C	8.53618	10.29484	-4.24123	H	15.86927	4.34032	5.88564
H	7.92409	9.78572	-4.99336	H	17.30337	5.38049	5.80703
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H	9.47443	9.73858	-4.13501	H	17.21024	2.77024	7.41559
C	9.61154	11.73535	-5.9785	H	18.60044	3.84461	7.23709
H	9.05271	11.24347	-6.78152	H	18.77273	2.12504	6.876
H	9.87629	12.74396	-6.31297	C	19.01061	3.60305	4.55962
C	9.70035	12.43543	-3.58054	H	18.80607	3.86785	3.51813
H	9.21274	12.44442	-2.60154	H	19.53659	4.44643	5.02136
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H	9.92175	13.47277	-3.85268	C	16.73358	0.89763	5.30785
C	6.64444	12.63195	-3.66265	C	16.07664	-0.17806	4.6819
H	6.93306	12.18618	-2.71588	C	15.84424	-1.48489	5.46527
C	4.46834	14.69167	-1.89267	C	17.20378	-2.06336	5.92462
C	5.35949	15.78531	-2.18703	H	17.74643	-1.3679	6.57167
H	6.10183	15.7791	-2.97085	H	17.84372	-2.28825	5.06509
C	5.11152	16.75427	-1.26838	H	17.052	-2.99128	6.48772
C	4.02432	16.28429	-0.44764	C	14.96812	-1.19041	6.70648
C	3.39491	17.05878	0.52775	H	14.7986	-2.10844	7.28059
C	2.21925	16.63746	1.15203	H	15.43847	-0.46245	7.37429
N	1.62333	15.40248	1.00791	H	13.99262	-0.79014	6.41084
Ni	2.318	13.8588	0.02625	C	15.13074	-2.55645	4.61889
N	0.98174	12.714	0.88915	H	15.71338	-2.8323	3.73385
C	-0.13785	13.11752	1.58887	H	14.98881	-3.4632	5.216
C	-0.45317	14.43178	1.93446	H	14.14218	-2.22316	4.28657
C	-1.73104	14.71999	2.66033	H	17.05687	0.7743	6.33433
C	-2.76185	15.40238	2.01187	C	15.66098	-0.00852	3.3592
H	-2.61344	15.69711	0.97763	H	15.15903	-0.80922	2.82945
C	-3.96882	15.70082	2.66654	C	13.04118	1.17682	1.93272
C	-5.08236	16.44463	1.90391	H	13.2069	1.03473	2.98961
C	-5.52615	15.59314	0.69042	C	11.86426	1.15649	1.25561

H	-4.69716	15.40166	0.00297	H	10.86971	1.00662	1.64808
H	-5.92029	14.62462	1.0154	C	16.41122	1.40736	0.2502
H	-6.31337	16.10945	0.12923	C	17.80163	1.10336	0.47579
C	-6.32081	16.71168	2.78055	H	18.23691	0.89834	1.44209
H	-6.77514	15.78253	3.14001	C	18.40657	1.09788	-0.74011
H	-7.07837	17.24214	2.19442	H	19.44309	0.90579	-0.97285
H	-6.08074	17.33427	3.64897	C	19.0483	1.35873	-3.57259
C	-4.54477	17.80673	1.40383	C	19.94692	2.38981	-3.89408
H	-3.6878	17.68718	0.73455	H	19.62039	3.41334	-3.75417
H	-5.32455	18.34465	0.85283	C	21.22854	2.1082	-4.37309
H	-4.22768	18.43477	2.24308	C	22.24093	3.21223	-4.73613
C	-4.10222	15.29324	3.99688	C	21.68115	4.62589	-4.48821
C	-3.08638	14.60529	4.68659	H	22.43399	5.37294	-4.76034
C	-3.30732	14.19767	6.1564	H	21.42484	4.78405	-3.43559
C	-3.53885	15.46533	7.01317	H	20.78862	4.82348	-5.09075
H	-4.41181	16.03207	6.67562	C	23.51862	3.04627	-3.8793
H	-2.67085	16.13147	6.96896	H	24.24992	3.82247	-4.13187
H	-3.70385	15.19223	8.0617	H	23.28776	3.13204	-2.81232
C	-4.5473	13.27767	6.25756	H	23.9966	2.07538	-4.03993
H	-4.7172	12.98058	7.2987	C	22.61007	3.09747	-6.23452
H	-5.45509	13.77366	5.90159	H	23.04934	2.12445	-6.47339
H	-4.40878	12.36828	5.66346	H	23.33875	3.86899	-6.50837
C	-2.101	13.43866	6.74153	H	21.72498	3.22786	-6.86612
H	-1.19149	14.04807	6.73267	C	21.59226	0.75689	-4.52352
H	-2.30596	13.16843	7.7826	H	22.58334	0.52988	-4.89764
H	-1.89649	12.5124	6.19448	C	20.72956	-0.29661	-4.20769
H	-5.02233	15.51401	4.52419	C	21.12507	-1.77746	-4.36714
C	-1.90298	14.32733	3.99811	C	21.04782	-2.47885	-2.98986
H	-1.08706	13.80801	4.48629	H	21.73916	-2.01722	-2.2769
C	-0.91285	11.97287	1.99526	H	20.04262	-2.42687	-2.56155
H	-1.84726	12.02119	2.53335	H	21.31507	-3.53753	-3.08468
C	-0.23059	10.87075	1.59031	C	22.55513	-1.95134	-4.91285
H	-0.50068	9.83316	1.71659	H	23.30405	-1.51115	-4.2461
C	0.4325	15.48487	1.69794	H	22.67184	-1.50124	-5.90432
C	0.27385	16.79833	2.26874	H	22.78487	-3.01761	-5.00684
H	-0.57659	17.11519	2.85329	C	20.14923	-2.4684	-5.34944
C	1.39179	17.50252	1.95415	H	20.18853	-1.9964	-6.33672
H	1.63742	18.52148	2.21254	H	19.11434	-2.42095	-4.9984
C	3.93667	18.41464	0.85935	H	20.41266	-3.52563	-5.46774
C	3.85182	19.47131	-0.0626	C	19.45055	0.0308	-3.72693
H	3.38264	19.27655	-1.01939	H	18.74539	-0.75388	-3.47114
C	4.34705	20.74084	0.24491	H	17.97952	2.54351	-5.75261
C	4.26381	21.92478	-0.73874	N	15.42466	2.53342	-3.59401
C	3.59516	21.53358	-2.07034	H	9.43449	2.5663	-3.14932
H	3.55991	22.40355	-2.73424	N	12.76141	2.50775	-2.80199
H	2.56652	21.18861	-1.9238	C	12.17029	1.44081	-0.12362

H	4.14917	20.74457	-2.58937	C	9.33749	0.03212	-0.6107
C	3.43549	23.06672	-0.10287	H	10.04968	-0.77318	-0.76527
H	3.37272	23.9194	-0.78854	C	8.01874	-0.26492	-0.27576
H	2.41604	22.73389	0.11854	H	7.71999	-1.30225	-0.15663
H	3.88025	23.42285	0.83115	H	3.32928	-18.4551	3.61734
C	5.69001	22.43854	-1.0499	H	4.27593	-15.6279	6.72252
H	6.20794	22.77827	-0.14814	N	2.24007	-18.465	6.94192
H	5.64765	23.28275	-1.74752	N	11.5489	-10.5032	-9.16963
H	6.29843	21.6512	-1.50722	H	11.49481	-9.38794	-5.85382
C	4.93576	20.92847	1.50946	H	9.79791	-13.0035	-7.46
H	5.32371	21.90948	1.75559	H	-12.1445	-2.94892	-9.74645
C	5.03559	19.9037	2.45477	H	-12.0398	1.09036	-10.0448
C	5.67962	20.10374	3.84041	H	10.54434	11.17941	-5.83909
C	4.63496	19.79962	4.94072	H	10.68041	3.94702	-11.4865
H	3.77755	20.47656	4.86343				
H	4.25805	18.77501	4.87374				
H	5.07959	19.92705	5.93428				
C	6.1924	21.54092	4.05166				
H	5.38412	22.27718	3.98954				
H	6.96041	21.81196	3.31967				
H	6.64098	21.62838	5.04658				
C	6.8798	19.13869	3.99279				
H	7.64106	19.33744	3.23112				
H	6.5765	18.09233	3.89564				
H	7.34471	19.26097	4.97775				
C	4.52158	18.64328	2.10618				
H	4.57744	17.81669	2.80781				
H	5.60105	17.70953	-1.15506				
N	3.65481	15.00946	-0.82691				
H	3.41012	9.07204	-1.69613				
N	3.01108	12.3113	-0.96349				
C	0.93374	11.33707	0.8798				
C	2.0011	8.39197	1.54313				
H	2.43528	8.99283	2.33687				

**Cogwheel 12:**

Calculation Type = FOPT. Calculation Method = RB3LYP. Basis Set = 6-31G(d,p). Charge = 0. Spin = Singlet. Electronic Energy = -19172.511 Hartree. RMS Gradient Norm = 6.6084251e-07 Hartree/Bohr. Dipole Moment = 5.8520514 Debye.



**Figure S11.** Frontier orbitals of cogwheel **12**.

Cartesian coordinates:

C	-0.30363	0.01343	0.36971	H	-7.2577	7.72761	17.29995
H	-0.32795	0.06515	1.46323	C	-9.46514	6.05359	18.11074
H	0.74519	-0.02393	0.06078	C	-9.91392	7.39234	17.60451
H	-0.77514	-0.9273	0.06344	C	-10.4112	8.35738	18.48283
C	-1.04672	1.21782	-0.25626	H	-10.4619	8.11388	19.53949
C	-2.52077	1.15363	0.18711	C	-10.8275	9.61963	18.0272
H	-2.62146	1.1993	1.27628	C	-11.363	10.65323	19.03711
H	-2.96454	0.20972	-0.14596	C	-12.6233	10.08472	19.73225
H	-3.11224	1.96742	-0.24496	H	-13.4138	9.88036	19.00227
C	-1.00415	1.10145	-1.79867	H	-13.0137	10.80258	20.46273
H	-1.48777	0.17335	-2.12411	H	-12.4103	9.15232	20.26327
H	0.02112	1.09312	-2.18009	C	-11.7456	11.98734	18.36846
H	-1.52868	1.93998	-2.26863	H	-12.5401	11.85996	17.62574
C	-0.35991	2.52644	0.18144	H	-12.113	12.68661	19.12658
C	0.9893	2.74773	-0.15181	H	-10.8879	12.45706	17.87566
C	1.67691	3.90815	0.21583	C	-10.2788	10.94433	20.10209
C	0.97338	4.87797	0.94983	H	-10.6475	11.67487	20.83119
H	1.46493	5.79802	1.25009	H	-9.99329	10.04237	20.65104
C	-0.36476	4.69389	1.30405	H	-9.37462	11.35314	19.63924
C	-1.10933	5.73593	2.08116	C	-10.7306	9.87931	16.65684

C	-2.06017	6.51076	1.41465	H	-11.0454	10.84566	16.2817
N	-2.87215	7.46939	1.98214	C	-10.2382	8.93348	15.73843
Ni	-2.99553	7.94756	3.88171	C	-10.1671	9.29211	14.24093
N	-1.4042	6.85738	4.26443	C	-9.60897	8.13673	13.38806
C	-0.67328	6.82605	5.43457	H	-8.59196	7.8627	13.6867
C	0.439	5.91867	5.30625	H	-9.57301	8.43971	12.3363
H	1.17458	5.72934	6.07288	H	-10.2368	7.24213	13.45217
C	0.34416	5.34972	4.07733	C	-9.24533	10.51987	14.04822
H	0.9868	4.60411	3.63504	H	-8.23128	10.30679	14.40228
C	-0.99532	7.49335	6.61744	H	-9.61142	11.3954	14.59244
C	-2.19628	8.19008	6.76848	H	-9.18371	10.78866	12.98731
C	-2.69258	8.63997	8.04488	C	-11.5857	9.629	13.72301
H	-2.1584	8.55516	8.97903	H	-11.5517	9.88891	12.6586
C	-3.94441	9.12099	7.83383	H	-12.0259	10.47577	14.25802
H	-4.6379	9.52231	8.55701	H	-12.2584	8.7732	13.84178
C	-4.19866	9.01911	6.41955	C	-9.83247	7.69226	16.23431
C	-5.34386	9.52047	5.80144	H	-9.44906	6.92878	15.5683
C	-5.46915	9.56643	4.4123	C	-10.4561	5.18012	18.60765
C	-6.51292	10.29201	3.73433	C	-11.8728	5.47097	18.64668
C	-6.23954	10.22594	2.40589	H	-12.3315	6.38274	18.29466
H	-6.79479	10.65342	1.58479	C	-12.4894	4.39118	19.20335
C	-5.0492	9.42654	2.26294	H	-13.5435	4.26303	19.39863
C	-4.53447	9.02959	1.0277	C	-11.4611	3.41595	19.49577
C	-5.13691	9.60086	-0.21856	C	-11.6899	2.15008	20.07678
C	-4.90716	10.93542	-0.55778	C	-10.6945	1.19645	20.37936
H	-4.28157	11.533	0.09821	C	-10.9506	-0.12461	20.91097
C	-5.45914	11.50181	-1.71934	H	-11.9269	-0.52389	21.14188
C	-5.17159	12.97816	-2.05429	C	-9.74585	-0.7486	21.03449
C	-3.6457	13.18235	-2.21153	H	-9.55573	-1.75216	21.38468
H	-3.42375	14.23024	-2.44358	C	-8.73515	0.18077	20.5783
H	-3.10324	12.92136	-1.29823	C	-7.35375	-0.10092	20.51142
H	-3.2496	12.56338	-3.02336	C	-6.90184	-1.43518	21.02778
C	-5.85258	13.43	-3.36017	C	-6.94805	-1.71086	22.40459
H	-5.61997	14.48276	-3.55104	H	-7.31083	-0.93435	23.06709
H	-5.50371	12.8542	-4.22381	C	-6.53228	-2.9444	22.91137
H	-6.94243	13.33863	-3.30501	C	-6.56283	-3.27651	24.4161
C	-5.69168	13.8756	-0.90593	C	-7.47418	-4.50388	24.65559
H	-5.48608	14.93001	-1.1231	H	-8.49841	-4.30072	24.32557
H	-5.21502	13.63333	0.04829	H	-7.11959	-5.38795	24.11753
H	-6.77322	13.76034	-0.77796	H	-7.50453	-4.75364	25.72235
C	-6.25373	10.68214	-2.52613	C	-7.10307	-2.10839	25.26319
H	-6.68887	11.09599	-3.4278	H	-8.12843	-1.84292	24.98574
C	-6.51696	9.33513	-2.21433	H	-6.48046	-1.21297	25.16766
C	-7.40859	8.49649	-3.15096	H	-7.11043	-2.39322	26.32038
C	-6.74525	8.40865	-4.54634	C	-5.1298	-3.59931	24.90293
H	-5.76474	7.92497	-4.48342	H	-5.13593	-3.84409	25.97114

H	-7.36964	7.82236	-5.23027	H	-4.4644	-2.74249	24.75476
H	-6.60082	9.39753	-4.99149	H	-4.6992	-4.4518	24.36892
C	-8.79688	9.16643	-3.28553	C	-6.06575	-3.90716	21.99701
H	-8.72633	10.17612	-3.70068	C	-6.00547	-3.67213	20.62021
H	-9.2922	9.23931	-2.31173	C	-5.49944	-4.72453	19.61445
H	-9.44016	8.57873	-3.95031	C	-5.09106	-6.04384	20.29696
C	-7.62083	7.06259	-2.62877	H	-4.74615	-6.75734	19.54146
H	-6.6774	6.51366	-2.54357	H	-5.93031	-6.50597	20.82727
H	-8.10981	7.05455	-1.6491	H	-4.27308	-5.89853	21.01055
H	-8.26197	6.5093	-3.32273	C	-4.26404	-4.16775	18.86718
C	-5.94714	8.81132	-1.05156	H	-3.45142	-3.94586	19.56717
H	-6.12427	7.78225	-0.76336	H	-3.8946	-4.90005	18.14011
H	-7.32831	10.799	4.22774	H	-4.49663	-3.24757	18.32334
C	-6.43885	10.10264	6.64148	C	-6.61726	-5.03948	18.59193
C	-6.26244	11.33059	7.30084	H	-7.50492	-5.43965	19.09291
H	-5.31418	11.84122	7.18304	H	-6.27152	-5.78451	17.86625
C	-7.27962	11.88403	8.08211	H	-6.92262	-4.14923	18.03457
C	-7.12373	13.22774	8.8206	H	-5.74141	-4.86676	22.38133
C	-5.73646	13.86075	8.60001	C	-6.432	-2.41734	20.15344
H	-4.93085	13.21404	8.96277	H	-6.40834	-2.1925	19.09169
H	-5.67241	14.80638	9.14799	C	-6.36542	0.76325	19.99384
H	-5.54992	14.07873	7.5434	C	-4.95344	0.45702	19.9236
C	-7.31222	13.00554	10.34049	H	-4.49689	-0.46043	20.26324
H	-6.56002	12.3121	10.73085	C	-4.33725	1.52952	19.35282
H	-8.29883	12.59427	10.57438	H	-3.28649	1.64042	19.13113
H	-7.21155	13.95418	10.87989	N	-6.58038	2.02174	19.48089
C	-8.19311	14.22413	8.31241	N	-9.34154	1.3508	20.18498
H	-8.09588	15.18479	8.83089	C	-13.1105	1.78303	20.38889
H	-8.07977	14.40505	7.23842	C	-13.5392	1.67466	21.72257
H	-9.20904	13.85573	8.48331	H	-12.8171	1.86691	22.50687
C	-8.48926	11.17236	8.18625	C	-14.8584	1.33791	22.0345
H	-9.28287	11.59464	8.79062	C	-15.3645	1.21696	23.48533
C	-8.70404	9.94968	7.54366	C	-16.5099	2.231	23.71867
C	-10.0251	9.16495	7.66207	H	-16.8826	2.15535	24.74657
C	-10.6443	8.98429	6.25538	H	-16.1626	3.25697	23.55814
H	-10.8667	9.95428	5.79815	H	-17.354	2.05546	23.0453
H	-11.5801	8.41764	6.32013	C	-15.8926	-0.21699	23.72987
H	-9.97388	8.44326	5.58129	H	-16.7129	-0.47166	23.05231
C	-11.0587	9.88171	8.55118	H	-15.0979	-0.95626	23.58447
H	-11.3264	10.86666	8.15446	H	-16.265	-0.31639	24.75581
H	-11.9763	9.28667	8.60227	C	-14.257	1.50086	24.51822
H	-10.694	10.01304	9.57561	H	-13.8601	2.51667	24.42194
C	-9.74248	7.77443	8.27928	H	-14.6625	1.39983	25.53032
H	-10.6718	7.20036	8.36845	H	-13.4227	0.79791	24.42545
H	-9.3063	7.87136	9.27922	C	-15.7485	1.10919	20.96865
H	-9.04801	7.19053	7.66849	H	-16.7737	0.84834	21.20191

C	-7.65537	9.42933	6.76631	C	-15.361	1.20623	19.62909
H	-7.77496	8.4818	6.25008	C	-16.3304	0.95357	18.458
C	-0.08638	7.38279	7.79964	C	-15.8072	-0.22518	17.60269
C	0.59722	8.50958	8.28206	H	-14.8128	-0.02252	17.19459
C	1.42601	8.4237	9.39849	H	-15.7432	-1.14223	18.19765
H	1.96303	9.30703	9.7314	H	-16.4822	-0.41294	16.7599
C	1.60222	7.20798	10.08047	C	-17.7534	0.60477	18.93413
C	0.91726	6.08115	9.59468	H	-17.7709	-0.30999	19.53577
H	1.00552	5.1345	10.11964	H	-18.1958	1.41288	19.52611
C	2.46766	7.11537	11.28238	H	-18.4008	0.44021	18.06652
C	3.25112	5.97433	11.52913	C	-16.417	2.22388	17.57865
H	3.25768	5.16325	10.8069	H	-16.7964	3.07389	18.1557
C	4.04178	5.87869	12.67046	H	-15.4419	2.5056	17.17082
H	4.64526	4.98928	12.83038	H	-17.0955	2.05747	16.7341
C	4.08284	6.91754	13.61644	C	-14.0247	1.54669	19.36009
C	4.91134	6.7621	14.84562	H	-13.6781	1.62664	18.33454
C	4.41892	6.33337	16.14555	N	-10.2381	3.92486	19.12572
C	5.54615	6.05245	16.9879	Zn	-8.40926	2.97385	19.30542
C	5.43388	5.33467	18.29215	C	-5.86629	6.08828	17.73791
C	5.22364	5.9671	19.52405	H	-4.89075	6.49791	17.52347
H	5.17335	7.04834	19.56483	C	-5.35982	2.51879	19.08771
C	5.08475	5.22796	20.69836	C	-1.42751	4.62866	18.84817
H	4.95461	5.75269	21.64021	H	-0.68854	4.70076	19.64058
C	5.13869	3.82583	20.68919	C	0.94501	4.82841	15.97295
C	4.99722	3.04094	21.94045	H	0.39575	4.17724	15.29966
C	4.11108	3.4415	22.95448	C	2.24397	5.20194	15.64091
H	3.49453	4.32349	22.80857	H	2.67226	4.84583	14.71163
C	3.9833	2.70612	24.13024	C	6.35622	6.67177	14.87981
H	3.28384	3.03002	24.89528	C	7.22218	6.75643	13.67605
C	4.73299	1.5378	24.3393	C	6.93085	7.61284	12.59739
C	4.59316	0.77035	25.61442	H	6.09411	8.29712	12.66556
C	5.06077	1.35531	26.79391	C	7.70644	7.61183	11.44204
C	5.86473	2.55112	26.81608	H	7.46729	8.31193	10.64719
H	6.12189	3.1376	25.94707	C	8.80294	6.7455	11.29806
C	6.2572	2.73879	28.10216	C	9.62962	6.74578	10.06681
H	6.89009	3.51696	28.50023	C	11.01817	6.53779	10.12545
C	5.64716	1.69292	28.8829	H	11.49788	6.39589	11.08941
C	5.70788	1.62764	30.27548	C	11.79576	6.53953	8.97002
C	4.9574	0.6988	30.99969	H	12.86814	6.38321	9.04165
C	4.78522	0.75932	32.42904	C	11.21678	6.74581	7.70824
C	3.90914	-0.22299	32.76286	C	12.06996	6.75606	6.48031
H	3.53518	-0.48414	33.7412	C	12.93955	7.83203	6.28611
C	3.57058	-0.91292	31.54437	C	12.89685	9.03527	7.07862
C	2.80336	-2.07828	31.51015	H	12.26233	9.18434	7.93921
C	2.16228	-2.55214	32.77833	C	13.74521	9.92146	6.49618
C	1.05324	-1.88025	33.29518	H	13.95605	10.93809	6.7911

H	0.66756	-1.0252	32.74871	C	14.35916	9.24341	5.38297
C	0.43839	-2.29243	34.48974	C	15.38794	9.78624	4.61248
C	-0.79133	-1.52555	35.01434	C	16.09264	9.01633	3.68461
C	-1.9254	-1.59715	33.96385	C	17.32504	9.44219	3.07136
H	-2.8064	-1.04857	34.31609	C	17.79453	8.38737	2.35589
H	-1.62291	-1.16238	33.00687	H	18.69535	8.3262	1.76427
H	-2.2227	-2.63489	33.77972	C	16.82882	7.32646	2.49171
C	-1.32767	-2.10445	36.33713	C	16.89658	6.12725	1.77927
H	-2.19641	-1.52505	36.66615	C	18.1317	5.83456	0.98554
H	-1.64906	-3.14542	36.22697	C	19.32134	5.51681	1.64379
H	-0.57972	-2.05879	37.13566	H	19.31486	5.4779	2.72861
C	-0.41185	-0.04521	35.25777	C	20.50247	5.24466	0.93334
H	-1.28045	0.51533	35.62181	C	21.78779	4.88761	1.70468
H	-0.06125	0.44281	34.34382	C	21.5473	3.60302	2.53358
H	0.383	0.03742	36.00661	H	22.45076	3.33605	3.09366
C	0.97922	-3.40016	35.14881	H	20.73376	3.72825	3.25409
H	0.52409	-3.73542	36.0728	H	21.28977	2.76072	1.88297
C	2.0972	-4.10269	34.6619	C	22.98603	4.63659	0.76974
C	2.63769	-5.31067	35.45242	H	23.87192	4.39166	1.36463
C	1.52819	-6.38168	35.5821	H	22.80464	3.79791	0.08946
H	1.20491	-6.73173	34.59618	H	23.22727	5.5197	0.16874
H	1.89762	-7.2465	36.14496	C	22.1577	6.04973	2.6572
H	0.64751	-5.99712	36.10495	H	23.06522	5.80597	3.2212
C	3.07143	-4.84957	36.86446	H	21.36302	6.25505	3.38031
H	2.23863	-4.41563	37.42577	H	22.34491	6.97139	2.09604
H	3.86229	-4.09466	36.80352	C	20.44839	5.30682	-0.4621
H	3.45606	-5.69819	37.44157	H	21.34671	5.10203	-1.03186
C	3.8536	-5.96338	34.76792	C	19.27078	5.62691	-1.16319
H	3.60768	-6.33653	33.76837	C	19.29353	5.67932	-2.70333
H	4.69311	-5.26678	34.67509	C	19.70068	4.29406	-3.25982
H	4.19709	-6.81578	35.36308	H	18.98402	3.52418	-2.95508
C	2.67714	-3.66123	33.47021	H	19.72904	4.31669	-4.35517
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C	2.68968	-2.84933	30.35326	C	20.31857	6.74018	-3.17044
N	3.18829	-2.51814	29.10964	H	21.32982	6.51322	-2.82009
Ni	4.05413	-0.83779	28.58227	H	20.05076	7.73402	-2.79679
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C	3.50357	-2.56296	26.17891	C	17.9204	6.04726	-3.29726
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C	0.03245	-6.41809	23.98413	C	15.81613	5.24555	1.72579
C	-1.18189	-6.17133	24.91128	N	14.63665	5.37316	2.43162
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C	-0.13665	-7.80335	23.33169	C	12.57463	4.00801	2.49698
H	-1.07073	-7.82954	22.76103	C	11.79851	2.9241	1.81469
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H	0.67935	-8.0303	22.63758	H	12.12815	1.47459	3.35134
C	0.04082	-5.35565	22.85922	C	10.93864	0.6377	1.74832
H	-0.88215	-5.41539	22.27111	C	10.81516	-0.74326	2.42136
H	0.11464	-4.33962	23.2576	C	12.22641	-1.34811	2.61398
H	0.88563	-5.51142	22.17993	H	12.72985	-1.48041	1.65053
C	2.23456	-7.3653	24.94312	H	12.15876	-2.32862	3.09901
H	2.02276	-8.3039	24.44533	H	12.86104	-0.7114	3.23718
C	3.4119	-7.26538	25.70741	C	9.97914	-1.73261	1.58746
C	4.35577	-8.47914	25.81433	H	9.91512	-2.69232	2.11051
C	5.57782	-8.19386	26.70776	H	10.42799	-1.92224	0.60682
H	6.18871	-7.37467	26.31487	H	8.95648	-1.37304	1.43251
H	6.21331	-9.08411	26.75738	C	10.13405	-0.58413	3.80183
H	5.28426	-7.94018	27.7316	H	10.0468	-1.55698	4.29872
C	4.86884	-8.85932	24.40485	H	10.70193	0.07647	4.46359
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H	4.04883	-9.11613	23.72761	C	10.36635	0.92893	0.50642
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C	3.58852	-9.67837	26.42084	C	10.48886	2.18832	-0.10944
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C	3.67525	-6.04976	26.34367	H	9.59181	3.9832	-2.97905
H	4.56802	-5.92021	26.94371	H	11.14266	4.06366	-2.1373
C	3.47986	-2.52144	24.73911	C	8.2972	2.22565	-1.35379
H	3.22697	-3.3555	24.1026	H	7.86709	2.92597	-0.62992
C	3.78887	-1.25028	24.37605	H	8.04862	1.21227	-1.02506
H	3.8423	-0.83674	23.38072	H	7.80862	2.39178	-2.32079
C	2.91684	-3.60411	28.30496	C	10.39479	1.43323	-2.51445
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H	1.92769	-5.58192	28.65361	H	10.21461	0.39457	-2.22193
C	2.07819	-4.15363	30.31734	H	11.47564	1.56453	-2.63128
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N	4.20772	-0.32953	30.46895	C	10.93503	4.07725	4.3858
C	6.53216	2.62547	31.02735	H	10.29468	3.27945	4.04236
C	6.18216	3.98631	31.0416	C	10.86519	4.76619	5.55398
H	5.29746	4.29114	30.49599	H	10.15326	4.64618	6.35611
C	6.94384	4.92241	31.74467	C	13.82333	4.35771	1.978
C	6.59013	6.42213	31.78001	C	14.50251	3.58402	0.96967
C	5.32605	6.74651	30.96096	H	14.08196	2.72698	0.46564
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H	4.44461	6.22305	31.34561	H	17.77223	10.41591	3.20267
C	7.76482	7.24137	31.19389	N	15.79582	7.72178	3.31483
H	7.95708	6.95982	30.15326	C	15.81194	11.20455	4.83689
H	8.69033	7.08903	31.7569	C	16.47441	11.5838	6.0164
H	7.53285	8.31217	31.21805	H	16.67229	10.82038	6.75924
C	6.33918	6.86024	33.24273	C	16.87705	12.90493	6.22649
H	6.08993	7.92667	33.28378	C	17.60622	13.35743	7.50682
H	5.50689	6.29988	33.68128	C	17.8319	12.19678	8.49449
H	7.21855	6.69999	33.87342	H	16.88742	11.75115	8.82339
C	8.0736	4.45881	32.44442	H	18.34942	12.56751	9.38524
H	8.66981	5.17863	32.99209	H	18.45025	11.40474	8.05972
C	8.4512	3.11291	32.46004	C	16.76347	14.43976	8.22302
C	9.68525	2.60058	33.22854	H	15.783	14.04521	8.50985
C	9.23394	1.57208	34.29307	H	16.59784	15.31491	7.58782
H	8.55165	2.03188	35.016	H	17.27209	14.77915	9.1325
H	10.0999	1.18587	34.84282	C	18.98787	13.94632	7.13457
H	8.71772	0.71906	33.84306	H	19.51632	14.27833	8.03548
C	10.44331	3.73224	33.94746	H	19.60967	13.19721	6.6333
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C	10.66229	1.91946	32.24064	C	15.94802	13.50633	4.02781
H	11.54127	1.54112	32.77483	C	15.6398	14.53338	2.92091
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C	7.65791	2.20486	31.7387	H	16.10432	14.80903	0.80389
H	7.91433	1.15017	31.71912	H	15.97941	13.10922	1.27326
N	4.9389	0.83506	28.06407	C	16.14386	15.94624	3.27116
C	4.08111	-0.52788	25.58862	H	17.22928	15.96768	3.41422
C	5.62233	1.1381	23.3293	H	15.9057	16.63501	2.45412
H	6.23289	0.25266	23.47888	H	15.67058	16.33637	4.17832
C	5.75008	1.87383	22.15356	C	14.10958	14.60817	2.70294
H	6.46938	1.55767	21.40371	H	13.87147	15.32899	1.91243
C	5.32522	3.19014	19.4495	H	13.59963	14.92697	3.61805
H	5.32689	2.10536	19.39853	H	13.69187	13.64102	2.40852
C	5.46559	3.92896	18.27913	C	15.56122	12.16652	3.85652
H	5.57621	3.40909	17.33118	H	15.04972	11.85696	2.95044
C	6.76429	6.28857	16.2109	N	13.84027	7.97061	5.25302
C	8.1636	6.06826	16.66692	C	11.91675	5.7514	5.52263
C	9.13171	7.08244	16.55064	C	9.8307	6.95953	7.6474
H	8.83314	8.05605	16.17689	H	9.36116	7.12969	6.68316
C	10.45121	6.86867	16.93397	C	9.05296	6.95772	8.80287
H	11.16301	7.68521	16.85665	H	7.97996	7.10394	8.72139
C	10.86779	5.63325	17.46094	C	9.08217	5.87582	12.36511
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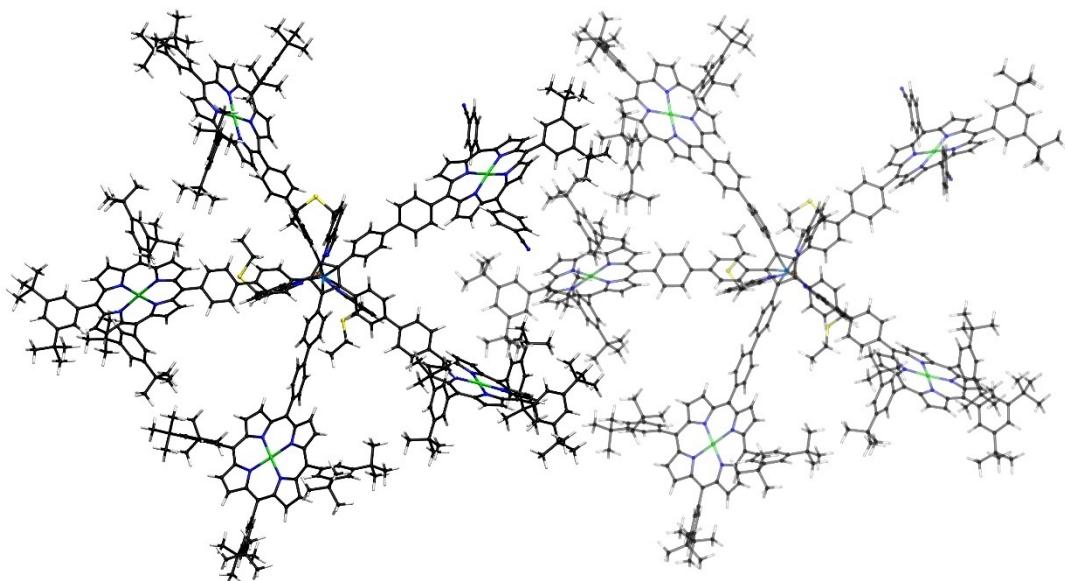
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C	18.84578	2.71577	17.45446	C	8.21369	14.26708	15.10297
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H	18.62902	2.42805	12.53851	H	6.41541	15.54609	13.26088
H	19.41434	2.33208	10.95971	C	5.30132	17.4043	13.11134
H	20.32562	2.91181	12.35705	H	5.43636	18.4734	13.30234
C	18.90993	-0.20912	11.77541	H	5.05794	17.27876	12.05116
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H	21.17027	0.66237	10.45012	H	5.66393	12.39495	18.02068
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H	23.48794	-2.01831	16.04187	C	0.66656	11.08806	16.961
H	23.06418	-3.39974	17.06928	H	-0.13228	10.44756	16.59904
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C	20.07736	1.44673	14.78114	C	0.36726	13.7436	22.45472
H	19.77122	2.4501	14.51066	H	-0.54172	13.14238	22.35791
C	21.25894	2.75503	17.80113	H	1.01428	13.2609	23.19487
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H	24.50562	3.32941	18.06003	H	3.5458	13.4364	18.27056
C	22.59673	3.99731	19.02056	N	6.34361	10.32117	18.5865
C	23.10423	4.80838	20.03744	C	7.06001	10.58881	19.71943
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H	24.50053	6.376	18.37233	H	9.01292	8.46866	21.5946
C	26.52766	6.19684	19.11209	C	8.65803	10.55069	21.98813
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C	26.8453	6.54396	16.63713	C	5.06196	14.13933	23.12102
H	27.24482	7.20583	15.86029	H	5.51917	14.44063	22.17336
H	25.77596	6.41458	16.44657	H	3.99225	13.98386	22.93587
H	27.32465	5.56532	16.52816	H	5.17223	14.96843	23.82553
C	27.31204	5.58763	20.09569	C	7.32518	8.44175	19.13917
H	28.37771	5.78148	20.11249	H	7.59994	7.40293	19.05077
C	26.7747	4.72512	21.06935	C	7.21811	11.78455	20.44858
C	27.7088	4.07753	22.11049	H	6.73744	12.70191	20.12539
C	28.43074	5.18303	22.91763	N	6.51789	9.00821	18.24434
H	27.7105	5.81449	23.44834	N	3.98646	9.58062	16.79622
H	29.10155	4.73619	23.66015	C	3.32087	8.06509	13.3604
H	29.0324	5.83193	22.27445	H	3.35644	8.88956	14.06354
C	28.76001	3.20413	21.38487	C	2.52639	8.16001	12.21875
H	29.36525	3.78968	20.68638	H	1.9232	9.05014	12.06608
H	28.27661	2.40274	20.81633	H	0.4829	9.45908	7.76733
H	29.44034	2.74313	22.11006	C	0.08916	6.16663	8.47831
C	26.94599	3.18101	23.10425	H	-0.44791	5.28631	8.13796
H	26.19736	3.74428	23.67108	N	-3.12666	8.42889	5.78007
H	26.43912	2.35203	22.59984	N	-4.58217	9.03474	3.50003
H	27.64824	2.74866	23.82449	C	-3.5347	8.0616	0.92553
C	25.39917	4.4833	21.03964	C	-3.10402	7.48419	-0.3225
H	24.93823	3.82017	21.76181	H	-3.45178	7.79265	-1.29657
C	22.29004	5.29991	21.05857	C	-2.21954	6.50037	-0.0173
N	20.91847	5.16408	21.1319	H	-1.68531	5.84654	-0.68993
Ni	19.72171	4.42124	19.7676	C	-0.78036	5.96331	3.41773

N	18.17036	5.16474	20.71596	C	3.15242	4.15799	-0.15305
C	18.14924	5.70884	21.98395	C	3.25706	5.44088	-1.01191
C	19.25808	5.91096	22.8056	H	2.68535	5.33721	-1.94017
C	19.06426	6.45119	24.18974	H	4.30193	5.63872	-1.27677
C	18.72507	7.78865	24.4024	H	2.87643	6.3189	-0.48215
C	18.55365	8.3027	25.69905	C	3.76489	2.99403	-0.95494
C	18.73663	7.42702	26.77346	H	4.8111	3.21775	-1.18805
C	19.08093	6.07357	26.60068	H	3.24351	2.83275	-1.90437
C	19.26375	5.17068	27.83645	H	3.74744	2.05584	-0.39045
C	19.63288	3.72442	27.45538	C	3.98241	4.33819	1.14046
H	18.85433	3.25075	26.84865	H	5.03423	4.52488	0.89575
H	19.75475	3.12397	28.36284	H	3.62684	5.18129	1.74017
H	20.57513	3.67679	26.89986	H	3.93447	3.43944	1.76457
C	17.9466	5.13254	28.64779	H	1.51147	1.98536	-0.71714
H	17.12675	4.73025	28.04371	C	-1.02249	3.51675	0.91086
H	17.65018	6.12755	28.99283	H	-2.06089	3.39454	1.1949
H	18.06238	4.49467	29.53144				
C	20.39644	5.73688	28.7258				
H	20.53139	5.1109	29.61521				
H	20.17947	6.75411	29.06507				
H	21.34616	5.7618	28.18121				
H	18.61037	7.80083	27.78234				
C	18.18101	9.78665	25.8853				
C	19.28577	10.67602	25.26632				
H	20.24918	10.50117	25.75668				
H	19.03237	11.73584	25.38369				
H	19.4153	10.48151	24.19775				
C	18.02945	10.17508	27.36831				
H	17.76632	11.23499	27.44591				
H	18.95948	10.02576	27.92682				
H	17.23738	9.60231	27.8619				
C	16.83638	10.07141	25.17417				
H	16.55918	11.12537	25.2893				
H	16.88809	9.8569	24.10273				
H	16.03221	9.46139	25.59913				
H	18.60123	8.43353	23.53792				
C	19.24232	5.60357	25.29503				
H	19.50558	4.56954	25.10673				
C	16.81795	6.14533	22.32006				
H	16.53611	6.59552	23.25969				
C	16.04194	5.91938	21.22903				
H	14.9942	6.14336	21.09913				
C	20.56031	5.70357	22.34861				
C	21.72606	6.17568	23.05173				
H	21.70815	6.64643	24.02312				
C	22.79097	5.96151	22.23684				

H	23.82689	6.2097	22.41032
H	22.86371	1.77837	16.5831
N	21.26854	3.68633	18.81794
N	18.53146	3.66884	18.40311
C	16.87622	5.27	20.24904
C	13.90869	4.40364	19.37809
H	14.12299	3.78925	20.24755
C	12.58729	4.61954	18.99416
H	11.78509	4.18741	19.58514
C	9.90056	4.62333	17.58408
H	10.19042	3.64683	17.96075
C	8.57909	4.83419	17.19429
H	7.86862	4.02179	17.28663
C	3.01114	6.01182	16.49604
C	2.4179	6.42518	17.70131
H	2.96961	7.07028	18.37376
C	1.11775	6.05376	18.0299
H	0.68175	6.42425	18.9527
C	0.34845	5.24827	17.17333
C	-1.04262	4.86496	17.51729
C	-2.02548	4.73153	16.52162
H	-1.76825	4.92856	15.48516
C	-3.33358	4.37891	16.8423
H	-4.07394	4.28434	16.05358
C	-3.71822	4.14939	18.17321
C	-2.73734	4.28103	19.16932
H	-3.00895	4.10933	20.20659
C	-5.13036	3.78848	18.51278
C	-6.12425	4.75396	18.23573
N	-7.47709	4.59751	18.42621
C	-8.08262	5.77578	18.05444
C	-7.07031	6.71524	17.62511

**System of two intertwined cogwheels **11** with a Ru-Ru distance of 35.3 Å**



**Figure S12.** Optimised geometry of two intertwined cogwheels **11** with a Ru-Ru distance of 35.3 Å

Cartesian coordinates:

Ru	0.47904636807140	-1.65212905787971	3.81123186839740
Ni	-11.56912514342715	5.61536384920190	-1.41836398699484
S	2.71163252151581	0.21932283593090	11.80559199673120
S	-2.83698800070021	-7.46113968330502	9.66197958249614
N	-12.99474765096283	5.52348089328820	-2.77017698783026
N	-0.94342818891489	-0.64742624177308	5.00697644202213
N	-10.67644868921090	4.06514738661039	-2.24295352042129
C	-1.99727865807869	-0.13364554944713	6.86192408381545
S	-5.73345475763747	0.40589907601594	9.87149594098014
C	-9.45748334415482	3.53897581616580	-1.90670050525972
C	1.31943289373363	-2.62135649607196	1.88864930513672
C	-1.12267856910186	-3.28953274281477	1.20398359430946
C	-1.51234322851545	-0.26745428433540	1.30891559058926
N	-12.39990455658541	7.22990313392547	-0.66092035044013
N	1.32833422831215	-1.46797898763789	6.70609726567123
C	1.07476328418800	3.39294679322056	2.53623503739761
C	-13.42103131136518	7.96520868448292	-1.20177193904838
H	-13.68068202112351	0.14701019313166	-7.87146273815996
C	1.74149778847413	3.84014491128316	1.39818451827802
C	-12.79078147040166	9.09761538821184	0.61978800305609
C	-3.44964882466947	0.90903590910691	8.42719336781652
N	0.02730307232939	-3.38261314939772	4.93139168569128
C	-8.52697790623566	4.99058764061003	1.42147519490192
C	-15.33412904884279	8.48719390024546	-2.67177073109992
N	-0.23565194394900	-3.29197544552036	6.24310687057965
C	-14.88027221289689	5.95473194029068	-4.01220301631541

C	-9.07824287505991	2.52775099723358	-2.84684064831499
C	2.19542335969395	2.89918636178624	0.47574374939191
C	1.99458413584543	-1.36111208459485	1.99672972442568
C	-17.70019867131267	8.89789070629183	-2.87950572740439
C	-0.27456824523741	-0.94224749759531	1.71127070422487
C	-13.65688308150456	9.13899412141327	-0.41726754678140
C	-12.31069386270989	3.49670694714665	-3.99259724160001
C	2.53122428298110	-5.98094511700002	0.70308051984748
C	-8.71915574852522	3.83931600652015	-0.76892124306409
C	-10.22198424406934	6.41786691071961	1.13244272972050
C	-15.06258198526277	9.74126902804037	-3.19376302764027
C	-1.47732276690258	0.79332915533318	0.40440870787147
C	-14.02495205931453	6.40617710398384	-2.95717033183524
C	-13.39137730745143	0.82711500574071	-7.08866448707283
C	-12.33741588951995	1.70170137004574	-7.30553067469858
C	-14.37225584370405	4.78345866932990	-4.45500936785148
C	-1.09442234839298	-6.88111361177406	9.59798719842916
N	1.78568431317787	-1.32752189423412	5.45226795974739
C	1.99910048536809	-3.92291140802433	1.83213351940950
C	-11.98365191012491	2.56651466304624	-6.27494643637731
C	-2.27204963403851	-4.25210298071392	-0.67932742535852
C	2.35702014655368	-1.29820076505249	7.57071890590121
N	-1.05152826914261	-0.93464936516502	6.31192741571295
C	-3.91340671332026	-0.05140096183324	1.40403376086851
C	4.24763419833782	-1.92449410792279	1.11023183858311
C	-14.10315082794633	0.79598928498999	-5.89046964962932
C	-0.66757865068092	-4.98658435003510	8.03905762918061
C	-3.01153258470462	-4.74082455635022	1.54466793404223
C	-19.32052353872498	7.08195960969976	-2.15228661308835
C	3.52334333785812	-1.03639886065871	6.80557394200446
C	-11.04255774358993	7.51042676714730	1.37550997890234
C	-0.39166392857861	-4.54108250207090	6.74573892334145
C	1.79613856542288	-4.81384423503714	0.78073879249451
C	0.04614959865310	-4.64593556527361	4.55904617119715
C	-10.10763936727377	2.39138271455007	-3.71204500850117
C	3.70459110440933	-1.13224890798097	11.06581502412790
C	3.48235560707932	-6.29971955976835	1.67048858440976
C	-3.51686102825767	1.62630217414292	6.10698948113812
C	-17.39708107420118	10.15382594666129	-3.40252856775345
C	-16.65158050354814	8.07034865342277	-2.51349497093202
C	-2.75314252764693	-0.68757183950053	1.79037470904453
C	-7.47323248147667	1.71906351626373	-0.34261892449332
C	-11.09713057116604	3.35390837134759	-3.33489191377703
C	-0.61024259415763	-7.25555147402103	7.17867278435106
C	2.91341429437594	-4.26501329279728	2.83092492790361
C	-6.27631533236996	3.79388169601004	-0.31387186720431
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C	-2.47241866119536	-0.02850399178922	8.16970976358335
C	-6.30949044787957	1.04500045237886	-0.03124432037047
C	0.84416266552788	2.04657407953526	2.73339996740281
C	-1.78807934010505	0.30896101320141	4.68349407680698

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C	-9.19800784602226	5.99030055838228	2.03566645793747
C	-13.73239484546538	1.67522275922269	-4.88668570914625
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C	-4.01699504622681	1.05093898394919	9.79962189260994
C	4.74693641418195	-0.80932450873545	7.44253563501869
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C	-7.47452319422426	3.10434118987407	-0.48265004127895
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C	1.97324247733879	1.55239997975582	0.67385625641560
C	3.64077649976202	-5.43166760812248	2.75206673482731
C	2.94655185352846	2.94304251225978	11.52290163573301
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C	-14.94253120489176	12.74530266656572	-3.07692794988314
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C	-5.11305829442229	3.11849691925815	-0.00638003069778
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H	-0.53336457952041	1.11831325265343	-0.00640462557872
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H	-0.95776826052221	-6.13819555977251	10.38245659101314
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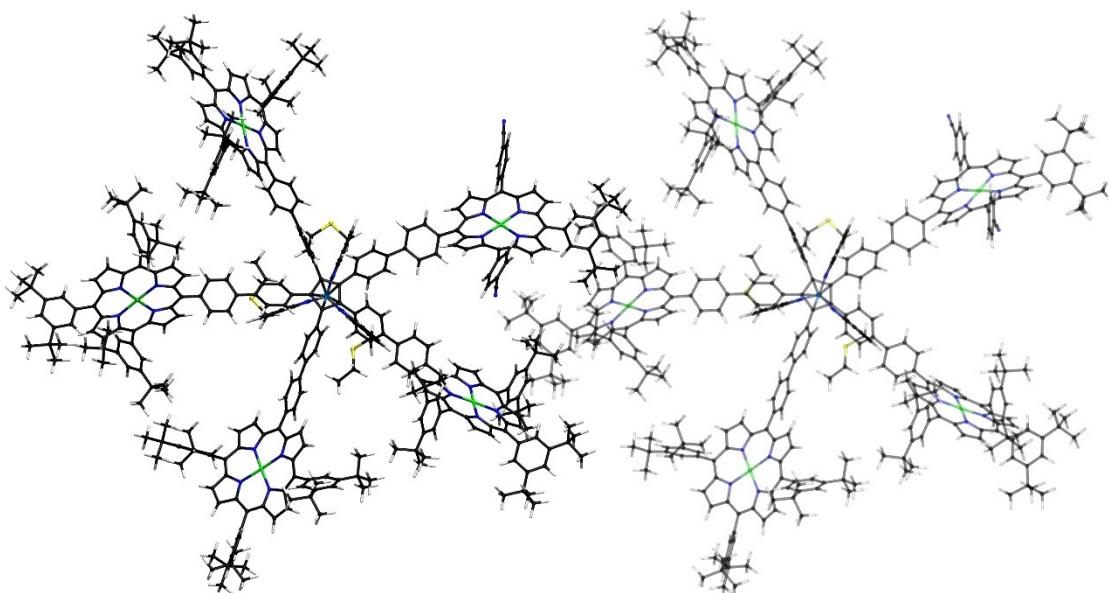
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H	45.08283411615464	-36.32966818853382	1.35728119456745
H	43.80750193613015	-37.54117796064882	1.27681534112489
H	43.53065491750090	-36.02220459555626	2.13287316451044
C	45.05025184233850	-33.89652877733057	0.08899822659264
H	45.83881475638199	-34.62741586722984	0.14017948101527
C	45.37497262734325	-32.54861108148282	0.11234357620152
C	46.80722551911682	-32.04352123735499	0.19952656008543
C	47.10680853188613	-31.18719151581693	-1.03915446940287
H	46.97856327922801	-31.77724294520062	-1.94471988644562
H	46.44646942890538	-30.32612153731151	-1.09652614219405
H	48.13271371438852	-30.82665169374426	-1.00602716795487
C	47.83537653815242	-33.17648390490069	0.25557169994271
H	47.78622164386806	-33.79614122913605	-0.63711359497861
H	47.68509781666394	-33.79978200407474	1.13424690068865
H	48.83614649184652	-32.75325057573119	0.31361255350404
C	46.96044905865870	-31.19518418498647	1.46947265681187
H	46.72799105573154	-31.79080144993063	2.35005742772221
H	46.29632457421189	-30.33546202285657	1.45542087989803
H	47.98286406654157	-30.83380350352308	1.55743700824938
C	44.33553888943910	-31.62720741188887	0.04579552985603
H	44.53397116368468	-30.56623963573329	0.07008635379396
H	41.62219799831804	-32.69930569155901	2.14709472859546
N	39.93525134299136	-30.09987827739650	0.95911767997349
H	36.17763204683484	-25.66200932661878	2.37115472156176
N	38.24543169332198	-27.89525507611522	1.04534389537253
C	38.47597969624670	-25.95284316832398	-1.13414762225942
C	37.76715907522694	-23.23611127326026	0.21110800270904
H	38.84616165402768	-23.27276318523932	0.16443851308155
C	37.11909229739917	-22.02423611008130	0.33560209455234
H	37.69535542651157	-21.11105488818993	0.36726578004839
C	38.94680491008141	-14.29485454597412	-0.95036208934910
C	39.28524628893005	-12.97560376963107	-1.24644929698863
H	38.53145915088339	-12.20415142253841	-1.18306694880056
C	40.56673257556564	-12.64619114034452	-1.63761796436931
H	40.81977088798204	-11.61812395669637	-1.85358023622588
C	41.55125814020630	-13.62593989386086	-1.73270655963303
C	42.93060637902083	-13.26680606311915	-2.10731854921705
C	43.17290601085468	-12.65759450397803	-3.33139896530876
C	42.14325616453801	-12.36857710956479	-4.28355662597562
C	42.71039356986014	-11.62549776337726	-5.25976373498646
H	42.25115476958339	-11.20231929478528	-6.13153207640808
C	44.09676316642579	-11.49519971127105	-4.92908972560469
C	44.99514574094830	-10.75951511721144	-5.68856692422799
C	44.49874244226984	-9.99008869237473	-6.84959602251529

C	44.47373854666862	-8.60119088364516	-6.79515664359233
H	44.82203944444804	-8.12453260071733	-5.89335195147954
C	44.00410999398756	-7.86458116431880	-7.87025979516088
C	43.95135640525981	-6.34392284852673	-7.86513535428565
C	44.86028355038873	-5.81088187043910	-8.98154365026925
H	45.88367488370428	-6.14633835108757	-8.82571383669889
H	44.53368614409749	-6.15733269652292	-9.95832125747232
H	44.85103185588279	-4.72284369921325	-8.98536874806479
C	42.50680321501032	-5.88544597300767	-8.10731161730015
H	42.45476607851096	-4.79884096373489	-8.09278928741892
H	42.13381760744978	-6.22947826293815	-9.06798074649311
H	41.85409380098063	-6.27427666058206	-7.32833883560263
C	44.42205785839747	-5.74317160451053	-6.53785039393804
H	45.45904056120489	-6.00081932571786	-6.33506259431246
H	44.34951904050019	-4.65815407572365	-6.58522297931572
H	43.80314089216953	-6.08814870465765	-5.71238416005311
C	43.57101291482347	-8.55362349271826	-9.00180802525234
H	43.21127475778284	-7.98280975527499	-9.84071864385815
C	43.58893924867610	-9.93755915316327	-9.08389267718428
C	43.11555205241051	-10.70049294692111	-10.31201504866133
C	41.96121684190930	-11.62789740629302	-9.90621223816759
H	41.13935408907905	-11.04665550536251	-9.49207800570197
H	42.27696110206658	-12.35222058021618	-9.16029844178139
H	41.59478869956476	-12.17240018361298	-10.77400020343370
C	42.61649495981174	-9.78015733614671	-11.42919686166402
H	41.76941871728388	-9.18367889499231	-11.09746361874021
H	43.40757097209731	-9.11870510201580	-11.77554057433735
C	44.28280893163231	-11.53143274968063	-10.86242024361978
H	44.63988421750626	-12.24870932813388	-10.12867065583463
H	43.96859500607309	-12.07870007009644	-11.74877951888892
H	45.11209789238762	-10.88118068714546	-11.13409348427453
C	44.05980450623733	-10.64913622571430	-7.98543807523832
H	44.10177909072846	-11.72794576516030	-8.00061170783242
C	46.35535461631749	-10.75991655261021	-5.41344844043650
C	47.31494055696107	-10.11534745436622	-6.25747896701876
H	47.06384537259908	-9.49656087794764	-7.09679399238102
C	48.53691610270216	-10.47817004995119	-5.80833318529761
C	48.32813927931718	-11.32104347423934	-4.67020891314518
C	49.36216250288327	-11.92492923418994	-3.96713627654852
C	49.12490710798889	-12.66898127407447	-2.81873033066646
N	47.91302750288393	-12.86044617680455	-2.20955307361440
Ni	46.14020281938239	-12.45342532678303	-2.95255275860546
N	45.29089230429778	-13.31765673429664	-1.40516373361987
C	45.90507431058577	-13.71082241229064	-0.24515770739293
C	47.27250887514853	-13.84170287691427	-0.04247416410199
C	47.76912318174409	-14.38709273870562	1.23444243351351
C	48.62062938134549	-13.62964486613733	2.02361304824437
H	48.88852114726868	-12.64050709844349	1.68381481300965
C	49.10632775399469	-14.12398123684010	3.22899922299987
C	50.04752757459873	-13.26146023556007	4.05656324292654
C	49.32754659080048	-11.96045506532145	4.43719709978338

H	49.03384507589872	-11.39723553331938	3.55581670048047
H	48.43171369533913	-12.18132495016708	5.01424954478088
H	49.98057999734453	-11.33297572731925	5.04030080916524
C	50.50560646695347	-13.94809020706517	5.34606966953531
H	49.66051592732848	-14.17092926513357	5.99368850920164
H	51.17711093319993	-13.28596759062939	5.88915052832214
H	51.04510037304301	-14.86786759940624	5.13081949328879
C	51.29285500369282	-12.94181091870401	3.21738656834594
H	51.03415151741191	-12.39501249446630	2.31472810126403
H	51.98843567976051	-12.33591325146536	3.79435722001159
H	51.79673202667144	-13.86176288220146	2.92668801075653
C	48.70858151068254	-15.39421074604732	3.61787687659151
C	47.85364253508116	-16.17923826860736	2.84595525039645
C	47.46411168849134	-17.56226244979873	3.34728548063373
C	48.73069606463450	-18.41483047679391	3.50514680403637
H	49.41421944949676	-17.98156593629724	4.23018030935630
H	49.25006712029859	-18.49525283782272	2.55231675172786
H	48.46911148522650	-19.41611394024089	3.84116653604614
C	46.75736698228366	-17.42280730259212	4.70308659676413
H	46.45200543837967	-18.40109763212831	5.06868189042048
H	47.40766957649350	-16.97093159971169	5.44697577123617
H	45.87025539494199	-16.80047759899038	4.60252985043450
C	46.51589709658555	-18.28964336017242	2.39018950729234
H	46.98046841145645	-18.44207099069389	1.41868178702459
H	46.26680402280033	-19.26679000633449	2.79971918976370
H	45.58931228335898	-17.73512340673128	2.25856025210053
H	49.07088770370439	-15.79652955702092	4.54840891237357
C	47.39154345561120	-15.66117051587218	1.64767639061087
H	46.74513933563654	-16.23189090609785	1.00118530650949
C	44.92637095318408	-14.06070601387022	0.73865904905041
H	45.15242654257261	-14.34957932889389	1.74629269487225
C	43.71648501371190	-13.94018364682521	0.14778532464283
H	42.74612917303477	-14.11019456791893	0.57205387323033
C	48.18879198507017	-13.49281779884695	-1.02782508640090
C	49.59298389225839	-13.74492558138842	-0.91558143264938
H	50.05550243709067	-14.25550456374545	-0.09378862199695
C	50.17303671843900	-13.23505719024492	-2.02510600543165
H	51.21200967806940	-13.22104340979658	-2.28996332287580
C	50.75431713849870	-11.74932493617384	-4.42860859013806
C	51.34972753592636	-10.49295337821199	-4.39309337334597
H	50.76904191151733	-9.66805654374327	-4.01362685094196
C	52.65643966906083	-10.32161342368688	-4.81934699797434
C	53.35404882439405	-8.96923106411609	-4.80657680495240
C	52.45280882525390	-7.84674510446129	-4.28495757292113
H	52.99928166544792	-6.90575385307021	-4.30208941400056
H	52.14405531551712	-8.03630752568105	-3.25949555827448
H	51.56823663961440	-7.73194642688460	-4.90747334495333
C	54.58954253990682	-9.05035629584026	-3.89926828522543
H	55.08981957555951	-8.08494045404702	-3.86013537887610
H	54.29557876359732	-9.32799035917320	-2.88902520827384
H	55.30154905655814	-9.78686911239783	-4.26143888286748

C	53.78059923009155	-8.61163894344859	-6.23737803963307
H	54.47802846808494	-9.34123410738190	-6.63950270212700
H	54.26359269830863	-7.63678372986730	-6.25154080091829
H	52.91125806441267	-8.57496160555076	-6.89094239017285
C	53.35257026629909	-11.43922388546360	-5.27664529182781
H	54.36913596327010	-11.30825612148632	-5.60581233941296
C	52.78526777879771	-12.70371094688797	-5.31913099835932
C	53.53799348393090	-13.93296286323213	-5.80585488876942
C	53.59330635996554	-14.96273838915145	-4.66836427922698
H	54.09840674046274	-14.53963029216851	-3.80196188587706
H	52.59720998684366	-15.27299166592554	-4.36469901744825
H	54.14134621319594	-15.84638986491340	-4.98875262776696
C	54.97393408980035	-13.62059190381322	-6.23552151903532
H	55.55321959490344	-13.21911906879909	-5.40689679461129
H	54.99117729607046	-12.91312312688501	-7.06158600899348
H	55.45839267599252	-14.53603262781363	-6.56949087684598
C	52.79669552413260	-14.52727317214263	-7.01128857178283
H	52.73521300786746	-13.79453251094387	-7.81351281744796
H	51.78653783334165	-14.82746983977274	-6.74720946919743
H	53.32582518320461	-15.40242579640546	-7.38281901958003
C	51.47022266463420	-12.84246527009857	-4.88844002155050
H	50.97876844096756	-13.80355754382416	-4.91103874800137
H	49.49913054623802	-10.21824469574969	-6.20357697816772
N	46.98848707832131	-11.47726058657926	-4.43441842893720
H	41.12474680102733	-12.69356819601954	-4.19861457969893
N	44.37149720826884	-12.15428223277563	-3.76095814259472
C	43.95123201950480	-13.49243090086690	-1.19119226986486
C	41.21565347362205	-14.94545230802617	-1.44307999707151
H	41.97248427606577	-15.71286783148897	-1.52097715583430
C	39.92972835662751	-15.27596236591144	-1.06543399993221
H	39.68840666053241	-16.30227428872038	-0.82874999542944
H	35.49165813529133	-33.05649711087852	4.54947973883683
H	36.93551147829005	-29.92133494434588	7.08272190505320
N	34.94495582063125	-32.61665509523166	7.93113068149197
N	42.18563726061966	-26.40575560488163	-9.85712852552755
H	42.40925097351029	-25.05581153333832	-6.68545953941550
H	40.69227972953358	-28.79810509891902	-7.85965947803304
H	20.28499154242096	-14.46999830856823	-5.46881646136173
H	19.59085213131993	-12.58939954357570	-10.22395871339991
H	41.97054595676867	-4.00353536337849	-5.26706821890474
H	42.29063417460202	-10.38244420260755	-12.27494324804499

**System of two intertwined cogwheels **11** with a Ru-Ru distance of 37.5 Å**



**Figure S13.** Optimised geometry of two intertwined cogwheels **11** with a Ru-Ru distance of 37.5 Å

Cartesian coordinates:

Ru	0.63121973107275	-1.76508772971725	3.80219919798458
Ni	-11.85598096212376	5.50152073780093	-0.61653406410306
S	3.96934068801599	0.36604108049171	11.32620831230118
S	-1.88996118140571	-7.33751973057583	10.25723479800497
N	-13.35853556844976	5.37465094119007	-1.88049222258986
N	-0.60127850496394	-0.71332778413420	5.15547441552957
N	-11.03507771037738	3.90074351408088	-1.42023772889188
C	-1.38233003020685	-0.13364715141158	7.12201855707451
S	-4.65150038097257	0.50670803798089	10.61199291390829
C	-9.81028132714796	3.36392850927672	-1.12476300961937
C	1.16584826642027	-2.81026880274678	1.82495688717166
C	-1.33953536777672	-3.47293162150658	1.49241562532264
C	-1.68513098046223	-0.43048478765799	1.53998499056303
N	-12.61674513057769	7.16352328531250	0.11330845711220
N	1.88701836591607	-1.49912550019805	6.53706464576225
C	1.10793632743704	3.21422595986778	2.33038975263643
C	-13.66136606640530	7.88767990241097	-0.39690038788955
H	-14.33962839622368	-0.15528867195474	-6.77099960083830
C	1.62653928217352	3.62812085079176	1.10578742752417
C	-12.89886894959709	9.09865974931179	1.32059962191505
C	-2.60092744517196	0.96524177175782	8.84067614211629
N	0.31628571373610	-3.45023414036471	5.02735112851997
C	-8.66596487453581	4.94890280342950	2.07316676309235

C	-15.65570645762410	8.37012234067635	-1.77003393214019
N	0.25728882030162	-3.32003309299367	6.36045114100435
C	-15.30881427796107	5.78105886954006	-3.02751723440112
C	-9.49788660334587	2.30822072752932	-2.04021075337553
C	1.93492081299037	2.66250218606859	0.14926866663571
C	1.86274107468797	-1.55908446913267	1.77540862765296
C	-18.02517437406411	8.80356088166011	-1.85872278379625
C	-0.41691998603312	-1.11378124279770	1.80874958782165
C	-13.83107724242080	9.10196766664021	0.34171241191596
C	-12.76534686695565	3.29610853434435	-3.06249046984115
C	2.30590450013092	-6.23313081025066	0.73536614885419
C	-9.00597945639347	3.69913342299172	-0.04301989669210
C	-10.34617989036545	6.39865354357751	1.81001340144804
C	-15.40138762008974	9.59521873446237	-2.36455117451020
C	-1.73913254307283	0.59602930252124	0.59718970806591
C	-14.38931902784770	6.26175580275495	-2.04155695478871
C	-14.01051685451286	0.54568717891856	-6.02310571757315
C	-12.96153407501687	1.40467069154651	-6.31387035145782
C	-14.83702758948427	4.58953794330165	-3.45602021332927
C	-0.16727838755084	-6.80347604438778	9.90609914199226
N	2.16021003693114	-1.39918004715144	5.22704556091117
C	1.84842119945303	-4.10906736221371	1.76864192559084
C	-12.55508262165161	2.29628869339701	-5.32663521772214
C	-2.65127105528566	-4.52357217255590	-0.22975284388350
C	3.02714572664497	-1.29917029118417	7.24044581424282
N	-0.52124148371398	-0.95448363367969	6.47151529172753
C	-4.05644564349531	-0.16766499651615	1.89834041669070
C	3.89207246959153	-2.20800945898569	0.51467362981836
C	-14.66694317450772	0.55604025774149	-4.79336848353061
C	0.05828827744570	-4.95773615989157	8.24833726950940
C	-3.18854710651122	-4.89776604712310	2.07384866352070
C	-19.62011642121109	7.04606817539350	-0.95360270872521
C	4.07130568298905	-1.06184437654486	6.30895459276535
C	-11.12903754271730	7.52057704858640	2.04418593509773
C	0.14396129987706	-4.55119512365860	6.91603472966022
C	1.52194090611476	-5.09940429218579	0.84562010804185
C	0.24147853978334	-4.72152227677027	4.69183879934246
C	-10.57103784426587	2.16027859163695	-2.84833260201636
C	4.85641807672781	-1.00943012131931	10.50077509782899
C	3.42955398205290	-6.40804845530848	1.53877688260117
C	-3.00098708886039	1.60008684858682	6.52996689801784
C	-17.73935805691508	10.03003257278463	-2.45612611560075
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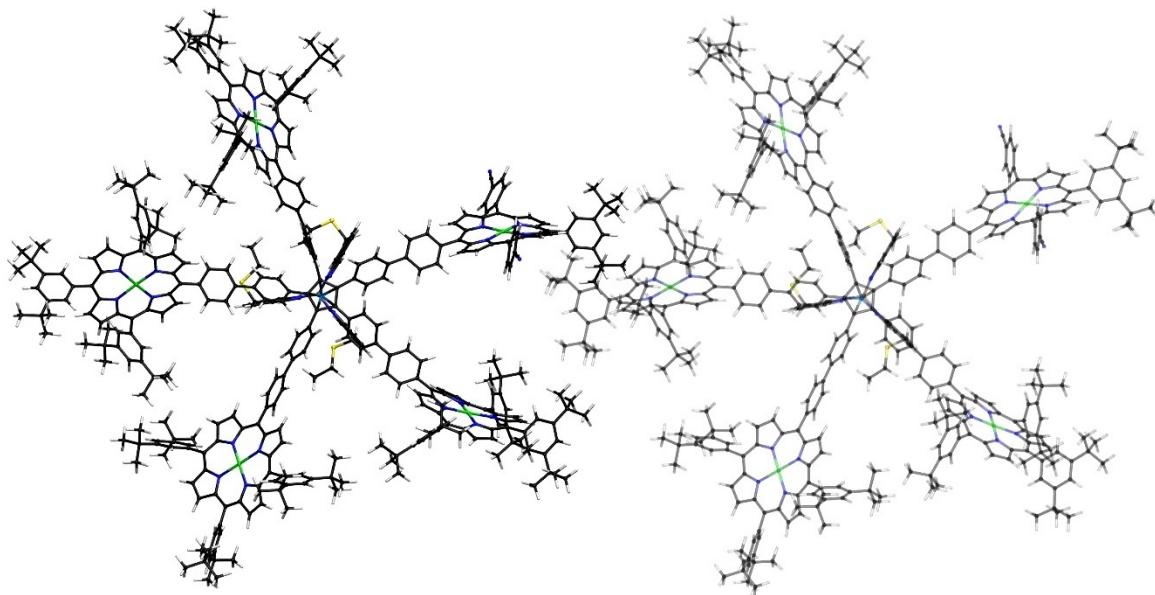
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C	55.47366163691675	-12.56462472616998	-5.80965501130274
H	56.14918330608049	-13.35268868564552	-6.13065810355965
H	55.97878784752919	-11.61002371507256	-5.94162626104142
H	54.59757091662268	-12.58294453790217	-6.45492710993256
C	54.99194199406921	-15.25041391784469	-4.52231225336597
H	56.00728458324315	-15.18349830224936	-4.87375409727647
C	54.39497452381883	-16.49701444658292	-4.41179458068970
C	55.11348040686995	-17.79251106023290	-4.75822353138690
C	55.15785512309753	-18.68374272810097	-3.50878769246772
H	55.68279021214542	-18.17509714231403	-2.70224299843272
H	54.15835589098825	-18.93172148404713	-3.16212667704739
H	55.68123864413877	-19.61196390201378	-3.72860268176873
C	56.55131242261306	-17.56732654900993	-5.23370765177772
H	57.14907514394874	-17.08610347051201	-4.46267954585075
H	56.57557308303831	-16.96171192507466	-6.13694433846730
H	57.01066943359116	-18.52697056171187	-5.46249856051234
C	54.34506994768651	-18.50502839540179	-5.87967592968656
H	54.29158233779445	-17.86952273619795	-6.76144756267307
H	53.33126178312854	-18.74772917285626	-5.57380727585422
H	54.84955516256695	-19.43013206395049	-6.15095247256061
C	53.08209051867805	-16.55254905562479	-3.95639720299130
H	52.56829601391720	-17.49747139352218	-3.86227164817067
H	51.16350902608667	-14.04022662295063	-5.54468621409022
N	48.64074861197918	-14.99983536696040	-3.61228409315355
H	42.73882075015096	-15.97096308735042	-3.21063555608094
N	46.01169070977939	-15.53493330388067	-2.85836085987236
C	45.58597355181031	-16.72235206656419	-0.21347741630817
C	42.82409152633223	-18.16347840138321	-0.43319773574364
H	43.57046731316302	-18.94265788110077	-0.49305714270977
C	41.52847866804230	-18.47062633952165	-0.06860835177717
H	41.26826615435250	-19.49082616323235	0.17446572089241
H	37.03587102639697	-36.32989828013280	4.63589936058794
H	38.11355135420727	-33.21973063105896	7.37390786228981
N	36.22086322642672	-36.04625587371283	7.98099720390107
N	44.31992531419554	-28.72383079777094	-8.99541352295994
H	44.37080748910514	-27.56285729891481	-5.74297940192468
H	42.71792752283702	-31.22345386747255	-7.22608394213077
H	21.63442043002856	-19.00175600795800	-8.24848499372417
H	20.88996053550963	-16.56882476465361	-9.19677979778647
H	44.18684929544423	-7.35440861712476	-4.98416963551927
H	43.74324071510404	-14.28001462253432	-11.39549884006272

**System of two intertwined cogwheels **11** with a Ru-Ru distance of 41.2 Å**



**Figure S14.** Optimised geometry of two intertwined cogwheels **11** with a Ru-Ru distance of 41.2 Å

Cartesian coordinates:

Ru	0.40335005207476	-1.05343890661140	3.79112489550819
Ni	-12.10131157852672	5.44803136075859	-1.35086640052651
S	2.86459691392013	1.59128578597754	11.49599072624094
S	-2.02996267295834	-6.68971312845225	10.23963126388304
N	-13.68516175048650	5.18405860921284	-2.48267892871870
N	-1.04359745999296	-0.10259398495763	5.00180825405350
N	-11.27388219881407	3.83240016959402	-2.11780492438070
C	-2.04070818407887	0.44370528632224	6.87822766026366
S	-5.63974917361607	0.81141435579875	10.06411750382564
C	-10.03382002176825	3.32510301258806	-1.83481688439581
C	1.20833652435998	-2.09913108404297	1.90420164270405
C	-1.21040097991045	-2.98526850502643	1.39478623102529
C	-1.80527832260596	-0.00528094483264	1.27581087171629
N	-12.85136329465068	7.14842395989959	-0.69439272645804
N	1.38974971550375	-0.57699501322423	6.60700954757198
C	0.47456159448873	3.88280518448841	2.31067061373553
C	-13.98369642807253	7.77671625545660	-1.13924382990678
H	-14.49630388744092	-0.44316071807385	-7.31867823475223
C	1.00358724587092	4.36660920421303	1.11689339861996
C	-13.03319403769947	9.22427913099820	0.27570733958567
C	-3.50700601248028	1.45075396380696	8.45392047614426
N	0.15894979239055	-2.72980576040763	5.05123484839117
C	-8.83799986605942	5.07270149348462	1.26143085720609
C	-16.17764439589919	8.00843423048559	-2.25239892362810

N	-0.01800690634758	-2.56802884819282	6.37037623468882
C	-15.77763309146211	5.38962778276349	-3.41165050227841
C	-9.70805972615495	2.27222341444292	-2.74789821840871
C	1.48704122031214	3.45332985485773	0.18126100256174
C	1.79183172910902	-0.78901791180232	1.86796562810930
C	-18.56245268295924	8.28640240662506	-2.04147305444876
C	-0.51262583871835	-0.55967117134888	1.68707960011415
C	-14.09773642839617	9.07368072981946	-0.54383213755437
C	-13.03521747021625	3.13754369528128	-3.68720105777483
C	2.61036709852310	-5.51086465293781	1.12786194388320
C	-9.22317442812548	3.69474182926809	-0.76960261661250
C	-10.45315881857374	6.56822702290775	0.87689103221280
C	-16.09749335789386	9.18208070273096	-2.98378418138535
C	-1.85674547849196	0.96200897957490	0.27251117565687
C	-14.79982864644304	5.97706794054586	-2.54659603789051
C	-14.19581066362891	0.28778061271959	-6.58759911205649
C	-13.22740922693164	1.22225014390254	-6.92184075450523
C	-15.24425036847320	4.24159245498603	-3.88444067040384
C	-0.35567813148248	-5.97129980233977	10.00226820112561
N	1.75342109669562	-0.47643043523025	5.31949248333331
C	1.98659392572409	-3.34289252810485	1.96718443595253
C	-12.85701562112935	2.15204472248141	-5.95608419863169
C	-2.37940822342778	-4.12416636101106	-0.37375176821731
C	2.44050544928672	-0.23170492853548	7.38885348641221
N	-1.04850537790798	-0.29880976649545	6.32799039841794
C	-4.21037795030371	0.08819322477994	1.43094226134756
C	3.99805960577241	-1.33137796141958	0.88654886402223
C	-14.80492533192847	0.25771195646504	-5.33402995847344
C	-0.19509105951182	-4.16143283332309	8.29796883587973
C	-3.0129900411209	-4.49426811482732	1.90553485136824
C	-19.88825167735737	6.52592617028304	-0.77857492985083
C	3.52126221349114	0.10508830913340	6.53262681571787
C	-11.17579534689434	7.74774146317849	1.00350978020281
C	-0.04753611067851	-3.78730278597302	6.96156472359743
C	1.78155645998130	-4.40468109268897	1.08941571725128
C	0.24009899952981	-4.01135174715947	4.75885390895546
C	-10.78435083350937	2.10083149724579	-3.54762786100455
C	3.96713533654269	0.32036723222830	10.76911221994535
C	3.66260751312689	-5.58733486495207	2.03632970154182
C	-3.77369104915726	1.98178425445204	6.09830567608963
C	-18.45106163527556	9.46593235615535	-2.77573521680778
C	-17.40917520907997	7.56381225721468	-1.78363911230259
C	-3.00524089827566	-0.44986788441843	1.83149182558770
C	-7.91370401020385	1.61855457414908	-0.28069580829693
C	-11.75874131543402	3.06949898321612	-3.14614826311912
C	-0.02853804019497	-6.47443124396685	7.58058013865295
C	2.99970341871057	-3.45039594963760	2.92436103628843
C	-6.76633444238689	3.71372184716117	-0.46797420433160

C	-3.06347278771590	1.49491897368759	-0.12744290581472
C	-2.45236170494051	0.59937836468333	8.20231935070682
C	-6.71859279304173	0.99368007068512	0.01759924076216
C	0.40149495898444	2.52534501722085	2.54710120025692
C	-1.99944341357050	0.73745039003486	4.66517004747406
C	5.31840383960373	-1.03237234485403	0.63329165480526
C	-4.16271483185425	2.12555091304088	7.40271073482996
C	3.19886255364583	-0.46558811196316	1.63764872986730
C	-9.38377482368871	6.20630520662955	1.75576701617473
C	-14.41540528736901	1.19771608060760	-4.39413052383346
C	-17.23655519513377	9.93250241771848	-3.25500611455889
C	3.00568680210273	-0.08237288376638	5.23386118956161
C	3.76243120496054	0.73804801593673	2.07086084365059
C	-4.26056898476895	1.08389309798451	0.45674433695410
C	-12.27921528897713	8.01039466947301	0.20270830378884
C	-2.69435372751816	1.13365126369931	5.82548318826644
C	3.54834968441454	3.06815606529561	10.66235630893976
C	-4.01359868525786	1.63345996218935	9.84501085516260
C	4.74579012900357	0.51143575511888	7.07100033058440
C	3.79370584535620	0.22265333813980	9.28804894432573
C	2.57710706868596	-0.17293860613068	8.77370979257688
C	-7.95600887201431	2.98992801264051	-0.51503990296958
C	-9.57177612188192	4.74101244162206	0.07786524662787
C	-0.17246873799452	-5.50694079319724	8.59770825160891
C	1.42281326327097	2.09562536990918	0.41877570415617
C	3.82584236200057	-4.54939251660838	2.95486217301604
C	2.75288132654243	4.30002040582891	11.04552506592002
C	-3.06821700891174	-5.21582957680192	9.96922961425089
C	-16.15537650988583	12.17122649356647	-3.30563506626735
N	-10.59563554365067	5.62912046492900	-0.10898401639772
C	-18.43749040801783	11.93980445196169	-4.25474938419321
C	4.86194333415374	0.56781193133126	8.43604376425888
C	-5.57380308762980	3.08829499093114	-0.17325810642615
C	-5.53057321861049	1.71888124925715	0.08648441593083
C	5.89262186309754	0.14775936083975	1.10407708739723
C	5.08475020360195	1.03558540995480	1.81073080078314
C	-13.44195542892816	2.14202020998013	-4.70095214432787
C	-3.21103860864516	-4.75217305899811	0.55156016401843
C	-16.52208155168219	10.89079020988741	-5.43620967208563
C	-17.10099073599151	11.22049677372676	-4.05343331206875
C	-1.39578536981077	-3.24959656630067	0.03978426851041
C	-2.02931560426498	-3.61908754241770	2.32082284098083
C	-20.85575299110444	7.64669948175649	-2.77037246063766
C	0.85835168119113	1.61621456123672	1.59959905913637
C	-19.93543500643092	7.84332154751825	-1.55730926385849
B	0.02140360954332	-1.16464875081742	7.00409818529985
C	0.11072505833140	-4.76250281221313	5.94378932973842
C	0.11434035947881	-6.12468167586681	6.26529678709444

C	-0.22073011459192	-1.95706294356116	1.77358380520147
C	0.71938701164527	0.16665461864141	1.82241022378552
C	-13.93620165865351	4.12590702879586	-3.31448083740654
C	-14.95377380098704	7.23060122016675	-1.96948438908654
C	-3.06772653197266	-4.27652238325510	11.16009928202229
C	-20.51448286187415	8.92395025583714	-0.63362204148906
C	-5.11063321531987	-0.92413952845821	9.84143109490728
C	-6.31260923903112	-1.84697833363817	9.88296575475471
H	0.09724874973152	4.57577749769455	3.04878924197163
H	-12.76821539694878	10.06872703395529	0.88132206860492
H	-8.02774255242228	4.49466460708248	1.66072533565475
H	-16.73283623328292	5.82418005910387	-3.63207342779588
H	-8.77543280614269	1.74282407051931	-2.76086211675811
H	1.93030159186640	3.81458014939865	-0.73567855988132
H	-14.89729842723297	9.76242116563511	-0.73398564724529
H	2.46096544717532	-6.30981030826771	0.41573340366369
H	-15.12960565229163	9.49490618812555	-3.345878949474960
H	-0.94564032878503	1.29229708313238	-0.20248725826290
H	-15.67071485371666	3.53806574771728	-4.57233076262123
H	-0.22898752373867	-5.16628739442501	10.72466414473700
H	0.31893270004823	-6.79043488055718	10.24776711329547
H	-12.11452698426464	2.90642037786800	-6.16935880093370
H	-2.53074536489069	-4.29490673559949	-1.42982560228548
H	-5.12227361604243	-0.24272447437538	1.90612131905926
H	3.57505139496036	-2.23780312619637	0.48076929660499
H	-0.30491093357426	-3.41534662386699	9.06941268468877
H	-3.63430842827879	-4.98488419287255	2.64078666339363
H	-19.50277512893768	5.71811149176138	-1.39662422083937
H	-20.89388886349029	6.25563592985903	-0.46224015421352
H	-19.27045150635745	6.61847536620579	0.11166466633542
H	0.98755436416756	-4.35275171596441	0.35864369262817
H	0.38403689418332	-4.36755926905423	3.75527524027529
H	-10.92397677833551	1.38895805101756	-4.33730888355232
H	4.99118916704510	0.57269886829704	11.04561208438481
H	3.67498333683620	-0.60415294440117	11.26698292567360
H	-19.34603940648561	10.03043448374536	-2.97406787660540
H	-17.43281527977124	6.65188198225508	-1.20962083525366
H	-2.98338153679093	-1.19544406915042	2.61414030438920
H	-8.83027476726436	1.04690485465127	-0.30799569364560
H	-0.03987195380047	-7.51556367497004	7.86753401922568
H	3.12245368830848	-2.65502001660832	3.65198831016133
H	-6.78575374775749	4.77603970921556	-0.66472301554077
H	-3.07861515668429	2.23322978876489	-0.91576406270619
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H	0.00384469896164	2.15172193891980	3.48385942257014
H	-2.17837152398134	1.03423672552311	3.64816014002013
H	5.90984852298785	-1.71262850000830	0.03779962704334

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H	-9.11185573225174	6.74937074224830	2.63956540787651
H	-14.84539815969158	1.21793872201750	-3.40604568743589
H	3.50633872162845	0.04953649473965	4.29252314342633
H	3.15879711573856	1.44629273034995	2.62102229286487
H	3.49961205748953	2.88363204133694	9.58804149544650
H	4.59137635136040	3.16174337461169	10.96993651335815
H	-4.21054925456291	2.68142337550526	10.06775323815971
H	-3.33127169856252	1.22178480635930	10.58884402824573
H	5.56927330925338	0.77496177785062	6.42468253295560
H	1.75658236106675	-0.41531343624946	9.42933662330040
H	1.80335087686088	1.39617899352094	-0.31366336760424
H	4.60050077320056	-4.61627252436055	3.70487929873516
H	1.71312541465574	4.18553814635436	10.74805397336953
H	3.16523854689613	5.17700928168620	10.55059795876140
H	2.78782065688388	4.45487704014841	12.12141284152159
H	-4.06665822493616	-5.61296800165287	9.78890414347579
H	-2.70899364009835	-4.72528790177443	9.06327039011532
H	-16.05676821533463	13.10768704501669	-3.85082307079395
H	-15.16489417351697	11.73896506624648	-3.19274772687079
H	-16.54815528290407	12.38966202756729	-2.31425827991080
H	-18.27473799750194	12.85159631742879	-4.82614625707670
H	-18.88123784412952	12.21754609488142	-3.30116549075010
H	-19.13771713003932	11.31887835158648	-4.80911389606896
H	5.79644247395267	0.88005854135469	8.88043322954672
H	-4.66759213512915	3.67317175376009	-0.11185736981709
H	5.50190936381408	1.96084690676774	2.18151172326218
H	-16.42690936050532	11.79809246303644	-6.02926790501926
H	-17.17783403636034	10.20069294578165	-5.96349523311190
H	-15.54042627724771	10.43227954782717	-5.35599047498357
H	-0.77765286850719	-2.74393761038443	-0.69032073925569
H	-1.90570209503290	-3.40186985441398	3.37498946835728
H	-21.83698347357139	7.30747446626519	-2.44485213660376
H	-20.43811106290104	6.89915024354180	-3.44192701926408
H	0.22894449338237	-6.86852562469637	5.49171138259834
H	-3.38266765872996	-4.80464395701521	12.05713661042768
H	-3.75435799686684	-3.45181512955105	10.98056419164956
H	-2.07558657796316	-3.86459488467074	11.33252809693844
H	-20.63512882445520	9.86983278380508	-1.15459136237456
H	-19.85396730034955	9.08429663709509	0.21611276418179
H	-21.48863987252367	8.61511533634593	-0.26012223387717
H	-4.40809294372671	-1.15114959376839	10.64594316900622
H	-4.59678743503513	-0.98696864783833	8.88064442775951
H	-6.81853454973876	-1.76982297097122	10.84257573760589
H	-5.99828622037158	-2.87830286809721	9.73242655774242
H	-7.01870184885708	-1.57968213243191	9.10040484350619
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