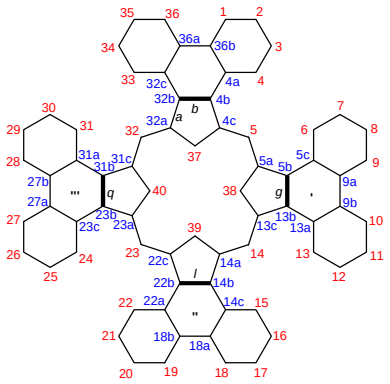
Peripherally Fused Porphyrins via the Scholl Reaction:
Synthesis, Self-assembly, and Mesomorphism

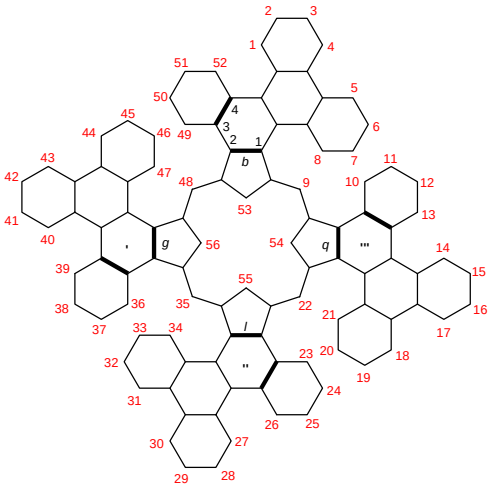
by Damian Myśliwiec, Bertrand Donnio, Piotr J. Chmielewski, Benoît Heinrich, and Marcin Stępień*

Supporting Information

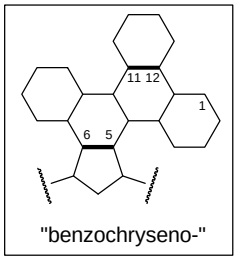
Table of contents



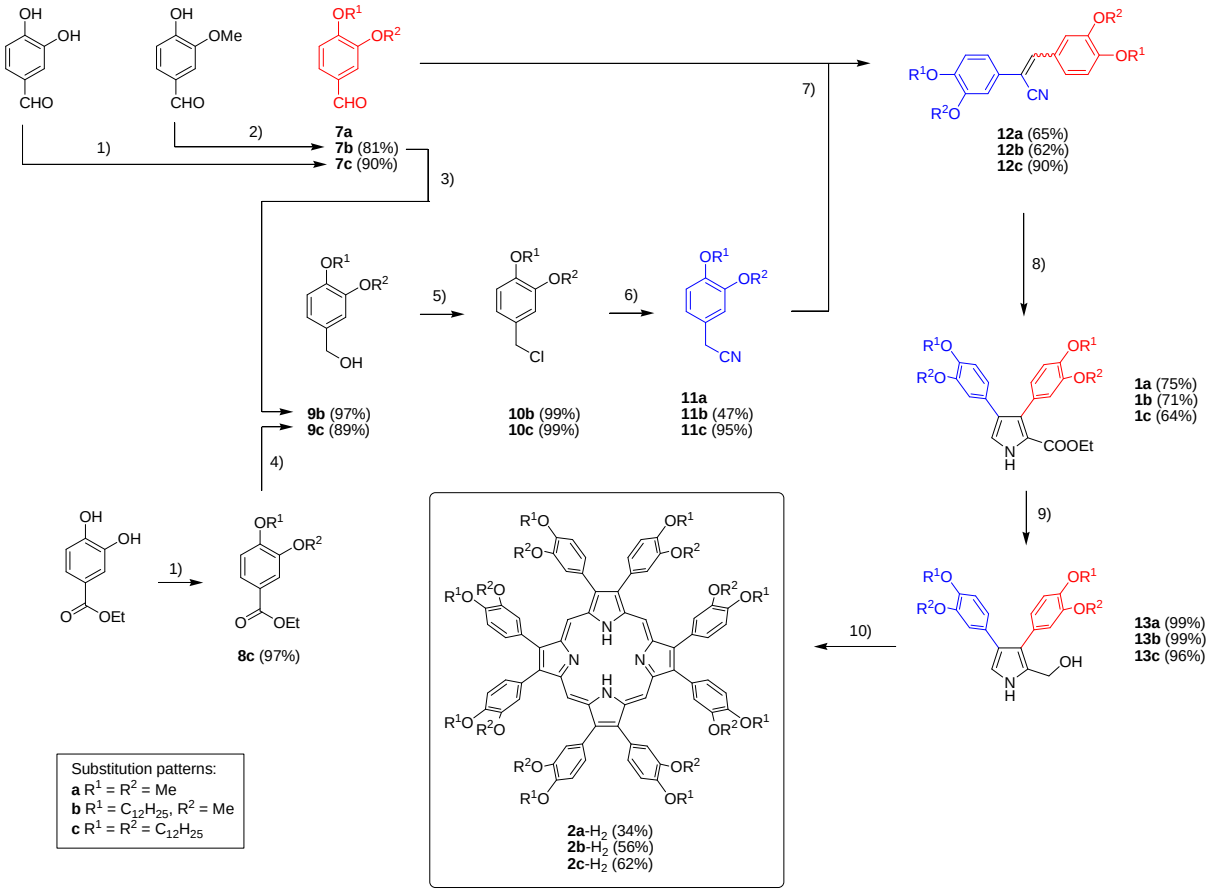
tetraphenantro-
[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrin



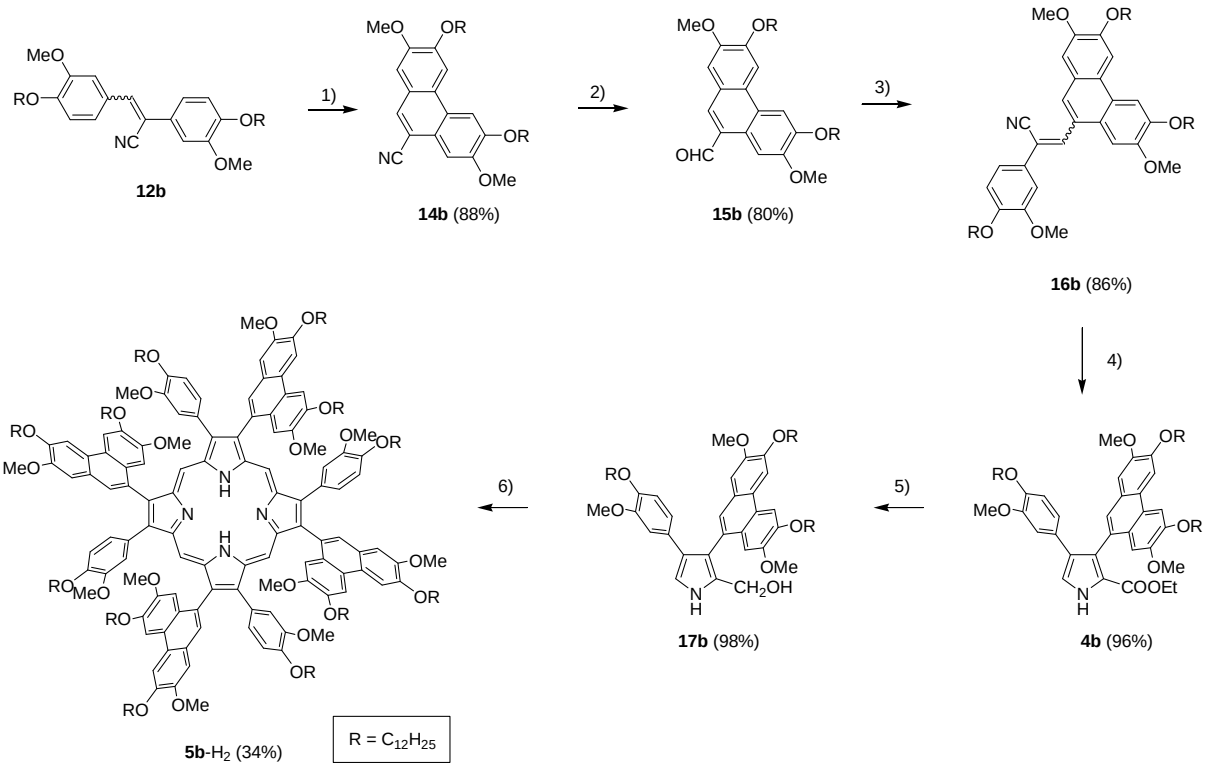
tetrabenzo[3,4:3',4':3'',4'':3''',4''']tetrakistriphenyleno-
[1,2-*b*:1',2'-*g*:1'',2''-*l*:1''',2'''-*q*]porphyrin
"tetra(benzochryseno)porphyrin"



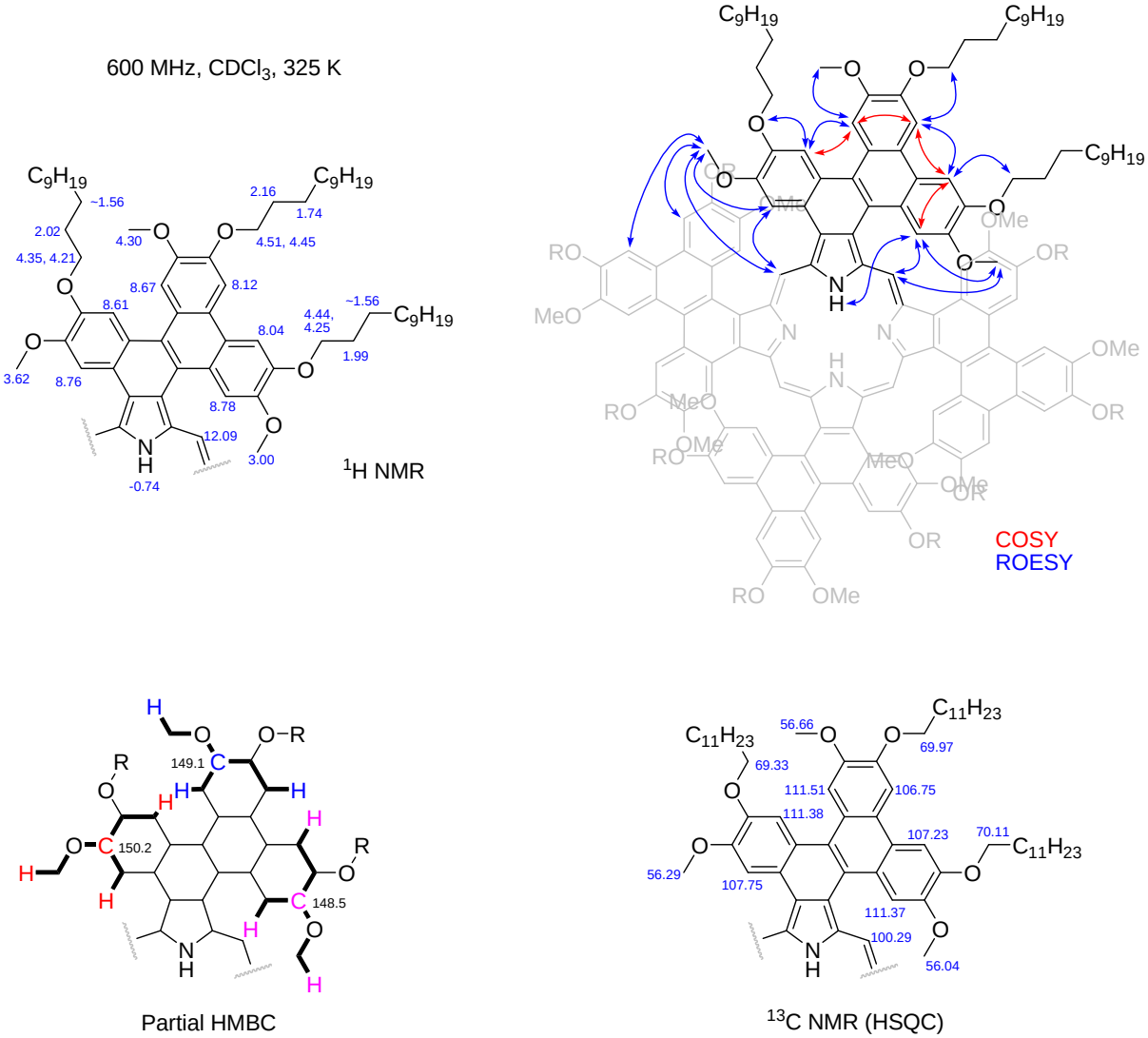
Scheme S1. Numbering scheme for tetraphenanthro- and tetra(benzochryseno)porphyrins. Thick lines show the boundaries of attached components. Locants for quaternary centers are indicated only for tetraphenanthroporphyrin.



Scheme S2. Synthesis of porphyrins **2a-c**-H_2. Reagents and conditions: 1) $C_{12}H_{25}Br$ (2.2 equiv.), K_2CO_3, DMF; 2) $C_{12}H_{25}Br$ (1.1 equiv.), K_2CO_3, DMF; 3) $NaBH_4$, THF; 4) $LiAlH_4$, THF; 5) $SOCl_2$, DCM; 6) KCN, water/DMF or NaCN, DMF; 7) EtONa, EtOH; 8) $CNCH_2COOEt$, *t*-BuOK, THF; 9) $LiAlH_4$, THF; 10) $BF_3{\cdot}Et_2O$, $CHCl_3$, then DDQ.



Scheme S3. Synthesis of porphyrins **2a-c**-H_2. Reagents and conditions: 1)$FeCl_3$, MCPBA, CH_2Cl_2; 2) DIBAL-H, CH_2Cl_2; 3) **11b**, EtONa, EtOH; 4) $CNCH_2COOEt$, *t*-BuOK, THF; 5) $LiAlH_4$, THF; 6) $BF_3{\cdot}Et_2O$, $CHCl_3$, then chloranil.



Scheme S4. Correlation data derived from COSY, ROESY, ^{1}H-^{13}C HSQC and HMBC spectra, used in the analysis of the ^{1}H NMR spectrum of tetra(benzochryseno)porphyrin **6b**-H_2.

Experimental

General. Tetrahydrofuran and N,N-dimethylformamide were dried using a commercial solvent purification system. Dichloromethane was distilled from calcium hydride when used as a reaction solvent. All other solvents and reagents were used as received. Compounds **7a** and **11a** are commercially available and were used as received. ^{1}H NMR spectra were recorded on high-field spectrometers (^{1}H frequency 500.13 or 600.13 MHz), equipped with broadband inverse gradient probeheads. Spectra were referenced to the residual solvent signals (chloroform-*d*, 7.24 ppm, toluene-d_8 2.09 ppm). Two-dimensional NMR spectra were recorded with 2048 data points in the t_2 domain and up to 2048 points in the t_1 domain, with a 1 s recovery delay. All 2D spectra were recorded with gradient selection, with the exception of NOESY and ROESY. NOESY mixing time and ROESY spinlock time were 500 ms and 300 ms, respectively. ^{13}C NMR spectra were recorded with ^{1}H broadband decoupling and referenced to solvent signals ($^{13}CDCl_3$, 77.0 ppm). High resolution mass spectra were recorded using electrospray ionization in the positive mode. Electrochemical measurements (CH_2Cl_2, 0.1M TBAP) were performed on an EA9C Multifunctional Electrochemical Analyzer using a glassy-carbon working electrode, platinum wire as the auxiliary electrode, and silver wire as a reference electrode. The voltammograms were referenced against the halfwave potential of Fc/Fc^+.

LC characterization. TGA measurements were carried out on a SDTQ 600 apparatus at scanning rate of 10°C min^{-1}. Transition temperatures and enthalpies were measured by differential scanning calorimetry with a TA Instruments DSC-Q1000 instrument operated at a scanning rates of 2 to 10 °C min^{-1} on heating and on cooling. The apparatus was calibrated with indium (156.6 °C; 28.4J·g^{-1}) and gallium (29.8 °C) as the standards. The XRD patterns were obtained with a transmission Debye-Scherrer-like (III) geometry. A linear monochromatic Cu-Kα_1 beam (λ = 1.5405Å) was obtained using a sealed-tube generator (900W) equipped with a bent quartz monochromator. The crude powder was filled in Lindemann capillaries of 1mm diameter and 10μm wall-thickness. In each case, exposure times were varied from 1 to 24h. The first set of diffraction patterns was recorded with a curved Inel CPS120 counter gas-filled detector linked to a data acquisition computer (periodicities up to 60Å) and can be measured on image plates (periodicities up to 100Å); the sample temperature controlled to within ±0.05°C in the 20 to 200°C temperature range. Derivation of cell parameters of the columnar phases and molecular volume estimation were performed using previously described methods[1] (see footnotes in tables for specific formulas).

Computational methods. Density functional theory (DFT and TD-DFT) calculations were performed using Gaussian 09.[2] DFT geometry optimizations were carried out in unconstrained C_1 symmetry,

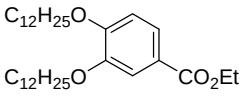
[1] Stępień, M.; Donnio, B.; Sessler, J. L. *Chem. Eur. J.* **2007**, *13*, 6853-6863.

[2] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

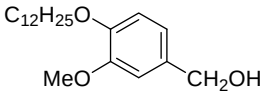
using MM+ models as starting geometries. DFT geometries were refined to meet standard convergence criteria, and whenever technically feasible, the existence of a local minimum was verified by a normal mode frequency calculation. DFT calculations were performed using the hybrid functional B3LYP,[3] combined with the 6-31G(d,p) basis set. The electronic spectra were simulated by means of time-dependent density functional theory (TD-DFT), using a variable number of states dependent on the convergence performance of the method. For these calculations the 6-311G(d,p) basis set was used in conjunction with geometries optimized at the lower level. The dimerization energies of [**3a**-Zn]$_2$ and [**3a**-H$_2$]$_2$ (ωB97XD/6-31G**), were calculated relative to monomer molecules, with all structures optimized at the same level of theory. The resulting energies contain a counterpoise correction but the y do not include. Molecular mechanics calculations were performed using the MM+ force field available in HyperChem.[4] Default atom types and parameters were used. Zinc centers were however restrained to yield slightly distorted square planar geometries observed in the DFT structures.

[3] Becke, A. D. *Phys. Rev.* **1988**, *38*, 3098. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev.* **1988**, *37*, 785.
[4] Hyperchem 8, Hypercube 2007.

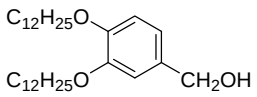
Synthesis



Ethyl 3,4-bis(dodecyloxy)benzoate (8c) was prepared following a literature procedure.[5] Yield 97%. **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 7.62 (dd, 1H, ^3J = 8.4 Hz, ^4J = 1.9 Hz), 7.52 (d, 1H, ^4J = 2.09 Hz), 6.84 (d, 1H, ^3J = 8.4 Hz), 4.32 (q, 2H, ^3J = 7.20 Hz), 4.02 (2 × t, 2 × 4H, ^3J = 6.61 Hz), 1.80 (m, 4H), 1.45 (m, 4H), 1.35 (t, 3H, ^3J = 7.04 Hz), 1.33 (m, 4H), 1.29–1.24 (m, 32H), 0.86 (t, 6H, ^3J = 6.96 Hz).**^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 166.54, 153.16, 148.52, 123.45, 122.81, 114.37, 111.97, 69.32, 69.03, 60.68, 31.92, 29.69, 29.67, 29.66, 29.63, 29.61, 29.42, 29.38, 29.36, 29.21, 29.09, 26.02, 25.98, 22.69, 14.41, 14.11.

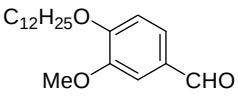


(4-(Dodecyloxy)-3-methoxyphenyl)methanol (9b). Sodium borohydride (14.17 g, 0.37 mol) was suspended in tetrahydrofuran (100 mL). The suspension was stirred under nitrogen and cooled to 0 °C. Compound **7b** (4 g, 0.012 mol) was then added in portions. The reaction mixture was allowed to warm to room temperature and was stirred for 48 h, after wihich time it became semi-solid. The mixture was heated so as to dissolve the solid and poured into water (100 mL). dilute hydrochloric acid was then added (1 M, 50 mL), and the mixture was extracted with dichloromethane. Combined extracts were dried with anhydrous sodium sulfate and filtered. Solvents were removed on a rotary evaporator yielding a white solid (19.53 g, 97%) which was used without further purification. **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 6.91 (d, 1H, ^3J = 1.75 Hz), 6.86–6.82 (m, 2H), 4.59 (b, 2H, ^3J = 6.1 Hz), 3.98 (t, 2H, ^3J = 6.9 Hz), 3.85 (s, 3H), 1.81 (m, 2H), 1.42 (m, 2H), 1.32 (m, 2H), 1.31–1.24 (m, 16H), 0.83 (t, 3H, ^3J = 6.8 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 149.58, 148.21, 133.52, 119.43, 112.89, 110.97, 69.18, 65.37, 55.96, 31.90, 29.64, 29.61, 29.58, 29.54, 29.39, 29.32, 29.16, 25.94, 22.66, 14.09.

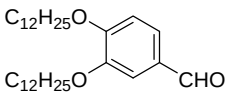


(3,4-Bis(dodecyloxy)phenyl)methanol (9c). In a round-bottomed flask equipped with a stirring bar, lithium aluminium hydride (15.37 g, 0.405 mol) was suspended in tetrahydrofuran (300 mL) and purged with nitrogen. A solution of **8b** (70 g, 0.135 mol) in tetrahydrofuran (500 mL) was prepared, purged with nitrogen, and added dropwise via a cannula to the well stirred reaction mixture. The mixture was stirred at room temperature for 1 h. Subsequently, the reaction was quenched by dropwise addition of water (13 mL), aqueous NaOH (15%, 18 mL) and again water (39 mL). The precipitate was filtered off and washed repeatedly with tetrahydrofuran. The filtrates were combined and the solvent was removed on a rotary evaporator. The crude product was crystallized from acetone, yielding colorless crystals (57.6 g, 89%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 6.90 (~s, 1H), 6.85–6.82 (~s, 2H), 4.58 (d, 2H, *J* = 6.0 Hz), 3.97 (m, 4H), 1.79 (m, 4H), 1.51 (t, 1H, ^3J = 6.14), 1.44 (m, 4H), 1.32 (m, 2H), 1.34–1.24 (m, 32H), 0.86 (t, 6H, ^3J = 6.9 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 149.40, 148.78, 133.74, 119.60, 113.96, 113.07, 69.47, 69.27, 65.38, 31.92, 29.69, 29.65, 29.63, 29.43, 29.36, 29.32, 26.04, 26.03, 22.68, 14.09.

[5] Percec, V.; Ahn, C. H.; Bera, T. K.; Ungar, G.; Yeardley, D. J. P. *Chem. Eur. J.* **1999**, *5*, 1070.

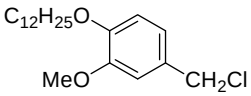


4-(Dodecyloxy)-3-methoxybenzaldehyde (7b) was obtained according to the procedure described for **7c**, using vanillin (20 g, 0.13 mol), 1-bromodecane (35 mL, 0.14 mol), N,N-dimethylformamide (660 mL), and anhydrous potassium carbonate (109 g, 0.79 mol). The reaction was carried out for 48 h at 65 °C, and the product was crystallized from ethanol. Colorless crystals (34.3 g, 81%). ^{1}H NMR (500 MHz, chloroform-*d*, 300 K): δ 9.83 (s, 1H), 7.41 (dd, 1H, ^{3}J = 8.10 Hz, ^{4}J = 1.9 Hz), 7.38 (d, 1H, ^{4}J = 1.9 Hz), 1.69 (d, 1H, ^{3}J = 8.2 Hz), 4.08 (t, 2H, ^{3}J = 6.9 Hz), 3.90 (s, 3H), 1.86 (m, 2H), 1.34 (m, 2H), 1.31–1.24 (m, 16H), 0.86 (t, 3H, ^{3}J = 6.9 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 190.93, 154.20, 149.84, 129.84, 126.81, 111.34, 109.23, 69.19, 56.03, 31.90, 29.63, 29.62, 29.56, 29.51, 29.33, 28.90, 25.88, 22.67, 14.10.



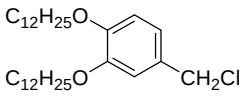
3,4-Bis(dodecyloxy)benzaldehyde (7c). 3,4-Dihydroxybenzaldehyde (4 g, 28.9 mmol) and 1-bromododecane (16 mL, 66 mmol) were dissolved in N,N-dimethylformamide (140 mL). The solution was purged with nitrogen for 15 min. and anhydrous potassium carbonate (15.9 g, 115. 6 mmol) was added. The mixture was stirred at 60 °C for 16 h. The mixture was allowed to cool to room temperature and poured into an ice-water mixture. A precipitate formed, which was filtered under reduced pressure and washed several times with water. The crude product was crystallized from acetone, yielding colorless crystals (12.4 g, 90%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ (9.8 (s, 1H), 7.39 (dd, 1H, ^{3}J = 8.2 Hz, ^{4}J = 1.9 Hz), 7.37 (d, 1H, ^{4}J = 1.9 Hz), 6.93 (d, 1H, ^{3}J = 8.2 Hz), 4.06 (t, 2H, ^{3}J = 6.7 Hz), 4.03 (t, 2H, ^{3}J = 6.7 Hz), 1.83 (m, 4H), 1.45 (m, 4H), 1.33 (m, 4H), 1.31–1.24 (m, 32H), 0.86 (t, 6H, *J* = 6.86 Hz). **^{13}C NMR** (151 MHz, chloroform-*d*, 300K): δ 190.99, 154.70, 149.46, 129.88, 126.57, 111.78, 111.01, 69.15, 69.13, 31.92, 29.69, 29.68, 29.65, 29.61, 29.60, 29.59, 29.38, 29.36, 29.07, 28.99, 25.99, 25.95, 22.68, 14.10.

General procedure for the synthesis of benzyl chlorides 10. Benzyl alcohol **9** was dissolved in freshly distilled dichloromethane, to which a catalytic amount of N,N-dimethylformamide was added. With continuous stirring, thionyl chloride (1.2 equiv.) was added to the reaction mixture. After 1 h of stirring, the solvent and excess thionyl chloride were removed on a rotary evaporator. The product was used in the next step without further purification.



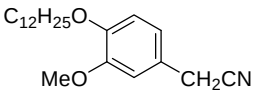
4-(Chloromethyl)-1-(dodecyloxy)-2-methoxybenzene (10b). Obtained from **9b** (19.53 g, 60.6 mmol) and thionyl chloride (7.3 mL, 101 mmol) in dichloromethane (190 mL, 0.1 mL N,N-dimethylformamide added). White solid (20.4 g, 99%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 6.90–6.87 (m, 2H), 6.80 (d, 1H, ^{3}J =6.8 Hz), 4.54 (s, 2H), 3.99 (t, 2H, ^{3}J = 6.81 Hz), 3.86 (s, 3H), 1.81 (m, 2H), 1.42 (m, 2H), 1.33–1.24 (m, 16H), 0.86 (t, 3H, ^{3}J =6.90 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 149.54, 148.87, 129.86, 121.16, 112.62, 112.21, 69.10, 56.03, 46.74, 31.91, 29.65, 29.62, 29.58, 29.55, 29.38, 29.33, 29.11, 25.94, 22.68, 14.10.

4-(Chloromethyl)-1,2-bis(dodecyloxy)benzene (10c). Obtained from **9c** (30 g, 63 mmol) and thionyl chloride (6.4 mL, 88 mmol) in dichloromethane (180 mL, 0.1 mL N,N-dimethylformamide added). White solid (30.9 g, 99%). ^{1}H NMR (500 MHz, chloroform-*d*, 300 K): δ 6.89 (d, 1H, ^4J = 2.1 Hz), 6.87 (dd, 1H, ^3J = 8.12 Hz, ^4J = 2.1 Hz), 6.80 (d, 1H, ^3J = 8.1 Hz), 4.53 (s, 2H), 3.97 (q, 4H, ^3J = 6.6 Hz), 1.78 (m, 4H), 1.44 (m, 4H), 1.32 (m, 2H), 1.31–1.24 (m, 32H), 0.86 (t, 6H, ^3J = 6.8 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 149.40, 149.27, 129.99, 121.25, 114.25, 113.51, 69.29, 69.28, 46.76, 31.92, 29.70, 29.66, 29.63, 29.42, 29.41, 29.36, 29.27, 29.23, 26.02, 22.69, 14.11.

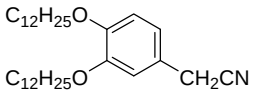


Warning: cyanides are highly toxic. All operations should be conducted in a well-ventilated hood and rubber gloves should be worn. Cyanide washings should be kept basic and disposed of properly.

2-(4-(Dodecyloxy)-3-methoxyphenyl)acetonitrile (11b).[6] Compound **10b** (20.37 g, 59.75 mmol) was dissolved in N,N-dimethylformamide (84 mL). Sodium cyanide (5.95 g, 122 mmol) was added and the mixture was heated at 100 °C for 2.5 h. The reaction mixture was cooled to room temperature, diluted with water, and extracted with dichloromethane. The extracts were dried over anhydrous sodium sulfate, filtered, and stripped of the solvent under reduced pressure. The brownish residue was crystallized from methanol/dichloromethane. The productwas isolated as pale yellow crystals (18.81 g, 95%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 6.84–6.78 (m, 3H), 3.98 (t, 2H, ^3J = 7.0 Hz), 3.86 (s, 3H), 3.68 (s, 2H), 1.81 (m, 2H), 1.42 (m, 2H), 1.33 (m, 2H), 1.31–1.24 (m, 16H), 0.86 (t, 3H, ^3J =6.9 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 149.85, 148.44, 122.01, 120.22, 118.12, 113.18, 111.44, 69.18, 56.07, 31.89, 29.63, 29.61, 29.56, 29.53, 29.37, 29.32, 29.10, 25.92, 23.19, 22.66, 14.08.

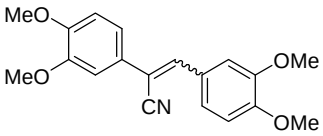


2-(3,4-Bis(dodecyloxy)phenyl)acetonitrile (11c). Compound **10c** (6.23 g, 12.6 mmol) was dissolved in N,N-dimethylformamide (10 mL). Potassium cyanide (1.63 g, 25.2 mmol) and water (2 mL) were added and the mixture was heated at 100 °C for 3 h. The reaction mixture was cooled to room temperature, diluted with water and extracted with dichloromethane. The extracts were dried over anhydrous sodium sulfate, filtered, and stripped of the solvent under reduced pressure. The crude product was purified by column chromatography (silicagel, 5% ethyl acetate in hexanes). The second fraction was collected and concentrated on a rotary evaporator to yield colorless crystals (2.89 g, 47%). Note: the method used for the synthesis of **11b** should give superior results. **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 6.84–6.78 (m, 3H), 3.96 (m, 4H), 3.96 (m, 4H), 1.78 (m, 4H), 1.44 (m, 4H), 1.31 (m, 4H), 1.30–1.24 (m, 32H), 0.86 (t, 6H, ^3J = 6.9 Hz).

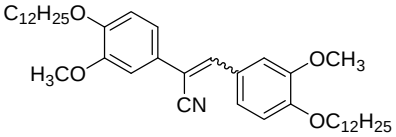


General procedure for the synthesis of diarylacrylonitriles (cyanostilbenes). Aldehyde **7** (1 equiv.) and the corresponding acetonitrile **11** (1 equiv.) were placed in a round-bottomed flask equipped with a magnetic stirring bar. Absolute ethyl alcohol (5 mL/mmol of **7**) was added followed by an ethanolic solution of sodium ethoxide (1 M, ca. 1 mL/mmol of **7**). The mixture was refluxed for 2 h, changing color to yellow. Towards the end of the reaction a yellow precipitate was usually formed. After cooling the reaction mixture to room temperature, the precipitate was filtered, washed with ethanol and dried. The product usually contained pure *Z* isomer of **11**.

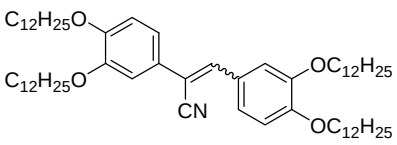
[6] Lee, J.; Lee, Ju-H.; Kim, S.; Perry, N. A.; Lewin, N. E.; Ayres, J. A,; Blumberg, P. M. *Bioorg. Med. Chem*. **2006**, *14,* 2022.



2,3-bis(3,4-dimethoxyphenyl)acrylonitrile (12a). Obtained from **7a** (2.02 g, 0.012 mmol) and **11a** (2.198 g, 0.012 mmol). Yellow crystals (3. 69 g, 65 %).**^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 7.65 (d, ^{1}H, *J* = 2.1 Hz), 7.34-7.32 (m, 2H), 7.21 (dd, 1H, *J* = 8.4 Hz, *J* = 2.2 Hz), 7.11 (dd, 1H *J* = 2.2 Hz), 6.90 (d, 1H, *J* = 8.5 Hz), 6.89 (d, 1H, *J* = 8.5 Hz), 3.95 (s, 3H), 3.94 (s, 3H), 3.92 (s, 3H),3.90 (s, 3H). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): d 150.92, 149.80, 149.30, 149.05, 140.43, 127.73, 126.91, 123.97, 118.80, 118.78, 111.35, 110.98, 110.76, 108.75, 108.62, 56.07, 56.04, 56.01, 55.98.



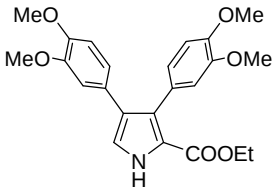
2,3-Bis(4-(dodecyloxy)-3-methoxyphenyl)acrylonitrile (12b). Obtained from **7b** (3 g, 9.05 mmol) and **11b** (2.90 g, 9.05 mmol). Yellow crystals (3.51 g, 62%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 7.62 (d, 1H, ^{3}*J* = 2.1 Hz), 7.30 (dd, 1H, ^{3}*J* = 8.4 Hz, ^{4}*J* = 2.1 Hz), 7.30 (s, 1H), 7.18 (dd, 1H, ^{3}*J* = 8.5 Hz, ^{4}*J* = 2.3 Hz), 7.10 (d, 1H, *J* =2.3 Hz), 6.89 (d, 1H, *J* = 8.5 Hz), 6.88 (d, 1H, ^{3}*J* = 8,5 Hz), 4.05 (t, 4H, ^{3}*J* = 6.9 Hz), 4.03 (t, 4H, ^{3}*J* = 6.9 Hz), 3.92 (s, 3H), 3.91 (s, 3H), 1.84 (m, 4H), 1.44 (m, 4H), 1.33 (m, 4H), 1.32–1.24 (m, 32H), 0.86 (m, 6H, ^{3}*J* = 6.9 Hz). **^{13}C NMR** (151 MHz, chloroform-*d*, 300K): δ 150.56, 149.65, 149.41, 149.33, 140.38, 127.62, 126.72, 123.89, 118.84, 118.78, 112.83, 112.23, 111.18, 109.23, 108.43, 69.17, 69.05, 56.21, 56.09, 31.91, 29.65, 29.63, 29.58, 29.54, 29.39, 29.38, 29.34, 29.10, 29.03, 25.94, 25.92, 22.68, 14.11.



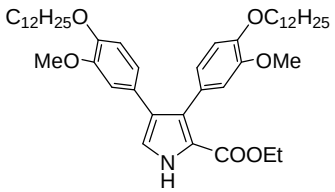
2,3-Bis(3,4-bis(dodecyloxy)phenyl)acrylonitrile (12c). Obtained from **7c** (1.67 g, 3.52 mmol) and **11c** (1.71 g, 3.52 mmol). Yellow crystals (2.98 g, 90%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 7.58 (d, 1H, ^{4}*J* = 2.2 Hz), 7.31 (dd, 1H, ^{3}*J* = 8.34 Hz, ^{4}*J* = 2.1 Hz), 7.28 (s, 1H), 7.17 (dd, 1H, ^{3}*J* = 8.4 Hz, ^{4}*J* = 2.2 Hz), 7.11 (d, 1H, *J* = 2.2 Hz), 6.88 (2 × d, 2H, ^{3}*J* = 8.5 Hz), 4.03 (m, 8H), 1.82 (m, 8H), 1.46 (m, 8H), 1.34 (m, 8H), 1.32–1.24 (m, 64H), 0.86 (m, 12H). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 151.07, 149.97, 149.37, 149.01, 140.40, 127.79, 126.84, 123.73, 118.88, 118.84, 113.63, 113.18, 112.88, 111.40, 108.37, 69.57, 69.30, 69.10, 31.93, 29.71, 29.70, 29.66, 29.63, 29.44, 29.42, 29.40, 29.37, 29.32, 29.23, 29.20, 29.14, 26.05, 26.02, 26.00, 22.69, 14.11.

General procedure for the synthesis of ethyl 3,4-diarylpyrrole-2-carboxylates (1a-c, 3).[7] In a dry flask equipped with magnetic stirring, appropriate cyanostilbene **12a-c** and ethyl isocyanoacetate (1 equiv.) were dissolved in dry tetrahydrofuran. The mixture was cooled to 0 °C and a solution of potassium *tert*-butoxide (1 M in tetrahydrofuran) was added. The mixture was stirred under argon until thin-layer chromatography showed complete consumption of the starting material. The mixture was diluted with water and extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate, filtered, and the solvents were removed on a rotary evaporator. The product was purified by column chromatography (silica gel, dichloromethane). The second fraction was collected, characterized by blue fluorescence under UV light. The solvent was removed on a rotary evaporator, to yield the product as a yellow-orange solid.

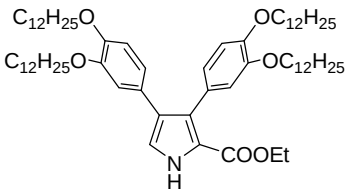
[7] Bullington, J. L.;Wolff, R. R.; Jackson, P. F. *J. Org. Chem.* **2002**, 67, 9439.

Ethyl 3,4-bis(3,4-dimethoxyphenyl)-1*H*-pyrrole-2-carboxylate (1a). 

Obtained from **12a** (1 g, 3.07 mmol) and ethyl isocyanoacetate (0.34 ml, 3.07 mmol) using tetrahydrofuran (4 mL) and potassium *tert*-butoxide solution (5.4 mL).Reaction time was 48 h.Yield: 0.95 g (75%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 9.14 (b, 1H), 7.05 (d, 1H, *J* = 3.2 Hz), 6.84-6.79 (m, 3H), 6.73 (m, 2H), 6.57 (t, 1H, *J* = 1.0 Hz), 4.19 (q, 2H, *J* = 7.1 Hz), 3.86 (s, 3H),3.82 (s, 3H),3.72 (s, 3H), 3.56 (s, 3H), 1.17 (t, 3H, *J* = 7.1 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 161.06, 148.40, 148.09, 147.97, 147.42, 128.85, 127.35, 126.99, 126.50, 123.30, 120.20, 119.85, 119.60, 114.38, 111.87, 111.07, 110.53, 60.15, 55.86, 55.82, 55.80, 55.48, 14.24.

Ethyl 3,4-bis(4-(dodecyloxy)-3-methoxyphenyl)-1*H*-pyrrole-2-carboxylate (1b). 

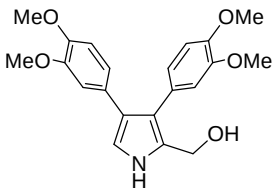
Obtained from **12b** (1 g, 1.577 mmol) and ethyl isocyanoacetate (181 µl, 1.577 mmol) using tetrahydrofuran (1.4 mL) and potassium *tert*-butoxide solution (2.8 mL). Reaction time was 24 h. Yield: 0.804 g (71%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 9.10 (b, 1H), 7.04 (d, 1H, *J* = 3.1 Hz), 6.79 (m, 3H), 6.72 (d, 1H, ^{3}J = 8.3 Hz), 6.70 (dd, 1H, ^{3}J = 8.3 Hz, 4H, ^{4}J = 1.7 Hz), 6.55 (d, 1H, ^{4}J = 1.7 Hz), 4.18 (q, 2H, ^{3}J = 7.2 Hz), 3.98 (t, 2H, ^{3}J = 6.9 Hz), 3.93 (t, 2H, ^{3}J = 6.9 Hz), 3.69 (s, 3H), 3.53 (s, 3H), 1.80 (m, 4H), 1.41 (m, 4H), 1.34–1.24 (m, 32H), 1.16 (t, 3H, ^{3}J = 7.13 Hz), 0.86 (m, 6H). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 161.13, 148.78, 148.50, 147.50, 146.94, 128.90, 127.28, 126.92, 126.58, 123.31, 120.15, 119.81, 119.56, 114.79, 112.73, 112.24, 69.06, 69.02, 60.14, 55.91, 55.57, 31.91, 29.66, 29.65, 29.63, 29.62, 29.61, 29.59, 29.56, 29.44, 29.42, 29.34, 29.21, 25.98, 25.96, 22.68, 14.24, 14.11.

Ethyl 3,4-bis(3,4-bis(dodecyloxy)phenyl)-1*H*-pyrrole-2-carboxylate (1c). 

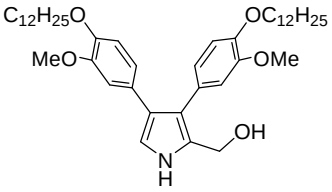
Obtained from **12c** (1 g, 1.06 mmol) and ethyl isocyanoacetate (116 µl, 1.06 mmol) using tetrahydrofuran (1.4 mL) and potassium *tert*-butoxide solution (1.9 mL).Reaction time was 20 h. Yield: 0.683 g (64%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 9.12 (d, 1H, ^{3}J = 2.41 Hz), 7.02 (d, 2H, ^{3}J = 3.05 Hz), 6.78–6.77 (m, 3H), 6.71 (d, 1H, ^{3}J = 8.3 Hz), 6.68 (dd, 1H, ^{3}J = 8.30, ^{4}J = 1.9 Hz), 6.57 (d, 1H, ^{4}J = 1.9 Hz), 4.17 (q, 2H, J = 7.14 Hz), 3.96 (t, 2H, *J* = 6.3 Hz), 3.90 (t, 2H, *J* = 6.64 Hz), 3.80 (t, 2H, *J* = 6.84 Hz), 3.63 (t, 2H, *J* = 6.7 Hz), 1.82–1.72 (m, 4H), 1.68 (m, 2H), 1.63 (m, 2H), 1.42 (m, 4H), 1.33 (m, 4H), 1.31–1.24 (m, 64H), 1.14 (t, 3H, *J* = 7.02 Hz), 0.86 (m, 12H). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K): δ 161.23, 148.63, 148.29, 148.13, 147.48, 128.98, 127.53, 127.20, 126.60, 123.42, 120.25, 119.82, 119.57, 116.95, 114.27, 113.81, 113.20, 69.33, 69.18, 68.88, 60.09, 31.93, 29.76, 29.74, 29.72, 29.70, 29.67, 29.66, 29.64, 29.52, 29.46, 29.43, 29.39, 29.37, 29.24, 29.20, 26.11, 26.05, 26.02, 22.69, 14.21, 14.09.

General procedure for the synthesis of pyrrol-2-ylmethanols (13a-c, 17b). In a round-bottomed flask equipped with a stirring bar, lithium aluminium hydride (10 equiv.) was suspended in tetrahydrofuran and purged with nitrogen. A solution of appropriate diarylpyrrole-2-carboxylate (**1a-c**, **3**) in tetrahydrofuran was prepared, purged with nitrogen, and added dropwise via a syringe to the well-stirred reaction mixture. The mixture was stirred at room temperature for 1 h, and the progress of the reaction was monitored with thin-layer chromatography. The reaction mixture was diluted with aqueous ammonium chloride and extracted with dichloromethane. The extracts were dried over anhydrous sodium sulfate and the solvent was removed on a rotary evaporator. The resulting pyrrolyl-2-methanol is unstable and was used directly for the next step.

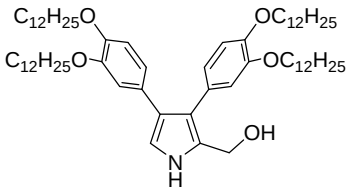
(3,4-Bis(3,4-dimethoxyphenyl)-1*H*-pyrrol-2-yl)methanol (13a). Obtained from **1a** (0.950 g, 2.31 mmol, in 50 mL of tetrahydrofuran) and lithium aluminium hydride (0.875 g, 23 mmol, in 25 mL of tetrahydrofuran). Reaction time: 1 h. Yellowish oil (0.85 g, 99%).



(3,4-Bis(4-(dodecyloxy)-3-methoxyphenyl)-1*H*-pyrrol-2-yl)methanol (13b). Obtained from **1b** (0.217 g, 0.302 mmol, in 10 mL of tetrahydrofuran) and lithium aluminium hydride (0.114 g, 3.02 mmol, in 5 mL of tetrahydrofuran). Reaction time: 2 h. Yellowish oil (0.200 g, 99%).

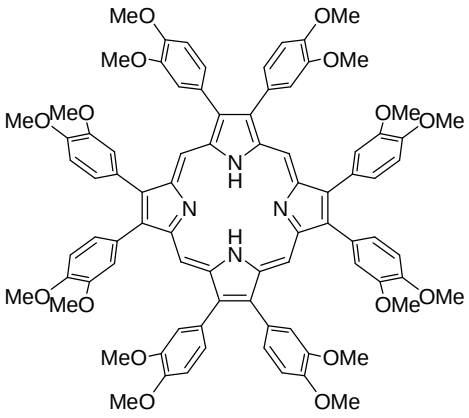


(3,4-Bis(3,4-bis(dodecyloxy)phenyl)-1*H*-pyrrol-2-yl)methanol (13c). Obtained from **1a** (0.899 g, 0.888 mmol, in 10 mL of tetrahydrofuran) and lithium aluminium hydride (0.337 g, 8.88 mmol, in 10 mL of tetrahydrofuran). Reaction time: 1 h. Yellowish oil (0.84 g, 96%).

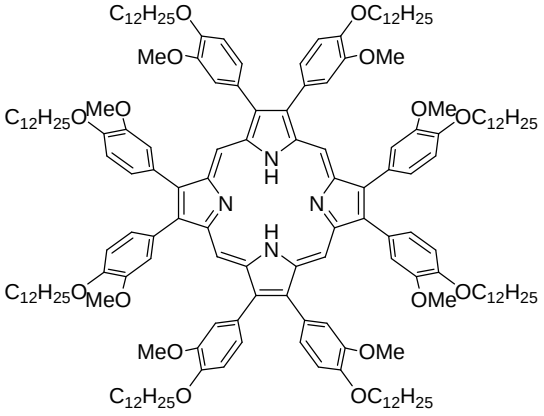


General procedure for the synthesis of porphyrins (2a-c-H_2, 4b-H_2). Appropriate pyrrol-2-ylmethanol (**13a-c**, **17b**) was dissolved in chloroform (ethanol content: 0.8%, 75 mL/mmol), which had been purged with argon for 5 min. Boron trifluoride diethyl etherate was added (0.33 equiv.), and the reaction mixture was stirred under argon for 1 h. Subsequently, 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ, 0.75 equiv.) was added, and the mixture was stirred for 10 min. The solvent was removed on a rotary evaporator. The residue was subjected to column chromatography (silica gel, dichloromethane). The first, red-colored fraction was collected. The product was crystallized from dichloromethane/methanol.

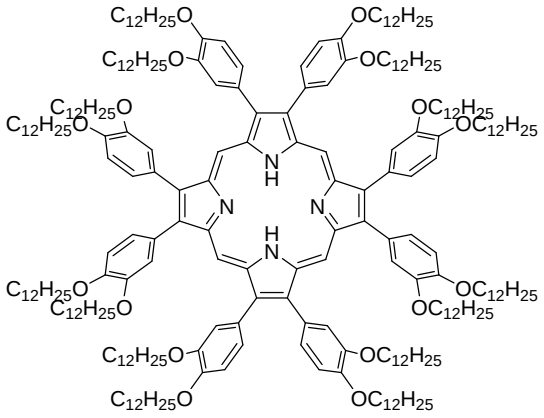
2,3,7,8,12,13,17,18-Octakis(3,4-dimethoxyphenyl)porphyrin (2a-H_2). Obtained from carbinol **13a** (0.85 g, 2.15 mmol), using chloroform (165 mL), boron trifluoride diethyl etherate (89 μL, 0.710 mmol), and DDQ (0.361 g, 1.59 mmol). Red crystals with violet lustre (0.27 g, 34%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.45 (s, 4H, meso), 7.56 (dd, 8H, *J* = 8.1 Hz, *J* = 2.1 Hz, β-aryl), 7.48 (d, 8H, *J* = 2.1 Hz, β-aryl), 7.12 (d, 8H, *J* = 8.1 Hz, β-aryl), 4.04 (s, 24H, OMe), 3.75 (s, 24H, OMe), –2.99 (b, 2H, NH). **^{13}C NMR** (151 MHz, chloroform-*d*, 325 K): δ 149.40, 149.10, 144.54, 141.04, 128.35, 125.30, 116.39, 111.89, 103.12, 56.25, 56.13. **HR-MS** (ESI+): *m*/*z* 1399.5412 [M-H$^+$], calcd. for $C_{84}H_{78}N_4O_{16}$: 1399.5486.



2,3,7,8,12,13,17,18-Octakis(4-(dodecyloxy)-3-methoxyphenyl)porphyrin (2b-H_2). Obtained from carbinol **13b** (0.202 g, 0.297 mmol), using chloroform (22 mL), boron trifluoride diethyl etherate (12.3 μL, 0.98 mmol), and DDQ (0.050 g, 0.219 mmol). Red crystals with violet lustre (0.111 g, 56%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.48 (s, 4H, H_{meso}), 7.56 (dd, 8H, ^3J = 8.2 Hz, ^4J = 1.9 Hz), 7.46 (d, 8H, J = 1.9 Hz), 7.12 (d, 8H, ^3J = 8.3 Hz), 4.16 (t, 8H, J = 6.82 Hz, dodecyl α–CH_2), 3.72 (s, 24H, CH_3), 1.96 (m, 16H, dodecyl β–CH_2), 1.55 (m, 16H, dodecyl β–CH_2), 1.43 (m, 16H, dodecyl γ–CH_2), 1.39–1.28 (m, 128H, dodecyl-(CH_2)$_8$), 0.87 (t, 24H, J = 7.05 Hz, dodecyl-CH_3), -3.01 (s, 2H, N*H*). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, one signal was not observed in the aromatic region, presumably due to dynamic broadening): δ 149.41, 148.29, 140.87, 128.04, 125.18, 116.29, 112.98, 103.05, 69.27, 31.95, 29.76, 29.72, 29.60, 29.44, 29.40, 26.17, 22.70, 14.12. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 427 (265000), 521 (22700), 558 (17100), 584 (12700), 639 (6470). **HR-MS** (ESI+): *m/z* 2632.9185 [M-H$^+$], calcd. for $C_{172}H_{254}N_4O_{16}$: 2632.9258. **Elemental analysis** calcd (%) for $C_{172}H_{254}N_4O_{16}$: C 78.43, H 9.72, N 2.13; found C 78.08, H 9.78, N 2.20.

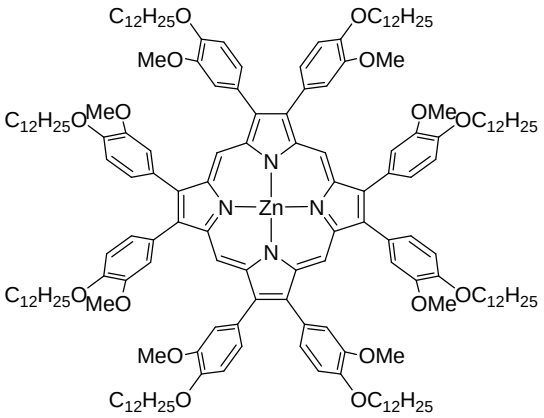


2,3,7,8,12,13,17,18-Octakis(3,4-bis(dodecyloxy)phenyl)porphyrin (2c-H_2). Obtained from carbinol **13c** (0.84 g, 0.85 mmol), using chloroform (62 mL), boron trifluoride diethyl etherate (35 μL, 0.28 mmol), and DDQ (0.143 g, 0.63 mmol). Red crystals with violet lustre (0.507 g, 62%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.45 (s, 4H, H_{meso}), 7.54 (dd, 8H, ^3J = 8.1 Hz, ^4J = 1.9 Hz), 7.44 (d, 8H, ^4J = 1.9 Hz), 7.09 (d, 8H, ^3J = 8.3 Hz), 4.12 (t, 8H, J = 6.8 Hz), 3.82 (t, 8H, ^3J = 6.8 Hz), 1.92 (m, 16H, dodecyl β–CH_2), 1.72 (m, 16H, dodecyl β–CH_2), 1.57 (m, 16H, dodecyl γ–CH_2) 1.43 (m, 16H, dodecyl γ–CH_2), 1.37–1.17 (m, 128H, dodecyl-(CH_2)$_8$), 0.87 (t, 24H, ^3J = 7.2 Hz, dodecyl-CH_3), 0.81 (t, 24H, ^3J = 7.1 Hz, dodecyl-CH_3), –3.05 (s, 2H, N*H*). **^{13}C NMR** (151 MHz, chloroform-*d*, 300K, two signals not observed in the aromatic region because of their low intensity): δ 149.12, 148.70, 128.22, 125.23, 118.14, 113.70, 103.09, 69.39, 69.32, 31.97, 31.90, 29.83, 29.80, 29.78, 29.76, 29.74, 29.71, 29.69, 29.63, 29.60, 29.44, 29.37, 26.30, 26.18, 22.72, 22.65, 14.12, 14.07. **HR-MS** (ESI+): *m/z* 1933.6839 [M-H_2^{2+}], calcd. for $C_{260}H_{432}N_4O_{16}$: 1933.6551. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 427 (267000), 522 (24100), 559 (18200), 584 (13500), 639 (6760). **Elemental analysis** calcd (%) for $C_{260}H_{430}N_4O_{16}$: C 80.73, H 11.20, N 1.45; found C 80.33, H 11.28, N 1.24.

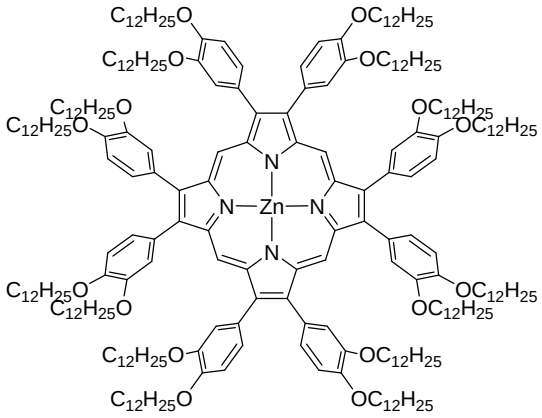


General procedure for the synthesis of Zn(II) complexes. Fee base porphyrin, tetraphenanthroporphyrin, or tetra(benzochryseno)porphyrin and zinc(II) acetate (10 equiv.) were dissolved in a 1:1 mixture of chloroform and methanol. The mixture was refluxed for 1 h. Subsequently, the mixture was diluted with water and extracted with dichloromethane. Organic extracts were dried over anhydrous sodium sulfate and stripped of the solvent on a rotary

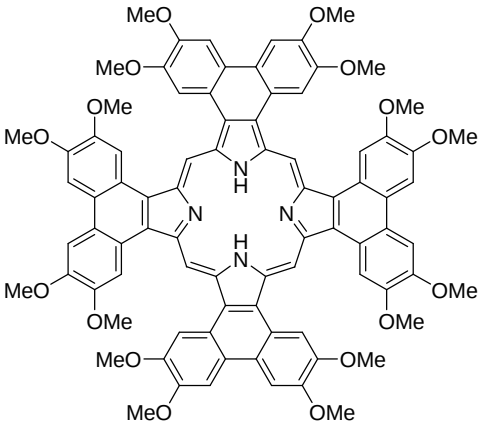
evaporator. The residue was crystallized from dichloromethane/methanol, providing the desired zinc complex in quantitative yield.



(2,3,7,8,12,13,17,18-Octakis(4-(dodecyloxy)-3-methoxyphenyl)porphyrinato)zinc(II) (2b-Zn). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.57 (s, 4H, H_{meso}), 7.58 (dd, 8H, ^{3}J = 8.2 Hz, ^{4}J = 1.9 Hz), 7.48 (d, 8H, *J* = 1.9 Hz), 7.13 (d, 8H, ^{3}J = 8.3 Hz), 4.17 (t, 8H, *J* = 6.82 Hz, dodecyl α–CH_2), 3.72 (s, 24H, CH_3), 1.97 (m, 16H, dodecyl β–CH_2), 1.55 (m, 16H, dodecyl β–CH_2), 1.43 (m, 16H, dodecyl γ–CH_2), 1.39–1.28 (m, 128H, dodecyl-(CH_2)$_8$), 0.87 (t, 24H, *J* = 7.05 Hz, dodecyl-CH_3). **^{13}C NMR** (125 MHz, chloroform-*d*, 300 K): δ 149.40, 148.19, 147.86, 141.84, 128.50, 125.18, 116.42, 113.03, 69.30, 56.06, 31.95, 29.76, 29.72, 29.70, 29.61, 29.45, 29.39, 26.18, 22.70, 14.11. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 431 (334000), 550 (29500), 589 (39500). **Elemental analysis** calcd (%) for $C_{172}H_{252}N_4O_{16}Zn$: C 76.59, H 9.42, N 2.08; found C 76.40, H 9.55, N 2.16.



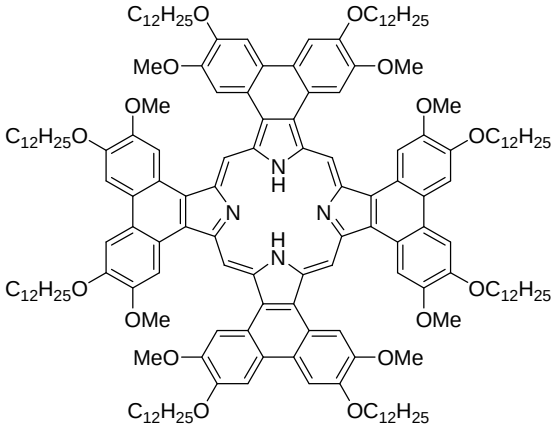
(2,3,7,8,12,13,17,18-Octakis(3,4-bis(dodecyloxy)phenyl)porphyrinato)zinc(II) (2c-Zn). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.54 (s, 4H), 7.55 (dd, 8H, ^{3}J = 8.2Hz, ^{4}J = 1.7 Hz), 7.46 (d, 8H, ^{4}J = 1.7 Hz), 7.11 (d, 8H, ^{3}J = 8.2 Hz), 4.13 (t, 8H, *J* = 6.7 Hz), 3.82 (t, 8H, ^{3}J = 6.5 Hz), 1.93 (m, 8H), 1.72 (m, 8H), 1.57 (m,) 1.44 (m, 8H), 1.42–1.17 (m, 256H), 0.87 (t, 24H, ^{3}J = 7.1 Hz), 0.81 (t, 24H, ^{3}J = 7.15 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300 K)]: δ 149.13, 148.61, 147.85, 141.72, 128.67, 125.24, 118.30, 113.79, 104.18, 69.45, 69.35, 31.97, 31.90, 29.83, 29.80, 29.78, 29.76, 29.73, 29.71, 29.68, 29.66, 29.60, 29.43, 29.39, 29.36, 26.31, 26.19, 22.71, 22.64, 14.11, 14.06. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 431 (334000), 550 (30100), 589 (40200). **Elemental analysis** calcd (%) for $C_{260}H_{428}N_4O_{16}Zn$: C 79.43, H 10.97, N 1.43; found C 78.91, H 11.14, N 1.25.



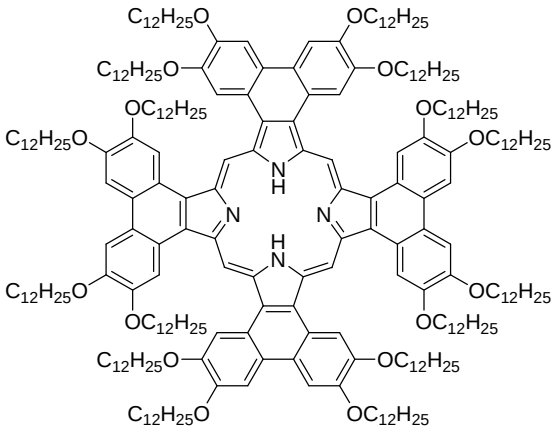
2,3,7,8,11,12,16,17,20,21,25,26,29,30,34,35-Hexadecamethoxytetraphenanthro[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrin (3a-H_2). Compound **2a**-H_2 (14 mg, 0.01 mmol) was dissolved in warm *o*-dichlorobenzene (5 mL). After cooling to room temperature, the mixture was purged with argon and anhydrous iron(III) chloride (16 mg, 0.1 mmol) was added in one portion. The reaction mixture became deep blue and a dark precipitate rapidly formed. The mixture was poured into water and extracted with dichloromethane.

Organic extracts were washed with water, dried over anhydrous sodium sulfate and stripped of solvents on a rotary evaporator. After column chromatography, the product was obtained as a dark green solid. Yield 13 mg (93%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 11.18 (s, 4H, H_{meso}), 8.88 (s, 8H), 8.24 (s, 8H), 4.38 (s, 24H, CH_3) 3.87 (s, 24H, CH_3), -4.53 (s, 2H, N*H*). **^{13}C NMR** (125 MHz, chloroform-*d*, 300 K) δ 150.51, 149.44, 131.07, 126.49, 122.93, 107.56, 106.54, 56.75, 55.58. **HR-MS** (ESI+): *m*/*z* 1391.4789 [M-H$^+$], calcd. for $C_{84}H_{70}N_4O_{16}$: 1391.4860. **UV-vis** (chloroform, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 471 (155000), 601 (14000), 648 (50000), 697 (42000).

2,8,11,17,20,26,29,35-Octakis(dodecyloxy)-3,7,12,16,21,25,30,34-octamethoxytetraphenanthro[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrin (3b-H_2). In a dry flask, compound **2b**-Zn (60 mg, 0.022 mmol) was dissolved in freshly distilled dichloromethane(2 mL). The solution was purged with argon and cooled to 0 °C. Solid anhydrous ferric chloride (43 mg, 0.26 mmol) was added under argon in one portion and the mixture was stirred for 3 h. During that time the color of the solution changes from dark red-brown to dark green. The reaction mixture was washed with water, the organic layer was separated and the aqueous layer was extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate, filtered, and concentrated on a rotary evaporator. The crude product was purified using column chromatography (silica gel, dichloromethane). The main fraction, which was deep green, was collected, and the solvent was removed on a rotary evaporator. The residue was crystallized from dichloromethane/acetone to yield dark green crystals (42 mg, 74%). **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K): δ 11.87 (s, 4H, H_{meso}), 9.41 (s, 8H, phenanthrene), 8.35 (s, 8H, phenanthrene), 4.49 (b, 16H, dodecyl α–CH_2), 4.25 (s, 24H, CH_3), 2.13 (m, 16H, dodecyl β–CH_2), 1.69 (m, 16H, dodecyl γ–CH_2), 1.34–1.23 (m, 128H, dodecyl-(CH_2)$_8$), 0.86 (b, 24H, CH_3), –1.53 (s, 2H, N*H*). **^{13}C NMR** (151 MHz, toluene-d_8, 300 K, partial, HSQC): δ 110.9, 110.3, 102.4, 70.9, 57.1, 30.5, 30.3-29.9, (multiple signals), 27.0. **HR-MS** (ESI+): *m*/*z* 1312.9352 [M-H_2^{2+}], calcd. for $C_{172}H_{246}N_4O_{16}$: 1312.9298. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 473 (199000), 603 (20300), 648 (71000), 698 (57500). **Elemental analysis** calcd (%) for $C_{172}H_{246}N_4O_{16}$: C 78.67, H 9.44, N 2.13; found C 78.46, H 9.59, N 2.13.

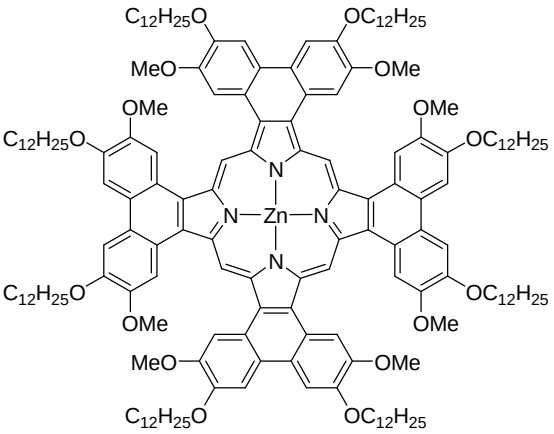


2,3,7,8,11,12,16,17,20,21,25,26,29,30,34,35-Hexadecakis(dodecyloxy)tetraphenantro[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrin (3c-H_2) was prepared from **2c**-Zn (200 mg, 0.050 mmol) and iron(III) chloride (99 mg, 0.61 mmol) in dichloromethane (2 mL), following the procedure described for **3b**-H_2. Dark-green crystals (191 mg, 97%). **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K): δ 11.88 (s, 4H, H_{meso}), 9.40 (s, 8H, phenanthrene), 8.35 (s, 8H, phenanthrene), 4.55 (t, 16H, ^3J = 6.5 Hz, dodecyl α–CH_2), 4.41 (t, 16H, ^3J = 6.2 Hz, dodecyl α–

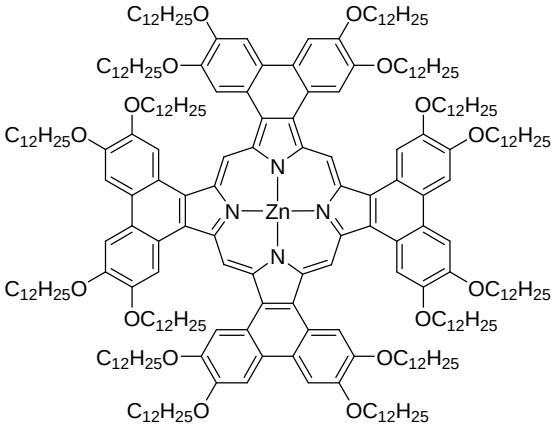


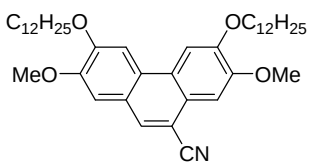
CH_2), 2.08 (m, 16H, dodecyl β–CH_2), 1.94 (m, 16H, dodecyl β–CH_2), 1.69 (m, 16H, dodecyl γ–CH_2), 1.43 (m, 16H, dodecyl γ–CH_2), 1.34–1.18 (m, 256H, dodecyl-(CH_2)$_8$), 0.87 (t, 24H, ^3J = 7.12 Hz, dodecyl-CH_3), 0.80 (t, 24H, ^3J = 7.12 Hz, dodecyl-CH_3), –1.54 (s, 2H, N*H*). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, broadened, one signal in the aromatic region was not identified): δ 150.48, 149.30, 131.21, 126.16, 122.93, 108.96, 108.09, 101.10, 77.21, 77.00, 76.79, 70.02, 69.24, 32.00, 31.97, 30.72, 29.90, 29.88, 29.82, 29.80, 29.58, 29.47, 28.59, 26.43, 26.16, 22.74, 22.70, 14.13, 14.09. **HR-MS** (ESI+): *m/z* 1929.6192 [M-H_2^{2+}], calcd. for $C_{260}H_{422}N_4O_{16}$: 1929.6238. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$):474 (201000), 603 (19700), 650 (80300), 698 (66100). **Elemental analysis** calcd (%) for $C_{260}H_{422}N_4O_{16}$: C 80.90, H 11.02, N 1.45; found C 80.78, H 11.21, N 1.25.

(2,8,11,17,20,26,29,35-Octakis(dodecyloxy)-3,7,12,16,21,25,30,34-octamethoxytetraphenanthro[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrinato)zinc(II) (3b-Zn). Obtained using the general procedure. Dark green crystals. **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K, dilute, broadened by aggregation): δ ~12.1 (s, 4H, H_{meso}), ~9.5 (s, 8H, phenanthrene), ~8.3 (s, 8H, phenanthrene), 4.48 (b, 16H, dodecyl α–CH_2), ~4.2 (b, 24H, CH_3), 2.13 (m, 16H, dodecyl β–CH_2), 1.70 (m, 16H, dodecyl γ–CH_2), 1.54–1.26 (m, 128H, dodecyl-(CH_2)$_8$), 0.87 (b, 24H, CH_3). Well-resolved ^{13}C NMR spectrum could not be recorded. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 473 (284000), 606 (20000), 661 (137000). **Elemental analysis** calcd (%) for $C_{172}H_{244}N_4O_{16}Zn$: C 76.82, H 9.15, N 2.08; found C 76.67, H 9.50, N 1.94.

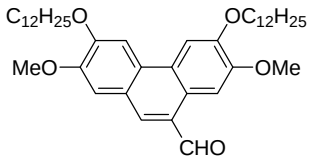


(2,3,7,8,11,12,16,17,20,21,25,26,29,30,34,35-Hexadecakis(dodecyloxy)tetraphenanthro[9,10-*b*:9',10'-*g*:9'',10''-*l*:9''',10'''-*q*]porphyrinato)zinc(II) (3c-Zn). Obtained using the general procedure. Dark green crystals. **^{1}H NMR** (600 MHz, toluen-d_8 380 K) δ 12.38, (s, 4H, H_{meso}), 9.93 (s, 8H, phenanthrene), 8.64 (s, 8H, phenanthrene), 4.67 (t, 16H, ^3J = 6.5 Hz, dodecyl α–CH_2), 4.51 (t, 16H, ^3J = 6.2 Hz, dodecyl α–CH_2), 2.12 (m, 16H, dodecyl β–CH_2), 1.79 (m, 16H), 1.68 (m, 16H), 1.59 (m, 16H), 1.53–1.23 (m, 256H, dodecyl-(CH_2)$_8$), 0.91 (t, 24H, ^3J = 7.08 Hz, dodecyl-CH_3), 0.83 (t, 24H, ^3J = 7.23 Hz, dodecyl-CH_3). **^{13}C NMR** (151 MHz, toluene-d_8, 380 K, some signals in the aromatic region not identified because of overlap with solvent lines) δ 152.32, 150.90, 146.70, 134.13, 111.88, 110.66, 71.26, 70.87, 32.67, 32.62, 30.95, 30.77, 30.61, 30.60, 30.56, 30.54, 30.53, 30.52, 30.50, 30.48, 30.44, 30.11, 30.07, 27.32, 27.17, 23.31, 23.26, 20.89, 20.76, 20.64, 20.51, 20.38, 20.25, 20.13, 14.33, 14.30. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 475 (205000), 611 (17600), 664 (95600).

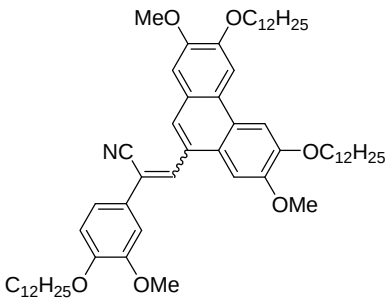


3,6-Bis(dodecyloxy)-2,7-dimethoxyphenanthrene-9-carbonitrile (14b). 

In a dry round-bottomed flask, compound **12b** (0.5 g, 0.8 mmol) was dissolved in dry dichloromethane and purged with argon. Solid anhydrous iron(III) chloride (1.3 mg, 8 μmol) was added under argon followed by *m*-chloroperoxybenzoic acid (50-60%, 0.136 g, ca. 0.8 mmol 50-60%). The mixture was stirred under argon for 1 hour. The reaction was quenched by pouring into a separatory funnel containing water. The organic layer was separated and the aqueous layer was washed extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate and stripped of the solvent on a rotary evaporator. The crude product was crystallized from dichloromethane/methanol to yield colorless crystals (0.44 g, 88%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 7.96 (s, 1H), 7.27 (s, 1H), 7.68 (s, 1H), 7.49 (s, 1H), 7.14 (s, 1H), 4.20 (2 × q, 4H, *J* = 7.3 Hz), 4.00 (s, 3H), 3.95 (s, 3H), 1.91 (m, 4H), 1.49 (m, 4H), 1.35 (m, 4H, 1.31-1.14 (m, 28H), 0.81 (t, 6H, *J* = 7.0 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K, partial overlap in the aliphatic region): δ 151.39, 150.52, 149.84, 149.83, 132.09, 126.78, 124.41, 124.25, 124.06, 118.93, 108.77, 105.92, 105.76, 104.68, 103.91, 69.47, 69.32, 56.14, 56.07, 31.92, 29.69, 29.66, 29.63, 29.61, 29.49, 29.47, 29.36, 14.11.

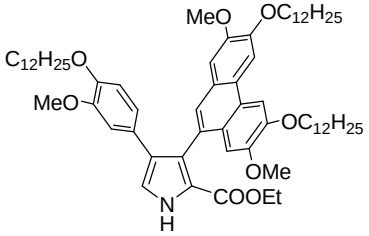
3,6-Bis(dodecyloxy)-2,7-dimethoxyphenanthrene-9-carbaldehyde (15b). 

In a dry two-necked round bottomed flask equipped with a thermometer, cyanophenanthrene **14b** (1.42 g, 2.25 mmol) was dissolved in dry dichloromethane (40 mL). The solution was stirred under argon and cooled to 0 °C in an ice-water mixture. A solution of diisobutylaluminium hydride (DIBAL, 1 M in hexane, 2.7 mL) was added dropwise to the reaction mixture over three hours. During the addition, the reaction mixture became yellow. The stirring was continued overnight. The reaction was stopped by portion-wise addition of dilute hydrochloric acid. The reaction mixture was extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate and the solvent was removed under reduced pressure. The crude product was purified by column chromatography (silica gel, dichloromethane:hexanes 1:1). The product eluted as the second band. After removal of solvents, the product was isolated in the form of brownish crystals (1.14 g, 80%). **^{1}H NMR** (500 MHz, chloroform-*d*, 300 K): δ 10.25 (s, 1H), 8.94 (s, 1H), 8.04 (s, 1H), 7.80 (s, 1H), 7.60 (s, 1H), 7.31 (s, 1H), 4.28 (t, 2H, *J* = 6.8 Hz), 4.24 (t, 2H, *J* = 6.8 Hz), 4.06 (s, 3H), 4.02 (s, 3H), 1.97 (m, 4H), 1.54 (m, 4H), 1.44-1.19 (m, 32H), 0.86 (2 × t, 6H, *J* = 6.9 Hz). **^{13}C NMR** (125 MHz, chloroform-*d*, 300K, partial overlap in the aliphatic region): δ 193.92, 151.92, 150.66, 149.57, 149.11, 139.30, 128.16, 128.01, 125.13, 124.58, 123.07, 109.66, 106.49, 104.56, 104.09, 69.30, 69.29, 56.07, 56.02, 31.93, 29.70, 29.66, 29.63, 29.61, 29.51, 29.48, 29.36, 29.23, 29.12, 26.14, 26.12, 22.69, 14.11**.**

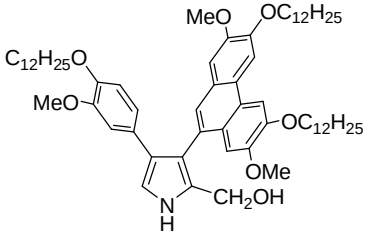
3-(3,6-Bis(dodecyloxy)-2,7-dimethoxyphenanthren-9-yl)-2-(4-(dodecyloxy)-3-methoxyphenyl)acrylonitrile (16b). 

Formylphenanthrene **15b** (1.1 g, 1.74 mmol) and nitrile **11b** were suspended in ethanol (9 mL) and heated to reflux, so as form a clear solution. To the heated reaction mixture a solution of sodium ethoxide in ethanol was added (1 M, 2 mL) and the reflux was continued for 3 hours. The reaction mixture was cooled to room temperature. A deep yellow precipitate formed, which was

filtered, washed with ethanol, and dried in air. The product was sufficiently pure for subsequent work (1.43 g, 86%). The compound slowly decomposes during storage. **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K, mixture of two isomers): δ 8.08 (s), 8.01 (d, *J* = 0.9 Hz), 7.84 (s), 7.79 (s), 7.77 (s), 7.75 (d, *J* = 1.0 Hz), 7.73 (s), 7.43 (s), 7.32 (dd, *J* = 8.3 Hz, *J* = 2.3 Hz), 7.27 (s), 7.24 (d, *J* = 2.3 Hz), 7.22 (s), 7.18 (s), 7.00 (dd, *J* = 8.3 Hz, *J* = 2.1 Hz), 6.98 (s), 6.96 (d, *J* = 8.5 Hz), 6.70 (d, *J* = 2.3 Hz), 6.67 (d, *J* = 8.6 Hz), 4.26-4.21 (m), 4.07 (t, *J* = 6.9 Hz), 4.01 (s), 3.97 (s), 3.95 (s), 3.93 (s), 3.89 (s), 3.21 (s), 1.99-1.85 (m), 1.58-1.20 (m), 0.88-0.84 (m). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, mixture of isomers, partial overlap in the alkyl region) δ 150.02, 149.86, 149.78, 149.73, 149.61, 149.50, 149.48, 149.42, 149.27, 149.07, 149.04, 148.77, 141.05, 139.16, 127.63, 127.57, 127.26, 125.97, 125.61, 125.61, 125.45, 125.43, 124.98, 124.86, 124.73, 124.63, 124.59, 123.58, 121.85, 120.30, 119.22, 118.20, 116.09, 114.12, 112.85, 112.06, 111.72, 109.79, 109.18, 108.70, 105.34, 105.29, 104.99, 104.93, 104.41, 104.26, 69.37, 69.36, 69.34, 69.21, 68.88, 56.25, 56.18, 56.01, 55.98, 55.95, 55.44, 31.91, 31.89, 29.68, 29.64, 29.62, 29.61, 29.55, 29.54, 29.49, 29.39, 29.34, 29.31, 29.22, 29.21, 29.09, 28.99, 26.12, 25.95, 25.86, 22.67, 14.09.

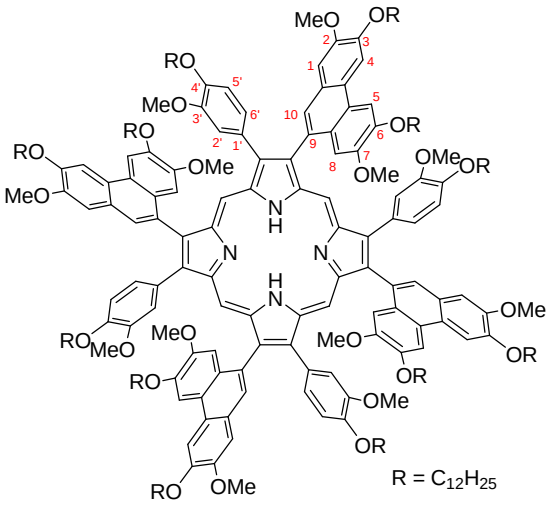


Ethyl 3-(3,6-bis(dodecyloxy)-2,7-dimethoxyphenanthren-9-yl)-4-(4-(dodecyloxy)-3-methoxyphenyl)-1*H*-pyrrole-2-carboxylate (4b). In a dry flask, cyanostilbene **16b** (0.35 g, 0.37 mmol) ad ethyl isocyanoacetate (43 μL, 0.37 mmol) was dissolved in dry THF (2 mL). The mixture was cooled to 0 °C and potassium *tert*-butoxide was added (1 M solution in THF, 0.6 mL). The reaction mixture was stirred under argon for 7 days. Subsequently, the mixture was transferred to a separatory funnel containing water and extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate and concentrated *in vacuo* to yield the product as a brown oil (0.367 g, 96%), which was sufficiently pure for further work. **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K, mixture of two isomers): δ 9.30 (bd, 1H, *J* = ca. 3 Hz), 7.793 (s, 1H), 7.791 (s, 1H), 7.43 (s, 1H), 7.26 (d, 1H, *J* = 3.0 Hz), 7.09 (s, 1H), 7.05 (s, 1H), 6.76 (dd, 1H, *J* = 8.5 Hz, *J* = 2.0 Hz), 6.59 (d, 1H, *J* = 8.5 Hz), 6.47 (d, 1H, *J* = 2.0 Hz), 4.24 (t, 2H, *J* = 6.9 Hz), 4.20 (t, 2H, *J* = 7.0 Hz), 3.94 (s, 3H), 3.92 (d, 2H, *J* = 7.1 Hz), 3.02 (d, 2H, *J* = 7.0 Hz), 3.67 (s, 3H), 3.01 (s, 3H), 1.99-1.92 (m, 4H), 1.72-1.68 (m, 2H), 1.58-1.17 (m, 74H), 0.90-0.82 (m, 9H), 0.68 (t, 3H, *J* = 7.0 Hz). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, partial overlap in the alkyl region) δ 161.31, 149.07, 148.84, 148.72, 148.61, 148.29, 146.79, 129.12, 127.28, 127.10, 127.03, 126.60, 126.32, 124.51, 124.12, 121.55, 119.43, 118.81, 112.63, 111.09, 108.60, 107.52, 104.64, 104.58, 69.41, 69.28, 68.84, 59.94, 55.86, 55.77, 55.06, 31.93, 29.70, 29.66, 29.61, 29.56, 29.52, 29.37, 29.33, 29.30, 29.14, 26.17, 26.16, 25.90, 22.69, 14.11, 13.67.

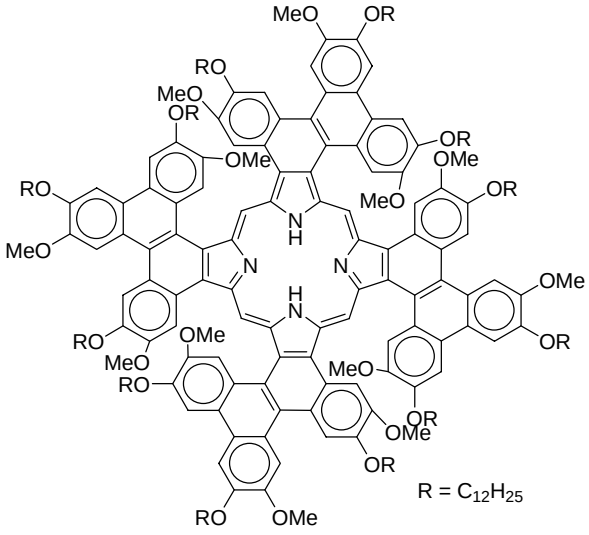


(3-(3,6-Bis(dodecyloxy)-2,7-dimethoxyphenanthren-9-yl)-4-(4-(dodecyloxy)-3-methoxyphenyl)-1*H*-pyrrol-2-yl)methanol (17b). Pyrrole **4b** (0.23 g, 23 mmol) was dissolved in dry THF (25 mL) and the solution was purged with argon. Lithium aluminum hydride (0.086 g, 2.3 mmol) was added and the suspension was stirred for 1 h under argon. The reaction was quenched with aqueous ammonium chloride and the mixture was extracted with dichloromethane. Combined organic extracts were dried over anhydrous sodium sulfate. The solvents were removed on a rotary evaporator yielding the product as a yellowish oil (0.22, 98%), which was used directly for the next step.

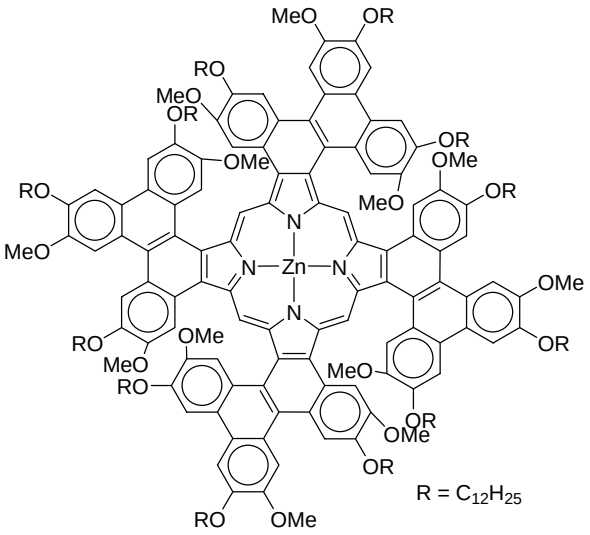
2,7,12,17-Tetrakis(3,6-bis(dodecyloxy)-2,7-dimethoxyphenanthren-9-yl)-3,8,13,18-tetrakis(4-(dodecyloxy)-3-methoxyphenyl)porphyrin (5b-H_2). Obtained from carbinol **17b** (33 mg, 0.033 mmol) using chloroform (2 mL), and boron trifluoride diethyl etherate (1.37 μL, 0.011 mmol). In the oxidation step, chloranil (60.1 mg, 0.25 mmol) was added and the reaction mixture was refluxed for 30 min. After workup, the product was obtained as dark red crystals (11 mg, 34%). **^{1}H NMR** (mixture of atropisomers, 500 MHz, chloroform-*d*, 300 K, partial assignment on the basis of 2D spectra): δ 10.39-10.30 (4H, meso), 8.21-7.94 (12H, 4,5,10-phenanthrene), 7.55-7.18 (16H, 1,8-phenanthrene, 2',6'-phenyl), 6.60-6.56 (4H, 5'-phenyl), 4.34-4.24 (16H, 3,6-α-CH_2), 4.02-3.96 (12H, 2-OMe), 3.86-3.76 (8H, 4'-α-CH_2), 3.20-3.04 (24H, 7-OMe, 3'-OMe), 2.06-1.19 (CH2), 0.89-0.82 (36H, CH_3).



3,6,12,16,19,25,29,32,38,42,45,51-Dodecakis(dodecyloxy)-2,7,11,15,20,24,28,33,37,41,46,50-dodecamethoxytetrabenzo[3,4:3',4':3'',4'':3''',4'''']tetrakistriphenyleno[1,2-*b*:1',2'-*g*:1'',2''-*l*:1''',2'''-*q*]porphyrin (6b-H_2). Compound **5b**-H_2 (5 mg, 1.2 μmol) was dissolved in freshly distilled dichloromethane (2 mL) and DDQ (1.2 mg, 5 μmol) was added. The reaction mixture was purged with argon and briefly brought to reflux. The reflux was stopped and boron trifluoride diethyl etherate was added (2.5 μL). After 15 minutes, the reaction was quenched by pouring the solution into water. The mixture was extracted with dichloromethane, the extracts were dried over anhydrous sodium sulfate, and the solvent was removed on a rotary evaporator. The crude product was purified by column chromatography (silica gel, dichloromethane) and crystallization (dichloromethane/acetone) yielding brown crystals with green luster (4 mg, 78%). **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K): δ 12.09 (s, 4H), 8.78 (s, 4H), 8.76 (s, 4H), 8.67 (s, 4H), 8.61 (s, 4H), 8.11 (s, 4H), 8.03 (s, 4H), 4.51 (m, 4H), 4.45 (m, 8H), 4.35 (m, 4H), 4.30 (s, 12H), 4.25 (m, 4H), 4.21 (m, 4H), 3.62 (s, 12H), 3.00 (t, 12H), 2.15 (m, 8H), 2.01 (m, 16H), 1.74 (m, 8H, 1.58 (m, 16H), 1.50-1.20 (m, 192H), 0.89 (m, 24H), 0.83 (t, 12H, *J* = 6.9 Hz), –0.74 (b, 2H). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, partially broadened, overlap in the alkyl region): δ 150.22, 149.34, 149.02, 148.96, 148.56, 148.40, 129.52, 126.83, 125.55, 124.39, 124.14, 123.67, 123.56, 123.43, 110.98, 110.87, 110.83, 107.41, 106.52, 106.04, 100.10, 69.72, 69.65, 69.04, 56.52, 56.16, 55.91, 31.97, 31.95, 31.90, 29.79, 29.73, 29.69, 29.65, 29.56, 29.52, 29.50, 29.42, 29.39, 29.34, 29.25, 26.31, 26.16, 26.05, 22.71, 22.66, 14.13, 14.07. **HR-MS** (ESI+): *m/z* 1941.3806 [M-H_2^{2+}], calcd. for $C_{256}H_{366}N_4O_{24}$: 1941.3844. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 307 (297000), 493 (239000), 630 (39700), 659 (55100), 686 (141000), 724 (136000).



3,6,12,16,19,25,29,32,38,42,45,51-Dodecakis(dodecyloxy)-2,7,11,15,20,24,28,33,37,41,46,50-dodecamethoxytetrabenzo[3,4:3',4':3'',4'':3''',4'''][tetrakistriphenyleno[1,2-*b*:1',2'-*g*:1'',2''-*l*:1''',2'''-*q*]porphyrinato zinc(II) (6b-Zn). Obtained using the general procedure. **^{1}H NMR** (600 MHz, chloroform-*d*, 300 K): δ 12.19 (s, 4H), 8.87 (s, 4H), 8.79 (s, 4H), 8.67 (s, 4H), 8.61 (s, 4H), 8.10 (s, 4H), 8.02 (s, 4H), 4.50 (m, 8H), 4.43 (m, 4H), 4.34 (m, 4H), 4.32 (s, 12H), 4.25-4.18 (m, 8H), 3.60 (s, 12H), 2.99 (t, 12H), 2.16 (m, 8H), 2.01 (m, 16H), 1.72 (m, 8H), 1.55 (m, 16H), 1.49-1.19 (m, 192H), 0.88 (m, 24H), 0.83 (t, 12H, *J* = 7.0 Hz). **^{13}C NMR** (151 MHz, chloroform-*d*, 300 K, overlap in the alkyl region): δ 150.10, 149.25, 148.93, 148.89, 148.40, 148.35, 146.00, 143.53, 133.18, 132.95, 129.20, 126.66, 125.47, 124.32, 124.22, 123.83, 123.68, 123.53, 111.06, 111.00, 110.84, 107.50, 106.58, 106.07, 101.56, 69.74, 69.64, 69.01, 56.53, 56.13, 55.79, 31.97, 31.95, 31.90, 29.79, 29.73, 29.69, 29.65, 29.63, 29.57, 29.51, 29.42, 29.39, 29.34, 29.25, 26.31, 26.18, 26.05, 22.71, 22.65, 14.12, 14.07. **UV-vis** (dichloromethane, 293 K) λ [nm] (ε in $M^{-1}cm^{-1}$): 299 (185000), 483 (198000), 620 (27200), 679 (183000).



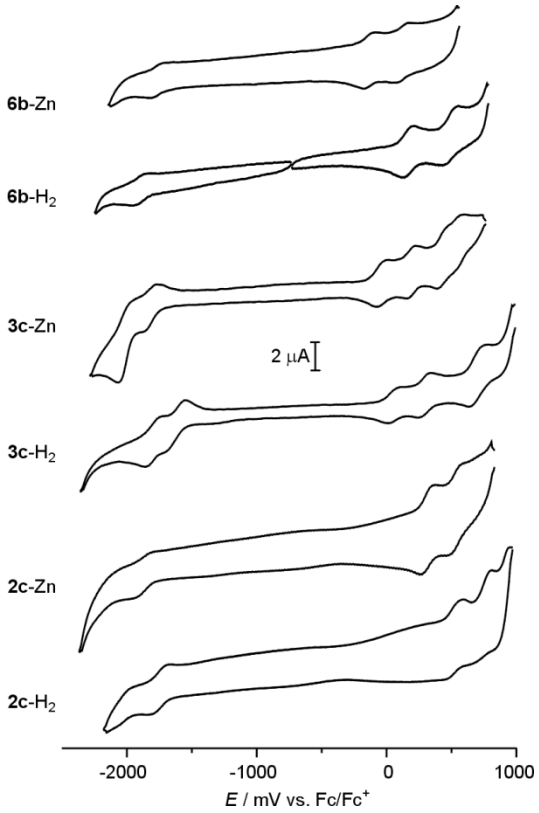


Figure S1. Cyclic voltammograms for compounds **2c**-H_2, **3c**-H_2, and **6b**-H_2, and their zinc(II) complexes.

Table S1. Electrochemical Data (CH_2Cl_2, tetrabutylammonium perchlorate) for compounds **2c**-H_2, **3c**-H_2, and **6b**-H_2, and their zinc(II) complexes.

System	$E_{ox,1}(\Delta E_{ac})$ [mV]	$E_{ox,2}(\Delta E_{ac})$ [mV]	$E_{ox,3}(\Delta E_{ac})$ [mV]	$E_{ox,4}(\Delta E_{ac})$ [mV]	$E_{red,1}(\Delta E_{ac})$ [mV]	$E_{red,2}(\Delta E_{ac})$ [mV]
2c-H_2	517(100)	741(104)	–	–	–1748(100)	–
2c-Zn	314(85)	524(70)	–	–	–1864(120)	–
3c-H_2	44(65)	290(75)	684(85)	–	–1616(120)	–1808(100)
3c-Zn	–43(60)	191(58)	417(58)	555(60)	–1803(77)	–2018(100)
6b-H_2	289(67)	567(90)	–	–	–1485(80)	–
6b-Zn	31(85)	309(90)	–	–	–1720(100)	–

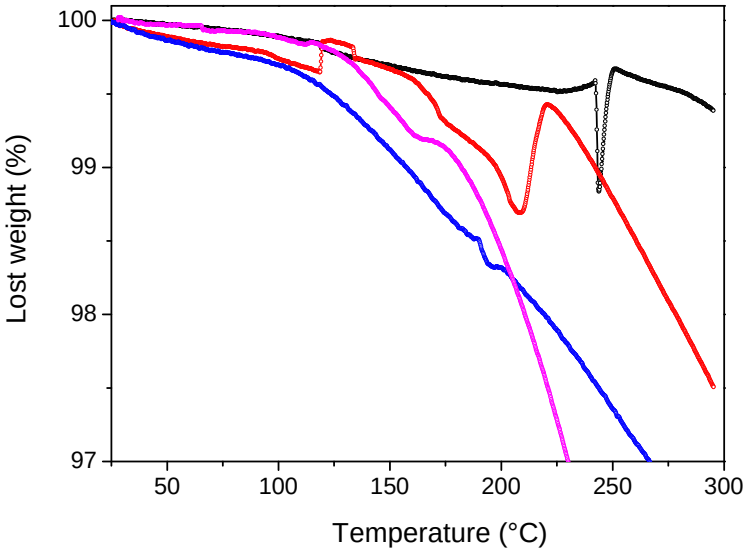


Figure S2. Thermogravimetric analyses for **2b**-H_2 (black), **2b**-Zn (red), **3b**-H_2 (blue) and **3b**-Zn (purple).

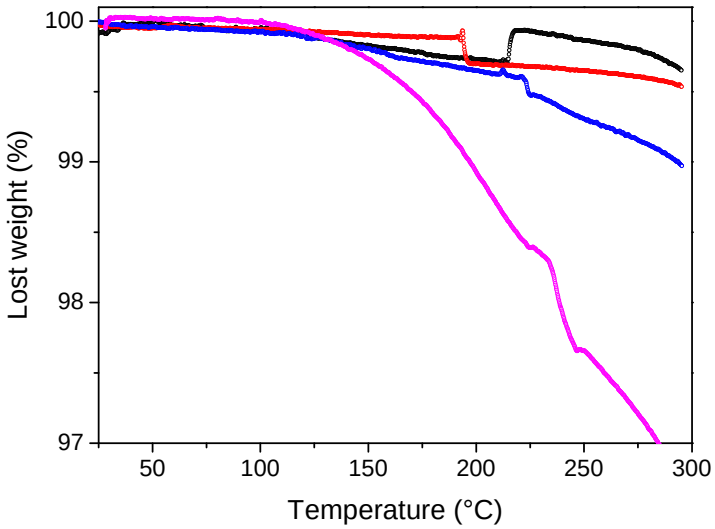


Figure S3. Thermogravimetric analyses for **2c**-H_2 (black), **2c**-Zn (red), **3c**-H_2 (blue) and **3c**-Zn (purple).

Table S2. Phase transitions observed by differential scanning calorimetry.[a]

Species	Heating/cooling runs: T_{ONSET}(°C)/T_{PEAK}(°C) [ΔH (J·g^{-1})]
2b-H_2	Cr 187.1/190.3 [0.6] Cr' 228.6/229.6 [3.86] Col_h 243.3/244.3 [5.82] I I 243.1/242.7 [-5.57] Col_h 226.7/227.0 [-3.58] Cr' 156.8/148.3 [-0.53] Cr
2b-Zn	Cr 166.1/172.8 [3.0] Col_h 201.9/209.8 [1.33] I I 205.8/201.9 [-2.0] Col_h 168.0/165.5 [-2.94] Cr
3b-H_2	[M] 150 [-] Cr 183.6/190.8 [8.3] I I 175.5/172.2 [-7.4] M + Cr
3b-Zn	Cr 110.5/118.6 [3.7] Col_h 155-160[b] [-] I I 150 [-] Col_h 130.8/125.0 [-0.55] Cr
2c-H_2	Cr 43.9/45.25 [16.0] Cr' 56.55/57.7 [7.0] Col_{r1} 142 [-] Col_{r2} 212.8/214.8 [8.0] I I 212.7/212.2 [-7.0] Col_{r2} 136 [-] Col_{r1} 56.7/56.2 [-8.5] Cr' 35.1/31.7 [-18.6] Cr
2c-Zn	Cr 31.1/32.5 [14.0] Col_{r1} 193.8/195.2 [7.5] I I 193.7/193.3 [-5.1] Col_{r1} 26.1/25.1 [16.5] Cr
3c-H_2	Cr 22.5/24.4 [17.0] Col_{r1} 217.8/222.9 [2.6] I I 219.7/218.3 [-8.0] Col_{r1} 5.2/2.0 [-7.0] Cr
3c-Zn	Cr 77.0/80.0 [2.0][c] Col_{r1} 245[b] I (no cooling run recorded due to decomposition)
6b-Zn	Cr ≈ 130[b] Mon 232[b] I

[*a*] Cr, Cr': crystalline and or semi-crystalline phases; Col_h: hexagonal columnar phase with *p6mm* planar group; Col_{r1}, $Colr_2$: rectangular columnar phases with *c2mm* planar group; Mon: monoclinic phase with $P2_1/m$ space group; M: unidentified monotropic phase (co-existence with Cr phase); I: isotropic liquid. [-]: transition enthalpy too weak to be accurately measured. [*b*] Transition temperature determined by POM. [*c*] Transition determined by TDA (TGA).

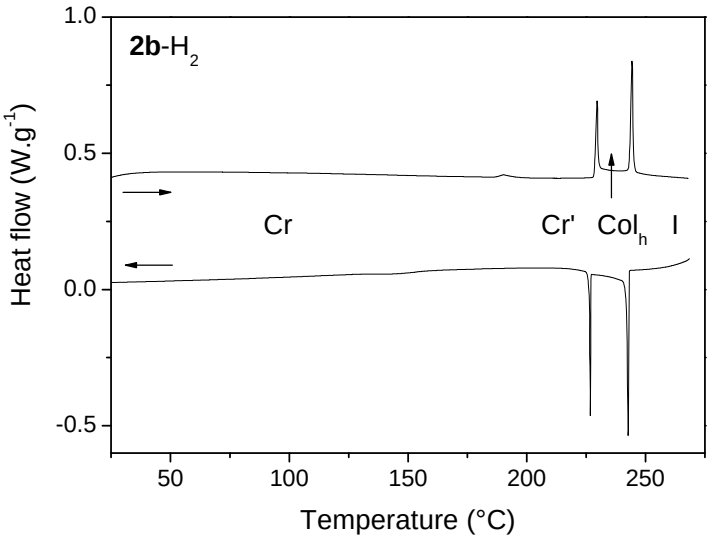


Figure S4. A differential scanning calorimetry scan for **2b**-H_2 (second cycle).

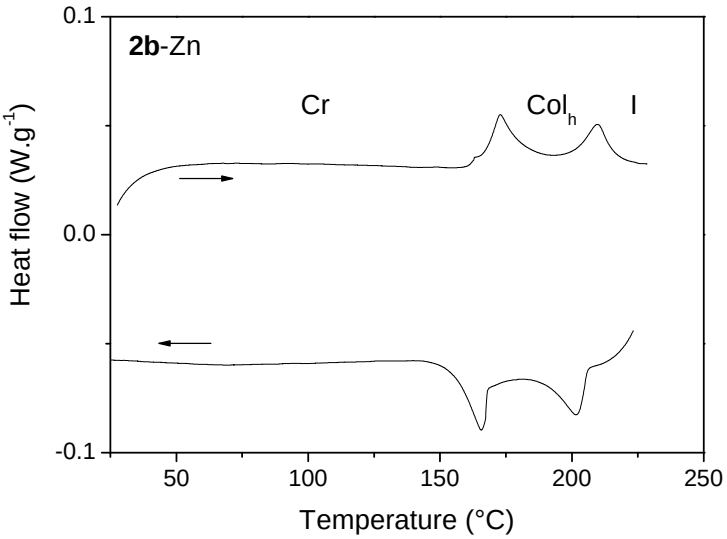


Figure S5. A differential scanning calorimetry scan for **2b**-Zn (second cycle).

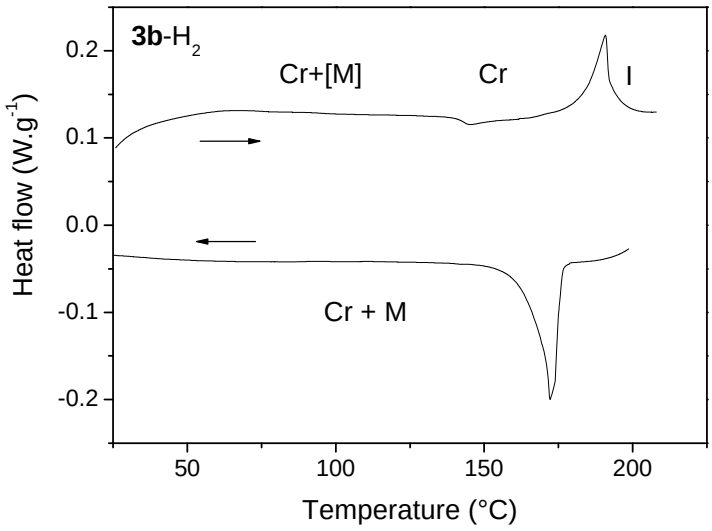


Figure S6. A differential scanning calorimetry scan for **3b**-H_2 (second cycle).

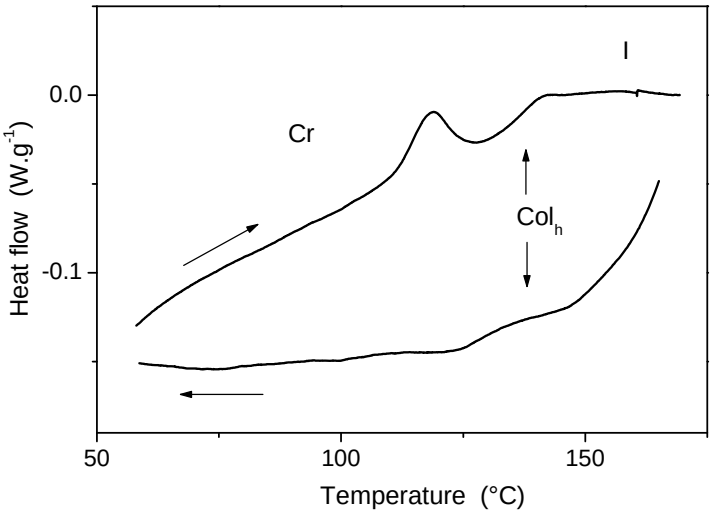


Figure S7. A differential scanning calorimetry scan for **3b**-Zn.

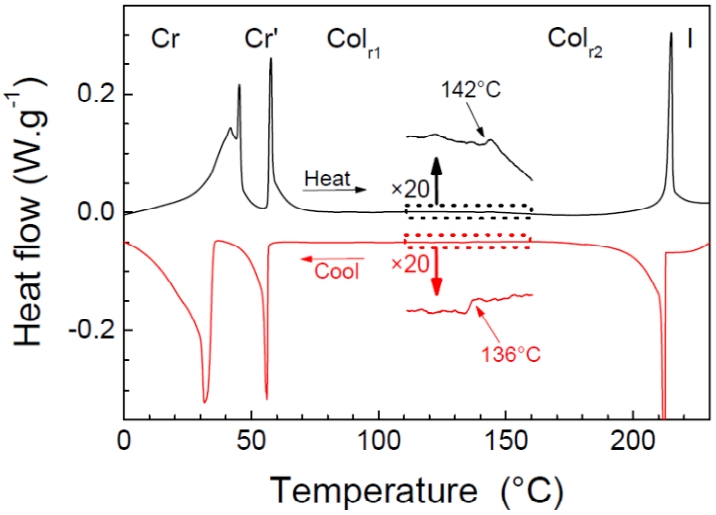


Figure S8. A differential scanning calorimetry scan for **2c**-H_2.

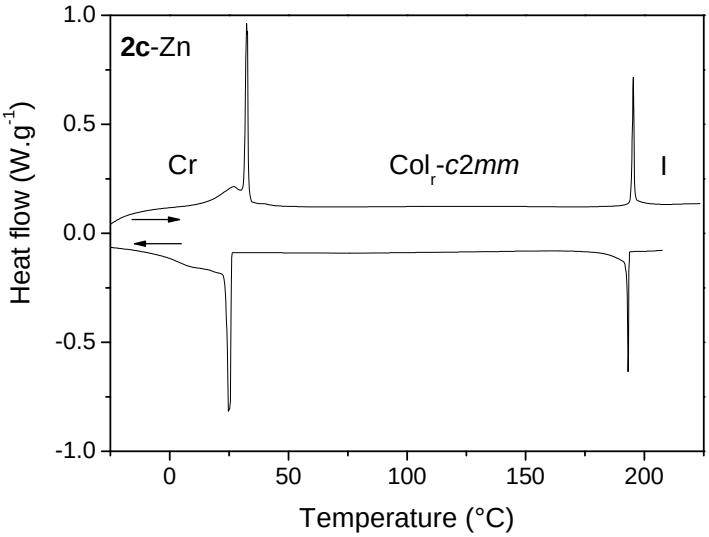


Figure S9. A differential scanning calorimetry scan for **2c**-Zn.

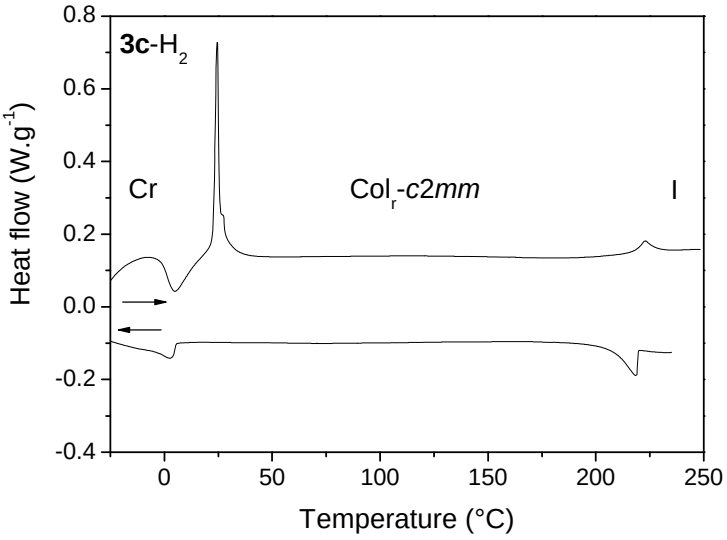


Figure S10. A differential scanning calorimetry scan for **3c**-H_2.

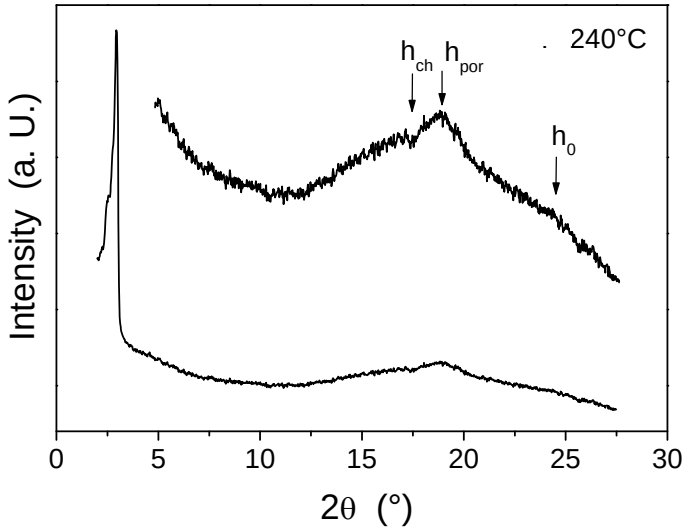


Figure S11. X-ray diffraction pattern for **2b**-H_2 at 240°C in the Col_h phase.

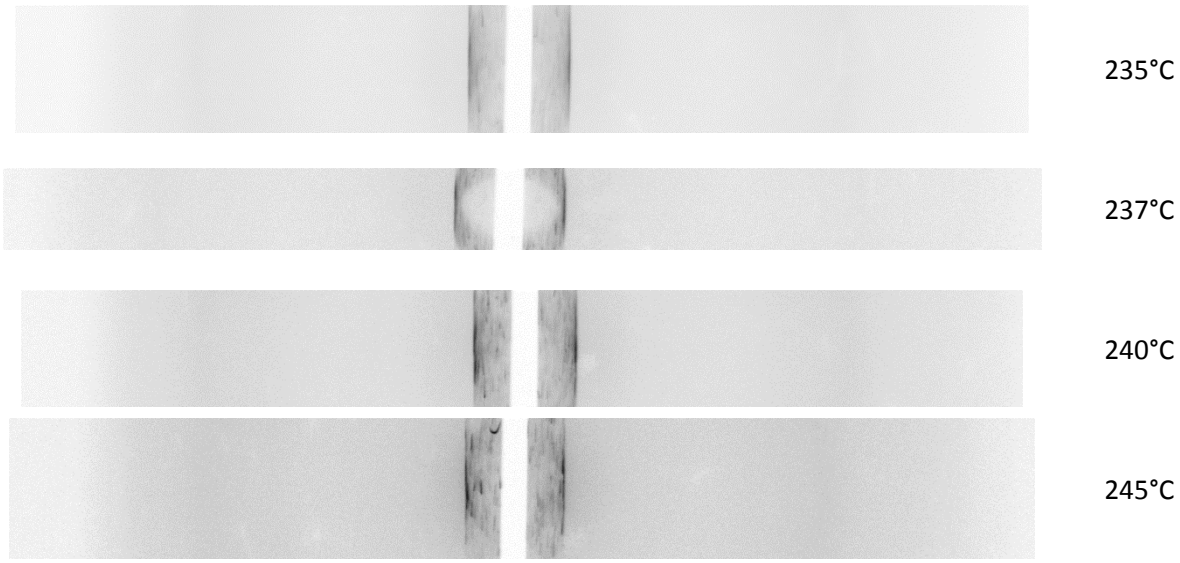


Figure S12. X-ray diffraction patterns of **2b**-H_2 at 235-245°C in the Col_h phase (only the fundamental small-angle reflection (10) of the hexagonal lattice is detected).

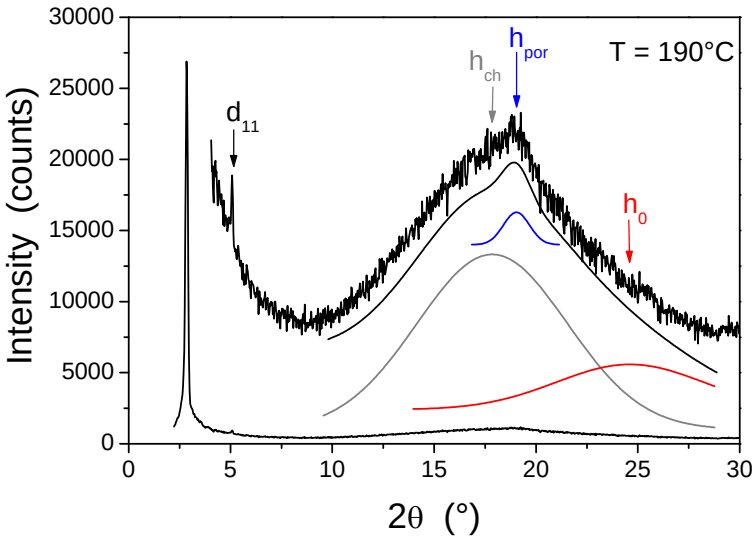


Figure S13. X-ray diffraction patterns for **2b**-Zn at 190°C in the Col_h phase.

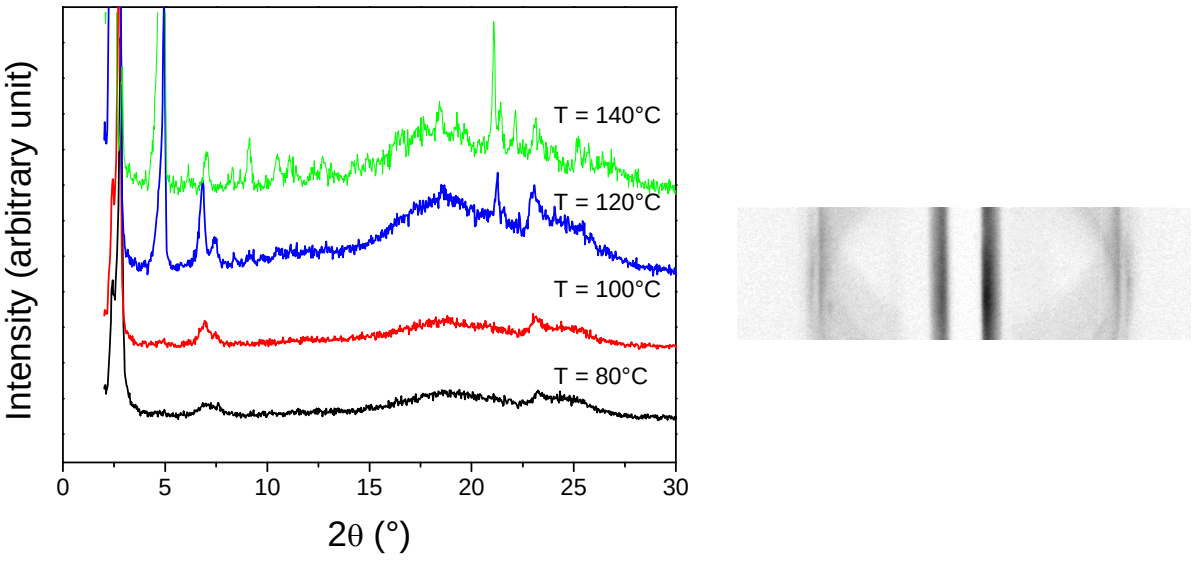


Figure S14. X-ray diffraction patterns for **3b**-H_2 observed during heating (left). Right: part of the small-angle X-ray pattern recorded at 80°C on cooling, showing two first order reflections with different line-shape, suggesting co-existence of crystalline phase and mesophase.

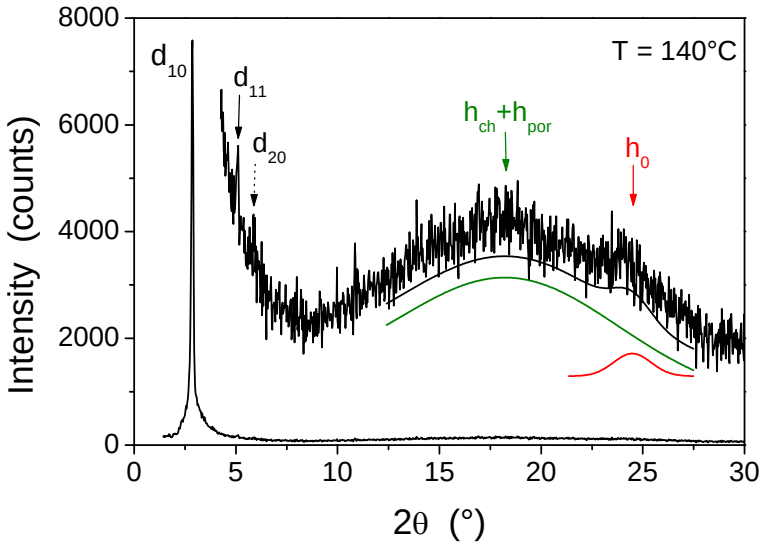


Figure S15. X-ray diffraction patterns for **3b**-Zn at 140°C in the Col_h phase.

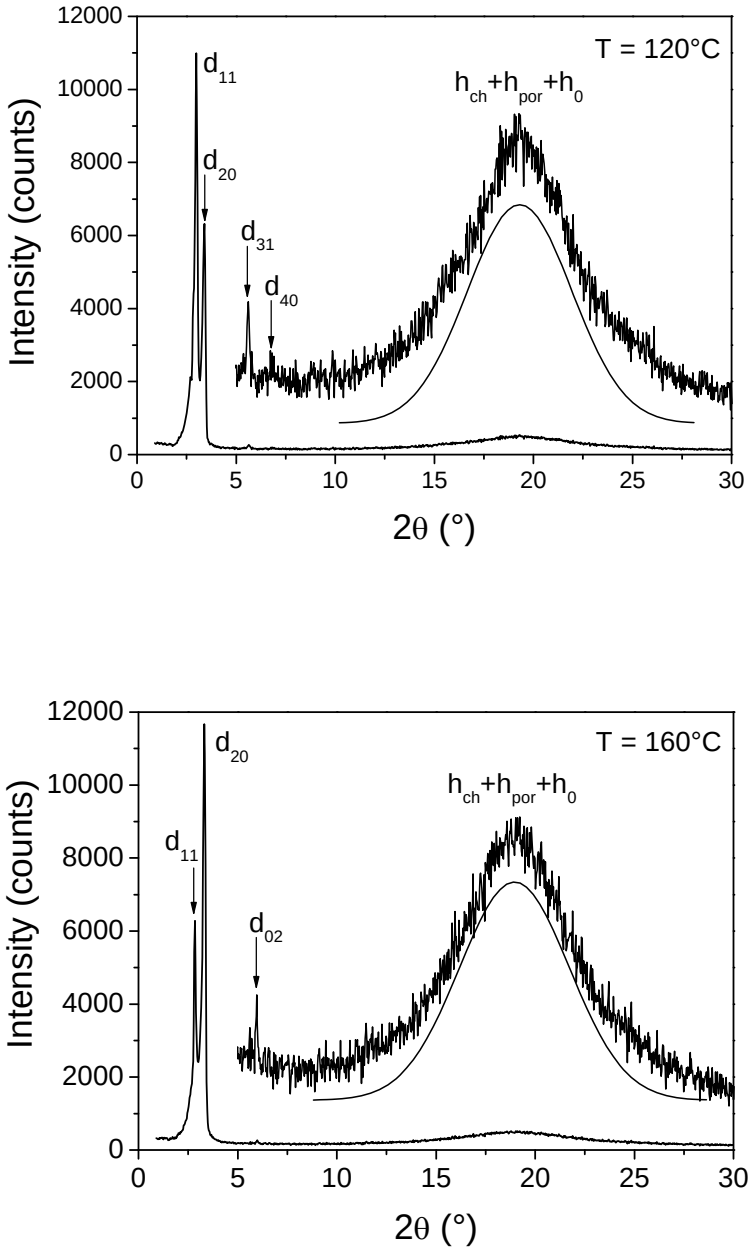


Figure S16. X-ray diffraction patterns for **2c**-H_2 at 120 and 160°C in the Col_r phases.

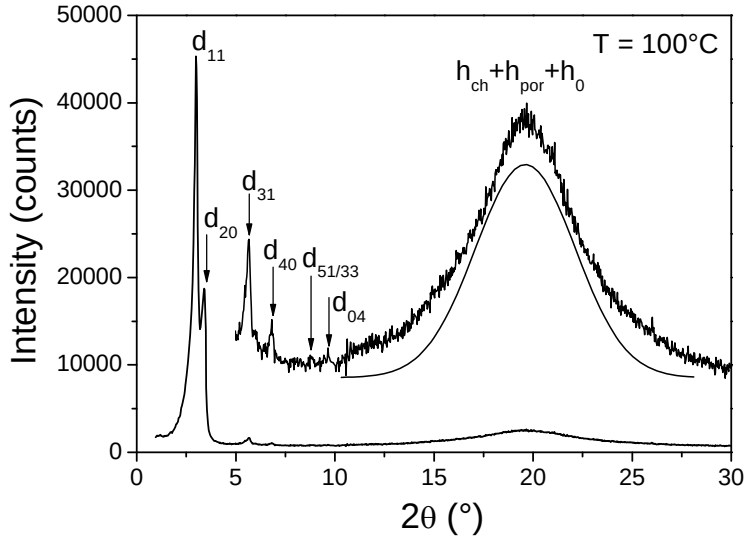


Figure S17. X-ray diffraction pattern for **2c**-Zn at 100°C in the Col_r phase.

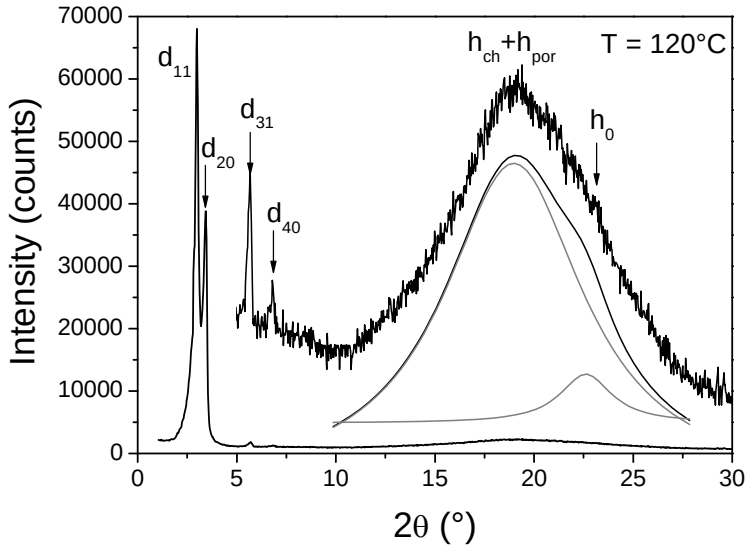


Figure S18. X-ray diffraction pattern for **3c**-H_2 at 120°C in the Col_r phase.

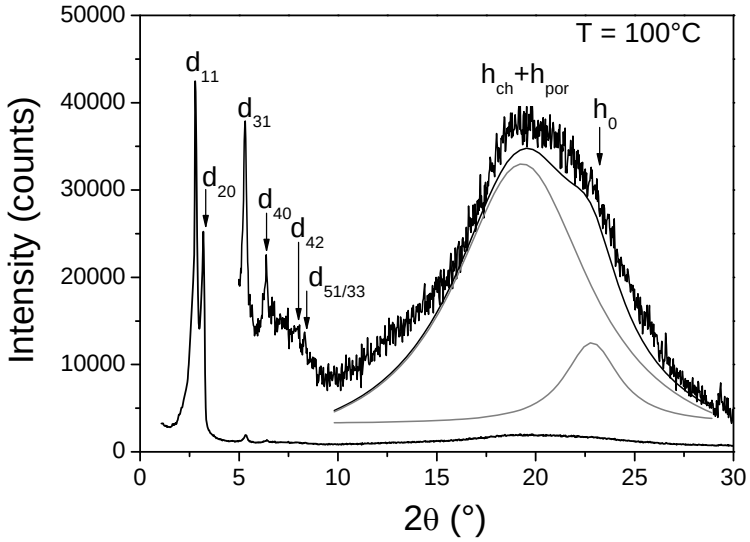


Figure S19. X-ray diffraction pattern for **3c**-Zn at 100°C in the Col_r phase.

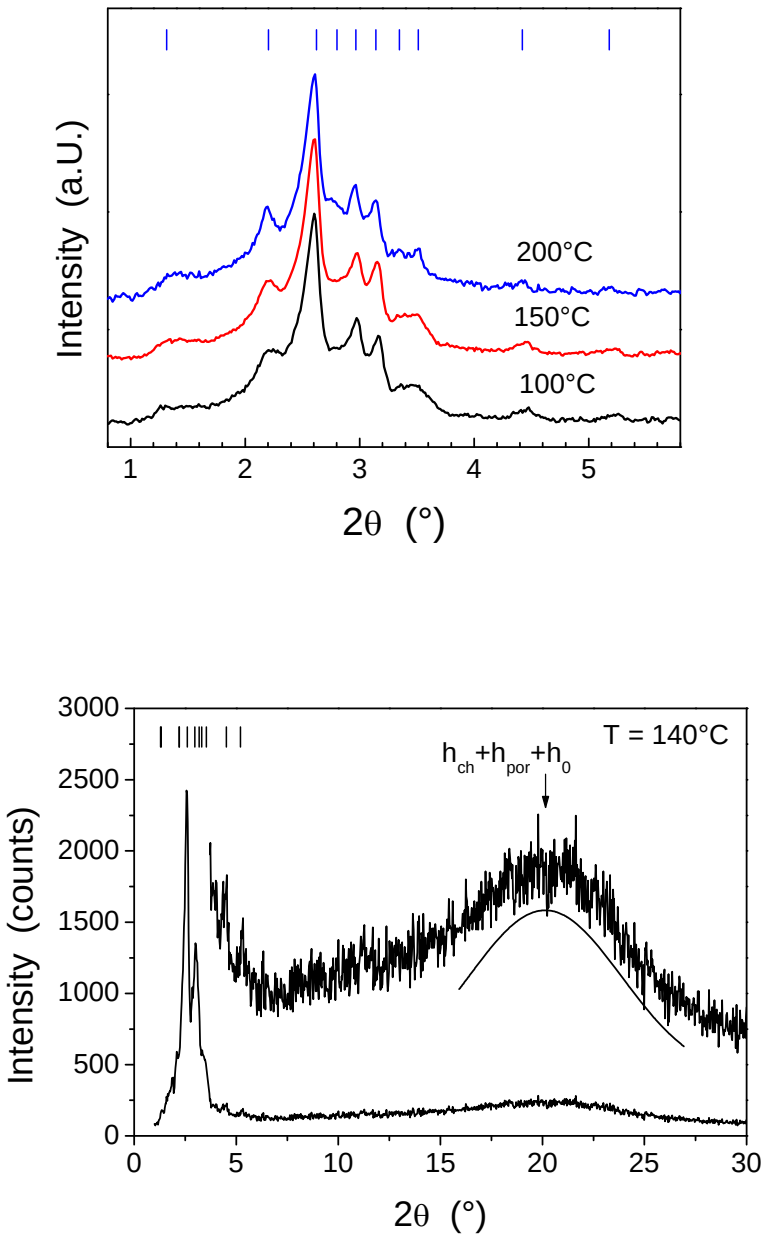


Figure S20. Small-angle (top) and full-angle range (bottom) XRD patterns of **6b**-Zn, at different temperatures.

Table S3. XRD data for liquid crystalline phases observed for **2b**-H_2 and for the series of Zn(II) complexes **2b**-Zn, **3b**-Zn and **6b**-Zn.

Sample T/°C	$d_{exp.}$/Å[a]	I (L)[b]	hk[c]	$d_{theo.}$/Å[a]	Parameters[d]
2b-H_2	29.91	VS (sh)	10	-	Col_h-*p6mm*
235	5.1-3.6	VS (br)	-	$h_{ch}+h_{por}+h_0$	T = 235, 240, 245°C
					a = 34.53, 34.47, 34.2 Å
	29.85	VS (sh)	10	-	S = 1033, 1030, 1015 Å^2
240	5.1	VS ($\xi \approx 10$ Å)	-	h_{ch}	V_M = 5450, 5465, 5479, ±400 Å^3
	4.68	M ($\xi \approx 30$ Å)	-	h_{por}	d = 0.802, 0.800, 0.798, ±0.060
	3.6	M ($\xi \approx 10$ Å)	-	h_0	h_M = 5.28, 5.31, 5.40, ±0.40 Å
					Z=1
	29.62	VS (sh)	10	-	
245	5.1-3.6	VS (br)	-	$h_{ch}+h_{por}+h_0$	
2b-Zn	30.14	VS (sh)	10	30.09	Col_h-*p6mm*
190	17.34	W (sh)	11	17.37	a = 34.75 Å,
	5.0	VS ($\xi \approx 10$ Å)	-	h_{ch}	S = 1045.5 Å^2
	4.66	M ($\xi \approx 50$ Å)	-	h_{por}	V_M = 5322±400 Å^3
	3.6	M ($\xi \approx 10$ Å)	-	h_0	d = 0.842±0.063
					h_M = 5.09 ± 0.40 Å
					Z=1
3b-Zn	29.87	VS (sh)	10	29.91	Col_h-*p6mm*
140	17.29	W (sh)	11	17.27	a = 34.52 Å
	4.9	VS (br)	-	$h_{ch}+h_{por}$	S = 1032 Å^2
	3.6	W (br)	-	h_0	$V_M \approx$ 5164 Å^3
					d ≈ 0.865
					$h_M \approx$ 5.00 Å
					Z=1
6b-Zn	69.0	W (sh)	100	67.84	Mon-$P2_1/m$
150	40.0	M (sh)	002	39.81	a = 68.2 Å; b = 39.0 Å
	33.7	VS (sh)	200/110	33.92	c = 81.0 Å; β =98.0°
	29.5	S (sh)	201	29.78	V = 213 10^3 Å^3 (N = 27.8)
	27.9	S (sh)	$20\bar{2}$	27.75	S = a×b/2 = 1331 Å^2
	26.4	VW (sh)	$11\bar{2}$	26.73	$V_M \approx$ 7689 Å^3
	25.2	VW (sh)	112	25.00	d ≈ 0.852
	19.6	M (sh)	020/310	19.58	$h_M \approx$ 5.73 Å
	16.7	W (sh)	400/220	16.96	Z=1
	4.4	VS (br)	-	$h_{ch}+h_{por}+h_0$	

[*a*] d_{exp} and d_{theo} are the experimentally measured and theoretical diffraction spacings, respectively. The distances are given in Å. d_{theor} is deduced from the following mathematical expression for the Col_h phase, $a = 2\sum d_{hk}\times(h^2+k^2+hk)^{½}/N_{hk}\sqrt{3}$, where N_{hk} is the number of *hk* reflections; h_{ch}: maximum of the diffuse scatering due to lateral distances between molten aliphatic tails, h_{por}: diffuse scattering due to the stacking of the porphyrin rings; h_0: diffuse scattering due to the π-π stacking of the aromatic side-groups. [b] Intensity (I) and width (L) of the reflections: VS very strong, S strong, M medium, W weak, VW very weak, br broad, sh sharp; ξ: correlation length (Scherrer formula). [c] Miller indices of the reflections. [d] V_M: molecular volume obtained from the combination of dilatometric data and single crystal structures by assuming the partial volume additivity and estimating the thermal expansion: the estimated maximum error and its repercussion on h_M and d are indicated for **2b**-H_2 and **2b**-Zn only, but the accurracy is similar in the other cases; d is the density in g.cm^{-3}; a is the lattice parameter in the Col_h phase (a=b; γ=120°); the columnar cross-section is given by $S = a^2\sqrt{3}/2$; Z is the number of molecules per columnar slice of thickness h_M: $h_M S = ZV_M$; a, b, c and β are the parameters of the monoclinic lattice, V is the lattice volume and N is the number of molecules contained in the lattice; S is the cross-section of a single molecular stack in the a×b plane (with 2 stacks per lattice); Z is the number of molecules per stack slice of thickness h_M.

Table S4. XRD data for liquid crystalline phases observed for compounds **2c**-H_2, **3c**-H_2 and their Zn(II) complexes.

Sample T/°C	$d_{exp.}$/Å[a]	I (L)[b]	hk[c]	$d_{theo.}$/Å[a]	Parameters[d]
2c-H_2	30.14	VS (sh)	11	-	Col_{r1}-*c*2*mm*
120	26.53	S (sh)	20	-	a = 53.06 Å
	15.8	W (sh)	31	15.93	b = 36.62 Å
	13.06	VW (sh)	40	13.26	S = 971.6 Å^2
	4.6	VS (br)	-	h_{ch}+h_{por}+h_0	V_M ≈ 7672 Å^3 (d ≈ 0.837)
					h_M ≈ 7.90 Å (Z=1)
160	31.72	S (sh)	20	-	Col_{r2}-*c*2*mm*
	27.13	VS (sh)	11	-	a = 63.45 Å
	15.04	W (sh)	02	15.01	b = 30.01 Å
	4.6	VS (br)	-	h_{ch}+h_{por}+h_0	S = 952.1 Å^2
					V_M ≈ 7858 Å^3 (d ≈ 0.831)
					h_M ≈ 8.25 Å (Z=1)
2c-Zn	30.07	VS (sh)	11	-	Col_{r1}-*c*2*mm*
100	26.32	S (sh)	20	-	a = 52.64 Å
	15.87	M (sh)	31	15.85	b = 36.64 Å
	13.07	W (sh)	40	13.18	S = 964.2 Å^2
	10.1	W (sh)	51/33	10.14/10.02	V_M ≈ 7579 Å^3 (d ≈ 0.861)
	9.19	VW (sh)	04	9.15	h_M ≈ 7.86 Å (Z=1)
	4.55	VS (br)	-	h_{ch}+h_{por}+h_0	
3c-H_2	30.35	VS (sh)	11	-	Col_{r1}-*c*2*mm*
120	26.27	S (sh)	20	-	a = 52.54 Å
	15.69	W (sh)	31	15.84	b = 37.18 Å
	13.07	VW (sh)	40	13.13	S = 976.7 Å^2
	4.55	VS (br)	-	h_{ch}+h_{por}	V_M ≈ 7658 Å^3 (d ≈ 0.837)
	4.1	VS (br)	-	h_0	h_M ≈ 7.84 Å (Z=1)
3c-Zn	31.5	VS (sh)	11	-	Col_{r1}-*c*2*mm*
100	28.0	S (sh)	20	-	a = 56.0 Å
	16.66	M (sh)	31	16.76	b = 38.1 Å
	13.81	M (sh)	40	14.0	S = 1066.8 Å^2
	11.3	VW (sh)	42	11.28	V_M ≈ 7565 Å^3 (d ≈ 0.861)
	10.6	VW (sh)	51/33	10.75/10.5	h_M ≈ 7.09 Å (Z=1)
	4.55	VS (br)	-	h_{ch}+h_{por}	
	4.0	VS (br)	-	h_0	

[*a*] d_{exp} and d_{theo} are the experimentally measured and theoretical diffraction spacings, respectively. The distances are given in Å. d_{theor} is deduced from the following mathematical expressions for the Col_{r1} and Col_{r2} phases: $1/d_{hk} = \sqrt{(h^2/a^2+k^2/b^2)}$; h_{ch}: maximum of the diffuse scatering due to lateral distances between molten aliphatic tails, h_{por}: diffuse scattering due to the stacking of the porphyrin rings; h_0: diffuse scattering due to the π-π stacking of the aromatic side-groups. [b] Intensity (I) and width (L) of the reflections: VS very strong, S strong, M medium, W weak, VW very weak, br broad, sh sharp. [c] Miller indices of the reflections. [d] V_M: molecular volume obtained from the combination of dilatometric data and single crystal structures by ussuming the partial volume additivity and estimating the thermal expansion; d is the density in g.cm^{-3}; a and b are the lattice parameters in the Col_{r1} and Col_{r2} phases (a≠b; γ=90°); the columnar cross-section is given by S = a.b/2; Z is the number of molecules per columnar slice of thickness h_M: $h_M S = ZV_M$.

Table S5. Indexation of the monoclinic phase of **6b**-Zn (small-angle peaks).

N°	$2\theta_{obs}$ [°]	d_{obs} [Å]	I	hkl	$2\theta_{cal}$ [°]	d_{cal} [Å]	Phase parameters[a]
1	1.28	68.9	W	100	1.311	67.31	T = 100°C, 1st heat
2	2.22	39.8	M	002	2.194	40.23	a = 67.9(065) Å
3	2.61	33.8	VS	200/110	2.623	33.66	b = 38.8(6) Å
5	2.99	29.5	S	201	2.974	29.68	c = 81.1(731) Å
6	3.16	27.9	S	20-2	3.189	27.68	α = 90°
7	3.35	26.4	VW	11-2	3.307	26.70	β =97.6°
8	3.51	25.2	M	112	3.530	25.01	γ = 90°
9	4.48	19.7	M	020/310	4.544	19.43	V = 212(321) Å^3
10	5.22	16.9	W	400/220	5.247	16.83	S = a×b/2 = 1319 Å^2
1	1.28	68.9	W	100	1.301	67.84	T = 150°C, 1st heat
2	2.20	40.0	M	002	2.217	39.81	a = 68.4(735) Å
3	2.62	33.7	VS	200/110	2.602	33.92	b = 39.1(70) Å
5	2.99	29.5	S	201	2.964	29.78	c = 80.3(736) Å
6	3.17	27.9	S	20-2	3.182	27.75	α = 90°
7	3.34	26.4	VW	11-2	3.302	26.73	β =97.8°
8	3.50	25.2	VW	112	3.531	25.00	γ = 90°
9	4.50	19.6	M	020/310	4.508	19.58	V = 213(576) Å^3
10	5.29	16.7	W	400/220	5.206	16.96	S = a×b/2 = 1341 Å^2
1	1.31	67.1	VW	100	1.306	67.57	T = 200°C, 1st heat
2	2.20	40.0	M	002	2.203	40.07	a = 68.2(34) Å
3	2.62	33.7	VS	200/110	2.613	33.78	b = 39.0(10) Å
4	2.80	31.5	VW	11-1	2.764	31.94	c = 80.9(75) Å
5	2.97	29.7	S	201	2.973	29.69	α = 90°
6	3.14	28.1	S	20-2	3.174	27.81	β =98.0°
7	3.34	26.4	VW	11-2	3.299	26.76	γ = 90°
8	3.51	25.1	W	112	3.533	24.98	V = 213(290) Å^3
							S = a×b/2 = 1331 Å^2

[*a*] S: half-lattice section area, corresponding to the cross-section area of the strings of discrete piled discs assemblies.

Table S6. Geometrical parameters of mesophases obtained from XRD.

Sample	T/°C	phase	a/(b√3)[a]	V_c/Å^3[b]	h_M/Å[c]	S_c/Å^2[d]	σ_c/Å^2[e]	ψ_c°[f]	d_c/D_c[g]	nC_{12}-mC_1[h]	N_{ch}[h]	D_c/Å[i]	d_c/Å[i]	Σ_c/Å^2[j]	S_{ch}/Å^2[k]	S_{ch}/σ_{ch}[l]
2b-H_2	235	Col_h	1	2194	5.28	415.7	415.7	0	1	8-8	16	23.01	-	381.3	23.83	0.967
2b-Zn	190	Col_h	1	2159	5.09	424.2	424.2	0	1	8-8	16	23.24	-	371.7	23.23	0.970
3b-Zn	140	Col_h	1	2107	5.00	421.1	421.1	0	1	8-8	16	23.15	-	364.0	22.75	0.983
6b-Zn	150	Mon	1.0093	3072	5.73	535.8	*614*	*29*	-	12-12	24	*27.96*[m]	*24.40*[m]	*472.1*[m]	*19.67*[m]	*0.844*[m]
2c-H_2	120	Col_{r1}	0.8365	2106	7.90	266.7	424.2	51.0	0.6287	16-0	16	23.24	14.61	475.6	29.73	1.302
	160	Col_{r2}	1.2207	2137	8.25	258.9	424.2	52.4	0.6102	16-0	16	23.24	14.18	492.2	30.77	1.311
2c-Zn	100	Col_{r1}	0.8295	2091	7.86	266.0	424.2	51.2	0.6270	16-0	16	23.24	14.57	473.1	29.57	1.314
3c-H_2	120	Col_{r1}	0.8159	2092	7.84	266.8	421.1	50.7	0.6336	16-0	16	23.15	14.67	471.7	29.48	1.292
3c-Zn	100	Col_{r1}	0.8486	2077	7.09	292.9	421.1	45.9	0.6955	16-0	16	23.15	16.10	440.8	27.55	1.224

[a] by using rectangular coordinates, the ratio a/(b√3) (q_{hex}) measures the deformation of the columnar lattice from the special case of hexagonally packed cylinders (a=b√3). [b] V_c: partial volume of the molecular core (i.e. the whole molecule except the aliphatic chains. [c] h_M: columnar slice thickness. [d] S_c: partial cross-section of the columnar cores, $S_C=V_c/h_M$. [e] σ_c: partial cross-section of the molecular cores (in the planes containing the stacked cores). For organizations with untilted piling (**2b** and **3b** series): $\sigma_c=S_c$. For the tilted organizations in the **2c** and **3c** series, σ_c was identified to the value of the corresponding Zinc complex in the **b** series. σ_c for **6b**-Zn was evaluated by assuming that h_M were the same than for **3b**-Zn, according to $\sigma_c=S_c\times h_M$[**6b**-Zn]/h_M[**3b**-Zn]. [f] ψ_c: tilt angle between the normal to the cores plane and the columnar axis deduced from the strectching degree of the columns: $\cos\psi_c=S_c/\sigma_c$. However in the **6b**-Zn special case, ψ_c does not traduce a regular tilting of the cores, but the elongation due to the pinching zones. [g] d_c/D_c: major and minor diameters ratio characterizing the elliptical columnar cross-section due to the tilting of the cores. [h] nC_{12}-mC_1: n $C_{12}H_{25}$ chains and m CH_3 groups, i.e. N_{ch}=n+m aliphatic tails, are grafted to the molecular core. [i] $D_c=[(4/\pi)\sigma_c]^{0.5}$: core's diameter (for circular cross-sections) or major diameter (for elliptical cross-sections). In latter case, the minor diameter is $d_c=D_c\cos\psi_c$. [j] Σ_c: area of the interface between the columnar cores and the aliphatic periphery. By assuming sharp interfaces with ideal circular or elliptical shape, the area is calculated from: $\Sigma_c=\pi D_c h_M\times[(1+\cos\psi_c)/2]\times[3-\{4-[(1-\cos\psi_c)/(1+\cos\psi_c)]^2\}^{0.5}]$. [k] $S_{ch}=\Sigma_c/N_{ch}$: partial interface area covered by a single chain. [l] the ratio S_{ch}/σ_{ch} (q_{ch}) evidences the agreement with the cross-section of a molten and stretched aliphatic chain according to $\sigma_{ch}=V_{CH2}/1.27$, the volume of a molten methylene unit being calculated from: $V_{CH2}(T)=26.5616+0.02023T$ (T in °C)). [m] In the **6b**-Zn special case, the fitting of the areas near to the interface does not occur over a regular tilting all along the columns, but over periodic pinching zones. Nevertheless, for the sake of comparison of both elongation mechanisms, the table contains values of D_c, d_c, Σ_c, and S_{ch} calculated for tilted columns with areas S_c and σ_c identical to the experimental ones.

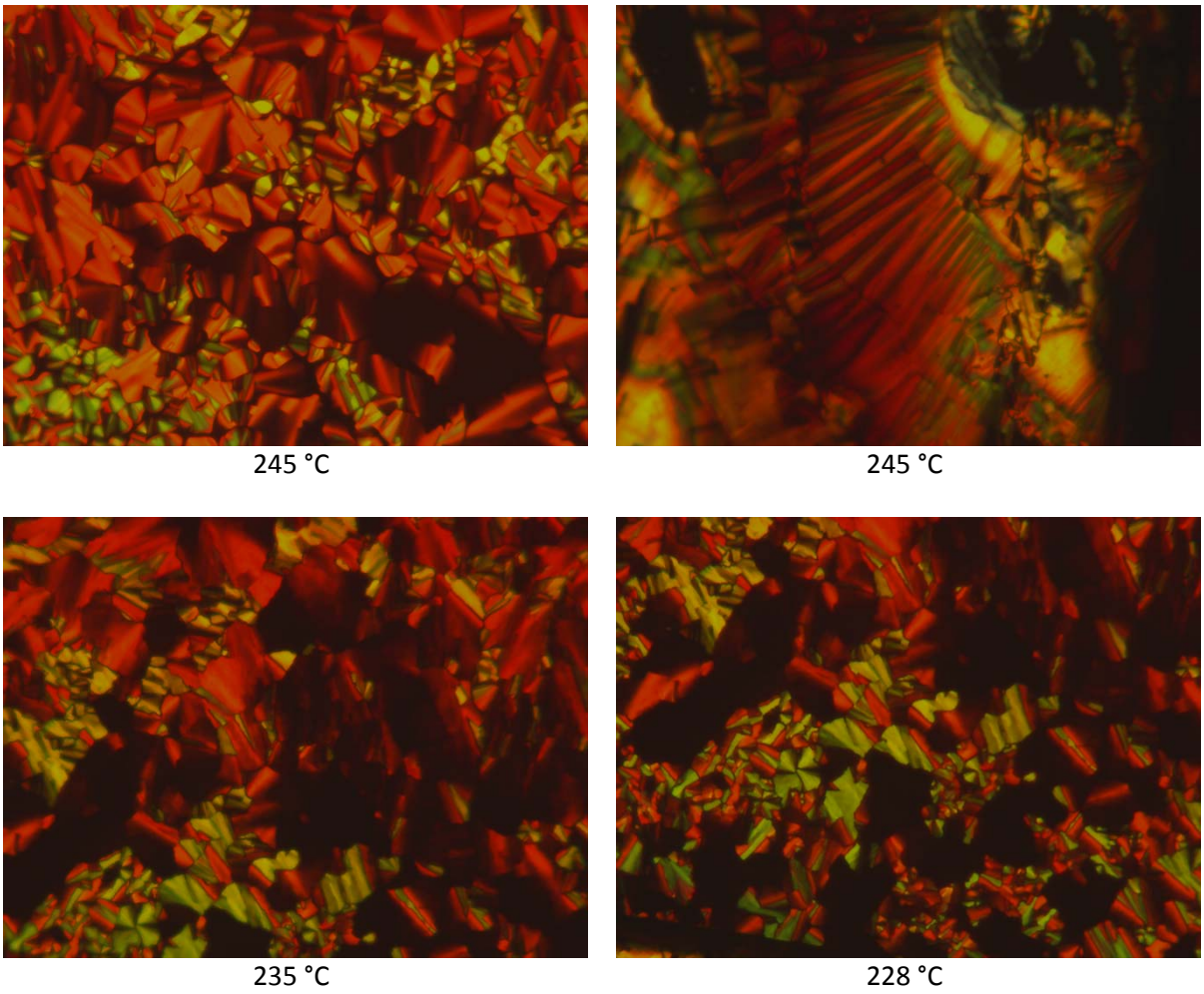


Figure S21. Polarizing optical microscopy images for **2b**-H_2 recorded on cooling.

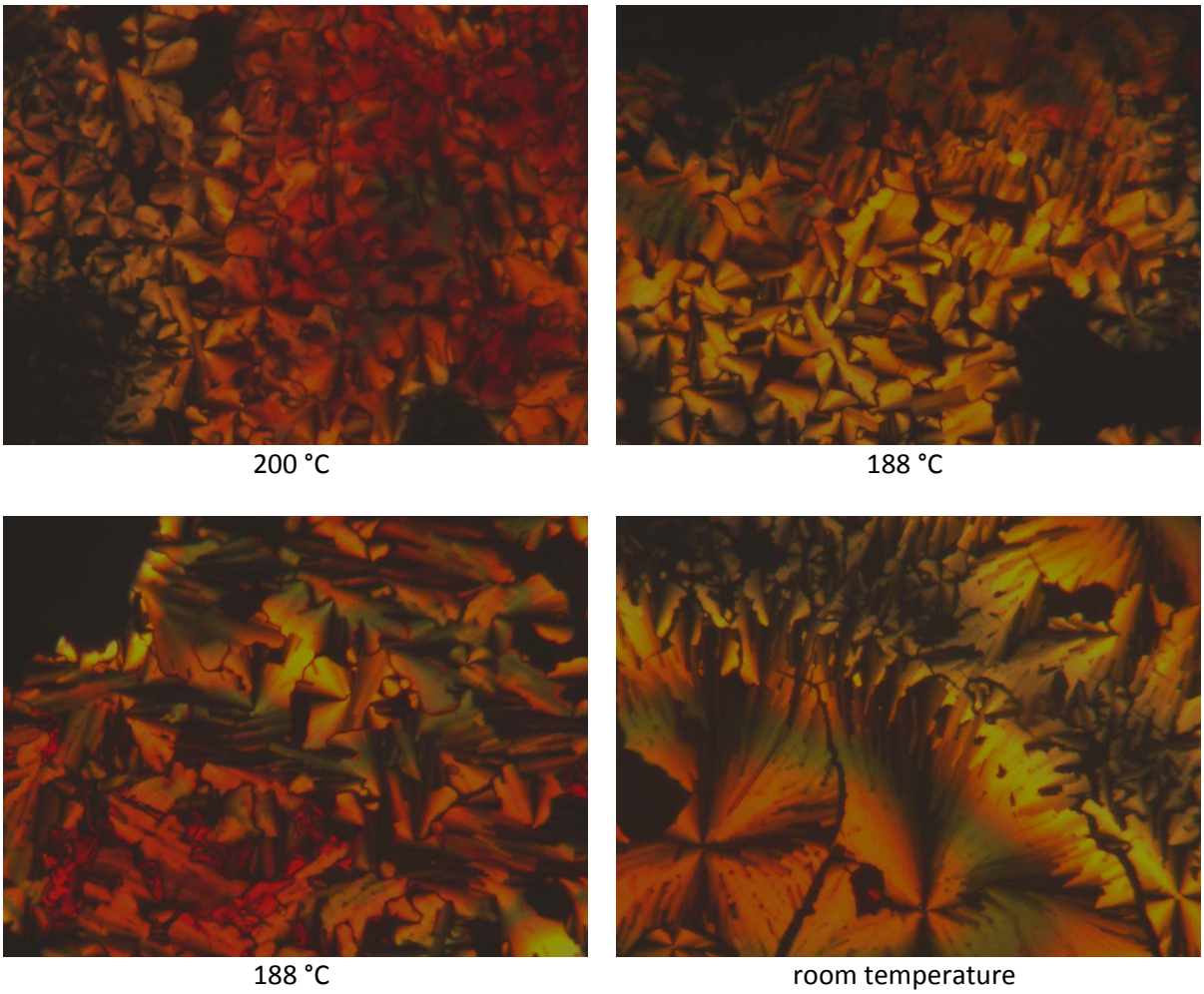
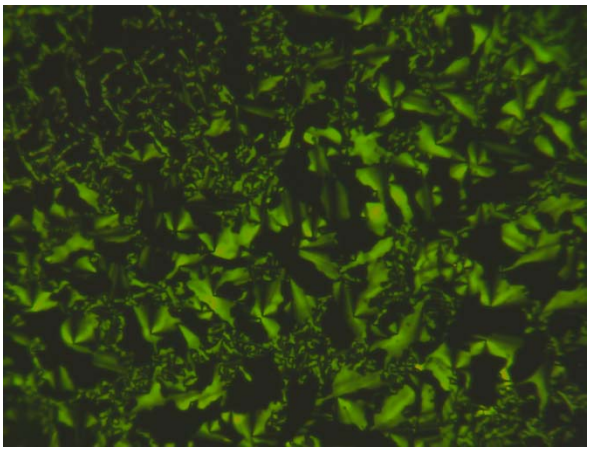
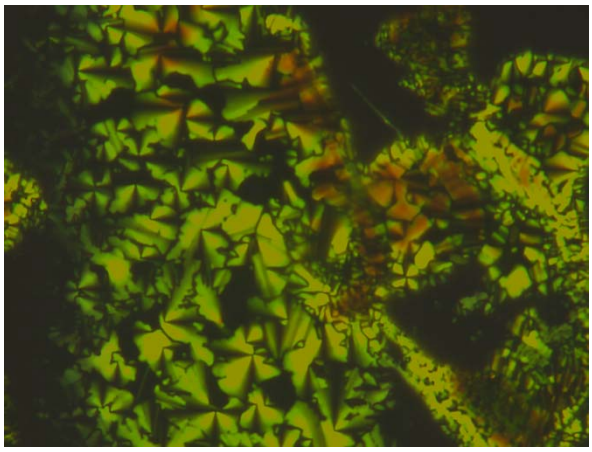


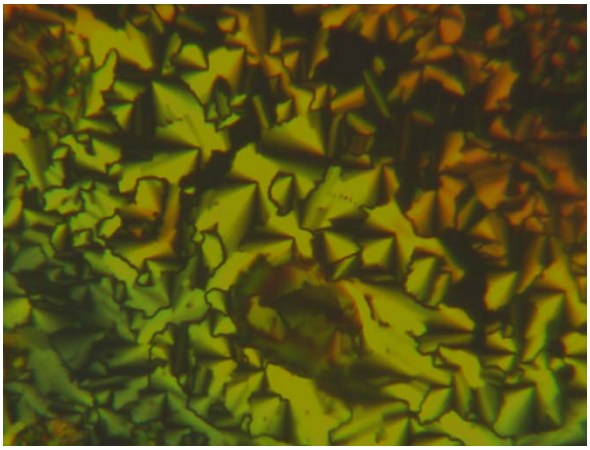
Figure S22. Polarizing optical microscopy textures for **2b**-Zn recorded on cooling.



160 °C



155 °C



room temperature

Figure S23. Polarizing optical microscopy textures for **3b**-Zn recorded on cooling.

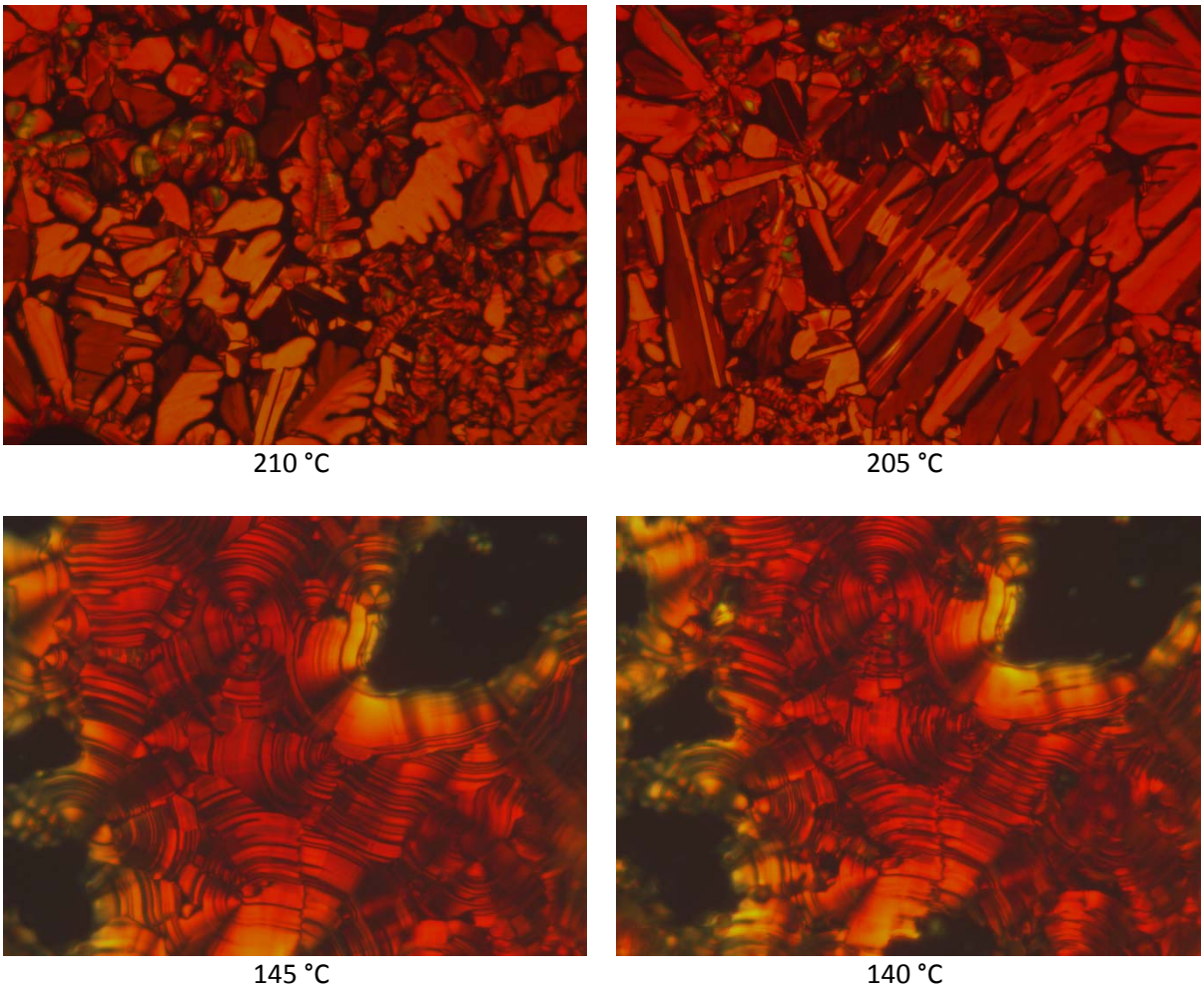


Figure S24. Polarizing optical microscopy images for **2c**-H_2 recorded on cooling.

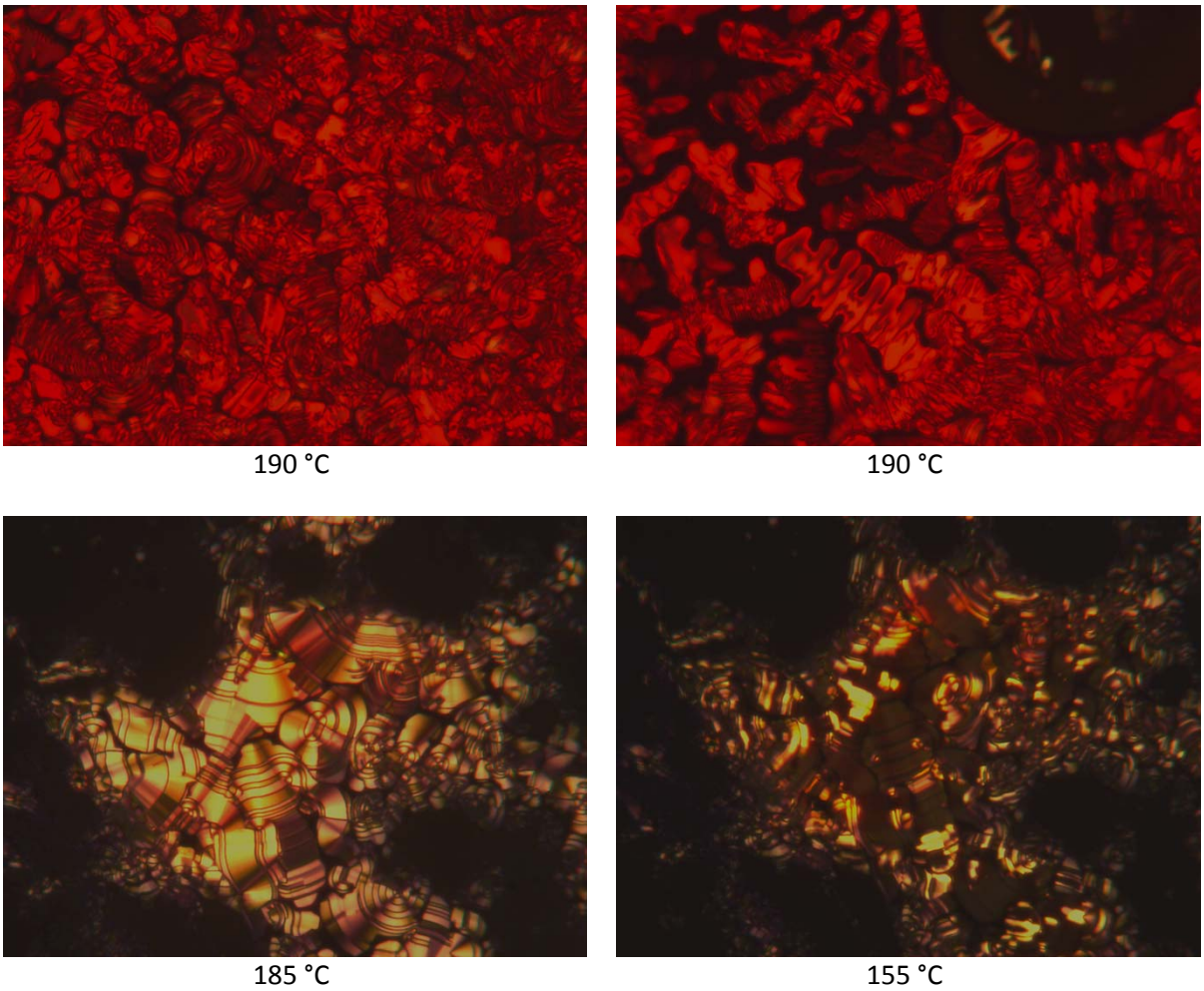


Figure S25. Polarizing optical microscopy images for **2c**-Zn recorded on cooling.

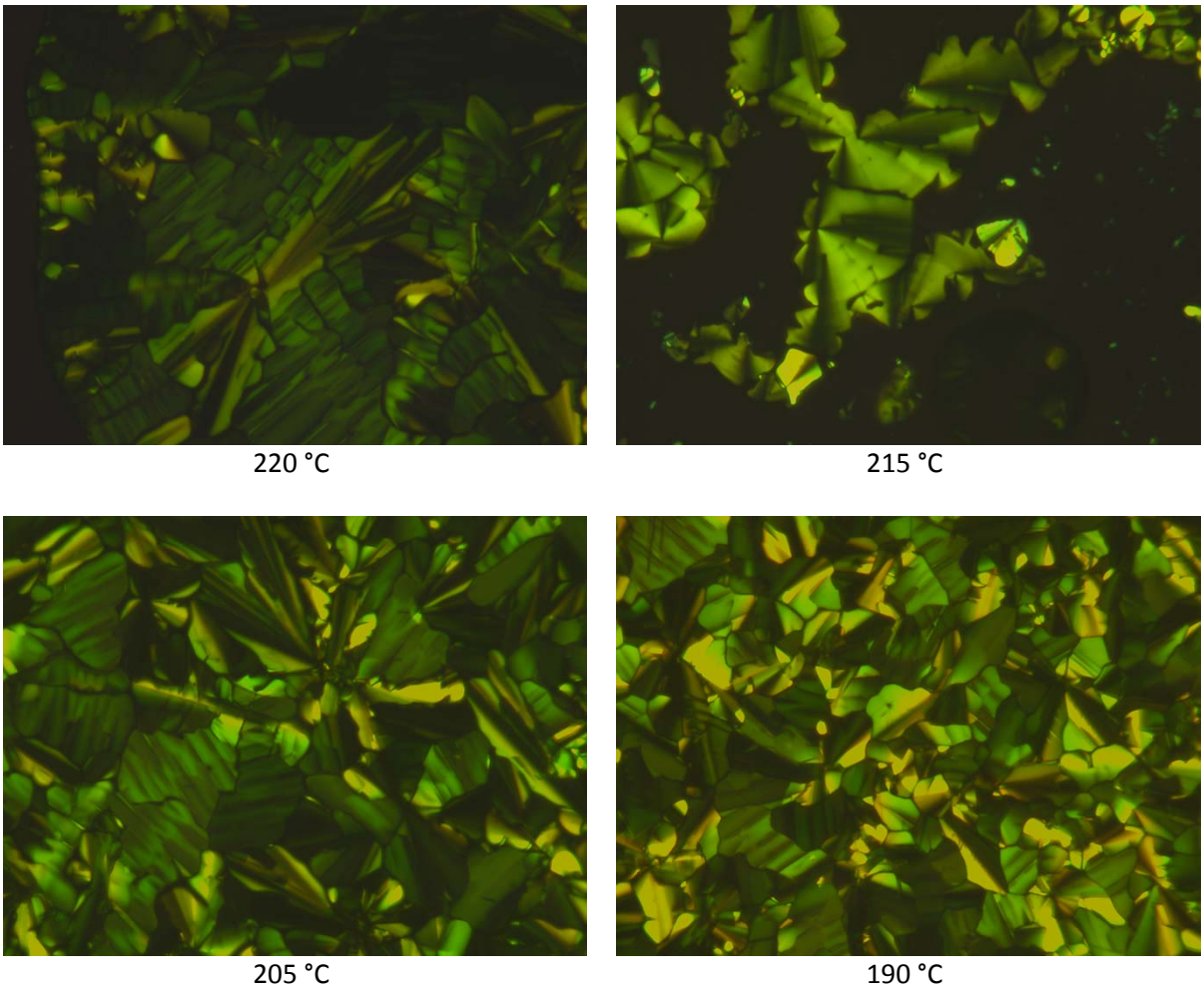
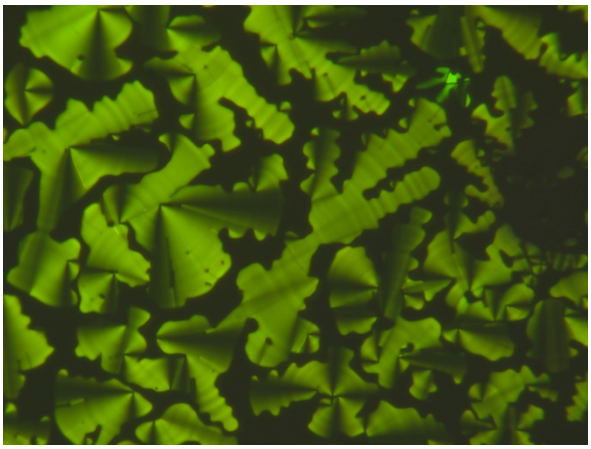
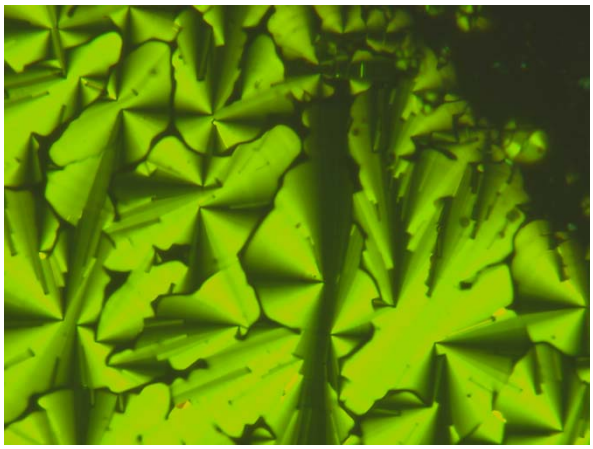


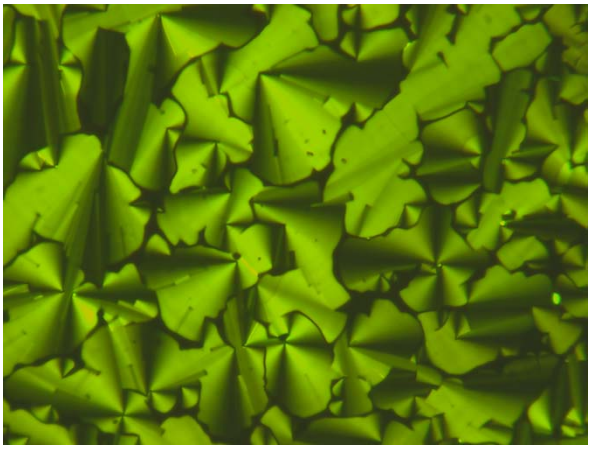
Figure S26. Polarizing optical microscopy images for **3c**-H_2 recorded on cooling.



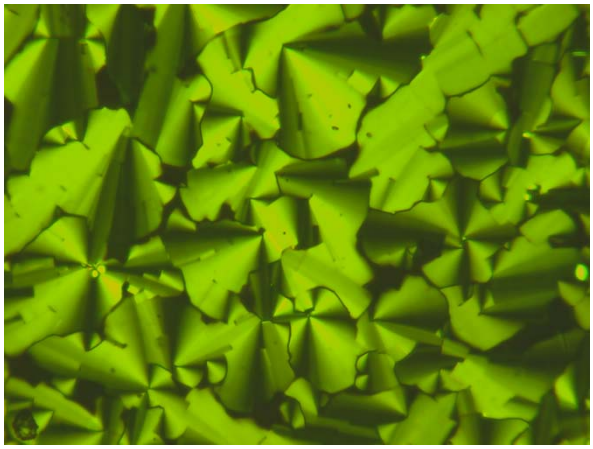
235 °C



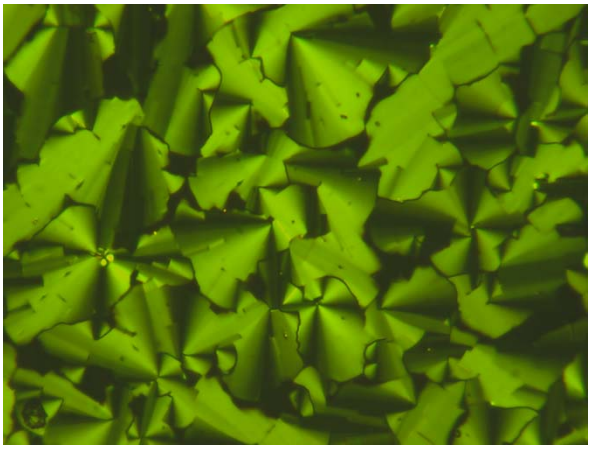
225 °C



210 °C



160 °C



145 °C

Figure S27. Polarizing optical microscopy images for **3c**-Zn recorded on cooling.

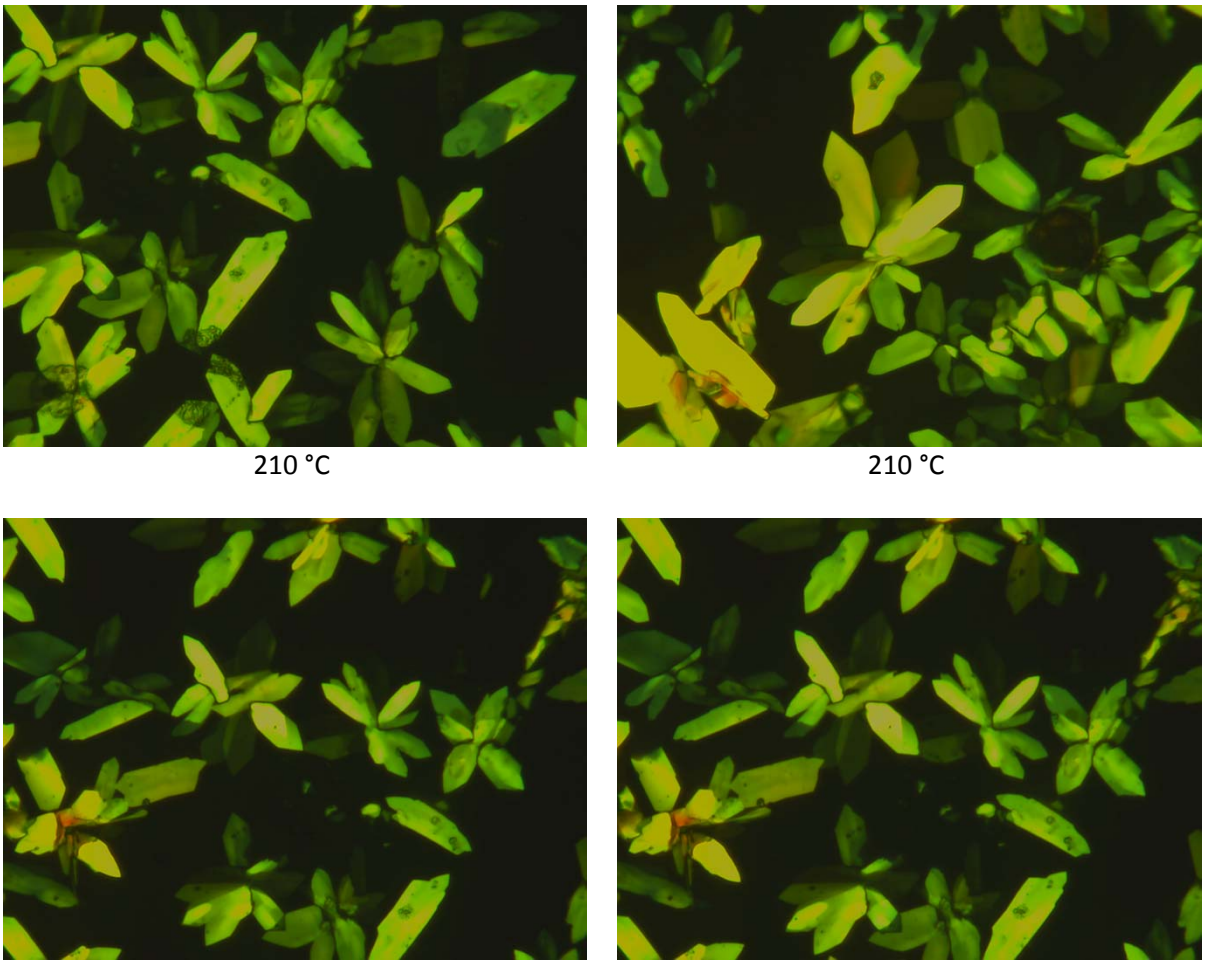
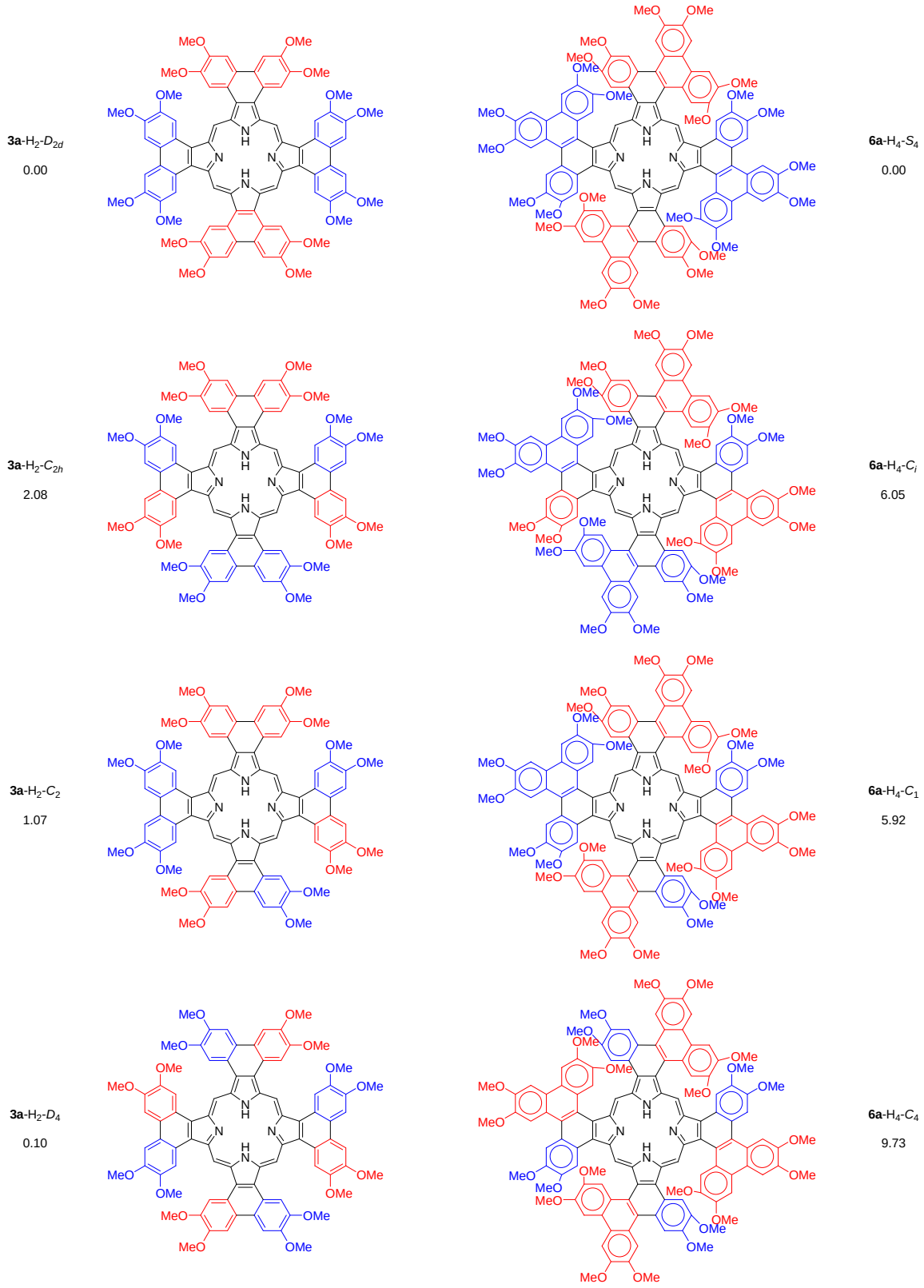


Figure S28. Polarizing optical microscopy images for **6b**-Zn recorded on cooling.

Table S7. Energies (Hartree unless indicated otherwise) for DFT-optimized structures.

System	E[a]	ZPV[a,b]	$E + ZPV$[a]	E_{rel}[c]	E_{hi}[d]
2a-H_2	-4670.445437	1.465044	-4668.980393		-4671.471796
2a-Zn	-6448.473289	1.442425	-6447.030864		-6449.676085
3a-H_2(-D_{2d})[e]	-4665.705213	1.380499	-4664.324714	0.00	-4666.714332
	-4664.235297[f]				
3a-H_2-C_{2h}	-4665.702893	1.381496	-4664.321397	2.08	
3a-H_2-C_2	-4665.703994	1.380989	-4664.323005	1.07	
3a-H_2-D_4	-4665.705714	1.381161	-4664.324553	0.10	
3a-Zn	-6443.734089	1.358548	-6442.375541		-6444.917833
	-6442.276967[f]				
3b-H_2	-8125.603038	[g]			
3c-H_2	-11585.506621	[g]			
6a-H_2(-S_4)	-6811.004383	2.015590	-6808.988793	0.00	-6812.473532
6a-H_2-C_4	-6810.988589	2.015302	-6808.973287	9.73	
6a-H_2-C_i	-6810.994827	2.015675	-6808.979152	6.05	
6a-H_2-C_1	-6810.995218	2.015858	-6808.97936	5.92	
6a-Zn	-8589.033409	1.993013	-8587.040396		-8590.676468
6b-H_2	-12000.850716	[g]			
[**3a**-H_2]$_2$-C_{2h}	-9328.592071[f,h]	[g]		-76.23[i]	
[**3a**-H_2]$_2$-C_2	-9328.578244[f,h]	[g]		-67.55[i]	
[**3a**-Zn]$_2$-C_{2h}	-12884.687628[f,h]	[g]		-83.89[i]	

[a] B3LYP/6-31G**// B3LYP/6-31G** unless noted otherwise. [b] Zero-point vibrational energy. [c] relative energies (kcal/mol). [d] B3LYP/6-311G**//B3LYP/6-31G**. [e] For symmetry designators see the following table. [f] ωB97XD/6-31G**//ωB97XD/6-31G**. [g] Frequency calculation was not possible because of technical limitations. [h] Conterpoise-corrected. [i] Energies relative to monomers including counterpoise correction.



Scheme S5. Relative energies for different conformers of **2a**-H_2 (left) and **6a**-H_2.Parts of molecules shown in red and blue are respectively above and below the mean plane of the macrocycle. Point group designations refer to effective symmetries in the limit of fast tautomerization. The choice of tautomers was arbitrary. Energies (including ZPV) are given relative to the most stable conformer.

Table S8. Lowest lying excited states for **2a**-H_2(TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      2.1043 eV  589.18 nm  f=0.0026  <S**2>=0.000
     368 -> 371        0.46503
     369 -> 370       -0.52256
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -4671.39447168
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      2.2291 eV  556.20 nm  f=0.0226  <S**2>=0.000
     368 -> 370       -0.53104
     369 -> 371       -0.46023

 Excited State   3:      Singlet-A      2.4930 eV  497.32 nm  f=0.0013  <S**2>=0.000
     366 -> 370        0.66934
     368 -> 371        0.18889

 Excited State   4:      Singlet-A      2.4985 eV  496.24 nm  f=0.0002  <S**2>=0.000
     367 -> 370        0.70012

 Excited State   5:      Singlet-A      2.5773 eV  481.07 nm  f=0.0256  <S**2>=0.000
     366 -> 371        0.70319

 Excited State   6:      Singlet-A      2.5829 eV  480.02 nm  f=0.0000  <S**2>=0.000
     367 -> 371        0.70449

 Excited State   7:      Singlet-A      2.7651 eV  448.38 nm  f=0.8241  <S**2>=0.000
     360 -> 371        0.13272
     364 -> 370        0.46467
     366 -> 370       -0.15698
     368 -> 371        0.34597
     369 -> 370        0.34354

 Excited State   8:      Singlet-A      2.7840 eV  445.35 nm  f=0.7562  <S**2>=0.000
     360 -> 370       -0.11945
     362 -> 370       -0.21707
     364 -> 371        0.45239
     368 -> 370       -0.30080
     369 -> 371        0.37227

 Excited State   9:      Singlet-A      2.7990 eV  442.96 nm  f=0.0000  <S**2>=0.000
     365 -> 370        0.69937

 Excited State  10:      Singlet-A      2.8010 eV  442.64 nm  f=0.0002  <S**2>=0.000
     365 -> 371        0.70136

 Excited State  11:      Singlet-A      2.8848 eV  429.78 nm  f=0.1890  <S**2>=0.000
     360 -> 370        0.14503
     362 -> 370        0.44784
     364 -> 371        0.47368
     368 -> 370        0.16916
     369 -> 371       -0.13183

 Excited State  12:      Singlet-A      2.9161 eV  425.17 nm  f=0.0000  <S**2>=0.000
     363 -> 370       -0.69312

 Excited State  13:      Singlet-A      2.9539 eV  419.73 nm  f=0.2035  <S**2>=0.000
     360 -> 371       -0.24420
     362 -> 371       -0.31013
     364 -> 370        0.46722
     366 -> 370        0.11055
     368 -> 371       -0.26920
     369 -> 370       -0.17637
```

Table S9. Lowest lying excited states for **2a**-Zn(TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      2.2206 eV  558.35 nm  f=0.0213  <S**2>=0.000
     382 -> 385        0.45368
     383 -> 384        0.52110
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -6449.59448075
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      2.2206 eV  558.34 nm  f=0.0212  <S**2>=0.000
     382 -> 384       -0.45377
     383 -> 385        0.52102

 Excited State   3:      Singlet-A      2.7196 eV  455.89 nm  f=0.0242  <S**2>=0.000
     381 -> 384        0.68466
     383 -> 385        0.10669

 Excited State   4:      Singlet-A      2.7198 eV  455.86 nm  f=0.0242  <S**2>=0.000
     381 -> 385        0.68467
     383 -> 384        0.10667

 Excited State   5:      Singlet-A      2.7266 eV  454.72 nm  f=0.0005  <S**2>=0.000
     379 -> 384        0.50022
     380 -> 385        0.49259

 Excited State   6:      Singlet-A      2.7376 eV  452.90 nm  f=0.0000  <S**2>=0.000
     379 -> 384        0.49137
     380 -> 385       -0.49902

 Excited State   7:      Singlet-A      2.7648 eV  448.44 nm  f=0.0000  <S**2>=0.000
     379 -> 385        0.49494
     380 -> 384        0.50117

 Excited State   8:      Singlet-A      2.7854 eV  445.12 nm  f=0.0000  <S**2>=0.000
     379 -> 385       -0.50175
     380 -> 384        0.49552

 Excited State   9:      Singlet-A      2.7910 eV  444.24 nm  f=0.6064  <S**2>=0.000
     378 -> 384        0.55996
     382 -> 384        0.34087
     383 -> 385        0.23987

 Excited State  10:      Singlet-A      2.7911 eV  444.21 nm  f=0.6071  <S**2>=0.000
     378 -> 385        0.55974
     382 -> 385        0.34109
     383 -> 384       -0.23997

 Excited State  11:      Singlet-A      2.9741 eV  416.88 nm  f=0.5932  <S**2>=0.000
     374 -> 384       -0.22309
     377 -> 384        0.42711
     378 -> 385        0.33016
     381 -> 385       -0.12830
     382 -> 385       -0.24307
     383 -> 384        0.25752

 Excited State  12:      Singlet-A      2.9742 eV  416.87 nm  f=0.5958  <S**2>=0.000
     374 -> 385        0.22370
     377 -> 385        0.42572
     378 -> 384        0.33030
     381 -> 384        0.12849
     382 -> 384       -0.24383
     383 -> 385       -0.25829

 Excited State  13:      Singlet-A      3.0333 eV  408.74 nm  f=0.1222  <S**2>=0.000
     369 -> 384        0.10101
     374 -> 384        0.20690
     377 -> 384        0.52404
     377 -> 385        0.12122
     378 -> 385       -0.19922
     382 -> 385        0.20984
     383 -> 384       -0.21287

 Excited State  14:      Singlet-A      3.0333 eV  408.74 nm  f=0.1211  <S**2>=0.000
     369 -> 385        0.10113
     374 -> 385       -0.20599
     377 -> 384       -0.12101
```

```
     377 -> 385        0.52519
     378 -> 384       -0.19838
     382 -> 384        0.20926
     383 -> 385        0.21234

 Excited State  15:      Singlet-A      3.0759 eV  403.09 nm  f=0.0000  <S**2>=0.000
     375 -> 385        0.49229
     376 -> 384        0.49803

 Excited State  16:      Singlet-A      3.1028 eV  399.59 nm  f=0.0000  <S**2>=0.000
     375 -> 384        0.49860
     376 -> 385        0.49742

 Excited State  17:      Singlet-A      3.1074 eV  399.00 nm  f=0.0000  <S**2>=0.000
     375 -> 385        0.49880
     376 -> 384       -0.49318

 Excited State  18:      Singlet-A      3.1193 eV  397.48 nm  f=0.0000  <S**2>=0.000
     375 -> 384       -0.49596
     376 -> 385        0.49708

 Excited State  19:      Singlet-A      3.3612 eV  368.87 nm  f=0.5203  <S**2>=0.000
     374 -> 384        0.61766
     378 -> 385        0.11542
     382 -> 385       -0.22281
     383 -> 384        0.16341

 Excited State  20:      Singlet-A      3.3613 eV  368.85 nm  f=0.5196  <S**2>=0.000
     374 -> 385        0.61774
     378 -> 384       -0.11526
     382 -> 384        0.22265
     383 -> 385        0.16329

 Excited State  21:      Singlet-A      3.5200 eV  352.23 nm  f=0.0000  <S**2>=0.000
     371 -> 385        0.45691
     372 -> 384        0.51524
     382 -> 386        0.11221

 Excited State  22:      Singlet-A      3.5221 eV  352.01 nm  f=0.0016  <S**2>=0.000
     371 -> 385        0.52072
     372 -> 384       -0.46313

 Excited State  23:      Singlet-A      3.5365 eV  350.58 nm  f=0.0000  <S**2>=0.000
     371 -> 384        0.15008
     372 -> 385       -0.14969
     383 -> 386        0.66577

 Excited State  24:      Singlet-A      3.5437 eV  349.87 nm  f=0.0518  <S**2>=0.000
     370 -> 384       -0.31293
     373 -> 384        0.61161

 Excited State  25:      Singlet-A      3.5439 eV  349.85 nm  f=0.0515  <S**2>=0.000
     370 -> 385        0.31302
     373 -> 385        0.61142

 Excited State  26:      Singlet-A      3.5633 eV  347.95 nm  f=0.0016  <S**2>=0.000
     365 -> 384        0.17954
     369 -> 384        0.65974
     377 -> 384       -0.13395

 Excited State  27:      Singlet-A      3.5635 eV  347.93 nm  f=0.0016  <S**2>=0.000
     365 -> 385       -0.17976
     369 -> 385       -0.65979
     377 -> 385        0.13395

 Excited State  28:      Singlet-A      3.5910 eV  345.27 nm  f=0.0000  <S**2>=0.000
     382 -> 386        0.67739

 Excited State  29:      Singlet-A      3.5968 eV  344.71 nm  f=0.0000  <S**2>=0.000
     371 -> 384        0.48124
     372 -> 385       -0.45961
     383 -> 386       -0.21102
 Excited State  30:      Singlet-A      3.6000 eV  344.40 nm  f=0.0000  <S**2>=0.000
     371 -> 384        0.48829
     372 -> 385        0.50888
```

Table S10. Lowest lying excited states for **3a**-H_2(TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      1.9158 eV  647.16 nm  f=0.1325  <S**2>=0.000
     364 -> 366        0.37132
     365 -> 367        0.59642
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -4666.64392706
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      1.9532 eV  634.79 nm  f=0.2474  <S**2>=0.000
     364 -> 367       -0.27915
     365 -> 366        0.64513

 Excited State   3:      Singlet-A      2.3946 eV  517.76 nm  f=0.1212  <S**2>=0.000
     362 -> 366        0.53187
     364 -> 366       -0.39889
     365 -> 367        0.21545

 Excited State   4:      Singlet-A      2.4338 eV  509.42 nm  f=0.0000  <S**2>=0.000
     363 -> 366        0.69905

 Excited State   5:      Singlet-A      2.5553 eV  485.20 nm  f=0.1026  <S**2>=0.000
     360 -> 366        0.40692
     362 -> 367        0.46372
     364 -> 367       -0.31741

 Excited State   6:      Singlet-A      2.5625 eV  483.83 nm  f=0.0015  <S**2>=0.000
     361 -> 366       -0.30966
     363 -> 367        0.63229

 Excited State   7:      Singlet-A      2.5910 eV  478.52 nm  f=0.2291  <S**2>=0.000
     360 -> 366        0.50063
     362 -> 367       -0.48789

 Excited State   8:      Singlet-A      2.6036 eV  476.21 nm  f=0.0307  <S**2>=0.000
     361 -> 366        0.62583
     363 -> 367        0.30392

 Excited State   9:      Singlet-A      2.6526 eV  467.41 nm  f=0.0000  <S**2>=0.000
     359 -> 366       -0.29828
     361 -> 367        0.63971

 Excited State  10:      Singlet-A      2.6611 eV  465.91 nm  f=0.4471  <S**2>=0.000
     356 -> 367        0.15898
     357 -> 366       -0.16360
     360 -> 367        0.37910
     362 -> 366        0.36978
     364 -> 366        0.33003
     365 -> 367       -0.23095

 Excited State  11:      Singlet-A      2.6707 eV  464.24 nm  f=0.6939  <S**2>=0.000
     356 -> 367       -0.11302
     360 -> 367        0.59150
     362 -> 366       -0.23294
     364 -> 366       -0.22618
     365 -> 367        0.15403

 Excited State  12:      Singlet-A      2.7021 eV  458.84 nm  f=0.0000  <S**2>=0.000
     358 -> 367       -0.10002
     359 -> 366        0.63184
     361 -> 367        0.29465

 Excited State  13:      Singlet-A      2.7550 eV  450.03 nm  f=0.0129  <S**2>=0.000
     358 -> 366        0.28604
     359 -> 367        0.63377
```

Table S11. Lowest lying excited states for **3a**-Zn(TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      1.9603 eV  632.49 nm  f=0.2122  <S**2>=0.000
     378 -> 381        0.29895
     379 -> 380        0.63413
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -6444.84579537
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      1.9604 eV  632.44 nm  f=0.2119  <S**2>=0.000
     378 -> 380       -0.29914
     379 -> 381        0.63403

 Excited State   3:      Singlet-A      2.6416 eV  469.36 nm  f=0.4578  <S**2>=0.000
     370 -> 381       -0.11448
     376 -> 380        0.52819
     377 -> 381        0.13781
     378 -> 380       -0.33629
     378 -> 381        0.14298
     379 -> 381       -0.17459

 Excited State   4:      Singlet-A      2.6418 eV  469.32 nm  f=0.4624  <S**2>=0.000
     370 -> 380       -0.11489
     376 -> 381        0.52575
     377 -> 380       -0.14225
     378 -> 380        0.14418
     378 -> 381        0.33722
     379 -> 380       -0.17481

 Excited State   5:      Singlet-A      2.6722 eV  463.97 nm  f=0.2017  <S**2>=0.000
     376 -> 381        0.28910
     377 -> 380        0.61896
     378 -> 381       -0.11455

 Excited State   6:      Singlet-A      2.6725 eV  463.93 nm  f=0.2083  <S**2>=0.000
     376 -> 380       -0.28582
     377 -> 381        0.61924
     378 -> 380       -0.11810

 Excited State   7:      Singlet-A      2.6758 eV  463.36 nm  f=0.0000  <S**2>=0.000
     372 -> 380       -0.27469
     372 -> 381       -0.39363
     373 -> 380        0.41986
     373 -> 381       -0.27275

 Excited State   8:      Singlet-A      2.6821 eV  462.27 nm  f=0.0000  <S**2>=0.000
     372 -> 381        0.45726
     373 -> 380        0.43547
     374 -> 380        0.20610
     375 -> 381       -0.19950

 Excited State   9:      Singlet-A      2.7040 eV  458.53 nm  f=0.0248  <S**2>=0.000
     372 -> 380        0.26456
     372 -> 381       -0.16179
     373 -> 380        0.18741
     373 -> 381        0.28164
     374 -> 381       -0.33537
     375 -> 380        0.39251

 Excited State  10:      Singlet-A      2.7060 eV  458.18 nm  f=0.0001  <S**2>=0.000
     372 -> 381        0.22239
     373 -> 380        0.19418
     374 -> 380       -0.38533
     374 -> 381        0.25068
     375 -> 380        0.19776
     375 -> 381        0.39643

 Excited State  11:      Singlet-A      2.7075 eV  457.93 nm  f=0.0000  <S**2>=0.000
     372 -> 380       -0.23837
     373 -> 381        0.21990
     374 -> 380        0.21836
     374 -> 381        0.39023
     375 -> 380        0.37381
     375 -> 381       -0.21176

 Excited State  12:      Singlet-A      2.7320 eV  453.82 nm  f=0.0268  <S**2>=0.000
```

```
     372 -> 380        0.30474
     372 -> 381       -0.21643
     373 -> 380        0.21600
     373 -> 381        0.30589
     374 -> 381        0.32159
     375 -> 380       -0.31398

 Excited State  13:      Singlet-A      2.7392 eV  452.62 nm  f=0.3397  <S**2>=0.000
     370 -> 381        0.14192
     371 -> 380        0.34329
     376 -> 380        0.23109
     376 -> 381       -0.13905
     377 -> 380        0.14102
     377 -> 381        0.24132
     378 -> 380        0.41609
     379 -> 381        0.16464

 Excited State  14:      Singlet-A      2.7395 eV  452.58 nm  f=0.3409  <S**2>=0.000
     370 -> 380       -0.14254
     371 -> 381        0.34283
     376 -> 380       -0.13849
     376 -> 381       -0.23226
     377 -> 380        0.23966
     377 -> 381       -0.14162
     378 -> 381        0.41656
     379 -> 380       -0.16477

 Excited State  15:      Singlet-A      2.7505 eV  450.77 nm  f=0.0001  <S**2>=0.000
     374 -> 380        0.47950
     374 -> 381       -0.11159
     375 -> 380        0.11024
     375 -> 381        0.48168

 Excited State  16:      Singlet-A      2.8098 eV  441.26 nm  f=0.0000  <S**2>=0.000
     372 -> 380       -0.43852
     373 -> 381        0.44022
     374 -> 381       -0.20795
     375 -> 380       -0.20837

 Excited State  17:      Singlet-A      2.8552 eV  434.24 nm  f=0.0314  <S**2>=0.000
     370 -> 381       -0.24579
     371 -> 380        0.57859
     376 -> 380       -0.19182
     376 -> 381        0.10071
     378 -> 380       -0.13374
     379 -> 381       -0.11430

 Excited State  18:      Singlet-A      2.8554 eV  434.21 nm  f=0.0311  <S**2>=0.000
     370 -> 380        0.24601
     371 -> 381        0.57884
     376 -> 380        0.10020
     376 -> 381        0.19195
     378 -> 381       -0.13312
     379 -> 380        0.11396

 Excited State  19:      Singlet-A      2.9681 eV  417.73 nm  f=0.0806  <S**2>=0.000
     379 -> 382        0.69747

 Excited State  20:      Singlet-A      3.1977 eV  387.73 nm  f=0.3284  <S**2>=0.000
     370 -> 381        0.61299
     371 -> 380        0.14406
     378 -> 380       -0.21784
     379 -> 381       -0.10468
```

Table S12. Lowest lying excited states for **6a**-H_2(TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      1.8246 eV  679.50 nm  f=0.2599  <S**2>=0.000
     528 -> 534        0.11232
     532 -> 534       -0.20075
     532 -> 535        0.12850
     533 -> 534        0.45249
     533 -> 535        0.45407
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -6812.40647778
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      1.8392 eV  674.12 nm  f=0.2732  <S**2>=0.000
     528 -> 534       -0.11770
     532 -> 534        0.15441
     532 -> 535        0.12798
     533 -> 534        0.48840
     533 -> 535       -0.43405

 Excited State   3:      Singlet-A      2.2277 eV  556.55 nm  f=0.1026  <S**2>=0.000
     528 -> 534        0.26698
     532 -> 534        0.61012
     533 -> 535        0.16726

 Excited State   4:      Singlet-A      2.2467 eV  551.86 nm  f=0.0021  <S**2>=0.000
     530 -> 534        0.13781
     531 -> 534        0.68318

 Excited State   5:      Singlet-A      2.3274 eV  532.71 nm  f=0.0077  <S**2>=0.000
     530 -> 534        0.65686
     531 -> 534       -0.14044
     531 -> 535       -0.18613

 Excited State   6:      Singlet-A      2.3340 eV  531.22 nm  f=0.0995  <S**2>=0.000
     528 -> 534       -0.19881
     529 -> 534        0.62979
     532 -> 535       -0.22411

 Excited State   7:      Singlet-A      2.3734 eV  522.39 nm  f=0.0011  <S**2>=0.000
     527 -> 534       -0.16292
     530 -> 534        0.16596
     530 -> 535       -0.14902
     531 -> 535        0.64209

 Excited State   8:      Singlet-A      2.3944 eV  517.80 nm  f=0.0045  <S**2>=0.000
     528 -> 535        0.45005
     529 -> 534        0.21686
     532 -> 535        0.47340

 Excited State   9:      Singlet-A      2.4088 eV  514.71 nm  f=0.0000  <S**2>=0.000
     527 -> 534        0.59896
     530 -> 535        0.29018
     531 -> 535        0.19780

 Excited State  10:      Singlet-A      2.4279 eV  510.66 nm  f=0.0157  <S**2>=0.000
     525 -> 534       -0.12307
     528 -> 534       -0.11706
     528 -> 535       -0.11780
     529 -> 535        0.65733
     532 -> 535        0.12327

 Excited State  11:      Singlet-A      2.4293 eV  510.37 nm  f=0.0001  <S**2>=0.000
     527 -> 534       -0.32144
     530 -> 535        0.61405

 Excited State  12:      Singlet-A      2.4640 eV  503.17 nm  f=0.6175  <S**2>=0.000
     524 -> 535       -0.13793
     525 -> 534       -0.32690
     528 -> 534       -0.50776
     529 -> 534       -0.11836
     529 -> 535       -0.15465
     532 -> 534        0.15978
     533 -> 535        0.16511

 Excited State  13:      Singlet-A      2.4711 eV  501.74 nm  f=0.0030  <S**2>=0.000
     526 -> 534       -0.36069
```

```
     527 -> 535       -0.59267

 Excited State  14:      Singlet-A      2.5251 eV  491.00 nm  f=0.2362  <S**2>=0.000
     524 -> 534       -0.13828
     525 -> 534        0.36916
     525 -> 535        0.33952
     528 -> 535        0.33558
     529 -> 534       -0.10330
     529 -> 535        0.14842
     532 -> 535       -0.14435
     533 -> 535        0.11470

 Excited State  15:      Singlet-A      2.5349 eV  489.10 nm  f=0.0055  <S**2>=0.000
     526 -> 534       -0.54864
     526 -> 535       -0.25065
     527 -> 535        0.33376

 Excited State  16:      Singlet-A      2.5625 eV  483.84 nm  f=0.0000  <S**2>=0.000
     526 -> 534        0.22384
     526 -> 535       -0.64197
     527 -> 535       -0.12953
```

Table S13. Lowest lying excited states for **6a**-Zn (TD-B3LYP/6-311G**//B3LYP/6-31G**).

```
Excited State   1:      Singlet-A      1.8599 eV  666.63 nm  f=0.2870  <S**2>=0.000
     546 -> 549       -0.23687
     547 -> 548        0.65375
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -8590.60812013
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      1.8604 eV  666.43 nm  f=0.2853  <S**2>=0.000
     546 -> 548        0.23714
     547 -> 549        0.65359

 Excited State   3:      Singlet-A      2.4138 eV  513.64 nm  f=0.0120  <S**2>=0.000
     540 -> 548        0.18729
     541 -> 549        0.18889
     543 -> 548        0.44482
     544 -> 549       -0.44980

 Excited State   4:      Singlet-A      2.4165 eV  513.07 nm  f=0.1723  <S**2>=0.000
     542 -> 548        0.29750
     545 -> 548        0.55442
     545 -> 549       -0.24005
     546 -> 548       -0.11858
     546 -> 549        0.10752

 Excited State   5:      Singlet-A      2.4174 eV  512.89 nm  f=0.1666  <S**2>=0.000
     542 -> 549        0.29997
     545 -> 548        0.24755
     545 -> 549        0.55682

 Excited State   6:      Singlet-A      2.4315 eV  509.91 nm  f=0.0000  <S**2>=0.000
     543 -> 549       -0.44089
     544 -> 548        0.51819

 Excited State   7:      Singlet-A      2.4421 eV  507.70 nm  f=0.0038  <S**2>=0.000
     540 -> 548       -0.27961
     541 -> 549       -0.28296
     543 -> 549        0.44256
     544 -> 548        0.35994

 Excited State   8:      Singlet-A      2.4513 eV  505.78 nm  f=0.0003  <S**2>=0.000
     540 -> 548        0.10798
     540 -> 549        0.28957
     541 -> 548        0.29973
     541 -> 549       -0.10664
     543 -> 548        0.38182
     544 -> 549        0.37475

 Excited State   9:      Singlet-A      2.4522 eV  505.61 nm  f=0.0437  <S**2>=0.000
     539 -> 548       -0.12025
     539 -> 549       -0.12841
     542 -> 548        0.57576
     542 -> 549       -0.10516
     545 -> 548       -0.30555

 Excited State  10:      Singlet-A      2.4528 eV  505.47 nm  f=0.0401  <S**2>=0.000
     539 -> 548       -0.12928
     539 -> 549        0.12062
     542 -> 548        0.10835
     542 -> 549        0.57288
     545 -> 549       -0.30985

 Excited State  11:      Singlet-A      2.4603 eV  503.94 nm  f=0.0001  <S**2>=0.000
     540 -> 548       -0.41223
     540 -> 549       -0.14238
     541 -> 548       -0.15298
     541 -> 549        0.40906
     543 -> 548        0.22680
     544 -> 549        0.22897

 Excited State  12:      Singlet-A      2.4837 eV  499.19 nm  f=0.0001  <S**2>=0.000
     540 -> 548        0.35896
     541 -> 549        0.35490
     543 -> 548       -0.20354
     543 -> 549        0.28221
```

```
     544 -> 548         0.27011
     544 -> 549         0.19621

 Excited State  13:      Singlet-A      2.5041 eV  495.12 nm  f=0.0040  <S**2>=0.000
     540 -> 549        -0.48118
     541 -> 548         0.49660
```

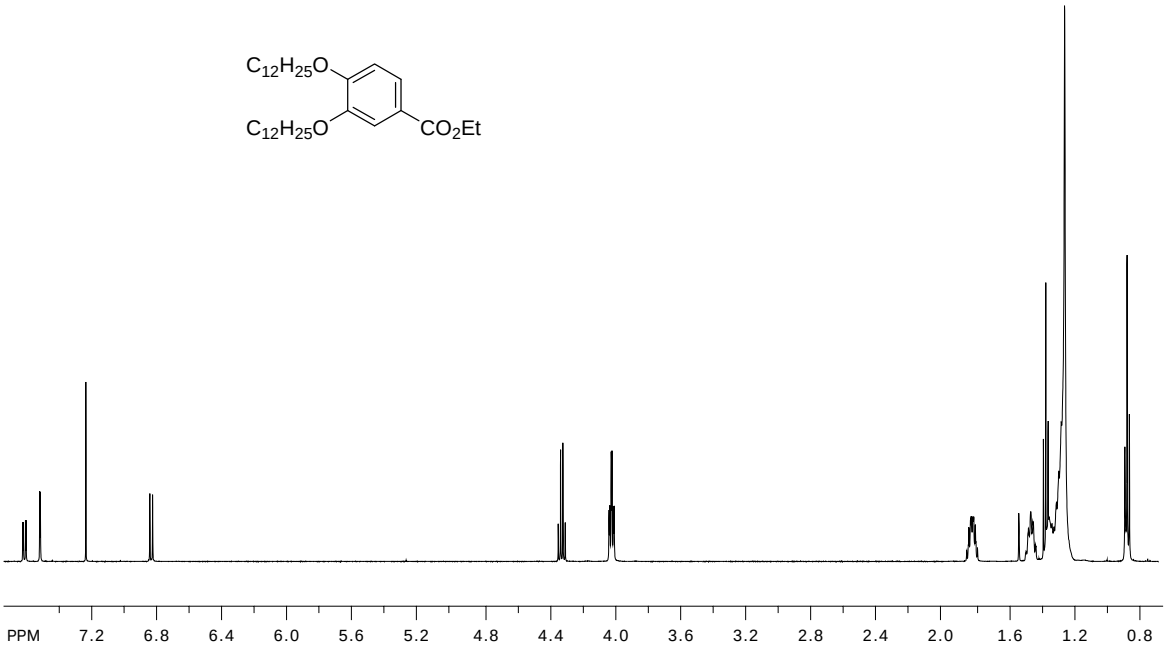


Figure S29. ^{1}H NMR spectrum of **8c** (chloroform-*d*, 500 MHz, 300 K).

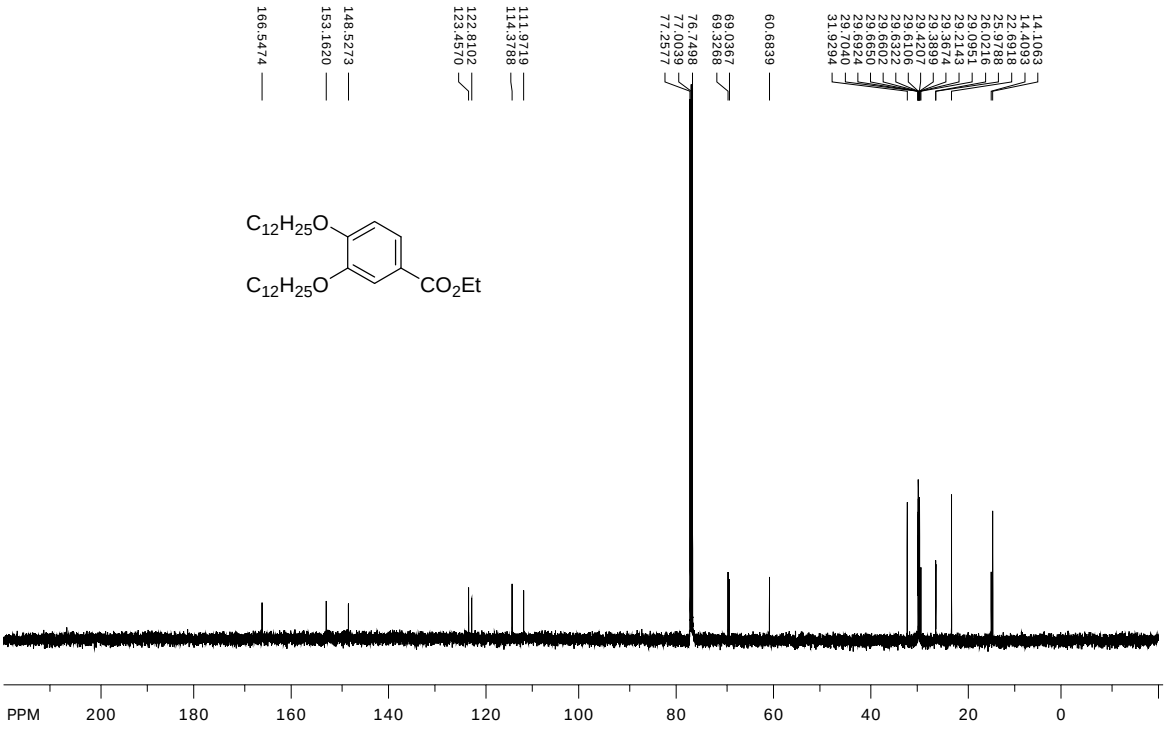


Figure S30. ^{13}C NMR spectrum of **8c** (chloroform-*d*, 125 MHz, 300 K).

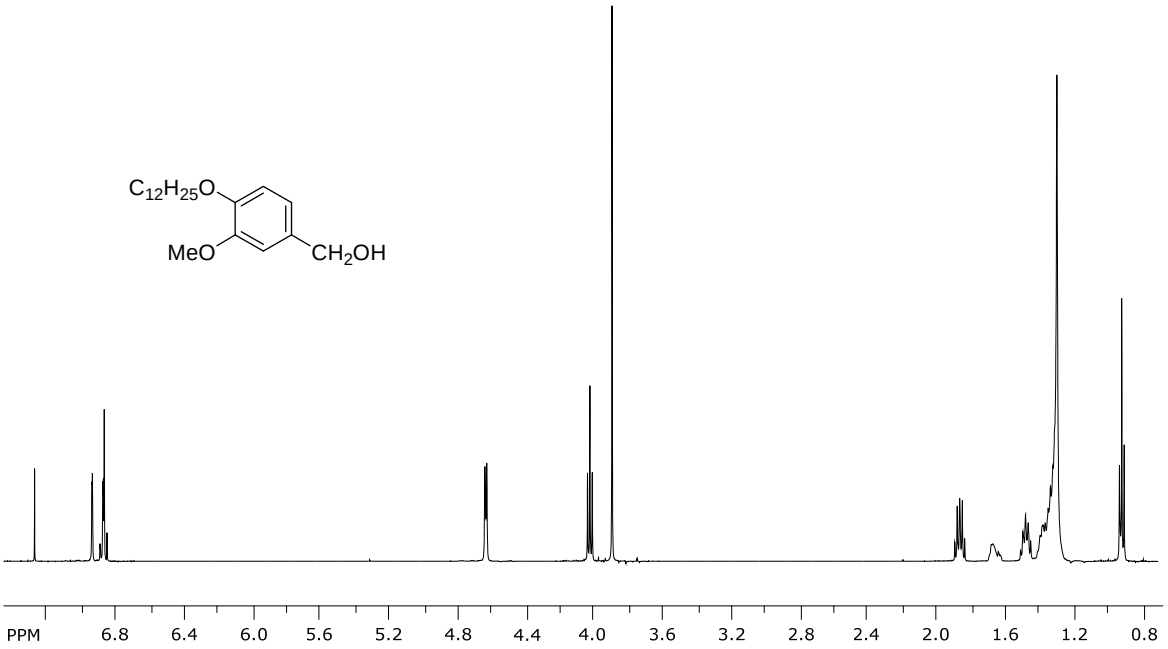


Figure S31. ^{1}H NMR spectrum of **9b** (chloroform-*d*, 500 MHz, 300 K).

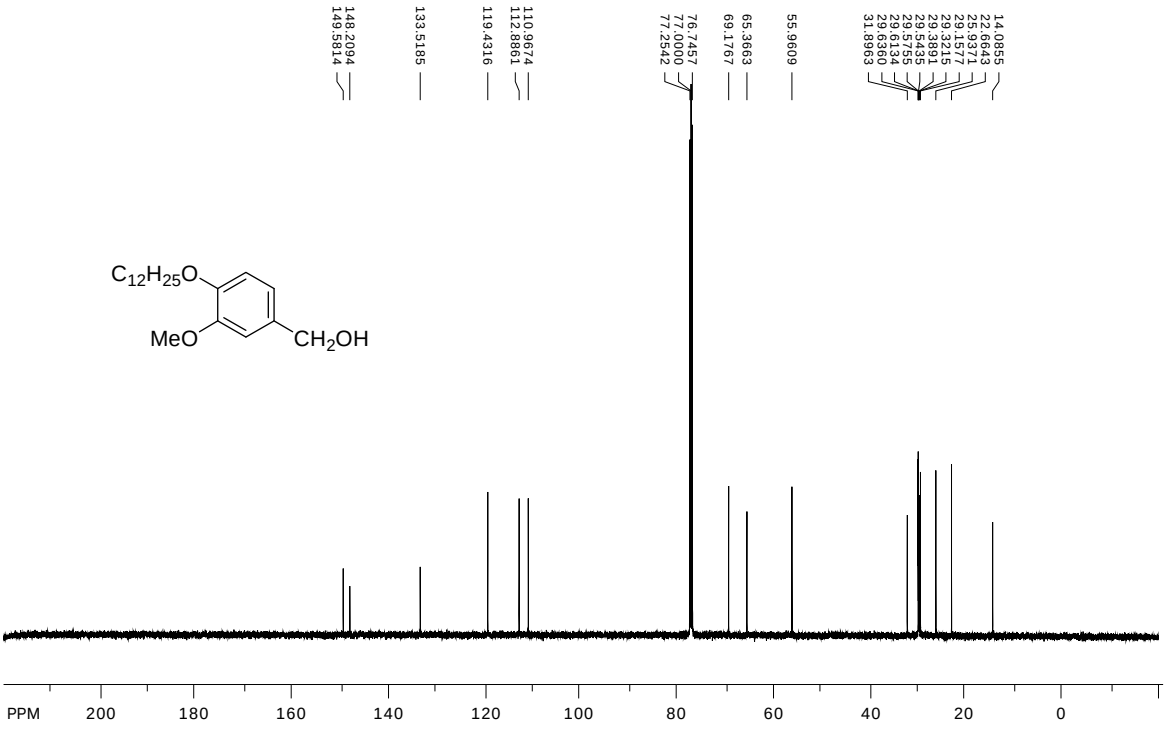


Figure S32. ^{13}C NMR spectrum of **9b** (chloroform-*d*, 125 MHz, 300 K).

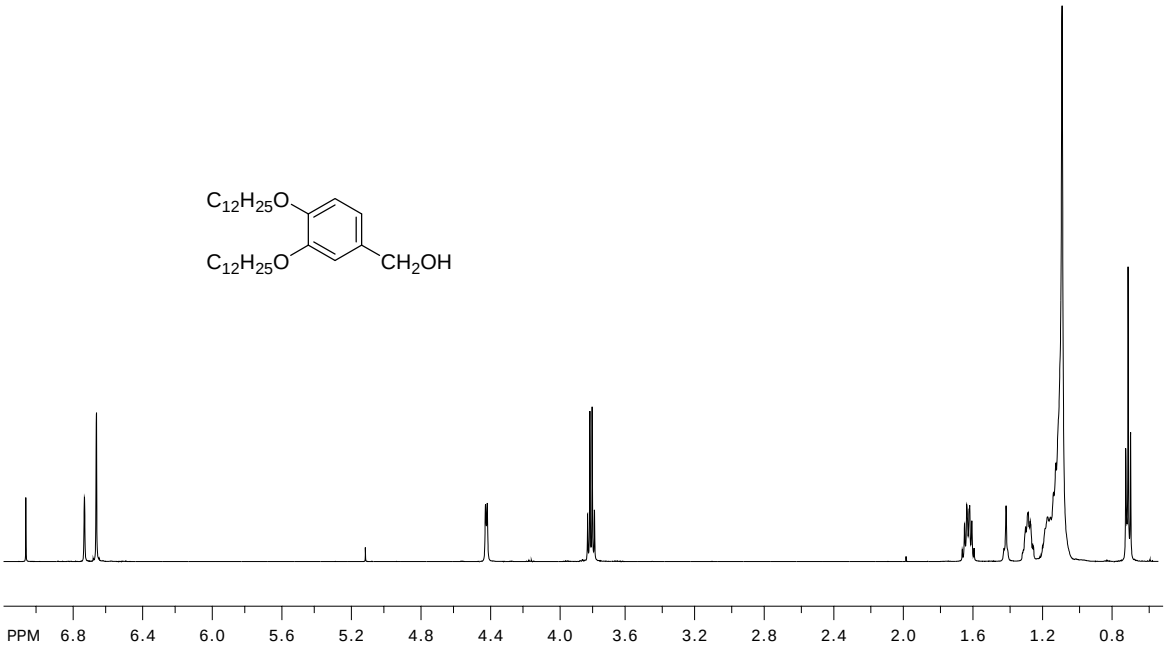


Figure S33. ^{1}H NMR spectrum of **9c** (chloroform-*d*, 500 MHz, 300 K).

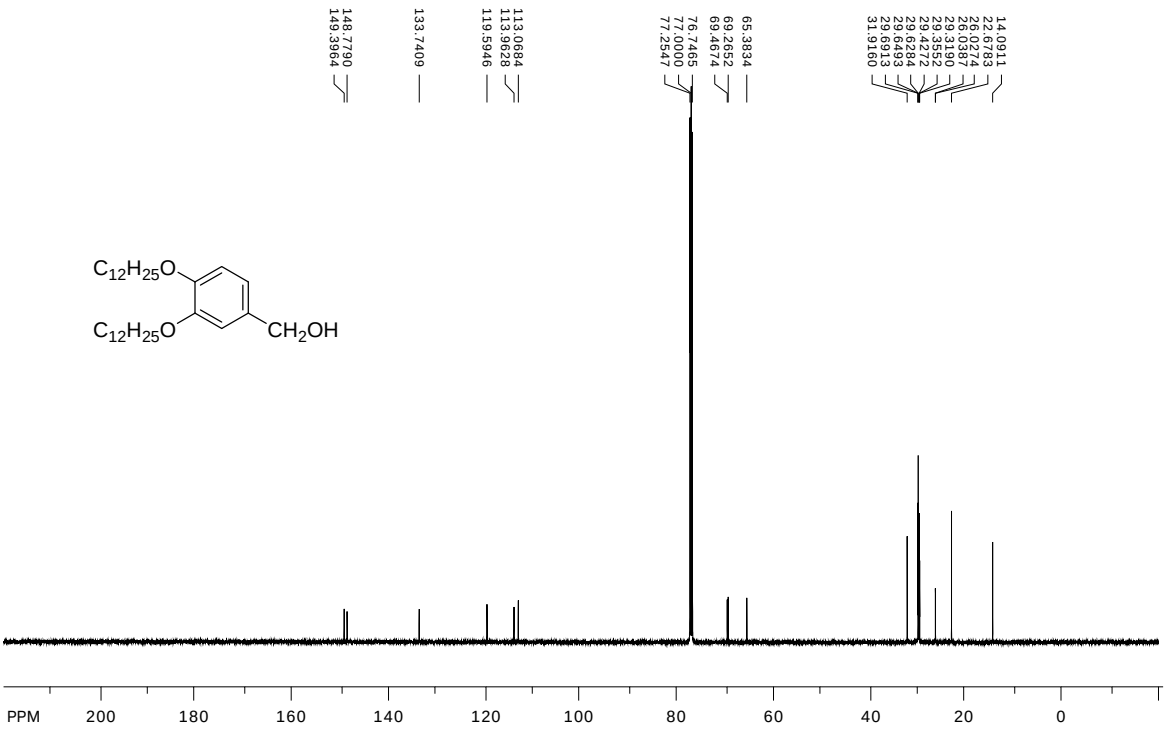


Figure S34. ^{13}C NMR spectrum of **9c** (chloroform-*d*, 125 MHz, 300 K).

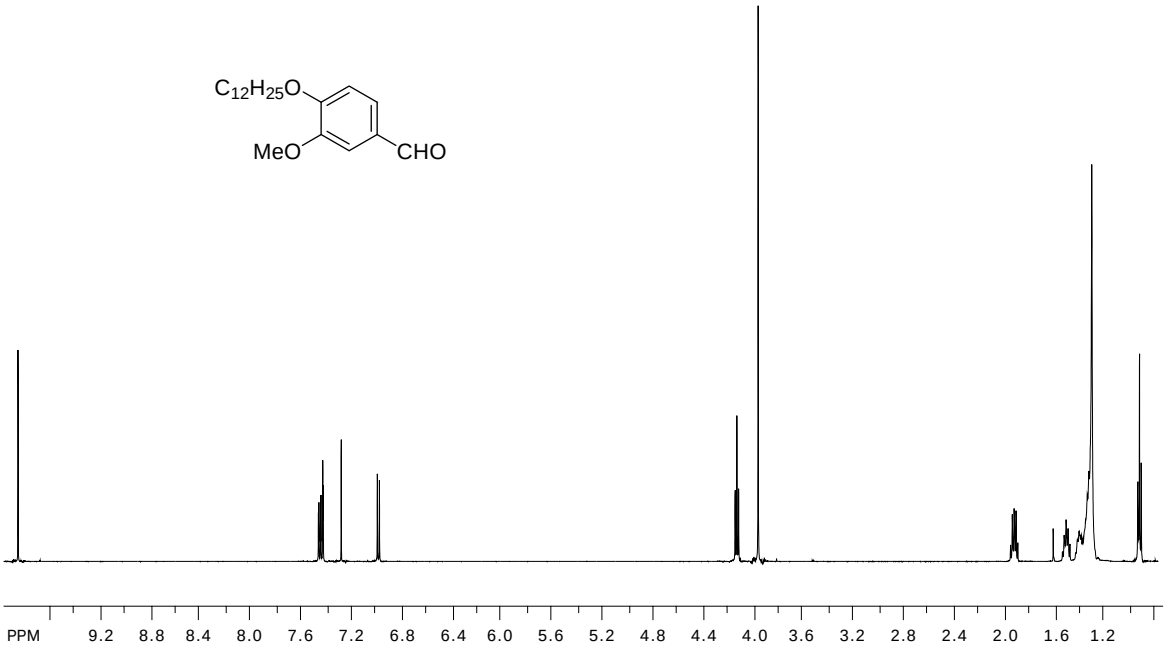


Figure S35. ^{1}H NMR spectrum of **7b** (chloroform-*d*, 500 MHz, 300 K).

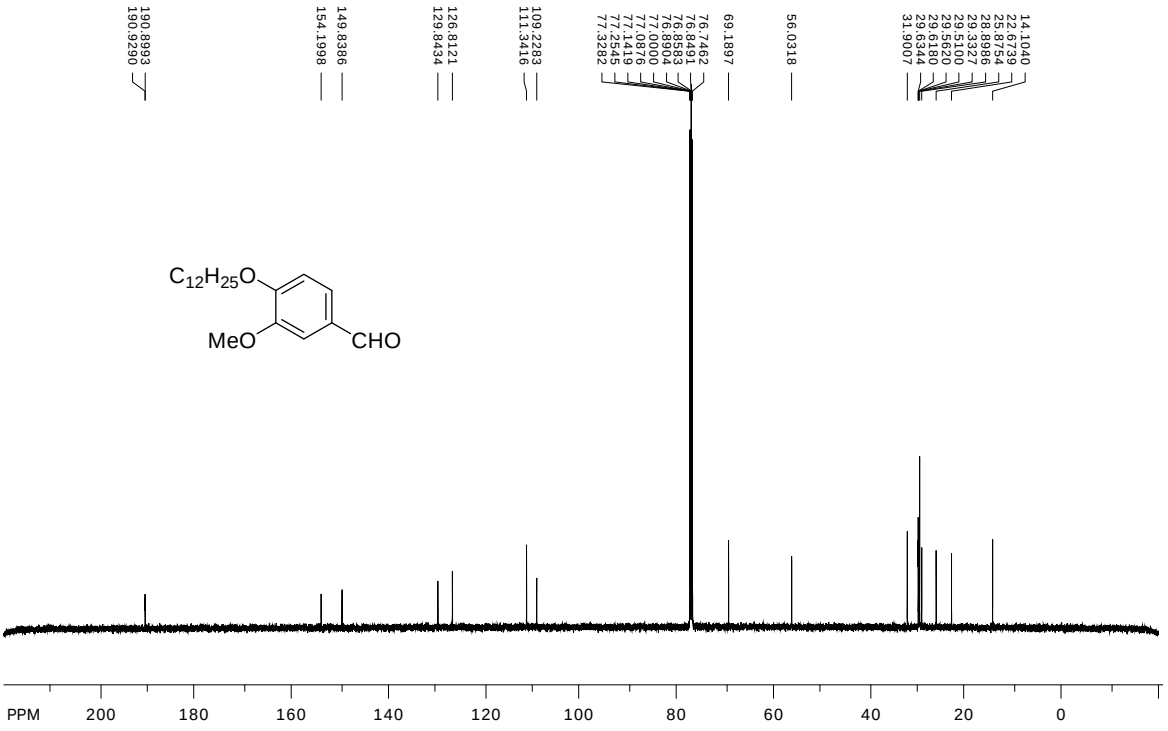


Figure S36. ^{13}C NMR spectrum of **7b** (chloroform-*d*, 125 MHz, 300 K).

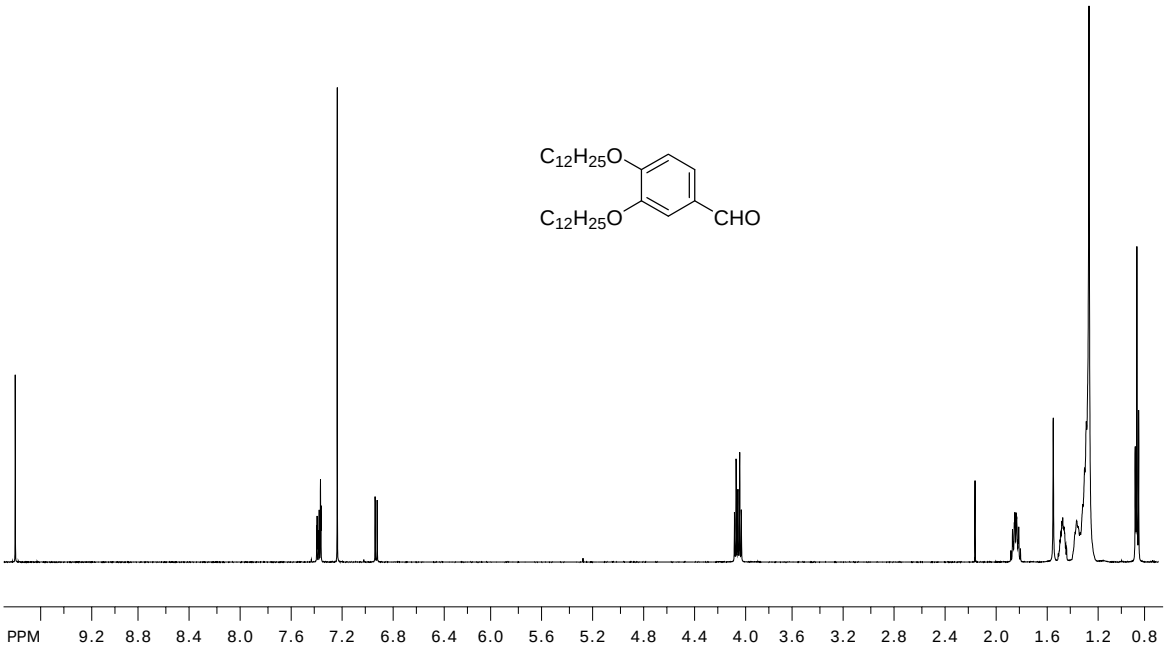


Figure S37. ^{1}H NMR spectrum of **7c** (chloroform-*d*, 500 MHz, 300 K).

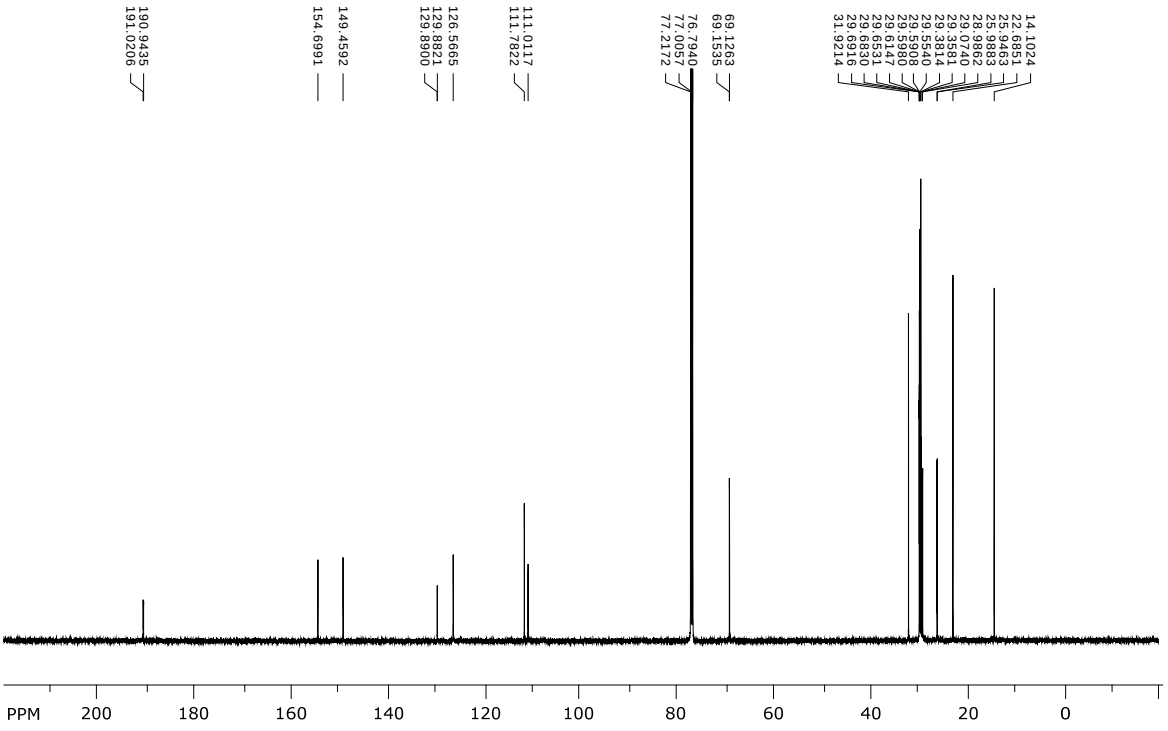


Figure S38. ^{13}C NMR spectrum of **7c** (chloroform-*d*, 151 MHz, 300 K).

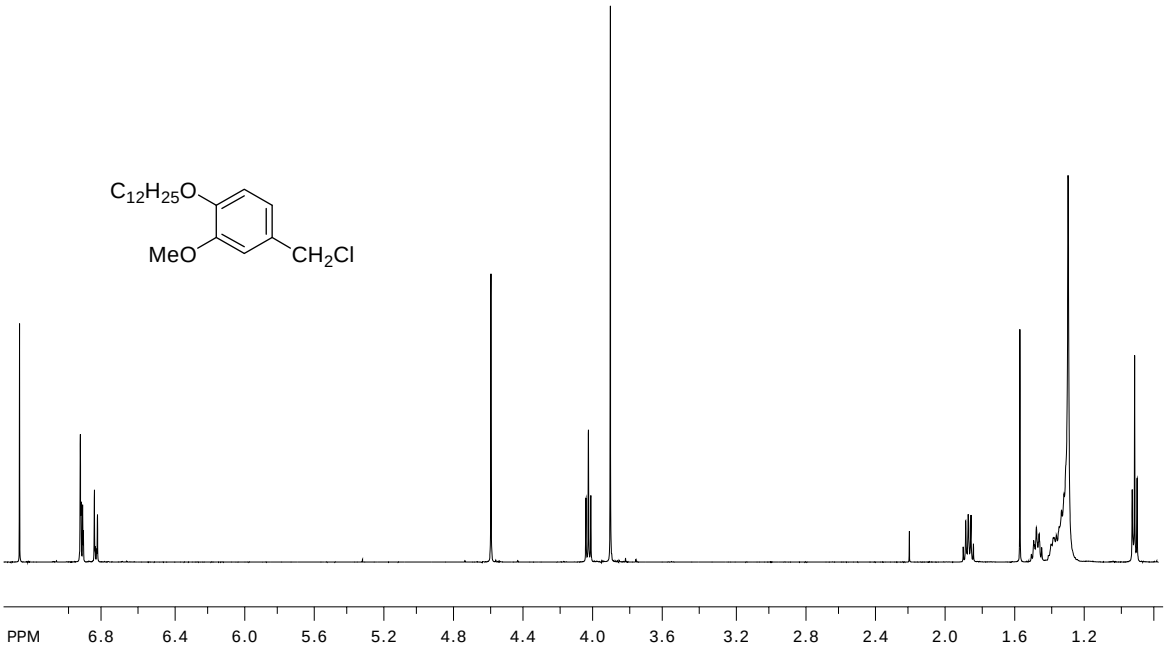


Figure S39. ^{1}H NMR spectrum of **10b** (chloroform-*d*, 500 MHz, 300 K).

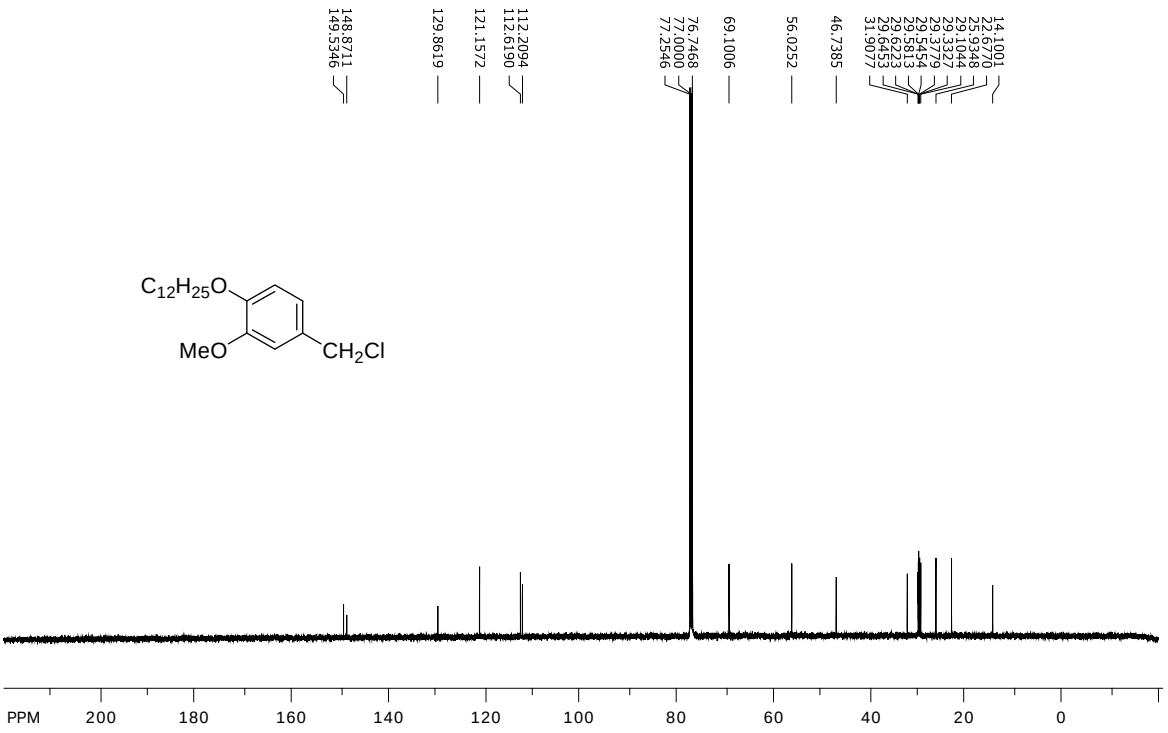


Figure S40. ^{13}C NMR spectrum of **10b** (chloroform-*d*, 125 MHz, 300 K).

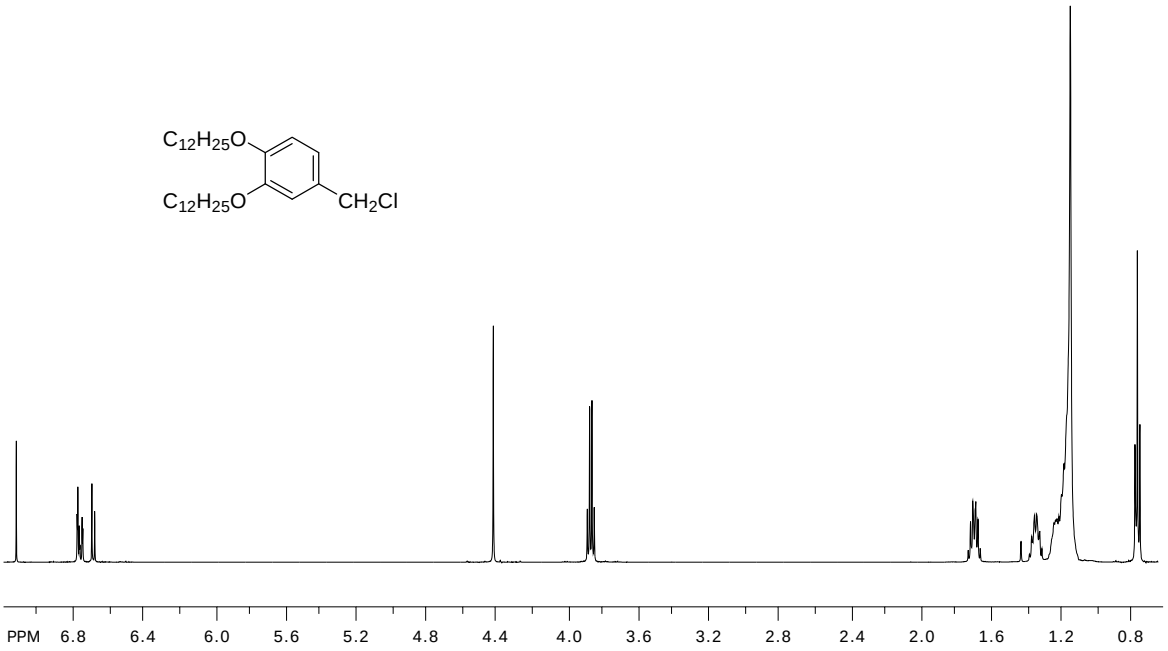


Figure S41. ^{1}H NMR spectrum of **10c** (chloroform-*d*, 500 MHz, 300 K).

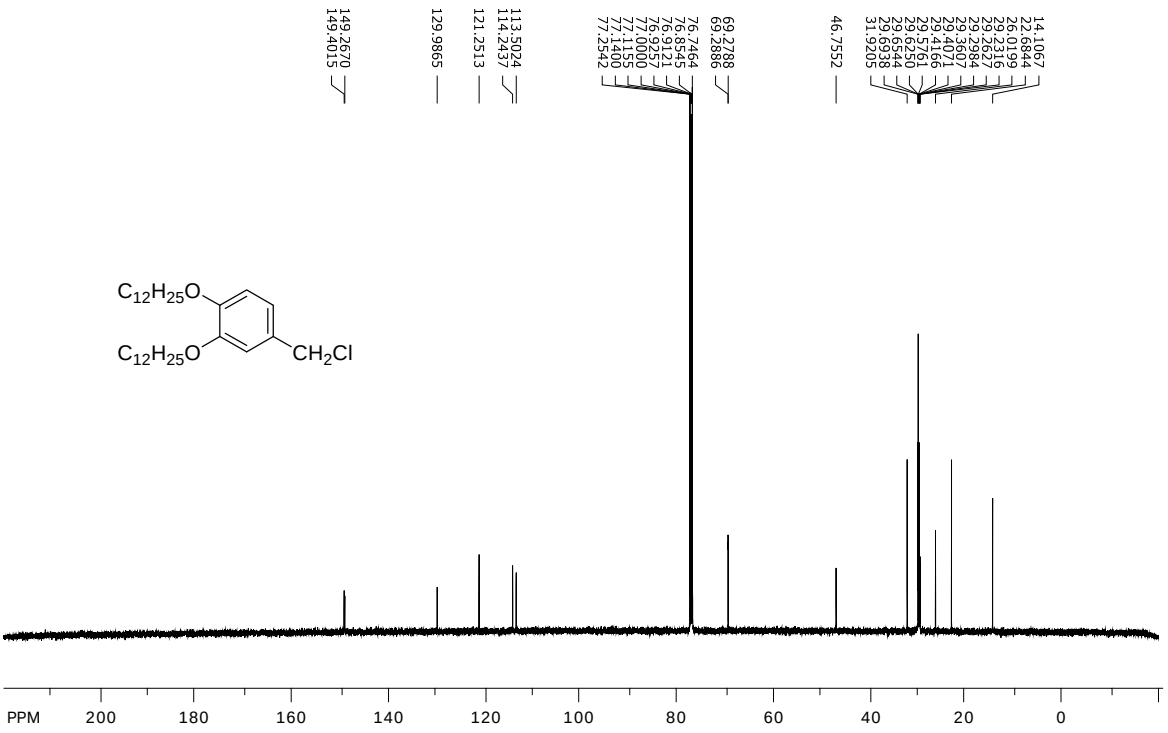


Figure S42. ^{13}C NMR spectrum of **10c** (chloroform-*d*, 125 MHz, 300 K).

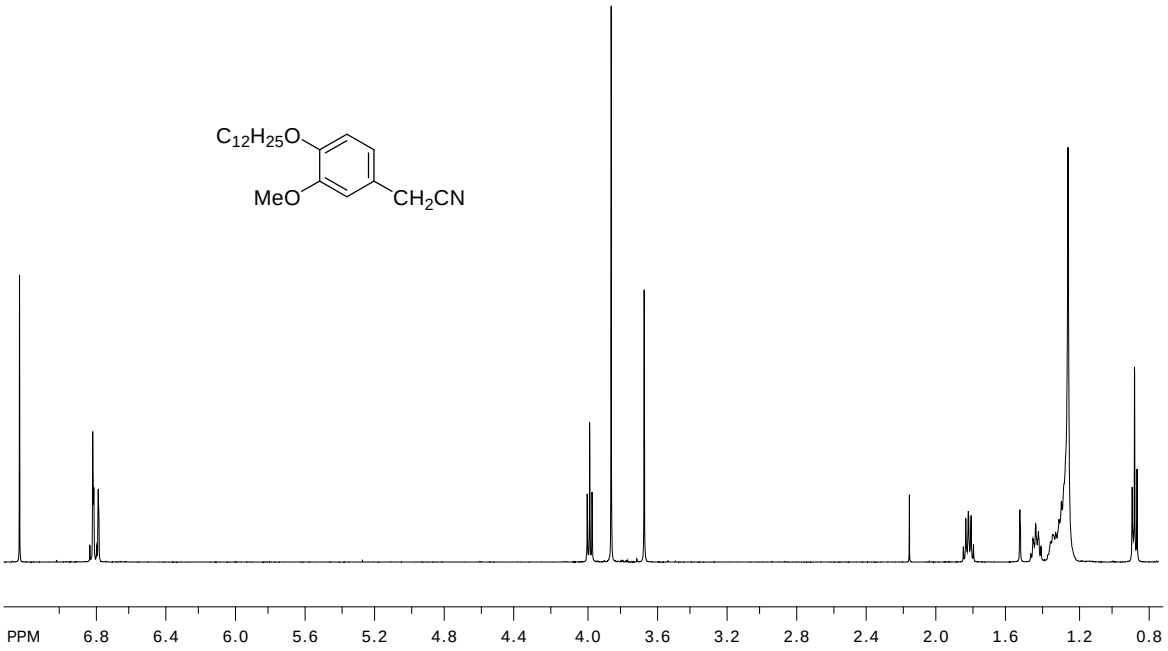


Figure S43. ^{1}H NMR spectrum of **11b** (chloroform-*d*, 500 MHz, 300 K).

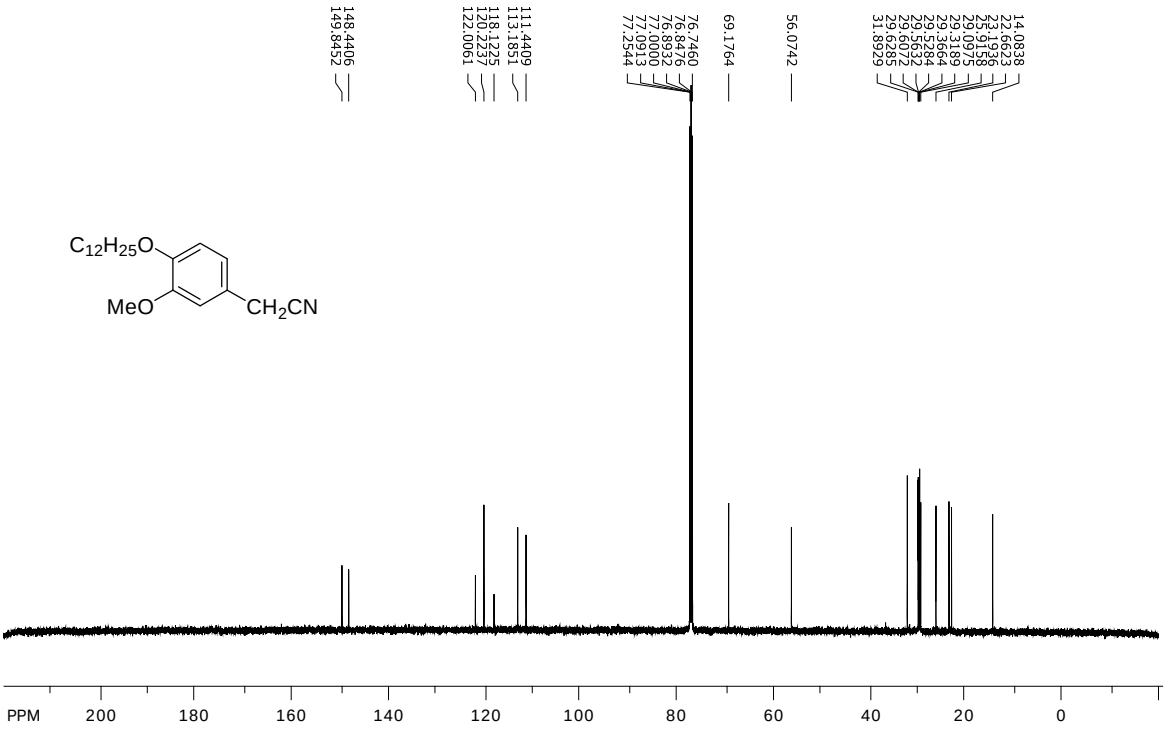


Figure S44. ^{13}C NMR spectrum of **11b** (chloroform-*d*, 125 MHz, 300 K).

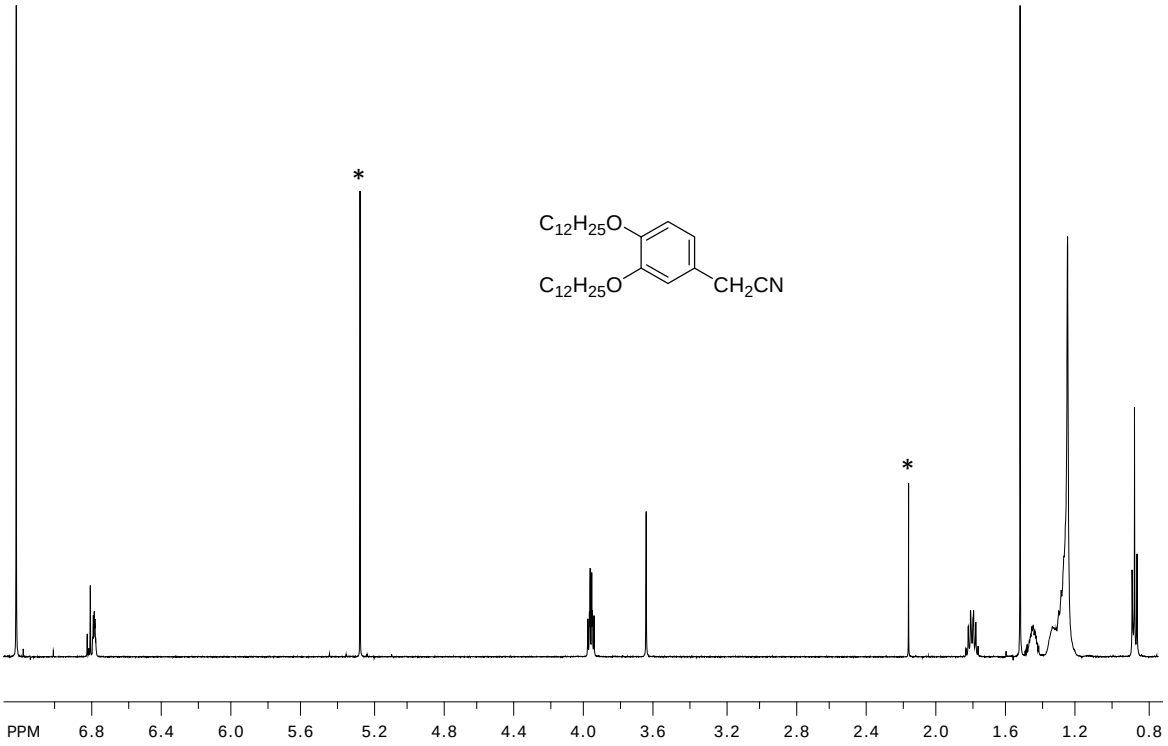


Figure S45. ^{1}H NMR spectrum of **11c** (chloroform-*d*, 500 MHz, 300 K).

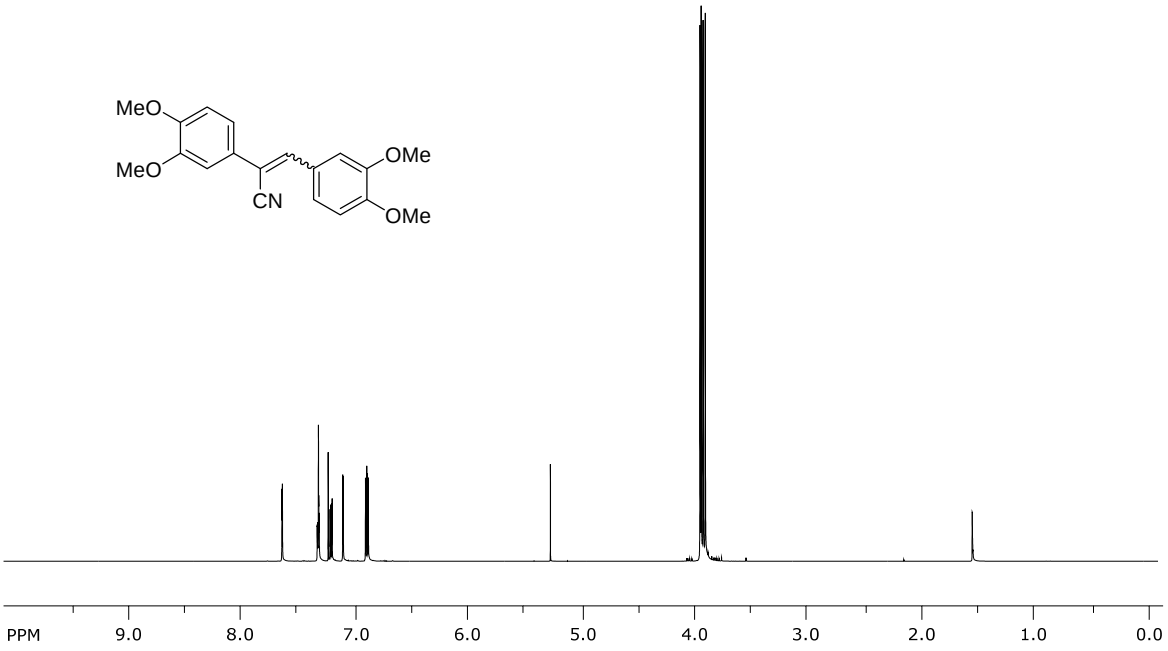


Figure S46. ^{1}H NMR spectrum of **12a** (chloroform-*d*, 600 MHz, 300 K).

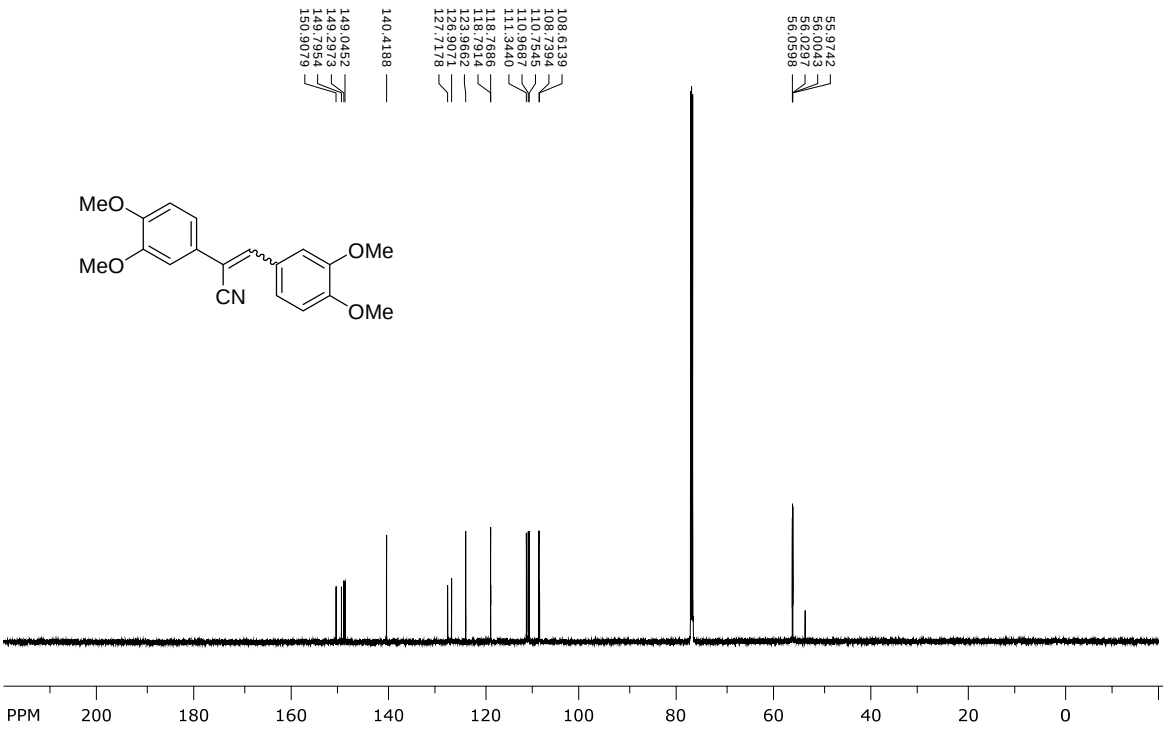


Figure S47. ^{13}C NMR spectrum of **12a** (chloroform-*d*, 151 MHz, 300 K).

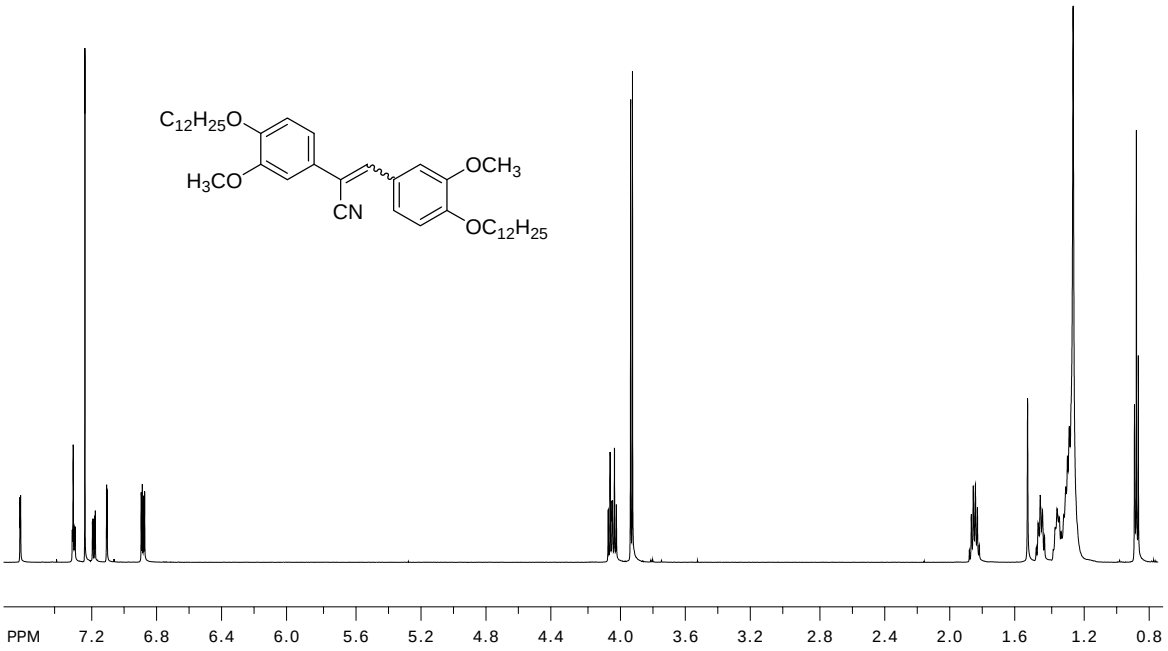


Figure S48. ^{1}H NMR spectrum of **12b** (chloroform-*d*, 500 MHz, 300 K).

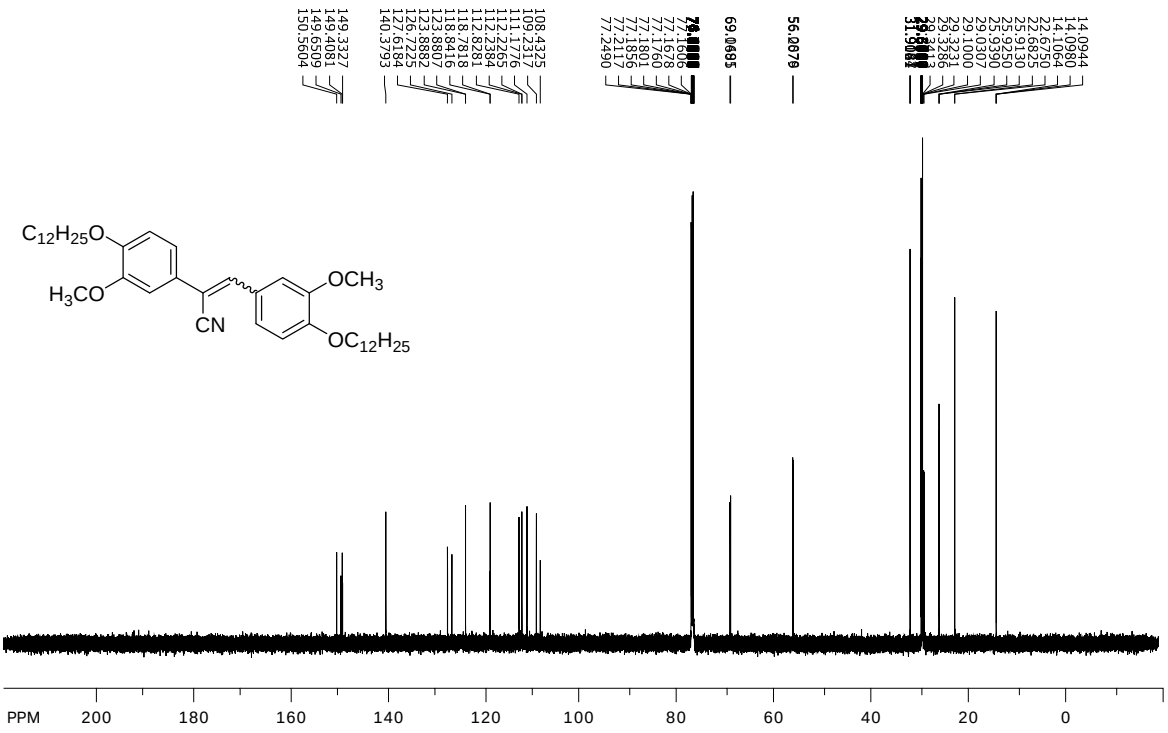


Figure S49. ^{13}C NMR spectrum of **12b** (chloroform-*d*, 125 MHz, 300 K).

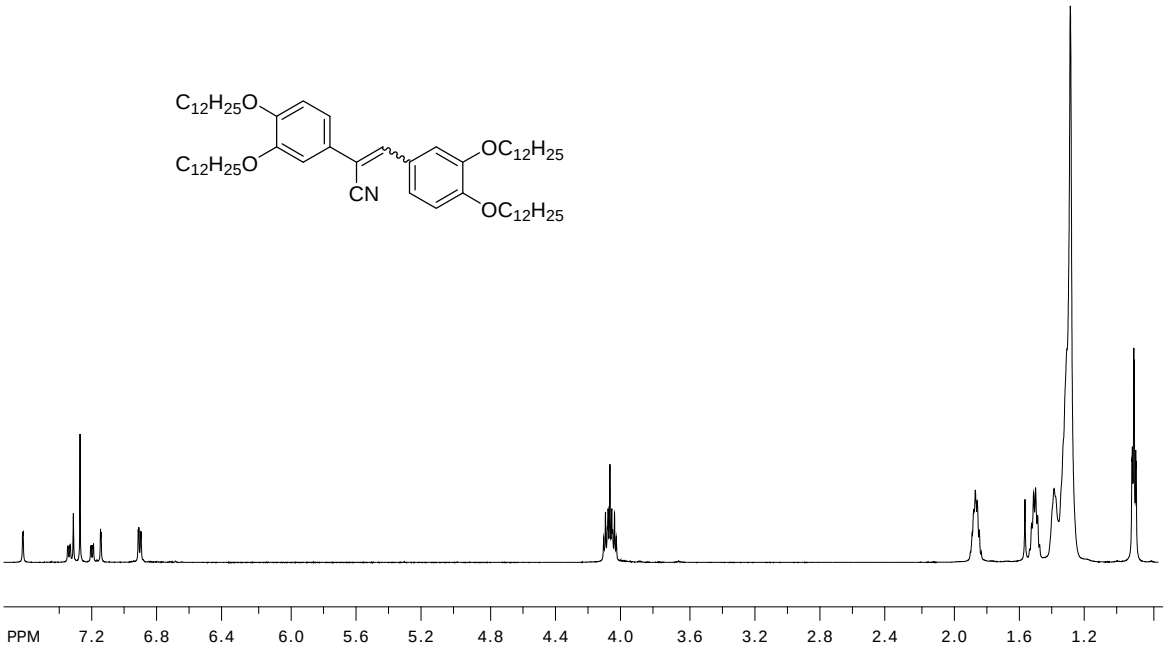


Figure S50. ^{1}H NMR spectrum of **12c** (chloroform-*d*, 500 MHz, 300 K).

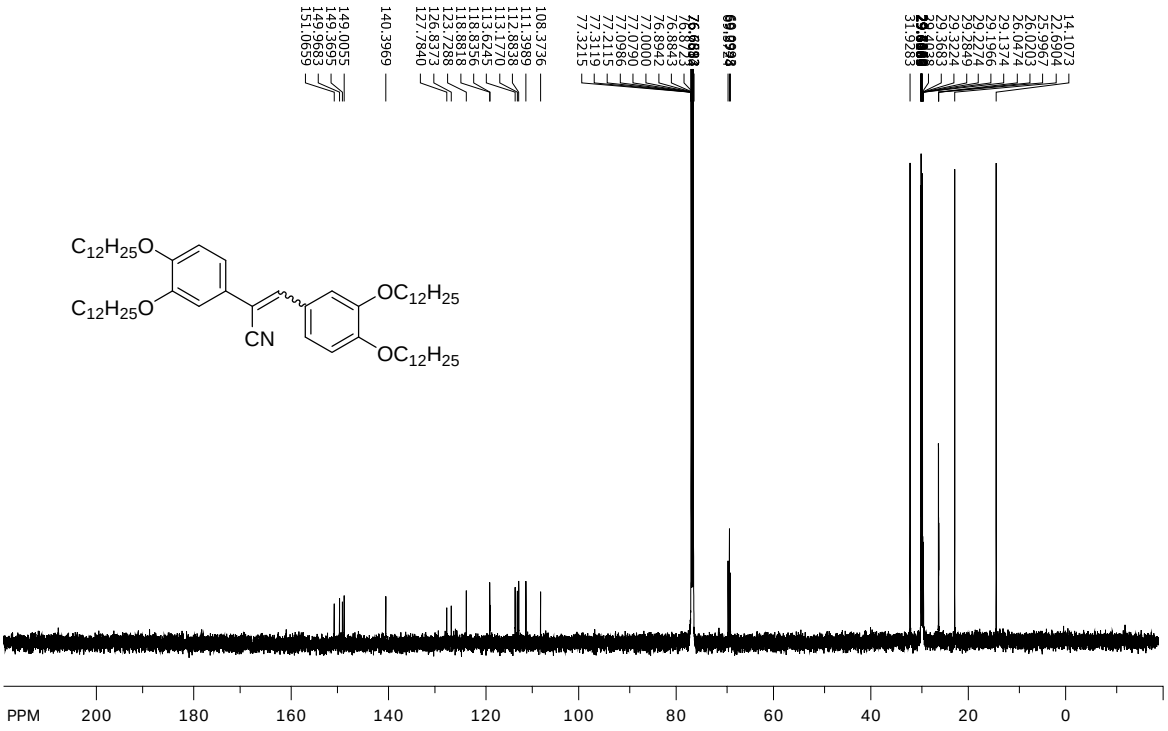


Figure S51. ^{13}C NMR spectrum of **12c** (chloroform-*d*, 125 MHz, 300 K).

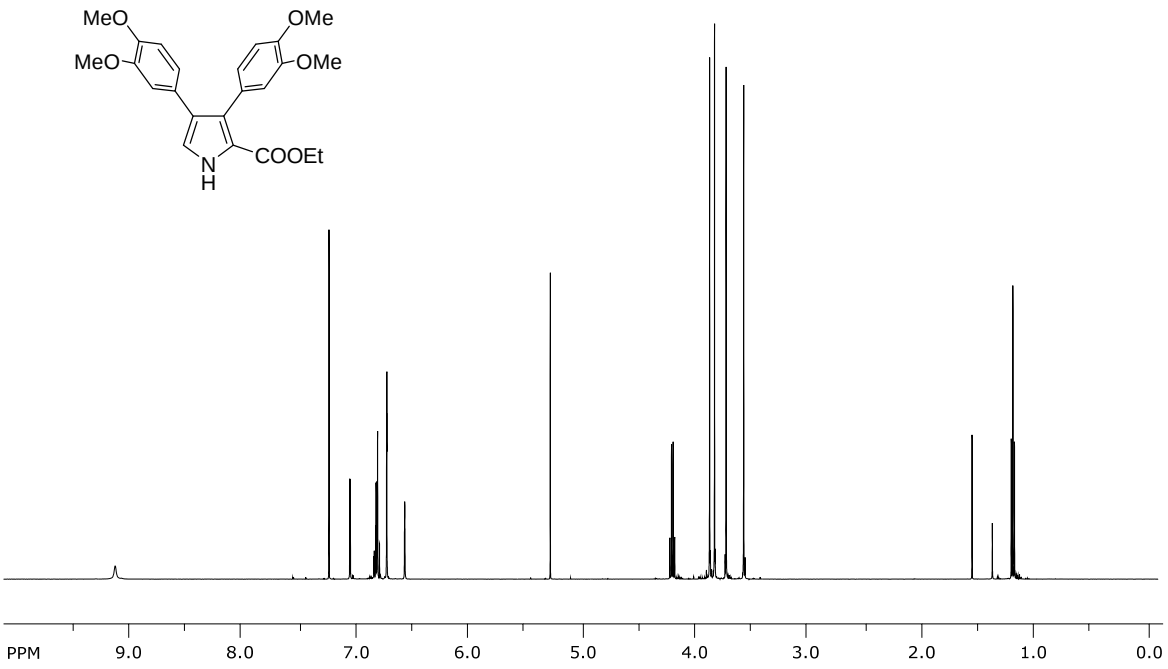


Figure S52. ^{1}H NMR spectrum of **1a** (chloroform-*d*, 500 MHz, 300 K).

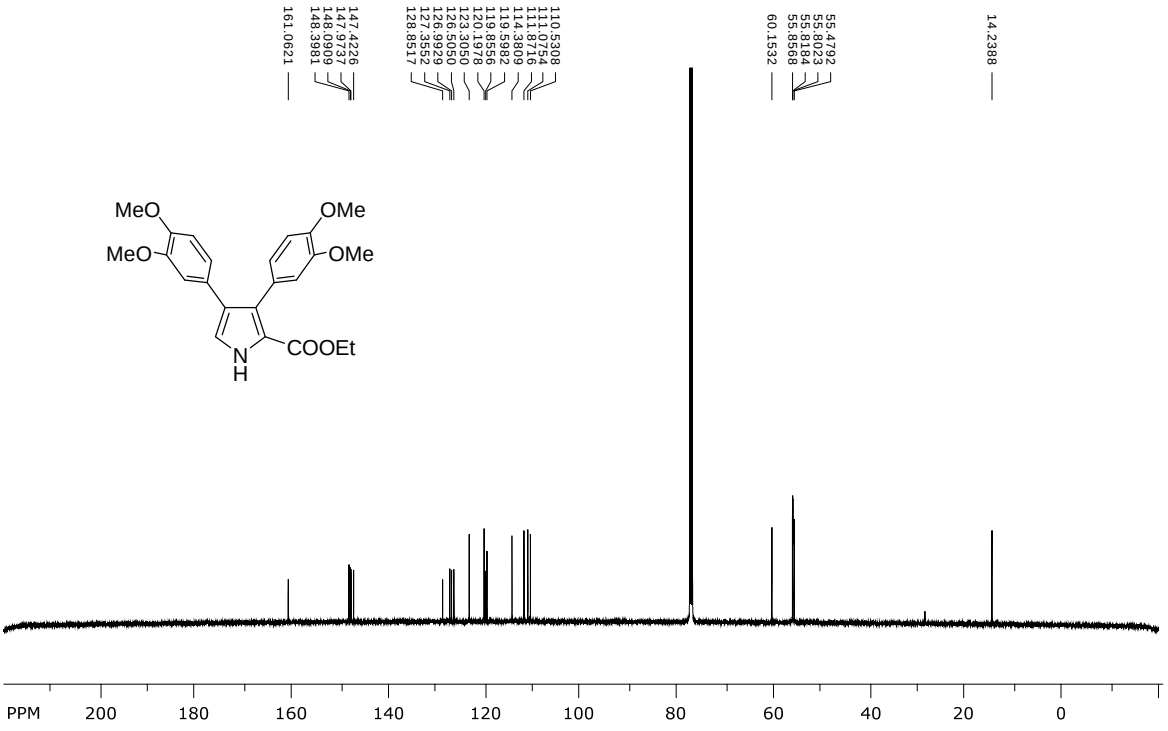


Figure S53. ^{13}C NMR spectrum of **1a** (chloroform-*d*, 125 MHz, 300 K).

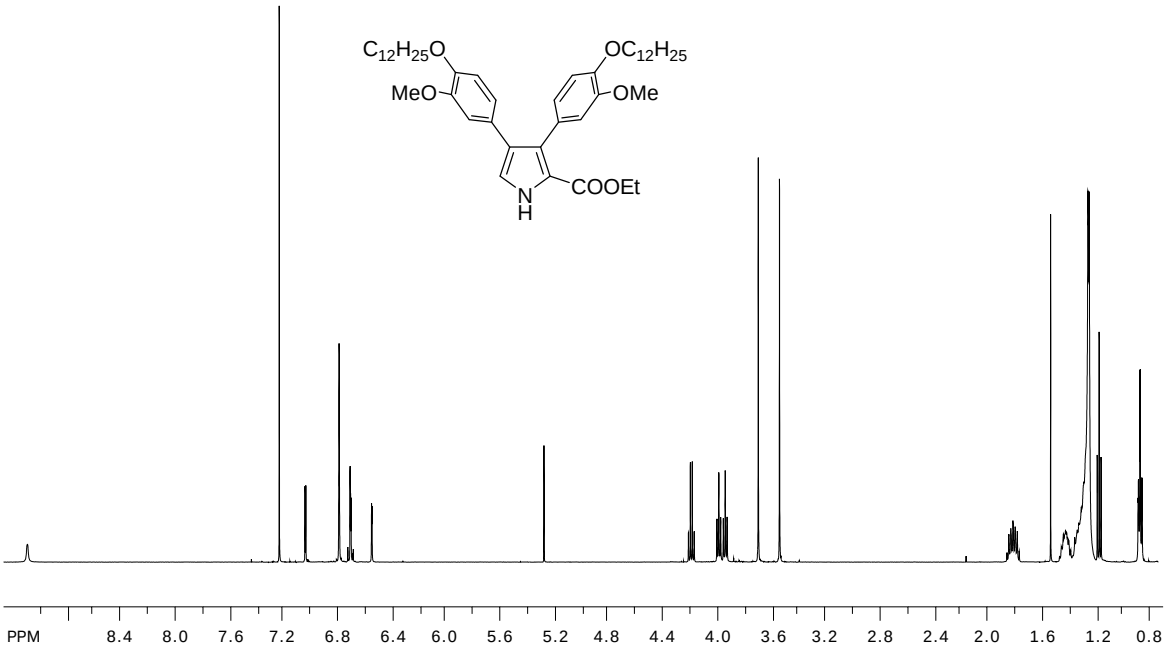


Figure S54. ^{1}H NMR spectrum of **1b** (chloroform-*d*, 500 MHz, 300 K).

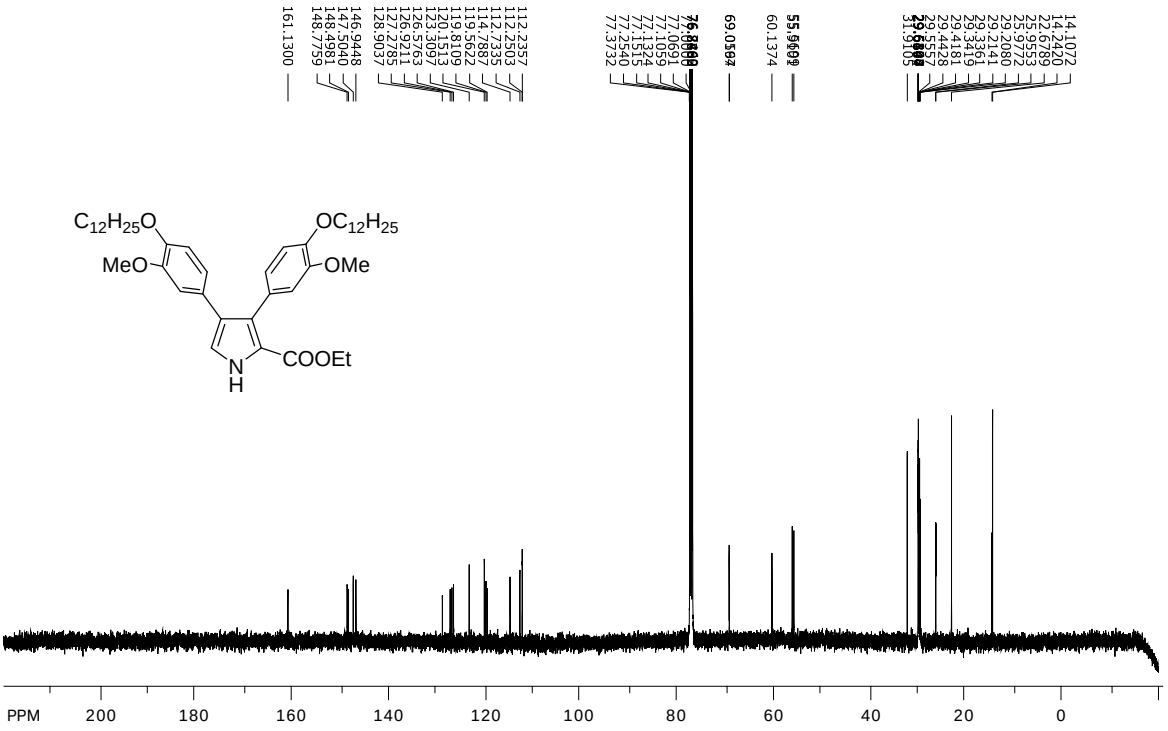


Figure S55. ^{13}C NMR spectrum of **1b** (chloroform-*d*, 125 MHz, 300 K).

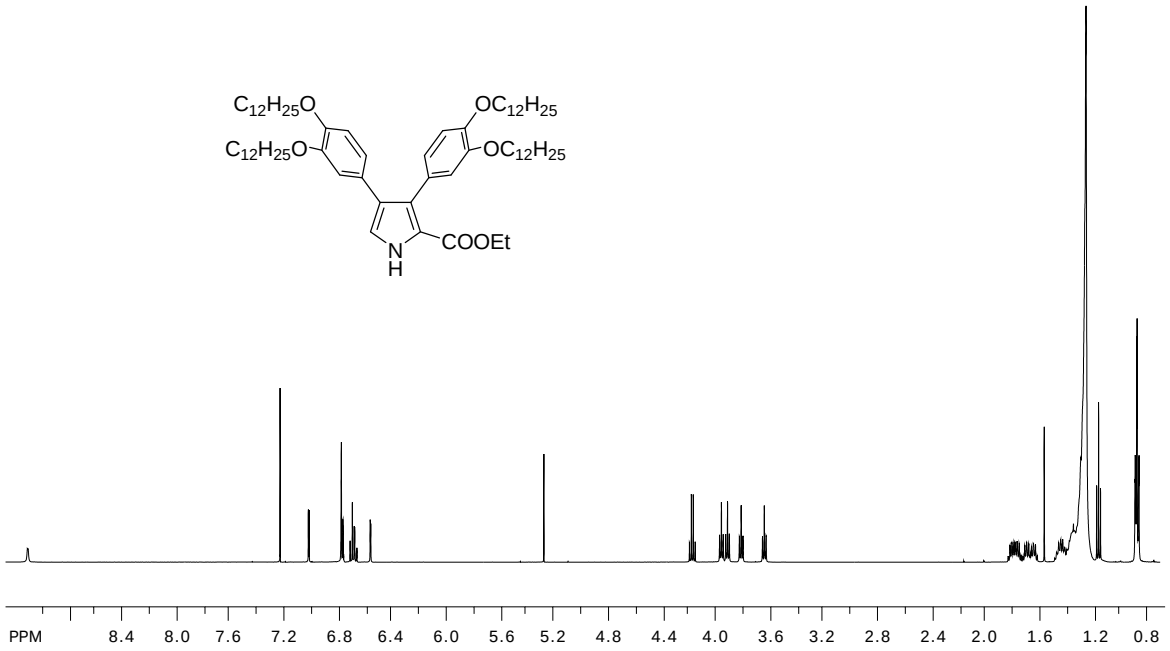


Figure S56. ^{1}H NMR spectrum of **1c** (chloroform-*d*, 500 MHz, 300 K).

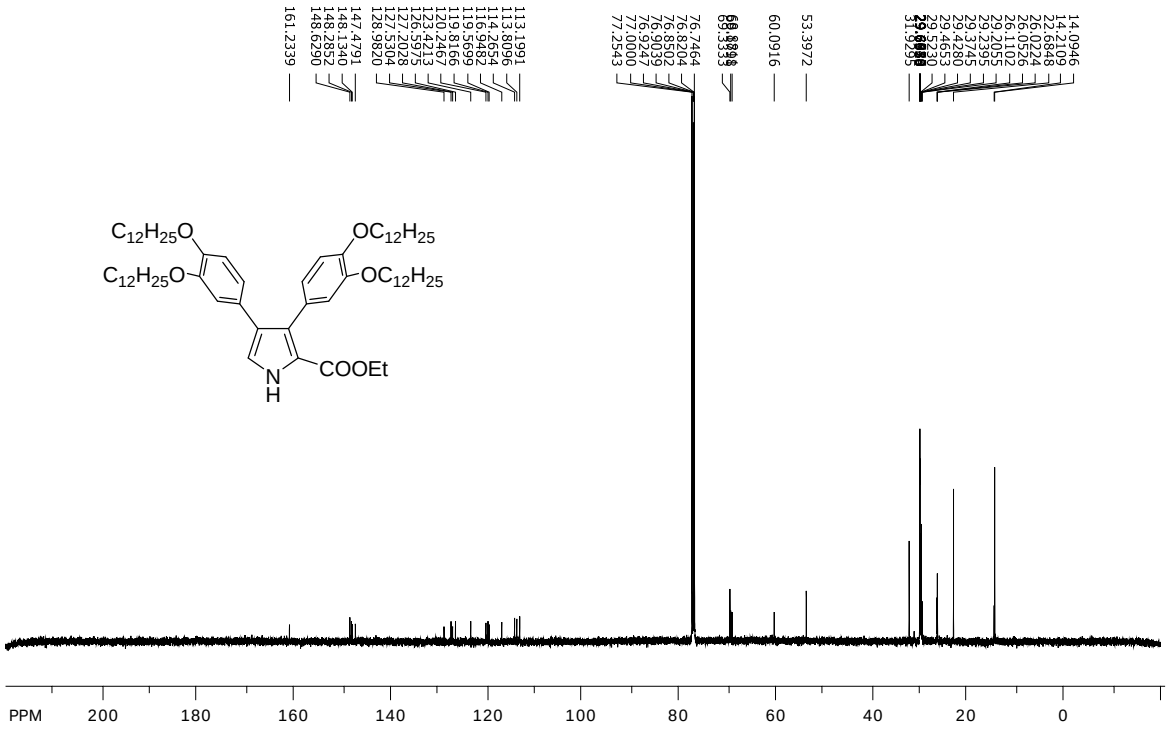


Figure S57. ^{13}C NMR spectrum of **1c** (chloroform-*d*, 125 MHz, 300 K).

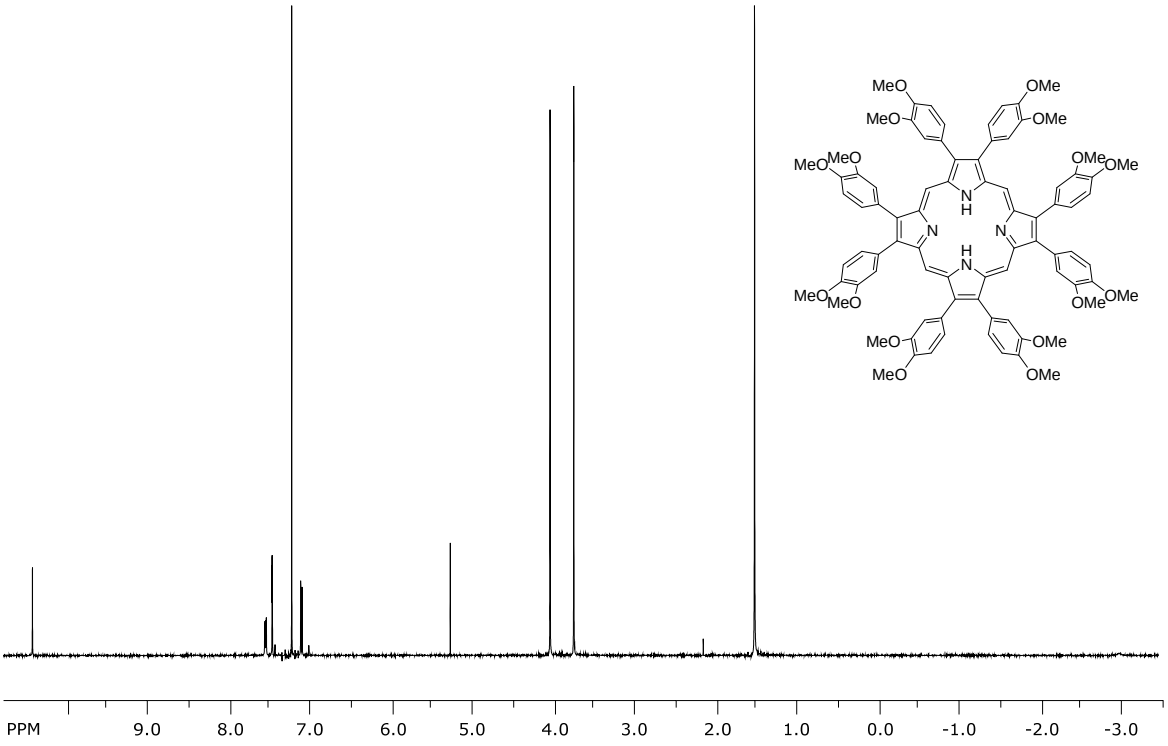


Figure S58. ^{1}H NMR spectrum of **2a**-H_2 (chloroform-*d*, 500 MHz, 300 K).

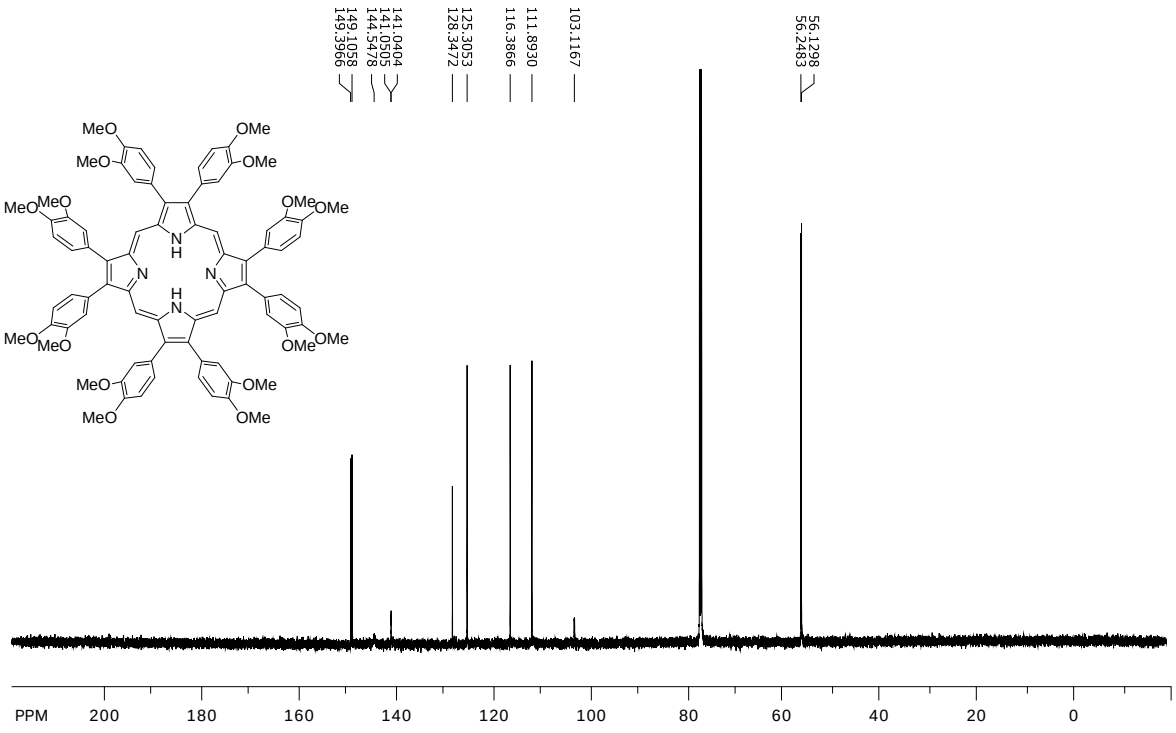


Figure S59. ^{13}C NMR spectrum of **2a**-H_2 (chloroform-*d*, 151 MHz, 325 K).

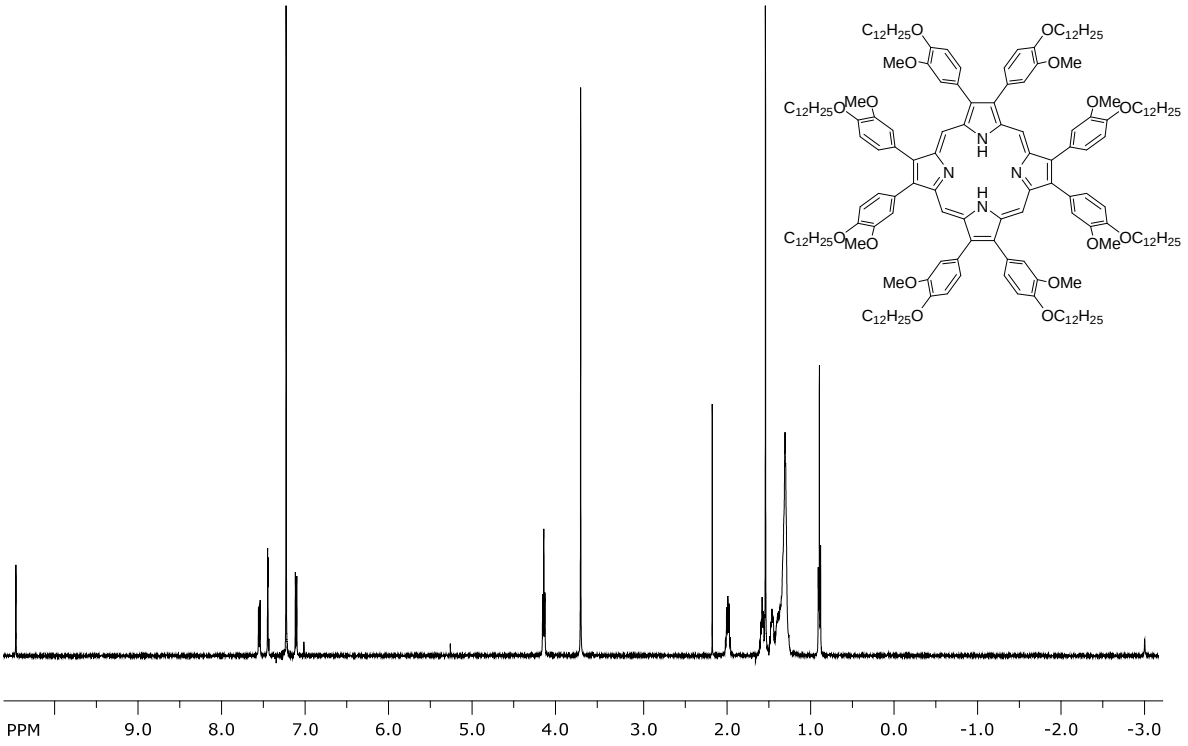


Figure S60. ^{1}H NMR spectrum of **2b**-H_2 (chloroform-*d*, 500 MHz, 300 K).

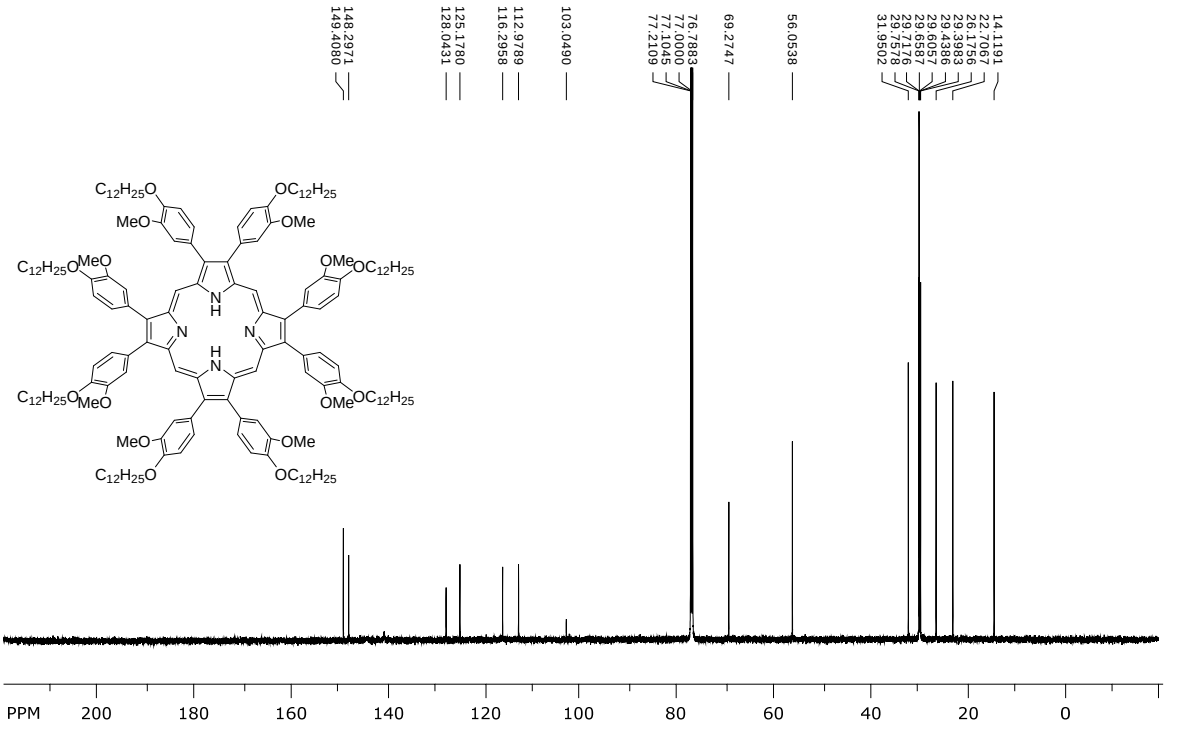


Figure S61. ^{13}C NMR spectrum of **2b**-H_2 (chloroform-*d*, 151 MHz, 300 K).

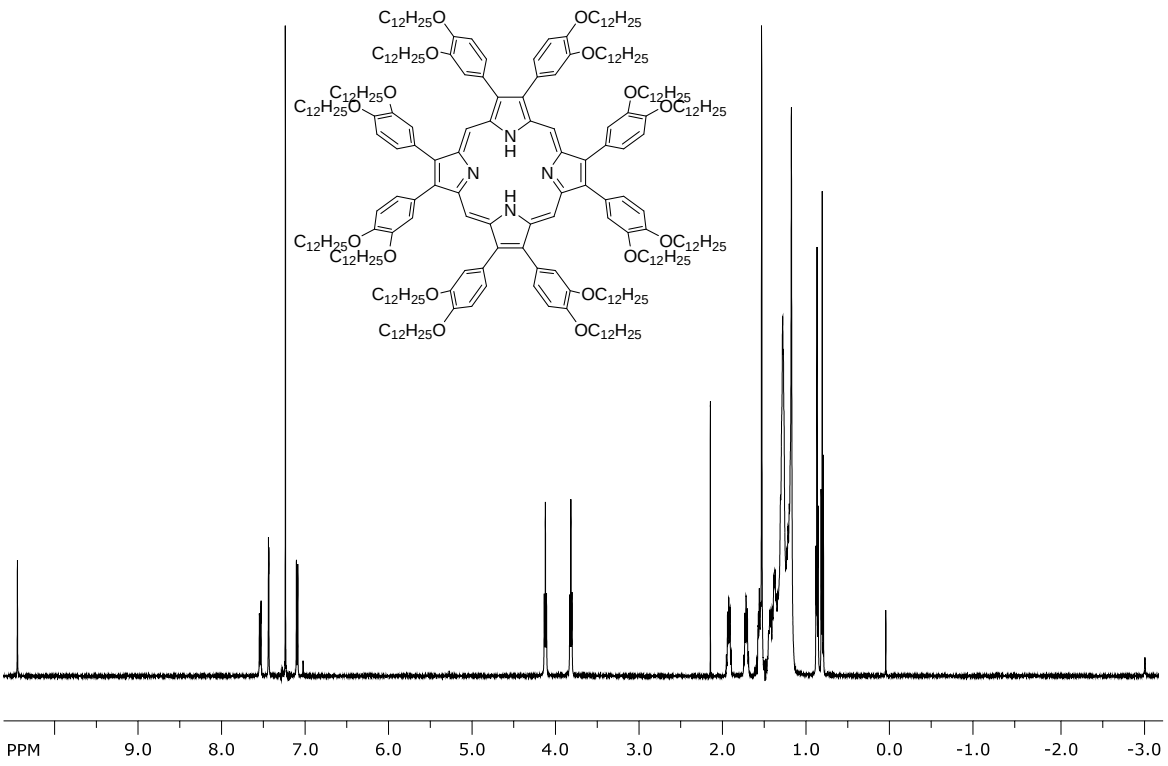


Figure S62. ^{1}H NMR spectrum of **2c**-H_2 (chloroform-*d*, 500 MHz, 300 K).

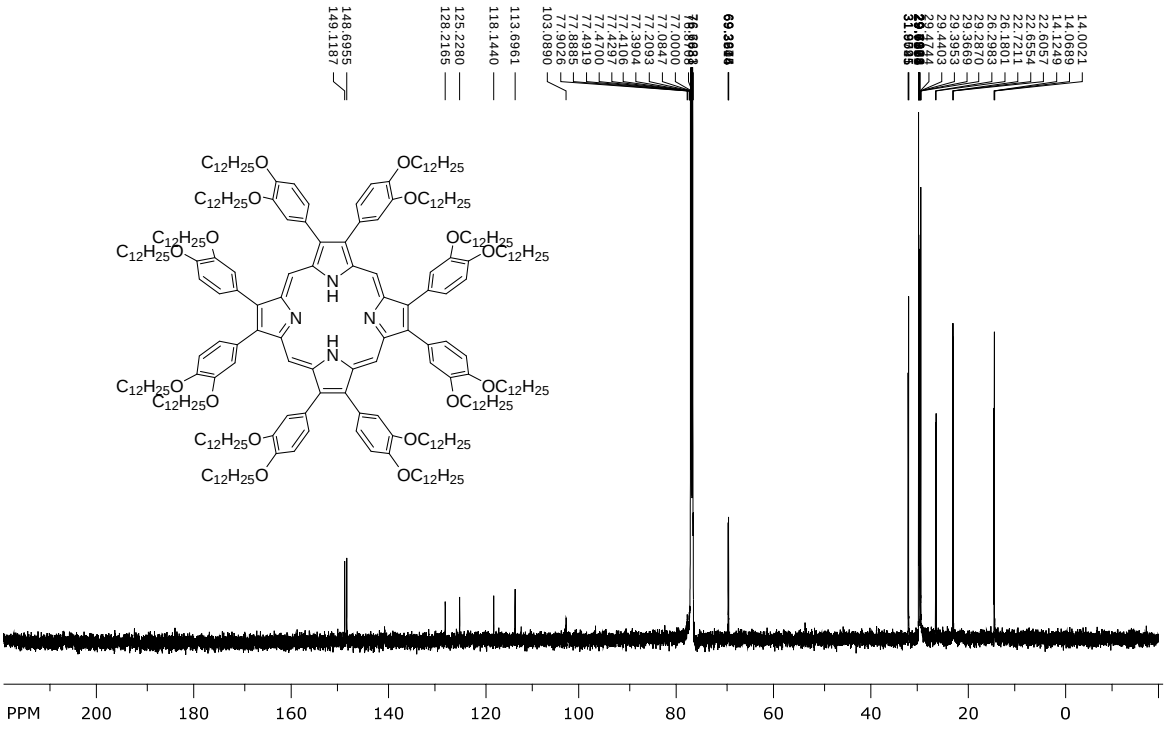


Figure S63. ^{13}C NMR spectrum of **2c**-H_2 (chloroform-*d*, 151 MHz, 300 K).

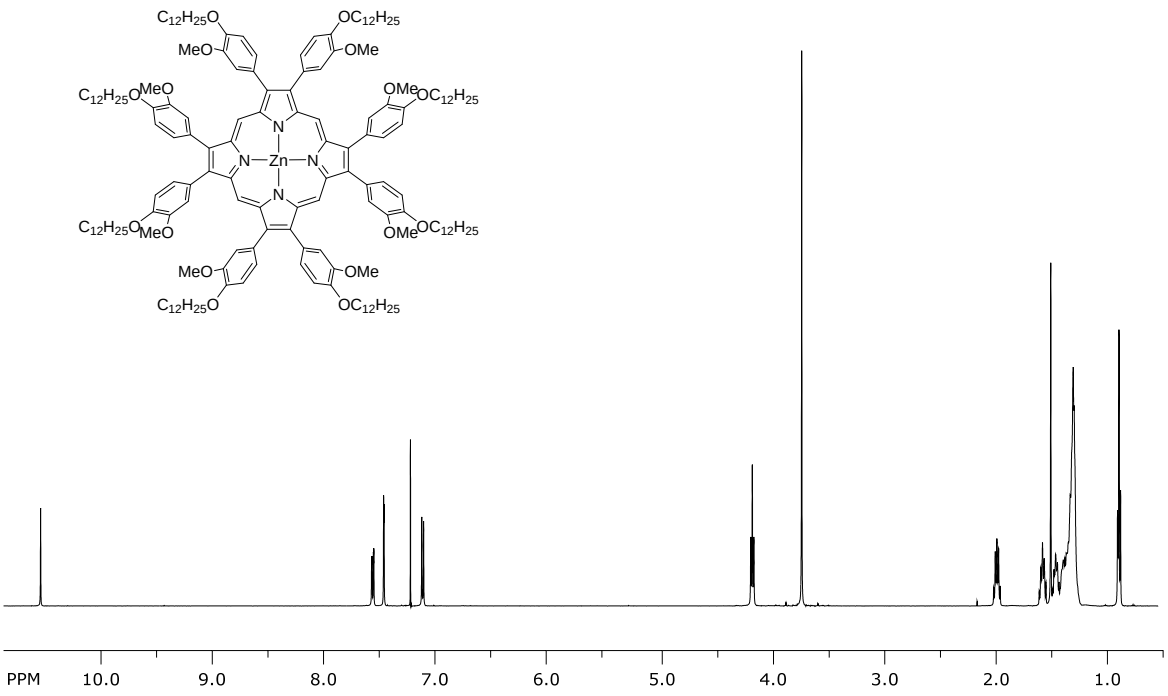


Figure S64. ^{1}H NMR spectrum of **2b**-Zn (chloroform-*d*, 500 MHz, 300 K).

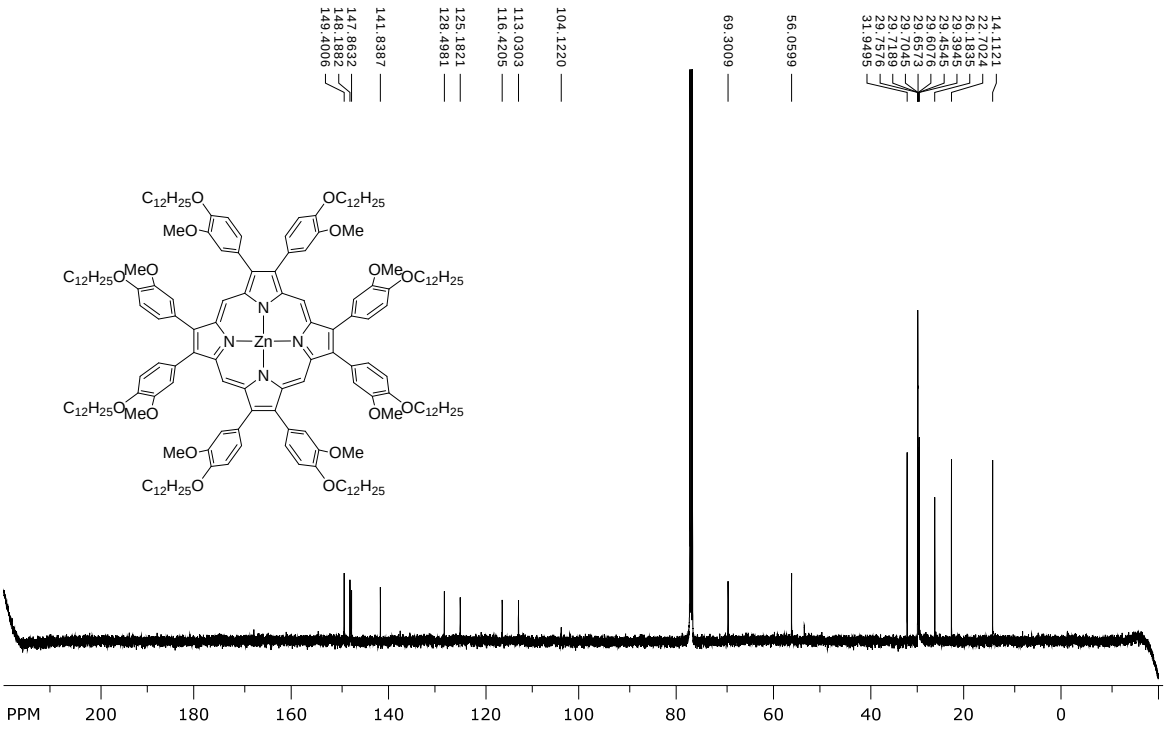


Figure S65. ^{13}C NMR spectrum of **2b**-Zn (chloroform-*d*, 125 MHz, 300 K).

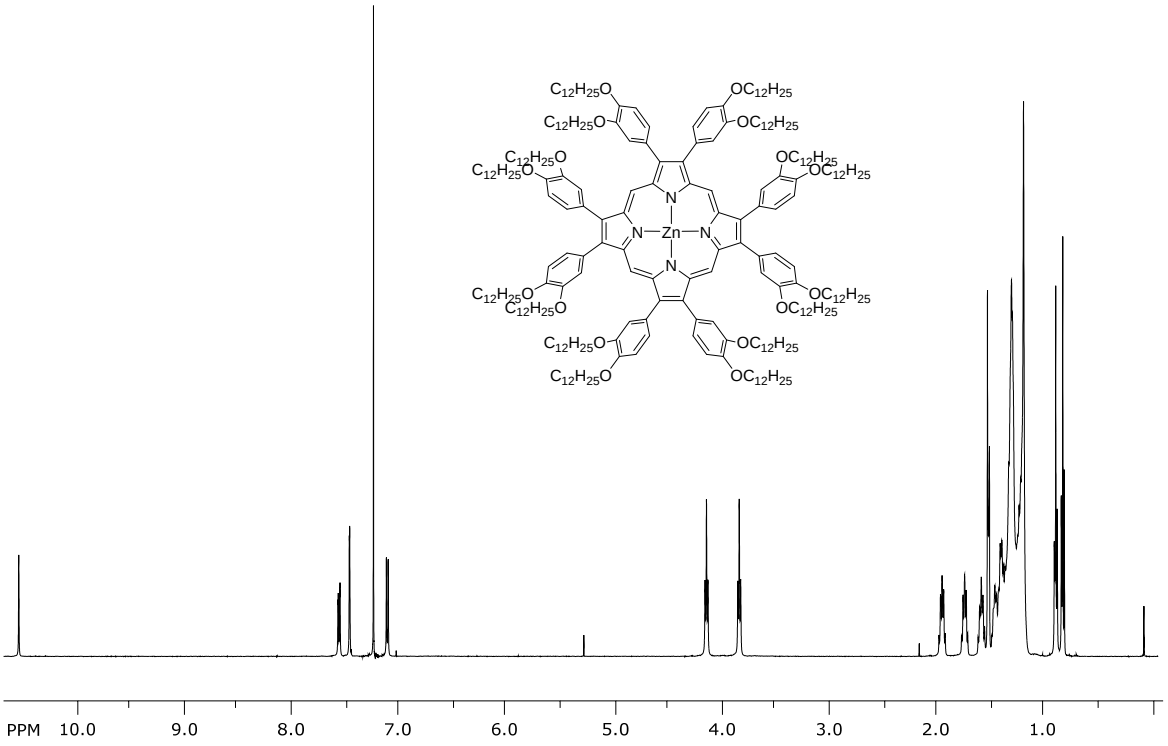


Figure S66. ^{1}H NMR spectrum of **2c**-Zn (chloroform-*d*, 500 MHz, 300 K).

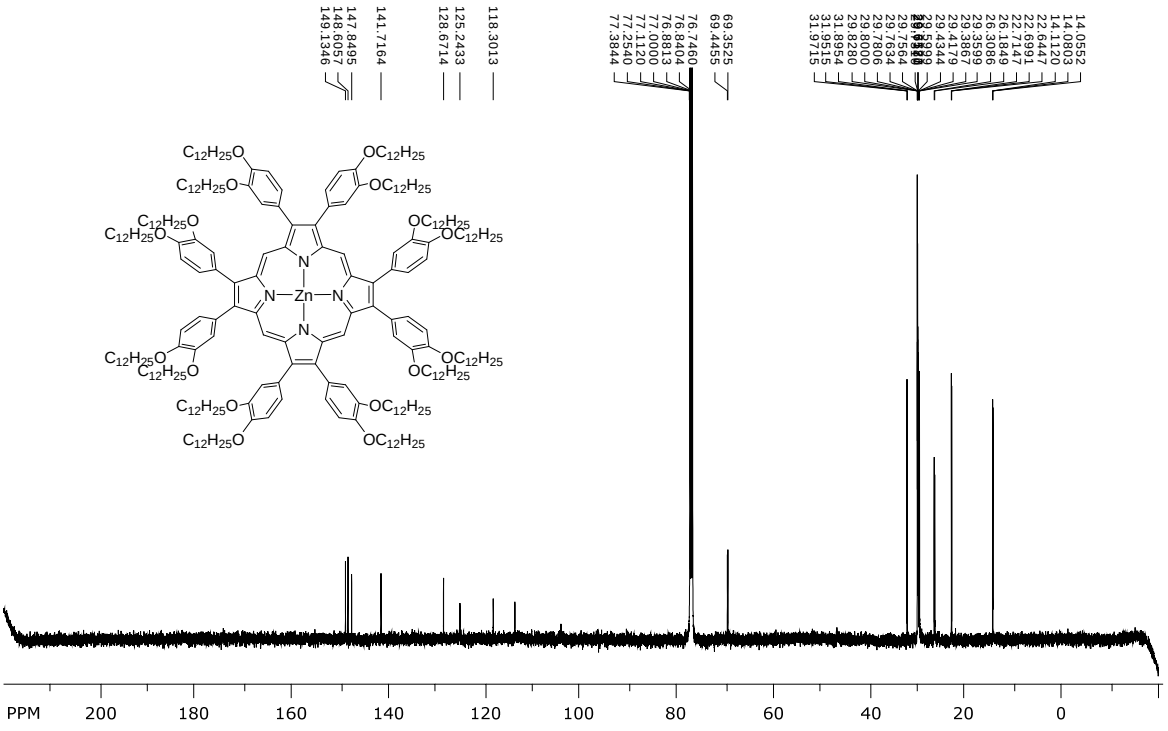


Figure S67. ^{13}C NMR spectrum of **2c**-Zn (chloroform-*d*, 500 MHz, 300 K).

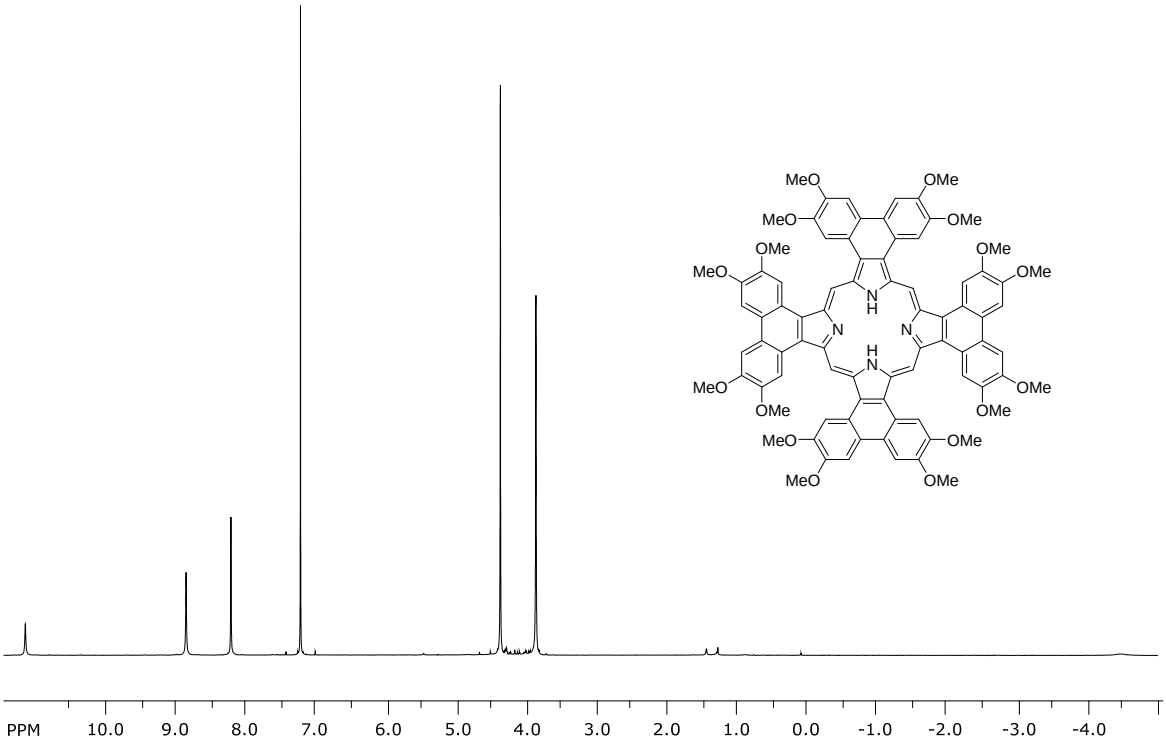


Figure S68. ^{1}H NMR spectrum of **3a**-H_2 (chloroform-*d*, 500 MHz, 300 K).

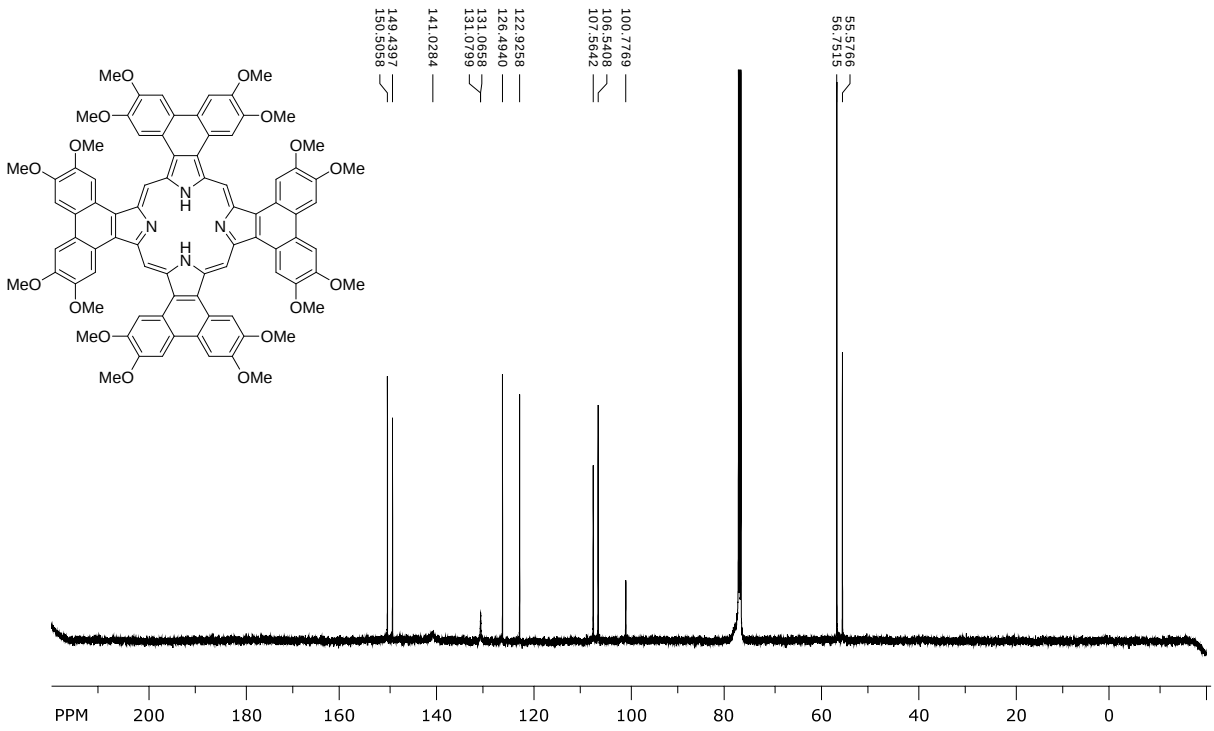


Figure S69. ^{13}C NMR spectrum of **3a**-H_2 (chloroform-*d*, 500 MHz, 300 K).

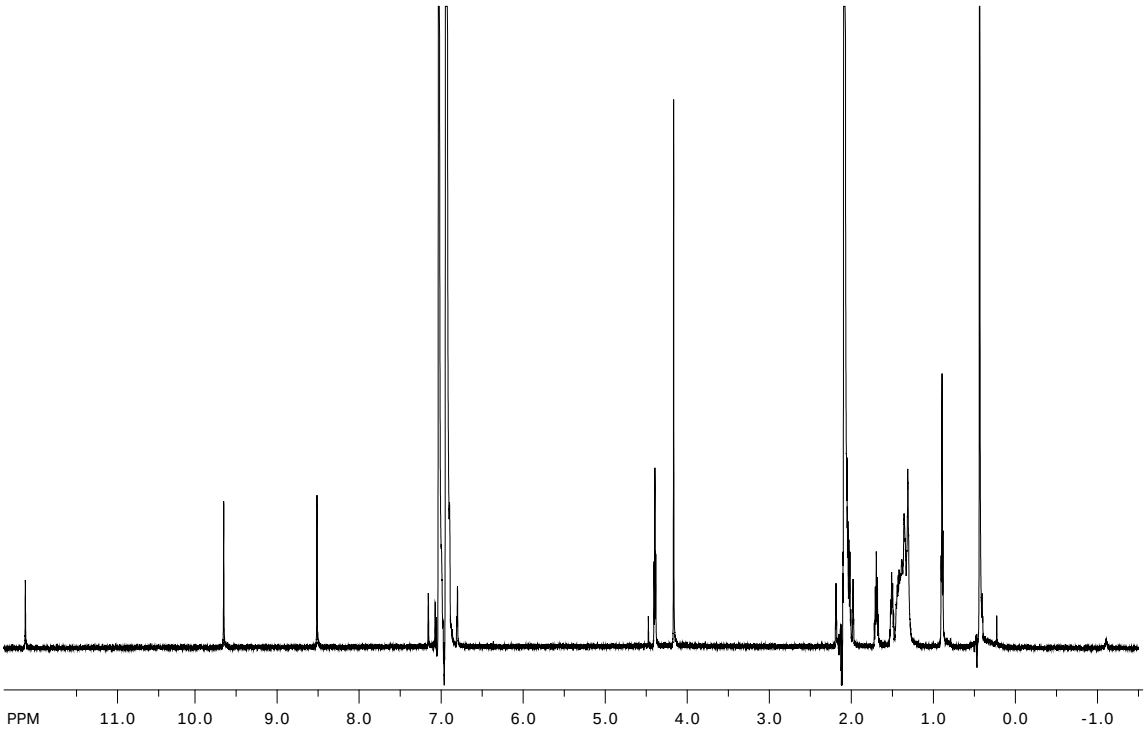


Figure S70. ^{1}H NMR spectrum of **3b**-H_2 (dilute in toluene-d_8, 600 MHz, 300 K).The spectrum becomes broad a higher concentrations.

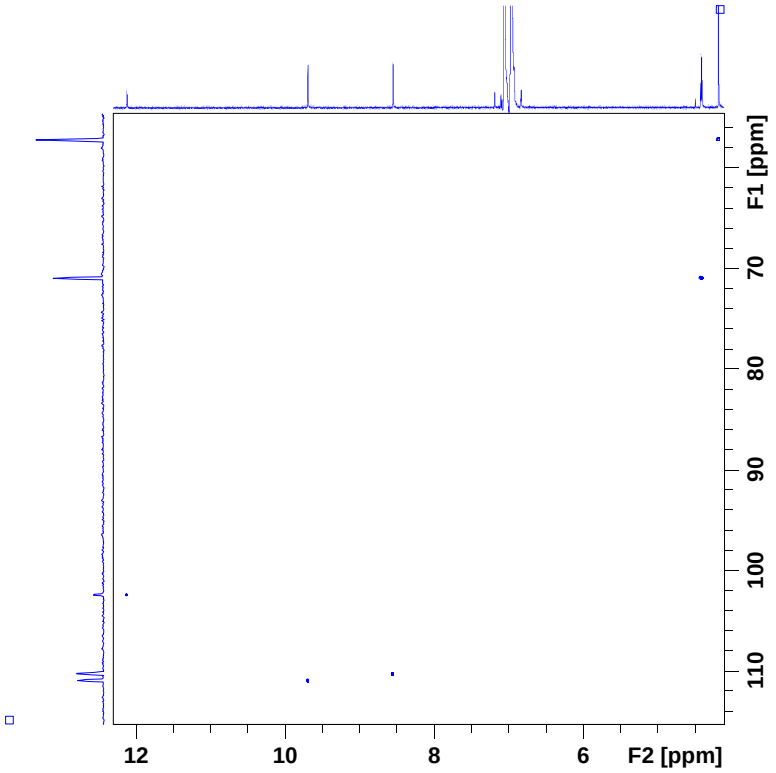


Figure S71. Partial ^{1}H-^{13}C HSQC spectrum of **3b**-H_2 (toluene-d_8, 600 MHz, 300 K).

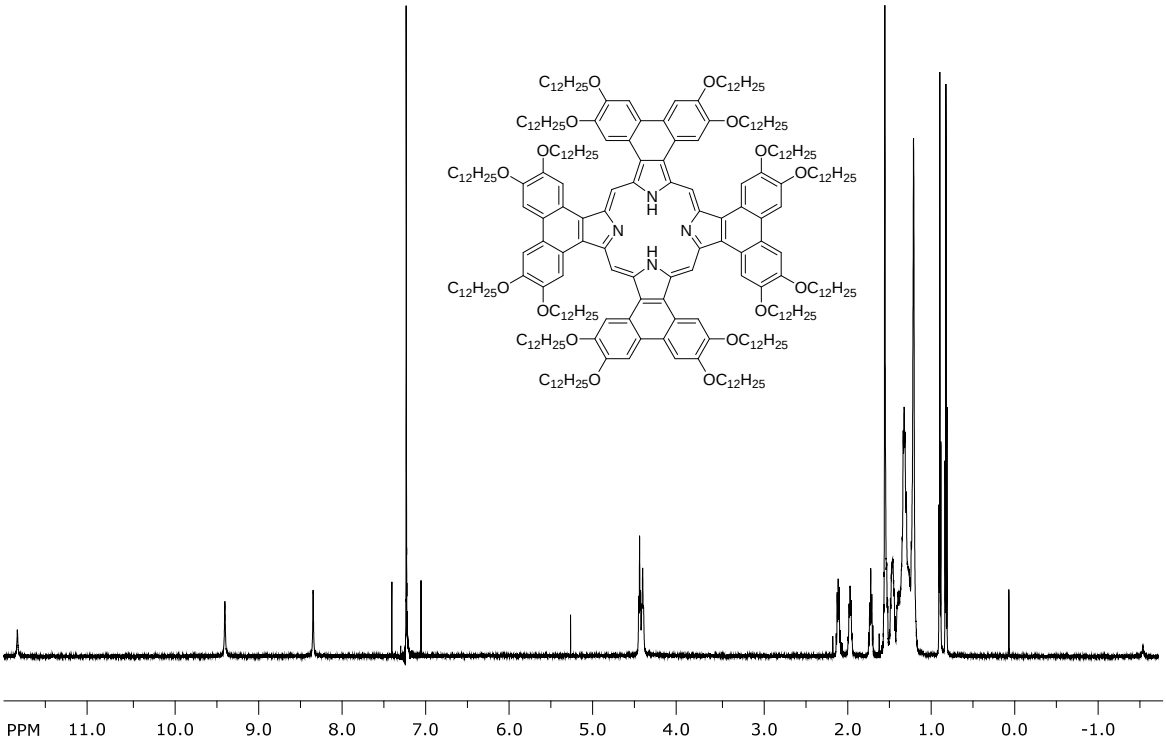


Figure S72. ^{1}H NMR spectrum of **3c**-H_2 (chloroform-*d*, 600 MHz, 300 K). High dilution was necessary to achieve narrow lines.

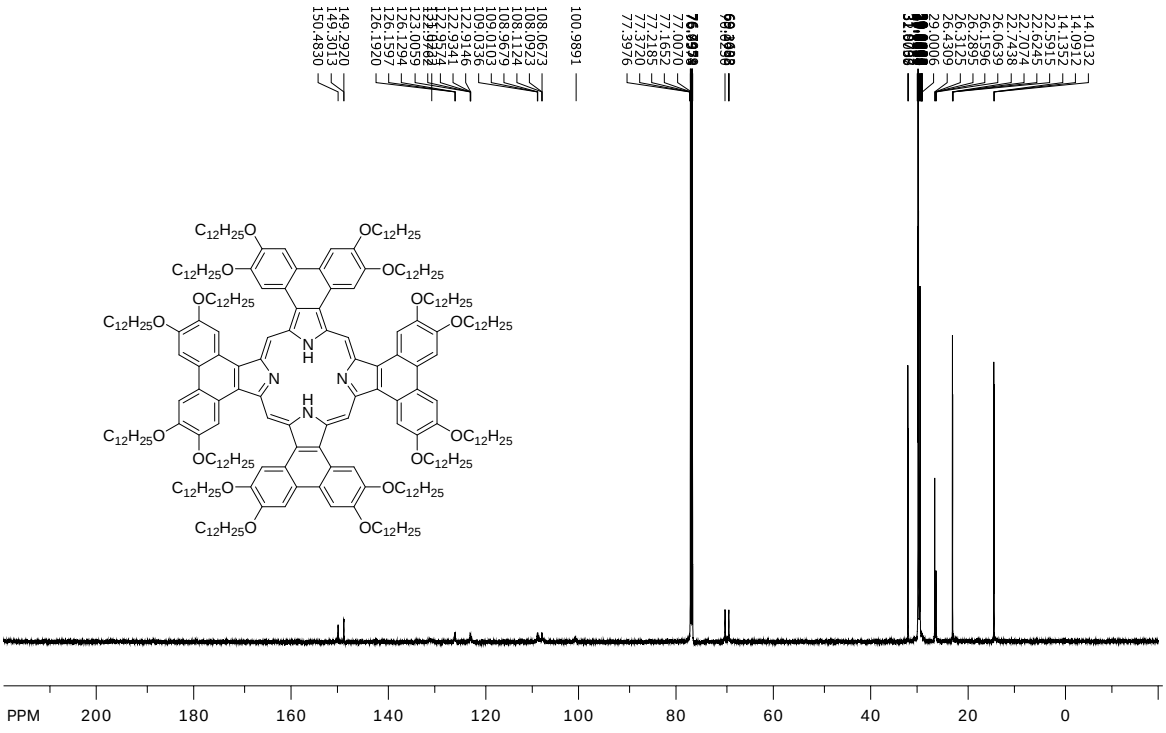


Figure S73. ^{13}C NMR spectrum of **3c**-H_2 (chloroform-*d*, 151 MHz, 300 K).

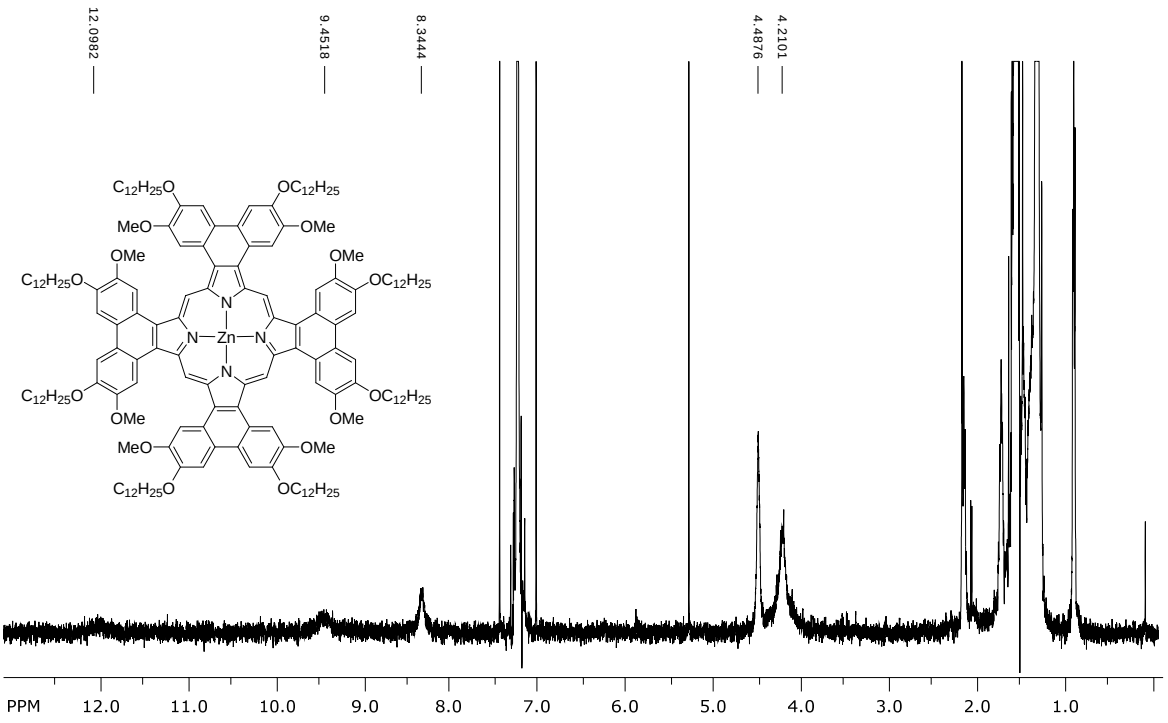


Figure S74. ^{1}H NMR spectrum of **3b**-Zn (dilute in chloroform-*d*, 500 MHz, 300 K). The spectrum becomes very broad at higher concentrations.

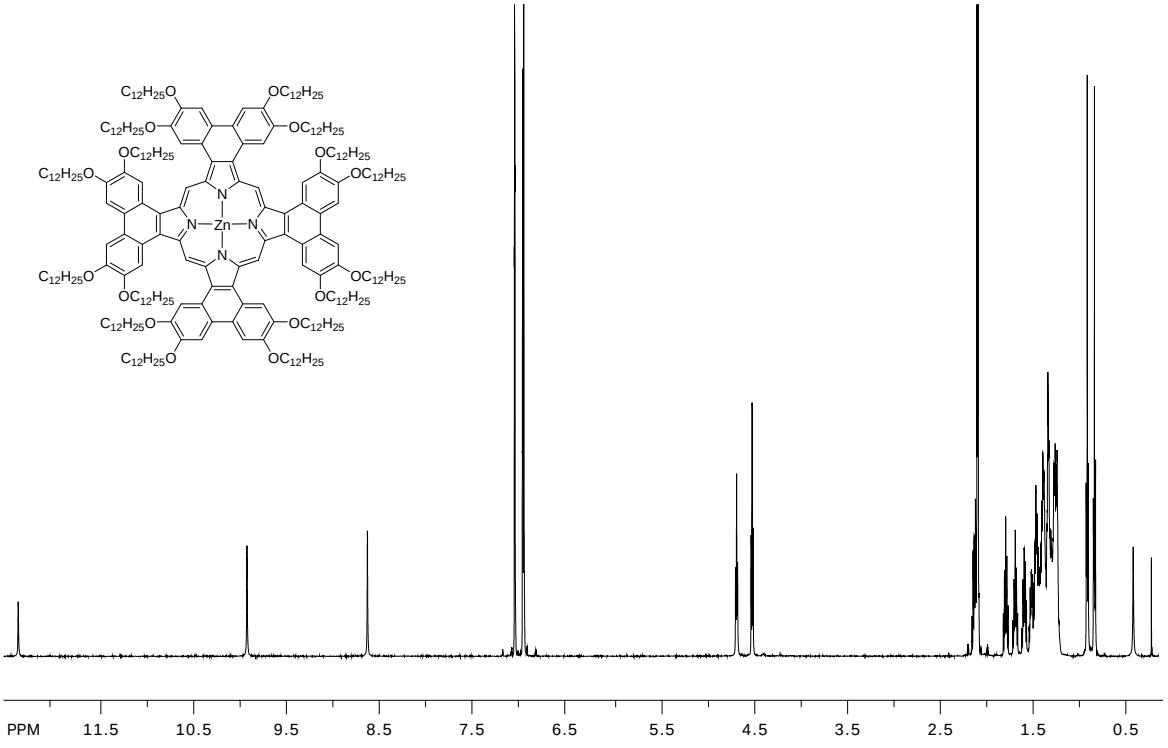


Figure S75. ^{1}H NMR spectrum of **3c**-Zn (toluene-d_8, 600 MHz, 380 K)

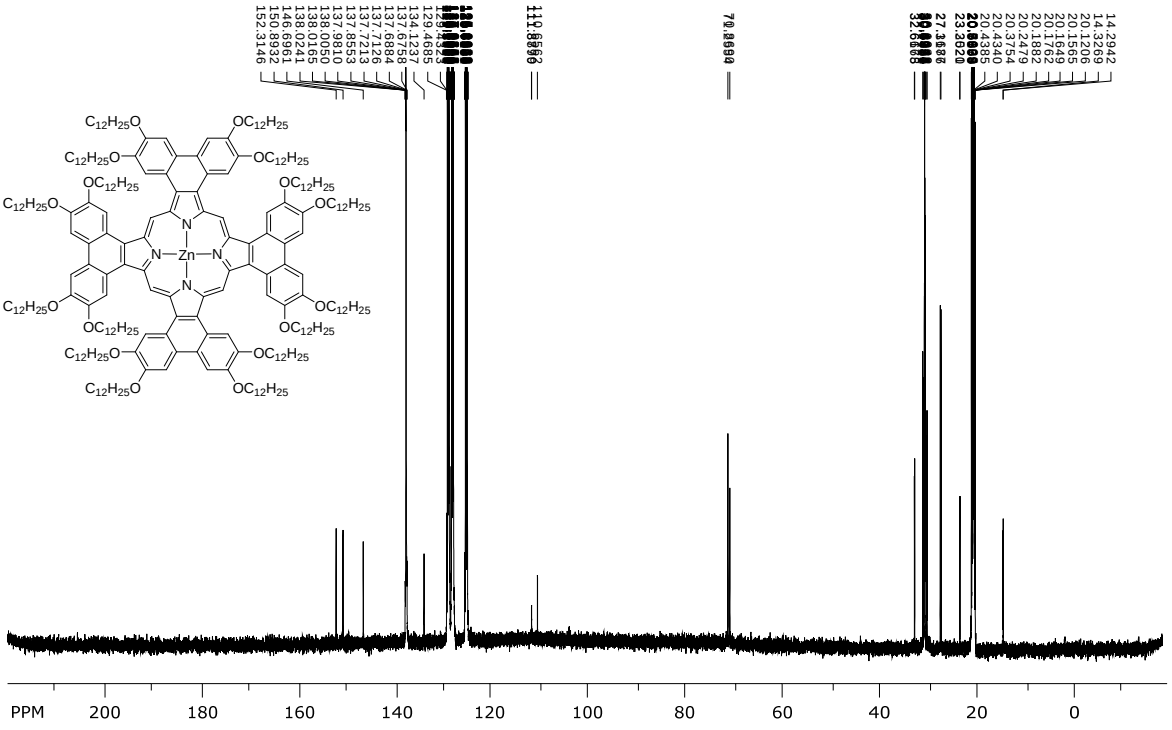


Figure S76. ^{13}C NMR spectrum of **3c**-Zn (toluene-d_8, 151 MHz, 380 K). Some signals overlap with the solvent lines.

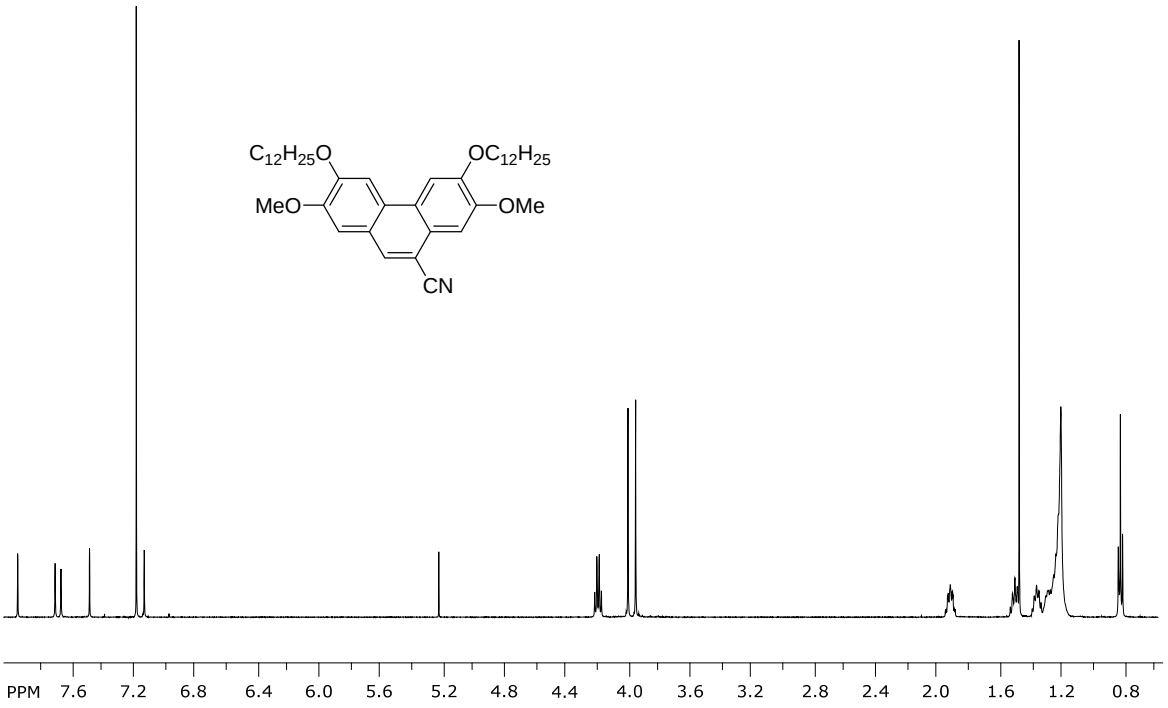


Figure S77. ^{1}H NMR spectrum of **14b** (chloroform-*d*, 500 MHz, 300 K).

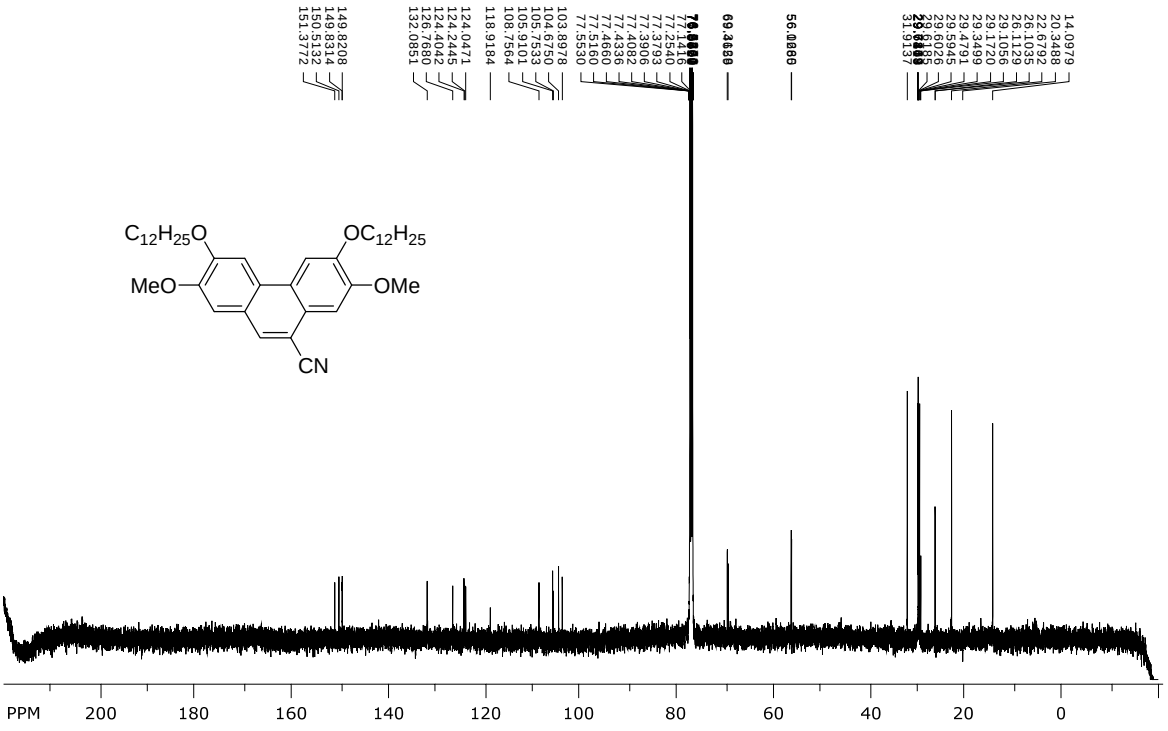


Figure S78. ^{13}C NMR spectrum of **14b** (chloroform-*d*, 125 MHz, 300 K).

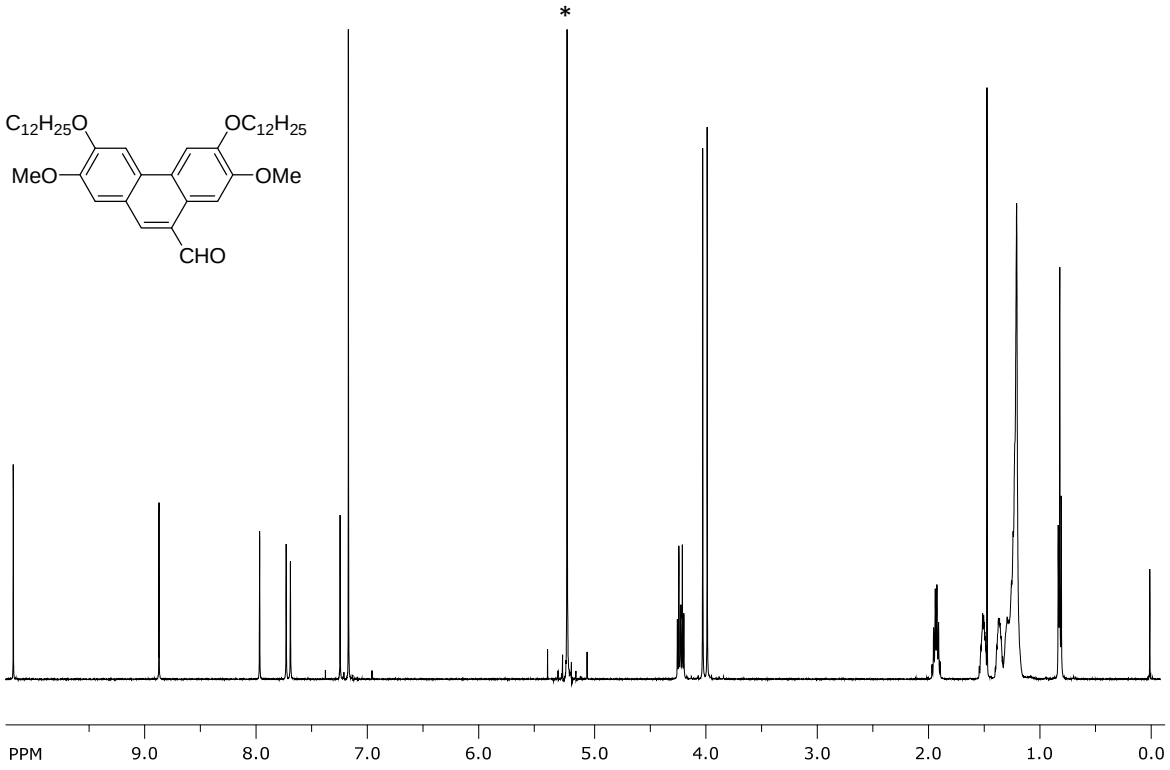


Figure S79. ^{1}H NMR spectrum of **15b** (chloroform-*d*, 500 MHz, 300 K).

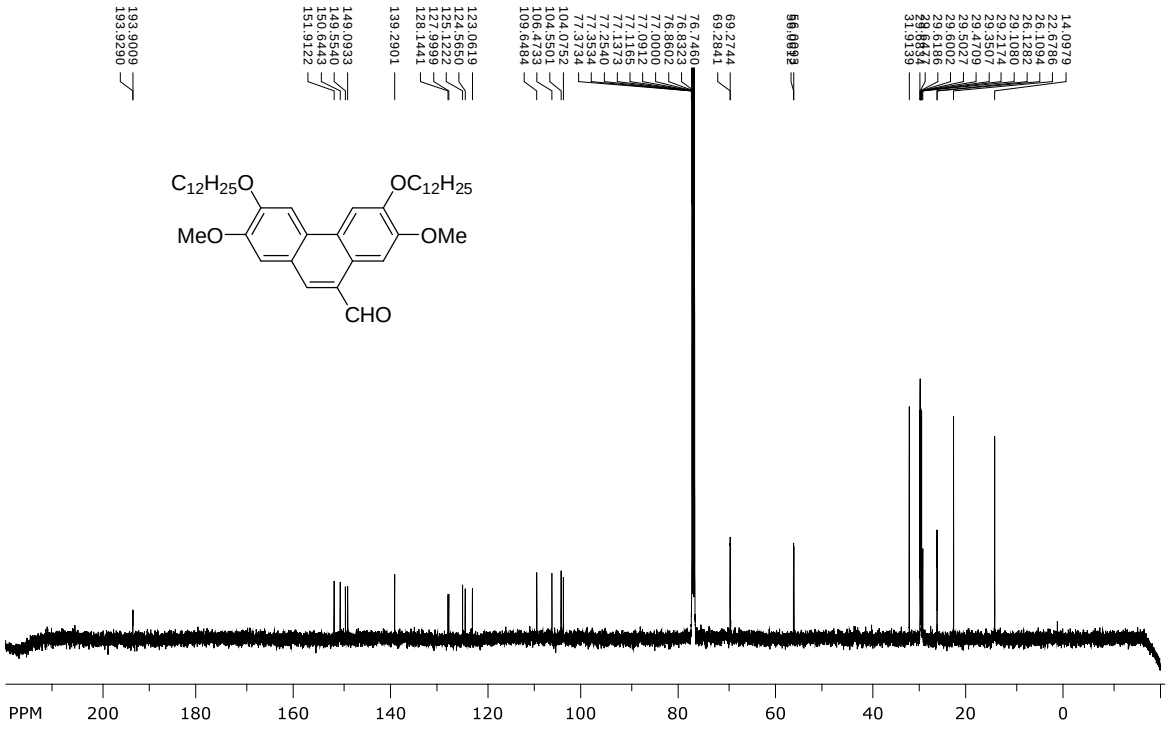


Figure S80. ^{13}C NMR spectrum of **15b** (chloroform-*d*, 125 MHz, 300 K).

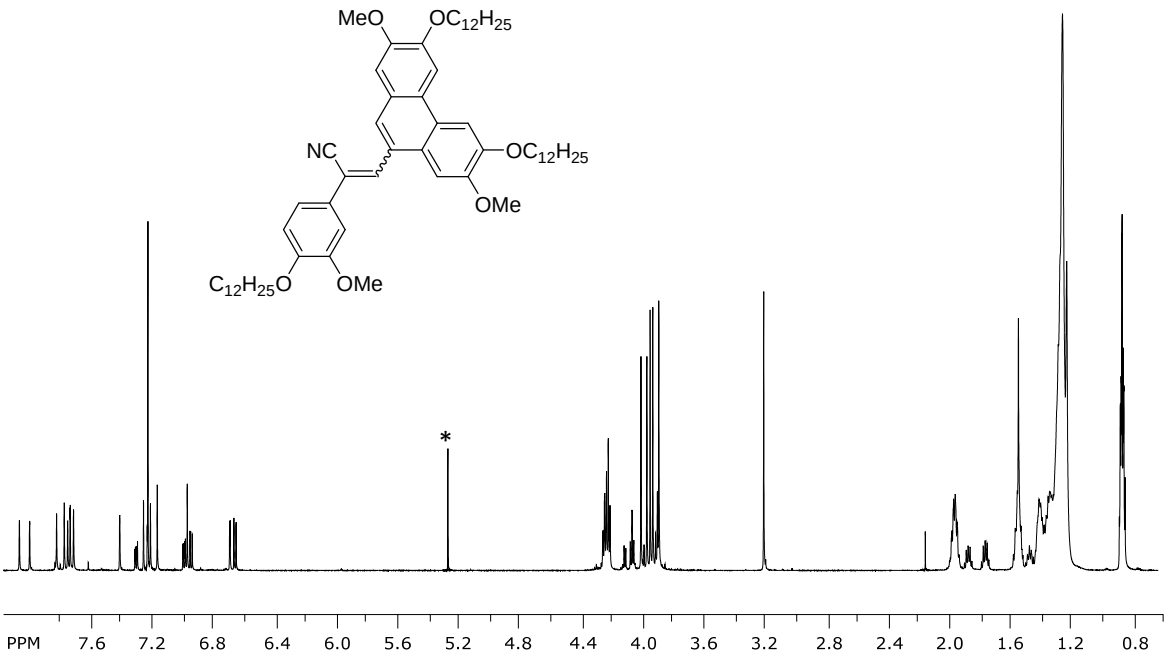


Figure S81. ^{1}H NMR spectrum of **16b** (ca. 1:1 mixture of isomers, chloroform-*d*, 600 MHz, 300 K).

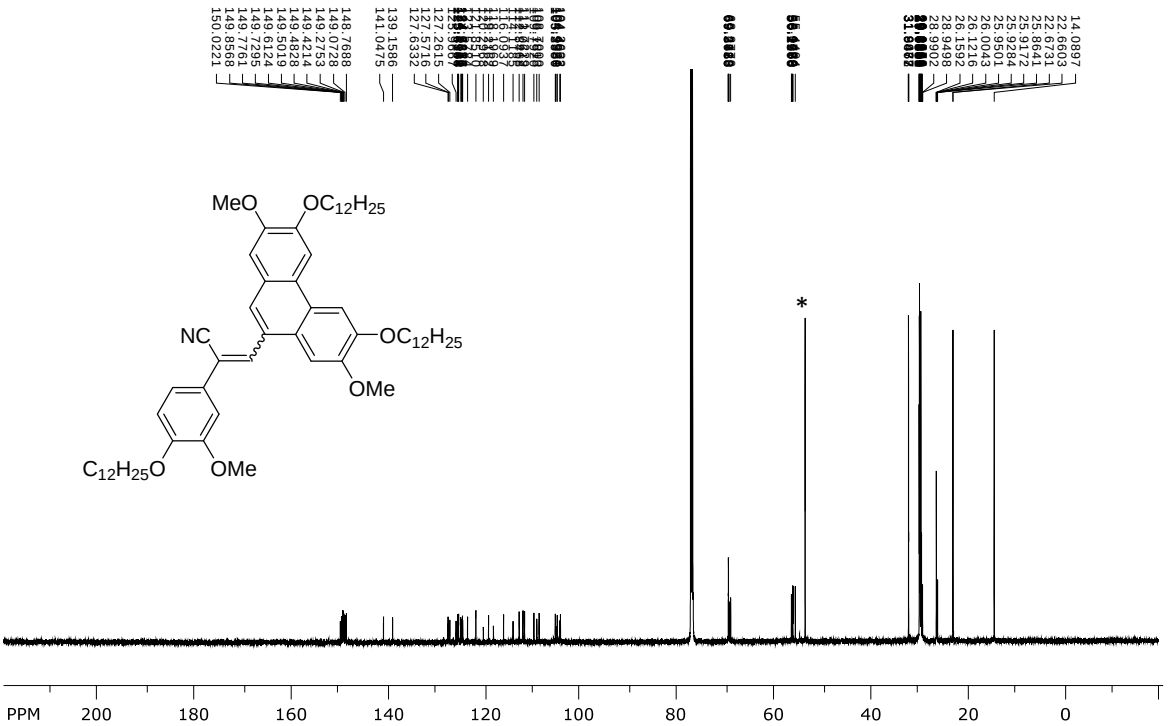


Figure S82. ^{13}C NMR spectrum of **16b** (ca. 1:1 mixture of isomers, chloroform-*d*, 151 MHz, 300 K).

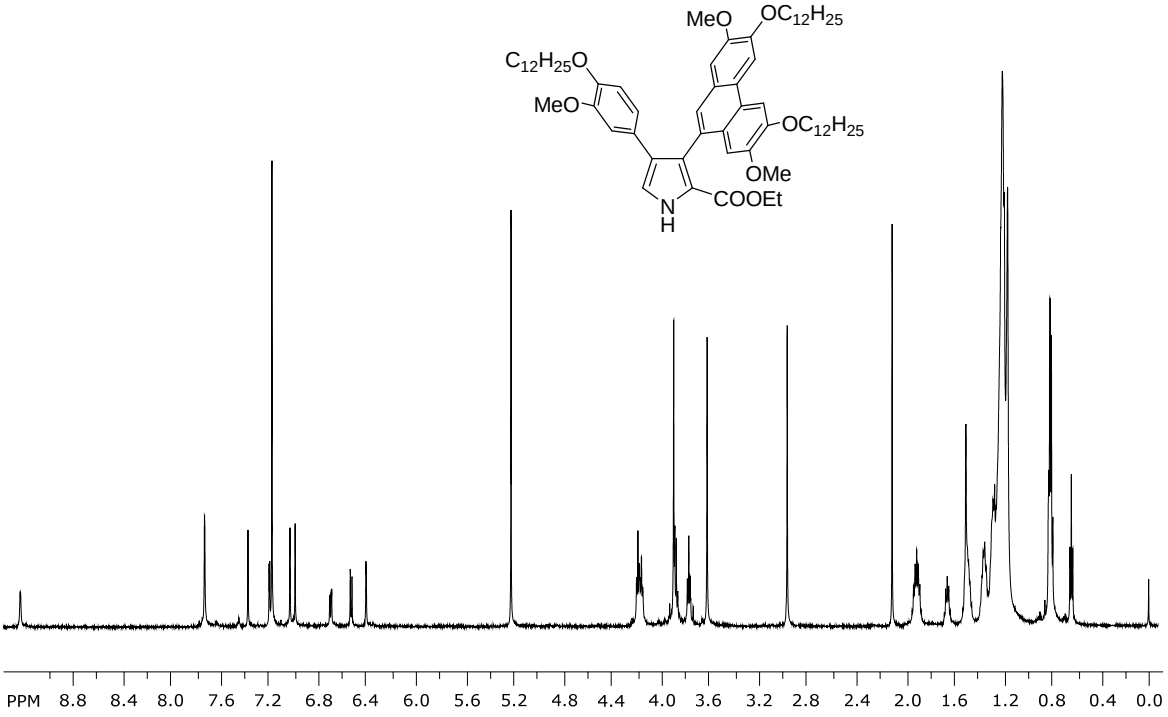


Figure S83. ^{1}H NMR spectrum of **4b** (chloroform-*d*, 600 MHz, 300 K).

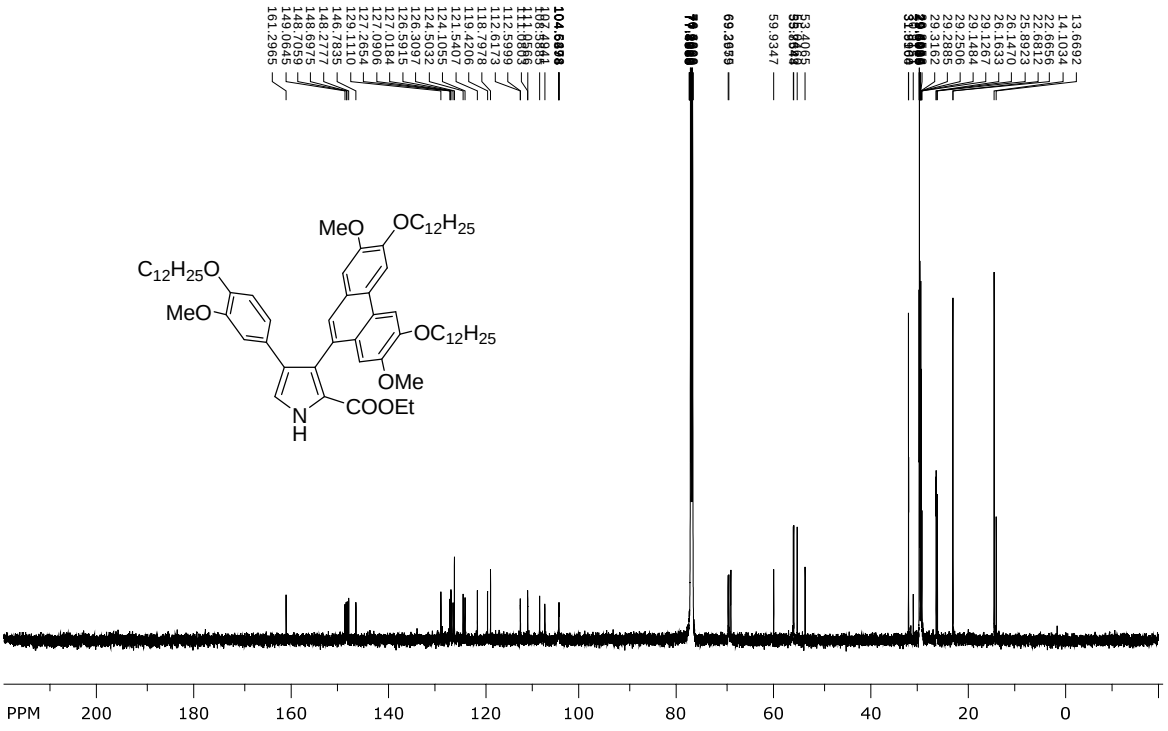


Figure S84. ^{13}C NMR spectrum of **4b** (chloroform-*d*, 151 MHz, 300 K).

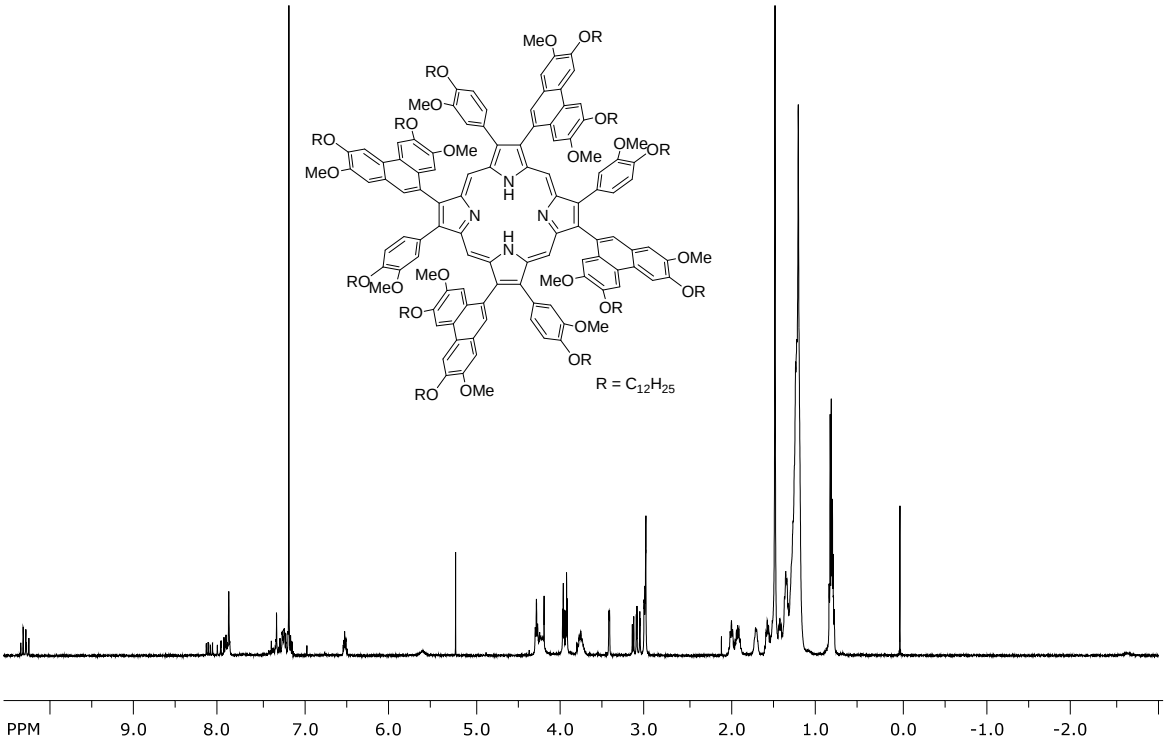


Figure S85. ^{1}H NMR spectrum of **5b**-H_2 (mixture of atropisomers, chloroform-*d*, 500 MHz, 300 K).

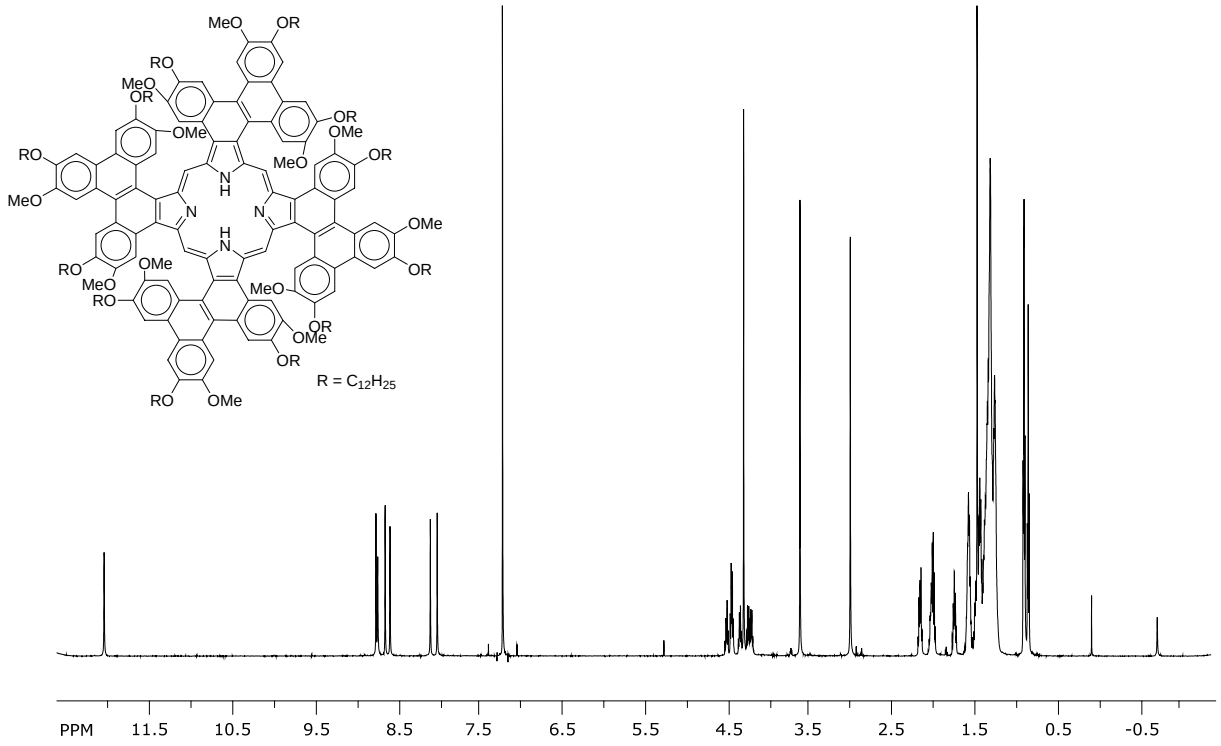


Figure S86. ^{1}H NMR spectrum of **6b**-H_2 (chloroform-*d*, 600 MHz, 325 K).

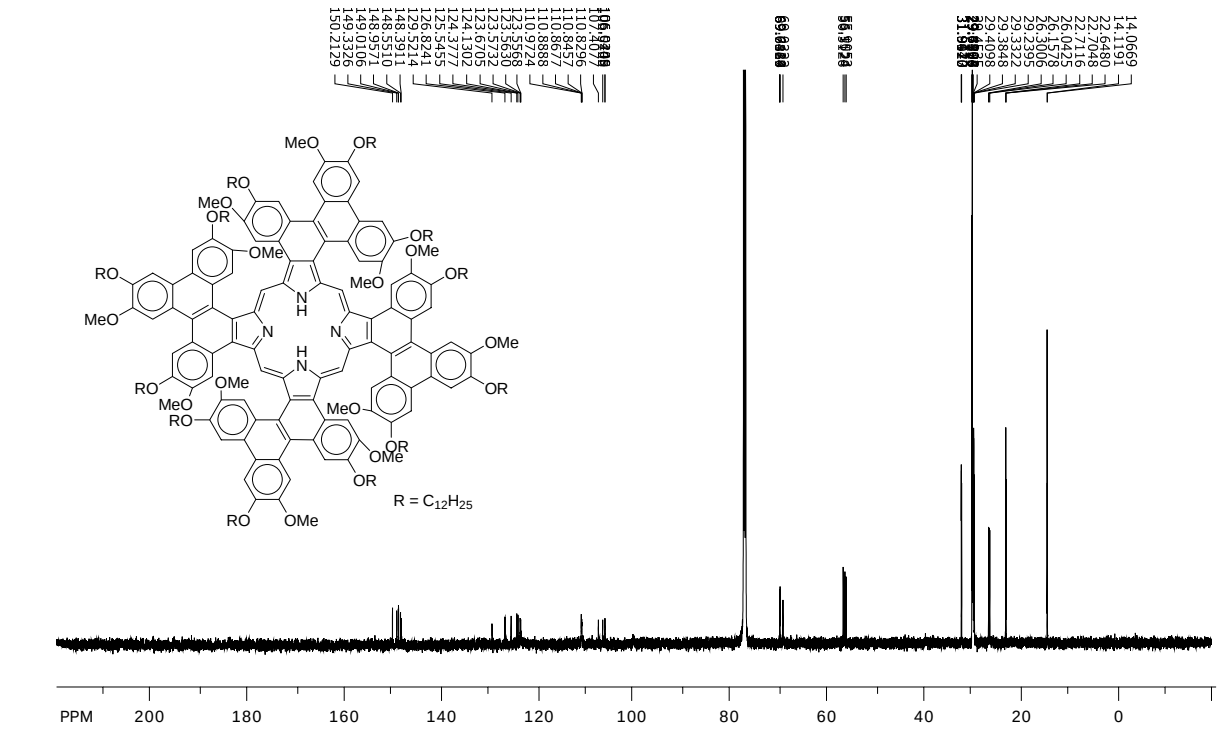


Figure S87. ^{13}C NMR spectrum of **6b**-H_2 (chloroform-*d*, 151 MHz, 300 K).

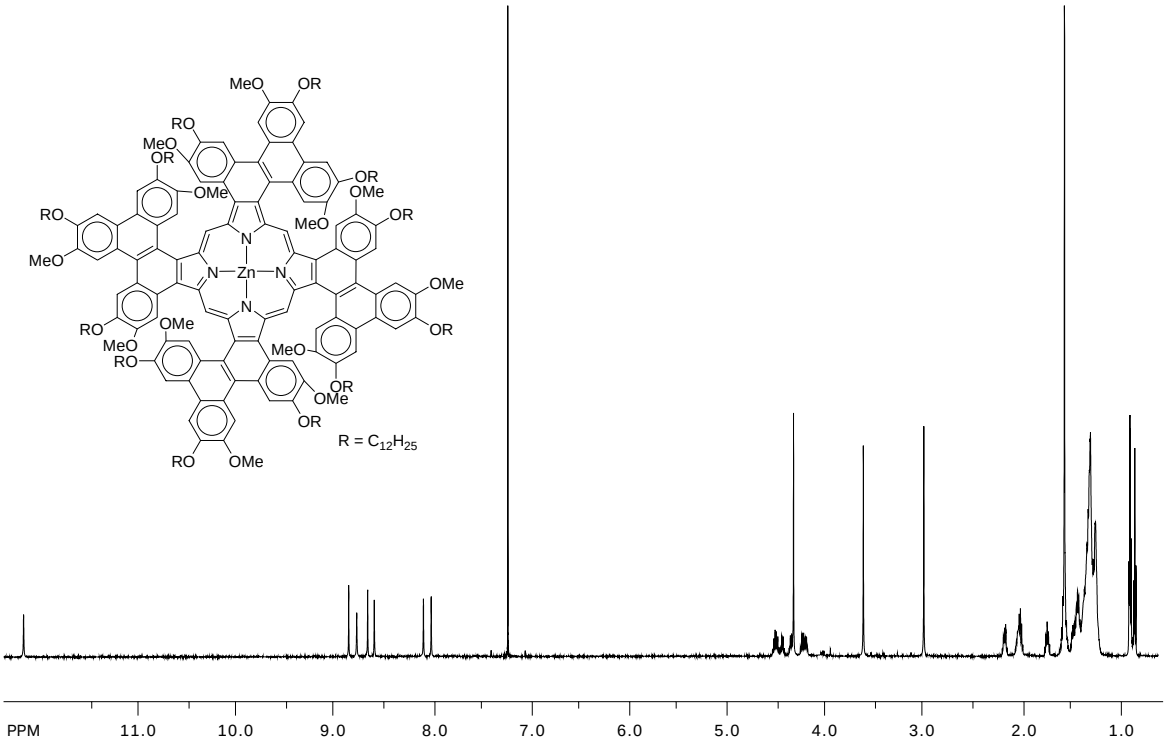


Figure S88. ^{1}H NMR spectrum of **6b**-Zn (chloroform-*d*, 600 MHz, 300 K).

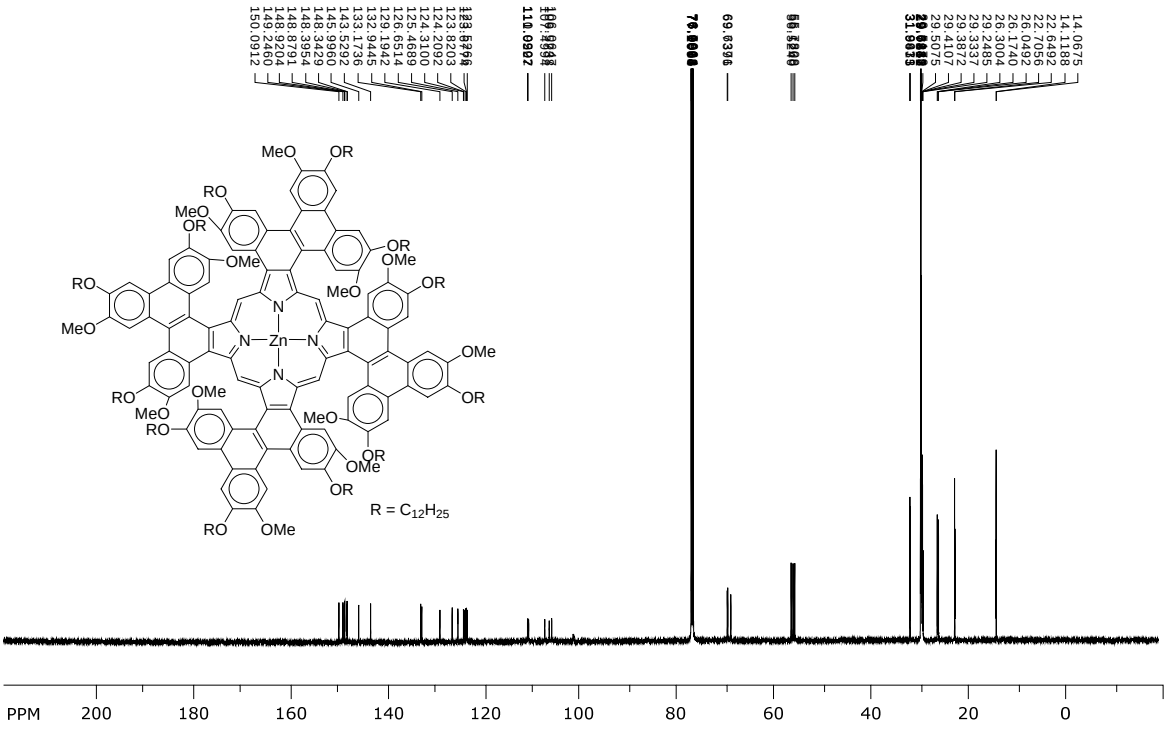


Figure S89. ^{13}C NMR spectrum of **6b**-Zn (chloroform-*d*, 151 MHz, 300 K).

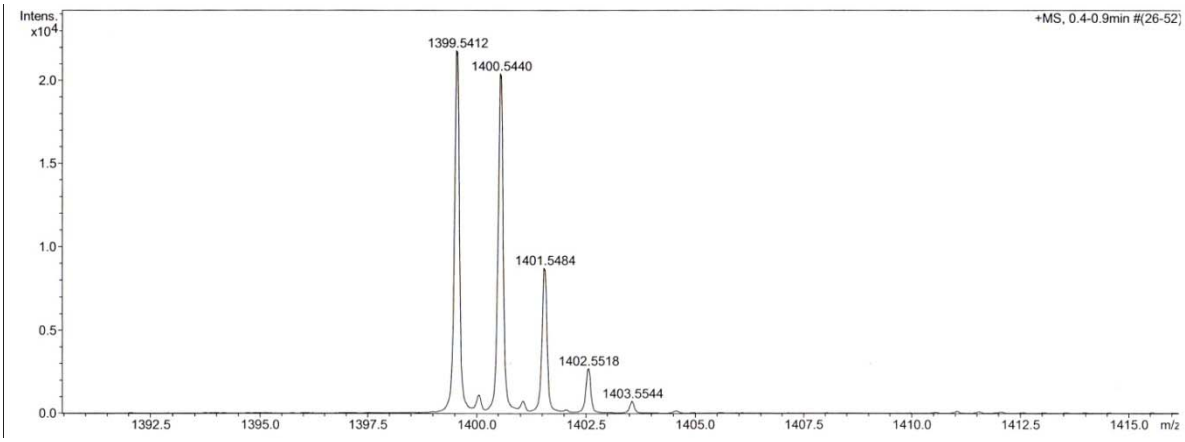


Figure S90. High resolution mass spectrum of **2a**-H_2 (ESI+).

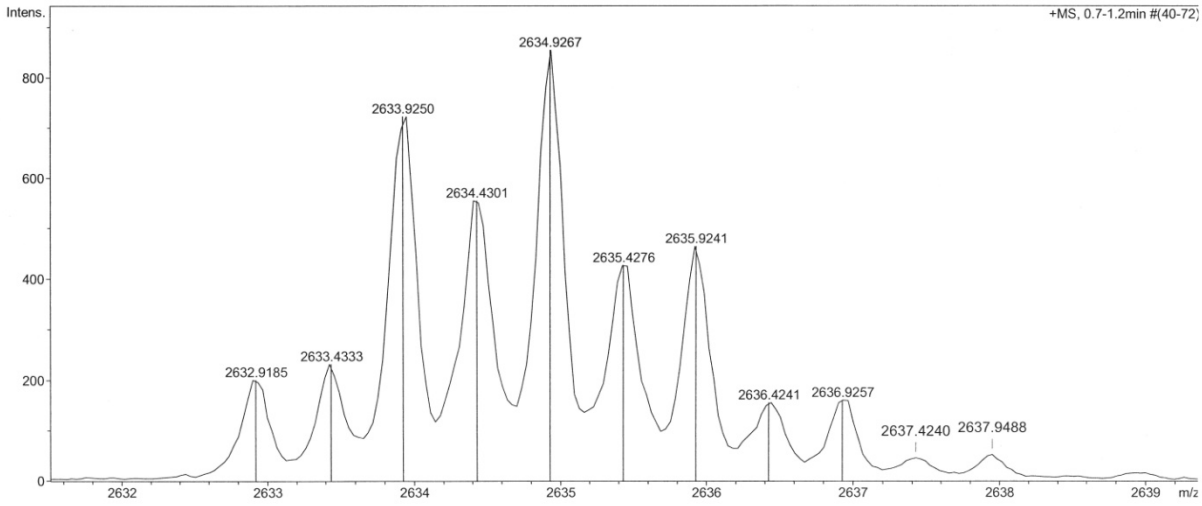


Figure S91. High resolution mass spectrum of **2b**-H_2 (ESI+).

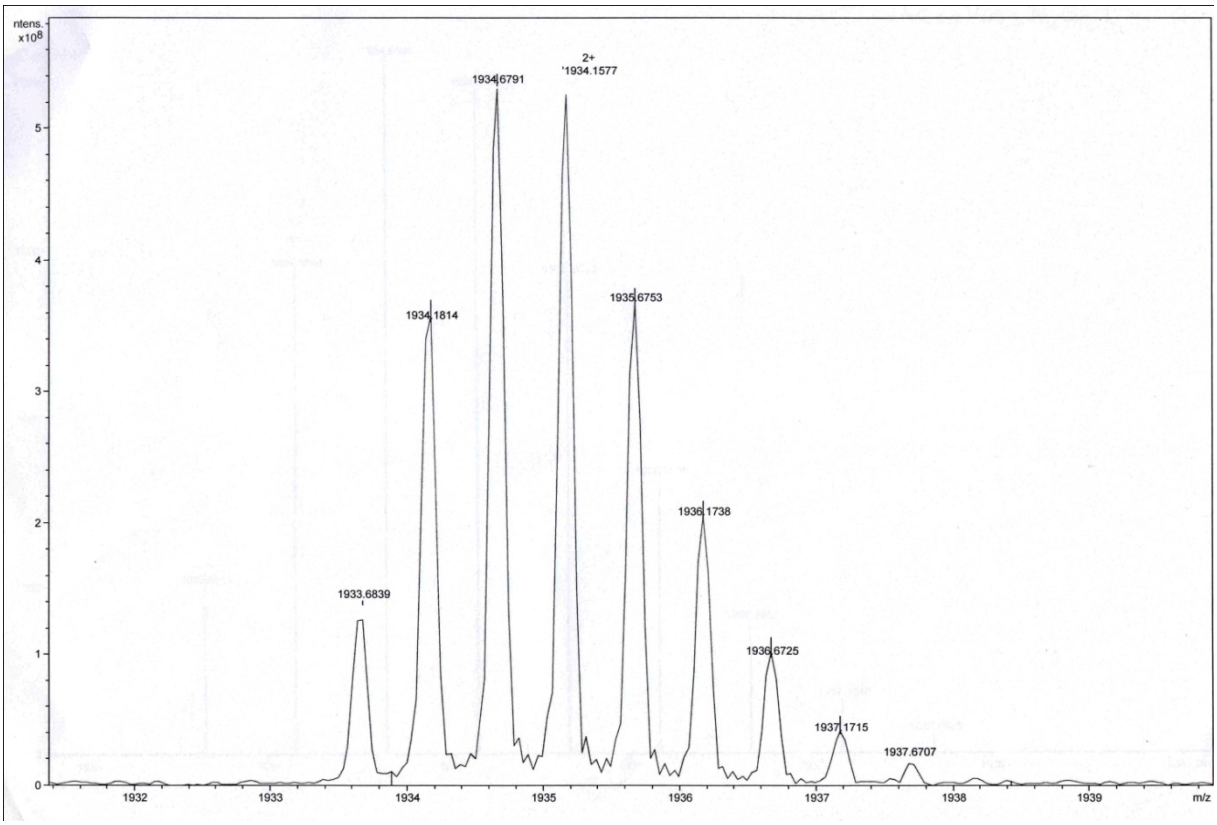


Figure S92. High resolution mass spectrum of **2c**-H_2 (ESI+).

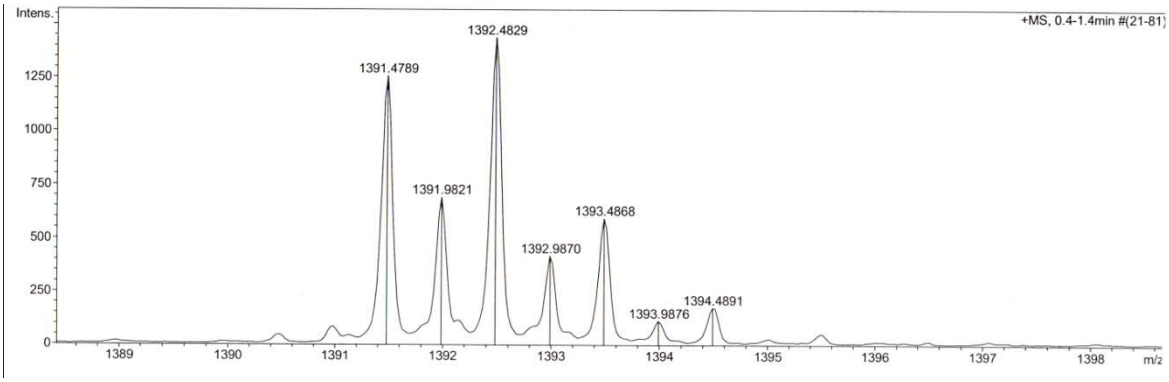


Figure S93. High resolution mass spectrum of **3a-H_2** (ESI+).

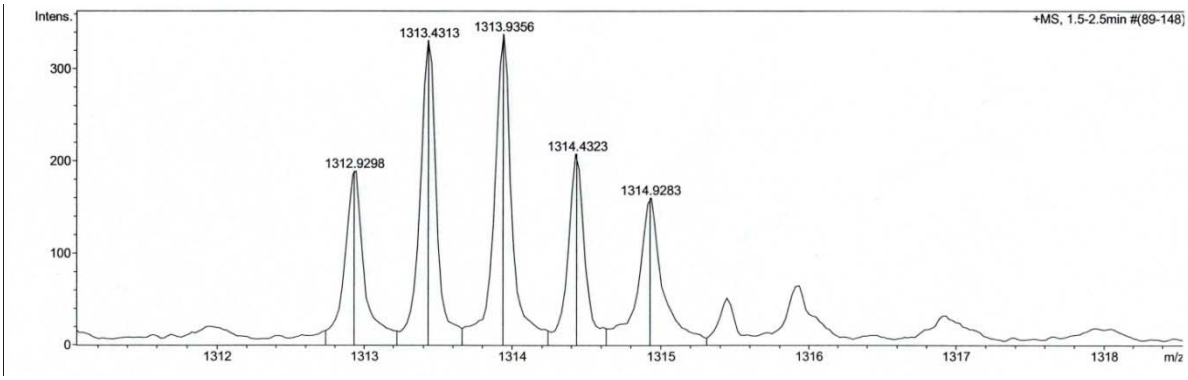


Figure S94. High resolution mass spectrum of **3b**-H_2 (ESI+).

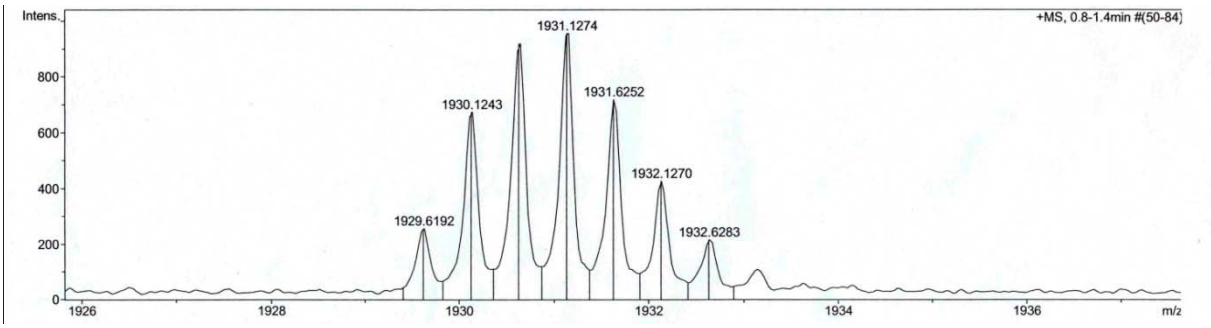


Figure S95. High resolution mass spectrum of **3c**-H_2 (ESI+).

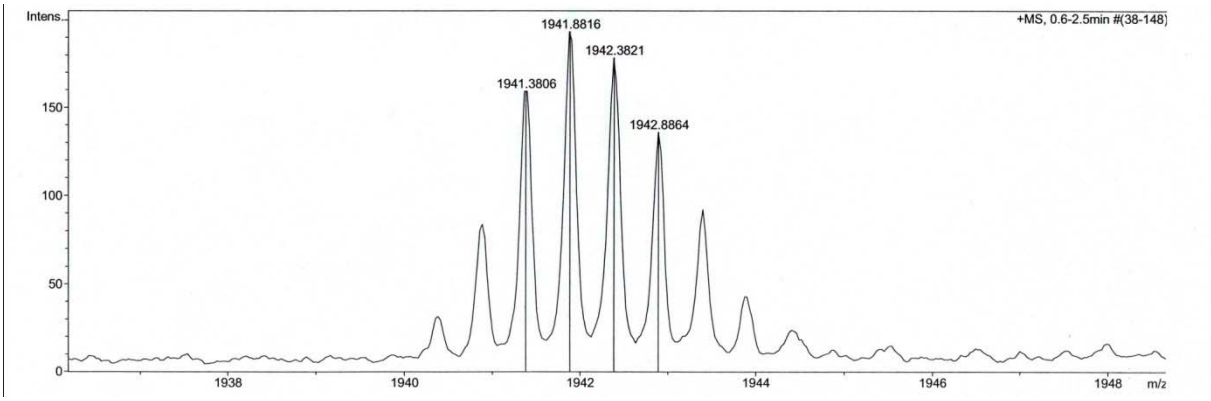


Figure S96. High resolution mass spectrum of **6b**-H_2 (ESI+). The observed peak corresponds to mixed modes of ionization (protonation and oxidation).

Table S14. Cartesian coordinates for the optimized structure of **2a**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.593747	2.277222	-0.890992
2	6	0	-7.690131	3.318413	0.069512
3	6	0	-6.668764	3.476356	1.002238
4	6	0	-5.556334	2.625793	0.995054
5	6	0	-5.443625	1.603043	0.050488
6	6	0	-6.481524	1.443912	-0.892424
7	6	0	-5.558459	-2.622234	-0.994021
8	6	0	-5.444642	-1.599552	-0.049515
9	6	0	-4.278521	-0.693903	-0.031517
10	6	0	-4.278080	0.696665	0.031946
11	6	0	-6.671435	-3.472091	-1.000663
12	6	0	-7.692252	-3.313491	-0.067446
13	6	0	-7.594729	-2.272370	0.893017
14	6	0	-6.481975	-1.439774	0.893912
15	6	0	-2.899027	1.130067	0.029545
16	7	0	-2.123709	0.000718	-0.000221
17	6	0	-2.899735	-1.128154	-0.029657
18	8	0	-8.636342	2.187412	-1.764139
19	8	0	-8.809805	4.091482	-0.008950
20	1	0	-6.727209	4.260264	1.747696
21	1	0	-6.730735	-4.255968	-1.746086
22	8	0	-8.812388	-4.085834	0.011571
23	8	0	-8.636833	-2.181901	1.766683
24	1	0	-1.109280	0.000419	-0.000371
25	6	0	2.306562	7.579735	-0.854867
26	6	0	3.329944	7.672735	0.124255
27	6	0	3.465844	6.651264	1.060158
28	6	0	2.610119	5.542601	1.037979
29	6	0	1.603005	5.431959	0.075334
30	6	0	1.468711	6.471074	-0.871050
31	6	0	-2.606566	5.544571	-1.038435
32	6	0	-1.599516	5.433048	-0.075823
33	6	0	-0.684904	4.275304	-0.043106
34	6	0	0.687607	4.274844	0.042408
35	6	0	-3.461509	6.653844	-1.060409
36	6	0	-3.324866	7.675059	-0.124333
37	6	0	-2.301544	7.581156	0.854763
38	6	0	-1.464483	6.471899	0.870746
39	6	0	1.085681	2.858420	0.038935
40	7	0	0.000618	2.037825	-0.000482
41	6	0	-1.083909	2.859141	-0.039801
42	8	0	2.237199	8.622473	-1.731017
43	8	0	4.110274	8.789828	0.059044
44	1	0	4.235724	6.707319	1.820489
45	1	0	-4.231361	6.710578	-1.820717
46	8	0	-4.104383	8.792708	-0.058910
47	8	0	-2.231430	8.623691	1.731094
48	6	0	2.421140	2.436296	0.007248
49	6	0	7.593396	-2.277354	-0.892916
50	6	0	7.690084	-3.318435	0.067677
51	6	0	6.669033	-3.476243	1.000771
52	6	0	5.556621	-2.625655	0.993869
53	6	0	5.443616	-1.603010	0.049227
54	6	0	6.481194	-1.444015	-0.894060
55	6	0	5.558166	2.622268	-0.995474
56	6	0	5.444636	1.599577	-0.050940
57	6	0	4.278509	0.693946	-0.032571
58	6	0	4.278075	-0.696619	0.030965
59	6	0	6.671164	3.472095	-1.002479
60	6	0	7.692291	3.313450	-0.069609
61	6	0	7.595063	2.272317	0.890870
62	6	0	6.482284	1.439757	0.892134
63	6	0	2.899023	-1.130016	0.028947
64	7	0	2.123701	-0.000667	-0.000684
65	6	0	2.899723	1.128202	-0.030375
66	8	0	8.635688	-2.187678	-1.766439
67	8	0	8.809708	-4.091547	-0.011081
68	1	0	6.727710	-4.260068	1.746298
69	1	0	6.730238	4.255979	-1.747912
70	8	0	8.812480	4.085754	0.009040
71	8	0	8.637466	2.181799	1.764175
72	1	0	1.109272	-0.000363	-0.000581
73	6	0	2.419624	-2.437816	-0.008499
74	6	0	-2.306689	-7.579763	-0.853933
75	6	0	-3.329891	-7.672705	0.125381
76	6	0	-3.465635	-6.651167	1.061234
77	6	0	-2.609926	-5.542496	1.038819
78	6	0	-1.602990	-5.431911	0.075982
79	6	0	-1.468858	-6.471092	-0.870352
80	6	0	2.606346	-5.544608	-1.038630
81	6	0	1.599491	-5.433005	-0.075824
82	6	0	0.684887	-4.275257	-0.043004
83	6	0	-0.687606	-4.274793	0.042800
84	6	0	3.461282	-6.653885	-1.060688
85	6	0	3.324824	-7.675025	-0.124505
86	6	0	2.301700	-7.581042	0.854790
87	6	0	1.464648	-6.471780	0.870855
88	6	0	-1.085681	-2.858370	0.039328
89	7	0	-0.000627	-2.037778	-0.000373
90	6	0	1.083891	-2.859095	-0.039875
91	8	0	-2.237471	-8.622566	-1.730017
92	8	0	-4.110217	-8.789814	0.060393
93	1	0	-4.235377	-6.707179	1.821708
94	1	0	4.230982	-6.710681	-1.821145
95	8	0	4.104352	-8.792671	-0.059148
96	8	0	2.231760	-8.623507	1.731219
97	6	0	-2.421145	-2.436246	0.007915
98	6	0	-2.419636	2.437865	-0.008098
99	1	0	3.176818	3.211124	0.009649
100	1	0	3.174830	-3.213102	-0.010954
101	1	0	-3.176824	-3.211072	0.010522
102	1	0	-3.174842	3.213152	-0.010431
103	6	0	-1.190768	-8.612970	-2.687811
104	6	0	-1.184624	8.613057	2.688765
105	6	0	8.621226	1.121315	2.707012
106	6	0	8.619990	-1.127328	-2.709433
107	6	0	-8.620953	1.126941	-2.707002
108	6	0	-8.620288	-1.121448	2.709549
109	6	0	1.190332	8.612809	-2.688631
110	6	0	1.185143	-8.612797	2.689096
111	1	0	-0.204140	-8.581446	-2.208678
112	1	0	-1.278837	-7.764011	-3.378371
113	1	0	-1.291373	-9.543037	-3.249333
114	1	0	-0.198073	8.580966	2.209509
115	1	0	-1.273225	7.763953	3.379079
116	1	0	-1.284496	9.543028	3.250576
117	1	0	8.585359	0.141953	2.213528
118	1	0	7.771981	1.204482	3.397705
119	1	0	9.551147	1.209079	3.270727
120	1	0	8.584953	-0.147865	-2.216090
121	1	0	7.770518	-1.209985	-3.399907
122	1	0	9.549711	-1.215849	-3.273357
123	1	0	-8.585704	0.147542	-2.213546
124	1	0	-7.771737	1.209535	-3.397799
125	1	0	-9.550884	1.215358	-3.270598
126	1	0	-8.584636	-0.142068	2.216085
127	1	0	-7.770787	-1.204609	3.399927
128	1	0	-9.550000	-1.209264	3.273600
129	1	0	0.203785	8.581341	-2.209326
130	1	0	1.278270	7.763789	-3.379132
131	1	0	1.290853	9.542826	-3.250249
132	1	0	0.198498	-8.580741	2.210032
133	1	0	1.273882	-7.763640	3.379326
134	1	0	1.285125	-9.542724	3.250959
135	6	0	5.141860	-8.930462	-1.013808
136	6	0	-5.147963	-8.926416	1.014968
137	6	0	-8.952870	-5.144560	-0.920295
138	6	0	-8.949002	5.150447	0.922839
139	6	0	-5.142070	8.930431	-1.013385
140	6	0	5.148187	8.926490	1.013430
141	6	0	8.952690	5.144481	-0.922865
142	6	0	8.949183	-5.150421	0.920771
143	1	0	5.638235	-9.874615	-0.784327
144	1	0	4.750109	-8.969217	-2.038840
145	1	0	5.870828	-8.112155	-0.944057
146	1	0	-5.645101	-9.870228	0.785737
147	1	0	-4.756374	-8.965161	2.040063
148	1	0	-5.876227	-8.107514	0.944850
149	1	0	-9.898432	-5.632637	-0.679664
150	1	0	-8.990576	-4.775067	-1.953457
151	1	0	-8.136546	-5.873589	-0.833547
152	1	0	-9.894294	5.639237	0.682594
153	1	0	-8.986506	4.781126	1.956071
154	1	0	-8.132139	5.878812	0.835597
155	1	0	-5.638398	9.874603	-0.783883
156	1	0	-4.750511	8.969107	-2.038494
157	1	0	-5.871029	8.112132	-0.943437
158	1	0	5.645299	9.870276	0.784038
159	1	0	4.756774	8.965323	2.038590
160	1	0	5.876427	8.107572	0.943252
161	1	0	9.898358	5.632513	-0.682556
162	1	0	8.990023	4.774996	-1.956043
163	1	0	8.136429	5.873548	-0.835829
164	1	0	9.894371	-5.639277	0.680248
165	1	0	8.987062	-4.780994	1.953950
166	1	0	8.132258	-5.878759	0.833887
167	1	0	-6.398049	0.654039	-1.627357
168	1	0	-6.397640	-0.649960	1.628810
169	1	0	0.692041	6.390457	-1.620296
170	1	0	-0.687860	6.390611	1.619966
171	1	0	6.397482	-0.654221	-1.629053
172	1	0	6.398180	0.649940	1.627054
173	1	0	-0.692330	-6.390521	-1.619750
174	1	0	0.688178	-6.390429	1.620227
175	1	0	-4.783676	2.757198	1.744905
176	1	0	-4.786249	-2.754133	-1.744247
177	1	0	2.723411	4.771024	1.792095
178	1	0	-2.720405	4.773214	-1.792694
179	1	0	4.784211	-2.756963	1.743993
180	1	0	4.785713	2.754190	-1.745445
181	1	0	-2.723088	-4.770869	1.792903
182	1	0	2.720035	-4.773311	-1.792973

Table S15. Cartesian coordinates for the optimized structure of **2a**-Zn (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.732892	-4.161941	0.858345
2	6	0	-6.560824	-5.175434	-0.120606
3	6	0	-5.534172	-5.049484	-1.052342
4	6	0	-4.677253	-3.942071	-1.026669
5	6	0	-4.829666	-2.939705	-0.065497
6	6	0	-5.872624	-3.070446	0.876684
7	6	0	-6.021894	1.112038	1.020011
8	6	0	-5.653326	0.155074	0.070970
9	6	0	-4.296700	-0.426800	0.046303
10	6	0	-3.941743	-1.760493	-0.031702
11	6	0	-7.314432	1.651205	1.033198
12	6	0	-8.264867	1.240885	0.102476
13	6	0	-7.908589	0.262977	-0.862702
14	6	0	-6.620584	-0.258764	-0.870320
15	6	0	-2.486492	-1.798261	-0.025926
16	7	0	-1.978667	-0.524846	0.011563
17	6	0	-3.051849	0.328510	0.046141
18	8	0	-7.761830	-4.358783	1.731037
19	8	0	-7.444796	-6.212023	-0.059433
20	1	0	-5.389833	-5.809606	-1.810762
21	1	0	-7.569044	2.391641	1.782029
22	8	0	-9.546035	1.702404	0.029730
23	8	0	-8.897099	-0.086632	-1.734354
24	6	0	4.161789	-6.732493	0.861513
25	6	0	5.175441	-6.560839	-0.117353
26	6	0	5.049648	-5.534616	-1.049576
27	6	0	3.942239	-4.677664	-1.024452
28	6	0	2.939740	-4.829683	-0.063380
29	6	0	3.070270	-5.872228	0.879274
30	6	0	-1.112345	-6.021589	1.021004
31	6	0	-0.155050	-5.653336	0.072169
32	6	0	0.426766	-4.296679	0.047319
33	6	0	1.760498	-3.941714	-0.030198
34	6	0	-1.651536	-7.314116	1.034403
35	6	0	-1.240953	-8.264815	0.104073
36	6	0	-0.262672	-7.908865	-0.860851
37	6	0	0.259144	-6.620890	-0.868647
38	6	0	1.798300	-2.486554	-0.024637
39	7	0	0.524825	-1.978633	0.012091
40	6	0	-0.328536	-3.051902	0.046416
41	8	0	4.358502	-7.761071	1.734650
42	8	0	6.211999	-7.444822	-0.055648
43	1	0	5.809877	-5.390651	-1.807957
44	1	0	-2.392217	-7.568503	1.783072
45	8	0	-1.702491	-9.545990	0.031530
46	8	0	0.087220	-8.897659	-1.732064
47	6	0	2.963482	-1.720265	0.010518
48	6	0	6.732596	4.161841	0.861123
49	6	0	6.560867	5.175434	-0.117790
50	6	0	5.534538	5.049575	-1.049891
51	6	0	4.677609	3.942157	-1.024623
52	6	0	4.829689	2.939698	-0.063499
53	6	0	5.872323	3.070346	0.879058
54	6	0	6.021539	-1.112161	1.022011
55	6	0	5.653302	-0.155099	0.072940
56	6	0	4.296686	0.426779	0.047858
57	6	0	3.941757	1.760480	-0.030131
58	6	0	7.314070	-1.651335	1.035591
59	6	0	8.264829	-1.240925	0.105241
60	6	0	7.908887	-0.262917	-0.859962
61	6	0	6.620890	0.258834	-0.867973
62	6	0	2.486503	1.798249	-0.024848
63	7	0	1.978665	0.524830	0.012321
64	6	0	3.051835	-0.328532	0.047172
65	8	0	7.761240	4.358597	1.734182
66	8	0	7.444822	6.212013	-0.056208
67	1	0	5.390457	5.809770	-1.808287
68	1	0	7.568418	-2.391850	1.784435
69	8	0	9.546017	-1.702445	0.032883
70	8	0	8.897700	0.086770	-1.731242
71	6	0	1.720258	2.963455	0.010095
72	6	0	-4.162043	6.732392	0.860958
73	6	0	-5.175372	6.560889	-0.118266
74	6	0	-5.049289	5.534793	-1.050589
75	6	0	-3.941898	4.677822	-1.025219
76	6	0	-2.939714	4.829691	-0.063794
77	6	0	-3.070541	5.872111	0.878959
78	6	0	1.111989	6.021450	1.022150
79	6	0	0.155020	5.653316	0.072937
80	6	0	-0.426784	4.296659	0.047709
81	6	0	-1.760490	3.941708	-0.030336
82	6	0	1.651170	7.313977	1.035900
83	6	0	1.240896	8.264799	0.105556
84	6	0	0.262946	7.908970	-0.859747
85	6	0	-0.258858	6.620992	-0.867891
86	6	0	-1.798296	2.486545	-0.024969
87	7	0	-0.524837	1.978617	0.012137
88	6	0	0.328518	3.051882	0.046895
89	8	0	-4.359020	7.760858	1.734167
90	8	0	-6.211940	7.444879	-0.056776
91	1	0	-5.809271	5.390940	-1.809238
92	1	0	2.391596	7.568273	1.784853
93	8	0	1.702456	9.545981	0.033338
94	8	0	-0.086653	8.897877	-1.730950
95	6	0	-2.963490	1.720247	0.009689
96	6	0	-1.720262	-2.963472	0.009143
97	1	0	3.898802	-2.264613	0.008903
98	1	0	2.264679	3.898732	0.008277
99	1	0	-3.898812	2.264589	0.007817
100	1	0	-2.264683	-3.898748	0.007019
101	6	0	-3.351034	8.009109	2.701486
102	6	0	1.101151	-8.613267	-2.683145
103	6	0	8.613565	1.101009	-2.682073
104	6	0	8.010233	3.349947	2.700626
105	6	0	-8.011222	-3.350177	2.697424
106	6	0	-8.612627	-1.100760	-2.685205
107	6	0	3.350160	-8.009516	2.701557
108	6	0	-1.100317	8.613627	-2.682366
109	1	0	-2.383972	8.228206	2.231631
110	1	0	-3.229992	7.161466	3.388471
111	1	0	-3.686109	8.881523	3.264471
112	1	0	2.042293	-8.326201	-2.197618
113	1	0	0.798223	-7.815578	-3.373906
114	1	0	1.250341	-9.536363	-3.245269
115	1	0	8.326357	2.041985	-2.196313
116	1	0	7.816070	0.798308	-3.373161
117	1	0	9.536812	1.250380	-3.243900
118	1	0	8.228885	2.383191	2.229947
119	1	0	7.163153	3.228496	3.388239
120	1	0	8.883123	3.684607	3.263120
121	1	0	-8.229687	-2.383401	2.226700
122	1	0	-7.164424	-3.228752	3.385390
123	1	0	-8.884339	-3.684867	3.259548
124	1	0	-8.325585	-2.041791	-2.199453
125	1	0	-7.814893	-0.797975	-3.375980
126	1	0	-9.535679	-1.250070	-3.247369
127	1	0	2.383279	-8.228549	2.231303
128	1	0	3.228851	-7.161995	3.388645
129	1	0	3.685051	-8.882021	3.264509
130	1	0	-2.041594	8.326491	-2.197146
131	1	0	-0.797189	7.816042	-3.373158
132	1	0	-1.249340	9.536808	-3.244393
133	6	0	2.684092	9.948623	0.972706
134	6	0	-7.251472	7.310869	-1.010534
135	6	0	-9.949112	2.684010	0.968939
136	6	0	-7.310723	-7.251305	-1.013447
137	6	0	-2.684520	-9.948716	0.970458
138	6	0	7.251927	-7.310559	-1.008943
139	6	0	9.948806	-2.684060	0.972212
140	6	0	7.311020	7.251433	-1.010120
141	1	0	2.911934	10.990173	0.741172
142	1	0	2.313046	9.881337	2.003867
143	1	0	3.600264	9.349723	0.885643
144	1	0	-7.969497	8.100788	-0.785092
145	1	0	-6.882380	7.441340	-2.036319
146	1	0	-7.750420	6.335729	-0.934491
147	1	0	-10.990601	2.911748	0.737025
148	1	0	-9.882169	2.312992	2.000132
149	1	0	-9.350275	3.600246	0.882086
150	1	0	-8.101073	-7.969062	-0.788664
151	1	0	-7.440474	-6.881822	-2.039180
152	1	0	-6.335842	-7.750712	-0.937040
153	1	0	-2.912337	-10.990215	0.738670
154	1	0	-2.313866	-9.881617	2.001772
155	1	0	-3.600615	-9.349740	0.883132
156	1	0	7.969931	-8.100445	-0.783318
157	1	0	6.883285	-7.440906	-2.034906
158	1	0	7.750741	-6.335381	-0.932533
159	1	0	10.990396	-2.911722	0.740678
160	1	0	9.881449	-2.313078	2.003389
161	1	0	9.350061	-3.600331	0.885099
162	1	0	8.101270	7.969185	-0.784969
163	1	0	7.441127	6.882101	-2.035862
164	1	0	6.336094	7.750785	-0.933957
165	1	0	-5.994862	-2.296343	1.622928
166	1	0	-6.340832	-0.998928	-1.608383
167	1	0	2.295949	-5.994173	1.625339
168	1	0	0.999630	-6.341385	-1.606483
169	1	0	5.994303	2.296163	1.625262
170	1	0	6.341398	0.999079	-1.606053
171	1	0	-2.296466	5.993946	1.625297
172	1	0	-0.999092	6.341580	-1.606016
173	1	0	-3.898350	-3.857831	-1.776936
174	1	0	-5.307047	1.432437	1.770223
175	1	0	3.858131	-3.899060	-1.775043
176	1	0	-1.432963	-5.306527	1.770911
177	1	0	3.898970	3.857994	-1.775173
178	1	0	5.306430	-1.432630	1.771944
179	1	0	-3.857553	3.899327	-1.775896
180	1	0	1.432351	5.306292	1.772075
181	30	0	0.000005	-0.000005	0.016260

Table S16. Cartesian coordinates for the optimized structure of **3a**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.482834	-3.550307	-1.713694
2	6	0	7.723823	-2.847984	-1.756415
3	6	0	7.731825	-1.475308	-1.607423
4	6	0	6.547562	-0.730236	-1.370411
5	6	0	5.328416	-1.447492	-1.218816
6	6	0	5.323579	-2.849206	-1.445719
7	6	0	6.547631	0.729554	-1.370443
8	6	0	5.328552	1.446933	-1.218886
9	6	0	4.149937	0.701872	-0.863441
10	6	0	4.149872	-0.702302	-0.863410
11	6	0	7.731967	1.474501	-1.607483
12	6	0	7.724096	2.847170	-1.756550
13	6	0	6.483172	3.549610	-1.713878
14	6	0	5.323850	2.848635	-1.445867
15	6	0	2.834402	-1.138341	-0.438891
16	7	0	2.084625	-0.000108	-0.287647
17	6	0	2.834509	1.138049	-0.438936
18	8	0	6.559484	-4.883870	-1.963695
19	8	0	8.819885	-3.621862	-1.985448
20	1	0	8.675588	-0.957302	-1.697637
21	1	0	8.675680	0.956401	-1.697660
22	8	0	8.820231	3.620933	-1.985624
23	8	0	6.559944	4.883149	-1.963970
24	1	0	1.114172	-0.000056	0.007029
25	6	0	-3.547063	-6.421985	1.723242
26	6	0	-2.846466	-7.662561	1.805132
27	6	0	-1.475199	-7.677248	1.652660
28	6	0	-0.728732	-6.501675	1.374017
29	6	0	-1.444773	-5.284945	1.178039
30	6	0	-2.847491	-5.273672	1.411661
31	6	0	0.728040	-6.501747	1.374066
32	6	0	1.444219	-5.285090	1.178136
33	6	0	0.695522	-4.125630	0.781301
34	6	0	-0.695934	-4.125563	0.781259
35	6	0	1.474365	-7.677398	1.652761
36	6	0	2.845622	-7.662855	1.805331
37	6	0	3.546352	-6.422353	1.723493
38	6	0	2.846922	-5.273966	1.411864
39	6	0	-1.093946	-2.790561	0.309928
40	7	0	-0.000089	-2.004933	0.111949
41	6	0	1.093683	-2.790668	0.309972
42	8	0	-4.880435	-6.488899	1.985181
43	8	0	-3.622224	-8.749605	2.074428
44	1	0	-0.957545	-8.617853	1.774029
45	1	0	0.956603	-8.617949	1.774094
46	8	0	3.621247	-8.749981	2.074687
47	8	0	4.879698	-6.489407	1.985530
48	6	0	-2.390959	-2.406046	-0.065086
49	6	0	-6.482813	3.550268	-1.713801
50	6	0	-7.723800	2.847941	-1.756547
51	6	0	-7.731800	1.475264	-1.607562
52	6	0	-6.547539	0.730195	-1.370533
53	6	0	-5.328399	1.447456	-1.218915
54	6	0	-5.323562	2.849170	-1.445809
55	6	0	-6.547601	-0.729594	-1.370571
56	6	0	-5.328523	-1.446970	-1.218982
57	6	0	-4.149919	-0.701902	-0.863511
58	6	0	-4.149859	0.702272	-0.863489
59	6	0	-7.731927	-1.474546	-1.607646
60	6	0	-7.724048	-2.847214	-1.756714
61	6	0	-6.483123	-3.549651	-1.714006
62	6	0	-5.323811	-2.848672	-1.445964
63	6	0	-2.834396	1.138321	-0.438965
64	7	0	-2.084620	0.000092	-0.287683
65	6	0	-2.834499	-1.138069	-0.438964
66	8	0	-6.559461	4.883832	-1.963797
67	8	0	-8.819860	3.621817	-1.985594
68	1	0	-8.675560	0.957256	-1.697789
69	1	0	-8.675640	-0.956449	-1.697851
70	8	0	-8.820173	-3.620980	-1.985820
71	8	0	-6.559886	-4.883191	-1.964099
72	1	0	-1.114172	0.000049	0.007010
73	6	0	-2.390742	2.406264	-0.065111
74	6	0	3.547030	6.422028	1.723113
75	6	0	2.846433	7.662608	1.804944
76	6	0	1.475170	7.677293	1.652442
77	6	0	0.728707	6.501712	1.373824
78	6	0	1.444751	5.284974	1.177905
79	6	0	2.847463	5.273705	1.411558
80	6	0	-0.728068	6.501786	1.373837
81	6	0	-1.444242	5.285120	1.177934
82	6	0	-0.695535	4.125647	0.781161
83	6	0	0.695920	4.125578	0.781150
84	6	0	-1.474402	7.677445	1.652469
85	6	0	-2.845663	7.662906	1.805002
86	6	0	-3.546390	6.422399	1.723189
87	6	0	-2.846950	5.274002	1.411621
88	6	0	1.093943	2.790561	0.309874
89	7	0	0.000088	2.004930	0.111889
90	6	0	-1.093688	2.790669	0.309873
91	8	0	4.880397	6.488946	1.985077
92	8	0	3.622188	8.749661	2.074217
93	1	0	0.957516	8.617903	1.773768
94	1	0	-0.956646	8.618001	1.773780
95	8	0	-3.621297	8.750040	2.074296
96	8	0	-4.879744	6.489459	1.985185
97	6	0	2.390964	2.406036	-0.065097
98	6	0	2.390741	-2.406274	-0.065010
99	1	0	-3.138946	-3.180164	-0.065442
100	1	0	-3.138659	3.180449	-0.065487
101	1	0	3.138952	3.180153	-0.065455
102	1	0	3.138656	-3.180459	-0.065357
103	6	0	5.609458	5.271811	2.062134
104	6	0	5.608897	-5.272352	2.062555
105	6	0	-5.347071	-5.619367	-2.058738
106	6	0	-5.346580	5.619906	-2.058388
107	6	0	5.346608	-5.619948	-2.058309
108	6	0	5.347130	5.619322	-2.058654
109	6	0	-5.609509	-5.271766	2.062161
110	6	0	-5.608935	5.272402	2.062247
111	1	0	5.627000	4.741487	1.102285
112	1	0	5.198016	4.606261	2.831451
113	1	0	6.628349	5.552261	2.331827
114	1	0	5.197499	-4.606714	2.831820
115	1	0	5.626541	-4.742080	1.102679
116	1	0	6.627744	-5.552905	2.332305
117	1	0	-4.796531	-5.626665	-1.110353
118	1	0	-4.697685	-5.221176	-2.848375
119	1	0	-5.638623	-6.639969	-2.308845
120	1	0	-4.697230	5.221709	-2.848051
121	1	0	-4.796040	5.627093	-1.110001
122	1	0	-5.638042	6.640551	-2.308428
123	1	0	4.697270	-5.221749	-2.847982
124	1	0	4.796050	-5.627143	-1.109933
125	1	0	5.638077	-6.640591	-2.308350
126	1	0	4.796559	5.626624	-1.110286
127	1	0	4.697771	5.221125	-2.848309
128	1	0	5.638689	6.639923	-2.308758
129	1	0	-5.627027	-4.741485	1.102288
130	1	0	-5.198094	-4.606178	2.831461
131	1	0	-6.628405	-5.552212	2.331838
132	1	0	-5.197548	4.606800	2.831549
133	1	0	-5.626555	4.742090	1.102393
134	1	0	-6.627790	5.552960	2.331965
135	6	0	-2.982062	10.007070	2.208920
136	6	0	2.983084	10.006757	2.208854
137	6	0	10.081685	2.981487	-2.076215
138	6	0	10.081395	-2.982535	-2.076084
139	6	0	2.982006	-10.007005	2.209338
140	6	0	-2.983120	-10.006695	2.209124
141	6	0	-10.081626	-2.981538	-2.076450
142	6	0	-10.081368	2.982487	-2.076253
143	1	0	-3.775592	10.727154	2.413445
144	1	0	-2.267041	10.011039	3.042239
145	1	0	-2.458823	10.297158	1.288123
146	1	0	3.776693	10.726760	2.413358
147	1	0	2.459852	10.296894	1.288069
148	1	0	2.268084	10.010801	3.042190
149	1	0	10.808352	3.775518	-2.253036
150	1	0	10.337897	2.456753	-1.146390
151	1	0	10.115196	2.268500	-2.910468
152	1	0	10.807991	-3.776641	-2.252861
153	1	0	10.114966	-2.269602	-2.910381
154	1	0	10.337658	-2.457767	-1.146293
155	1	0	3.775530	-10.727083	2.413910
156	1	0	2.266963	-10.010944	3.042638
157	1	0	2.458791	-10.297125	1.288538
158	1	0	-3.776731	-10.726693	2.413636
159	1	0	-2.459868	-10.296864	1.288360
160	1	0	-2.268137	-10.010708	3.042475
161	1	0	-10.808286	-3.775570	-2.253293
162	1	0	-10.337868	-2.456804	-1.146634
163	1	0	-10.115114	-2.268552	-2.910705
164	1	0	-10.807962	3.776592	-2.253037
165	1	0	-10.114923	2.269558	-2.910553
166	1	0	-10.337644	2.457714	-1.146467
167	1	0	4.379878	-3.371961	-1.467221
168	1	0	4.380197	3.371479	-1.467408
169	1	0	-3.370515	-4.329662	1.404091
170	1	0	3.370045	-4.330013	1.404345
171	1	0	-4.379861	3.371930	-1.467286
172	1	0	-4.380157	-3.371512	-1.467481
173	1	0	3.370485	4.329693	1.404033
174	1	0	-3.370071	4.330047	1.404118

Table S17. Cartesian coordinates for the optimized structure of **3a**-H_2 (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.528384	3.640371	-1.243861
2	6	0	-7.771797	2.961865	-1.108707
3	6	0	-7.784694	1.592836	-0.969328
4	6	0	-6.592973	0.830630	-0.902607
5	6	0	-5.364340	1.522838	-0.919445
6	6	0	-5.360864	2.919954	-1.149697
7	6	0	-6.613700	-0.630712	-0.907918
8	6	0	-5.405103	-1.357320	-0.925532
9	6	0	-4.183799	-0.629996	-0.701914
10	6	0	-4.163736	0.760309	-0.700099
11	6	0	-7.826037	-1.358367	-0.985848
12	6	0	-7.851341	-2.726470	-1.132754
13	6	0	-6.626925	-3.439880	-1.263601
14	6	0	-5.440211	-2.752974	-1.162023
15	6	0	-2.820377	1.175273	-0.369602
16	7	0	-2.081020	0.034174	-0.257316
17	6	0	-2.853316	-1.084608	-0.371750
18	8	0	-6.609805	4.971275	-1.461391
19	8	0	-8.868109	3.752115	-1.171274
20	1	0	-8.740545	1.090611	-0.924521
21	1	0	-8.767687	-0.829704	-0.944996
22	8	0	-8.968878	-3.485015	-1.207341
23	8	0	-6.744896	-4.767299	-1.484763
24	1	0	-1.098066	0.020554	-0.007750
25	6	0	3.638914	6.482689	1.269116
26	6	0	2.966507	7.731838	1.150939
27	6	0	1.599823	7.752286	0.999646
28	6	0	0.833472	6.563796	0.902286
29	6	0	1.520970	5.329743	0.896215
30	6	0	2.917208	5.319965	1.143516
31	6	0	-0.624660	6.587990	0.900571
32	6	0	-1.352632	5.377376	0.894902
33	6	0	-0.624178	4.165268	0.645630
34	6	0	0.753039	4.142496	0.645284
35	6	0	-1.351897	7.801015	0.993846
36	6	0	-2.718838	7.825679	1.142560
37	6	0	-3.432199	6.599461	1.262937
38	6	0	-2.748751	5.413712	1.140376
39	6	0	1.128092	2.772522	0.279639
40	7	0	0.029120	1.994881	0.129774
41	6	0	-1.044204	2.808301	0.280716
42	8	0	4.968831	6.555505	1.504562
43	8	0	3.761108	8.824154	1.243411
44	1	0	1.100301	8.710353	0.971746
45	1	0	-0.821868	8.742459	0.963899
46	8	0	-3.477917	8.943347	1.229921
47	8	0	-4.759164	6.716389	1.497049
48	6	0	2.420904	2.361482	-0.046740
49	6	0	6.526116	-3.640052	-1.253853
50	6	0	7.769980	-2.963017	-1.114675
51	6	0	7.783937	-1.594435	-0.970937
52	6	0	6.592715	-0.831492	-0.903378
53	6	0	5.363590	-1.522678	-0.923429
54	6	0	5.359161	-2.919027	-1.158439
55	6	0	6.614216	0.629761	-0.904871
56	6	0	5.406050	1.357132	-0.923016
57	6	0	4.184177	0.630075	-0.701930
58	6	0	4.163572	-0.759935	-0.702596
59	6	0	7.827180	1.356866	-0.978757
60	6	0	7.853493	2.725182	-1.123120
61	6	0	6.629702	3.439410	-1.256044
62	6	0	5.442339	2.753146	-1.157468
63	6	0	2.819860	-1.175311	-0.372317
64	7	0	2.080674	-0.033998	-0.259061
65	6	0	2.853246	1.084860	-0.371644
66	8	0	6.606582	-4.970257	-1.475953
67	8	0	8.865445	-3.754246	-1.178004
68	1	0	8.740189	-1.093154	-0.923272
69	1	0	8.768391	0.827435	-0.936742
70	8	0	8.971593	3.483356	-1.193350
71	8	0	6.749273	4.766906	-1.475992
72	1	0	1.097724	-0.020460	-0.009534
73	6	0	2.349199	-2.438470	-0.048062
74	6	0	-3.639253	-6.480660	1.273681
75	6	0	-2.966961	-7.730231	1.160582
76	6	0	-1.600351	-7.751407	1.008283
77	6	0	-0.833934	-6.563437	0.905777
78	6	0	-1.521094	-5.329270	0.897150
79	6	0	-2.917286	-5.318507	1.144459
80	6	0	0.624238	-6.588024	0.901556
81	6	0	1.352652	-5.377688	0.892728
82	6	0	0.624226	-4.165580	0.643254
83	6	0	-0.753007	-4.142609	0.644074
84	6	0	1.351063	-7.801206	0.995119
85	6	0	2.718303	-7.826349	1.141109
86	6	0	3.432389	-6.600339	1.258363
87	6	0	2.749244	-5.414438	1.135511
88	6	0	-1.128307	-2.772899	0.278255
89	7	0	-0.028829	-1.995245	0.127348
90	6	0	1.043878	-2.808638	0.277450
91	8	0	-4.969375	-6.552354	1.508369
92	8	0	-3.761562	-8.822027	1.258655
93	1	0	-1.100958	-8.709632	0.983881
94	1	0	0.820519	-8.742429	0.967248
95	8	0	3.477036	-8.944210	1.228604
96	8	0	4.759792	-6.717555	1.490137
97	6	0	-2.420601	-2.361681	-0.047518
98	6	0	-2.349205	2.438470	-0.044207
99	1	0	3.179349	3.123948	-0.048756
100	1	0	3.084479	-3.223290	-0.049709
101	1	0	-3.179265	-3.123904	-0.049301
102	1	0	-3.084686	3.223190	-0.044644
103	6	0	-5.644075	-5.351928	1.825522
104	6	0	-5.472098	5.541678	1.827684
105	6	0	5.576029	5.488745	-1.795603
106	6	0	5.412705	-5.654947	-1.800929
107	6	0	-5.416330	5.657934	-1.783818
108	6	0	-5.569736	-5.488010	-1.799854
109	6	0	5.643016	5.357104	1.830745
110	6	0	5.473555	-5.543053	1.819337
111	1	0	-5.612185	-4.628196	1.002854
112	1	0	-5.221617	-4.888088	2.725239
113	1	0	-6.681876	-5.628683	2.006953
114	1	0	-5.061378	5.073433	2.730380
115	1	0	-5.466712	4.809848	1.011760
116	1	0	-6.499263	5.855121	2.009698
117	1	0	4.843037	5.469407	-0.981113
118	1	0	5.109205	5.097078	-2.707555
119	1	0	5.892459	6.518309	-1.957145
120	1	0	4.958762	-5.243843	-2.710785
121	1	0	4.680001	-5.618894	-0.986691
122	1	0	5.697715	-6.692658	-1.968584
123	1	0	-4.961882	5.250104	-2.694876
124	1	0	-4.683853	5.619663	-0.969510
125	1	0	-5.702116	6.695962	-1.948137
126	1	0	-4.840456	-5.468578	-0.982028
127	1	0	-5.099320	-5.095278	-2.709457
128	1	0	-5.884654	-6.517670	-1.963525
129	1	0	5.611845	4.627427	1.013260
130	1	0	5.219609	4.899699	2.733419
131	1	0	6.680711	5.634883	2.011123
132	1	0	5.065125	-5.074862	2.723156
133	1	0	5.466409	-4.810941	1.003681
134	1	0	6.501165	-5.856572	1.998813
135	6	0	2.822485	-10.187780	1.147455
136	6	0	-3.147166	-10.086475	1.187004
137	6	0	-10.213164	-2.832140	-1.117509
138	6	0	-10.129033	3.133451	-1.070430
139	6	0	-2.824008	10.187169	1.145725
140	6	0	3.146474	10.088162	1.164730
141	6	0	10.215288	2.829732	-1.100285
142	6	0	10.127046	-3.137697	-1.072898
143	1	0	3.601052	-10.945519	1.233929
144	1	0	2.099387	-10.318779	1.962924
145	1	0	2.304867	-10.309529	0.187092
146	1	0	-3.948308	-10.819196	1.282801
147	1	0	-2.636625	-10.233032	0.226255
148	1	0	-2.425732	-10.232562	2.001464
149	1	0	-10.969989	-3.612072	-1.198568
150	1	0	-10.329082	-2.314844	-0.156294
151	1	0	-10.350648	-2.109783	-1.932523
152	1	0	-10.865638	3.933462	-1.141410
153	1	0	-10.294747	2.417449	-1.885820
154	1	0	-10.248851	2.616509	-0.109461
155	1	0	-3.602754	10.944676	1.232731
156	1	0	-2.099286	10.319535	1.959573
157	1	0	-2.308416	10.307775	0.184090
158	1	0	3.947515	10.821499	1.256389
159	1	0	2.635881	10.229238	0.203124
160	1	0	2.425044	10.238700	1.978430
161	1	0	10.972729	3.609409	-1.177563
162	1	0	10.327675	2.310940	-0.139480
163	1	0	10.355256	2.108568	-1.915897
164	1	0	10.862618	-3.938582	-1.144654
165	1	0	10.295468	-2.419673	-1.885981
166	1	0	10.245733	-2.623595	-0.110253
167	1	0	-4.419176	3.423245	-1.309446
168	1	0	-4.511997	-3.280997	-1.320585
169	1	0	3.416221	4.374296	1.294264
170	1	0	-3.277432	4.484486	1.292158
171	1	0	4.417146	-3.420850	-1.320936
172	1	0	4.514639	3.281818	-1.316769
173	1	0	-3.416091	-4.372341	1.292371
174	1	0	3.278685	-4.485272	1.284931

Table S18. Cartesian coordinates for the optimized structure of **3a**-Zn (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.157632	-7.275792	-1.683922
2	6	0	2.473686	-7.824886	-1.730971
3	6	0	3.562596	-6.989399	-1.583199
4	6	0	3.424970	-5.596781	-1.344682
5	6	0	2.110238	-5.073608	-1.186484
6	6	0	1.000131	-5.931386	-1.411591
7	6	0	4.576105	-4.701012	-1.348612
8	6	0	4.392479	-3.297577	-1.194398
9	6	0	3.080909	-2.827662	-0.839242
10	6	0	1.978421	-3.685591	-0.835113
11	6	0	5.891331	-5.177473	-1.590264
12	6	0	6.968056	-4.327585	-1.744590
13	6	0	6.758975	-2.916868	-1.702877
14	6	0	5.495448	-2.432963	-1.427832
15	6	0	0.835827	-2.887469	-0.404060
16	7	0	1.228578	-1.581653	-0.259476
17	6	0	2.590150	-1.522540	-0.410378
18	8	0	0.150405	-8.154371	-1.934311
19	8	0	2.534686	-9.165574	-1.961879
20	1	0	4.550691	-7.416406	-1.676923
21	1	0	6.062928	-6.240491	-1.679889
22	8	0	8.252102	-4.716438	-1.978340
23	8	0	7.856805	-2.157158	-1.960829
24	6	0	-7.276480	-1.158211	1.680725
25	6	0	-7.825197	-2.474359	1.728830
26	6	0	-6.989041	-3.563180	1.583856
27	6	0	-5.596488	-3.425335	1.345819
28	6	0	-5.073656	-2.110635	1.186443
29	6	0	-5.931940	-1.000495	1.409057
30	6	0	-4.700356	-4.576137	1.351905
31	6	0	-3.297070	-4.392183	1.197363
32	6	0	-2.827340	-3.081096	0.840016
33	6	0	-3.685677	-1.978937	0.834816
34	6	0	-5.176180	-5.890805	1.597176
35	6	0	-4.326140	-6.967077	1.754081
36	6	0	-2.915604	-6.757584	1.710525
37	6	0	-2.432157	-5.494577	1.431935
38	6	0	-2.887602	-0.836533	0.403801
39	7	0	-1.581748	-1.228972	0.258976
40	6	0	-1.522560	-2.590416	0.410349
41	8	0	-8.155639	-0.151002	1.929012
42	8	0	-9.165982	-2.535310	1.959487
43	1	0	-7.416025	-4.551240	1.678175
44	1	0	-6.239010	-6.062300	1.686998
45	8	0	-4.714682	-8.250523	1.991330
46	8	0	-2.155447	-7.854504	1.971495
47	6	0	-3.350810	0.418760	-0.006095
48	6	0	-1.159743	7.277624	-1.675123
49	6	0	-2.476099	7.825797	-1.722360
50	6	0	-3.564693	6.989014	-1.578882
51	6	0	-3.426231	5.596158	-1.343029
52	6	0	-2.111356	5.073370	-1.184403
53	6	0	-1.001625	5.932528	-1.406316
54	6	0	-4.576946	4.699734	-1.350064
55	6	0	-4.392333	3.296428	-1.197333
56	6	0	-3.081174	2.826872	-0.840016
57	6	0	-1.978966	3.685142	-0.834152
58	6	0	-5.891702	5.175589	-1.595029
59	6	0	-6.967373	4.324945	-1.752945
60	6	0	-6.757290	2.914333	-1.711690
61	6	0	-5.494161	2.431020	-1.433444
62	6	0	-0.836623	2.886692	-0.403530
63	7	0	-1.229181	1.580817	-0.259692
64	6	0	-2.590813	1.521828	-0.411146
65	8	0	-0.152710	8.157606	-1.921783
66	8	0	-2.537523	9.166938	-1.950680
67	1	0	-4.552898	7.415902	-1.672634
68	1	0	-6.063621	6.238528	-1.684078
69	8	0	-8.250843	4.713181	-1.990519
70	8	0	-7.854119	2.154094	-1.972945
71	6	0	0.418752	3.350252	0.005837
72	6	0	7.277243	1.158619	1.676788
73	6	0	7.825669	2.474962	1.722871
74	6	0	6.989631	3.563817	1.577575
75	6	0	5.596756	3.425561	1.341123
76	6	0	5.073698	2.110611	1.184112
77	6	0	5.932153	1.000699	1.407787
78	6	0	4.700591	4.576386	1.347000
79	6	0	3.297031	4.392378	1.194849
80	6	0	2.827003	3.080992	0.839093
81	6	0	3.685232	1.978618	0.834423
82	6	0	5.176867	5.891539	1.589597
83	6	0	4.326959	6.967954	1.745872
84	6	0	2.916219	6.758582	1.705099
85	6	0	2.432377	5.495044	1.429606
86	6	0	2.886890	0.836055	0.404062
87	7	0	1.581143	1.228652	0.259727
88	6	0	1.521980	2.590261	0.410390
89	8	0	8.156826	0.151695	1.925212
90	8	0	9.166739	2.536372	1.951480
91	1	0	7.417208	4.551790	1.670683
92	1	0	6.239937	6.063414	1.677923
93	8	0	4.716050	8.251896	1.980233
94	8	0	2.156665	7.856073	1.964877
95	6	0	3.350252	-0.419486	-0.005468
96	6	0	-0.419594	-3.350694	0.005535
97	1	0	-4.419089	0.551955	-0.009384
98	1	0	0.551909	4.418618	0.009102
99	1	0	4.418583	-0.553029	-0.007834
100	1	0	-0.553138	-4.419010	0.007920
101	6	0	7.647315	-1.171334	2.028295
102	6	0	-0.748482	-7.683846	2.077989
103	6	0	-7.683069	0.747371	-2.082200
104	6	0	1.170539	7.648914	-2.022933
105	6	0	-1.172385	-7.644281	-2.036261
106	6	0	7.686793	-0.750331	-2.070195
107	6	0	-7.646078	1.172138	2.029437
108	6	0	0.749813	7.685700	2.075382
109	1	0	7.210692	-1.517741	1.083886
110	1	0	6.893706	-1.248787	2.822140
111	1	0	8.502661	-1.800533	2.277015
112	1	0	-0.491525	-6.964444	2.865758
113	1	0	-0.301857	-7.354896	1.131911
114	1	0	-0.349074	-8.664945	2.337569
115	1	0	-7.353997	0.299525	-1.136891
116	1	0	-6.963322	0.491625	-2.869942
117	1	0	-8.663958	0.347983	-2.342605
118	1	0	1.250086	6.895596	-2.816586
119	1	0	1.516000	7.212432	-1.078311
120	1	0	1.799473	8.504693	-2.270297
121	1	0	-1.249920	-6.888163	-2.827568
122	1	0	-1.519047	-7.210114	-1.090964
123	1	0	-1.801497	-8.498973	-2.286903
124	1	0	7.354688	-0.301982	-1.126158
125	1	0	6.970303	-0.494054	-2.860743
126	1	0	8.668833	-0.351661	-2.327244
127	1	0	-7.211444	1.517217	1.083755
128	1	0	-6.890613	1.251357	2.821385
129	1	0	-8.501047	1.801631	2.278602
130	1	0	0.494713	6.967718	2.865072
131	1	0	0.300777	7.354741	1.131175
132	1	0	0.351437	8.667518	2.333820
133	6	0	6.104238	8.523023	2.064978
134	6	0	9.769150	3.815477	2.042490
135	6	0	8.522896	-6.104516	-2.064970
136	6	0	3.813613	-9.767949	-2.054711
137	6	0	-6.102698	-8.521442	2.079117
138	6	0	-9.767795	-3.814583	2.053571
139	6	0	-8.522672	6.101156	-2.076491
140	6	0	-3.816981	9.768507	-2.043716
141	1	0	6.189924	9.595642	2.244190
142	1	0	6.573399	7.980081	2.896126
143	1	0	6.624789	8.269047	1.132080
144	1	0	10.831104	3.635538	2.214703
145	1	0	9.645208	4.389277	1.114559
146	1	0	9.361213	4.397476	2.879402
147	1	0	9.595599	-6.190305	-2.243278
148	1	0	8.268196	-6.626360	-1.133080
149	1	0	7.980171	-6.572831	-2.896667
150	1	0	3.633604	-10.829545	-2.229629
151	1	0	4.395589	-9.357699	-2.890530
152	1	0	4.387279	-9.646055	-1.126606
153	1	0	-6.187967	-9.593743	2.260387
154	1	0	-6.570977	-7.976821	2.909735
155	1	0	-6.625143	-8.269117	1.146827
156	1	0	-10.829391	-3.634266	2.227199
157	1	0	-9.645222	-4.389805	1.126452
158	1	0	-9.358024	-4.395128	2.890573
159	1	0	-9.595062	6.186261	-2.257627
160	1	0	-8.270573	6.622868	-1.143696
161	1	0	-7.978283	6.570413	-2.906660
162	1	0	-3.637571	10.830710	-2.215318
163	1	0	-4.397478	9.360216	-2.881626
164	1	0	-4.391861	9.643861	-1.116607
165	1	0	0.007522	-5.507808	-1.427792
166	1	0	5.327569	-1.366997	-1.446806
167	1	0	-5.508127	-0.007931	1.423911
168	1	0	-1.366198	-5.326683	1.451178
169	1	0	-0.008571	5.509735	-1.421130
170	1	0	-5.326077	1.365061	-1.453589
171	1	0	5.508820	0.008005	1.424107
172	1	0	1.366483	5.326803	1.449844
173	30	0	-0.000144	-0.000138	-0.000106

Table S19. Cartesian coordinates for the optimized structure of **3a**-Zn (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.062228	6.709699	-1.492449
2	6	0	-4.474299	6.887317	-1.515438
3	6	0	-5.297314	5.791246	-1.398492
4	6	0	-4.789148	4.481826	-1.209738
5	6	0	-3.390782	4.325612	-1.094395
6	6	0	-2.551506	5.449666	-1.293860
7	6	0	-5.661171	3.310830	-1.214653
8	6	0	-5.111221	2.015541	-1.102785
9	6	0	-3.711957	1.905214	-0.796738
10	6	0	-2.885154	3.014913	-0.793218
11	6	0	-7.060441	3.423053	-1.409753
12	6	0	-7.873782	2.320747	-1.536368
13	6	0	-7.298747	1.018754	-1.516708
14	6	0	-5.946169	0.889916	-1.311296
15	6	0	-1.567878	2.545851	-0.394012
16	7	0	-1.595165	1.188941	-0.261867
17	6	0	-2.887320	0.775372	-0.399194
18	8	0	-2.328296	7.828062	-1.685591
19	8	0	-4.889564	8.162968	-1.694505
20	1	0	-6.365245	5.942344	-1.469548
21	1	0	-7.510855	4.403190	-1.478040
22	8	0	-9.213930	2.353339	-1.721945
23	8	0	-8.158425	-0.004361	-1.719429
24	6	0	6.709438	3.062172	1.494016
25	6	0	6.886913	4.474273	1.516948
26	6	0	5.790776	5.297191	1.399654
27	6	0	4.481397	4.788900	1.210831
28	6	0	4.325352	3.390537	1.095552
29	6	0	5.449461	2.551358	1.295194
30	6	0	3.310335	5.660816	1.215302
31	6	0	2.015007	5.110822	1.103195
32	6	0	1.904976	3.711420	0.797277
33	6	0	3.014798	2.884722	0.794134
34	6	0	3.422647	7.060122	1.409985
35	6	0	2.320431	7.873637	1.535345
36	6	0	1.018420	7.298716	1.515221
37	6	0	0.889460	5.946078	1.311026
38	6	0	2.546045	1.567214	0.395112
39	7	0	1.189192	1.594389	0.262336
40	6	0	0.775528	2.886475	0.399322
41	8	0	7.827818	2.328316	1.687349
42	8	0	8.162491	4.889633	1.696248
43	1	0	5.941793	6.365167	1.470251
44	1	0	4.402809	7.510420	1.479140
45	8	0	2.353122	9.213917	1.720288
46	8	0	-0.004546	8.158777	1.716457
47	6	0	3.325230	0.484488	-0.002870
48	6	0	3.062360	-6.708925	-1.497415
49	6	0	4.474455	-6.886660	-1.519775
50	6	0	5.297628	-5.790813	-1.400601
51	6	0	4.789557	-4.481476	-1.210812
52	6	0	3.391252	-4.325382	-1.095829
53	6	0	2.551792	-5.449009	-1.296743
54	6	0	5.661463	-3.310384	-1.214389
55	6	0	5.111318	-2.015113	-1.102208
56	6	0	3.711834	-1.905268	-0.796577
57	6	0	2.885261	-3.015119	-0.793916
58	6	0	7.060826	-3.422552	-1.408668
59	6	0	7.874276	-2.320233	-1.533549
60	6	0	7.299207	-1.018299	-1.513580
61	6	0	5.946493	-0.889466	-1.309753
62	6	0	1.567518	-2.546835	-0.395105
63	7	0	1.594609	-1.189949	-0.261887
64	6	0	2.886724	-0.776144	-0.398313
65	8	0	2.328182	-7.826807	-1.692962
66	8	0	4.889552	-8.162111	-1.700243
67	1	0	6.365590	-5.942018	-1.470390
68	1	0	7.511213	-4.402654	-1.478001
69	8	0	9.214649	-2.352774	-1.717912
70	8	0	8.159237	0.004779	-1.714558
71	6	0	0.484791	-3.326374	0.002678
72	6	0	-6.709436	-3.062397	1.494536
73	6	0	-6.887274	-4.474471	1.516998
74	6	0	-5.791396	-5.297706	1.398759
75	6	0	-4.481966	-4.789725	1.209473
76	6	0	-4.325711	-3.391422	1.094298
77	6	0	-5.449392	-2.551895	1.294647
78	6	0	-3.310909	-5.661690	1.214016
79	6	0	-2.015688	-5.111608	1.101891
80	6	0	-1.905536	-3.712341	0.795813
81	6	0	-3.015256	-2.885648	0.792719
82	6	0	-3.422956	-7.060914	1.409474
83	6	0	-2.320523	-7.874073	1.536170
84	6	0	-1.018610	-7.298866	1.516337
85	6	0	-0.889931	-5.946337	1.310472
86	6	0	-2.546607	-1.568188	0.393659
87	7	0	-1.189667	-1.595416	0.261076
88	6	0	-0.775975	-2.887606	0.397895
89	8	0	-7.827439	-2.328155	1.689224
90	8	0	-8.162868	-4.889511	1.696722
91	1	0	-5.942666	-6.365632	1.469007
92	1	0	-4.403021	-7.511401	1.478208
93	8	0	-2.352925	-9.214188	1.722017
94	8	0	0.004634	-8.158321	1.719475
95	6	0	-3.326039	-0.485500	-0.004440
96	6	0	-0.485208	3.324971	0.004306
97	1	0	4.389410	0.639626	-0.004599
98	1	0	0.640032	-4.390782	0.004396
99	1	0	-4.390362	-0.641013	-0.006572
100	1	0	-0.640634	4.389088	0.006449
101	6	0	-7.677348	-0.930667	1.838798
102	6	0	-1.300582	7.614967	1.868228
103	6	0	7.615214	1.300643	-1.866736
104	6	0	0.930671	-7.676538	-1.841698
105	6	0	-0.930538	7.679565	-1.836134
106	6	0	-7.613321	-1.299799	-1.869720
107	6	0	7.679235	0.930552	1.837779
108	6	0	1.299913	-7.612855	1.869103
109	1	0	-7.271641	-0.458725	0.935736
110	1	0	-7.028628	-0.690361	2.689975
111	1	0	-8.677854	-0.540092	2.020122
112	1	0	-1.342835	6.920831	2.715900
113	1	0	-1.640441	7.095498	0.964730
114	1	0	-1.960002	8.460945	2.055087
115	1	0	7.095231	1.640470	-0.963414
116	1	0	6.921449	1.342635	-2.714818
117	1	0	8.461207	1.960220	-2.053376
118	1	0	0.690057	-7.026927	-2.692122
119	1	0	0.459234	-7.271754	-0.937904
120	1	0	0.539974	-8.676859	-2.024005
121	1	0	-0.689819	7.032147	-2.687614
122	1	0	-0.457391	7.273452	-0.934604
123	1	0	-0.540983	8.680261	-2.015762
124	1	0	-7.094984	-1.638467	-0.964483
125	1	0	-6.917750	-1.341547	-2.716733
126	1	0	-8.458735	-1.960124	-2.058428
127	1	0	7.273039	0.457521	0.936133
128	1	0	7.031803	0.689864	2.689342
129	1	0	8.679978	0.540940	2.017401
130	1	0	1.341592	-6.916552	2.715500
131	1	0	1.638198	-7.095242	0.963294
132	1	0	1.960504	-8.457931	2.058583
133	6	0	-3.613948	-9.832881	1.815965
134	6	0	-8.394191	-6.274710	1.794524
135	6	0	-9.832433	3.614439	-1.816056
136	6	0	-6.274557	8.393831	-1.795585
137	6	0	3.614094	9.832018	1.817820
138	6	0	8.393255	6.274665	1.797113
139	6	0	9.832966	-3.613680	-1.814959
140	6	0	6.274805	-8.393340	-1.797548
141	1	0	-3.418743	-10.893788	1.971866
142	1	0	-4.192036	-9.443507	2.664048
143	1	0	-4.197630	-9.704495	0.895152
144	1	0	-9.467289	-6.391586	1.945065
145	1	0	-8.098706	-6.800430	0.877242
146	1	0	-7.859971	-6.713654	2.647156
147	1	0	-10.893371	3.419376	-1.971903
148	1	0	-9.703922	4.198249	-0.895349
149	1	0	-9.442971	4.192295	-2.664248
150	1	0	-6.391509	9.466967	-1.945756
151	1	0	-6.710911	7.859960	-2.649655
152	1	0	-6.802549	8.097581	-0.879949
153	1	0	3.418980	10.892972	1.973449
154	1	0	4.189388	9.442087	2.667411
155	1	0	4.200361	9.703643	0.898755
156	1	0	9.466336	6.391686	1.947631
157	1	0	8.097287	6.802438	0.881240
158	1	0	7.859066	6.711190	2.650920
159	1	0	10.893991	-3.418451	-1.969973
160	1	0	9.704122	-4.199858	-0.895896
161	1	0	9.443629	-4.189145	-2.664709
162	1	0	6.391745	-9.466323	-1.948860
163	1	0	6.714179	-7.858455	-2.649559
164	1	0	6.800050	-8.098553	-0.879759
165	1	0	-1.483182	5.304702	-1.347574
166	1	0	-5.500088	-0.091474	-1.366837
167	1	0	5.304550	1.483021	1.348827
168	1	0	-0.092216	5.500614	1.366742
169	1	0	1.483595	-5.303162	-1.350212
170	1	0	5.500881	0.092134	-1.365591
171	1	0	-5.303607	-1.483697	1.348240
172	1	0	0.091348	-5.500010	1.365899
173	30	0	-0.000282	-0.000552	-0.000080

Table S20. Cartesian coordinates for the optimized structure of **3b**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.524972	-3.469986	-1.808891
2	6	0	7.754821	-2.748795	-1.864970
3	6	0	7.739509	-1.374009	-1.732974
4	6	0	6.544174	-0.646435	-1.497933
5	6	0	5.337802	-1.381773	-1.330724
6	6	0	5.355323	-2.785702	-1.542944
7	6	0	6.520757	0.813209	-1.511854
8	6	0	5.292421	1.512365	-1.351124
9	6	0	4.128853	0.751359	-0.980700
10	6	0	4.149821	-0.652739	-0.973083
11	6	0	7.690420	1.574125	-1.769542
12	6	0	7.661116	2.946321	-1.924635
13	6	0	6.409610	3.629358	-1.869424
14	6	0	5.263946	2.912613	-1.585090
15	6	0	2.843436	-1.105719	-0.537878
16	7	0	2.078089	0.022343	-0.387541
17	6	0	2.810575	1.170445	-0.548253
18	8	0	6.621884	-4.805650	-2.044086
19	8	0	8.862350	-3.506609	-2.086785
20	1	0	8.674042	-0.841623	-1.832896
21	1	0	8.639908	1.069553	-1.872052
22	8	0	8.742063	3.734709	-2.170099
23	8	0	6.462471	4.963559	-2.125879
24	1	0	1.109437	0.009324	-0.087358
25	6	0	-3.463320	-6.455797	1.676774
26	6	0	-2.746208	-7.685506	1.780314
27	6	0	-1.374290	-7.682446	1.629281
28	6	0	-0.644471	-6.501345	1.330757
29	6	0	-1.376601	-5.296941	1.118523
30	6	0	-2.779733	-5.302254	1.349769
31	6	0	0.812282	-6.483174	1.324777
32	6	0	1.512497	-5.259897	1.113169
33	6	0	0.748154	-4.113582	0.708052
34	6	0	-0.643343	-4.131922	0.709416
35	6	0	1.573844	-7.647512	1.609007
36	6	0	2.946407	-7.617066	1.750973
37	6	0	3.630791	-6.368156	1.655591
38	6	0	2.916234	-5.230422	1.339239
39	6	0	-1.059423	-2.805690	0.229045
40	7	0	0.023736	-2.006895	0.025170
41	6	0	1.128084	-2.776996	0.226332
42	8	0	-4.796941	-6.536858	1.936649
43	8	0	-3.506450	-8.778227	2.066027
44	1	0	-0.843774	-8.613215	1.768066
45	1	0	1.067927	-8.592730	1.741167
46	8	0	3.736047	-8.693324	2.019323
47	8	0	4.967287	-6.416639	1.909324
48	6	0	-2.361369	-2.439859	-0.147980
49	6	0	-6.539676	3.459930	-1.782474
50	6	0	-7.769699	2.738719	-1.834410
51	6	0	-7.754079	1.364204	-1.700102
52	6	0	-6.558053	0.636928	-1.467467
53	6	0	-5.351343	1.372413	-1.303907
54	6	0	-5.369448	2.776075	-1.518156
55	6	0	-6.534531	-0.822686	-1.480199
56	6	0	-5.306601	-1.522132	-1.317432
57	6	0	-4.141977	-0.760436	-0.951530
58	6	0	-4.162561	0.643785	-0.948128
59	6	0	-7.703984	-1.583126	-1.739964
60	6	0	-7.675431	-2.955422	-1.893799
61	6	0	-6.424920	-3.639682	-1.831951
62	6	0	-5.279222	-2.923200	-1.546861
63	6	0	-2.854099	1.097768	-0.520365
64	7	0	-2.088250	-0.029949	-0.370467
65	6	0	-2.821649	-1.178441	-0.524109
66	8	0	-6.637118	4.795164	-2.019775
67	8	0	-8.877707	3.496214	-2.054807
68	1	0	-8.689073	0.831810	-1.795467
69	1	0	-8.652616	-1.077831	-1.846326
70	8	0	-8.756312	-3.742461	-2.144120
71	8	0	-6.478376	-4.974524	-2.084795
72	1	0	-1.118138	-0.016221	-0.075130
73	6	0	-2.426933	2.370733	-0.144046
74	6	0	3.468150	6.463449	1.611120
75	6	0	2.750584	7.693232	1.710629
76	6	0	1.377035	7.686747	1.575657
77	6	0	0.645630	6.501853	1.296881
78	6	0	1.377194	5.297065	1.084955
79	6	0	2.782728	5.306208	1.301377
80	6	0	-0.811037	6.481172	1.309595
81	6	0	-1.511849	5.256450	1.108905
82	6	0	-0.750120	4.109648	0.700373
83	6	0	0.641325	4.128842	0.689702
84	6	0	-1.570659	7.644556	1.602643
85	6	0	-2.941418	7.612479	1.760686
86	6	0	-3.625537	6.362909	1.672565
87	6	0	-2.913072	5.225645	1.349753
88	6	0	1.053914	2.800578	0.211724
89	7	0	-0.030555	2.000663	0.019692
90	6	0	-1.133458	2.771215	0.226772
91	8	0	4.804371	6.548665	1.855912
92	8	0	3.512396	8.789986	1.975931
93	1	0	0.846792	8.618326	1.709856
94	1	0	-1.064284	8.590088	1.730539
95	8	0	-3.728803	8.687720	2.039702
96	8	0	-4.959236	6.410013	1.940740
97	6	0	2.352975	2.433132	-0.173284
98	6	0	2.418824	-2.377644	-0.155208
99	1	0	-3.099076	-3.223875	-0.147198
100	1	0	-3.184970	3.134994	-0.139842
101	1	0	3.090924	3.216815	-0.180278
102	1	0	3.177036	-3.141742	-0.154009
103	6	0	5.552381	5.342163	1.911591
104	6	0	5.680376	-5.189585	1.974996
105	6	0	-5.253656	-5.693010	-2.154862
106	6	0	-5.435723	5.550230	-2.106890
107	6	0	5.420246	-5.560698	-2.128361
108	6	0	5.236931	5.679583	-2.207210
109	6	0	-5.543074	-5.329011	1.986546
110	6	0	-5.670260	5.182241	2.014216
111	1	0	5.564773	4.820781	0.946716
112	1	0	5.161776	4.663075	2.680041
113	1	0	5.264465	-4.524821	2.742640
114	1	0	5.685690	-4.664478	1.012166
115	1	0	-4.720151	-5.689075	-1.196690
116	1	0	-4.595474	-5.288192	-2.933863
117	1	0	-4.778983	5.168224	-2.898505
118	1	0	-4.886231	5.558927	-1.157871
119	1	0	4.762270	-5.179487	-2.919333
120	1	0	4.872343	-5.568279	-1.178424
121	1	0	4.697761	5.680336	-1.252251
122	1	0	4.584194	5.269115	-2.987801
123	1	0	-5.563102	-4.817352	1.016527
124	1	0	-5.145178	-4.642550	2.744652
125	1	0	-5.245818	4.518215	2.777829
126	1	0	-5.684850	4.656675	1.051686
127	6	0	-3.113158	9.963961	2.186817
128	6	0	2.864713	10.048094	2.140699
129	6	0	10.024655	3.123145	-2.281489
130	6	0	10.127151	-2.857680	-2.190561
131	6	0	3.122653	-9.971415	2.159711
132	6	0	-2.858762	-10.035221	2.239308
133	6	0	-10.035464	-3.127065	-2.273528
134	6	0	-10.142300	2.846902	-2.158729
135	6	0	-4.212237	10.982396	2.455287
136	1	0	-2.392238	9.939832	3.017859
137	1	0	-2.559084	10.223008	1.272048
138	6	0	3.941035	11.092483	2.401710
139	1	0	2.291075	10.298709	1.235668
140	1	0	2.156744	9.999071	2.981689
141	6	0	11.045531	4.226912	-2.519210
142	1	0	10.258738	2.568770	-1.360313
143	1	0	10.026104	2.403821	-3.114163
144	6	0	11.182748	-3.933412	-2.404080
145	1	0	10.117163	-2.148141	-3.031471
146	1	0	10.333639	-2.286438	-1.273148
147	6	0	4.225251	-10.991513	2.406638
148	1	0	2.409977	-9.956440	2.998088
149	1	0	2.559716	-10.221373	1.247838
150	6	0	-3.934053	-11.074734	2.523143
151	1	0	-2.294462	-10.297374	1.331653
152	1	0	-2.142364	-9.977213	3.072568
153	6	0	-11.056607	-4.226940	-2.527482
154	1	0	-10.281243	-2.572687	-1.355299
155	1	0	-10.022676	-2.407028	-3.105505
156	6	0	-11.197158	3.921807	-2.379784
157	1	0	-10.130397	2.133737	-2.996480
158	1	0	-10.350977	2.279676	-1.239334
159	1	0	4.420482	-3.324518	-1.552986
160	1	0	4.312150	3.420851	-1.598280
161	1	0	-3.316094	-4.366005	1.327726
162	1	0	3.428155	-4.280476	1.320102
163	1	0	-4.434729	3.314940	-1.531523
164	1	0	-4.327969	-3.432486	-1.556904
165	1	0	3.320323	4.370618	1.281160
166	1	0	-3.423888	4.274986	1.337846
167	6	0	-3.663212	12.400638	2.651953
168	1	0	-4.918781	10.963139	1.616739
169	1	0	-4.772227	10.666931	3.343822
170	6	0	3.360896	12.495466	2.617399
171	1	0	4.520822	10.784244	3.280036
172	1	0	4.636434	11.097027	1.553659
173	6	0	12.471339	3.684975	-2.677124
174	1	0	10.752513	4.787021	-3.415334
175	1	0	10.999365	4.931847	-1.680345
176	6	0	12.595165	-3.353380	-2.546969
177	1	0	11.144620	-4.632203	-1.559680
178	1	0	10.918428	-4.509350	-3.299100
179	6	0	3.680385	-12.413600	2.586371
180	1	0	4.925971	-10.958872	1.563618
181	1	0	4.790821	-10.687699	3.295714
182	6	0	-3.354521	-12.476435	2.748658
183	1	0	-4.504529	-10.755509	3.403667
184	1	0	-4.637911	-11.087503	1.682148
185	6	0	-12.478427	-3.679091	-2.701218
186	1	0	-10.754251	-4.785047	-3.421868
187	1	0	-11.023543	-4.934872	-1.690422
188	6	0	-12.609319	3.341669	-2.524419
189	1	0	-11.161377	4.624367	-1.538519
190	1	0	-10.930011	4.493584	-3.276542
191	6	0	-4.760924	13.443958	2.894799
192	1	0	-2.962436	12.408863	3.498965
193	1	0	-3.076371	12.693585	1.769420
194	6	0	4.437512	13.559962	2.862812

195	1	0	2.760411	12.784269	1.742881	298	1	0	17.826385	-3.770025	-2.374686
196	1	0	2.667457	12.479295	3.470218	299	6	0	5.909124	-18.401269	3.600456
197	6	0	13.514554	4.788451	-2.892440	300	1	0	4.122629	-17.373730	4.252692
198	1	0	12.743600	3.099979	-1.786862	301	1	0	4.204112	-17.630337	2.518523
199	1	0	12.506004	2.984146	-3.523439	302	6	0	-5.458802	-18.467141	3.988673
200	6	0	13.668904	-4.430467	-2.746105	303	1	0	-3.764428	-17.705661	2.882360
201	1	0	12.621643	-2.654899	-3.395540	304	1	0	-3.694731	-17.379861	4.605976
202	1	0	12.841258	-2.758569	-1.655659	305	6	0	-18.461247	-5.896851	-3.767206
203	6	0	4.781407	-13.457565	2.810163	306	1	0	-17.697101	-4.221899	-2.634168
204	1	0	2.983181	-12.435222	3.436009	307	1	0	-17.440292	-4.087574	-4.365241
205	1	0	3.090640	-12.695691	1.702386	308	6	0	-18.651858	5.450547	-3.467798
206	6	0	-4.431328	-13.536522	3.012006	309	1	0	-17.604611	3.672733	-4.112911
207	1	0	-2.760952	-12.774889	1.872553	310	1	0	-17.841830	3.769223	-2.376554
208	1	0	-2.654768	-12.453129	3.596209	311	6	0	-5.334359	19.795899	3.984848
209	6	0	-13.522069	-4.777175	-2.941155	312	1	0	-6.559220	18.372815	2.912948
210	1	0	-12.761430	-3.100907	-1.809672	313	1	0	-6.480488	18.084711	4.642957
211	1	0	-12.499109	-2.970756	-3.541891	314	6	0	4.896160	19.903873	4.047298
212	6	0	-13.681355	4.418046	-2.735729	315	1	0	6.078751	18.203159	4.664177
213	1	0	-12.632756	2.637465	-3.368156	316	1	0	6.137403	18.523391	2.939842
214	1	0	-12.859463	2.753251	-1.630150	317	6	0	19.888366	5.398721	-3.821290
215	6	0	-4.219123	14.863194	3.104737	318	1	0	18.187723	6.535910	-4.519802
216	1	0	-5.456031	13.441640	2.043249	319	1	0	18.432803	6.614242	-2.783754
217	1	0	-5.355056	13.147819	3.771027	320	6	0	20.063767	-4.903323	-3.607637
218	6	0	3.868279	14.964999	3.093549	321	1	0	18.622855	-6.147034	-2.582728
219	1	0	5.044680	13.266814	3.730732	322	1	0	18.391796	-6.073226	-4.321059
220	1	0	5.125504	13.581801	2.006091	323	6	0	5.373750	-19.826632	3.783889
221	6	0	14.941929	4.255103	-3.064964	324	1	0	6.595632	-18.379630	2.742164
222	1	0	13.238143	5.380693	-3.776149	325	1	0	6.513180	-18.125220	4.476458
223	1	0	13.485863	5.483539	-2.041521	326	6	0	-4.896932	-19.873115	4.232892
224	6	0	15.085119	-3.862945	-2.901213	327	1	0	-6.073054	-18.167560	4.850116
225	1	0	13.646233	-5.124628	-1.894210	328	1	0	-6.141033	-18.493703	3.126737
226	1	0	13.418693	-5.030843	-3.632126	329	6	0	-19.889854	-5.362501	-3.927697
227	6	0	4.244447	-14.881861	2.996135	330	1	0	-18.185120	-6.469788	-4.664133
228	1	0	5.475370	-13.438676	1.958184	331	1	0	-18.433329	-6.611868	-2.932432
229	1	0	5.375527	-13.174638	3.690414	332	6	0	-20.071109	4.892991	-3.631402
230	6	0	-3.863356	-14.940894	3.250144	333	1	0	-18.631486	6.145736	-2.616489
231	1	0	-5.031248	-13.234624	3.882121	334	1	0	-18.393656	6.049890	-4.352453
232	1	0	-5.126060	-13.564230	2.160761	335	6	0	-6.432548	20.842692	4.207849
233	6	0	-14.946627	-4.238137	-3.119119	336	1	0	-4.649381	19.799708	4.845150
234	1	0	-13.238748	-5.357788	-3.830444	337	1	0	-4.727473	20.086626	3.115003
235	1	0	-13.502865	-5.484045	-2.099687	338	6	0	5.977045	20.966591	4.279296
236	6	0	-15.097464	3.850957	-2.892454	339	1	0	4.275880	20.198830	3.188881
237	1	0	-13.661455	5.118413	-1.889118	340	1	0	4.219887	19.879398	4.913665
238	1	0	-13.426996	5.011467	-3.625028	341	6	0	20.934312	6.502357	-4.018868
239	6	0	-5.316700	15.909630	3.334295	342	1	0	20.161136	4.793129	-2.945129
240	1	0	-3.529933	14.865708	3.961777	343	1	0	19.916434	4.714318	-4.681267
241	1	0	-3.616704	15.154742	2.231888	344	6	0	21.131804	-5.987733	-3.794448
242	6	0	4.946171	16.029612	3.331630	345	1	0	20.086643	-4.219390	-4.468298
243	1	0	3.256068	15.255747	2.227883	346	1	0	20.317377	-4.291855	-2.729680
244	1	0	3.183988	14.942842	3.953673	347	6	0	6.474248	-20.874549	3.988155
245	6	0	15.987355	5.358575	-3.267935	348	1	0	4.687922	-19.848784	4.642791
246	1	0	15.214251	3.654993	-2.184751	349	1	0	4.768909	-20.101987	2.908108
247	1	0	14.970705	3.565745	-3.921075	350	6	0	-5.979227	-20.933168	4.471925
248	6	0	16.157450	-4.942576	-3.092755	351	1	0	-4.280498	-20.171692	3.372532
249	1	0	15.108096	-3.172441	-3.756610	352	1	0	-4.216907	-19.847654	5.096741
250	1	0	15.333220	-3.257671	-2.017398	353	6	0	-20.932288	-6.460971	-4.169588
251	6	0	5.344792	-15.928721	3.207956	354	1	0	-20.166200	-4.791645	-3.029228
252	1	0	3.555329	-14.901103	3.852478	355	1	0	-19.918164	-4.645504	-4.761013
253	1	0	3.643394	-15.160313	2.118682	356	6	0	-21.135472	5.977451	-3.837453
254	6	0	-4.942228	-16.001642	3.501396	357	1	0	-20.092035	4.197839	-4.482790
255	1	0	-3.256367	-15.239092	2.383091	358	1	0	-20.330035	4.294052	-2.746622
256	1	0	-3.174203	-14.913924	4.106465	359	6	0	-5.895135	22.264119	4.414996
257	6	0	-15.991210	-5.335582	-3.356384	360	1	0	-7.119441	20.837446	3.349106
258	1	0	-15.227883	-3.655903	-2.229814	361	1	0	-7.038037	20.554533	5.079495
259	1	0	-14.965218	-3.531353	-3.961071	362	6	0	5.415633	22.372890	4.522347
260	6	0	-16.167257	4.930110	-3.099578	363	1	0	6.597996	20.672107	5.137551
261	1	0	-15.117155	3.152653	-3.741274	364	1	0	6.653359	20.991764	3.412855
262	1	0	-15.350680	3.254437	-2.004406	365	6	0	22.362997	5.972363	-4.191914
263	6	0	-4.775818	17.328854	3.548287	366	1	0	20.663996	7.106596	-4.896773
264	1	0	-6.003723	15.908600	2.475473	367	1	0	20.905031	7.188687	-3.160406
265	1	0	-5.921635	15.616560	4.204867	368	6	0	22.551671	-5.431964	-3.959938
266	6	0	4.380119	17.434731	3.570473	369	1	0	21.109431	-6.671774	-2.933788
267	1	0	5.561739	15.735611	4.193647	370	1	0	20.878526	-6.599730	-4.672201
268	1	0	5.627323	16.054365	2.469220	371	6	0	5.940110	-22.300789	4.168832
269	6	0	17.414642	4.826338	-3.446094	372	1	0	7.161246	-20.851941	3.130043
270	1	0	15.712849	5.961631	-4.145321	373	1	0	7.078647	-20.601089	4.864977
271	1	0	15.960619	6.045266	-2.409717	374	6	0	-5.419441	-22.340197	4.714980
272	6	0	17.575027	-4.379806	-3.254483	375	1	0	-6.595866	-20.635833	5.332689
273	1	0	16.135852	-5.630548	-2.235352	376	1	0	-6.659734	-20.958584	3.608354
274	1	0	15.906085	-5.550622	-3.973660	377	6	0	-22.362908	-5.928974	-4.320621
275	6	0	4.808692	-17.353486	3.393977	378	1	0	-20.660084	-7.028601	-5.071630
276	1	0	6.033006	-15.909226	2.351012	379	1	0	-20.900250	-7.181550	-3.339191
277	1	0	5.946840	-15.650218	4.084536	380	6	0	-22.556218	5.423319	-4.000028
278	6	0	-4.377813	-17.406760	3.744707	381	1	0	-21.114178	6.673465	-2.986666
279	1	0	-5.552042	-15.701237	4.365591	382	1	0	-20.877374	6.576128	-4.722771
280	1	0	-5.628825	-16.029852	2.643116	383	6	0	-6.999288	23.302418	4.635755
281	6	0	-17.417689	-4.798984	-3.527344	384	1	0	-5.209483	22.270186	5.273431
282	1	0	-15.712088	-5.915062	-4.247960	385	1	0	-5.290742	22.552149	3.543885
283	1	0	-15.968767	-6.044729	-2.516672	386	6	0	6.502834	23.426974	4.752298
284	6	0	-17.585007	4.368284	-3.261841	387	1	0	4.795359	22.667505	3.664912
285	1	0	-16.148278	5.626539	-2.249309	388	1	0	4.740712	22.347835	5.388711
286	1	0	-15.911012	5.528668	-3.985275	389	6	0	23.400247	7.081568	-4.390324
287	6	0	-5.873824	18.375878	3.773011	390	1	0	22.633698	5.370513	-3.313726
288	1	0	-4.090886	17.330597	4.408857	391	1	0	22.392556	5.285994	-5.049046
289	1	0	-4.168516	17.620625	2.678819	392	6	0	23.610529	-6.523073	-4.145054
290	6	0	5.459741	18.498369	3.805017	393	1	0	22.574665	-4.749368	-4.820475
291	1	0	3.762503	17.728312	2.709698	394	1	0	22.805035	-4.820805	-3.082858
292	1	0	3.701078	17.410435	4.434634	395	6	0	7.046379	-23.340275	4.371684
293	6	0	18.460718	5.930084	-3.643908	396	1	0	5.254262	-22.323921	5.026589
294	1	0	17.687753	4.220454	-2.570136	397	1	0	5.336786	-22.574185	3.292479
295	1	0	17.441885	4.142110	-4.306341	398	6	0	-6.507932	-23.392023	4.950813
296	6	0	18.645072	-5.462255	-3.442698	399	1	0	-4.803107	-22.637284	3.855161
297	1	0	17.597490	-3.693823	-4.113538	400	1	0	-4.740663	-22.315183	5.578780

401	6	0	-23.396420	-7.033464	-4.562722
402	1	0	-22.635222	-5.363651	-3.418233
403	1	0	-22.395536	-5.208377	-5.149823
404	6	0	-23.611026	6.514493	-4.206135
405	1	0	-22.577865	4.727902	-4.850009
406	1	0	-22.814851	4.826438	-3.114886
407	1	0	-6.584655	24.305801	4.777239
408	1	0	-7.682214	23.342317	3.779477
409	1	0	-7.597382	23.061985	5.522171
410	1	0	6.071154	24.418609	4.922552
411	1	0	7.117686	23.178053	5.624721
412	1	0	7.172635	23.499777	3.887953
413	1	0	24.408542	6.671797	-4.508976
414	1	0	23.176941	7.677905	-5.282257
415	1	0	23.417923	7.765108	-3.533888
416	1	0	24.612032	-6.095592	-4.259202
417	1	0	23.634631	-7.201522	-3.284614
418	1	0	23.403932	-7.128219	-5.035176
419	1	0	6.633683	-24.346684	4.496488
420	1	0	7.728765	-23.364744	3.514451
421	1	0	7.644587	-23.113779	5.261605
422	1	0	-6.077331	-24.384329	5.120205
423	1	0	-7.118584	-23.141016	5.825936
424	1	0	-7.181949	-23.464370	4.089310
425	1	0	-24.406582	-6.622715	-4.662160
426	1	0	-23.172838	-7.591967	-5.479521
427	1	0	-23.409419	-7.752216	-3.734752
428	1	0	-24.613327	6.088279	-4.317542
429	1	0	-23.636447	7.206011	-3.356394
430	1	0	-23.399302	7.105231	-5.104555
431	1	0	6.570726	5.635173	2.170070
432	1	0	6.704558	-5.454608	2.240495
433	1	0	-5.525377	-6.718710	-2.406766
434	1	0	-5.742159	6.568344	-2.349561
435	1	0	5.726192	-6.579120	-2.370367
436	1	0	5.508488	6.704291	-2.463273
437	1	0	-6.559479	-5.618121	2.256807
438	1	0	-6.691945	5.446255	2.290134

Table S21. Cartesian coordinates for the optimized structure of **3c**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.690348	-6.485279	1.687331
2	6	0	-5.114948	-6.548399	1.632753
3	6	0	-5.841338	-5.379745	1.497609
4	6	0	-5.221555	-4.112524	1.347578
5	6	0	-3.802191	-4.075632	1.258070
6	6	0	-3.068175	-5.267978	1.486098
7	6	0	-5.988418	-2.869498	1.371918
8	6	0	-5.319638	-1.616791	1.294600
9	6	0	-3.919020	-1.621766	0.967444
10	6	0	-3.180351	-2.814136	0.954638
11	6	0	-7.394761	-2.857069	1.561199
12	6	0	-8.106648	-1.685598	1.740985
13	6	0	-7.408380	-0.442419	1.800659
14	6	0	-6.047223	-0.429197	1.564624
15	6	0	-1.826345	-2.483525	0.559265
16	7	0	-1.787805	-1.118657	0.426586
17	6	0	-3.027233	-0.550725	0.573895
18	8	0	-3.052861	-7.658121	1.950342
19	8	0	-5.649390	-7.794753	1.758329
20	1	0	-6.919576	-5.440932	1.526637
21	1	0	-7.934560	-3.792594	1.589603
22	8	0	-9.455517	-1.602650	1.908846
23	8	0	-8.162856	0.646768	2.107195
24	1	0	-0.960195	-0.603436	0.146732
25	6	0	6.432671	-3.613728	-1.377459
26	6	0	6.510342	-5.038605	-1.346342
27	6	0	5.351822	-5.777931	-1.205097
28	6	0	4.080665	-5.170964	-1.023858
29	6	0	4.031586	-3.751725	-0.902980
30	6	0	5.216152	-3.004723	-1.142285
31	6	0	2.844290	-5.943064	-1.045742
32	6	0	1.587149	-5.281341	-0.933929
33	6	0	1.593018	-3.890237	-0.578093
34	6	0	2.770789	-3.152154	-0.567353
35	6	0	2.838042	-7.345598	-1.266277
36	6	0	1.670663	-8.061387	-1.450902
37	6	0	0.422687	-7.369223	-1.479928
38	6	0	0.402058	-6.015270	-1.208190
39	6	0	2.389505	-1.799570	-0.135966
40	7	0	1.042432	-1.711723	0.038314
41	6	0	0.536884	-2.961976	-0.149218
42	8	0	7.596077	-2.963733	-1.658211
43	8	0	7.762262	-5.554353	-1.500615
44	1	0	5.422695	-6.855218	-1.253650
45	1	0	3.777519	-7.876495	-1.318483
46	8	0	1.597685	-9.407674	-1.654663
47	8	0	-0.666637	-8.122271	-1.799069
48	6	0	3.281870	-0.777896	0.222259
49	6	0	3.642991	6.474912	1.682047
50	6	0	5.067492	6.540558	1.627333
51	6	0	5.795836	5.373654	1.489728
52	6	0	5.178037	4.105688	1.338053
53	6	0	3.758723	4.065893	1.250548
54	6	0	3.022515	5.256839	1.480364
55	6	0	5.947935	2.864640	1.357245
56	6	0	5.282291	1.610266	1.278778
57	6	0	3.879733	1.611823	0.958843
58	6	0	3.139067	2.803005	0.948094
59	6	0	7.355029	2.856265	1.541463
60	6	0	8.071768	1.686602	1.713157
61	6	0	7.377970	0.440981	1.769106
62	6	0	6.015781	0.424360	1.539342
63	6	0	1.784584	2.470328	0.555929
64	7	0	1.746905	1.105326	0.425853
65	6	0	2.987193	0.538742	0.570746
66	8	0	3.005224	7.647109	1.945444
67	8	0	5.599526	7.787802	1.754455
68	1	0	6.873966	5.436788	1.517464
69	1	0	7.891688	3.793502	1.572392
70	8	0	9.421298	1.606906	1.876346
71	8	0	8.136935	-0.647434	2.067219
72	1	0	0.918986	0.588693	0.149439
73	6	0	0.730857	3.308000	0.195682
74	6	0	-6.467840	3.599773	-1.412311
75	6	0	-6.543342	5.025063	-1.387680
76	6	0	-5.384810	5.763151	-1.239074
77	6	0	-4.115775	5.155353	-1.047413
78	6	0	-4.069565	3.736151	-0.922307
79	6	0	-5.253773	2.989899	-1.166104
80	6	0	-2.878434	5.926402	-1.064964
81	6	0	-1.623265	5.261545	-0.950563
82	6	0	-1.632647	3.872116	-0.590315
83	6	0	-2.811125	3.135518	-0.579361
84	6	0	-2.867298	7.329613	-1.283247
85	6	0	-1.696538	8.040828	-1.465478
86	6	0	-0.451328	7.343748	-1.498474
87	6	0	-0.435489	5.990131	-1.226336
88	6	0	-2.431582	1.784435	-0.141693
89	7	0	-1.084609	1.696134	0.035271
90	6	0	-0.578126	2.945128	-0.155976
91	8	0	-7.630637	2.950371	-1.697455
92	8	0	-7.792602	5.543542	-1.555173
93	1	0	-5.453329	6.840374	-1.292160
94	1	0	-3.804462	7.865178	-1.334144
95	8	0	-1.615151	9.387275	-1.662328
96	8	0	0.640326	8.092232	-1.820392
97	6	0	-3.323842	0.764442	0.220812
98	6	0	-0.773006	-3.322940	0.200937
99	1	0	4.326552	-1.036193	0.227978
100	1	0	0.954549	4.360906	0.189283
101	1	0	-4.369000	1.021819	0.226583
102	1	0	-0.997883	-4.375614	0.196545
103	6	0	-7.571987	1.540540	-1.945598
104	6	0	-1.900523	-7.441083	-2.056414
105	6	0	7.465209	-1.888986	2.317331
106	6	0	1.595296	7.606179	2.202753
107	6	0	-1.645420	-7.612705	2.221364
108	6	0	-7.489438	1.889208	2.347980
109	6	0	7.533806	-1.557287	-1.923976
110	6	0	1.871274	7.405388	-2.076704
111	1	0	-7.304001	1.008724	-1.021814
112	1	0	-6.793509	1.335200	-2.692897
113	6	0	-8.930138	1.079422	-2.456695
114	1	0	-1.723627	-6.629768	-2.775378
115	1	0	-2.281723	-6.993862	-1.127460
116	6	0	-2.902232	-8.437386	-2.622867
117	1	0	7.004918	-2.257224	1.389940
118	1	0	6.665800	-1.727193	3.052957
119	6	0	8.476562	-2.891532	2.853398
120	1	0	1.390956	6.862254	2.984690
121	1	0	1.058293	7.300876	1.293929
122	6	0	1.143881	8.988754	2.652663
123	1	0	-1.451785	-6.866489	3.003820
124	1	0	-1.100315	-7.307063	1.317449
125	6	0	-1.190786	-8.991635	2.678502
126	1	0	-7.015745	2.241934	1.421174
127	1	0	-6.700351	1.735732	3.096585
128	6	0	-8.507148	2.904294	2.849440
129	1	0	7.270467	-1.013861	-1.005740
130	1	0	6.750514	-1.362904	-2.669122
131	6	0	8.886473	-1.100998	-2.452153
132	1	0	1.690709	6.592429	-2.792869
133	1	0	2.251416	6.959678	-1.146571
134	6	0	2.876614	8.395427	-2.647547
135	6	0	-2.819848	10.148122	-1.644237
136	6	0	-7.950054	6.959529	-1.529467
137	6	0	-10.221695	-2.804310	1.867191
138	6	0	-7.067189	-7.932726	1.697812
139	6	0	2.811745	-10.153606	-1.657283
140	6	0	7.921931	-6.970210	-1.495178
141	6	0	10.182853	2.811901	1.854693
142	6	0	7.017155	7.928279	1.696451
143	6	0	-2.451531	11.616985	-1.797639
144	1	0	-3.481474	9.823735	-2.461557
145	1	0	-3.354221	9.981885	-0.696989
146	6	0	-9.436190	7.265081	-1.650998
147	1	0	-7.546839	7.364423	-0.589229
148	1	0	-7.387793	7.416535	-2.357675
149	6	0	-11.690587	-2.427379	1.996159
150	1	0	-10.040492	-3.331681	0.918880
151	1	0	-9.915413	-3.473080	2.685505
152	6	0	-7.399857	-9.416065	1.765049
153	1	0	-7.533646	-7.389328	2.533208
154	1	0	-7.445724	-7.495205	0.762145
155	6	0	2.468641	-11.625375	-1.838097
156	1	0	3.464686	-9.804110	-2.471202
157	1	0	3.348984	-9.998353	-0.709750
158	6	0	9.411190	-7.268819	-1.593978
159	1	0	7.503370	-7.392556	-0.569521
160	1	0	7.375495	-7.413622	-2.341284
161	6	0	11.653167	2.437710	1.975208
162	1	0	9.999346	3.355329	0.915959
163	1	0	9.874609	3.465053	2.684865
164	6	0	7.347261	9.412010	1.768049
165	1	0	7.483143	7.383462	2.531170
166	1	0	7.397849	7.493835	0.760226
167	1	0	-1.993363	-5.210971	1.558788
168	1	0	-5.509619	0.502660	1.645008
169	1	0	5.150117	-1.929395	-1.199497
170	1	0	-0.535185	-5.483934	-1.266128
171	1	0	1.947844	5.198187	1.554254
172	1	0	5.482583	-0.510030	1.617038
173	1	0	-5.188764	1.914179	-1.217960
174	1	0	0.499385	5.454662	-1.284494
175	6	0	-3.681797	12.532433	-1.777695
176	1	0	-1.767591	11.890101	-0.984945
177	1	0	-1.895577	11.747245	-2.733756
178	6	0	-9.734763	8.768504	-1.605025
179	1	0	-9.810406	6.831594	-2.586235
180	1	0	-9.961998	6.753396	-0.835685
181	6	0	-12.616863	-3.648751	1.947672
182	1	0	-11.834170	-1.878213	2.934296
183	1	0	-11.942739	-1.734163	1.184620
184	6	0	-8.908648	-9.679670	1.680568
185	1	0	-6.883222	-9.924610	0.941975
186	1	0	-6.991909	-9.829466	2.695179
187	6	0	3.720628	-12.511230	-1.841632
188	1	0	1.794402	-11.928892	-1.028064
189	1	0	1.911864	-11.748464	-2.774667
190	6	0	9.713641	-8.771947	-1.611152
191	1	0	9.806211	-6.792459	-2.499215
192	1	0	9.916201	-6.793639	-0.744079
193	6	0	12.573896	3.664237	1.968107
194	1	0	11.797006	1.860153	2.896013

195	1	0	11.910232	1.771347	1.142948	298	6	0	-13.365005	12.396812	-1.543284
196	6	0	8.855770	9.677767	1.686273	299	1	0	-13.494360	10.481194	-2.537906
197	1	0	6.831034	9.921857	0.945530	300	1	0	-13.534934	10.380225	-0.786007
198	1	0	6.937450	9.822345	2.698703	301	6	0	-17.470713	-5.317762	1.860649
199	6	0	-10.073568	1.245211	-1.449692	302	1	0	-16.754120	-3.533496	2.849831
200	1	0	-9.160435	1.625164	-3.380481	303	1	0	-16.730663	-3.436891	1.097414
201	1	0	-8.828134	0.021378	-2.734326	304	6	0	-12.627986	-13.199515	1.374261
202	6	0	-3.298248	-9.560080	-1.657217	305	1	0	-10.602143	-13.387373	0.645884
203	1	0	-3.794298	-7.864998	-2.912131	306	1	0	-10.736111	-13.436668	2.395554
204	1	0	-2.489789	-8.862512	-3.546621	307	6	0	5.634240	-17.260831	-2.030354
205	6	0	9.590111	-3.266508	1.868410	308	1	0	3.718710	-16.679735	-1.214404
206	1	0	8.911427	-2.489486	3.777282	309	1	0	3.801569	-16.595131	-2.966075
207	1	0	7.914689	-3.791745	3.137675	310	6	0	13.357367	-12.387850	-1.656457
208	6	0	1.315877	10.080350	1.590670	311	1	0	13.543158	-10.378502	-2.431923
209	1	0	0.085621	8.905781	2.935333	312	1	0	13.456643	-10.461793	-0.680506
210	1	0	1.692075	9.258728	3.564189	313	6	0	17.414920	5.367286	1.952347
211	6	0	-1.333324	-10.086069	1.615035	314	1	0	16.727746	3.493810	2.784479
212	1	0	-0.137871	-8.898751	2.977851	315	1	0	16.672682	3.558607	1.031087
213	1	0	-1.750499	-9.266048	3.581634	316	6	0	12.573408	13.198683	1.387348
214	6	0	-9.605050	3.243682	1.835192	317	1	0	10.548242	13.386898	0.657016
215	1	0	-8.954009	2.525821	3.777491	318	1	0	10.680399	13.436034	2.406826
216	1	0	-7.950309	3.812834	3.116408	319	6	0	-5.083596	18.846959	-1.846251
217	6	0	10.043167	-1.244449	-1.456587	320	1	0	-6.086910	17.125315	-2.686147
218	1	0	9.109715	-1.660441	-3.369512	321	1	0	-6.021223	17.127781	-0.932181
219	1	0	8.778493	-0.047903	-2.746037	322	6	0	-14.867237	12.705401	-1.528304
220	6	0	3.273777	9.523578	-1.688883	323	1	0	-12.900622	12.816971	-0.639716
221	1	0	3.767626	7.818625	-2.931288	324	1	0	-12.895749	12.914171	-2.392232
222	1	0	2.467391	8.815791	-3.574908	325	6	0	-18.955061	-4.933577	1.829327
223	6	0	-3.329104	14.022479	-1.867596	326	1	0	-17.230056	-5.905122	0.962990
224	1	0	-4.351882	12.266898	-2.607600	327	1	0	-17.284515	-5.983209	2.715706
225	1	0	-4.254398	12.354879	-0.856136	328	6	0	-12.978434	-14.688815	1.272988
226	6	0	-11.233732	9.086327	-1.673140	329	1	0	-13.149011	-12.760864	2.237264
227	1	0	-9.319125	9.195876	-0.681322	330	1	0	-13.016615	-12.675848	0.489085
228	1	0	-9.217742	9.273498	-2.433267	331	6	0	5.346492	-18.765953	-2.093405
229	6	0	-14.104061	-3.277647	2.005267	332	1	0	6.281715	-16.979638	-2.873211
230	1	0	-12.424720	-4.217306	1.026546	333	1	0	6.211283	-17.041239	-1.120669
231	1	0	-12.377807	-4.326761	2.779156	334	6	0	14.856172	-12.698027	-1.558825
232	6	0	-9.263192	-11.171505	1.673118	335	1	0	12.827830	-12.902866	-0.842082
233	1	0	-9.416748	-9.189215	2.522942	336	1	0	12.958881	-12.810258	-2.590059
234	1	0	-9.310388	-9.212592	0.769969	337	6	0	18.899716	5.002637	1.832296
235	6	0	3.411610	-14.008066	-1.970237	338	1	0	17.141514	6.043235	1.129573
236	1	0	4.383036	-12.206732	-2.664364	339	1	0	17.252931	5.937600	2.878062
237	1	0	4.289263	-12.341983	-0.916067	340	6	0	12.924552	14.687670	1.284384
238	6	0	11.215956	-9.081490	-1.621272	341	1	0	13.093309	12.761003	2.251512
239	1	0	9.255256	-9.249604	-0.733384	342	1	0	12.962941	12.673761	0.503314
240	1	0	9.240572	-9.232689	-2.489886	343	6	0	-6.312014	19.763761	-1.800226
241	6	0	14.063283	3.298224	1.993239	344	1	0	-4.430425	19.073659	-0.991177
242	1	0	12.369642	4.270755	1.074166	345	1	0	-4.493751	19.074804	-2.745502
243	1	0	12.340708	4.304960	2.830212	346	6	0	-15.186361	14.203054	-1.446282
244	6	0	9.208766	11.169966	1.681652	347	1	0	-15.334267	12.283446	-2.429565
245	1	0	9.363208	9.186496	2.528570	348	1	0	-15.333413	12.188802	-0.676836
246	1	0	9.259399	9.212666	0.775497	349	6	0	-19.900762	-6.137614	1.741717
247	6	0	-4.555633	14.942301	-1.832810	350	1	0	-19.197629	-4.345760	2.726059
248	1	0	-2.657048	14.283564	-1.037932	351	1	0	-19.137638	-4.267353	0.973743
249	1	0	-2.759437	14.207349	-2.788995	352	6	0	-14.482186	-14.959183	1.139365
250	6	0	-11.546470	10.585929	-1.603706	353	1	0	-12.454434	-15.124908	0.410173
251	1	0	-11.652532	8.668145	-2.599161	354	1	0	-12.591890	-15.214405	2.157803
252	1	0	-11.747333	8.571380	-0.848950	355	6	0	6.611728	-19.632154	-2.071119
253	6	0	-15.041712	-4.489154	1.937617	356	1	0	4.700180	-19.046414	-1.249143
254	1	0	-14.302989	-2.712592	2.926573	357	1	0	4.769571	-18.988418	-3.002309
255	1	0	-14.335686	-2.595152	1.175358	358	6	0	15.179858	-14.195470	-1.628750
256	6	0	-10.769383	-11.440112	1.564460	359	1	0	15.389387	-12.173718	-2.364825
257	1	0	-8.747450	-11.658422	0.833408	360	1	0	15.250033	-12.285692	-0.618485
258	1	0	-8.871556	-11.644278	2.584620	361	6	0	19.834396	6.217899	1.867140
259	6	0	4.667945	-14.887239	-1.960009	362	1	0	19.172109	4.312013	2.643010
260	1	0	2.749022	-14.311473	-1.147412	363	1	0	19.060424	4.448055	0.896646
261	1	0	2.847270	-14.186084	-2.896218	364	6	0	14.428602	14.956678	1.151590
262	6	0	11.533755	-10.581087	-1.657605	365	1	0	12.401558	15.122800	0.420465
263	1	0	11.683138	-8.589084	-2.485625	366	1	0	12.537557	15.214780	2.168077
264	1	0	11.679740	-8.634064	-0.730767	367	6	0	-5.965425	21.257562	-1.796109
265	6	0	14.993581	4.517322	1.993377	368	1	0	-6.960405	19.543832	-2.660415
266	1	0	14.272268	2.679726	2.877186	369	1	0	-6.906714	19.527609	-0.906171
267	1	0	14.291999	2.668670	1.121743	370	6	0	-16.688336	14.509745	-1.409603
268	6	0	10.714952	11.439531	1.575368	371	1	0	-14.708258	14.627147	-0.551724
269	1	0	8.693802	11.657698	0.841933	372	1	0	-14.731401	14.718239	-2.304336
270	1	0	8.815558	11.641020	2.593346	373	6	0	-21.383531	-5.750372	1.689915
271	6	0	-4.205276	16.434806	-1.876512	374	1	0	-19.650090	-6.731166	0.850870
272	1	0	-5.217014	14.698425	-2.676410	375	1	0	-19.727599	-6.798514	2.603071
273	1	0	-5.137139	14.734664	-0.923166	376	6	0	-14.830047	-16.447793	1.021409
274	6	0	-13.047742	10.898702	-1.624335	377	1	0	-15.006304	-14.531410	2.006026
275	1	0	-11.102987	11.005946	-0.689609	378	1	0	-14.869562	-14.425967	0.259332
276	1	0	-11.055083	11.100059	-2.441992	379	6	0	6.328595	-21.138538	-2.119054
277	6	0	-16.527997	-4.110944	1.942170	380	1	0	7.254137	-19.356834	-2.919800
278	1	0	-14.819322	-5.068335	1.029984	381	1	0	7.192310	-19.401772	-1.166341
279	1	0	-14.832655	-5.159835	2.783191	382	6	0	16.676499	-14.508117	-1.510270
280	6	0	-11.123113	-12.930627	1.499664	383	1	0	14.635819	-14.721748	-0.831192
281	1	0	-11.284495	-10.979737	2.419606	384	1	0	14.797630	-14.604545	-2.575121
282	1	0	-11.162222	-10.937589	0.668935	385	6	0	21.316122	5.857449	1.706088
283	6	0	4.372479	-16.389526	-2.049479	386	1	0	19.544509	6.920854	1.073190
284	1	0	5.321694	-14.595422	-2.794330	387	1	0	19.692004	6.757283	2.814384
285	1	0	5.240981	-14.686794	-1.043387	388	6	0	14.777780	16.444637	1.029822
286	6	0	13.035129	-10.889528	-1.601633	389	1	0	14.951521	14.530818	2.019905
287	1	0	11.031478	-11.079161	-0.815936	390	1	0	14.816423	14.420775	0.273388
288	1	0	11.104806	-11.021461	-2.569036	391	6	0	-7.195068	22.173048	-1.751087
289	6	0	16.481700	4.150352	1.937849	392	1	0	-5.318945	21.478312	-0.934407
290	1	0	14.748709	5.159672	1.135412	393	1	0	-5.369483	21.495725	-2.688870
291	1	0	14.799284	5.123089	2.889890	394	6	0	-17.008338	16.007639	-1.332647
292	6	0	11.068361	12.930106	1.511299	395	1	0	-17.169026	14.082613	-2.301407
293	1	0	11.229029	10.979144	2.431126	396	1	0	-17.142221	13.998289	-0.548421
294	1	0	11.109313	10.937403	0.680291	397	6	0	-22.330770	-6.953186	1.600133
295	6	0	-5.432434	17.353448	-1.832793	398	1	0	-21.636162	-5.156440	2.579999
296	1	0	-3.543334	16.675140	-1.032085	399	1	0	-21.556215	-5.089606	0.828004
297	1	0	-3.624420	16.646556	-2.785438	400	6	0	-16.333382	-16.719385	0.885643

401	1	0	-14.305750	-16.875509	0.154484	504	1	0	-10.018622	5.253328	2.525283
402	1	0	-14.443620	-16.982520	1.900943	505	6	0	12.550333	-0.876539	-1.046567
403	6	0	7.595699	-22.002107	-2.096604	506	1	0	11.605141	-1.249493	-2.953434
404	1	0	5.687593	-21.414915	-1.269434	507	1	0	11.262757	0.337403	-2.286269
405	1	0	5.747763	-21.371316	-3.023105	508	6	0	4.729097	11.602396	-1.331913
406	6	0	17.000594	-16.005158	-1.588622	509	1	0	5.259274	9.849359	-2.481911
407	1	0	17.223054	-13.977752	-2.303477	510	1	0	4.023357	10.847055	-3.229972
408	1	0	17.057712	-14.104986	-0.560641	511	6	0	-13.917388	0.379950	-1.464031
409	6	0	22.251954	7.071282	1.758929	512	1	0	-12.307604	0.450558	-0.023917
410	1	0	21.604983	5.143580	2.490646	513	1	0	-12.670394	1.999287	-0.762716
411	1	0	21.459538	5.330524	0.751775	514	6	0	-5.873255	-12.536503	-1.819040
412	6	0	16.281535	16.714289	0.894663	515	1	0	-3.862575	-12.245178	-1.079284
413	1	0	14.254748	16.870324	0.161150	516	1	0	-5.059615	-11.215597	-0.314351
414	1	0	14.391047	16.982247	1.907453	517	6	0	12.594968	-5.809498	2.014789
415	6	0	-6.841105	23.663127	-1.741037	518	1	0	11.261724	-5.014593	0.509999
416	1	0	-7.839014	21.955011	-2.613925	519	1	0	12.282263	-3.804019	1.266717
417	1	0	-7.791618	21.932651	-0.860475	520	6	0	0.437348	13.913851	1.376869
418	6	0	-18.510154	16.304541	-1.287995	521	1	0	2.082471	12.643556	0.784897
419	1	0	-16.524026	16.435674	-0.444435	522	1	0	0.552313	12.222792	0.037832
420	1	0	-16.559939	16.517371	-2.196271	523	6	0	-0.338856	-13.890677	1.404378
421	6	0	-23.808815	-6.556384	1.540836	524	1	0	-2.020889	-12.675617	0.798247
422	1	0	-22.075793	-7.548237	0.712592	525	1	0	-0.498491	-12.202041	0.066515
423	1	0	-22.162056	-7.611054	2.463515	526	6	0	-12.662298	5.727812	1.742898
424	6	0	-16.671252	-18.208220	0.763741	527	1	0	-11.256818	4.863941	0.350273
425	1	0	-16.856812	-16.294982	1.753271	528	1	0	-12.272870	3.685691	1.159467
426	1	0	-16.719619	-16.183223	0.008026	529	6	0	13.871879	-0.326674	-1.597510
427	6	0	7.306323	-23.505542	-2.138451	530	1	0	12.309635	-0.367707	-0.102211
428	1	0	8.234235	-21.728553	-2.947658	531	1	0	12.675228	-1.938670	-0.792427
429	1	0	8.177259	-21.766625	-1.194798	532	6	0	5.860601	12.488906	-1.866199
430	6	0	18.496029	-16.309929	-1.460343	533	1	0	3.837499	12.219512	-1.152282
431	1	0	16.449996	-16.535879	-0.799725	534	1	0	5.017972	11.198607	-0.350870
432	1	0	16.625891	-16.406155	-2.540459	535	6	0	-15.053445	0.591250	-0.455344
433	6	0	23.728071	6.704687	1.578865	536	1	0	-14.183758	0.856204	-2.418314
434	1	0	21.955990	7.789937	0.982779	537	1	0	-13.818593	-0.693809	-1.680143
435	1	0	22.116937	7.589580	2.717894	538	6	0	-6.249438	-13.677303	-0.864909
436	6	0	16.620977	18.202299	0.767882	539	1	0	-6.764412	-11.924719	-2.021288
437	1	0	16.803573	16.292353	1.764316	540	1	0	-5.571006	-12.957785	-2.788433
438	1	0	16.668103	16.174660	0.019332	541	6	0	13.741987	-6.179730	1.066100
439	1	0	-7.738951	24.288781	-1.706289	542	1	0	13.011423	-5.499822	2.983969
440	1	0	-6.224873	23.917967	-0.871256	543	1	0	11.991291	-6.705604	2.219516
441	1	0	-6.275896	23.942703	-2.637419	544	6	0	0.669044	14.990401	0.309054
442	1	0	-18.704787	17.380726	-1.236694	545	1	0	-0.641419	13.817888	1.568023
443	1	0	-19.017329	15.917257	-2.178975	546	1	0	0.883978	14.239591	2.327154
444	1	0	-18.980450	15.839951	-0.413904	547	6	0	-0.512511	-14.971719	0.330114
445	1	0	-24.458064	-7.435473	1.474442	548	1	0	0.732487	-13.755836	1.613002
446	1	0	-24.104199	-5.991873	2.432558	549	1	0	-0.787923	-14.235964	2.346597
447	1	0	-24.014536	-5.924854	0.669024	550	6	0	-13.776372	5.967187	0.715969
448	1	0	-17.750306	-18.368424	0.670457	551	1	0	-13.108292	5.484367	2.717741
449	1	0	-16.191998	-18.652700	-0.115973	552	1	0	-12.097135	6.659122	1.892800
450	1	0	-16.327056	-18.765646	1.642342	553	6	0	15.049975	-0.459018	-0.624619
451	1	0	8.230549	-24.092278	-2.120412	554	1	0	14.116704	-0.843204	-2.536564
452	1	0	6.698837	-23.816346	-1.280843	555	1	0	13.740025	0.732414	-1.862856
453	1	0	6.757137	-23.778735	-3.046675	556	6	0	6.216836	13.654204	-0.934393
454	1	0	18.693760	-17.385025	-1.523660	557	1	0	6.755299	11.871801	-2.033628
455	1	0	19.069983	-15.819025	-2.254733	558	1	0	5.579599	12.885337	-2.852347
456	1	0	18.891903	-15.955090	-0.501783	559	6	0	-16.404418	0.026924	-0.911603
457	1	0	24.369771	7.590423	1.627416	560	1	0	-14.775394	0.129268	0.502971
458	1	0	24.062296	6.009605	2.357399	561	1	0	-15.159702	1.666269	-0.250622
459	1	0	23.901494	6.222001	0.610393	562	6	0	-7.393499	-14.559613	-1.378897
460	1	0	17.700294	18.361091	0.675175	563	1	0	-5.364016	-14.301664	-0.678579
461	1	0	16.143213	18.644151	-0.113967	564	1	0	-6.530094	-13.254725	0.110706
462	1	0	16.276437	18.763266	1.644076	565	6	0	14.628572	-7.316027	1.590037
463	6	0	-11.417893	0.723639	-1.972751	566	1	0	13.326138	-6.466867	0.089522
464	1	0	-9.816773	0.723293	-0.517532	567	1	0	14.361242	-5.290635	0.880055
465	1	0	-10.167141	2.306428	-1.193019	568	6	0	0.065255	16.356151	0.657321
466	6	0	-4.375001	-10.489796	-2.230281	569	1	0	1.749300	15.103618	0.138696
467	1	0	-2.405598	-10.142931	-1.403439	570	1	0	0.248976	14.645309	-0.646782
468	1	0	-3.658115	-9.120489	-0.716718	571	6	0	0.134515	-16.314765	0.688574
469	6	0	10.538166	-4.333443	2.429095	572	1	0	-1.584463	-15.123930	0.139236
470	1	0	9.142486	-3.627731	0.932323	573	1	0	-0.087404	-14.609301	-0.617070
471	1	0	10.158372	-2.365060	1.611941	574	6	0	-14.741422	7.102448	1.078625
472	6	0	0.792487	11.450468	2.039227	575	1	0	-13.321927	6.182353	-0.262020
473	1	0	2.378713	10.159372	1.335343	576	1	0	-14.347328	5.037047	0.582348
474	1	0	0.798754	9.776938	0.670122	577	6	0	16.366245	0.102633	-1.176386
475	6	0	-0.781074	-11.443522	2.067286	578	1	0	14.802928	0.054669	0.315689
476	1	0	-2.392266	-10.188791	1.352137	579	1	0	15.188037	-1.517579	-0.361948
477	1	0	-0.816622	-9.771573	0.697982	580	6	0	7.375257	14.519886	-1.444521
478	6	0	-10.574796	4.325693	2.326170	581	1	0	5.328612	14.285020	-0.786989
479	1	0	-9.141263	3.570644	0.894354	582	1	0	6.472536	13.258100	0.059052
480	1	0	-10.163820	2.330317	1.601566	583	6	0	-17.530590	0.244593	0.106716
481	6	0	11.372469	-0.723305	-2.016414	584	1	0	-16.686598	0.484918	-1.870288
482	1	0	9.797568	-0.706490	-0.530546	585	1	0	-16.299012	-1.049386	-1.111136
483	1	0	10.147451	-2.300260	-1.182020	586	6	0	-7.772305	-15.694089	-0.418476
484	6	0	4.358843	10.442322	-2.264288	587	1	0	-8.277556	-13.932679	-1.565205
485	1	0	2.382965	10.113324	-1.444655	588	1	0	-7.115764	-14.985462	-2.353626
486	1	0	3.626399	9.090091	-0.742835	589	6	0	15.778492	-7.685792	0.644809
487	6	0	-12.568805	0.926702	-0.979896	590	1	0	15.040338	-7.034349	2.569714
488	1	0	-11.662720	1.225411	-2.919919	591	1	0	14.007071	-8.205318	1.769398
489	1	0	-11.327655	-0.346130	-2.212011	592	6	0	0.308212	17.421225	-0.419289
490	6	0	-4.753980	-11.635390	-1.283495	593	1	0	-1.016835	16.243288	0.817997
491	1	0	-5.274181	-9.902278	-2.467129	594	1	0	0.477141	16.705200	1.615043
492	1	0	-4.027965	-10.908786	-3.185747	595	6	0	-0.032508	-17.381593	-0.400655
493	6	0	11.682312	-4.701032	1.476147	596	1	0	1.205823	-16.159760	0.882529
494	1	0	10.960330	-3.983242	3.382077	597	1	0	-0.291510	-16.685319	1.631827
495	1	0	9.962501	-5.239311	2.669486	598	6	0	-15.842263	7.311420	0.031401
496	6	0	1.006385	12.544595	0.986034	599	1	0	-15.200604	6.896227	2.055940
497	1	0	-0.279632	11.373884	2.272456	600	1	0	-14.174734	8.036744	1.202209
498	1	0	1.285912	11.745141	2.976556	601	6	0	17.543724	-0.014041	-0.200806
499	6	0	-0.950567	-12.541176	1.009632	602	1	0	16.617553	-0.415782	-2.112668
500	1	0	0.285651	-11.338855	2.314007	603	1	0	16.223487	1.158998	-1.446603
501	1	0	-1.277929	-11.753206	2.997946	604	6	0	7.725178	15.687492	-0.513311
502	6	0	-11.700389	4.609509	1.323726	605	1	0	8.264635	13.888206	-1.583487
503	1	0	-11.011469	4.021438	3.288279	606	1	0	7.125976	14.911947	-2.440897

607	6	0	-18.878488	-0.344899	-0.325284
608	1	0	-17.236547	-0.196249	1.070034
609	1	0	-17.647833	1.322016	0.291494
610	6	0	-8.931869	-16.563332	-0.919218
611	1	0	-6.892446	-16.329086	-0.241811
612	1	0	-8.037405	-15.266865	0.559277
613	6	0	18.857520	0.551444	-0.753973
614	1	0	17.291846	0.505026	0.735077
615	1	0	17.688487	-1.069960	0.069017
616	6	0	8.900733	16.538482	-1.008186
617	1	0	6.840713	16.328117	-0.387234
618	1	0	7.958933	15.295394	0.486897
619	6	0	-20.003118	-0.111550	0.691140
620	1	0	-19.171451	0.083838	-1.294469
621	1	0	-18.764231	-1.425392	-0.495764
622	6	0	-9.309695	-17.697094	0.042394
623	1	0	-9.812664	-15.927959	-1.092428
624	1	0	-8.671340	-16.990254	-1.898396
625	6	0	20.037381	0.431908	0.218337
626	1	0	19.108535	0.036402	-1.692387
627	1	0	18.714064	1.608847	-1.020078
628	6	0	9.244072	17.710925	-0.080761
629	1	0	9.787695	15.898850	-1.125358
630	1	0	8.673864	16.925426	-2.012091
631	6	0	-21.341103	-0.724868	0.268099
632	1	0	-19.702652	-0.525915	1.663151
633	1	0	-20.128446	0.968363	0.848798
634	6	0	-10.476369	-18.553516	-0.458386
635	1	0	-8.432038	-18.336062	0.210017
636	1	0	-9.564268	-17.269798	1.021817
637	6	0	21.344723	0.999052	-0.343088
638	1	0	19.787251	0.948034	1.155139
639	1	0	20.180787	-0.624406	0.483809
640	6	0	10.428132	18.547614	-0.574154
641	1	0	8.360869	18.354826	0.029027
642	1	0	9.463311	17.324247	0.923779
643	1	0	-22.122553	-0.533740	1.010821
644	1	0	-21.683165	-0.311782	-0.687746
645	1	0	-21.257954	-1.811037	0.146454
646	1	0	-10.717766	-19.354726	0.247633
647	1	0	-11.380420	-17.949154	-0.595592
648	1	0	-10.242109	-19.019039	-1.422510
649	1	0	22.167702	0.893344	0.371260
650	1	0	21.636526	0.483606	-1.265204
651	1	0	21.245262	2.064747	-0.579184
652	1	0	10.644176	19.377588	0.106418
653	1	0	11.336501	17.939358	-0.654182
654	1	0	10.228550	18.972807	-1.564413
655	6	0	16.647227	-8.840788	1.157134
656	1	0	15.367137	-7.952011	-0.339423
657	1	0	16.410450	-6.801621	0.478948
658	6	0	-0.324885	18.780692	-0.100605
659	1	0	1.390572	17.549538	-0.563512
660	1	0	-0.082849	17.058244	-1.380635
661	6	0	0.634626	-18.719803	-0.062525
662	1	0	-1.103495	-17.546545	-0.585915
663	1	0	0.381749	-17.000994	-1.345214
664	6	0	-16.804785	8.460365	0.355218
665	1	0	-15.376933	7.496966	-0.947306
666	1	0	-16.415270	6.379711	-0.079864
667	6	0	17.804787	-9.203473	0.218576
668	1	0	17.051137	-8.582222	2.146619
669	1	0	16.016071	-9.728001	1.312036
670	6	0	-0.071667	19.842628	-1.177839
671	1	0	-1.409134	18.653681	0.033001
672	1	0	0.057064	19.145031	0.864043
673	6	0	0.475075	-19.778480	-1.160897
674	1	0	1.705118	-18.553255	0.126572
675	1	0	0.219173	-19.106435	0.879132
676	6	0	-17.901343	8.652122	-0.699487
677	1	0	-17.270954	8.282714	1.335077
678	1	0	-16.234634	9.395240	0.457315
679	6	0	18.658643	-10.366901	0.731216
680	1	0	17.401499	-9.454926	-0.771790
681	1	0	18.440349	-8.319704	0.071020
682	6	0	-0.722989	21.192796	-0.864333
683	1	0	1.011229	19.978511	-1.303255
684	1	0	-0.443508	19.472990	-2.143221
685	6	0	1.150044	-21.110300	-0.821096
686	1	0	-0.593827	-19.948087	-1.348414
687	1	0	0.888586	-19.389024	-2.101038
688	6	0	-18.852756	9.810249	-0.384179
689	1	0	-17.433573	8.819773	-1.679182
690	1	0	-18.476635	7.721140	-0.794937
691	1	0	19.478080	-10.597300	0.042632
692	1	0	19.099764	-10.135595	1.707535
693	1	0	18.058439	-11.276558	0.848685
694	1	0	-0.517991	21.928998	-1.648485
695	1	0	-1.811267	21.096490	-0.775840
696	1	0	-0.350735	21.602631	0.081634
697	1	0	1.018607	-21.842330	-1.624506
698	1	0	2.227139	-20.979502	-0.665389
699	1	0	0.734584	-21.544045	0.095672
700	1	0	-19.625179	9.915788	-1.153035
701	1	0	-19.358648	9.657909	0.576107
702	1	0	-18.312269	10.761952	-0.324385

Table S22. Cartesian coordinates for the optimized structure of **6a**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.709450	-3.153004	0.944676
2	6	0	-7.725212	-1.782640	0.581715
3	6	0	-6.570290	-0.939086	0.869543
4	6	0	-5.340664	-1.582111	1.126223
5	6	0	-6.628833	0.515006	0.933306
6	6	0	-5.430210	1.286865	0.911489
7	6	0	-4.201524	0.577448	0.700472
8	6	0	-4.149326	-0.820952	0.853635
9	6	0	-7.847407	1.197349	1.204918
10	6	0	-7.897551	2.561578	1.412347
11	6	0	-6.695555	3.328462	1.372017
12	6	0	-5.496228	2.683909	1.141579
13	6	0	-8.806054	-3.973100	0.583035
14	6	0	-8.814369	-1.310662	-0.200914
15	1	0	-8.750760	0.618636	1.325701
16	8	0	-9.023128	3.268658	1.709109
17	8	0	-6.841354	4.654952	1.618757
18	1	0	-4.577725	3.247554	1.198931
19	6	0	-9.879651	-3.485840	-0.137787
20	6	0	-9.870406	-2.125761	-0.560485
21	8	0	-10.926578	-1.750618	-1.335429
22	8	0	-10.962139	-4.212657	-0.529043
23	6	0	-11.014615	-5.579646	-0.158041
24	6	0	-10.940312	-0.428782	-1.846914
25	6	0	-10.242964	2.558822	1.835480
26	6	0	-5.671691	5.464575	1.618683
27	1	0	-8.784673	-5.022573	0.842985
28	1	0	-8.780425	-0.299435	-0.578971
29	1	0	-10.994668	-5.704171	0.932542
30	1	0	-11.960039	-5.960113	-0.546984
31	1	0	-10.187130	-6.151584	-0.598069
32	1	0	-11.849986	-0.347465	-2.443465
33	1	0	-10.968722	0.318078	-1.042235
34	1	0	-10.069175	-0.230065	-2.484064
35	1	0	-11.001285	3.305622	2.074950
36	1	0	-10.516804	2.053121	0.899846
37	1	0	-10.199421	1.814996	2.641244
38	1	0	-6.012649	6.481056	1.818564
39	1	0	-4.971578	5.158864	2.406338
40	1	0	-5.161883	5.437302	0.649228
41	6	0	-3.696219	6.460273	-1.679394
42	6	0	-0.961653	6.535369	-0.860889
43	6	0	-1.584599	5.284889	-1.077945
44	6	0	-2.917634	5.277661	-1.671241
45	6	0	0.488316	6.610287	-0.912458
46	6	0	1.274011	5.417678	-0.850100
47	6	0	0.576217	4.191268	-0.608916
48	6	0	-0.808242	4.118629	-0.764865
49	6	0	1.160354	7.830567	-1.208207
50	6	0	2.524226	7.890991	-1.407049
51	6	0	3.304006	6.698053	-1.332375
52	6	0	2.673558	5.498223	-1.073520
53	6	0	-1.169412	2.740254	-0.380270
54	7	0	-0.054190	2.005107	-0.117249
55	6	0	1.010311	2.851082	-0.195638
56	6	0	-4.936171	6.460831	-2.364901
57	6	0	-3.386862	4.156983	-2.405043
58	1	0	0.572286	8.723464	-1.358593
59	8	0	3.221975	9.016715	-1.729136
60	8	0	4.630705	6.853812	-1.579492
61	1	0	3.249449	4.586077	-1.105791
62	6	0	-5.398453	5.346828	-3.040335
63	6	0	-4.597776	4.168350	-3.069774
64	8	0	-6.570617	5.273360	-3.728744
65	8	0	-5.103434	3.137575	-3.799550
66	6	0	-7.405790	6.417832	-3.742347
67	6	0	-4.356378	1.930275	-3.848173
68	6	0	2.499119	10.224016	-1.891174
69	6	0	5.450765	5.693043	-1.558143
70	6	0	-2.469231	2.302721	-0.082436
71	1	0	-5.518447	7.371439	-2.397793
72	1	0	-2.756354	3.283086	-2.472586
73	1	0	-8.286502	6.139927	-4.323081
74	1	0	-7.715911	6.704454	-2.728872
75	1	0	-6.913417	7.274260	-4.221688
76	1	0	-4.949809	1.236585	-4.445297
77	1	0	-3.380903	2.077488	-4.329241
78	1	0	-4.202397	1.510694	-2.846754
79	1	0	3.238311	10.985036	-2.145692
80	1	0	1.760532	10.151323	-2.699804
81	1	0	1.984054	10.516136	-0.966093
82	1	0	5.431992	5.202602	-0.578430
83	1	0	5.149086	4.973162	-2.329555
84	1	0	6.463590	6.038809	-1.768975
85	6	0	-2.796666	-1.233549	0.514516
86	7	0	-2.082819	-0.080551	0.301444
87	6	0	-2.880856	1.034995	0.325701
88	1	0	-1.106758	-0.076699	0.024739
89	6	0	-2.308931	-2.503433	0.209753
90	6	0	3.696183	-6.460327	-1.679448
91	6	0	0.961625	-6.535409	-0.860923
92	6	0	1.584586	-5.284934	-1.077969
93	6	0	2.917619	-5.277705	-1.671250
94	6	0	-0.488354	-6.610300	-0.912507
95	6	0	-1.274021	-5.417673	-0.850101
96	6	0	-0.576204	-4.191285	-0.608916
97	6	0	0.808248	-4.118662	-0.764890
98	6	0	-1.160441	-7.830533	-1.208345
99	6	0	-2.524317	-7.890897	-1.407190
100	6	0	-3.304062	-6.697940	-1.332442
101	6	0	-2.673569	-5.498150	-1.073518
102	6	0	1.169440	-2.740294	-0.380299
103	7	0	0.054233	-2.005148	-0.117209
104	6	0	-1.010280	-2.851105	-0.195620
105	6	0	4.936139	-6.460873	-2.364947
106	6	0	3.386882	-4.156984	-2.404963
107	1	0	-0.572416	-8.723443	-1.358801
108	8	0	-3.222103	-9.016578	-1.729344
109	8	0	-4.630760	-6.853631	-1.579593
110	1	0	-3.249426	-4.585974	-1.105712
111	6	0	5.398447	-5.346840	-3.040318
112	6	0	4.597800	-4.168338	-3.069683
113	8	0	6.570621	-5.273353	-3.728704
114	8	0	5.103496	-3.137522	-3.799376
115	6	0	7.405770	-6.417841	-3.742378
116	6	0	4.356472	-1.930199	-3.847916
117	6	0	-2.499296	-10.223904	-1.891401
118	6	0	-5.450810	-5.692858	-1.557958
119	6	0	2.469276	-2.302762	-0.082539
120	1	0	5.518407	-7.371485	-2.397870
121	1	0	2.756398	-3.283062	-2.472436
122	1	0	6.913382	-7.274227	-4.221780
123	1	0	8.286494	-6.139915	-4.323084
124	1	0	7.715878	-6.704539	-2.728920
125	1	0	4.949930	-1.236477	-4.444976
126	1	0	3.381000	-2.077350	-4.329006
127	1	0	4.202489	-1.510692	-2.846465
128	1	0	-3.238518	-10.984889	-2.145938
129	1	0	-1.760701	-10.151229	-2.700025
130	1	0	-1.984250	-10.516060	-0.966321
131	1	0	-5.431892	-5.202562	-0.578175
132	1	0	-5.149242	-4.972871	-2.329313
133	1	0	-6.463668	-6.038587	-1.768697
134	6	0	7.709466	3.152975	0.944740
135	6	0	7.725241	1.782637	0.581700
136	6	0	6.570325	0.939048	0.869508
137	6	0	5.340697	1.582056	1.126200
138	6	0	6.628885	-0.515040	0.933230
139	6	0	5.430262	-1.286904	0.911372
140	6	0	4.201577	-0.577490	0.700363
141	6	0	4.149365	0.820905	0.853577
142	6	0	7.847455	-1.197393	1.204856
143	6	0	7.897595	-2.561625	1.412256
144	6	0	6.695599	-3.328510	1.371891
145	6	0	5.496278	-2.683954	1.141436
146	6	0	2.796696	1.233500	0.514475
147	7	0	2.082863	0.080499	0.301370
148	6	0	2.880911	-1.035040	0.325594
149	6	0	8.806050	3.973110	0.583124
150	6	0	8.814362	1.310730	-0.201019
151	1	0	8.750804	-0.618684	1.325682
152	8	0	9.023166	-3.268711	1.709028
153	8	0	6.841393	-4.655001	1.618625
154	1	0	4.577777	-3.247603	1.198759
155	1	0	1.106801	0.076637	0.024669
156	6	0	9.879628	3.485913	-0.137771
157	6	0	9.870379	2.125867	-0.560570
158	8	0	10.926518	1.750795	-1.335598
159	8	0	10.962094	4.212772	-0.529014
160	6	0	11.014573	5.579730	-0.157901
161	6	0	10.940242	0.428997	-1.847180
162	6	0	10.242997	-2.558876	1.835454
163	6	0	5.671733	-5.464628	1.618499
164	6	0	2.308958	2.503389	0.209740
165	1	0	8.784655	5.022571	0.843121
166	1	0	8.780416	0.299532	-0.579151
167	1	0	10.994657	5.704163	0.932694
168	1	0	11.959984	5.960234	-0.546841
169	1	0	10.187074	6.151702	-0.597857
170	1	0	11.849890	0.347732	-2.443779
171	1	0	10.968696	-0.317924	-1.042558
172	1	0	10.069079	0.230319	-2.484306
173	1	0	11.001313	-3.305681	2.074929
174	1	0	10.516865	-2.053151	0.899841
175	1	0	10.199428	-1.815071	2.641235
176	1	0	4.971603	-5.158946	2.406150
177	1	0	5.161945	-5.437326	0.649036
178	1	0	6.012689	-6.481114	1.818358
179	1	0	-3.252629	3.035883	-0.188861
180	1	0	-3.020532	-3.307501	0.306747
181	1	0	3.252670	-3.035924	-0.189019
182	1	0	3.020556	3.307449	0.306796
183	6	0	-6.563525	-3.680021	1.666699
184	6	0	-5.368385	-2.920516	1.702156
185	6	0	-6.602746	-4.928657	2.335361
186	6	0	-4.275016	-3.418479	2.458311
187	6	0	-5.515218	-5.418375	3.033685
188	6	0	-4.324111	-4.637987	3.104925
189	8	0	-5.478661	-6.599834	3.707058
190	8	0	-3.321751	-5.171300	3.852056
191	6	0	-6.633136	-7.421083	3.673128
192	6	0	-2.098302	-4.452105	3.932533
193	1	0	-7.522809	-5.496523	2.335241
194	1	0	-3.391853	-2.805708	2.558657

195	1	0	-6.892679	-7.710891	2.646528
196	1	0	-6.382800	-8.314327	4.247045
197	1	0	-7.497233	-6.925832	4.135349
198	1	0	-1.429280	-5.069868	4.532916
199	1	0	-1.658075	-4.293315	2.941026
200	1	0	-2.232706	-3.480963	4.425776
201	6	0	6.563539	3.679949	1.666809
202	6	0	5.368397	2.920438	1.702189
203	6	0	6.602761	4.928531	2.335554
204	6	0	4.274999	3.418400	2.458286
205	6	0	5.515219	5.418244	3.033866
206	6	0	4.324076	4.637885	3.104951
207	8	0	5.478644	6.599697	3.707242
208	8	0	3.321653	5.171221	3.851969
209	6	0	6.633129	7.420909	3.673439
210	6	0	2.098227	4.452002	3.932441
211	1	0	7.522834	5.496375	2.335448
212	1	0	3.391798	2.805671	2.558556
213	1	0	7.497199	6.925628	4.135687
214	1	0	6.892757	7.710774	2.646871
215	1	0	6.382798	8.314126	4.247403
216	1	0	1.429195	5.069725	4.532855
217	1	0	1.657984	4.293235	2.940936
218	1	0	2.232656	3.480843	4.425647
219	6	0	-3.194394	7.635893	-0.985913
220	6	0	-1.827348	7.685285	-0.614170
221	6	0	-4.036797	8.726797	-0.661446
222	6	0	-1.381108	8.805458	0.138675
223	6	0	-3.574041	9.830030	0.030500
224	6	0	-2.217202	9.857839	0.460307
225	8	0	-1.865126	10.944466	1.204494
226	8	0	-4.323694	10.910201	0.386434
227	6	0	-5.689042	10.924962	0.007691
228	6	0	-0.544135	11.001901	1.714096
229	1	0	-5.083866	8.678052	-0.927666
230	1	0	-0.372245	8.801293	0.524504
231	1	0	-6.247002	10.098372	0.467217
232	1	0	-6.090729	11.872760	0.368745
233	1	0	-5.808028	10.872823	-1.082545
234	1	0	-0.480882	11.932538	2.279846
235	1	0	-0.327257	10.156921	2.380055
236	1	0	0.201886	11.018179	0.908258
237	6	0	3.194363	-7.635945	-0.985962
238	6	0	1.827325	-7.685324	-0.614181
239	6	0	4.036778	-8.726832	-0.661480
240	6	0	1.381131	-8.805441	0.138775
241	6	0	3.574054	-9.830025	0.030548
242	6	0	2.217240	-9.857805	0.460428
243	8	0	1.865210	-10.944372	1.204723
244	8	0	4.323728	-10.910169	0.386521
245	6	0	5.689059	-10.924952	0.007719
246	6	0	0.544240	-11.001790	1.714379
247	1	0	5.083840	-8.678091	-0.927728
248	1	0	0.372297	-8.801247	0.524672
249	1	0	6.247036	-10.098327	0.467162
250	1	0	6.090765	-11.872724	0.368822
251	1	0	5.807995	-10.872891	-1.082525
252	1	0	0.481020	-11.932389	2.280194
253	1	0	0.327377	-10.156769	2.380290
254	1	0	-0.201811	-11.018131	0.908570

Table S23. Cartesian coordinates for the optimized structure of **6a**-Zn (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.600168	-3.310544	-0.999924
2	6	0	7.655813	-1.940312	-0.640494
3	6	0	6.516134	-1.068853	-0.909072
4	6	0	5.265064	-1.682310	-1.138682
5	6	0	6.607566	0.382137	-0.973945
6	6	0	5.425915	1.181535	-0.931248
7	6	0	4.184841	0.500004	-0.709514
8	6	0	4.098613	-0.890203	-0.856241
9	6	0	7.837458	1.036802	-1.264968
10	6	0	7.916144	2.399273	-1.470983
11	6	0	6.733209	3.194299	-1.406478
12	6	0	5.522938	2.578323	-1.158058
13	6	0	8.682585	-4.156991	-0.656857
14	6	0	8.770841	-1.494366	0.120514
15	1	0	8.724499	0.437109	-1.402711
16	8	0	9.052627	3.080829	-1.788182
17	8	0	6.907656	4.518604	-1.651138
18	1	0	4.617218	3.164189	-1.198312
19	6	0	9.781219	-3.695165	0.042631
20	6	0	9.813290	-2.334659	0.461908
21	8	0	10.893325	-1.983942	1.215670
22	8	0	10.852492	-4.448321	0.416362
23	6	0	10.864569	-5.816286	0.046499
24	6	0	10.951598	-0.660348	1.719172
25	6	0	10.252257	2.342631	-1.940088
26	6	0	5.759994	5.357505	-1.620763
27	1	0	8.630019	-5.206092	-0.913963
28	1	0	8.769591	-0.481662	0.496217
29	1	0	10.822892	-5.941742	-1.043422
30	1	0	11.806777	-6.219966	0.419699
31	1	0	10.030774	-6.367409	0.501257
32	1	0	11.876193	-0.598891	2.294869
33	1	0	10.980578	0.081402	0.909713
34	1	0	10.100271	-0.436164	2.374561
35	1	0	11.022930	3.071355	-2.195463
36	1	0	10.533930	1.830029	-1.010493
37	1	0	10.174389	1.600189	-2.744641
38	1	0	6.122527	6.366614	-1.821008
39	1	0	5.035432	5.075973	-2.395378
40	1	0	5.269782	5.336141	-0.640825
41	6	0	3.812302	6.411017	1.703848
42	6	0	1.072245	6.510503	0.905503
43	6	0	1.683158	5.256884	1.128577
44	6	0	3.022567	5.235461	1.704997
45	6	0	-0.379018	6.602957	0.965417
46	6	0	-1.179788	5.422425	0.913378
47	6	0	-0.499374	4.181727	0.686167
48	6	0	0.890398	4.093589	0.835618
49	6	0	-1.033897	7.831767	1.260704
50	6	0	-2.397018	7.910766	1.462411
51	6	0	-3.193006	6.728991	1.389805
52	6	0	-2.577139	5.519816	1.136688
53	6	0	1.246103	2.721611	0.470179
54	7	0	0.100010	1.999128	0.253755
55	6	0	-0.966989	2.860076	0.291893
56	6	0	5.060084	6.400154	2.375348
57	6	0	3.492264	4.108842	2.429734
58	1	0	-0.433976	8.717419	1.405910
59	8	0	-3.078643	9.046284	1.782321
60	8	0	-4.517627	6.902872	1.632035
61	1	0	-3.164237	4.614674	1.170593
62	6	0	5.521379	5.281056	3.042666
63	6	0	4.712001	4.108285	3.077922
64	8	0	6.700367	5.196356	3.717506
65	8	0	5.219604	3.070957	3.796330
66	6	0	7.546500	6.333167	3.723570
67	6	0	4.471039	1.864053	3.838005
68	6	0	-2.339537	10.244000	1.943456
69	6	0	-5.356316	5.754924	1.600218
70	6	0	2.516367	2.248743	0.122703
71	1	0	5.650526	7.305693	2.402928
72	1	0	2.856158	3.239438	2.502754
73	1	0	8.431929	6.045158	4.292076
74	1	0	7.846109	6.619868	2.706998
75	1	0	7.068181	7.192446	4.211961
76	1	0	5.069974	1.162142	4.419853
77	1	0	3.501479	2.006978	4.332118
78	1	0	4.305402	1.457690	2.832982
79	1	0	-3.068361	11.014117	2.199983
80	1	0	-1.600290	10.161070	2.750422
81	1	0	-1.823147	10.530207	1.017276
82	1	0	-5.336078	5.267051	0.619358
83	1	0	-5.073671	5.028692	2.372962
84	1	0	-6.365226	6.116778	1.802425
85	6	0	2.724470	-1.245635	-0.498034
86	7	0	2.000166	-0.099420	-0.288279
87	6	0	2.860897	0.967716	-0.323558
88	6	0	2.250448	-2.515071	-0.149522
89	6	0	-3.811756	-6.406663	1.708186
90	6	0	-1.072829	-6.508438	0.905871
91	6	0	-1.682554	-5.254367	1.129686
92	6	0	-3.021147	-5.231717	1.707833
93	6	0	0.378516	-6.601730	0.964217
94	6	0	1.180089	-5.421662	0.912070
95	6	0	0.500352	-4.180197	0.686820
96	6	0	-0.889278	-4.091507	0.836626
97	6	0	1.032926	-7.831108	1.258317
98	6	0	2.396214	-7.911271	1.458209
99	6	0	3.192993	-6.730109	1.385035
100	6	0	2.577689	-5.520309	1.133230
101	6	0	-1.244546	-2.719242	0.471773
102	7	0	-0.098221	-1.996875	0.255829
103	6	0	0.968444	-2.858176	0.294326
104	6	0	-5.058346	-6.394695	2.381903
105	6	0	-3.488622	-4.104514	2.433106
106	1	0	0.432592	-8.716337	1.404126
107	8	0	3.077293	-9.047567	1.776646
108	8	0	4.517745	-6.905279	1.625434
109	1	0	3.165564	-4.615651	1.166441
110	6	0	-5.517387	-5.275148	3.050062
111	6	0	-4.707116	-4.102922	3.083584
112	8	0	-6.694941	-5.189481	3.727436
113	8	0	-5.212371	-3.065024	3.802940
114	6	0	-7.541625	-6.325956	3.735896
115	6	0	-4.462390	-1.858926	3.842654
116	6	0	2.337366	-10.244756	1.937694
117	6	0	5.357254	-5.757916	1.594223
118	6	0	-2.514551	-2.246757	0.123187
119	1	0	-5.649494	-7.299761	2.410729
120	1	0	-2.851679	-3.235591	2.504787
121	1	0	-7.062408	-7.185205	4.223459
122	1	0	-8.425563	-6.037310	4.306411
123	1	0	-7.843674	-6.612880	2.720093
124	1	0	-5.059486	-1.156130	4.425307
125	1	0	-3.492119	-2.002732	4.335026
126	1	0	-4.298165	-1.453284	2.837118
127	1	0	3.065800	-11.015726	2.192851
128	1	0	1.598968	-10.161788	2.745466
129	1	0	1.819814	-10.529910	1.011891
130	1	0	5.336828	-5.269117	0.613859
131	1	0	5.075577	-5.032233	2.367804
132	1	0	6.365944	-6.120796	1.795510
133	6	0	-7.601625	3.307310	-0.996338
134	6	0	-7.655754	1.936027	-0.640744
135	6	0	-6.514887	1.066831	-0.911069
136	6	0	-5.264420	1.682272	-1.139077
137	6	0	-6.604725	-0.384060	-0.978795
138	6	0	-5.422315	-1.182114	-0.935604
139	6	0	-4.182345	-0.499278	-0.711987
140	6	0	-4.097008	0.891091	-0.858091
141	6	0	-7.833473	-1.039469	-1.272922
142	6	0	-7.910260	-2.401680	-1.481110
143	6	0	-6.726709	-3.195723	-1.414850
144	6	0	-5.517405	-2.578786	-1.163962
145	6	0	-2.722869	1.247190	-0.500495
146	7	0	-1.998479	0.101174	-0.289197
147	6	0	-2.858707	-0.966273	-0.324901
148	6	0	-8.685107	4.151515	-0.651046
149	6	0	-8.770538	1.486357	0.118411
150	1	0	-8.720923	-0.440438	-1.411157
151	8	0	-9.045354	-3.083923	-1.801998
152	8	0	-6.899398	-4.520068	-1.660767
153	1	0	-4.610957	-3.163635	-1.203402
154	6	0	-9.783361	3.686256	0.046797
155	6	0	-9.814078	2.324403	0.461886
156	8	0	-10.894036	1.970061	1.214117
157	8	0	-10.855687	4.436990	0.422498
158	6	0	-10.869441	5.805980	0.056231
159	6	0	-10.950640	0.644854	1.713599
160	6	0	-10.244974	-2.346414	-1.957675
161	6	0	-5.751240	-5.357985	-1.625802
162	6	0	-2.248654	2.516969	-0.153532
163	1	0	-8.633788	5.201454	-0.905007
164	1	0	-8.768283	0.472428	0.490820
165	1	0	-10.827630	5.934344	-1.033345
166	1	0	-11.812351	6.207355	0.430235
167	1	0	-10.036508	6.357051	0.512713
168	1	0	-11.875455	0.580247	2.288635
169	1	0	-10.978033	-0.094465	0.901877
170	1	0	-10.099269	0.420019	2.368667
171	1	0	-11.014146	-3.075312	-2.216920
172	1	0	-10.530516	-1.835063	-1.028558
173	1	0	-10.164258	-1.603052	-2.761024
174	1	0	-5.024402	-5.076911	-2.398294
175	1	0	-5.264201	-5.335114	-0.644323
176	1	0	-6.112445	-6.367467	-1.826150
177	1	0	3.325656	2.954687	0.222925
178	1	0	2.956990	-3.324263	-0.244539
179	1	0	-3.323902	-2.952630	0.223433
180	1	0	-2.955019	3.326193	-0.250138
181	6	0	6.427238	-3.811618	-1.697114
182	6	0	5.250265	-3.023958	-1.709732
183	6	0	6.422988	-5.062366	-2.363097
184	6	0	4.129459	-3.498926	-2.439857
185	6	0	5.309331	-5.528485	-3.035962
186	6	0	4.135249	-4.721472	-3.082472
187	8	0	5.230898	-6.710824	-3.705325
188	8	0	3.103479	-5.234205	-3.804826
189	6	0	6.372795	-7.550484	-3.707728
190	6	0	1.896053	-4.487280	-3.859192
191	1	0	7.329567	-5.651576	-2.381332
192	1	0	3.259513	-2.864635	-2.521622
193	1	0	6.656004	-7.851032	-2.690255
194	1	0	6.092532	-8.436292	-4.279539

195	1	0	7.231641	-7.065994	-4.191012
196	1	0	1.199847	-5.089030	-4.444844
197	1	0	1.480982	-4.318875	-2.858186
198	1	0	2.041926	-3.519173	-4.355188
199	6	0	-6.429460	3.811134	-1.692844
200	6	0	-5.251469	3.025108	-1.707310
201	6	0	-6.427348	5.062534	-2.357461
202	6	0	-4.131772	3.502394	-2.437666
203	6	0	-5.315343	5.530232	-3.031975
204	6	0	-4.140537	4.724552	-3.080974
205	8	0	-5.239524	6.712755	-3.701092
206	8	0	-3.111684	5.237866	-3.807112
207	6	0	-6.383055	7.550002	-3.701764
208	6	0	-1.905086	4.490060	-3.868891
209	1	0	-7.334607	5.650586	-2.373970
210	1	0	-3.260979	2.869437	-2.520149
211	1	0	-7.241805	7.063520	-4.182907
212	1	0	-6.664785	7.850545	-2.683979
213	1	0	-6.105519	8.435879	-4.274721
214	1	0	-1.211758	5.091971	-4.457795
215	1	0	-1.484655	4.320209	-2.870356
216	1	0	-2.054654	3.522637	-4.365226
217	6	0	3.315460	7.590058	1.013738
218	6	0	1.946795	7.650926	0.649261
219	6	0	4.165132	8.673790	0.683359
220	6	0	1.506295	8.773301	-0.104175
221	6	0	3.708266	9.779395	-0.008429
222	6	0	2.349648	9.817455	-0.432752
223	8	0	2.003767	10.904946	-1.178217
224	8	0	4.464614	10.852876	-0.369127
225	6	0	5.833047	10.855333	-0.000252
226	6	0	0.681294	10.972112	-1.683235
227	1	0	5.212938	8.616866	0.944541
228	1	0	0.495498	8.777101	-0.484741
229	1	0	6.379248	10.021625	-0.460984
230	1	0	6.241263	11.797986	-0.367447
231	1	0	5.959038	10.805778	1.089236
232	1	0	0.623331	11.902881	-2.249392
233	1	0	0.455677	10.128387	-2.347770
234	1	0	-0.061578	10.994730	-0.874754
235	6	0	-3.316754	-7.586290	1.017697
236	6	0	-1.948674	-7.648340	0.651062
237	6	0	-4.167794	-8.669585	0.689368
238	6	0	-1.510350	-8.771554	-0.102540
239	6	0	-3.712866	-9.776107	-0.002278
240	6	0	-2.354940	-9.815500	-0.428707
241	8	0	-2.010958	-10.904171	-1.173454
242	8	0	-4.470553	-10.849450	-0.360787
243	6	0	-5.838562	-10.850196	0.010072
244	6	0	-0.688890	-10.973567	-1.679347
245	1	0	-5.215150	-8.611589	0.952196
246	1	0	-0.500254	-8.776440	-0.484993
247	1	0	-6.384484	-10.016148	-0.450401
248	1	0	-6.248243	-11.792669	-0.356026
249	1	0	-5.962956	-10.799894	1.099723
250	1	0	-0.632504	-11.905100	-2.244459
251	1	0	-0.462640	-10.130915	-2.344974
252	1	0	0.054420	-10.996163	-0.871299
253	30	0	0.000563	0.001395	-0.022277

Table S24. Cartesian coordinates for the optimized structure of **6b**-H_2 (B3LYP/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.059983	-2.079322	-0.973565
2	6	0	7.893473	-0.720932	-0.604219
3	6	0	6.636063	-0.037886	-0.889013
4	6	0	5.503331	-0.837814	-1.149434
5	6	0	6.499317	1.411179	-0.946248
6	6	0	5.208648	2.016751	-0.919855
7	6	0	4.085675	1.148259	-0.711857
8	6	0	4.221396	-0.243874	-0.872429
9	6	0	7.616275	2.249163	-1.217711
10	6	0	7.486567	3.609068	-1.420784
11	6	0	6.193124	4.209317	-1.374631
12	6	0	5.089465	3.411535	-1.143619
13	6	0	9.254690	-2.749053	-0.614317
14	6	0	8.910680	-0.112815	0.181286
15	1	0	8.587151	1.794741	-1.342694
16	8	0	8.508709	4.458063	-1.717799
17	8	0	6.162274	5.544567	-1.617432
18	1	0	4.104350	3.849380	-1.196669
19	6	0	10.255028	-2.128441	0.110317
20	6	0	10.065039	-0.783091	0.537944
21	8	0	11.063150	-0.274312	1.314819
22	8	0	11.422833	-2.708926	0.498679
23	6	0	11.670378	-4.058636	0.113035
24	6	0	10.905927	1.038780	1.823920
25	6	0	9.819549	3.920331	-1.866513
26	6	0	4.896964	6.194357	-1.610081
27	1	0	9.371945	-3.790529	-0.879535
28	1	0	8.743667	0.884026	0.562445
29	1	0	11.629590	-4.148257	-0.982796
30	6	0	13.044885	-4.451909	0.635462
31	1	0	10.894341	-4.717718	0.530379
32	1	0	11.799751	1.239885	2.416301
33	1	0	10.832478	1.781095	1.017855
34	1	0	10.019372	1.123617	2.465277
35	6	0	10.764787	5.070438	-2.184998
36	1	0	10.126552	3.414039	-0.938699
37	1	0	9.830445	3.171298	-2.671844
38	1	0	5.101347	7.247209	-1.808414
39	1	0	4.238935	5.802139	-2.395736
40	1	0	4.399477	6.099170	-0.638645
41	6	0	2.774078	6.917442	1.635496
42	6	0	0.054960	6.609097	0.823795
43	6	0	0.844297	5.457968	1.047714
44	6	0	2.166502	5.638642	1.638066
45	6	0	-1.391309	6.483662	0.875236
46	6	0	-2.006113	5.194642	0.815947
47	6	0	-1.144994	4.074939	0.581735
48	6	0	0.236152	4.194234	0.741300
49	6	0	-2.222668	7.602044	1.167361
50	6	0	-3.582728	7.478326	1.364655
51	6	0	-4.192353	6.189765	1.289645
52	6	0	-3.404659	5.085396	1.035051
53	6	0	0.785121	2.877373	0.363683
54	7	0	-0.217521	1.994949	0.099322
55	6	0	-1.388580	2.686455	0.172258
56	6	0	4.003102	7.094753	2.317139
57	6	0	2.787525	4.599351	2.378856
58	1	0	-1.760624	8.566181	1.315811
59	8	0	-4.426358	8.499548	1.684206
60	8	0	-5.529061	6.165238	1.532599
61	1	0	-3.852195	4.103702	1.067268
62	6	0	4.617029	6.061479	3.000824
63	6	0	3.986276	4.784002	3.040690
64	8	0	5.788265	6.158761	3.686922
65	8	0	4.631113	3.838713	3.777257
66	6	0	6.478388	7.404994	3.674439
67	6	0	4.062497	2.538323	3.830850
68	6	0	-3.880622	9.802583	1.862663
69	6	0	-6.186918	4.905665	1.504451
70	6	0	2.133935	2.621539	0.071700
71	1	0	4.453981	8.076992	2.340595
72	1	0	2.283926	3.646742	2.452296
73	6	0	7.757160	7.243274	4.484483
74	1	0	6.707426	7.694968	2.638049
75	1	0	5.844002	8.191891	4.109279
76	1	0	4.748462	1.937302	4.429412
77	1	0	3.076433	2.547614	4.312829
78	1	0	3.968414	2.097622	2.831041
79	6	0	-5.025999	10.747222	2.199938
80	1	0	-3.132863	9.791668	2.669266
81	1	0	-3.370649	10.127552	0.942901
82	1	0	-6.097786	4.424498	0.524128
83	1	0	-5.797155	4.230194	2.276593
84	1	0	-7.238085	5.112908	1.709503
85	6	0	2.937221	-0.836552	-0.534548
86	7	0	2.074820	0.208718	-0.315570
87	6	0	2.715112	1.421888	-0.336057
88	1	0	1.106937	0.080362	-0.039847
89	6	0	2.626576	-2.162170	-0.235118
90	6	0	-2.774228	-6.916803	1.633541
91	6	0	-0.055182	-6.608625	0.821419
92	6	0	-0.844310	-5.457463	1.045886
93	6	0	-2.166333	-5.638153	1.636655
94	6	0	1.391117	-6.483386	0.872710
95	6	0	2.006064	-5.194411	0.813690
96	6	0	1.145062	-4.074522	0.579972
97	6	0	-0.236085	-4.193731	0.739613
98	6	0	2.222410	-7.601916	1.164497
99	6	0	3.582513	-7.478400	1.361593
100	6	0	4.192282	-6.189894	1.286745
101	6	0	3.404666	-5.085380	1.032550
102	6	0	-0.784945	-2.876745	0.362248
103	7	0	0.217762	-1.994250	0.098397
104	6	0	1.388760	-2.685862	0.171108
105	6	0	-4.003193	-7.094153	2.315288
106	6	0	-2.786762	-4.599211	2.378436
107	1	0	1.760289	-8.566020	1.312896
108	8	0	4.426066	-8.499770	1.680851
109	8	0	5.529026	-6.165581	1.529497
110	1	0	3.852312	-4.103739	1.064954
111	6	0	-4.616574	-6.061159	2.999880
112	6	0	-3.985343	-4.783949	3.040539
113	8	0	-5.787658	-6.158477	3.686235
114	8	0	-4.629650	-3.838972	3.777968
115	6	0	-6.478995	-7.404015	3.672026
116	6	0	-4.060610	-2.538795	3.832281
117	6	0	3.880159	-9.802653	1.859848
118	6	0	6.187040	-4.906085	1.501430
119	6	0	-2.133633	-2.620774	0.069868
120	1	0	-4.454394	-8.076258	2.338193
121	1	0	-2.282826	-3.646830	2.452438
122	1	0	-5.844767	-8.192552	4.104162
123	6	0	-7.756364	-7.242773	4.484397
124	1	0	-6.709868	-7.691417	2.635314
125	1	0	-4.746150	-1.938001	4.431549
126	1	0	-3.074355	-2.548740	4.313848
127	1	0	-3.966799	-2.097393	2.832759
128	6	0	5.025479	-10.747280	2.197379
129	1	0	3.132496	-9.791305	2.666530
130	1	0	3.370025	-10.127916	0.940280
131	1	0	6.097722	-4.424716	0.521225
132	1	0	5.797557	-4.230717	2.273805
133	1	0	7.238231	-5.113499	1.706175
134	6	0	-8.060052	2.079454	-0.973943
135	6	0	-7.893292	0.720776	-0.605781
136	6	0	-6.635644	0.038314	-0.890862
137	6	0	-5.503037	0.838735	-1.150391
138	6	0	-6.498540	-1.410674	-0.949105
139	6	0	-5.207734	-2.015896	-0.922607
140	6	0	-4.085085	-1.147257	-0.713645
141	6	0	-4.221001	0.244955	-0.873407
142	6	0	-7.615163	-2.248804	-1.221517
143	6	0	-7.484961	-3.608557	-1.425341
144	6	0	-6.191359	-4.208469	-1.379060
145	6	0	-5.088025	-3.410507	-1.147186
146	6	0	-2.936975	0.837582	-0.534745
147	7	0	-2.074500	-0.207727	-0.316187
148	6	0	-2.714645	-1.420941	-0.337572
149	6	0	-9.255008	2.748564	-0.614360
150	6	0	-8.910540	0.111697	0.178927
151	1	0	-8.586130	-1.794593	-1.346621
152	8	0	-8.506695	-4.457718	-1.723256
153	8	0	-6.160034	-5.543569	-1.622633
154	1	0	-4.102744	-3.847998	-1.200121
155	1	0	-1.106728	-0.079395	-0.040071
156	6	0	-10.255347	2.127070	0.109511
157	6	0	-10.065124	0.781377	0.535963
158	8	0	-11.063268	0.271678	1.312194
159	8	0	-11.423376	2.706934	0.498134
160	6	0	-11.671177	4.056878	0.113488
161	6	0	-10.905873	-1.041840	1.820137
162	6	0	-9.817722	-3.920473	-1.872012
163	6	0	-4.894560	-6.193035	-1.615038
164	6	0	-2.626360	2.162998	-0.234404
165	1	0	-9.372464	3.790240	-0.878691
166	1	0	-8.743384	-0.885457	0.559201
167	1	0	-11.630385	4.147294	-0.982280
168	6	0	-13.045766	4.449566	0.636148
169	1	0	-10.895268	4.715806	0.531313
170	1	0	-11.799806	-1.243693	2.412102
171	1	0	-10.832043	-1.783403	1.013413
172	1	0	-10.019466	-1.127061	2.461648
173	6	0	-10.762482	-5.071016	-2.190360
174	1	0	-10.124945	-3.414227	-0.944245
175	1	0	-9.828893	-3.171511	-2.677406
176	1	0	-4.236272	-5.800242	-2.400187
177	1	0	-4.397536	-6.098217	-0.643326
178	1	0	-5.098576	-7.245838	-1.813999
179	1	0	2.810373	3.454207	0.180597
180	1	0	3.439976	-2.862180	-0.338001
181	1	0	-2.810157	-3.453453	0.178150
182	1	0	-3.439716	2.863098	-0.336928
183	6	0	6.995008	-2.750180	-1.700263
184	6	0	5.709149	-2.157311	-1.733287
185	6	0	7.201772	-3.978247	-2.375779
186	6	0	4.693315	-2.792800	-2.494543
187	6	0	6.191070	-4.605628	-3.080205
188	6	0	4.906305	-3.990803	-3.148435
189	8	0	6.316131	-5.775978	-3.761194
190	8	0	3.984739	-4.649205	-3.900650
191	6	0	7.567584	-6.456449	-3.719134
192	6	0	2.675019	-4.102271	-3.974640
193	1	0	8.189155	-4.418533	-2.376539
194	1	0	3.735750	-2.303147	-2.590503

195	1	0	7.834785	-6.682554	-2.676096	298	1	0	7.491084	6.945018	5.505715
196	6	0	7.431530	-7.736032	-4.532339	299	1	0	8.340022	6.418293	4.057774
197	1	0	8.359145	-5.816061	-4.136324	300	1	0	8.864830	8.805431	3.478919
198	1	0	2.094958	-4.799991	-4.580037	301	1	0	7.985027	9.356264	4.895379
199	1	0	2.218494	-4.012954	-2.981779	302	1	0	9.599581	8.149511	6.382950
200	1	0	2.675646	-3.117742	-4.459587	303	1	0	10.475888	7.570528	4.976520
201	6	0	-6.995120	2.751188	-1.699882	304	1	0	11.000772	9.933639	4.317901
202	6	0	-5.709122	2.158627	-1.733288	305	1	0	10.104373	10.527369	5.704883
203	6	0	-7.202087	3.979779	-2.374390	306	1	0	11.698210	9.351974	7.247990
204	6	0	-4.693404	2.794928	-2.494019	307	1	0	12.593276	8.741884	5.867258
205	6	0	-6.191478	4.607945	-3.078241	308	1	0	13.123864	11.093901	5.164365
206	6	0	-4.906589	3.993441	-3.146909	309	1	0	12.216651	11.712304	6.533043
207	8	0	-6.316745	5.778812	-3.758309	310	1	0	13.796001	10.554391	8.108154
208	8	0	-3.985115	4.652647	-3.898533	311	1	0	14.703040	9.928508	6.742747
209	6	0	-7.568415	6.458866	-3.716028	312	1	0	15.235505	12.275389	6.016989
210	6	0	-2.675305	4.105989	-3.972973	313	1	0	14.322075	12.905169	7.376213
211	1	0	-8.189542	4.419902	-2.374815	314	1	0	15.894840	11.755612	8.967414
212	1	0	-3.735758	2.305529	-2.590397	315	1	0	16.808884	11.124462	7.609305
213	1	0	-8.359667	5.818576	-4.133943	316	1	0	17.338895	13.469262	6.876027
214	1	0	-7.835976	6.684087	-2.672891	317	1	0	16.423481	14.100935	8.231697
215	6	0	-7.432538	7.739056	-4.528293	318	1	0	18.871909	14.089679	8.757963
216	1	0	-2.095379	4.804263	-4.577860	319	1	0	18.020381	12.980773	9.840193
217	1	0	-2.218728	4.016005	-2.980197	320	1	0	18.943515	12.345982	8.474505
218	1	0	-2.675785	3.121826	-4.458660	321	6	0	-4.546432	12.184717	2.434046
219	6	0	2.114002	8.008154	0.935631	322	6	0	-5.688167	13.166418	2.725748
220	6	0	0.752674	7.866061	0.567817	323	6	0	-5.206758	14.601502	2.971024
221	6	0	2.797284	9.202318	0.601464	324	6	0	-6.343651	15.598449	3.226289
222	6	0	0.154806	8.908682	-0.191003	325	6	0	-5.855053	17.031046	3.473076
223	6	0	2.186353	10.226913	-0.097474	326	6	0	-6.988132	18.038112	3.704122
224	6	0	0.837716	10.063321	-0.523255	327	6	0	-6.494575	19.469339	3.949054
225	8	0	0.336872	11.085511	-1.274662	328	6	0	-7.625014	20.482248	4.165944
226	8	0	2.780456	11.396557	-0.461899	329	6	0	-7.129639	21.913180	4.409102
227	6	0	4.133190	11.620116	-0.074293	330	6	0	-8.264554	22.920035	4.618269
228	6	0	-0.980338	10.954888	-1.779932	331	1	0	-5.755509	10.719520	1.381310
229	1	0	3.841172	9.301047	0.865548	332	1	0	-5.540943	10.369398	3.091368
230	1	0	-0.845718	8.763026	-0.571351	333	1	0	-3.832058	12.201034	3.269053
231	1	0	4.782967	10.844381	-0.506788	334	1	0	-3.989438	12.534087	1.552797
232	6	0	4.540251	12.999188	-0.573770	335	1	0	-6.395453	13.158169	1.884453
233	1	0	4.224682	11.558450	1.020487	336	1	0	-6.254259	12.816829	3.600561
234	1	0	-1.174674	11.864496	-2.350265	337	1	0	-4.516152	14.610841	3.826230
235	1	0	-1.078671	10.084513	-2.441302	338	1	0	-4.618653	14.938538	2.105310
236	1	0	-1.719416	10.870588	-0.971908	339	1	0	-7.030421	15.592102	2.367821
237	6	0	-2.114459	-8.007365	0.933149	340	1	0	-6.936231	15.262636	4.089277
238	6	0	-0.753175	-7.865383	0.565116	341	1	0	-5.179376	17.039170	4.340235
239	6	0	-2.797966	-9.201370	0.598860	342	1	0	-5.249065	17.358845	2.616199
240	6	0	-0.155666	-8.907866	-0.194188	343	1	0	-7.662188	18.030685	2.835615
241	6	0	-2.187310	-10.225911	-0.100383	344	1	0	-7.595969	17.712118	4.560290
242	6	0	-0.838778	-10.062361	-0.526527	345	1	0	-5.826854	19.478023	4.822433
243	8	0	-0.338248	-11.084434	-1.278267	346	1	0	-5.879222	19.790609	3.096373
244	8	0	-2.781569	-11.395504	-0.464737	347	1	0	-8.292546	20.474457	3.292237
245	6	0	-4.133977	-11.619343	-0.076111	348	1	0	-8.241505	20.163213	5.018746
246	6	0	0.978871	-10.953875	-1.783821	349	1	0	-6.466128	21.921936	5.284564
247	1	0	-3.841803	-9.300034	0.863159	350	1	0	-6.511054	22.230430	3.558460
248	1	0	0.844759	-8.762231	-0.574790	351	1	0	-7.878597	23.930299	4.789077
249	1	0	-4.784289	-10.843951	-0.508410	352	1	0	-8.924789	22.959851	3.744357
250	6	0	-4.540943	-12.998726	-0.574814	353	1	0	-8.880523	22.649050	5.483376
251	1	0	-4.224700	-11.557350	1.018708	354	6	0	-8.721271	8.569824	-4.527042
252	1	0	1.172935	-11.863382	-2.354404	355	6	0	-8.620996	9.845195	-5.373226
253	1	0	1.077156	-10.083354	-2.445005	356	6	0	-9.901178	10.688961	-5.356468
254	1	0	1.718139	-10.869860	-0.975944	357	6	0	-9.815988	11.952440	-6.221586
255	6	0	5.983174	13.355650	-0.196400	358	6	0	-11.093333	12.800521	-6.193512
256	6	0	6.417182	14.736230	-0.704367	359	6	0	-11.016837	14.056610	-7.070105
257	6	0	7.854134	15.104538	-0.315641	360	6	0	-12.292761	14.906655	-7.036202
258	6	0	8.295549	16.479998	-0.830492	361	6	0	-12.220968	16.158523	-7.918935
259	6	0	9.728850	16.852063	-0.431303	362	6	0	-13.496166	17.009713	-7.883498
260	6	0	10.174699	18.224202	-0.951127	363	6	0	-13.416753	18.256093	-8.770081
261	6	0	11.605553	18.598454	-0.545249	364	1	0	-6.602655	8.326774	-4.118148
262	6	0	12.054081	19.968475	-1.067877	365	1	0	-7.152881	7.474578	-5.555193
263	6	0	13.483808	20.344134	-0.659220	366	1	0	-9.554536	7.956698	-4.899241
264	6	0	13.924341	21.712864	-1.186620	367	1	0	-8.981220	8.840442	-3.493852
265	1	0	4.415385	13.028158	-1.662944	368	1	0	-7.779144	10.453692	-5.014167
266	1	0	3.846588	13.740374	-0.158857	369	1	0	-8.377305	9.572917	-6.409655
267	1	0	6.095132	13.321264	0.896648	370	1	0	-10.745837	10.073477	-5.697783
268	1	0	6.667043	12.593255	-0.595851	371	1	0	-10.134238	10.973164	-4.320371
269	1	0	6.316170	14.767438	-1.798275	372	1	0	-8.966252	12.564903	-5.887782
270	1	0	5.728025	15.498567	-0.314722	373	1	0	-9.592582	11.666550	-7.259246
271	1	0	7.951121	15.078662	0.779166	374	1	0	-11.944629	12.184621	-6.517104
272	1	0	8.541907	14.336768	-0.697959	375	1	0	-11.310687	13.094127	-5.156603
273	1	0	8.206074	16.503040	-1.925914	376	1	0	-10.162975	14.670993	-6.750483
274	1	0	7.603558	17.247230	-0.454869	377	1	0	-10.804578	13.761996	-8.107740
275	1	0	9.816048	16.833355	0.664476	378	1	0	-13.147395	14.290445	-7.350419
276	1	0	10.420309	16.081912	-0.802073	379	1	0	-12.501876	15.205527	-5.999051
277	1	0	10.092328	18.241067	-2.047265	380	1	0	-11.365754	16.775154	-7.606755
278	1	0	9.480620	18.993993	-0.584589	381	1	0	-12.014066	15.859965	-8.956722
279	1	0	11.686631	18.584167	0.551091	382	1	0	-14.350794	16.393341	-8.194267
280	1	0	12.299332	17.826985	-0.908989	383	1	0	-13.701548	17.309975	-6.846936
281	1	0	11.975908	19.982682	-2.164523	384	1	0	-14.340801	18.841522	-8.723519
282	1	0	11.359823	20.740641	-0.706251	385	1	0	-12.593071	18.910025	-8.461569
283	1	0	13.561408	20.331649	0.436508	386	1	0	-13.246813	17.986041	-9.818589
284	1	0	14.177319	19.572236	-1.019880	387	6	0	-13.419414	5.889342	0.263561
285	1	0	14.947557	21.951421	-0.878592	388	6	0	-14.798325	6.312833	0.784961
286	1	0	13.890870	21.745121	-2.281606	389	6	0	-15.178454	7.747687	0.400099
287	1	0	13.270810	22.509944	-0.814177	390	6	0	-16.553728	8.180807	0.922594
288	6	0	8.594430	8.527491	4.507475	391	6	0	-16.934513	9.612607	0.526375
289	6	0	9.870687	8.408448	5.349976	392	6	0	-18.307418	10.051396	1.050290
290	6	0	10.717742	9.686483	5.350974	393	6	0	-18.688614	11.481079	0.646818
291	6	0	11.982485	9.587954	6.212818	394	6	0	-20.059926	11.923181	1.171626
292	6	0	12.831667	10.864685	6.198932	395	6	0	-20.441743	13.351876	0.765097
293	6	0	14.088965	10.778301	7.072768	396	6	0	-21.811851	13.786176	1.294112
294	6	0	14.938368	12.054754	7.051944	397	1	0	-13.787270	3.749403	0.232885
295	6	0	16.191518	11.974770	7.931980	398	1	0	-13.056115	4.324855	1.725647
296	6	0	17.040667	13.251382	7.910219	399	1	0	-12.658585	6.579436	0.655175
297	6	0	18.288459	13.164092	8.793842	400	1	0	-13.397154	6.001741	-0.829790

401	1	0	-15.559543	5.619026	0.401427	504	1	0	-8.206173	-16.505002	-1.922223
402	1	0	-14.819087	6.210966	1.879024	505	1	0	-7.602327	-17.248006	-0.451111
403	1	0	-14.412733	8.439846	0.778577	506	1	0	-9.814241	-16.834419	0.669475
404	1	0	-15.159330	7.845719	-0.694772	507	1	0	-10.419828	-16.084152	-0.797142
405	1	0	-17.319167	7.485272	0.549859	508	1	0	-10.091701	-18.243932	-2.041211
406	1	0	-16.571000	8.090180	2.018025	509	1	0	-9.478719	-18.995687	-0.578449
407	1	0	-16.166731	10.307478	0.895674	510	1	0	-11.684179	-18.586146	0.558401
408	1	0	-16.919328	9.701073	-0.569371	511	1	0	-12.298151	-17.830091	-0.901746
409	1	0	-19.074993	9.354370	0.684682	512	1	0	-11.974581	-19.986390	-2.156210
410	1	0	-18.321327	9.967707	2.146376	513	1	0	-11.357261	-20.743228	-0.697859
411	1	0	-17.919667	12.177739	1.010395	514	1	0	-13.558319	-20.334512	0.446037
412	1	0	-18.676080	11.563533	-0.449453	515	1	0	-14.175461	-19.576188	-1.010418
413	1	0	-20.829633	11.226219	0.809937	516	1	0	-14.944621	-21.955605	-0.867315
414	1	0	-20.072636	11.843618	2.268200	517	1	0	-13.888832	-21.749689	-2.271075
415	1	0	-19.672368	14.048046	1.126028	518	1	0	-13.267595	-22.513403	-0.803550
416	1	0	-20.430438	13.430893	-0.330555	519	6	0	4.545802	-12.184472	2.432995
417	1	0	-22.054863	14.808761	0.987448	520	6	0	5.687566	-13.165998	2.725213
418	1	0	-22.606540	13.129790	0.921547	521	6	0	5.206128	-14.600674	2.972726
419	1	0	-21.843114	13.751340	2.389096	522	6	0	6.343088	-15.597278	3.229075
420	6	0	-12.206937	-4.598179	-2.393659	523	6	0	5.854520	-17.029392	3.478660
421	6	0	-13.189364	-5.743487	-2.668288	524	6	0	6.987709	-18.036050	3.711025
422	6	0	-14.630561	-5.266897	-2.885524	525	6	0	6.494225	-19.466757	3.959101
423	6	0	-15.627778	-6.406324	-3.128058	526	6	0	7.624804	-20.479277	4.177193
424	6	0	-17.065785	-5.921462	-3.349393	527	6	0	7.129527	-21.909709	4.423456
425	6	0	-18.072525	-7.056541	-3.571908	528	6	0	8.264585	-22.916194	4.633759
426	6	0	-19.508642	-6.566150	-3.793376	529	1	0	5.754647	-10.720404	1.378424
427	6	0	-20.520816	-7.698323	-4.004586	530	1	0	5.540873	-10.368769	3.088249
428	6	0	-21.956377	-7.205870	-4.225248	531	1	0	3.831785	-12.199888	3.268318
429	6	0	-22.962221	-8.342449	-4.430180	532	1	0	3.988387	-12.534619	1.552324
430	1	0	-10.400780	-5.582803	-3.090222	533	1	0	6.394330	-13.158935	1.883466
431	1	0	-10.713648	-5.801151	-1.373334	534	1	0	6.254267	-12.815354	3.599214
432	1	0	-12.540807	-4.044740	-1.504197	535	1	0	4.515846	-14.608710	3.828211
433	1	0	-12.243553	-3.882003	-3.226506	536	1	0	4.617669	-14.938943	2.107727
434	1	0	-12.854335	-6.306659	-3.550634	537	1	0	7.029408	-15.592461	2.370227
435	1	0	-13.162413	-6.452170	-1.828586	538	1	0	6.936164	-15.260010	4.091170
436	1	0	-14.954259	-4.683547	-2.011549	539	1	0	5.179241	-17.035915	4.346156
437	1	0	-14.657735	-4.572866	-3.737591	540	1	0	5.248115	-17.358722	2.622651
438	1	0	-15.304409	-6.994537	-3.998741	541	1	0	7.661266	-18.030364	2.842099
439	1	0	-15.604951	-7.096261	-2.272424	542	1	0	7.596079	-17.708392	4.566203
440	1	0	-17.382324	-5.321655	-2.483985	543	1	0	5.827097	-19.473702	4.832970
441	1	0	-17.089610	-5.240720	-4.212308	544	1	0	5.878257	-19.789665	3.107459
442	1	0	-17.757107	-7.658479	-4.436161	545	1	0	8.291754	-20.473203	3.303005
443	1	0	-18.050402	-7.735466	-2.707454	546	1	0	8.241904	-20.158614	5.028973
444	1	0	-19.820144	-5.957917	-2.932009	547	1	0	6.466611	-21.916776	5.299411
445	1	0	-19.531508	-5.892293	-4.661783	548	1	0	6.510329	-22.228567	3.573833
446	1	0	-20.211224	-8.307798	-4.865868	549	1	0	7.878702	-23.926142	4.806590
447	1	0	-20.499358	-8.371947	-3.135790	550	1	0	8.924325	-22.957579	3.759522
448	1	0	-22.264538	-6.594876	-3.365821	551	1	0	8.881070	-22.643687	5.498053
449	1	0	-21.978692	-6.535726	-5.095403	552	6	0	8.720055	-8.567121	-4.531397
450	1	0	-23.975827	-7.958497	-4.584904	553	6	0	8.619499	-9.842215	-5.377998
451	1	0	-22.700475	-8.950771	-5.303501	554	6	0	9.899273	-10.686621	-5.360805
452	1	0	-22.988656	-9.009618	-3.561036	555	6	0	9.814136	-11.949612	-6.226663
453	6	0	-8.595726	-8.525689	4.504494	556	6	0	11.090760	-12.798775	-6.197215
454	6	0	-9.869258	-8.407930	5.351390	557	6	0	11.014867	-14.053875	-7.075287
455	6	0	-10.719875	-9.683660	5.347245	558	6	0	12.289699	-14.905485	-7.039084
456	6	0	-11.980333	-9.587526	6.215830	559	6	0	12.219013	-16.155856	-7.924031
457	6	0	-12.834735	-10.860836	6.194161	560	6	0	13.492828	-17.008976	-7.885654
458	6	0	-14.086051	-10.778135	7.077232	561	6	0	13.414756	-18.253598	-8.774829
459	6	0	-14.942456	-12.049997	7.045727	562	1	0	6.601443	-8.323848	-4.122720
460	6	0	-16.188158	-11.974844	7.937125	563	1	0	7.152095	-7.470775	-5.559103
461	6	0	-17.045785	-13.245931	7.902256	564	1	0	9.553484	-7.954057	-4.903366
462	6	0	-18.285235	-13.164168	8.798556	565	1	0	8.979914	-8.838168	-3.498278
463	1	0	-7.488271	-6.948166	5.506202	566	1	0	7.777172	-10.450413	-5.019457
464	1	0	-8.338544	-6.415467	4.061163	567	1	0	8.376413	-9.569544	-6.414495
465	1	0	-8.869635	-8.798833	3.475483	568	1	0	10.744505	-10.071351	-5.701192
466	1	0	-7.986595	-9.357229	4.887144	569	1	0	10.131443	-10.971488	-4.324657
467	1	0	-9.594392	-8.155768	6.385215	570	1	0	8.963424	-12.561565	-5.894287
468	1	0	-10.473273	-7.566022	4.984565	571	1	0	9.592353	-11.663010	-7.264513
469	1	0	-11.008386	-9.922681	4.313524	572	1	0	11.943170	-12.183220	-6.518634
470	1	0	-10.107211	-10.528999	5.692418	573	1	0	11.306002	-13.093643	-5.160194
471	1	0	-11.690286	-9.361959	7.252083	574	1	0	10.159478	-14.667589	-6.758403
472	1	0	-12.589391	-8.735629	5.880587	575	1	0	10.805499	-13.757909	-8.113147
473	1	0	-13.134554	-11.078143	5.158749	576	1	0	13.145984	-14.289792	-7.349845
474	1	0	-12.220941	-11.714774	6.515642	577	1	0	12.495442	-15.206239	-6.001794
475	1	0	-13.785153	-10.568592	8.113941	578	1	0	11.361854	-16.771726	-7.615716
476	1	0	-14.697794	-9.920529	6.761530	579	1	0	12.016038	-15.855342	-8.962029
477	1	0	-15.249130	-12.254930	6.009651	580	1	0	14.349466	-16.393300	-8.192224
478	1	0	-14.328071	-12.908668	7.353639	581	1	0	13.694057	-17.311452	-6.848928
479	1	0	-15.881693	-11.773417	8.974095	582	1	0	14.337712	-18.840548	-8.725955
480	1	0	-16.802694	-11.115030	7.632181	583	1	0	12.588932	-18.906802	-8.470561
481	1	0	-17.354693	-13.445312	6.866636	584	1	0	13.249108	-17.981364	-9.823454
482	1	0	-16.431183	-14.105264	8.204864	585	6	0	13.418274	-5.891575	0.262174
483	1	0	-18.875451	-14.085365	8.752149	586	6	0	14.797196	-6.315422	0.783244
484	1	0	-18.006544	-13.000208	9.846203	587	6	0	15.177045	-7.750280	0.398120
485	1	0	-18.937576	-12.335589	8.498453	588	6	0	16.552411	-8.183563	0.920220
486	6	0	-5.983444	-13.355583	-0.196168	589	6	0	16.932895	-9.615465	0.524084
487	6	0	-6.417231	-14.736631	-0.703058	590	6	0	18.305955	-10.054270	1.047557
488	6	0	-7.853756	-15.105334	-0.313069	591	6	0	18.686830	-11.484131	0.644411
489	6	0	-8.294904	-16.481318	-0.826756	592	6	0	20.058336	-11.926159	1.168745
490	6	0	-9.727785	-16.853764	-0.426350	593	6	0	20.439806	-13.355086	0.762696
491	6	0	-10.173364	-18.226428	-0.945028	594	6	0	21.810135	-13.789270	1.291201
492	6	0	-11.603811	-18.601044	-0.537985	595	1	0	13.786530	-3.751690	0.232558
493	6	0	-12.052072	-19.971573	-1.059519	596	1	0	13.055268	-4.327758	1.725022
494	6	0	-13.481403	-20.347589	-0.649739	597	1	0	12.657407	-6.581731	0.653596
495	6	0	-13.921677	-21.716811	-1.176082	598	1	0	13.395869	-6.003507	-0.831218
496	1	0	-4.416926	-13.028039	-1.664074	599	1	0	15.558463	-5.621684	0.399697
497	1	0	-3.846691	-13.739511	-0.160172	600	1	0	14.818169	-6.213735	1.877315
498	1	0	-6.094589	-13.320668	0.896945	601	1	0	14.411356	-8.442381	0.776746
499	1	0	-6.667926	-12.593692	-0.595518	602	1	0	15.157617	-7.848214	-0.696748
500	1	0	-6.317099	-14.768402	-1.797019	603	1	0	17.317829	-7.488186	0.547171
501	1	0	-5.727477	-15.498456	-0.313478	604	1	0	16.570040	-8.092806	2.015628
502	1	0	-7.949966	-15.078829	0.781789	605	1	0	16.165197	-10.310188	0.893802
503	1	0	-8.542134	-14.338111	-0.695383	606	1	0	16.917281	-9.704123	-0.571631

607	1	0	19.073458	-9.357461	0.681411
608	1	0	18.320330	-9.970226	2.143602
609	1	0	17.917995	-12.180580	1.008593
610	1	0	18.673784	-11.566982	-0.451816
611	1	0	20.827940	-11.229455	0.806369
612	1	0	20.071586	-11.846092	2.265269
613	1	0	19.670556	-14.050998	1.124357
614	1	0	20.427927	-13.434628	-0.332903
615	1	0	22.052858	-14.812054	0.984971
616	1	0	22.604692	-13.133193	0.917848
617	1	0	21.841993	-13.753828	2.386138
618	6	0	12.209039	4.596872	-2.388146
619	6	0	13.191843	5.741573	-2.663999
620	6	0	14.632835	5.264129	-2.881024
621	6	0	15.630315	6.402910	-3.125620
622	6	0	17.068086	5.917128	-3.346929
623	6	0	18.074992	7.051582	-3.572039
624	6	0	19.510788	6.560258	-3.794006
625	6	0	20.523065	7.691837	-4.008032
626	6	0	21.958212	7.198494	-4.229750
627	6	0	22.964116	8.334459	-4.437716
628	1	0	10.403337	5.582171	-3.085004
629	1	0	10.716265	5.800795	-1.368138
630	1	0	12.542864	4.044068	-1.498262
631	1	0	12.245227	3.879965	-3.220401
632	1	0	12.856872	6.304002	-3.546880
633	1	0	13.165304	6.451116	-1.824961
634	1	0	14.956665	4.681922	-2.006272
635	1	0	14.659467	4.568823	-3.732139
636	1	0	15.306728	6.989970	-3.997085
637	1	0	15.608110	7.094159	-2.270931
638	1	0	17.385000	5.318689	-2.480599
639	1	0	17.091183	5.234833	-4.208755
640	1	0	17.758999	7.652297	-4.437047
641	1	0	18.053834	7.731934	-2.708559
642	1	0	19.822963	5.953286	-2.931875
643	1	0	19.532612	5.884930	-4.661421
644	1	0	20.212597	8.300202	-4.869873
645	1	0	20.502876	8.366761	-3.140118
646	1	0	22.267317	6.588679	-3.369773
647	1	0	21.979179	6.527001	-5.098963
648	1	0	23.977374	7.949907	-4.593363
649	1	0	22.701275	8.941636	-5.311535
650	1	0	22.992040	9.002860	-3.569522

Table S25. Cartesian coordinates for the optimized structure of [**3a**-H_2]$_2$-C_{2h} (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.320317	3.521266	-1.896107
2	6	0	5.391144	2.831526	-2.526621
3	6	0	5.331623	1.464899	-2.658027
4	6	0	4.192755	0.727012	-2.265897
5	6	0	3.071796	1.437758	-1.792349
6	6	0	3.179891	2.827250	-1.559703
7	6	0	4.192264	-0.732470	-2.264643
8	6	0	3.070649	-1.441600	-1.790325
9	6	0	1.854137	-0.695623	-1.598524
10	6	0	1.854671	0.693033	-1.599174
11	6	0	5.330647	-1.471941	-2.655162
12	6	0	5.389019	-2.838392	-2.521322
13	6	0	4.317618	-3.526227	-1.889658
14	6	0	3.177504	-2.830753	-1.555203
15	6	0	0.479201	1.127993	-1.609025
16	7	0	-0.285898	-0.000568	-1.557673
17	6	0	0.478420	-1.129661	-1.608448
18	8	0	4.529454	4.839571	-1.675987
19	8	0	6.435070	3.604153	-2.913406
20	1	0	6.194476	0.949173	-3.053317
21	1	0	6.194076	-0.957643	-3.051056
22	8	0	6.432322	-3.612482	-2.906916
23	8	0	4.525933	-4.844130	-1.666478
24	1	0	-1.300226	-0.000237	-1.573108
25	6	0	-6.101956	6.430080	-2.712682
26	6	0	-5.419275	7.678792	-2.686538
27	6	0	-4.043764	7.698110	-2.679350
28	6	0	-3.274477	6.508827	-2.638621
29	6	0	-3.960424	5.279613	-2.526230
30	6	0	-5.373481	5.267757	-2.629497
31	6	0	-1.825222	6.520916	-2.802984
32	6	0	-1.102732	5.306544	-2.817606
33	6	0	-1.799797	4.116396	-2.415286
34	6	0	-3.172191	4.101798	-2.291834
35	6	0	-1.116573	7.720163	-3.060606
36	6	0	0.215997	7.722082	-3.400545
37	6	0	0.900530	6.484305	-3.557197
38	6	0	0.245003	5.314268	-3.254917
39	6	0	-3.515309	2.761156	-1.816492
40	7	0	-2.410534	1.984527	-1.721316
41	6	0	-1.350786	2.777769	-2.021002
42	8	0	-7.447954	6.502669	-2.818280
43	8	0	-6.218090	8.771282	-2.712672
44	1	0	-3.541975	8.654680	-2.719512
45	1	0	-1.639602	8.665416	-3.023627
46	8	0	0.955566	8.826131	-3.660726
47	8	0	2.171360	6.573418	-4.011109
48	6	0	-4.775435	2.388933	-1.346604
49	6	0	-8.777743	-3.556425	0.390393
50	6	0	-9.999420	-2.843836	0.554080
51	6	0	-10.003428	-1.471105	0.464215
52	6	0	-8.832936	-0.729714	0.165765
53	6	0	-7.641764	-1.446189	-0.076708
54	6	0	-7.635228	-2.854378	0.084033
55	6	0	-8.832638	0.731582	0.166566
56	6	0	-7.641218	1.447926	-0.075246
57	6	0	-6.478787	0.695986	-0.466195
58	6	0	-6.479092	-0.694258	-0.466887
59	6	0	-10.002835	1.473016	0.466027
60	6	0	-9.998332	2.845630	0.557527
61	6	0	-8.776455	3.557991	0.394427
62	6	0	-7.634233	2.855944	0.086944
63	6	0	-5.189187	-1.127645	-0.951827
64	7	0	-4.448069	0.000694	-1.139331
65	6	0	-5.188618	1.129231	-0.950656
66	8	0	-8.853693	-4.887839	0.578139
67	8	0	-11.078772	-3.611152	0.833984
68	1	0	-10.934509	-0.949772	0.634279
69	1	0	-10.934041	0.951789	0.635720
70	8	0	-11.077357	3.612980	0.838606
71	8	0	-8.851986	4.889223	0.583639
72	1	0	-3.498312	0.000695	-1.495293
73	6	0	-4.776865	-2.387199	-1.349107
74	6	0	0.897366	-6.486389	-3.556563
75	6	0	0.211281	-7.723517	-3.401579
76	6	0	-1.121820	-7.720354	-3.063745
77	6	0	-1.829633	-6.520492	-2.806672
78	6	0	-1.105806	-5.306872	-2.819500
79	6	0	0.242596	-5.315817	-3.254742
80	6	0	-3.279136	-6.506972	-2.644532
81	6	0	-3.963872	-5.277154	-2.531459
82	6	0	-3.174633	-4.100429	-2.295131
83	6	0	-1.802125	-4.116243	-2.417301
84	6	0	-4.049699	-7.695325	-2.688159
85	6	0	-5.425180	-7.674445	-2.697171
86	6	0	-6.106445	-6.424942	-2.722154
87	6	0	-5.376773	-5.263559	-2.636444
88	6	0	-1.352279	-2.778214	-2.021804
89	7	0	-2.411568	-1.984250	-1.722477
90	6	0	-3.516903	-2.759889	-1.818972
91	8	0	2.168840	-6.576656	-4.008450
92	8	0	0.950111	-8.828224	-3.661041
93	1	0	-1.645828	-8.665108	-3.027874
94	1	0	-3.548966	-8.652402	-2.729279
95	8	0	-6.225177	-8.766000	-2.726144
96	8	0	-7.452417	-6.495881	-2.829241
97	6	0	-0.021131	-2.400400	-1.854009
98	6	0	-0.019765	2.398994	-1.854338
99	1	0	-5.512355	3.169137	-1.286443
100	1	0	-5.514382	-3.166919	-1.289952
101	1	0	0.717120	-3.176336	-1.961768
102	1	0	0.718841	3.174525	-1.962498
103	6	0	2.776457	-5.391422	-4.485283
104	6	0	2.776801	5.387764	-4.489676
105	6	0	-7.639572	5.631641	0.593739
106	6	0	-7.641752	-5.631051	0.584971
107	6	0	3.514387	5.564702	-1.001521
108	6	0	3.508419	-5.568071	-0.994362
109	6	0	-8.156815	5.295816	-3.014078
110	6	0	-8.159821	-5.287889	-3.023200
111	1	0	2.877718	-4.632444	-3.703506
112	1	0	2.204104	-4.969367	-5.320397
113	1	0	3.772047	-5.677824	-4.821719
114	1	0	2.202362	4.966706	-5.323859
115	1	0	2.878825	4.628352	-3.708420
116	1	0	3.772025	5.673288	-4.827929
117	1	0	-7.117783	5.567454	-0.366811
118	1	0	-6.971902	5.288915	1.388514
119	1	0	-7.933539	6.667175	0.761409
120	1	0	-6.972919	-5.290925	1.379890
121	1	0	-7.120999	-5.564625	-0.375965
122	1	0	-7.936188	-6.666832	0.750268
123	1	0	3.306351	5.135075	-0.018400
124	1	0	2.589658	5.598621	-1.587834
125	1	0	3.899770	6.576202	-0.880531
126	1	0	2.586345	-5.604086	-1.584714
127	1	0	3.295569	-5.135999	-0.013325
128	1	0	3.893970	-6.578949	-0.868858
129	1	0	-8.048542	4.609960	-2.165146
130	1	0	-7.827981	4.787648	-3.928930
131	1	0	-9.205145	5.576851	-3.107324
132	1	0	-7.829574	-4.778100	-3.936640
133	1	0	-8.051675	-4.603953	-2.172691
134	1	0	-9.208347	-5.567643	-3.118121
135	6	0	-5.607170	-10.030591	-2.729276
136	6	0	0.312848	-10.078846	-3.562380
137	6	0	7.556809	-2.971870	-3.470717
138	6	0	7.559538	2.961590	-3.475007
139	6	0	0.319785	10.077375	-3.560427
140	6	0	-5.598663	10.035182	-2.714369
141	6	0	-12.312576	2.965124	1.027077
142	6	0	-12.313813	-2.963103	1.022966
143	1	0	-6.415279	-10.761874	-2.739094
144	1	0	-4.981258	-10.172668	-3.619981
145	1	0	-4.992831	-10.182286	-1.832106
146	1	0	1.074527	-10.825153	-3.788230
147	1	0	-0.078221	-10.254941	-2.551610
148	1	0	-0.508687	-10.172880	-4.284626
149	1	0	8.287997	-3.759565	-3.651953
150	1	0	7.299116	-2.481010	-4.417817
151	1	0	7.989223	-2.237003	-2.781187
152	1	0	8.291682	3.748279	-3.656745
153	1	0	7.990490	2.227311	-2.783941
154	1	0	7.302347	2.469521	-4.421622
155	1	0	1.081906	10.822996	-3.787057
156	1	0	-0.502759	10.172662	-4.281358
157	1	0	-0.069550	10.253346	-2.548964
158	1	0	-6.405960	10.767390	-2.721829
159	1	0	-4.982978	10.184582	-1.817738
160	1	0	-4.973758	10.178141	-3.605640
161	1	0	-13.040061	3.752587	1.223294
162	1	0	-12.616994	2.406302	0.132611
163	1	0	-12.283706	2.279458	1.884308
164	1	0	-13.041602	-3.750552	1.218104
165	1	0	-12.284887	-2.278459	1.881011
166	1	0	-12.617856	-2.403125	0.129096
167	1	0	2.385448	3.331735	-1.027485
168	1	0	2.382301	-3.333593	-1.022551
169	1	0	-5.886707	4.320007	-2.696562
170	1	0	0.749039	4.372340	-3.415948
171	1	0	-6.698752	-3.389313	0.052872
172	1	0	-6.697651	3.390711	0.055632
173	1	0	0.747876	-4.374346	-3.414510
174	1	0	-5.888828	-4.315115	-2.702659
175	6	0	-4.320037	3.521793	1.895906
176	6	0	-5.390891	2.832209	2.526559
177	6	0	-5.331556	1.465581	2.658034
178	6	0	-4.192755	0.727540	2.265959
179	6	0	-3.071726	1.438159	1.792382
180	6	0	-3.179690	2.827636	1.559558
181	6	0	-4.192341	-0.731946	2.264865
182	6	0	-3.070711	-1.441181	1.790729
183	6	0	-1.854152	-0.695296	1.598872
184	6	0	-1.854630	0.693360	1.599355
185	6	0	-5.330802	-1.471329	2.655369
186	6	0	-5.389111	-2.837818	2.521888
187	6	0	-4.317680	-3.525784	1.890420
188	6	0	-3.177580	-2.830372	1.555815
189	6	0	-0.479147	1.128273	1.609228
190	7	0	0.285910	-0.000318	1.558043
191	6	0	-0.478445	-1.129382	1.608863
192	8	0	-4.529095	4.840078	1.675615
193	8	0	-6.434649	3.605033	2.913409
194	1	0	-6.194450	0.949997	3.053435

195	1	0	-6.194317	-0.956935	3.050955
196	8	0	-6.432406	-3.611882	2.907565
197	8	0	-4.526009	-4.843728	1.667498
198	1	0	1.300241	-0.000029	1.573326
199	6	0	6.102183	6.430127	2.712871
200	6	0	5.419554	7.678862	2.686727
201	6	0	4.044039	7.698236	2.679485
202	6	0	3.274706	6.508988	2.638725
203	6	0	3.960612	5.279748	2.526374
204	6	0	5.373660	5.267832	2.629660
205	6	0	1.825439	6.521127	2.803048
206	6	0	1.102909	5.306778	2.817744
207	6	0	1.799948	4.116590	2.415492
208	6	0	3.172334	4.101948	2.292030
209	6	0	1.116811	7.720411	3.060550
210	6	0	-0.215775	7.722391	3.400430
211	6	0	-0.900351	6.484651	3.557164
212	6	0	-0.244833	5.314570	3.255018
213	6	0	3.515411	2.761317	1.816633
214	7	0	2.410615	1.984719	1.721454
215	6	0	1.350895	2.777990	2.021158
216	8	0	7.448186	6.502643	2.818476
217	8	0	6.218413	8.771321	2.712907
218	1	0	3.542291	8.654828	2.719631
219	1	0	1.639854	8.665654	3.023501
220	8	0	-0.955320	8.826487	3.660471
221	8	0	-2.171208	6.573843	4.010982
222	6	0	4.775525	2.389056	1.346736
223	6	0	8.777454	-3.556535	-0.390533
224	6	0	9.999015	-2.843929	-0.555007
225	6	0	10.003032	-1.471184	-0.465382
226	6	0	8.832660	-0.729765	-0.166532
227	6	0	7.641602	-1.446220	0.076580
228	6	0	7.635054	-2.854455	-0.083829
229	6	0	8.832387	0.731535	-0.167458
230	6	0	7.641107	1.447927	0.074920
231	6	0	6.478775	0.696024	0.466233
232	6	0	6.479054	-0.694223	0.467016
233	6	0	10.002457	1.472928	-0.467509
234	6	0	9.997972	2.845548	-0.558977
235	6	0	8.776236	3.557972	-0.395142
236	6	0	7.634137	2.855956	-0.087158
237	6	0	5.189196	-1.127545	0.952153
238	7	0	4.448121	0.000822	1.139652
239	6	0	5.188666	1.129329	0.950822
240	8	0	8.853395	-4.887982	-0.578014
241	8	0	11.078246	-3.611264	-0.835330
242	1	0	10.934030	-0.949862	-0.635930
243	1	0	10.933544	0.951669	-0.637754
244	8	0	11.076875	3.612843	-0.840675
245	8	0	8.851726	4.889206	-0.584356
246	1	0	3.498387	0.000857	1.495679
247	6	0	4.776851	-2.387039	1.349580
248	6	0	-0.897450	-6.486331	3.556534
249	6	0	-0.211318	-7.723426	3.401508
250	6	0	1.121807	-7.720190	3.063769
251	6	0	1.829609	-6.520288	2.806845
252	6	0	1.105754	-5.306676	2.819753
253	6	0	-0.242684	-5.315717	3.254879
254	6	0	3.279113	-6.506735	2.644775
255	6	0	3.963831	-5.276888	2.531928
256	6	0	3.174584	-4.100174	2.295617
257	6	0	1.802067	-4.115999	2.417702
258	6	0	4.049703	-7.695081	2.688214
259	6	0	5.425181	-7.674160	2.697378
260	6	0	6.106410	-6.424639	2.722741
261	6	0	5.376720	-5.263263	2.637113
262	6	0	1.352241	-2.777950	2.022251
263	7	0	2.411553	-1.983993	1.722948
264	6	0	3.516872	-2.759639	1.819481
265	8	0	-2.168972	-6.576649	4.008299
266	8	0	-0.950121	-8.828178	3.660836
267	1	0	1.645872	-8.664916	3.027971
268	1	0	3.548985	-8.652180	2.729027
269	8	0	6.225211	-8.765694	2.726179
270	8	0	7.452361	-6.495579	2.830054
271	6	0	0.021099	-2.400117	1.854478
272	6	0	0.019863	2.399270	1.854496
273	1	0	5.512460	3.169242	1.286545
274	1	0	5.514322	-3.166805	1.290492
275	1	0	-0.717159	-3.176040	1.962272
276	1	0	-0.718709	3.174842	1.962613
277	6	0	-2.776464	-5.391543	4.485629
278	6	0	-2.776755	5.388251	4.489578
279	6	0	7.639378	5.631723	-0.593672
280	6	0	7.641522	-5.631319	-0.584163
281	6	0	-3.513834	5.565112	1.001318
282	6	0	-3.508639	-5.567644	0.995124
283	6	0	8.156965	5.295769	3.014450
284	6	0	8.159767	-5.287578	3.023952
285	1	0	-2.877867	-4.632311	3.704113
286	1	0	-2.203931	-4.969777	5.320764
287	1	0	-3.771999	-5.678026	4.822157
288	1	0	-2.202360	4.967165	5.323778
289	1	0	-2.878837	4.628828	3.708340
290	1	0	-3.771952	5.673875	4.827824
291	1	0	7.118059	5.567348	0.367119
292	1	0	6.971239	5.289309	-1.388195
293	1	0	7.933357	6.667276	-0.761208
294	1	0	6.972415	-5.291687	-1.379062
295	1	0	7.121014	-5.564460	0.376867
296	1	0	7.936035	-6.667152	-0.748995
297	1	0	-3.305712	5.135500	0.018207
298	1	0	-2.589180	5.598859	1.587757
299	1	0	-3.899064	6.576669	0.880347
300	1	0	-2.586218	-5.603153	1.584962
301	1	0	-3.296505	-5.135844	0.013819
302	1	0	-3.893941	-6.578694	0.870263
303	1	0	8.048962	4.609966	2.165433
304	1	0	7.827833	4.787552	3.929165
305	1	0	9.205267	5.576788	3.108069
306	1	0	7.829534	-4.777747	3.937374
307	1	0	8.051608	-4.603683	2.173408
308	1	0	9.208292	-5.567330	3.118874
309	6	0	5.607248	-10.030310	2.728634
310	6	0	-0.312712	-10.078746	3.562419
311	6	0	-7.556740	-2.971229	3.471605
312	6	0	-7.559103	2.962745	3.475342
313	6	0	-0.319488	10.077695	3.560056
314	6	0	5.599045	10.035249	2.714757
315	6	0	12.311951	2.964936	-1.029907
316	6	0	12.313122	-2.963199	-1.025337
317	1	0	6.415382	-10.761569	2.738202
318	1	0	4.981234	-10.172836	3.619196
319	1	0	4.993020	-10.181592	1.831319
320	1	0	-1.074338	-10.825102	3.788288
321	1	0	0.078487	-10.254941	2.551717
322	1	0	0.508752	-10.172587	4.284770
323	1	0	-8.287655	-3.758979	3.653696
324	1	0	-7.298664	-2.479779	4.418294
325	1	0	-7.989686	-2.236838	2.781899
326	1	0	-8.290902	3.749658	3.657508
327	1	0	-7.990599	2.228749	2.784315
328	1	0	-7.301711	2.470436	4.421774
329	1	0	-1.081593	10.823370	3.786564
330	1	0	0.503026	10.173035	4.281014
331	1	0	0.069899	10.253533	2.548590
332	1	0	6.406376	10.767419	2.722344
333	1	0	4.983400	10.184806	1.818125
334	1	0	4.974116	10.178112	3.606026
335	1	0	13.039350	3.752371	-1.226547
336	1	0	12.616884	2.406082	-0.135636
337	1	0	12.282534	2.279289	-1.887135
338	1	0	13.040793	-3.750653	-1.220897
339	1	0	12.283526	-2.278686	-1.883463
340	1	0	12.617819	-2.403076	-0.131780
341	1	0	-2.385203	3.331961	1.027253
342	1	0	-2.382396	-3.333292	1.023215
343	1	0	5.886855	4.320063	2.696676
344	1	0	-0.748899	4.372663	3.416083
345	1	0	6.698615	-3.389427	-0.052137
346	1	0	6.697605	3.390780	-0.055408
347	1	0	-0.747986	-4.374275	3.414750
348	1	0	5.888716	-4.314803	2.703582

Table S26. Cartesian coordinates for the optimized structure of [**3a**-H_2]$_2$-C_{2h} (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.058797	4.330020	1.108262
2	6	0	-4.352218	3.814717	1.382417
3	6	0	-4.492108	2.486977	1.718589
4	6	0	-3.400479	1.597569	1.772235
5	6	0	-2.112108	2.127767	1.545789
6	6	0	-1.969788	3.489244	1.213591
7	6	0	-3.587311	0.157383	1.924498
8	6	0	-2.519183	-0.721476	1.653593
9	6	0	-1.196273	-0.154626	1.611721
10	6	0	-0.999847	1.218914	1.614004
11	6	0	-4.836699	-0.399815	2.277609
12	6	0	-5.049271	-1.759751	2.262593
13	6	0	-4.030901	-2.621985	1.768423
14	6	0	-2.787878	-2.102174	1.493377
15	6	0	0.417512	1.461974	1.741213
16	7	0	1.020389	0.239766	1.737698
17	6	0	0.105023	-0.773945	1.733449
18	8	0	-2.978320	5.623870	0.713966
19	8	0	-5.496274	4.530927	1.167126
20	1	0	-5.508006	2.132044	1.846834
21	1	0	-5.644298	0.253534	2.578495
22	8	0	-6.186436	-2.377594	2.647087
23	8	0	-4.390145	-3.919983	1.619111
24	1	0	2.020170	0.095307	1.819959
25	6	0	7.495796	6.147251	1.769405
26	6	0	6.897734	7.431890	1.637224
27	6	0	5.541041	7.567294	1.818216
28	6	0	4.701561	6.453957	2.068106
29	6	0	5.281194	5.166554	2.046637
30	6	0	6.690443	5.052332	1.967207
31	6	0	3.293656	6.614115	2.406278
32	6	0	2.492058	5.478187	2.649795
33	6	0	3.050841	4.193775	2.343676
34	6	0	4.392814	4.038803	2.079932
35	6	0	2.697496	7.891016	2.554766
36	6	0	1.388307	8.046424	2.950284
37	6	0	0.618000	6.899342	3.291342
38	6	0	1.178391	5.652418	3.151601
39	6	0	4.565438	2.623438	1.739731
40	7	0	3.384237	1.958752	1.821761
41	6	0	2.441860	2.880790	2.116719
42	8	0	8.846705	6.119402	1.684857
43	8	0	7.758559	8.444593	1.374596
44	1	0	5.110712	8.557985	1.770778
45	1	0	3.287065	8.777494	2.366983
46	8	0	0.747407	9.231790	3.089544
47	8	0	-0.636050	7.146818	3.736207
48	6	0	5.727674	2.059500	1.225415
49	6	0	8.681825	-4.398476	-0.700742
50	6	0	10.012273	-3.909216	-0.833442
51	6	0	10.262485	-2.565844	-0.658328
52	6	0	9.241551	-1.654139	-0.292156
53	6	0	7.962082	-2.177251	-0.020775
54	6	0	7.695068	-3.540185	-0.281779
55	6	0	9.441418	-0.206408	-0.347689
56	6	0	8.349407	0.669501	-0.160065
57	6	0	7.126740	0.109647	0.352129
58	6	0	6.947708	-1.266201	0.429647
59	6	0	10.687168	0.357166	-0.714493
60	6	0	10.835606	1.702302	-0.963763
61	6	0	9.697450	2.554505	-0.910162
62	6	0	8.487846	2.036165	-0.507240
63	6	0	5.652522	-1.506430	1.009632
64	7	0	5.084344	-0.283340	1.202900
65	6	0	5.944331	0.729101	0.895194
66	8	0	8.488994	-5.694754	-1.026314
67	8	0	10.933070	-4.835361	-1.188008
68	1	0	11.263300	-2.200524	-0.841363
69	1	0	11.549884	-0.285677	-0.819601
70	8	0	11.993112	2.310215	-1.312367
71	8	0	9.911798	3.836584	-1.276961
72	1	0	4.165145	-0.134945	1.603575
73	6	0	5.106755	-2.708248	1.437727
74	6	0	-1.074375	-5.984005	3.665533
75	6	0	-0.605958	-7.310181	3.446346
76	6	0	0.694740	-7.513818	3.047531
77	6	0	1.580021	-6.437530	2.791745
78	6	0	1.072507	-5.124940	2.895854
79	6	0	-0.241788	-4.926755	3.386206
80	6	0	2.996576	-6.652271	2.519048
81	6	0	3.878580	-5.551050	2.434369
82	6	0	3.296365	-4.238850	2.347435
83	6	0	1.943333	-4.046973	2.524272
84	6	0	3.543237	-7.954715	2.407520
85	6	0	4.895016	-8.172551	2.282034
86	6	0	5.788794	-7.065530	2.319583
87	6	0	5.274636	-5.792904	2.398031
88	6	0	1.687562	-2.646253	2.187049
89	7	0	2.840766	-2.001116	1.902618
90	6	0	3.826565	-2.934503	1.932729
91	8	0	-2.333157	-5.881371	4.148592
92	8	0	-1.507331	-8.287252	3.704795
93	1	0	1.052694	-8.530059	2.960088
94	1	0	2.882643	-8.810308	2.420599
95	8	0	5.485118	-9.384354	2.154352
96	8	0	7.102675	-7.376921	2.270706
97	6	0	0.416548	-2.094675	2.000668
98	6	0	1.067981	2.657286	1.997034
99	1	0	6.546834	2.728600	1.031373
100	1	0	5.750788	-3.563762	1.339477
101	1	0	-0.419057	-2.768069	2.083787
102	1	0	0.427969	3.516713	2.099615
103	6	0	-2.764256	-4.607396	4.586490
104	6	0	-1.396373	6.046987	4.194710
105	6	0	8.773561	4.655305	-1.458282
106	6	0	7.145477	-6.133538	-1.144189
107	6	0	-1.697873	6.162035	0.453182
108	6	0	-3.426348	-4.813029	1.086655
109	6	0	9.498022	4.914746	2.034253
110	6	0	8.032582	-6.326447	2.440117
111	1	0	-2.769595	-3.870241	3.775977
112	1	0	-2.130286	-4.237930	5.401799
113	1	0	-3.784751	-4.742052	4.942625
114	1	0	-0.906568	5.549474	5.040580
115	1	0	-1.575706	5.310051	3.401453
116	1	0	-2.351916	6.458440	4.518865
117	1	0	8.213383	4.798821	-0.527916
118	1	0	8.094472	4.229117	-2.206386
119	1	0	9.149666	5.619465	-1.799349
120	1	0	6.581640	-5.501261	-1.840149
121	1	0	6.633512	-6.138676	-0.174013
122	1	0	7.198431	-7.154921	-1.519413
123	1	0	-1.203303	5.627949	-0.364771
124	1	0	-1.063073	6.143454	1.345235
125	1	0	-1.862512	7.193326	0.144280
126	1	0	-2.562062	-4.915026	1.750569
127	1	0	-3.089248	-4.491221	0.098178
128	1	0	-3.926056	-5.777654	1.000318
129	1	0	9.232825	4.089717	1.362995
130	1	0	9.263067	4.624975	3.065799
131	1	0	10.565113	5.112321	1.940019
132	1	0	7.915603	-5.849179	3.421057
133	1	0	7.940533	-5.564535	1.657861
134	1	0	9.018303	-6.784625	2.370014
135	6	0	4.652389	-10.518769	2.140665
136	6	0	-1.091767	-9.621178	3.538775
137	6	0	-7.239710	-1.578017	3.140619
138	6	0	-5.622660	5.805596	1.783277
139	6	0	1.466390	10.402774	2.784998
140	6	0	7.225280	9.741983	1.263160
141	6	0	13.148702	1.511987	-1.411853
142	6	0	12.258444	-4.402874	-1.381685
143	1	0	5.313502	-11.377801	2.026281
144	1	0	4.089654	-10.618835	3.078104
145	1	0	3.946089	-10.491666	1.300403
146	1	0	-1.956859	-10.239507	3.778352
147	1	0	-0.778433	-9.821255	2.505532
148	1	0	-0.267595	-9.876254	4.217774
149	1	0	-8.075082	-2.257562	3.310145
150	1	0	-6.955334	-1.090335	4.081808
151	1	0	-7.547192	-0.816875	2.415844
152	1	0	-6.571710	6.214091	1.432141
153	1	0	-5.648157	5.703815	2.875933
154	1	0	-4.816623	6.477994	1.490758
155	1	0	0.775321	11.231206	2.940628
156	1	0	2.333898	10.528931	3.445606
157	1	0	1.808083	10.407157	1.741371
158	1	0	8.067272	10.397503	1.040899
159	1	0	6.490289	9.808810	0.450050
160	1	0	6.752583	10.067159	2.199207
161	1	0	13.959485	2.187062	-1.685194
162	1	0	13.388207	1.026756	-0.456798
163	1	0	13.042947	0.742699	-2.187956
164	1	0	12.831571	-5.292337	-1.642988
165	1	0	12.330576	-3.674373	-2.200000
166	1	0	12.676213	-3.958302	-0.468997
167	1	0	-0.997471	3.855230	0.920237
168	1	0	-2.020826	-2.743652	1.084027
169	1	0	7.147411	4.084413	2.107324
170	1	0	0.619784	4.783393	3.466964
171	1	0	6.669433	-3.878218	-0.277836
172	1	0	7.615463	2.676252	-0.508488
173	1	0	-0.573999	-3.921180	3.600613
174	1	0	5.955137	-4.959246	2.480783
175	6	0	3.059480	4.332754	-1.110944
176	6	0	4.352347	3.817418	-1.387429
177	6	0	4.492246	2.489454	-1.722062
178	6	0	3.400595	1.599888	-1.773062
179	6	0	2.112399	2.130210	-1.545515
180	6	0	1.970281	3.491932	-1.213856
181	6	0	3.587672	0.159658	-1.924154
182	6	0	2.519743	-0.719112	-1.652371
183	6	0	1.196830	-0.152279	-1.610137
184	6	0	1.000083	1.221250	-1.612574
185	6	0	4.837180	-0.397590	-2.276905
186	6	0	5.049988	-1.757466	-2.261005
187	6	0	4.031594	-2.619573	-1.766687
188	6	0	2.788566	-2.099741	-1.491715
189	6	0	-0.417498	1.463883	-1.739362
190	7	0	-1.019939	0.241451	-1.735545
191	6	0	-0.104275	-0.771968	-1.731442
192	8	0	2.980515	5.626953	-0.717557
193	8	0	5.495623	4.535984	-1.175650
194	1	0	5.508003	2.134674	-1.851883

195	1	0	5.644715	0.255636	-2.578204
196	8	0	6.187400	-2.375416	-2.644631
197	8	0	4.390845	-3.917534	-1.617205
198	1	0	-2.019692	0.096668	-1.817593
199	6	0	-7.500043	6.142872	-1.768478
200	6	0	-6.903362	7.428148	-1.636325
201	6	0	-5.546769	7.564973	-1.817101
202	6	0	-4.706061	6.452477	-2.066886
203	6	0	-5.284418	5.164516	-2.045914
204	6	0	-6.693558	5.048861	-1.966602
205	6	0	-3.298124	6.613972	-2.404265
206	6	0	-2.495323	5.478870	-2.647770
207	6	0	-3.052983	4.193800	-2.342205
208	6	0	-4.394940	4.037613	-2.079037
209	6	0	-2.703175	7.891500	-2.551992
210	6	0	-1.394002	8.048368	-2.946961
211	6	0	-0.622496	6.902167	-3.288268
212	6	0	-1.181682	5.654616	-3.149116
213	6	0	-4.566515	2.622175	-1.738675
214	7	0	-3.384702	1.958493	-1.820355
215	6	0	-2.442912	2.881286	-2.115049
216	8	0	-8.850890	6.113519	-1.683294
217	8	0	-7.765335	8.439891	-1.373754
218	1	0	-5.117480	8.556104	-1.769445
219	1	0	-3.293728	8.777308	-2.364148
220	8	0	-0.754290	9.234467	-3.085471
221	8	0	0.631374	7.151067	-3.732877
222	6	0	-5.728484	2.057624	-1.224227
223	6	0	-8.679050	-4.401934	0.703052
224	6	0	-10.010109	-3.913827	0.833789
225	6	0	-10.261262	-2.570712	0.658041
226	6	0	-9.240658	-1.658241	0.292761
227	6	0	-7.960500	-2.180370	0.022861
228	6	0	-7.692522	-3.542929	0.284981
229	6	0	-9.441660	-0.210640	0.347607
230	6	0	-8.350216	0.666100	0.160374
231	6	0	-7.126791	0.107078	-0.350914
232	6	0	-6.946693	-1.268680	-0.427626
233	6	0	-10.688055	0.352035	0.713567
234	6	0	-10.837615	1.697060	0.962810
235	6	0	-9.699989	2.550052	0.909986
236	6	0	-8.489866	2.032709	0.507272
237	6	0	-5.651293	-1.508180	-1.007394
238	7	0	-5.083877	-0.284800	-1.200966
239	6	0	-5.944561	0.727185	-0.893761
240	8	0	-8.485605	-5.697936	1.029370
241	8	0	-10.930532	-4.840771	1.187302
242	1	0	-11.262637	-2.206232	0.839673
243	1	0	-11.550361	-0.291444	0.818142
244	8	0	-11.995834	2.304095	1.310611
245	8	0	-9.915328	3.831855	1.277187
246	1	0	-4.164685	-0.135897	-1.601476
247	6	0	-5.104831	-2.709667	-1.435399
248	6	0	1.077852	-5.980283	-3.665957
249	6	0	0.609975	-7.306927	-3.448493
250	6	0	-0.690604	-7.511622	-3.049841
251	6	0	-1.576322	-6.436040	-2.792631
252	6	0	-1.069394	-5.123112	-2.895257
253	6	0	0.244800	-4.923763	-3.385358
254	6	0	-2.992786	-6.651743	-2.520235
255	6	0	-3.875276	-5.551010	-2.434440
256	6	0	-3.293643	-4.238685	-2.346028
257	6	0	-1.940733	-4.045934	-2.522705
258	6	0	-3.538941	-7.954529	-2.410292
259	6	0	-4.890687	-8.173049	-2.285625
260	6	0	-5.784920	-7.066371	-2.322465
261	6	0	-5.271257	-5.793452	-2.399024
262	6	0	-1.685822	-2.645212	-2.184884
263	7	0	-2.839385	-2.000905	-1.900078
264	6	0	-3.824562	-2.934912	-1.930563
265	8	0	2.336565	-5.876456	-4.148889
266	8	0	1.511690	-8.283276	-3.708410
267	1	0	-1.048186	-8.528113	-2.963839
268	1	0	-2.877981	-8.809822	-2.423947
269	8	0	-5.480346	-9.385217	-2.159535
270	8	0	-7.098710	-7.378341	-2.274918
271	6	0	-0.415177	-2.092855	-1.998624
272	6	0	-1.068810	2.658799	-1.995168
273	1	0	-6.547898	2.726396	-1.029932
274	1	0	-5.748269	-3.565610	-1.337128
275	1	0	0.420801	-2.765734	-2.081999
276	1	0	-0.429379	3.518698	-2.097644
277	6	0	2.767048	-4.601691	-4.585036
278	6	0	1.392586	6.052287	-4.192371
279	6	0	-8.777750	4.651584	1.457964
280	6	0	-7.141955	-6.135865	1.148478
281	6	0	1.700790	6.165829	-0.454556
282	6	0	3.426750	-4.810674	-1.085496
283	6	0	-9.500955	4.907858	-2.031500
284	6	0	-8.028872	-6.328056	-2.444137
285	1	0	2.771627	-3.865559	-3.773623
286	1	0	2.133132	-4.231581	-5.400096
287	1	0	3.787752	-4.735246	-4.940968
288	1	0	0.903241	5.555286	-5.038809
289	1	0	1.572349	5.314646	-3.399892
290	1	0	2.347871	6.464780	-4.515953
291	1	0	-8.218446	4.795556	0.527109
292	1	0	-8.097684	4.226148	2.205661
293	1	0	-9.154560	5.615387	1.799318
294	1	0	-6.579283	-5.503458	1.845230
295	1	0	-6.629022	-6.140367	0.178841
296	1	0	-7.194604	-7.157368	1.523411
297	1	0	1.207409	5.632079	0.364313
298	1	0	1.064400	6.147438	-1.345493
299	1	0	1.866487	7.197075	-0.146131
300	1	0	2.563408	-4.913388	-1.750531
301	1	0	3.088132	-4.488476	-0.097683
302	1	0	3.926784	-5.774999	-0.997850
303	1	0	-9.234433	4.083625	-1.359740
304	1	0	-9.266162	4.617612	-3.062960
305	1	0	-10.568225	5.104282	-1.936838
306	1	0	-7.911307	-5.849835	-3.424555
307	1	0	-7.937746	-5.566805	-1.661128
308	1	0	-9.014483	-6.786683	-2.375312
309	6	0	-4.647125	-10.519245	-2.146041
310	6	0	1.096702	-9.617567	-3.544069
311	6	0	7.241572	-1.576079	-3.136579
312	6	0	5.621880	5.803689	-1.805795
313	6	0	-1.474563	10.404522	-2.780360
314	6	0	-7.233634	9.737940	-1.262635
315	6	0	-13.151098	1.505133	1.408179
316	6	0	-12.256675	-4.409613	1.378612
317	1	0	-5.307910	-11.378641	-2.032600
318	1	0	-4.083776	-10.618483	-3.083182
319	1	0	-3.941334	-10.492321	-1.305350
320	1	0	1.962049	-10.235215	-3.784431
321	1	0	0.783462	-9.819078	-2.511090
322	1	0	0.272629	-9.872135	-4.223381
323	1	0	8.077112	-2.255799	-3.304608
324	1	0	6.958834	-1.088457	-4.078258
325	1	0	7.548053	-0.814951	-2.411383
326	1	0	6.562509	6.223918	-1.445548
327	1	0	5.664621	5.688675	-2.896834
328	1	0	4.806468	6.473891	-1.533738
329	1	0	-0.784353	11.233789	-2.935357
330	1	0	-2.342088	10.530165	-3.441049
331	1	0	-1.816460	10.407923	-1.736788
332	1	0	-8.076422	10.392478	-1.040466
333	1	0	-6.498679	9.805861	-0.449594
334	1	0	-6.761415	10.063466	-2.198801
335	1	0	-13.962702	2.179634	1.680529
336	1	0	-13.388887	1.020038	0.452611
337	1	0	-13.046067	0.735661	2.184209
338	1	0	-12.829324	-5.299625	1.639139
339	1	0	-12.330961	-3.681013	2.196647
340	1	0	-12.673322	-3.965674	0.465101
341	1	0	0.998276	3.857998	-0.919459
342	1	0	2.021631	-2.741156	-1.082058
343	1	0	-7.149484	4.080460	-2.106734
344	1	0	-0.622107	4.786259	-3.464611
345	1	0	-6.666582	-3.880002	0.282355
346	1	0	-7.617979	2.673518	0.508484
347	1	0	0.576551	-3.917801	-3.598585
348	1	0	-5.952055	-4.959975	-2.481071

Table S27. Cartesian coordinates for the optimized structure of [**3a**-Zn]$_2$ (ωB97XD/6-31G**).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.311498	-3.523782	-1.916711
2	6	0	-5.376899	-2.833287	-2.555878
3	6	0	-5.314116	-1.467257	-2.689977
4	6	0	-4.178476	-0.729507	-2.288640
5	6	0	-3.062757	-1.440458	-1.801683
6	6	0	-3.174257	-2.830168	-1.569183
7	6	0	-4.178502	0.729360	-2.288667
8	6	0	-3.062817	1.440365	-1.801703
9	6	0	-1.850087	0.693501	-1.581903
10	6	0	-1.850062	-0.693541	-1.581906
11	6	0	-5.314160	1.467051	-2.690073
12	6	0	-5.376992	2.833078	-2.556016
13	6	0	-4.311643	3.523629	-1.916822
14	6	0	-3.174389	2.830076	-1.569220
15	6	0	-0.456233	-1.102785	-1.590055
16	7	0	0.340822	0.000008	-1.538170
17	6	0	-0.456259	1.102785	-1.590043
18	8	0	-4.522591	-4.841877	-1.699955
19	8	0	-6.418846	-3.604749	-2.947973
20	1	0	-6.173567	-0.951661	-3.092451
21	1	0	-6.173572	0.951415	-3.092582
22	8	0	-6.418945	3.604504	-2.948156
23	8	0	-4.522811	4.841715	-1.700124
24	6	0	6.110081	-6.417661	-2.677552
25	6	0	5.428187	-7.666133	-2.645459
26	6	0	4.052186	-7.686266	-2.640604
27	6	0	3.282747	-6.497655	-2.608424
28	6	0	3.967803	-5.268542	-2.502919
29	6	0	5.380053	-5.255119	-2.602038
30	6	0	1.832428	-6.512085	-2.777890
31	6	0	1.109171	-5.299777	-2.803915
32	6	0	1.802749	-4.103786	-2.407499
33	6	0	3.179235	-4.086694	-2.279250
34	6	0	1.126514	-7.712849	-3.032111
35	6	0	-0.204827	-7.717721	-3.379003
36	6	0	-0.889303	-6.481917	-3.546303
37	6	0	-0.235685	-5.309559	-3.246639
38	6	0	3.532830	-2.757658	-1.812570
39	7	0	2.413837	-1.985021	-1.746559
40	6	0	1.338175	-2.778916	-2.029118
41	8	0	7.455809	-6.489780	-2.779079
42	8	0	6.227146	-8.758346	-2.663405
43	1	0	3.551129	-8.643365	-2.676433
44	1	0	1.650006	-8.657476	-2.987437
45	8	0	-0.941703	-8.823885	-3.636522
46	8	0	-2.157566	-6.573978	-4.006135
47	6	0	4.776800	-2.367991	-1.323217
48	6	0	8.768180	3.555876	0.420167
49	6	0	9.991272	2.843975	0.578043
50	6	0	9.995823	1.471926	0.485985
51	6	0	8.824094	0.729916	0.191011
52	6	0	7.630095	1.445458	-0.047090
53	6	0	7.624907	2.854373	0.116787
54	6	0	8.824088	-0.729917	0.190947
55	6	0	7.630077	-1.445422	-0.047181
56	6	0	6.467003	-0.691228	-0.426498
57	6	0	6.467008	0.691301	-0.426473
58	6	0	9.995812	-1.471974	0.485827
59	6	0	9.991237	-2.844032	0.577766
60	6	0	8.768125	-3.555898	0.419874
61	6	0	7.624857	-2.854348	0.116584
62	6	0	5.154273	1.100531	-0.904262
63	7	0	4.373826	0.000042	-1.088141
64	6	0	5.154272	-1.100448	-0.904275
65	8	0	8.845002	4.887795	0.609811
66	8	0	11.071574	3.612288	0.854767
67	1	0	10.927924	0.950807	0.651492
68	1	0	10.927929	-0.950887	0.651342
69	8	0	11.071532	-3.612390	0.854392
70	8	0	8.844921	-4.887835	0.609395
71	6	0	4.776784	2.368072	-1.323198
72	6	0	-0.889412	6.482042	-3.545996
73	6	0	-0.204940	7.717834	-3.378606
74	6	0	1.126412	7.712945	-3.031765
75	6	0	1.832339	6.512167	-2.777660
76	6	0	1.109093	5.299854	-2.803748
77	6	0	-0.235771	5.309662	-3.246451
78	6	0	3.282660	6.497740	-2.608242
79	6	0	3.967727	5.268629	-2.502811
80	6	0	3.179177	4.086764	-2.279164
81	6	0	1.802691	4.103848	-2.407396
82	6	0	4.052087	7.686358	-2.640400
83	6	0	5.428090	7.666235	-2.645318
84	6	0	6.109987	6.417768	-2.677490
85	6	0	5.379971	5.255218	-2.601972
86	6	0	1.338141	2.778952	-2.029051
87	7	0	2.413818	1.985073	-1.746501
88	6	0	3.532799	2.757729	-1.812520
89	8	0	-2.157701	6.574154	-4.005755
90	8	0	-0.941830	8.824017	-3.635997
91	1	0	1.649900	8.657574	-2.987028
92	1	0	3.551016	8.643453	-2.676162
93	8	0	6.227043	8.758454	-2.663248
94	8	0	7.455711	6.489889	-2.779060
95	6	0	0.017909	2.385715	-1.851295
96	6	0	0.017940	-2.385705	-1.851345
97	1	0	5.526110	-3.137019	-1.271771
98	1	0	5.526086	3.137105	-1.271775
99	1	0	-0.726622	3.154613	-1.966144
100	1	0	-0.726591	-3.154606	-1.966211
101	6	0	-2.760436	5.391608	-4.495763
102	6	0	-2.760262	-5.391334	-4.495949
103	6	0	7.633034	-5.629717	0.624948
104	6	0	7.633134	5.629710	0.625339
105	6	0	-3.515519	-5.566191	-1.013169
106	6	0	-3.515819	5.566103	-1.013298
107	6	0	8.165340	-5.282533	-2.972995
108	6	0	8.165222	5.282639	-2.973024
109	1	0	-2.865220	4.626628	-3.720443
110	1	0	-2.182023	4.977203	-5.330474
111	1	0	-3.754347	5.679057	-4.836107
112	1	0	-2.181841	-4.976814	-5.330597
113	1	0	-2.865003	-4.626476	-3.720500
114	1	0	-3.754188	-5.678690	-4.836330
115	1	0	7.104564	-5.562172	-0.331700
116	1	0	6.969716	-5.289650	1.424557
117	1	0	7.927410	-6.666055	0.787351
118	1	0	6.969758	5.289618	1.424887
119	1	0	7.104724	5.562231	-0.331346
120	1	0	7.927531	6.666031	0.787816
121	1	0	-3.316969	-5.132864	-0.029881
122	1	0	-2.584961	-5.603075	-1.589979
123	1	0	-3.903365	-6.576713	-0.892217
124	1	0	-2.585236	5.603029	-1.590063
125	1	0	-3.317304	5.132826	-0.029978
126	1	0	-3.903725	6.576610	-0.892402
127	1	0	8.050146	-4.594811	-2.126716
128	1	0	7.842648	-4.777458	-3.891686
129	1	0	9.214431	-5.563188	-3.057704
130	1	0	7.842483	4.777582	-3.891709
131	1	0	8.050060	4.594903	-2.126752
132	1	0	9.214311	5.563286	-3.057782
133	6	0	5.608460	10.022841	-2.657111
134	6	0	-0.305147	10.074223	-3.526942
135	6	0	-7.545529	2.960296	-3.504493
136	6	0	-7.545438	-2.960579	-3.504340
137	6	0	-0.305033	-10.074107	-3.527559
138	6	0	5.608562	-10.022732	-2.657348
139	6	0	12.307183	-2.964455	1.037600
140	6	0	12.307205	2.964312	1.037966
141	1	0	6.416340	10.754407	-2.657854
142	1	0	4.985427	10.172616	-3.548554
143	1	0	4.991316	10.166278	-1.760530
144	1	0	-1.065465	10.821571	-3.753809
145	1	0	0.079441	10.245172	-2.512827
146	1	0	0.520814	10.171862	-4.243572
147	1	0	-8.278808	3.746386	-3.683972
148	1	0	-7.291907	2.467780	-4.451788
149	1	0	-7.972666	2.226811	-2.810417
150	1	0	-8.278692	-3.746692	-3.683821
151	1	0	-7.972607	-2.227092	-2.810284
152	1	0	-7.291810	-2.468070	-4.451638
153	1	0	-1.065348	-10.821427	-3.754525
154	1	0	0.520955	-10.171686	-4.244166
155	1	0	0.079514	-10.245155	-2.513445
156	1	0	6.416440	-10.754300	-2.658080
157	1	0	4.991373	-10.166203	-1.760803
158	1	0	4.985571	-10.172472	-3.548828
159	1	0	13.035745	-3.751618	1.231332
160	1	0	12.608118	-2.405787	0.141784
161	1	0	12.281851	-2.278144	1.894511
162	1	0	13.035777	3.751446	1.231782
163	1	0	12.281830	2.277937	1.894825
164	1	0	12.608157	2.405706	0.142117
165	1	0	-2.383797	-3.336626	-1.032653
166	1	0	-2.383990	3.336582	-1.032647
167	1	0	5.892119	-4.306866	-2.670717
168	1	0	-0.739078	-4.368264	-3.413556
169	1	0	6.688114	3.389303	0.089305
170	1	0	6.688050	-3.389260	0.089086
171	1	0	-0.739159	4.368379	-3.413428
172	1	0	5.892048	4.306971	-2.670668
173	30	0	2.357700	0.000013	-1.317689
174	6	0	4.311558	-3.523727	1.916702
175	6	0	5.376945	-2.833230	2.555891
176	6	0	5.314154	-1.467201	2.689994
177	6	0	4.178511	-0.729457	2.288653
178	6	0	3.062801	-1.440413	1.801683
179	6	0	3.174313	-2.830122	1.569170
180	6	0	4.178524	0.729410	2.288683
181	6	0	3.062838	1.440414	1.801719
182	6	0	1.850114	0.693542	1.581911
183	6	0	1.850104	-0.693502	1.581904
184	6	0	5.314177	1.467105	2.690093
185	6	0	5.377007	2.833135	2.556051
186	6	0	4.311663	3.523684	1.916847
187	6	0	3.174414	2.830125	1.569237
188	6	0	0.456280	-1.102763	1.590047
189	7	0	-0.340785	0.000021	1.538158
190	6	0	0.456280	1.102809	1.590047
191	8	0	4.522673	-4.841817	1.699942
192	8	0	6.418886	-3.604691	2.948002
193	1	0	6.173599	-0.951603	3.092479
194	1	0	6.173587	0.951470	3.092606

195	8	0	6.418958	3.604548	2.948227
196	8	0	4.522830	4.841772	1.700137
197	6	0	-6.110045	-6.417598	2.677542
198	6	0	-5.428179	-7.666084	2.645403
199	6	0	-4.052175	-7.686249	2.640528
200	6	0	-3.282710	-6.497655	2.608368
201	6	0	-3.967747	-5.268532	2.502892
202	6	0	-5.379993	-5.255072	2.602023
203	6	0	-1.832390	-6.512098	2.777850
204	6	0	-1.109124	-5.299794	2.803924
205	6	0	-1.802685	-4.103790	2.407494
206	6	0	-3.179167	-4.086697	2.279235
207	6	0	-1.126488	-7.712874	3.032046
208	6	0	0.204840	-7.717763	3.378985
209	6	0	0.889308	-6.481969	3.546379
210	6	0	0.235709	-5.309596	3.246721
211	6	0	-3.532769	-2.757673	1.812554
212	7	0	-2.413784	-1.985026	1.746545
213	6	0	-1.338114	-2.778913	2.029111
214	8	0	-7.455771	-6.489685	2.779157
215	8	0	-6.227160	-8.758280	2.663349
216	1	0	-3.551138	-8.643359	2.676338
217	1	0	-1.649978	-8.657499	2.987304
218	8	0	0.941707	-8.823939	3.636475
219	8	0	2.157545	-6.574062	4.006275
220	6	0	-4.776748	-2.368034	1.323207
221	6	0	-8.768181	3.555804	-0.420095
222	6	0	-9.991276	2.843904	-0.577954
223	6	0	-9.995822	1.471852	-0.485927
224	6	0	-8.824082	0.729838	-0.191001
225	6	0	-7.630083	1.445382	0.047091
226	6	0	-7.624900	2.854301	-0.116752
227	6	0	-8.824064	-0.729998	-0.190963
228	6	0	-7.630050	-1.445502	0.047165
229	6	0	-6.466977	-0.691301	0.426476
230	6	0	-6.466991	0.691227	0.426447
231	6	0	-9.995782	-1.472058	-0.485860
232	6	0	-9.991200	-2.844116	-0.577812
233	6	0	-8.768091	-3.555981	-0.419907
234	6	0	-7.624828	-2.854430	-0.116600
235	6	0	-5.154255	1.100474	0.904211
236	7	0	-4.373797	-0.000005	1.088096
237	6	0	-5.154235	-1.100503	0.904247
238	8	0	-8.845006	4.887728	-0.609708
239	8	0	-11.071588	3.612220	-0.854631
240	1	0	-10.927928	0.950738	-0.651413
241	1	0	-10.927898	-0.950975	-0.651388
242	8	0	-11.071490	-3.612472	-0.854463
243	8	0	-8.844888	-4.887917	-0.609446
244	6	0	-4.776783	2.368021	1.323138
245	6	0	0.889295	6.482040	3.546116
246	6	0	0.204828	7.717827	3.378673
247	6	0	-1.126508	7.712930	3.031765
248	6	0	-1.832419	6.512146	2.777639
249	6	0	-1.109161	5.299841	2.803762
250	6	0	0.235679	5.309655	3.246533
251	6	0	-3.282738	6.497705	2.608174
252	6	0	-3.967790	5.268585	2.502737
253	6	0	-3.179213	4.086731	2.279124
254	6	0	-1.802730	4.103827	2.407385
255	6	0	-4.052178	7.686315	2.640300
256	6	0	-5.428181	7.666177	2.645173
257	6	0	-6.110066	6.417702	2.677339
258	6	0	-5.380037	5.255158	2.601860
259	6	0	-1.338152	2.778945	2.029039
260	7	0	-2.413813	1.985050	1.746468
261	6	0	-3.532805	2.757693	1.812468
262	8	0	2.157551	6.574159	4.005962
263	8	0	0.941700	8.824015	3.636091
264	1	0	-1.649993	8.657557	2.986990
265	1	0	-3.551120	8.643415	2.676072
266	8	0	-6.227151	8.758385	2.663060
267	8	0	-7.455793	6.489816	2.778869
268	6	0	-0.017910	2.385731	1.851305
269	6	0	-0.017883	-2.385689	1.851333
270	1	0	-5.526051	-3.137075	1.271796
271	1	0	-5.526094	3.137048	1.271715
272	1	0	0.726606	3.154641	1.966173
273	1	0	0.726656	-3.154583	1.966186
274	6	0	2.760258	5.391615	4.496010
275	6	0	2.760250	-5.391458	4.496176
276	6	0	-7.633009	-5.629816	-0.624974
277	6	0	-7.633143	5.629651	-0.625256
278	6	0	3.515614	-5.566160	1.013175
279	6	0	3.515844	5.566149	1.013296
280	6	0	-8.165253	-5.282439	2.973273
281	6	0	-8.165311	5.282558	2.972763
282	1	0	2.865100	4.626638	3.720695
283	1	0	2.181790	4.977204	5.330681
284	1	0	3.754142	5.679071	4.836429
285	1	0	2.181776	-4.976938	5.330789
286	1	0	2.865090	-4.626584	3.720760
287	1	0	3.754130	-5.678870	4.836644
288	1	0	-7.104567	-5.562299	0.331690
289	1	0	-6.969663	-5.289748	-1.424556
290	1	0	-7.927395	-6.666147	-0.787404
291	1	0	-6.969764	5.289559	-1.424801
292	1	0	-7.104721	5.562187	0.331424
293	1	0	-7.927549	6.665968	-0.787742
294	1	0	3.317053	-5.132855	0.029879
295	1	0	2.585057	-5.603054	1.589985
296	1	0	3.903477	-6.576678	0.892238
297	1	0	2.585261	5.603090	1.590059
298	1	0	3.317311	5.132851	0.029988
299	1	0	3.903750	6.576653	0.892378
300	1	0	-8.050097	-4.594610	2.127076
301	1	0	-7.842489	-4.777490	3.892007
302	1	0	-9.214347	-5.563074	3.058018
303	1	0	-7.842593	4.777456	3.891430
304	1	0	-8.050139	4.594870	2.126455
305	1	0	-9.214400	5.563207	3.057518
306	6	0	-5.608592	10.022784	2.656936
307	6	0	0.305021	10.074220	3.526987
308	6	0	7.545529	2.960306	3.504554
309	6	0	7.545480	-2.960516	3.504358
310	6	0	0.305036	-10.074154	3.527441
311	6	0	-5.608602	-10.022679	2.657261
312	6	0	-12.307138	-2.964536	-1.037681
313	6	0	-12.307218	2.964240	-1.037814
314	1	0	-6.416485	10.754335	2.657638
315	1	0	-4.985599	10.172580	3.548405
316	1	0	-4.991412	10.166225	1.760380
317	1	0	1.065326	10.821571	3.753887
318	1	0	-0.079512	10.245157	2.512849
319	1	0	-0.520979	10.171866	4.243571
320	1	0	8.278815	3.746381	3.684071
321	1	0	7.291888	2.467758	4.451829
322	1	0	7.972663	2.226838	2.810457
323	1	0	8.278728	-3.746630	3.683859
324	1	0	7.972655	-2.227047	2.810285
325	1	0	7.291853	-2.467984	4.451645
326	1	0	1.065339	-10.821487	3.754407
327	1	0	-0.520979	-10.171756	4.244013
328	1	0	-0.079474	-10.245163	2.513306
329	1	0	-6.416495	-10.754230	2.658000
330	1	0	-4.991434	-10.166150	1.760702
331	1	0	-4.985596	-10.172445	3.548726
332	1	0	-13.035697	-3.751698	-1.231428
333	1	0	-12.608084	-2.405876	-0.141863
334	1	0	-12.281795	-2.278217	-1.894586
335	1	0	-13.035801	3.751372	-1.231596
336	1	0	-12.281860	2.277882	-1.894686
337	1	0	-12.608145	2.405614	-0.141968
338	1	0	2.383862	-3.336582	1.032628
339	1	0	2.384017	3.336630	1.032663
340	1	0	-5.892033	-4.306803	2.670714
341	1	0	0.739104	-4.368314	3.413685
342	1	0	-6.688114	3.389245	-0.089268
343	1	0	-6.688023	-3.389341	-0.089087
344	1	0	0.739063	4.368373	3.413533
345	1	0	-5.892104	4.306903	2.670550
346	30	0	-2.357667	-0.000001	1.317673