

# Time-resolved imaging and analysis of the electron beam-induced formation of an open-cage metallo-azafullerene

---

In the format provided by the authors and unedited

---

## **This PDF file includes:**

Captions for Supplementary Video 1 to 3, Supplementary Synthetic Details, Supplementary Description of Cross-Section Calculation, Supplementary Computational Details, XYZ Coordinates, NMR and MS Spectral Appendix, Supplementary Text, Supplementary Figures 1 to 36, Supplementary Tables 1 to 19, Supplementary References.

## **Other Supplementary Materials for this manuscript include the following:**

Supplementary Video 1 to 3

## **Content**

1	CAPTION FOR VIDEOS	2
2	SYNTHETIC SECTION	3
2.1	General methods and materials	3
2.2	Synthetic details	4
3	ELECTRON MICROSCOPY SECTION	11
3.1	Elastic scattering-induced processes	11
3.2	Inelastic scattering-induced processes	13
3.3	Secondary electron flux	15
3.4	Supplementary Video 1 – Transformation of 1Pb to Pb@(FP-Pb) and Pb@(FP)	16
3.5	Supplementary Video 2 – Decomposition of Pb@(FP) under the electron beam	19
3.6	Supplementary Video 3 – Detachment of empty hemi-FP from graphene monolayer	22
3.7	STEM/EDS analysis	26
4	COMPUTATIONAL SECTION	27
4.1	Thermochemical analysis	27
4.2	Homolytic bond dissociation analysis	39
4.3	Orbital energies of 1 for ionization cross-section	42
4.4	Calculated energies for fullerophyrin metal complexes	50
4.5	XYZ Coordinates from thermochemistry	57
5	SPECTRAL APPENDIX (NMR, MS)	105
6	SUPPLEMENTARY REFERENCES	125

## 1 Caption for Videos

**Supplementary Video 1: Transformation of 1Pb to Pb@(FP-Pb) and Pb@(FP) on graphene.** 80 kV, magnification 1 000 000x,  $t_{\text{exp}} = 500$  ms, drift corrected, bandpass filtered, and contrast corrected. Video displayed at 6 fps, 1-86-Frames. The video displays the motion 3 times faster than the actual recording.

**Supplementary Video 2: Decomposition of Pb@(FP) under the electron beam.** 80 kV, magnification 1 000 000x,  $t_{\text{exp}} = 500$  ms, drift corrected, bandpass filtered, and contrast corrected. Video displayed at 12 fps, 87-200-Frames. The video displays the motion 6 times faster than the actual recording.

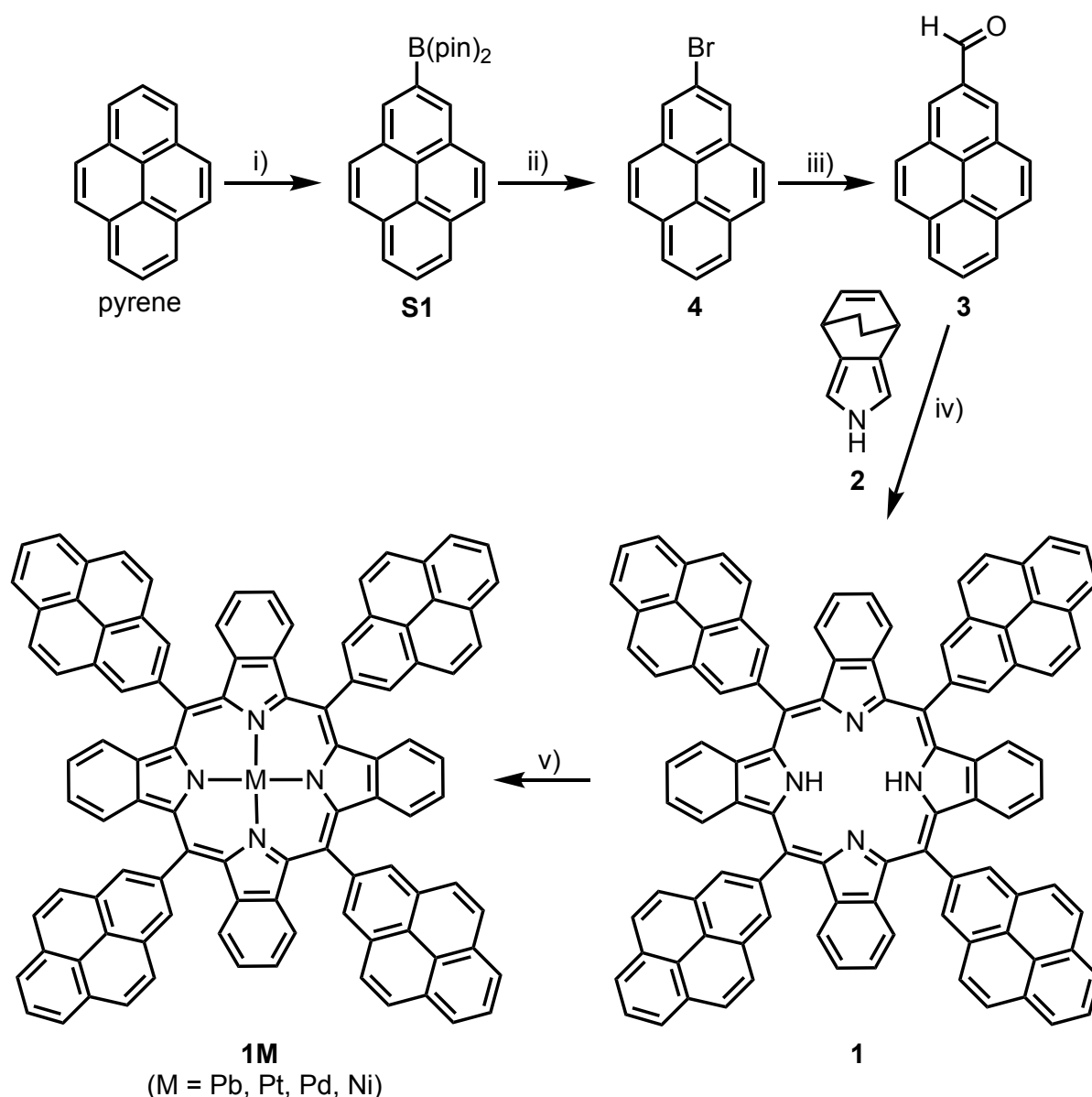
**Supplementary Video 3: Detachment of empty hemi-FP from graphene monolayer.** 80 kV, magnification 2 000 000x,  $t_{\text{exp}} = 500$  ms, drift corrected, bandpass filtered, and contrast corrected. Video displayed at 10 fps, 1-140-Frames. The video displays the motion 5 times faster than the actual recording.

## 2 Synthetic Section

### 2.1 General methods and materials

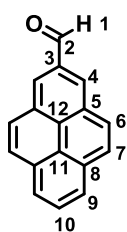
**Chemicals** were purchased from Sigma-Aldrich and used without any further purification. Solvents were distilled prior to usage.  $\text{CH}_2\text{Cl}_2$  was neutralized with  $\text{K}_2\text{CO}_3$  prior to distillation.  $\text{Et}_2\text{O}$  was dried over  $\text{CaH}_2$  and distilled prior to usage. **Reactions** were carried out under a dry  $\text{N}_2$  or Ar atmosphere, using standard Schlenk techniques. Reaction vessels were heated with polymer-coated heat-on blocks from Radleys. Microwave reactions were carried out in a Biotage initiator<sup>+</sup> mono-mode microwave reactor, using the respective reaction vials at a stirring rate of 600 rpm and fixed hold time. **Thin-layer chromatography** (TLC) was performed on Merck silica gel 60 F524, which was detected by UV light (254nm, 366nm). **Column chromatography** was performed on Macherey-Nagel silica gel 60 M (230-400 mesh, 0.04–0.063 mm). **NMR spectroscopy** was performed on a Bruker Avance 400 ( $^1\text{H}$ : 400 MHz,  $^{13}\text{C}$ : 100 MHz) and Bruker Avance 600 Ascend LH with Cryo Probe DCH ( $^1\text{H}$ : 600 MHz,  $^{13}\text{C}$ : 150 MHz). Deuterated solvents were purchased from Sigma Aldrich and used as received. Chemical shifts are referenced to residual solvent peaks or to the deuterated solvent itself ( $\delta$  in parts per million (ppm):  $\text{CDCl}_3$ :  $^1\text{H}$ : 7.24 ppm,  $^{13}\text{C}$ : 77.0 ppm;  $\text{THF-D}_8$ :  $^1\text{H}$ : 1.73 ppm, 3.58 ppm,  $^{13}\text{C}$ : 25.5 ppm, 67.7 ppm. The resonance multiplicities are indicated as “s” (singlet), “d” (doublet), “t” (triplet), “q” (quartet), and “m” (multiplet). Signals referred to as “br s” (broad singlet) are not clearly resolved or significantly broadened. **Mass spectrometry** was performed on a Bruker ultrafleXreme spectrometer LDI/MALDI-TOF (nitrogen UV-laser, 337 nm) instrument with (*E*)-2-(3-(4-(*tert*-butyl)phenyl)-2-methylallylidene)-malononitrile (DCTB) as matrices. ESI/APPI-TOF mass spectrometry was carried out on a Bruker maXis 4G UHR TOF MS/MS-spectrometer or a Bruker micrOTOF II focus TOF MS-spectrometer. **IR spectroscopy** was performed on a Bruker FT-IR Tensor 27 and Pike MIRacle ATR unit. The ATR unit was equipped with a diamond crystal plate and a high-pressure clamp. Spectra were recorded as solid samples directly from the diamond crystal. All absorptions  $\tilde{\nu}$  are given in wave numbers [ $\text{cm}^{-1}$ ]. **UV/vis spectroscopy** was carried out on a Varian Cary 5000 UV-Vis-NIR spectrometer, and **fluorescence spectroscopy** was performed on a Shimadzu RF-5301PC spectrofluorophotometer. Spectra were recorded at room temperature using quartz cuvettes with a light-path length of 1 cm.

## 2.2 Synthetic details



**Supplementary Fig. 1. Synthetic scheme to benzoporphyrin 1M.** i)  $B_2\text{pin}_2$  (1.1 equiv),  $[\{\text{Ir}(\mu\text{-OMe})\text{cod}\}_2]$  (1 mol%), dtbpy (2 mol%), hexanes,  $80^\circ\text{C}$ , 16 h (**S1** 65%); ii)  $\text{CuBr}_2$  (3.0 equiv),  $\text{MeOH}/\text{H}_2\text{O}$  (1:1),  $90^\circ\text{C}$ , 16 h (**4** 83%); iii) 1.  $n\text{-BuLi}$  (2.2 equiv),  $\text{Et}_2\text{O}$ ,  $-20^\circ\text{C}$ , 1 h, then 30 min, rt; 2. DMF (40 equiv), rt, 1 h; 3. 10% HCl (**3** 53%). iv) 1. 4,7-dihydro-2H-ethanoisindole **2**,  $\text{BF}_3\cdot\text{OEt}_2$ ,  $\text{CH}_2\text{Cl}_2$ , rt, 20 h; 2. DDQ, reflux, 2 h; 3.  $200^\circ\text{C}$ , 1.5 h (**1** 81%); v) **1Pb**:  $\text{Pb}(\text{OAc})_2\cdot 3\text{H}_2\text{O}$  (15 equiv), DMF,  $140^\circ\text{C}$ , 2 h; **1Pt**:  $\text{Pt}(\text{acac})_2$  (15 equiv), PhCN,  $180^\circ\text{C}$ , 3 h; **1Pd**:  $\text{PdCl}_2$  (15 equiv), PhCN,  $180^\circ\text{C}$ , 3 h; **1Ni**:  $\text{Ni}(\text{acac})_2$  (20 equiv), toluene,  $130^\circ\text{C}$ , 1 h.  $B_2\text{pin}_2$  = bis(pinacolato)diboron; cod = cyclooctadiene; dtbpy = 4,4'-di-*tert*-butyl-2,2'-dipyridyl; DMF = *N,N*-dimethylformamide; DDQ = 2,3-dichloro-5,6-dicyano-1,4-benzoquinone; acac = acetylacetonate.

Synthesis of pyrene-2-carbaldehyde 3:



2-Bromopyrene **4** (1.0 g, 3.56 mmol) was suspended in Et<sub>2</sub>O (50 mL) under N<sub>2</sub> in a 250 mL Schlenk flask and cooled to -20 °C (ice water/salt mixture). *n*-BuLi 1.6 M in hexanes (5.0 mL, 8.0 mmol, 2.2 equiv) was added slowly under N<sub>2</sub>, and the reaction mixture was stirred for 1 h at -20 °C. Then the bath was removed and the mixture was stirred for another 30 min at rt. After the addition of DMF (10 mL, 144 mmol, 40 equiv), the mixture was stirred for 1 h at rt. The reaction was quenched carefully with 10% HCl solution, and the organic layer was evaporated. The mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> (2x150 mL), and the combined organic layers were washed with water (2x150 mL) and brine (150 mL) before they were dried over MgSO<sub>4</sub> and filtered. The solvent was removed by rotary evaporation. The crude product was adsorbed on silica gel and purified via column chromatography (SiO<sub>2</sub>, diameter: 5 cm, height: 30 cm, CH<sub>2</sub>Cl<sub>2</sub>:hexanes = 3:2). The product was isolated as a light-yellow solid in 53% yield (0.43 g, 1.87 mmol).

**R<sub>f</sub>** (SiO<sub>2</sub>): 0.33 (CH<sub>2</sub>Cl<sub>2</sub>:hexanes = 3:2).

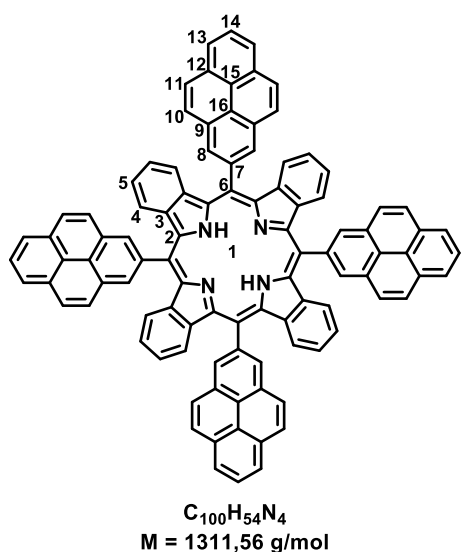
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>, rt): δ = 10.4 (s, 1H, 1), 8.58 (s, 2H, 4), 8.20 (d, 2H, <sup>3</sup>J = 7.6Hz, 9), 8.11 (d, 2H, <sup>3</sup>J = 9.2Hz, 6/7), 8.09 (d, 2H, <sup>3</sup>J = 9.3Hz, 6/7), 8.08-8.04 (m, 1H, 10).

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>, rt): δ = 192.9, 133.3, 131.9, 131.3, 128.6, 127.8, 127.7, 127.4, 125.7, 125.5, 124.2.

**HRMS** (APPI, CH<sub>2</sub>Cl<sub>2</sub>/THF): *m/z* calc. for C<sub>17</sub>H<sub>11</sub>O [M+H]<sup>+</sup>: 231.0804; found: 231.0800.

**IR** (ATR, rt):  $\tilde{\nu}$  = 3036, 2360, 2339, 1995, 1694, 1595, 1555, 1451, 1365, 1316, 1277, 1179, 1152, 1130, 982, 964, 874, 841, 821, 760, 708, 686, 587, 549, 526, 507, 490, 470.

## Synthesis of 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrin **1**:



Pyrene-2-carbaldehyde **3** (0.489 g; 2.12 mmol) and 4,7-dihydro-2*H*-ethanoisindole **2** (0.307 g; 2.11 mmol) were dissolved in  $CH_2Cl_2$  (125 mL) in a 250 mL Schlenk flask under  $N_2$ . The solution was purged with  $N_2$  for 15 min before  $BF_3 \cdot OEt_2$  (0.075 mL, 0.61 mmol) was added. The mixture was stirred for 20 h at rt under light exclusion. Then DDQ (0.475 g; 2.09 mmol) was added, and the mixture was brought to reflux for 2 h under  $N_2$ . After cooling to rt, the mixture was washed with a solution of 10%

aqueous  $Na_2SO_3$  (125 mL) and 10%  $Na_2CO_3$  (125 mL). The phases were separated, and the solvent was removed under vacuum. Then the crude product was heated under vacuum to 200 °C for 1.5 h. After cooling to rt, the solid was dissolved in  $CH_2Cl_2$  and purified by plug filtration ( $SiO_2$ , diameter 4 cm; height: 8 cm;  $CH_2Cl_2$  + 1% TFA). The final purification was carried out by recrystallization ( $MeOH/CH_2Cl_2$ ). The product was isolated as a dark-green solid in 81% yield (0.565 g; 0.431 mmol).

$R_f$  ( $SiO_2$ ): 0.88 ( $CH_2Cl_2$ ).

$^1H$  NMR (400 MHz,  $CDCl_3$ , rt):  $\delta$  = 9.30 (s, 8H, 8), 8.37-8.28 (m, 24H, 10, 11, 13), 8.16 (t, 4H,  $^3J$  = 8.0 Hz, 14), 6.76-6.64 (br s, 16H, 4, 5), -0.64 - -0.74 (br s, 2H, 1).

$^1H$  NMR (600 MHz,  $THF-D_8$ , rt):  $\delta$  = 9.32 (s, 8H, 8), 8.40 (d,  $^3J$  = 7.5 Hz, 16H), 8.35 (d,  $^3J$  = 8.8 Hz, 8H), 8.17 (t, 4H,  $^3J$  = 7.8 Hz, 14), 6.73 (br s, 16H, 4, 5), -0.38 - -0.49 (br s, 2H, 1).

$^{13}C$  NMR (100 MHz,  $CDCl_3$ , rt):  $\delta$  = 139.4, 131.7, 131.6, 131.0, 128.3, 128.2, 126.5, 125.9, 125.5, 125.0, 124.9, 124.2, 116.1.

$^{13}C$  NMR (150 MHz,  $THF-D_8$ , rt):  $\delta$  = 140.6, 132.7, 132.6, 131.7, 129.1, 128.7, 127.3, 126.3, 125.7, 125.5, 124.9, 117.1.

MS (MALDI, DCTB):  $m/z$  (rel. Int.) = 1311.4392 [ $M$ ] $^+$  (100).

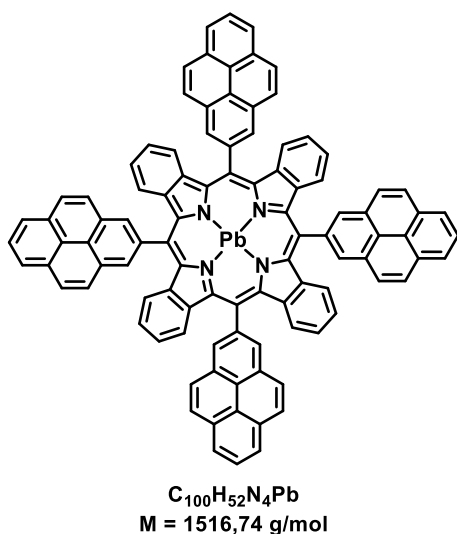
HRMS (MALDI, DCTB):  $m/z$  calc. for  $C_{100}H_{54}N_4$  [ $M$ ] $^+$ : 1310.4343; found: 1310.4328.

IR (ATR, rt):  $\tilde{\nu}$  = 3035, 2929, 2856, 2090, 1597, 1550, 1447, 1391, 1315, 1258, 1178, 1137, 1121, 1044, 1003, 976, 889, 841, 826, 754, 710, 601, 541, 515, 497, 477, 449.

**UV/Vis** (CH<sub>2</sub>Cl<sub>2</sub>, rt):  $\lambda$  ( $\epsilon$ ) = 246 (122406), 268 (79882), 278 (90161), 311 (49987), 324 (75598), 340 (93691), 472 (302650), 550 (5770), 594 (12137), 644 (31778), 698 (6984).

**Fluo** (CH<sub>2</sub>Cl<sub>2</sub>, rt, 310nm):  $\lambda_{max}$  (rel. int.) = 706 (100), 785 (21); (CH<sub>2</sub>Cl<sub>2</sub>, rt, 320nm):  $\lambda_{max}$  (rel. int.) = 706 (100), 785 (21); (CH<sub>2</sub>Cl<sub>2</sub>, rt, 340nm):  $\lambda_{max}$  (rel. int.) = 705 (100), 787 (20); (CH<sub>2</sub>Cl<sub>2</sub>, rt, 470nm):  $\lambda_{max}$  (rel. int.) = 719 (100), 781 (36).

Synthesis of 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrinato-lead(II) **1Pb**:



In a flame-dried Schlenk tube, Pb(OAc)<sub>2</sub>·3H<sub>2</sub>O (22 mg; 57  $\mu$ mol, 15 equiv) was dissolved in DMF (1.0 mL) under N<sub>2</sub> and heated to 135 °C for 5 min. 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrin **1** (5.0 mg; 3.8  $\mu$ mol) was added, and the mixture was heated to 140 °C for 2 h. The reaction was cooled to rt, and the solvent was removed in vacuum. The crude product was re-dissolved in a small amount of CH<sub>2</sub>Cl<sub>2</sub> and precipitated with MeOH. The precipitate was filtered and washed several times with MeOH. The

brownish, slightly purple product (around 4 mg) was collected and stored in vacuum on a hydrophobic PTFE filter paper, until used for TEM experiments.

**<sup>1</sup>H NMR** (600 MHz, THF-D<sub>8</sub>, rt):  $\delta$  = 9.40 (s, 4H), 9.33 (s, 4H), 8.42-8.39 (m, 16H), 8.36 (d, <sup>3</sup>J = 8.7 Hz, 8H), 8.18 (t, 4H, <sup>3</sup>J = 7.8 Hz, 14), 6.73-6.64 (m, 16H, 4, 5).

**<sup>13</sup>C NMR** (150 MHz, THF-D<sub>8</sub>, rt):  $\delta$  = 161.4, 161.1, 160.9, 145.4, 141.8, 139.8, 132.8, 132.6, 132.5, 132.3, 132.0, 129.1, 128.8, 128.78, 128.73, 128.4, 127.2, 126.2, 126.1, 125.8, 125.4, 125.1, 119.2, 117.7, 98.2, 98.1.

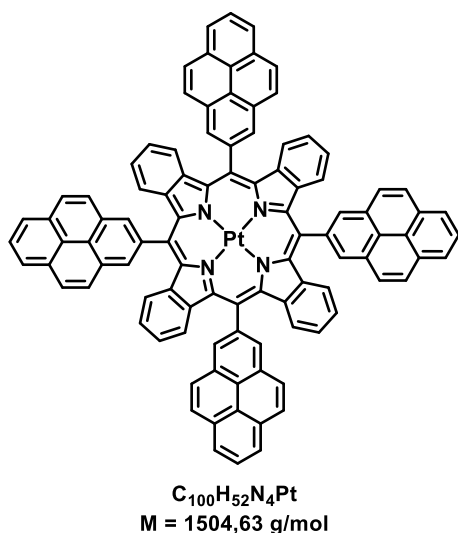
**MS** (MALDI, DCTB):  $m/z$  (rel. Int.) = 1311.4716 [M-Pb+2H]<sup>+</sup> (100), 1516.4201 [M]<sup>+</sup>.

**HRMS** (MALDI, DCTB):  $m/z$  calc. for C<sub>100</sub>H<sub>52</sub>N<sub>4</sub>Pb [M]<sup>+</sup>: 1516.3953; found: 1516.4015.

**UV/Vis** (CH<sub>2</sub>Cl<sub>2</sub>, rt):  $\lambda$  (rel. Int.) = 245 (1.3), 266 (0.98), 277 (0.99), 312 (0.65), 325 (0.94), 341 (1.2), 471 (0.27), 524 (1), 535 (shoulder), 666 (0.18), 709 (0.15).



Synthesis of 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrinato-platinum(II) **1Pt**:



In a flame-dried Schlenk tube  $Pt(acac)_2$  (22.4 mg; 57  $\mu\text{mol}$ , 15 equiv) was dissolved in PhCN (1.5 mL) under  $N_2$  and heated to 180 °C for 15 min. 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrin **1** (5.0 mg; 3.8  $\mu\text{mol}$ ) was added, and the mixture was heated to 180 °C for 3 h. The reaction was cooled to rt, and the solvent was distilled off in vacuum. The crude product was re-dissolved in a small amount of  $CH_2Cl_2$  and precipitated with MeOH. The precipitate was filtered and washed several times with MeOH. The

product was isolated as a dark greenish (slightly blue) solid after drying in vacuum, which is greenish/turquoise in  $CH_2Cl_2$  solution. The product (around 4-5 mg) was collected and stored on a hydrophobic PTFE filter paper in vacuum, until used for TEM experiments.

$R_f$  ( $SiO_2$ ): 0.66 (hexanes: $CH_2Cl_2$  = 1:1).

$^1H$  NMR (600 MHz, THF- $D_8$ , rt):  $\delta$  = 9.22 (s, 8H), 8.41-8.35 (m, 24H), 8.18 (t, 4H,  $^3J$  = 7.8 Hz, 14), 6.72-6.70 (m, 8H), 6.56-6.54 (m, 8H).

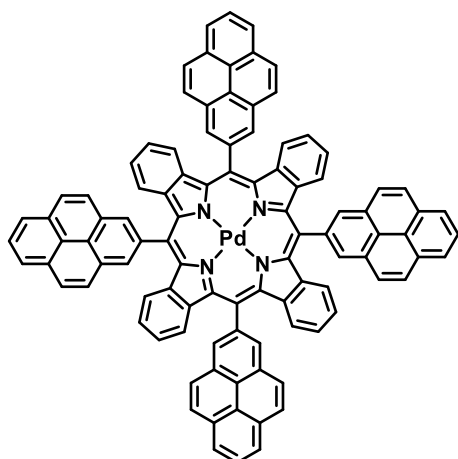
$^{13}C$  NMR (150 MHz, THF- $D_8$ , rt):  $\delta$  = 140.0, 138.6, 137.4, 132.9, 132.7, 130.9, 129.2, 128.6, 127.3, 126.3, 126.1, 125.7, 125.6, 124.8, 119.7.

MS (MALDI, DCTB):  $m/z$  (rel. Int.) = 1504.4242 [ $M$ ] $^+$  (100) 1311.4683 [ $M-Pt+2H$ ] $^+$  (20).

HRMS (MALDI, DCTB):  $m/z$  calc. for  $C_{100}H_{52}N_4Pt$  [ $M$ ] $^+$ : 1503.3834; found: 1503.3841.

UV/Vis ( $CH_2Cl_2$ , rt):  $\lambda$  (rel. Int.) = 247 (0.79), 269 (0.61), 278 (0.74), 311 (0.30), 324 (0.46), 339 (0.58), 436 (1), 469 (0.29), 568 (0.072), 616 (0.5).

Synthesis of 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrinato-palladium(II) **1Pd**:



$C_{100}H_{52}N_4Pd$   
 $M = 1415,96 \text{ g/mol}$

In a flame-dried Schlenk tube  $PdCl_2$  (10 mg; 57  $\mu\text{mol}$ , 15 equiv) was dissolved in PhCN (1.5 mL) under  $N_2$  and heated to 180  $^\circ\text{C}$  for 15 min. 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrin **1** (5.0 mg; 3.8  $\mu\text{mol}$ ) was added, and the mixture was heated to 180  $^\circ\text{C}$  for 3 h. The reaction was cooled to rt, and the solvent was distilled off in vacuum. The crude product was re-dissolved in a small amount of  $CH_2Cl_2$  and precipitated with MeOH. The precipitate was filtered and washed several times with MeOH. The product was isolated as

a greenish/blueish solid after drying in vacuum, which is green in solution ( $CH_2Cl_2$ ). The product (around 4-5 mg) was collected and stored on a hydrophobic PTFE filter paper in vacuum, until used for TEM experiments.

$R_f$  ( $SiO_2$ ): 0.59 (hexanes: $CH_2Cl_2$  = 1:1).

$^1H$  NMR (600 MHz, THF- $D_8$ , rt):  $\delta$  = 9.26 (s, 8H), 8.45-8.38 (m, 24H), 8.22 (t, 4H,  $^3J$  = 7.8 Hz, 14), 6.77-6.75 (m, 8H), 6.63-6.62 (m, 8H).

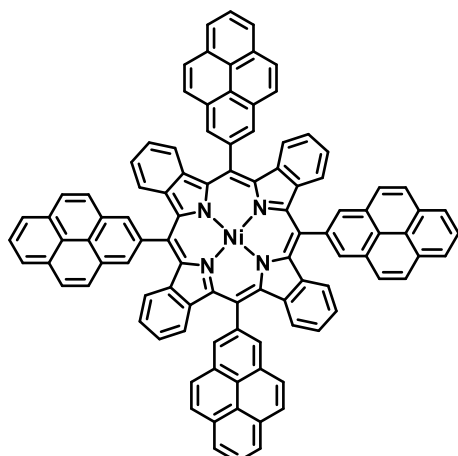
$^{13}C$  NMR (150 MHz, THF- $D_8$ , rt):  $\delta$  = 161.4, 161.2, 160.9, 140.2, 139.7, 139.0, 132.82, 132.75, 131.1, 129.2, 128.6, 127.3, 126.3, 126.0, 125.7, 125.6, 124.6, 119.4, 98.2, 98.1.

MS (MALDI, DCTB):  $m/z$  (rel. Int.) = 1414.3523 [ $M$ ] $^+$  (100).

HRMS (MALDI, DCTB):  $m/z$  calc. for  $C_{100}H_{52}N_4Pd$  [ $M$ ] $^+$ : 1414.3221; found: 1414.3224.

UV/Vis ( $CH_2Cl_2$ , rt):  $\lambda$  (rel. Int.) = 248 (0.52), 269 (0.42), 277 (0.45), 311 (shoulder), 324 (0.28), 340 (0.36), 421 (0.20), 448 (1), 583 (0.051), 630 (0.34).

Synthesis of 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrinato-nickel(II) **1Ni**:



$C_{100}H_{52}N_4Ni$   
 $M = 1368,24 \text{ g/mol}$

In a 5 mL microwave vial  $Ni(acac)_2$  (39 mg; 0.152 mmol, 20 equiv) and 5,10,15,20-tetrakis(2-pyrenyl)tetrabenzoporphyrins **1** (10 mg; 7.6  $\mu\text{mol}$ ) were dissolved in toluene (1.0 mL). The mixture was heated in a microwave reactor: 130 °C, 1 h, low absorption level. The solvent was removed, and the crude product was purified by plug filtration ( $SiO_2$ , diameter: 3.5 cm; height: 10 cm;  $CH_2Cl_2$ ). After removal of the solvent, the product was isolated as a dark green solid in 71% yield (7.4 mg; 5.4  $\mu\text{mol}$ ).

$R_f$  ( $SiO_2$ ): 0.63 (hexanes: $CH_2Cl_2$  = 1:1).

$^1H$  NMR (600 MHz, THF- $D_8$ , rt):  $\delta$  = 9.01 (s, 8H), 8.39-8.30 (m, 24H), 8.16 (t, 4H,  $^3J$  = 7.8 Hz, 14), 6.72-6.70 (m, 8H), 6.62-6.61 (m, 8H).

$^{13}C$  NMR (150 MHz, THF- $D_8$ , rt):  $\delta$  = 140.5, 139.7, 139.1, 132.7, 130.6, 129.0, 128.6, 127.2, 126.2, 125.7, 125.5, 124.03, 124.0, 116.8.

MS (MALDI, DCTB):  $m/z$  (rel. Int.) = 1367.3560  $[M]^+$  (100).

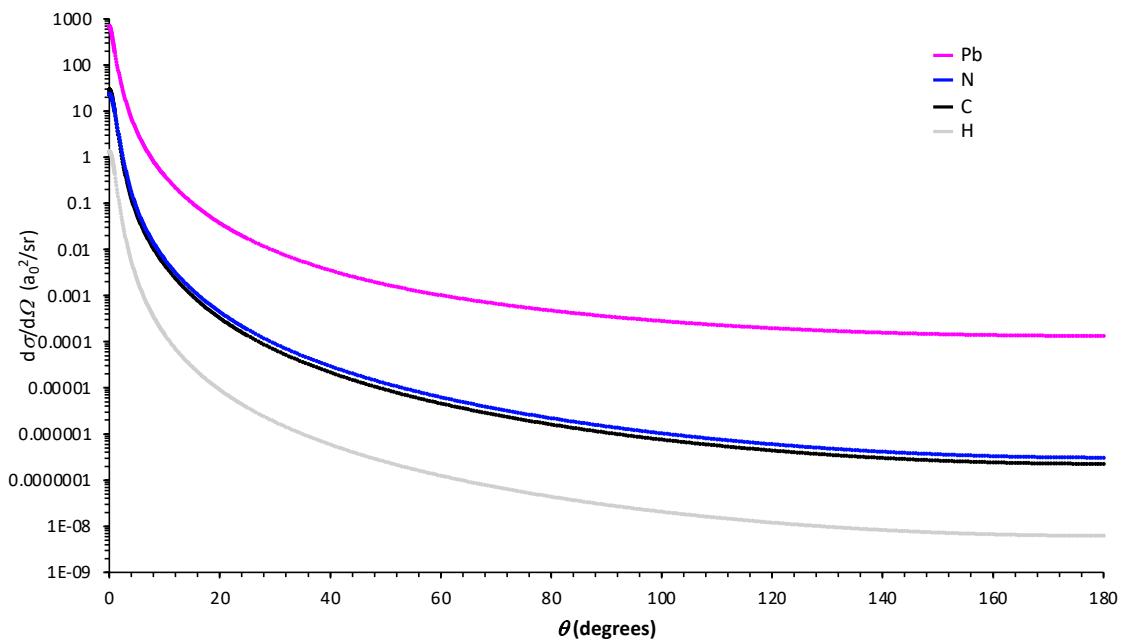
HRMS (MALDI, DCTB):  $m/z$  calc. for  $C_{100}H_{52}N_4Ni$   $[M]^+$ : 1366.3540; found: 1366.3528.

UV/Vis ( $CH_2Cl_2$ , rt):  $\lambda$  (rel. Int.) = 245 (0.77), 268 (0.54), 278 (0.65), 310 (shoulder), 325 (0.44), 340 (0.55), 452 (1), 594 (0.063), 646 (0.35).

## 3 Electron Microscopy Section

### 3.1 Elastic scattering-induced processes

Elastic scattering of electrons is a coherent process and is responsible for phase and Z-contrast in transmission electron microscopy imaging. It occurs without significant energy loss of the primary electron, as opposed to inelastic scattering, in which a substantial amount of energy of the primary electron is transferred to the observed atoms/molecules. The total differential elastic-scattering cross-sections for H, C, N, and Pb at 80 keV are shown in Supplementary Fig. 2.<sup>1</sup>



**Supplementary Fig. 2. Differential elastic-scattering cross-section of H, C, N, and Pb at 80 keV.**  $a_0$  = Bohr radius ( $a_0^2 = 2.8002852 \times 10^{-21} \text{ m}^2$ ); Total cross-section: H =  $1.55 \times 10^{-3} a_0^2$ ; C =  $3.42 \times 10^{-2} a_0^2$ ; N =  $3.68 \times 10^{-2} a_0^2$ ; Pb =  $9.56 \times 10^{-1} a_0^2$ .

Elastic scattering of high-energetic primary electrons (e-beam) can lead to a so-called knock-on kinetic energy transfer from the accelerated electron to the nucleus of the atom or molecule. Depending on the amount of transferred energy, derived from the scattering angle  $\theta$ , this can cause bond vibrations or even homolytic bond cleavages in the molecule, called knock-on displacement. The transferrable kinetic energy  $E_T$  from the primary electron beam to the sample is dependent on the kinetic energy of the primary electron  $E_0$ , the atomic mass number  $A$  and the scattering angle  $\theta$ , as described in Supplementary Equation 1.<sup>2</sup>

$$E_T = \frac{E_0 \left(1.02 + \frac{E_0}{106}\right)}{465.7A} \sin^2 \frac{\theta}{2} \quad \text{Supplementary Eq. 1}$$

The maximum transferred energy  $E_{\max}$  is obtained at a scattering angle of  $180^\circ$  (least probable case), which gives  $\sin^2 \frac{\theta}{2} = 1$  (compare Supplementary Equation 2). At 80 kV acceleration voltage, the maximum transferable kinetic energy  $E_{\max}$  for hydrogen is around 187.5 eV, for carbon 15.7 eV, for nitrogen 13.5 eV, and for lead 0.91 eV.

$$E_{\max} = \frac{E_0 \left(1.02 + \frac{E_0}{10^6}\right)}{465.7A} \quad \text{Supplementary Eq. 2}$$

From  $E_{\max}$  and the threshold energy (displacement energy) for a homolytic bond cleavage  $E_d$ , which is further dependent on the binding strength of the atom within the molecule, the smallest electron scattering angle  $\theta_{\min}$  for an irreversible bond dissociation, can be determined in Supplementary Equation 3.

$$\theta_{\min} = 2 \sin^{-1} \left( \sqrt{\frac{E_d}{E_{\max}}} \right) \quad \text{Supplementary Eq. 3}$$

With these intrinsic molecular parameters, the knock-on-induced displacement cross-section  $\sigma_d$  for a physical fragmentation of the molecule can be approximated by the McKinley-Feshbach approximation for light to mid-heavy elements, as described in Supplementary Equation 4.<sup>3</sup>

$$\sigma_d = \int_{E_T > E_d} \sigma(E_T) \frac{4\pi}{E_{\max}} dE_T = 4\pi \left( \frac{Ze^2}{8\pi\epsilon_0\gamma m_e c^2 \beta^2} \right)^2 \left[ \left( \frac{E_{\max}}{E_d} - 1 \right) - \beta^2 \ln \left( \frac{E_{\max}}{E_d} \right) + \pi Z \alpha \beta \left\{ 2 \left( \left( \frac{E_{\max}}{E_d} \right)^{1/2} - 1 \right) - \ln \left( \frac{E_{\max}}{E_d} \right) \right\} \right] \quad \text{Supplementary Eq. 4}$$

The total electron dose ( $TED_{ev}$ ) until an elastic scattering induced displacement event should occur is approximated with Supplementary Eq. 5 and Supplementary Eq. 6.<sup>4</sup>

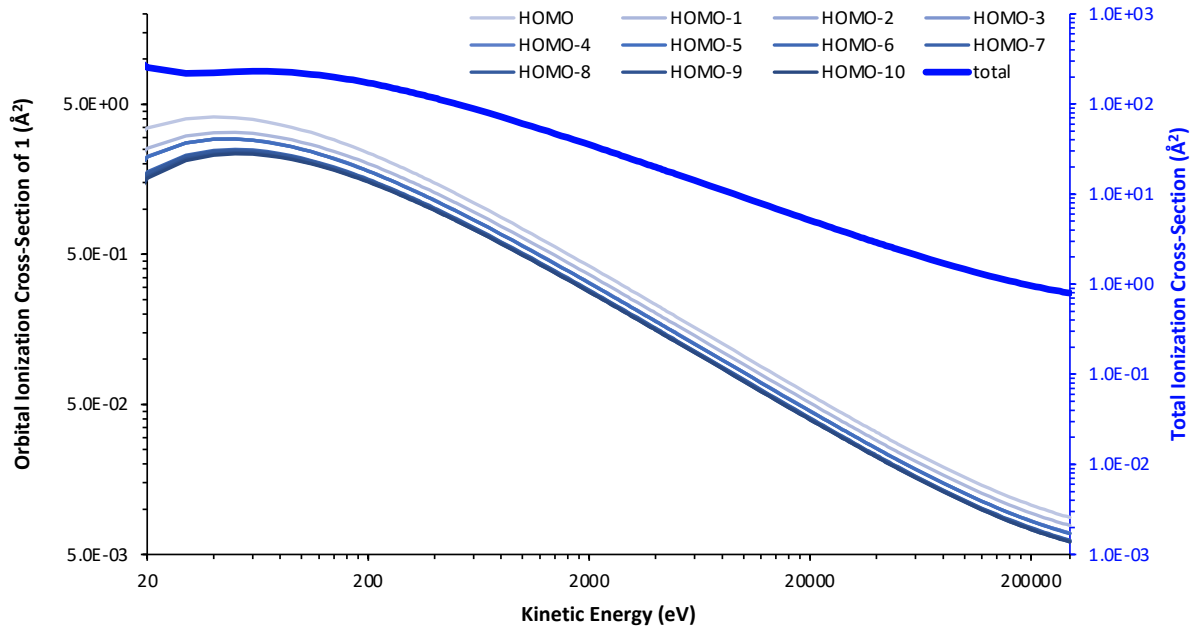
$$t_d = \frac{1}{jn\sigma_d} \quad \text{Supplementary Eq. 5}$$

$$TED_{ev} = \frac{1}{n\sigma_d} \quad \text{Supplementary Eq. 6}$$

$E_T$ : transferable kinetic energy;  $E_0$ : kinetic energy of primary electron;  $A$ : atomic mass number;  $\theta$ : elastic scattering angle;  $\theta_{\min}$ : minimum scattering angle for knock-on removal;  $E_d$ : threshold displacement energy for knock-on event;  $E_{\max}$ : maximum transferable kinetic energy;  $\sigma_d$ : knock-on displacement cross-section;  $Z$ : nuclear charge;  $\epsilon_0$ : vacuum permittivity ( $55.26349406 \text{ e}^2 \text{ GeV}^{-1} \text{ fm}^{-1}$ );  $m_e$ : mass of electron;  $\gamma$ : Lorentz factor ( $1/\sqrt{1-\beta^2}$ );  $c$ : speed of light;  $\beta$ : relativistic factor for the electron ( $\sqrt{1 - (1 + E_0/m_e c^2)^{-2}}$ );  $\alpha$ : fine structure constant ( $7.2973525693 \cdot 10^{-3}$ );  $j$ : electron flux;  $n$ : number of equivalent atoms;  $t_d$ : time until first knock-on displacement event;  $TED_{ev}$ : total electron dose until first knock-on displacement event occurs.

### 3.2 Inelastic scattering-induced processes

Inelastic scattering is an incoherent process, meaning the scattering occurs with significant energy loss of the primary electron. The total inelastic scattering cross-section is approximately proportional to the nuclear charge  $Z$  and occurs from interactions between the primary electrons with the shell electrons of the specimen (atoms/molecules/substrate). Besides phonon and plasmon excitation, electron-impact ionization of the specimen can occur through inelastic scattering.<sup>5</sup> The total electron-impact ionization cross-section  $\sigma_{rBEB}$  of **1** is shown in Supplementary Fig. 3, and is derived from the Binary Encounter Bethe model (Supplementary Eq. 7), which needs to be modified for electrons  $>20$  keV to the relativistic Binary Encounter Bethe (rBEB) model (Supplementary Eq. 8).<sup>6</sup> Hereby, the cross-section is dependent on the kinetic energy of the primary electron  $E_0$ , the kinetic and potential energy of the electron in the respective orbital  $U$  and  $B$  of the atom/molecule, as well as the orbital occupation number  $N$  (typically  $N = 2$ ). The total ionization cross-section is derived from the sum of all cross-sections of all occupied orbitals.



**Supplementary Fig. 3. Electron-impact ionization cross-section of 1.** Calculated with the relativistic Binary Encounter Bethe model for the valence orbitals HOMO – HOMO-10, and the total ionization cross-section over all orbitals.

$$\sigma_{rBEB} = \frac{4\pi a_0^2 N \left(\frac{R}{B}\right)^2}{t+u+1} \left[ \frac{\ln(t)}{2} \left(1 - \frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{\ln(t)}{t+1} \right] \quad \text{Supplementary Eq. 7}$$

$$\sigma_{rBEB} = \frac{4\pi a_0^2 \alpha^4 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2) 2b'} \left\{ \frac{1}{2} \left[ \ln \left( \frac{\beta_t^2}{1 - \beta_t^2} \right) - \beta_t^2 - \ln(2b') \right] \left(1 - \frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{\ln(t)}{t+1} \frac{1+2t'}{(1+\frac{t'}{2})^2} + \frac{b'^2}{(1+\frac{t'}{2})^2} \frac{t-1}{2} \right\} \quad \text{Supplementary Eq. 8}$$

The variables  $b$ ,  $b'$ ,  $t$ ,  $t'$ ,  $u$ ,  $\beta_b^2$ ,  $\beta_t^2$ , and  $\beta_u^2$  are derived from Supplementary Equations 9 – 16.

$$t = \frac{E_0}{B} \quad \text{Supplementary Eq. 9}$$

$$u = \frac{U}{B} \quad \text{Supplementary Eq. 10}$$

$$\beta_t^2 = 1 - \frac{1}{(1+t')^2} \quad \text{Supplementary Eq. 11}$$

$$t' = \frac{E_0}{m_e c^2} \quad \text{Supplementary Eq. 12}$$

$$\beta_b^2 = 1 - \frac{1}{(1+b')^2} \quad \text{Supplementary Eq. 13}$$

$$b' = \frac{B}{m_e c^2} \quad \text{Supplementary Eq. 14}$$

$$\beta_u^2 = 1 - \frac{1}{(1+u')^2} \quad \text{Supplementary Eq. 15}$$

$$u' = \frac{U}{m_e c^2} \quad \text{Supplementary Eq. 16}$$

$\sigma_{rBEB}$ : ionization cross-section;  $E_0$ : kinetic energy of primary electron;  $B$ : binding energy of the electron in orbital;  $U$ : kinetic energy of the electron in orbital;  $R$ : Rydberg energy (13.6 eV);  $a_0$ : Bohr radius (0.527 Å);  $N$ : orbital occupation number (typically = 2);  $\alpha$ : fine structure constant ( $7.2973525693 \cdot 10^{-3}$ );  $m_e$ : mass of electron;  $c$ : speed of light;  $\beta$ : relativistic factors.

### 3.3 Secondary electron flux

The total ionization cross-section  $\sigma_{ion}$  for atomic carbon calculated with the modified relativistic binary encounter Bethe (MRBEB) model is approximately  $10^{-18} \text{ cm}^{-2}$ .<sup>7</sup> The areal density  $\rho_A$  of carbon atoms in graphene is  $0.382 \text{ \AA}^{-2}$ . The frequency of ionization of carbon atoms under the applied EDR,  $\tau^{-1}$ , can be estimated by  $\tau^{-1} = \sigma j$ , where  $j$  is the electron dose rate in the TEM. The number of electrons ejected from the carbon substrate by ionization, which is the secondary electron flux  $j(SE)$ , can be estimated by  $\tau^{-1} \times \rho_A$  (Supplementary Equation 17).

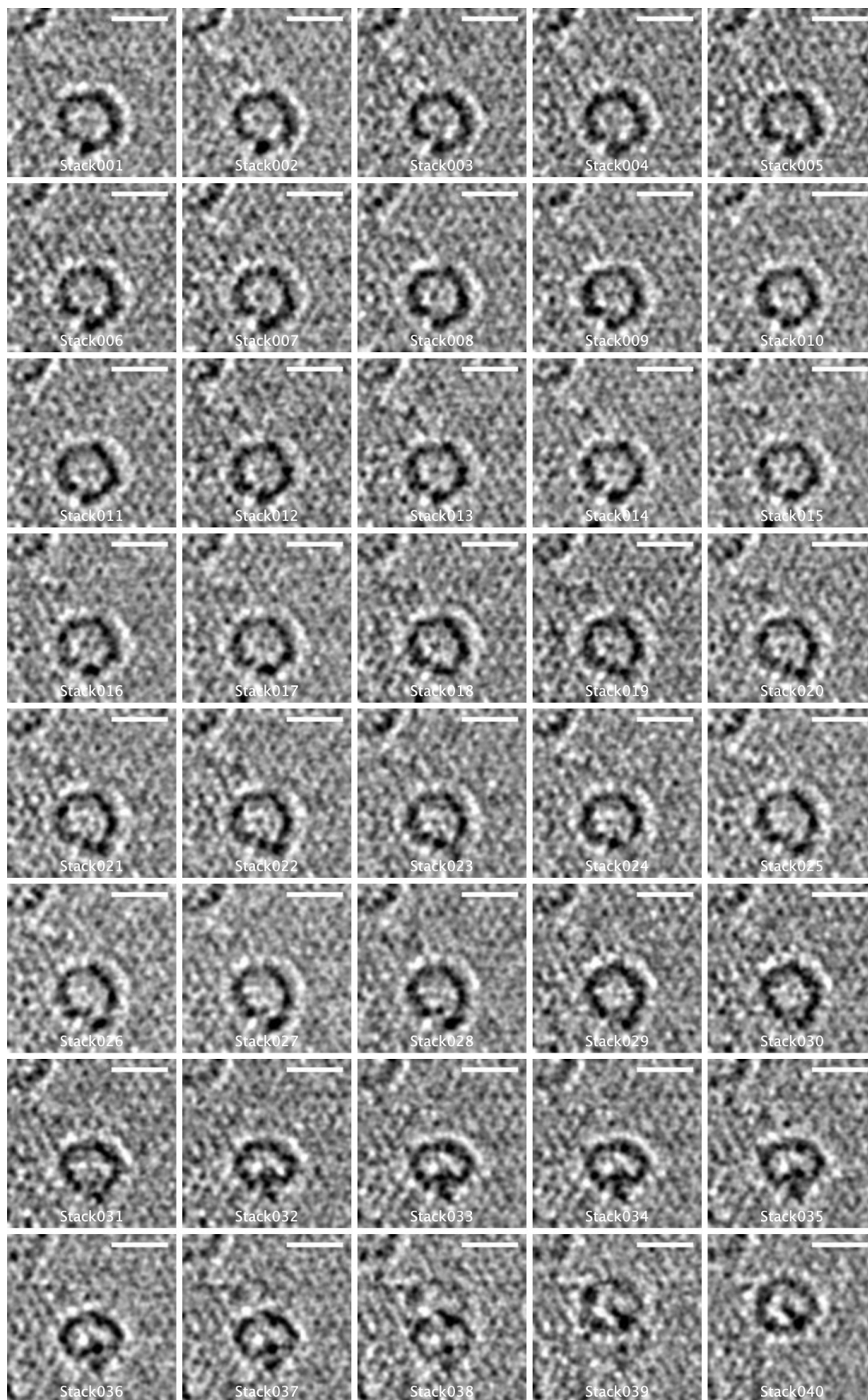
In our experiments,  $j$  is  $1.5 \times 10^6 \text{ e}^{-}\text{nm}^{-2}\text{s}^{-1}$  and the resulting  $j(SE)$  is approximated to be  $5.72 \times 10^3 \text{ e}^{-}\text{nm}^{-2}\text{s}^{-1}$ .

$$j(SE) = \sigma_{ion} \times j \times \rho_A$$

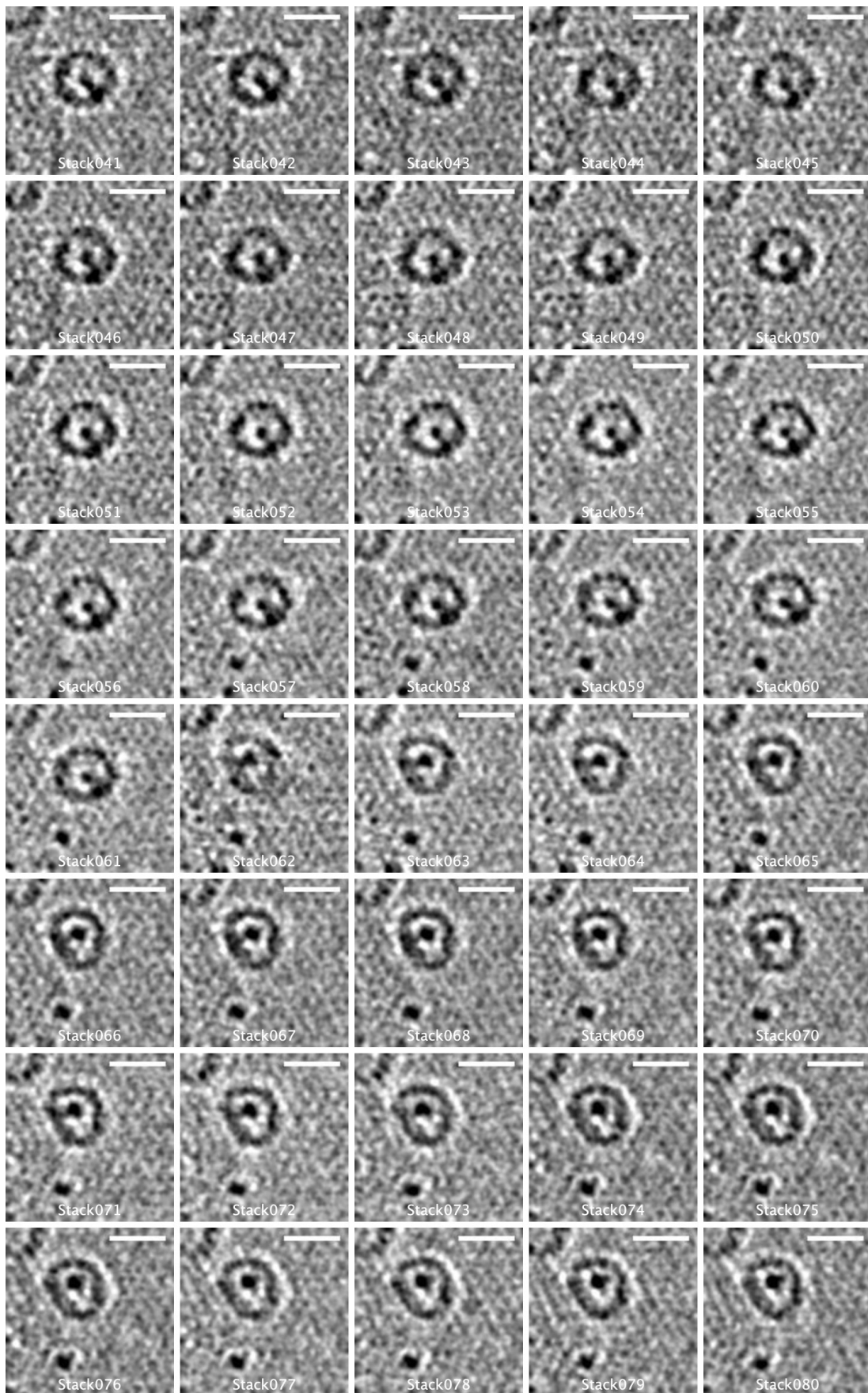
Supplementary Eq. 17



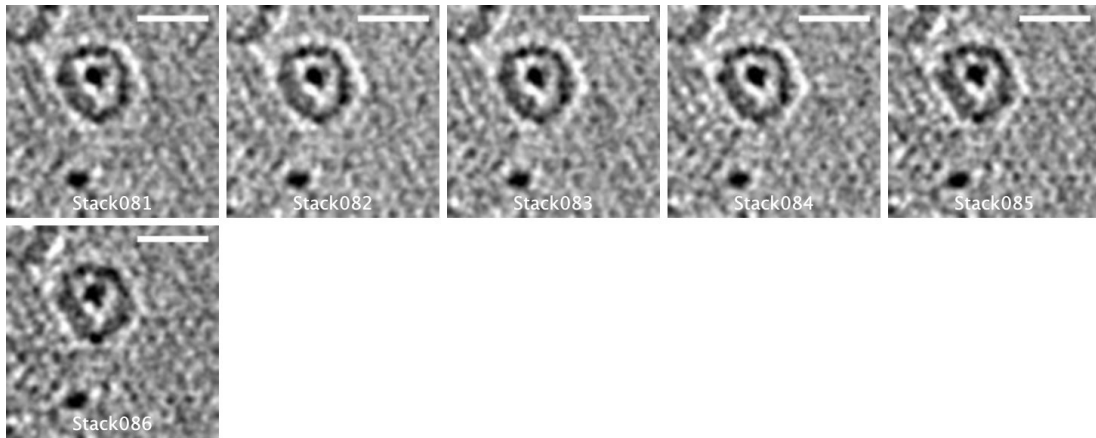
### 3.4 Supplementary Video 1 – Transformation of 1Pb to Pb@(FP-Pb) and Pb@(FP)



**Supplementary Fig. 4. Supplementary Video 1: SMART-EM video sequence.** Frames 1 – 40, scale bar 1nm.

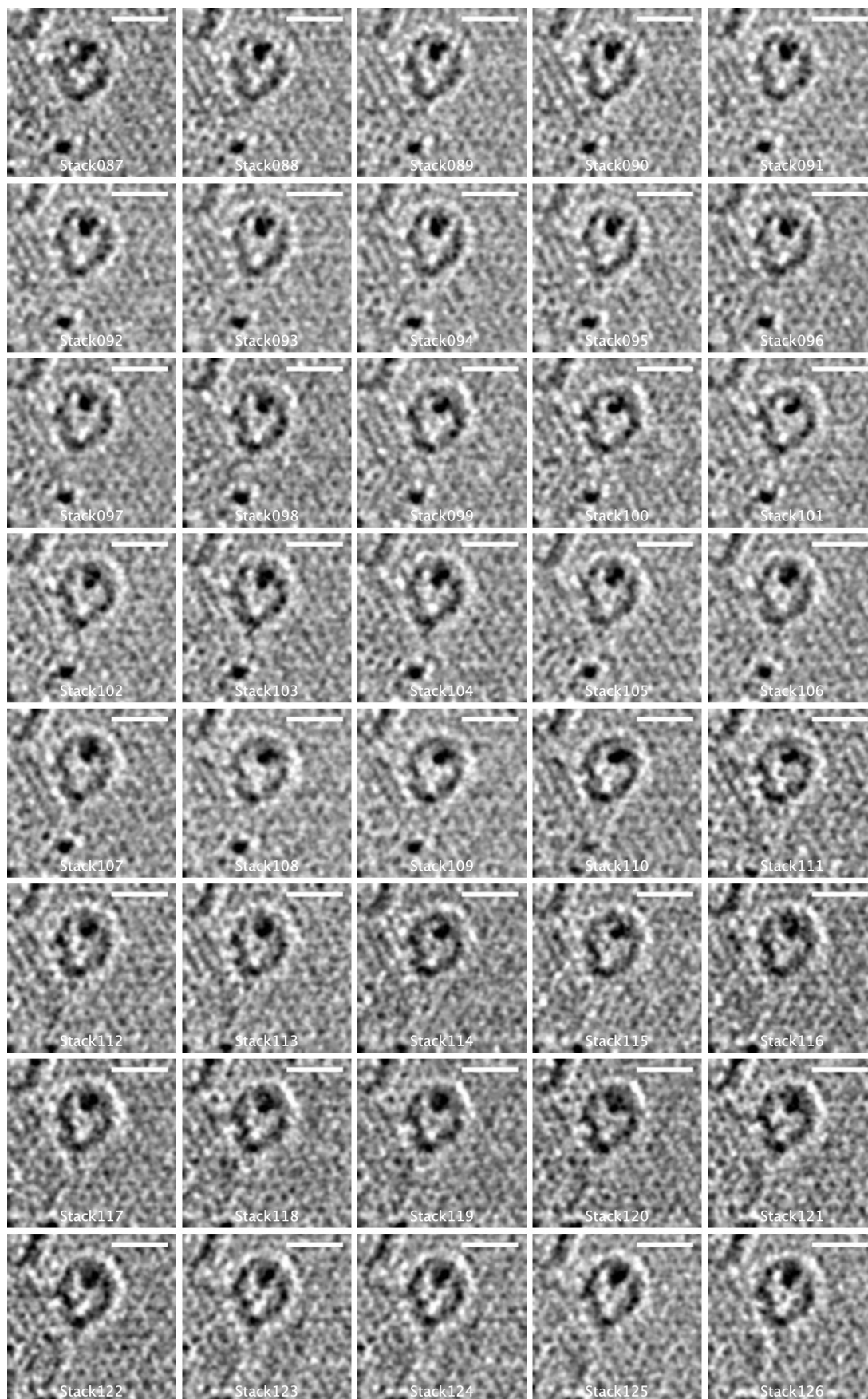


**Supplementary Fig. 5. Supplementary Video 1 (Continued): SMART-EM video sequence. Frames 41 – 80, scale bar 1nm.**

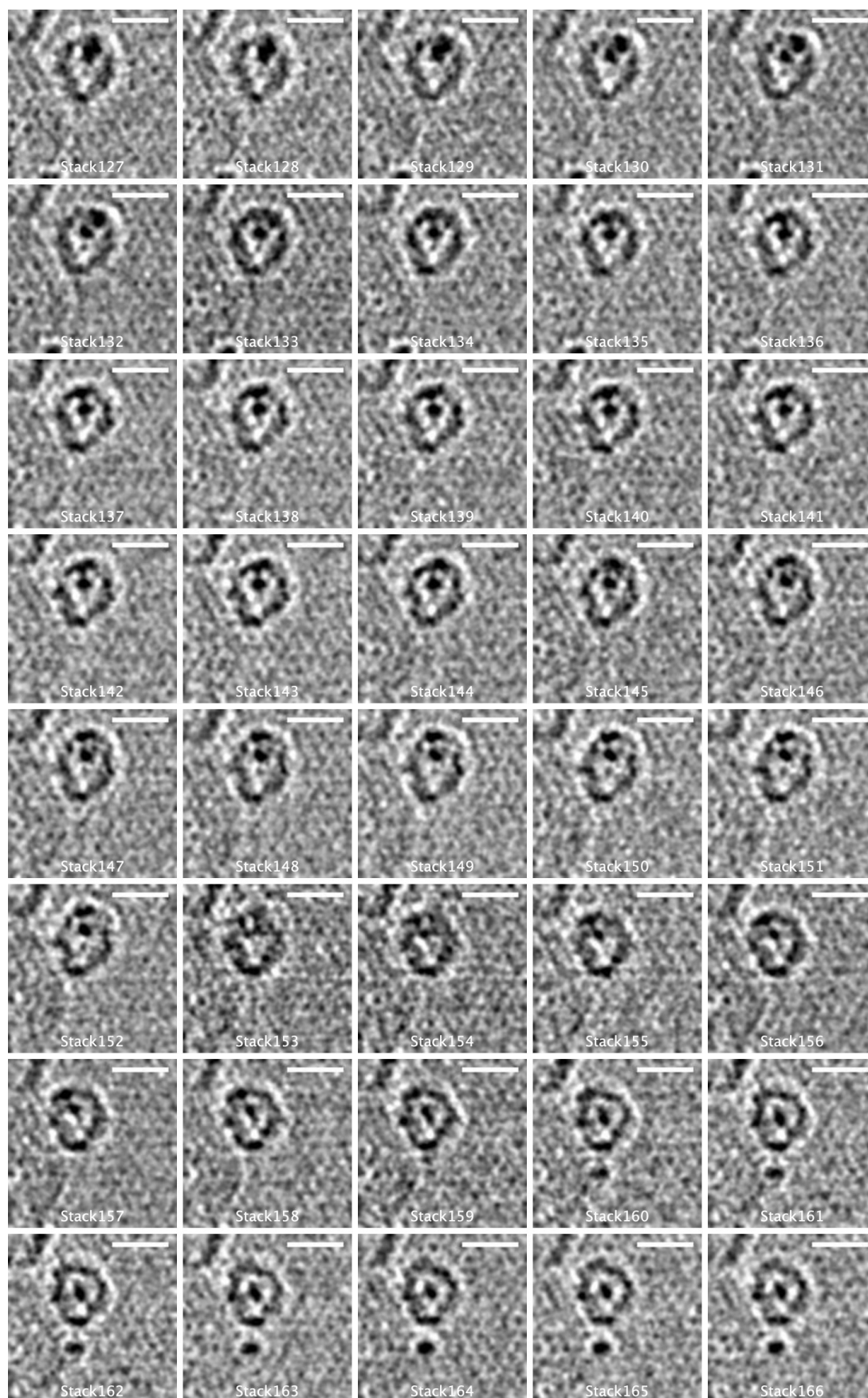


**Supplementary Fig. 6. Supplementary Video 1 (Continued): SMART-EM video sequence.** Frames 81 – 86, scale bar 1nm.

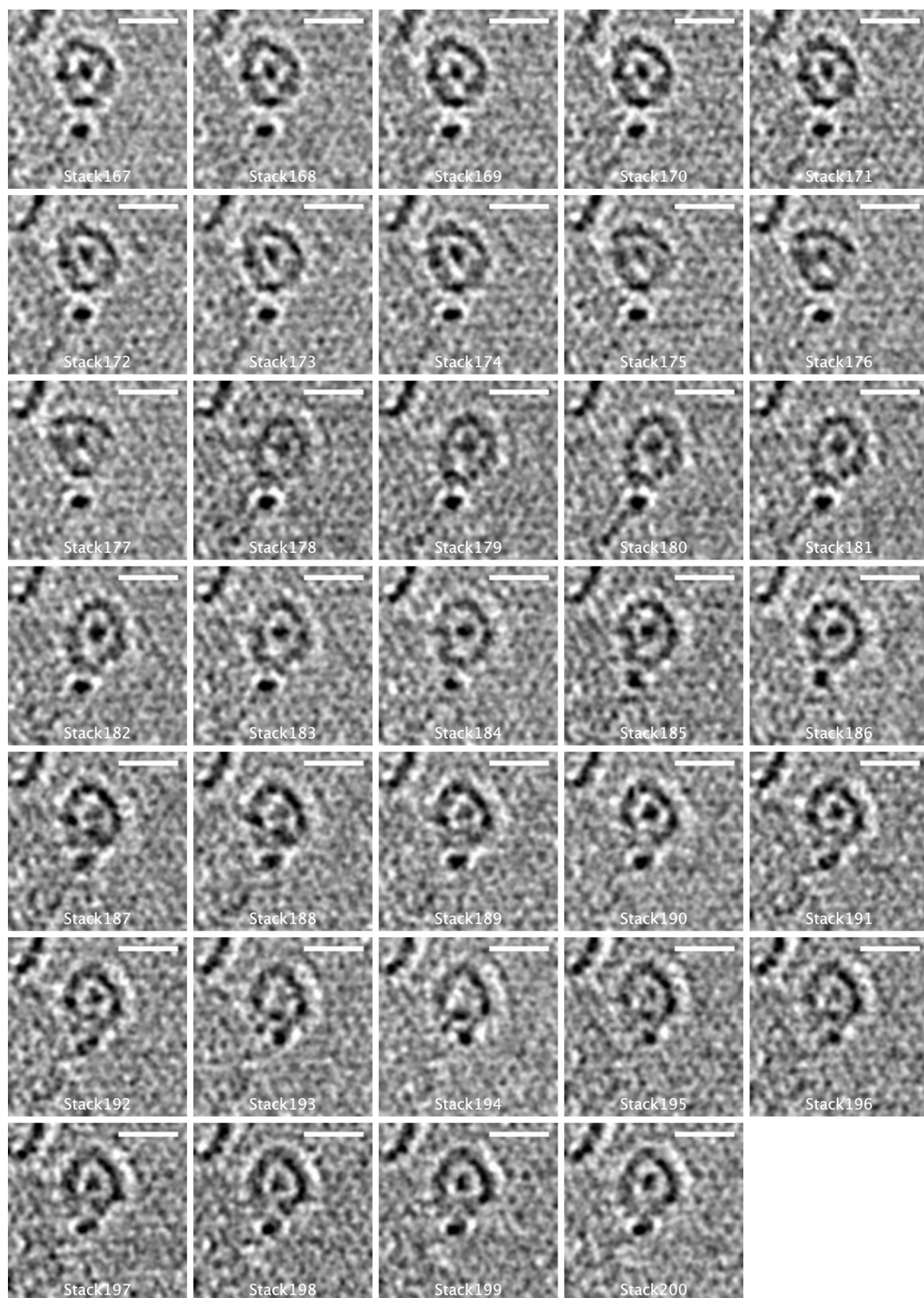
### 3.5 Supplementary Video 2 – Decomposition of Pb@(FP) under the electron beam



**Supplementary Fig. 7. Supplementary Video 2: SMART-EM video sequence.** Frames 87 –126, scale bar 1 nm.

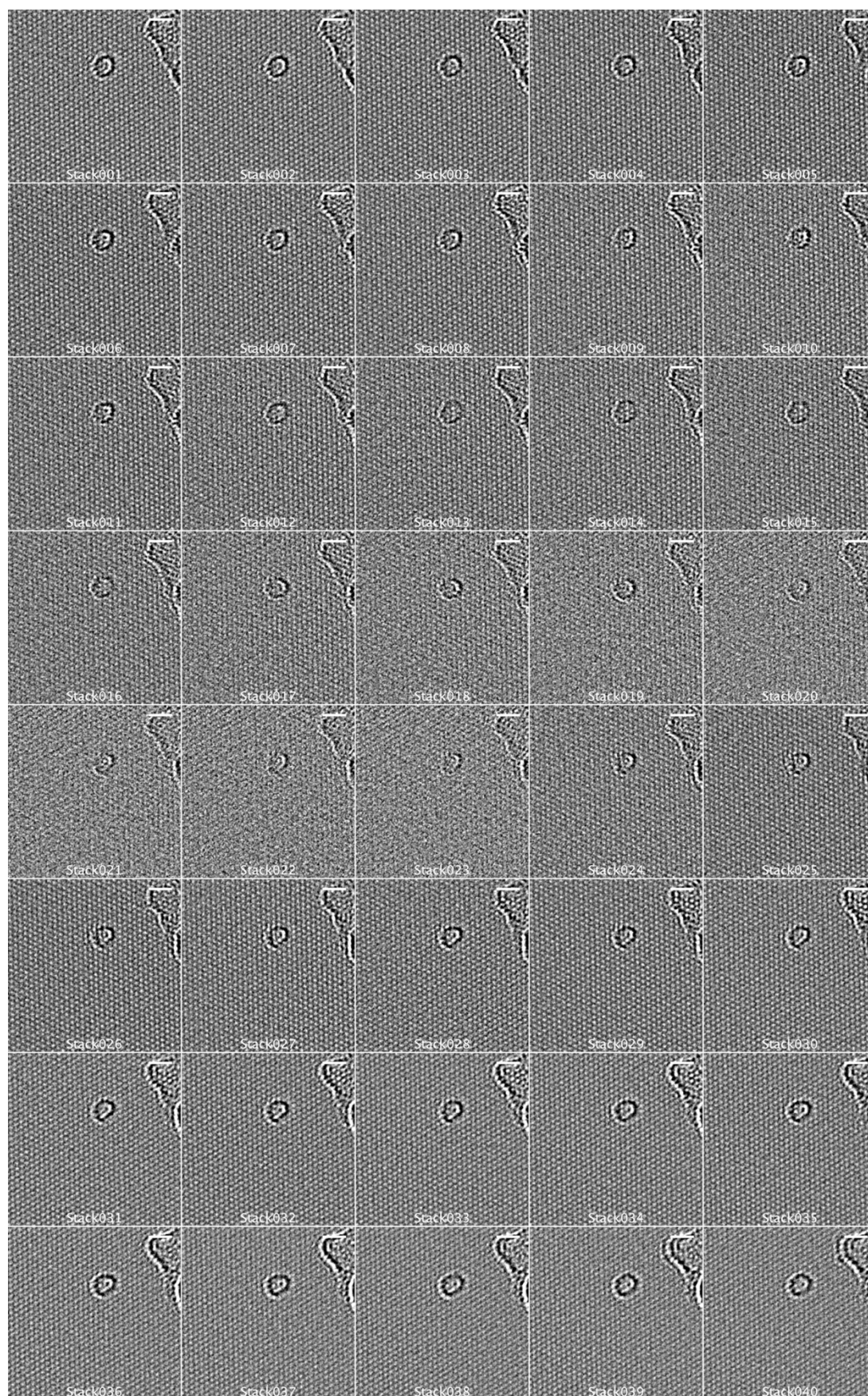


**Supplementary Fig. 8. Supplementary Video 2 (Continued): SMART-EM video sequence. Frames 127 –166, scale bar 1 nm.**

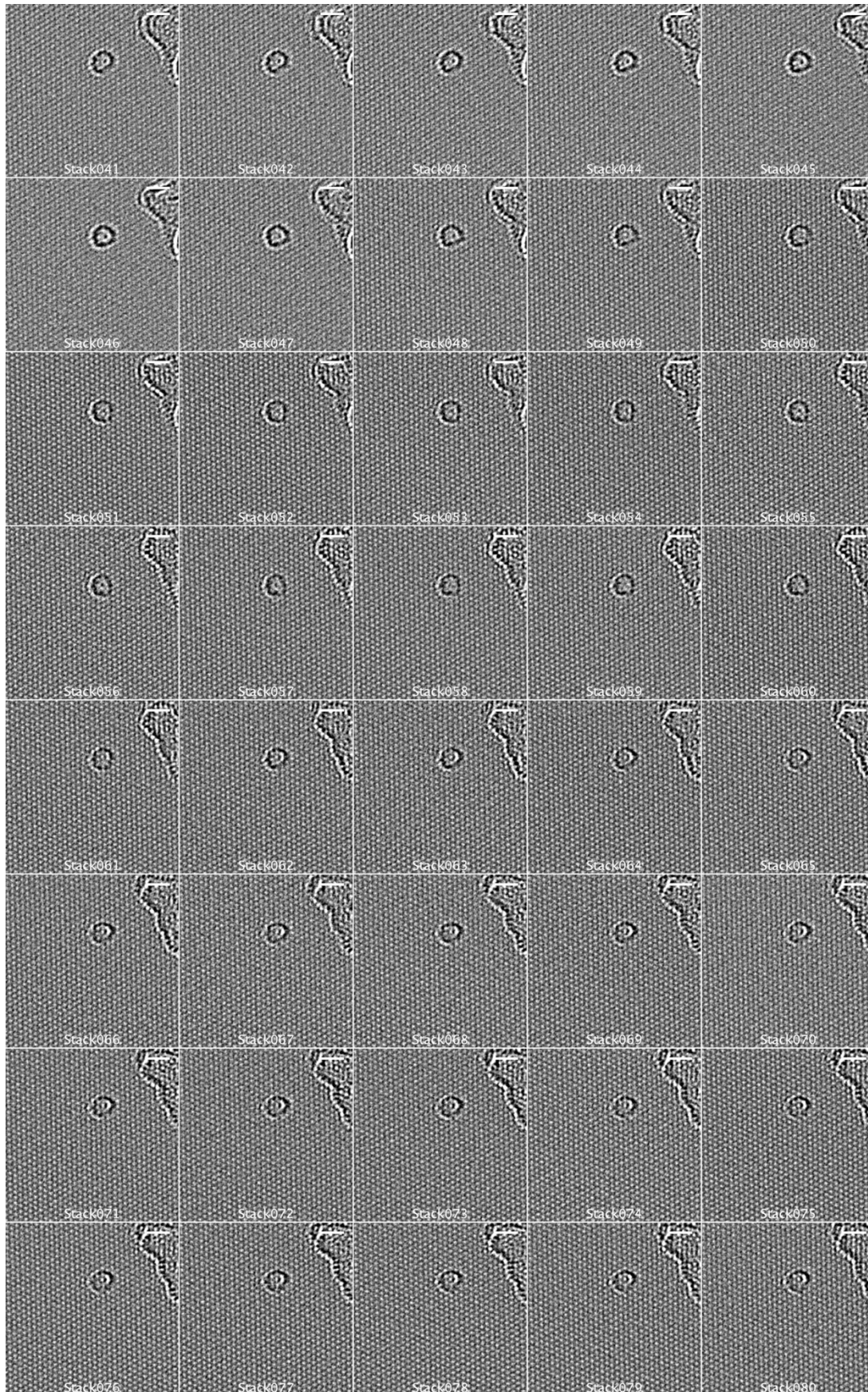


**Supplementary Fig. 9. Supplementary Video 2 (Continued): SMART-EM video sequence. Frames 167 –200, scale bar 1 nm.**

### 3.6 Supplementary Video 3 – Detachment of empty hemi-FP from graphene monolayer

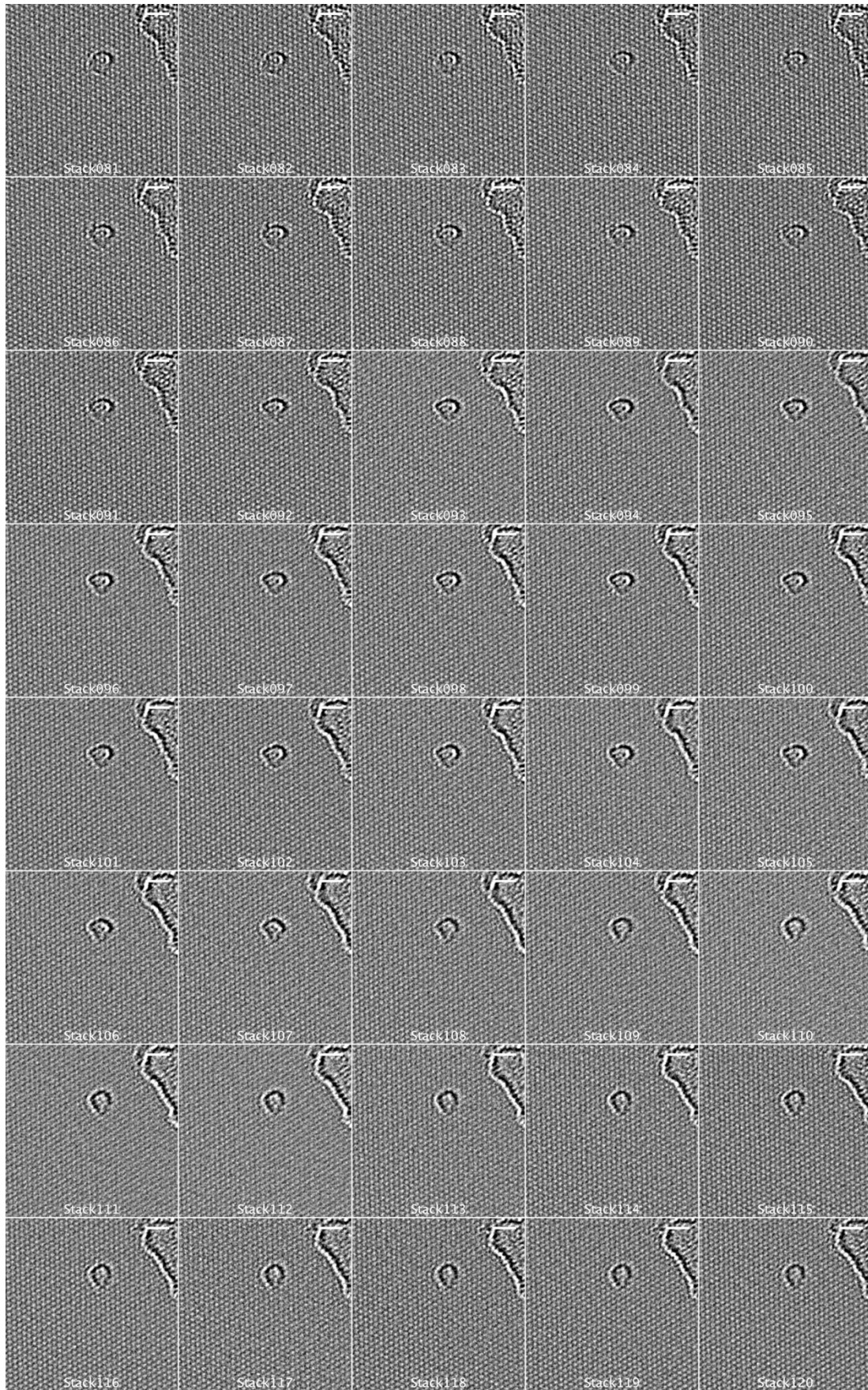


**Supplementary Fig. 10. Supplementary Video 3: SMART-EM video sequence. Frames 1–40, scale bar 1 nm.**

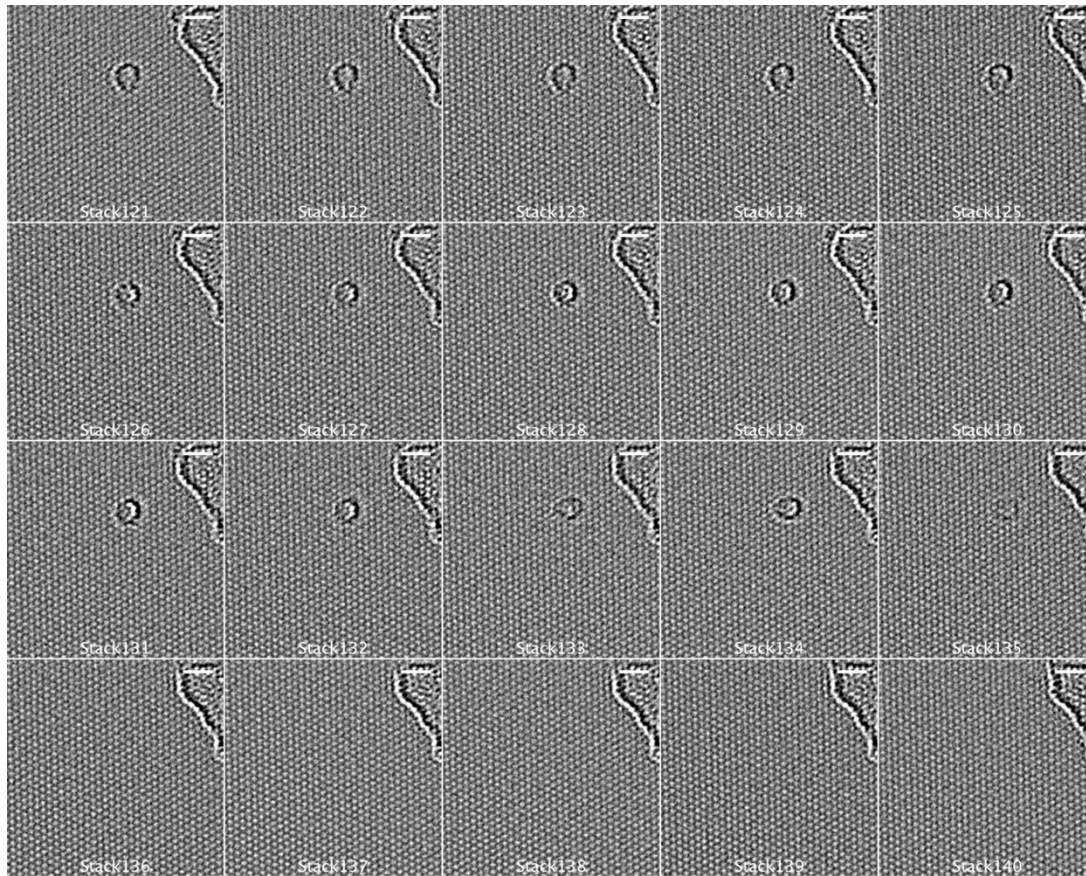


**Supplementary Fig. 11. Supplementary Video 3 (Continued): SMART-EM video sequence.** Frames 41–80, scale bar 1 nm.



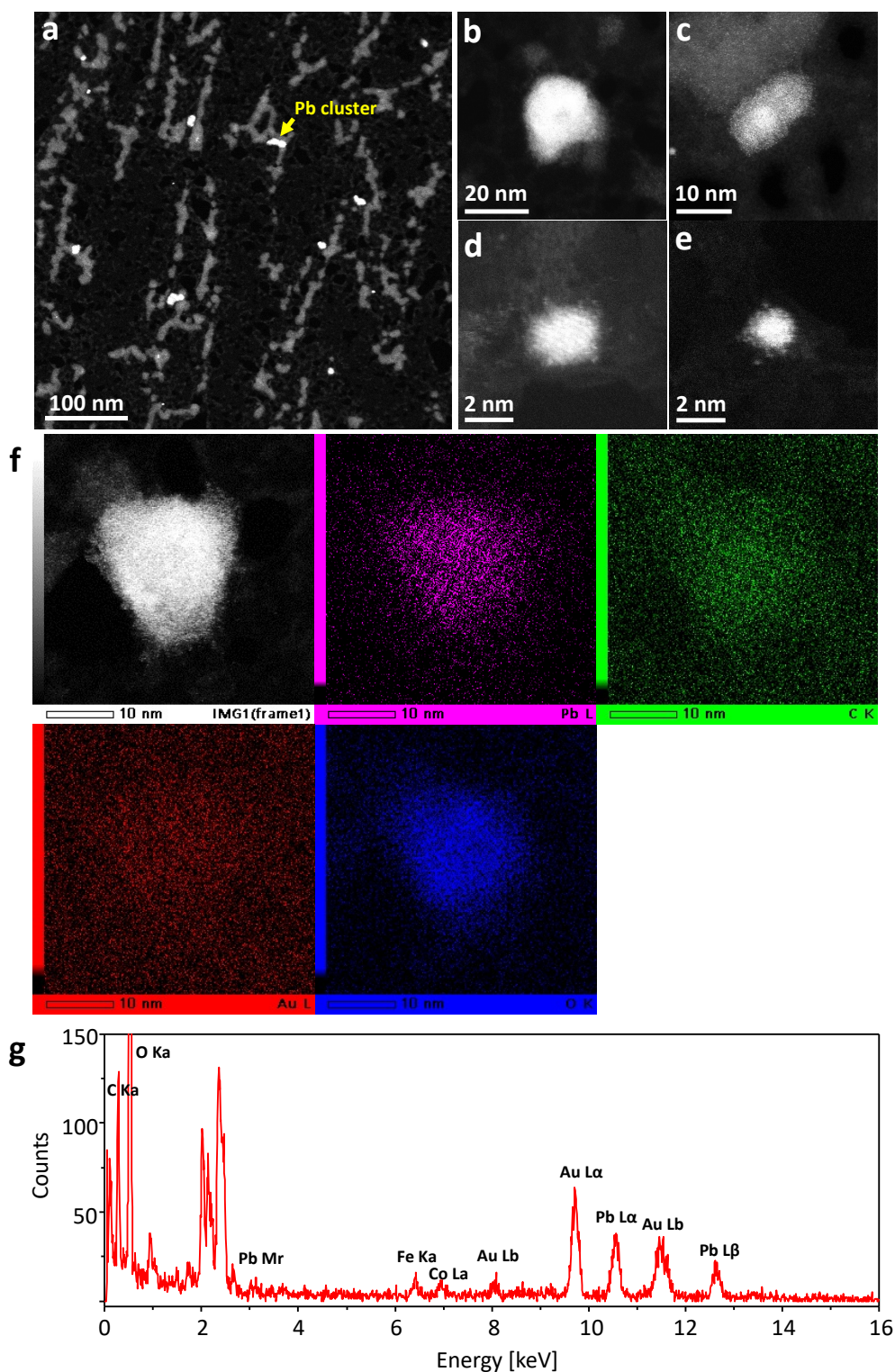


**Supplementary Fig. 12. Supplementary Video 3 (Continued): SMART-EM video sequence.** Frames 81 –120, scale bar 1 nm.



**Supplementary Fig. 13. Supplementary Video 3 (Continued): SMART-EM video sequence.** Frames 121 –140, scale bar 1 nm.

### 3.7 STEM/EDS analysis



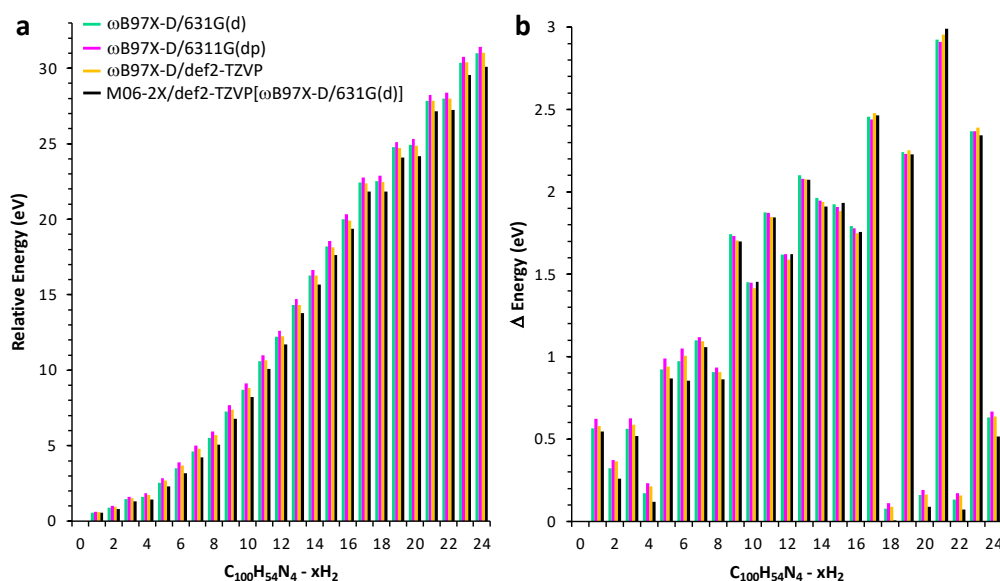
**Supplementary Fig. 14. STEM-EDX analysis of Pb aggregates.** a-e, HAADF-STEM images of the Pb aggregates. f, EDS elemental mapping of Pb. (g) EDX spectrum.

## 4 Computational Section

### 4.1 Thermochemical analysis

**Supplementary Table 1. Comparison of thermochemistry results obtained from different density functionals and basis sets.** Geometry optimization at the  $\omega$ B97X-D/6-31G(d) level of theory.

-nH <sub>2</sub>	Relative Energy (eV)				$\Delta$ Energy (eV)			
	$\omega$ B97X-D/ 631G(d)	$\omega$ B97X-D/ 6311G(d,p)	$\omega$ B97X-D/ def2-TZVP	M06-2X/ def2-TZVP	$\omega$ B97X-D/ 631G(d)	$\omega$ B97X-D/ 6311G(d,p)	$\omega$ B97X-D/ def2-TZVP	M06-2X/ def2-TZVP
0	0.000	0.000	0.000	0.000	0	0	0	0
1	0.564	0.622	0.580	0.546	0.564	0.622	0.580	0.546
2	0.887	0.996	0.943	0.804	0.323	0.373	0.363	0.258
3	1.450	1.621	1.531	1.322	0.563	0.626	0.588	0.518
4	1.621	1.852	1.744	1.441	0.171	0.231	0.212	0.118
5	2.544	2.843	2.684	2.308	0.923	0.990	0.941	0.868
6	3.517	3.891	3.689	3.163	0.972	1.049	1.005	0.854
7	4.615	5.010	4.783	4.219	1.099	1.119	1.094	1.057
8	5.522	5.945	5.689	5.081	0.906	0.934	0.905	0.862
9	7.265	7.677	7.394	6.779	1.743	1.732	1.706	1.699
10	8.717	9.124	8.811	8.233	1.452	1.448	1.416	1.454
11	10.592	10.998	10.658	10.079	1.875	1.873	1.848	1.846
12	12.211	12.619	12.248	11.700	1.619	1.621	1.590	1.621
13	14.311	14.698	14.323	13.772	2.100	2.078	2.076	2.073
14	16.275	16.646	16.263	15.687	1.964	1.948	1.939	1.911
15	18.201	18.556	18.147	17.619	1.926	1.910	1.884	1.933
16	19.993	20.334	19.897	19.376	1.792	1.778	1.750	1.757
17	22.448	22.774	22.376	21.840	2.455	2.440	2.478	2.464
18	22.527	22.885	22.465	21.847	0.079	0.110	0.089	0.007
19	24.770	25.115	24.719	24.076	2.243	2.230	2.254	2.229
20	24.931	25.307	24.882	24.165	0.161	0.192	0.164	0.089
21	27.855	28.218	27.836	27.155	2.924	2.911	2.953	2.990
22	27.989	28.391	27.994	27.227	0.134	0.173	0.158	0.071
23	30.356	30.760	30.384	29.569	2.367	2.369	2.390	2.342
24	30.986	31.428	31.020	30.084	0.630	0.668	0.636	0.515



**Supplementary Fig. 15. Comparison of density functionals and basis set on thermochemical results.**

**Supplementary Table 2. Thermochemically investigated intermediates, derived from a zipper-mechanism from 1 to FP.**

$1 - nH_2$	Isomers								
	A	B	C	D	E	F	G	H	
0									
1									
2									
3									
4									
5									
6									
7									
8									
9									
10									
11									
12									

**Supplementary Table 3. (Continued) Thermochemically investigated intermediates, derived from a zipper-mechanism from 1 to FP.**

1 - nH <sub>2</sub>	Isomers							
	A	B	C	D	E	F	G	H
13								
14								
15								
16								
17								
18								
19								
20								
21								
22								
23								
24								

**Supplementary Table 4. Thermochemical analysis of the successive cyclodehydrogenation via zipper-mechanism of 1 to FP. Calculated at the DFT  $\omega$ B97X-D/6-31G(d) level of theory;  $1 \rightarrow \text{FP} + n\text{H}_2 + E$ .**

Entry	Bonds	Isomer	Symmetry	$E$ (hartree)	Rel. $E$ (eV)	$\Delta E$ (eV)
1	--	H <sub>2</sub>	$D_{\text{th}}$	-1.17193	--	--
<b>2</b>	<b>0</b>		<b>C<sub>s</sub></b>	-4061.069046	0.000	0
<b>3</b>	<b>1</b>	<b>a</b>	<b>C<sub>1</sub></b>	-4059.876385	0.564	0.564
4	1	b	C <sub>1</sub>	-4059.874447	0.617	0.617
<b>5</b>	<b>2</b>	<b>a</b>	<b>C<sub>1</sub></b>	-4058.692577	0.887	0.323
6	2	b	C <sub>1</sub>	-4058.682162	1.171	0.607
7	2	c	C <sub>1</sub>	-4058.675828	1.343	0.779
8	2	d	C <sub>1</sub>	-4058.677583	1.295	0.731
9	2	e	C <sub>1</sub>	-4058.683044	1.147	0.583
10	2	f	C <sub>1</sub>	-4058.682162	1.171	0.607
11	2	g = a	C <sub>1</sub>	-4058.692577	0.887	0.323
12	2	h	C <sub>1</sub>	-4058.637644	2.382	1.818
13	3	a	C <sub>1</sub>	-4057.489237	1.742	0.855
14	3	b	C <sub>1</sub>	-4057.494952	1.587	0.699
15	3	c	C <sub>1</sub>	-4057.499896	1.452	0.565
<b>16</b>	<b>3</b>	<b>d</b>	<b>C<sub>1</sub></b>	-4057.499961	1.450	0.563
17	3	e	C <sub>1</sub>	-4057.496517	1.544	0.657
18	3	f	C <sub>1</sub>	-4057.491925	1.669	0.782
19	3	g	C <sub>1</sub>	-4057.450237	2.803	1.916
20	3	h	C <sub>1</sub>	-4057.450708	2.790	1.903
21	4	a	C <sub>1</sub>	-4056.297698	2.276	0.825
22	4	b	C <sub>1</sub>	-4056.298368	2.257	0.807
<b>23</b>	<b>4</b>	<b>c</b>	<b>C<sub>2</sub></b>	-4056.321747	1.621	0.171
24	4	d	C <sub>1</sub>	-4056.293463	2.391	0.941
25	4	e	C <sub>1</sub>	-4056.298581	2.252	0.801
26	4	f	C <sub>1</sub>	-4056.258051	3.354	1.904
27	4	g	C <sub>1</sub>	-4056.259576	3.313	1.863
28	4	h	C <sub>1</sub>	-4056.259877	3.305	1.855
29	5	a	C <sub>1</sub>	-4055.115496	2.555	0.934
<b>30</b>	<b>5</b>	<b>b</b>	<b>C<sub>1</sub></b>	-4055.115896	2.544	0.923
31	5	c	C <sub>1</sub>	-4055.079636	3.531	1.910
32	5	d	C <sub>1</sub>	-4055.080209	3.515	1.894
33	6	a	C <sub>1</sub>	-4053.906111	3.574	1.030
34	6	b	C <sub>1</sub>	-4053.905598	3.588	1.044
<b>35</b>	<b>6</b>	<b>c</b>	<b>C<sub>1</sub></b>	-4053.908235	3.517	0.972
36	6	d	C <sub>1</sub>	-4053.877238	4.360	1.816
37	6	e	C <sub>1</sub>	-4053.875879	4.397	1.853
38	6	f	C <sub>1</sub>	-4053.87034	4.548	2.003
39	6	g	C <sub>1</sub>	-4053.867297	4.631	2.086
40	6	h	C <sub>1</sub>	-4053.875076	4.419	1.875
41	7	a = b	C <sub>1</sub>	-4052.695759	4.620	1.103
<b>42</b>	<b>7</b>	<b>b = a</b>	<b>C<sub>1</sub></b>	-4052.695933	4.615	1.099
43	7	c	C <sub>1</sub>	-4052.657619	5.658	2.141
44	7	d	C <sub>1</sub>	-4052.66657	5.414	1.898
45	7	e	C <sub>1</sub>	-4052.659741	5.600	2.083
46	7	f	C <sub>1</sub>	-4052.657381	5.664	2.148
47	7	g	C <sub>1</sub>	-4052.66646	5.417	1.901
48	7	h	C <sub>1</sub>	-4052.659989	5.593	2.077

49	8	a	$C_{2v}$	-4051.490692	5.522	0.906
50	8	b	$C_1$	-4051.4541	6.517	1.902
51	8	c	$C_1$	-4051.459564	6.369	1.753
52	8	d	$C_1$	-4051.448621	6.666	2.051
53	8	e	$C_1$	-4051.44865	6.666	2.050
54	8	f	$C_1$	-4051.448468	6.671	2.055
55	8	g	$C_1$	-4051.450004	6.629	2.014
56	8	h	$C_1$	-4051.456312	6.457	1.842
57	9	a	$C_1$	-4050.254698	7.265	1.743
58	9	b	$C_1$	-4050.251648	7.348	1.826
59	10	a	$C_1$	-4049.000865	9.494	2.229
60	10	b	$C_1$	-4049.009145	9.268	2.003
61	10	c	$C_1$	-4049.013292	9.155	1.891
62	10	d	$C_1$	-4049.020793	8.951	1.686
63	10	e	$C_1$	-4049.017246	9.048	1.783
64	10	f	$C_1$	-4049.019425	8.988	1.724
65	10	g	$C_s$	-4049.029398	8.717	1.452
66	11	a	$C_1$	-4047.778623	10.863	2.145
67	11	b	$C_1$	-4047.783758	10.723	2.006
68	11	c	$C_1$	-4047.78858	10.592	1.875
69	11	d	$C_1$	-4047.763446	11.276	2.558
70	12	a	$C_1$	-4046.541065	12.648	2.057
71	12	b	$C_1$	-4046.538714	12.712	2.121
72	12	c	$C_1$	-4046.557145	12.211	1.619
73	12	d	$C_1$	-4046.543366	12.586	1.994
74	12	e	$C_1$	-4046.536479	12.773	2.182
75	12	f	$C_1$	-4046.522531	13.153	2.561
76	13	a=b=d=e	$C_1$	-4045.307894	14.315	2.104
77	13	b=a=d=e	$C_1$	-4045.308027	14.311	2.100
78	13	c=f	$C_1$	-4045.29005	14.800	2.590
79	13	d=a=b=e	$C_1$	-4045.307856	14.316	2.105
80	13	e=a=b=d	$C_1$	-4045.308046	14.311	2.100
81	13	f=c	$C_1$	-4045.290666	14.784	2.573
82	14	a	$C_1$	-4044.060659	16.364	2.053
83	14	b	$C_1$	-4044.050325	16.645	2.334
84	14	c	$C_s$	-4044.062652	16.310	1.999
85	14	d	$C_1$	-4044.063917	16.275	1.964
86	14	e	$C_1$	-4044.040369	16.916	2.605
87	15	a=c	$C_1$	-4042.821152	18.203	1.928
88	15	b=d	$C_1$	-4042.803863	18.673	2.398
89	15	c=a	$C_1$	-4042.821219	18.201	1.926
90	15	d=b	$C_1$	-4042.803813	18.675	2.399
91	16	a	$C_2$	-4041.583445	19.993	1.792
92	16	b	$C_1$	-4041.559576	20.642	2.441
93	16	c	$C_1$	-4041.55183	20.853	2.652
94	16	d	$C_1$	-4041.559347	20.649	2.447
95	17	a	$C_s$	-4040.321279	22.448	2.455
96	17	b	$C_s$	-4040.320209	22.477	2.485
97	18	a	$C_1$	-4039.053432	25.058	2.610
98	18	b	$C_{2v}$	-4039.070262	24.600	2.152
99	18	c	$C_1$	-4039.146456	22.527	0.079



100	19	a	$C_1$	-4037.880897	25.075	2.548
<b>101</b>	<b>19</b>	<b>b</b>	<b><math>C_s</math></b>	<b>-4037.892111</b>	<b>24.770</b>	<b>2.243</b>
102	19	c	$C_1$	-4037.88087	25.075	2.549
103	20	a	$C_1$	-4036.617178	27.572	2.803
<b>104</b>	<b>20</b>	<b>b</b>	<b><math>C_{2v}</math></b>	<b>-4036.714259</b>	<b>24.931</b>	<b>0.161</b>
<b>105</b>	<b>21</b>	<b>a</b>	<b><math>C_s</math></b>	<b>-4035.434873</b>	<b>27.855</b>	<b>2.924</b>
<b>106</b>	<b>22</b>	<b>a</b>	<b><math>C_s</math></b>	<b>-4034.258017</b>	<b>27.989</b>	<b>0.134</b>
107	22	b	$C_{2v}$	-4034.174027	30.274	2.420
<b>108</b>	<b>23</b>	<b>a</b>	<b><math>C_s</math></b>	<b>-4032.999104</b>	<b>30.356</b>	<b>2.367</b>
<b>109</b>	<b>24</b>	--	<b><math>C_{2v}</math></b>	<b>-4031.804004</b>	<b>30.986</b>	<b>0.630</b>

Supplementary Table 5. Thermochemical analysis of the successive cyclodehydrogenation via zipper-mechanism of **1** to FP. Calculated at the DFT  $\omega$ B97X-D/6-311G(d,p)[6-31G(d)] level of theory;  $\mathbf{1} \rightarrow \text{FP} + n\text{H}_2 + E$ .

Entry	Bonds	Isomer	Symmetry	$E$ (hartree)	Rel. $E$ (eV)	$\Delta E$ (eV)
110	--	H <sub>2</sub>	$D_{ih}$	-1.176081	--	--
<b>111</b>	<b>0</b>		<b><math>C_s</math></b>	<b>-4061.894656</b>	<b>0.000</b>	<b>0</b>
<b>112</b>	<b>1</b>	<b>a</b>	<b><math>C_1</math></b>	<b>-4060.695706</b>	<b>0.622</b>	<b>0.622</b>
113	1	b	$C_1$	-4060.693853	0.673	0.673
<b>114</b>	<b>2</b>	<b>a</b>	<b><math>C_1</math></b>	<b>-4059.505902</b>	<b>0.996</b>	<b>0.373</b>
115	2	b	$C_1$	-4059.495179	1.288	0.665
116	2	c	$C_1$	-4059.488681	1.464	0.842
117	2	d	$C_1$	-4059.490385	1.418	0.796
118	2	e	$C_1$	-4059.496059	1.264	0.641
119	2	f	$C_1$	-4059.495179	1.288	0.665
120	2	g = a	$C_1$	-4059.505902	0.996	0.373
121	2	h	$C_1$	-4059.451816	2.467	1.845
122	3	a	$C_1$	-4058.295839	1.920	0.925
123	3	b	$C_1$	-4058.301881	1.756	0.760
124	3	c	$C_1$	-4058.306601	1.628	0.632
<b>125</b>	<b>3</b>	<b>d</b>	<b><math>C_1</math></b>	<b>-4058.306834</b>	<b>1.621</b>	<b>0.626</b>
126	3	e	$C_1$	-4058.303374	1.715	0.720
127	3	f	$C_1$	-4058.298699	1.843	0.847
128	3	g	$C_1$	-4058.259224	2.917	1.921
129	3	h	$C_1$	-4058.259704	2.904	1.908
130	4	a	$C_1$	-4057.098047	2.511	0.890
131	4	b	$C_1$	-4057.098381	2.502	0.881
<b>132</b>	<b>4</b>	<b>c</b>	<b><math>C_2</math></b>	<b>-4057.12226</b>	<b>1.852</b>	<b>0.231</b>
133	4	d	$C_1$	-4057.09347	2.636	1.015
134	4	e	$C_1$	-4057.098854	2.489	0.868
135	4	f	$C_1$	-4057.060686	3.528	1.907
136	4	g	$C_1$	-4057.062068	3.490	1.869
137	4	h	$C_1$	-4057.061795	3.498	1.876
138	5	a	$C_1$	-4055.909269	2.857	1.004
<b>139</b>	<b>5</b>	<b>b</b>	<b><math>C_1</math></b>	<b>-4055.909788</b>	<b>2.843</b>	<b>0.990</b>
140	5	c	$C_1$	-4055.875521	3.775	1.923
141	5	d	$C_1$	-4055.876365	3.752	1.900
142	6	a	$C_1$	-4054.694717	3.904	1.061
143	6	b	$C_1$	-4054.692882	3.953	1.111
<b>144</b>	<b>6</b>	<b>c</b>	<b><math>C_1</math></b>	<b>-4054.695166</b>	<b>3.891</b>	<b>1.049</b>

145	6	d	C <sub>1</sub>	-4054.666467	4.672	1.830
146	6	e	C <sub>1</sub>	-4054.665253	4.705	1.863
147	6	f	C <sub>1</sub>	-4054.660519	4.834	1.992
148	6	g	C <sub>1</sub>	-4054.657724	4.910	2.068
149	6	h	C <sub>1</sub>	-4054.66476	4.719	1.876
150	7	a = b	C <sub>1</sub>	-4053.477796	5.015	1.124
<b>151</b>	<b>7</b>	<b>b = a</b>	<b>C<sub>1</sub></b>	<b>-4053.477958</b>	<b>5.010</b>	<b>1.119</b>
152	7	c	C <sub>1</sub>	-4053.441156	6.012	2.121
153	7	d	C <sub>1</sub>	-4053.449357	5.789	1.897
154	7	e	C <sub>1</sub>	-4053.443023	5.961	2.070
155	7	f	C <sub>1</sub>	-4053.440887	6.019	2.128
156	7	g	C <sub>1</sub>	-4053.449253	5.792	1.900
157	7	h	C <sub>1</sub>	-4053.443334	5.953	2.061
<b>158</b>	<b>8</b>	<b>a</b>	<b>C<sub>2v</sub></b>	<b>-4052.267551</b>	<b>5.945</b>	<b>0.934</b>
159	8	b	C <sub>1</sub>	-4052.232563	6.897	1.886
160	8	c	C <sub>1</sub>	-4052.237415	6.765	1.754
161	8	d	C <sub>1</sub>	-4052.226805	7.053	2.043
162	8	e	C <sub>1</sub>	-4052.227119	7.045	2.034
163	8	f	C <sub>1</sub>	-4052.227222	7.042	2.031
164	8	g	C <sub>1</sub>	-4052.228811	6.999	1.988
165	8	h	C <sub>1</sub>	-4052.234881	6.834	1.823
<b>166</b>	<b>9</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4051.027814</b>	<b>7.677</b>	<b>1.732</b>
167	9	b	C <sub>1</sub>	-4051.024893	7.756	1.812
168	10	a	C <sub>1</sub>	-4049.770966	9.874	2.198
169	10	b	C <sub>1</sub>	-4049.778393	9.672	1.996
170	10	c	C <sub>1</sub>	-4049.782424	9.563	1.886
171	10	d	C <sub>1</sub>	-4049.789921	9.359	1.682
172	10	e	C <sub>1</sub>	-4049.78659	9.449	1.773
173	10	f	C <sub>1</sub>	-4049.788642	9.393	1.717
<b>174</b>	<b>10</b>	<b>g</b>	<b>C<sub>s</sub></b>	<b>-4049.798528</b>	<b>9.124</b>	<b>1.448</b>
175	11	a	C <sub>1</sub>	-4048.544469	11.246	2.122
176	11	b	C <sub>1</sub>	-4048.548955	11.124	2.000
<b>177</b>	<b>11</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4048.553598</b>	<b>10.998</b>	<b>1.873</b>
178	11	d	C <sub>1</sub>	-4048.529743	11.647	2.523
179	12	a	C <sub>1</sub>	-4047.302667	13.035	2.037
180	12	b	C <sub>1</sub>	-4047.300515	13.093	2.095
<b>181</b>	<b>12</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4047.317939</b>	<b>12.619</b>	<b>1.621</b>
182	12	d	C <sub>1</sub>	-4047.304341	12.989	1.991
183	12	e	C <sub>1</sub>	-4047.298261	13.155	2.157
184	12	f	C <sub>1</sub>	-4047.284756	13.522	2.524
185	13	a=b=d=e	C <sub>1</sub>	-4046.065326	14.702	2.083
<b>186</b>	<b>13</b>	<b>b=a=d=e</b>	<b>C<sub>1</sub></b>	<b>-4046.065455</b>	<b>14.698</b>	<b>2.079</b>
187	13	c=f	C <sub>1</sub>	-4046.048108	15.170	2.551
188	13	d=a=b=e	C <sub>1</sub>	-4046.065285	14.703	2.084
189	13	e=a=b=d	C <sub>1</sub>	-4046.065476	14.698	2.078
190	13	f=c	C <sub>1</sub>	-4046.048711	15.154	2.535
191	14	a	C <sub>1</sub>	-4044.814569	16.734	2.036
192	14	b	C <sub>1</sub>	-4044.804402	17.010	2.312
193	14	c	C <sub>s</sub>	-4044.81659	16.679	1.981
<b>194</b>	<b>14</b>	<b>d</b>	<b>C<sub>1</sub></b>	<b>-4044.817793</b>	<b>16.646</b>	<b>1.948</b>
195	14	e	C <sub>1</sub>	-4044.794856	17.270	2.572

196	15	a=c	C <sub>1</sub>	-4043.571456	18.558	1.912
197	15	b=d	C <sub>1</sub>	-4043.554353	19.023	2.377
<b>198</b>	<b>15</b>	<b>c=a</b>	<b>C<sub>1</sub></b>	<b>-4043.571536</b>	<b>18.556</b>	<b>1.910</b>
199	15	d=b	C <sub>1</sub>	-4043.55431	19.024	2.378
<b>200</b>	<b>16</b>	<b>a</b>	<b>C<sub>2</sub></b>	<b>-4042.330102</b>	<b>20.334</b>	<b>1.778</b>
201	16	b	C <sub>1</sub>	-4042.306101	20.987	2.431
202	16	c	C <sub>1</sub>	-4042.298724	21.188	2.632
203	16	d	C <sub>1</sub>	-4042.306157	20.986	2.430
<b>204</b>	<b>17</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4041.064342</b>	<b>22.774</b>	<b>2.440</b>
205	17	b	C <sub>s</sub>	-4041.063088	22.808	2.474
206	18	a	C <sub>1</sub>	-4039.79266	25.376	2.601
207	18	b	C <sub>2v</sub>	-4039.809528	24.917	2.142
<b>208</b>	<b>18</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4039.884207</b>	<b>22.885</b>	<b>0.110</b>
209	19	a	C <sub>1</sub>	-4038.614847	25.423	2.538
<b>210</b>	<b>19</b>	<b>b</b>	<b>C<sub>s</sub></b>	<b>-4038.626159</b>	<b>25.115</b>	<b>2.230</b>
211	19	c	C <sub>1</sub>	-4038.614822	25.423	2.539
212	20	a	C <sub>1</sub>	-4037.347597	27.904	2.789
<b>213</b>	<b>20</b>	<b>b</b>	<b>C<sub>2v</sub></b>	<b>-4037.443033</b>	<b>25.307</b>	<b>0.192</b>
<b>214</b>	<b>21</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4036.159965</b>	<b>28.218</b>	<b>2.911</b>
<b>215</b>	<b>22</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4034.977527</b>	<b>28.391</b>	<b>0.173</b>
216	22	b	C <sub>2v</sub>	-4034.894777	30.643	2.425
<b>217</b>	<b>23</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4033.714377</b>	<b>30.760</b>	<b>2.369</b>
<b>218</b>	<b>24</b>	<b>--</b>	<b>C<sub>2v</sub></b>	<b>-4032.513742</b>	<b>31.428</b>	<b>0.668</b>

Supplementary Table 6. Thermochemical analysis of the successive cyclodehydrogenation via zipper-mechanism of **1** to FP. Calculated at the DFT  $\omega$ B97X-D/def2-TZVP[6-31G(d)] level of theory; **1**  $\rightarrow$  FP + nH<sub>2</sub> + E.

Entry	Bonds	Isomer	Symmetry	E (hartree)	Rel. E (eV)	$\Delta E$ (eV)
219	--	H <sub>2</sub>	D <sub>ih</sub>	-1.176081	--	--
<b>220</b>	<b>0</b>		<b>C<sub>s</sub></b>	<b>-4062.374763</b>	<b>0.000</b>	<b>0</b>
<b>221</b>	<b>1</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4061.177384</b>	<b>0.580</b>	<b>0.580</b>
222	1	b	C <sub>1</sub>	-4061.175135	0.641	0.641
<b>223</b>	<b>2</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4059.987946</b>	<b>0.943</b>	<b>0.363</b>
224	2	b	C <sub>1</sub>	-4059.977803	1.219	0.639
225	2	c	C <sub>1</sub>	-4059.971276	1.397	0.817
226	2	d	C <sub>1</sub>	-4059.973031	1.349	0.769
227	2	e	C <sub>1</sub>	-4059.979022	1.186	0.606
228	2	f	C <sub>1</sub>	-4059.977803	1.219	0.639
229	2	g = a	C <sub>1</sub>	-4059.987946	0.943	0.363
230	2	h	C <sub>1</sub>	-4059.934891	2.387	1.807
231	3	a	C <sub>1</sub>	-4058.779813	1.815	0.872
232	3	b	C <sub>1</sub>	-4058.78495	1.675	0.732
233	3	c	C <sub>1</sub>	-4058.790138	1.534	0.591
<b>234</b>	<b>3</b>	<b>d</b>	<b>C<sub>1</sub></b>	<b>-4058.790255</b>	<b>1.531</b>	<b>0.588</b>
235	3	e	C <sub>1</sub>	-4058.786461	1.634	0.691
236	3	f	C <sub>1</sub>	-4058.782686	1.737	0.794
237	3	g	C <sub>1</sub>	-4058.742829	2.822	1.879
238	3	h	C <sub>1</sub>	-4058.743551	2.802	1.859
239	4	a	C <sub>1</sub>	-4057.583151	2.375	0.844
240	4	b	C <sub>1</sub>	-4057.583121	2.376	0.845

<b>241</b>	<b>4</b>	<b>c</b>	<b>C<sub>2</sub></b>	<b>-4057.606365</b>	<b>1.744</b>	<b>0.212</b>
242	4	d	C <sub>1</sub>	-4057.578577	2.500	0.969
243	4	e	C <sub>1</sub>	-4057.584025	2.351	0.820
244	4	f	C <sub>1</sub>	-4057.545651	3.396	1.865
245	4	g	C <sub>1</sub>	-4057.547425	3.347	1.816
246	4	h	C <sub>1</sub>	-4057.546527	3.372	1.841
247	5	a	C <sub>1</sub>	-4056.39526	2.697	0.953
<b>248</b>	<b>5</b>	<b>b</b>	<b>C<sub>1</sub></b>	<b>-4056.395712</b>	<b>2.684</b>	<b>0.941</b>
249	5	c	C <sub>1</sub>	-4056.361659	3.611	1.867
250	5	d	C <sub>1</sub>	-4056.362337	3.592	1.849
251	6	a	C <sub>1</sub>	-4055.181705	3.716	1.032
252	6	b	C <sub>1</sub>	-4055.180612	3.746	1.062
<b>253</b>	<b>6</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4055.182705</b>	<b>3.689</b>	<b>1.005</b>
254	6	d	C <sub>1</sub>	-4055.154247	4.463	1.779
255	6	e	C <sub>1</sub>	-4055.1528	4.503	1.819
256	6	f	C <sub>1</sub>	-4055.14713	4.657	1.973
257	6	g	C <sub>1</sub>	-4055.144712	4.723	2.039
258	6	h	C <sub>1</sub>	-4055.152404	4.514	1.829
259	7	a = b	C <sub>1</sub>	-4053.966243	4.788	1.099
<b>260</b>	<b>7</b>	<b>b = a</b>	<b>C<sub>1</sub></b>	<b>-4053.966412</b>	<b>4.783</b>	<b>1.094</b>
261	7	c	C <sub>1</sub>	-4053.929938	5.776	2.087
262	7	d	C <sub>1</sub>	-4053.938433	5.545	1.856
263	7	e	C <sub>1</sub>	-4053.931123	5.744	2.054
264	7	f	C <sub>1</sub>	-4053.929624	5.784	2.095
265	7	g	C <sub>1</sub>	-4053.938297	5.548	1.859
266	7	h	C <sub>1</sub>	-4053.931462	5.734	2.045
<b>267</b>	<b>8</b>	<b>a</b>	<b>C<sub>2v</sub></b>	<b>-4052.757061</b>	<b>5.689</b>	<b>0.905</b>
268	8	b	C <sub>1</sub>	-4052.72225	6.636	1.853
269	8	c	C <sub>1</sub>	-4052.72755	6.492	1.708
270	8	d	C <sub>1</sub>	-4052.716201	6.801	2.017
271	8	e	C <sub>1</sub>	-4052.71688	6.782	1.999
272	8	f	C <sub>1</sub>	-4052.716666	6.788	2.005
273	8	g	C <sub>1</sub>	-4052.718185	6.747	1.963
274	8	h	C <sub>1</sub>	-4052.724547	6.573	1.790
<b>275</b>	<b>9</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4051.518293</b>	<b>7.394</b>	<b>1.706</b>
276	9	b	C <sub>1</sub>	-4051.515518	7.470	1.781
277	10	a	C <sub>1</sub>	-4050.261571	9.589	2.194
278	10	b	C <sub>1</sub>	-4050.269868	9.363	1.969
279	10	c	C <sub>1</sub>	-4050.273741	9.258	1.863
280	10	d	C <sub>1</sub>	-4050.281308	9.052	1.657
281	10	e	C <sub>1</sub>	-4050.277908	9.144	1.750
282	10	f	C <sub>1</sub>	-4050.279984	9.088	1.693
<b>283</b>	<b>10</b>	<b>g</b>	<b>C<sub>s</sub></b>	<b>-4050.290166</b>	<b>8.811</b>	<b>1.416</b>
284	11	a	C <sub>1</sub>	-4049.036227	10.929	2.119
285	11	b	C <sub>1</sub>	-4049.041526	10.785	1.974
<b>286</b>	<b>11</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4049.046188</b>	<b>10.658</b>	<b>1.848</b>
287	11	d	C <sub>1</sub>	-4049.019893	11.374	2.563
288	12	a	C <sub>1</sub>	-4047.795324	12.693	2.035
289	12	b	C <sub>1</sub>	-4047.793056	12.755	2.097
<b>290</b>	<b>12</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4047.811691</b>	<b>12.248</b>	<b>1.590</b>
291	12	d	C <sub>1</sub>	-4047.797785	12.626	1.968

292	12	e	C <sub>1</sub>	-4047.790911	12.813	2.155
293	12	f	C <sub>1</sub>	-4047.776019	13.219	2.560
294	13	a=b=d=e	C <sub>1</sub>	-4046.559146	14.329	2.081
<b>295</b>	<b>13</b>	<b>b=a=d=e</b>	<b>C<sub>1</sub></b>	<b>-4046.559304</b>	<b>14.324</b>	<b>2.076</b>
296	13	c=f	C <sub>1</sub>	-4046.540523	14.835	2.587
297	13	d=a=b=e	C <sub>1</sub>	-4046.55909	14.330	2.082
298	13	e=a=b=d	C <sub>1</sub>	-4046.559333	14.323	2.076
299	13	f=c	C <sub>1</sub>	-4046.541421	14.811	2.563
300	14	a	C <sub>1</sub>	-4045.309237	16.338	2.013
301	14	b	C <sub>1</sub>	-4045.296909	16.673	2.349
302	14	c	C <sub>s</sub>	-4045.310788	16.295	1.971
<b>303</b>	<b>14</b>	<b>d</b>	<b>C<sub>1</sub></b>	<b>-4045.311974</b>	<b>16.263</b>	<b>1.939</b>
304	14	e	C <sub>1</sub>	-4045.287671	16.924	2.600
305	15	a=c	C <sub>1</sub>	-4044.066578	18.149	1.886
306	15	b=d	C <sub>1</sub>	-4044.04732	18.673	2.410
<b>307</b>	<b>15</b>	<b>c=a</b>	<b>C<sub>1</sub></b>	<b>-4044.066653</b>	<b>18.147</b>	<b>1.884</b>
308	15	d=b	C <sub>1</sub>	-4044.04726	18.675	2.412
<b>309</b>	<b>16</b>	<b>a</b>	<b>C<sub>2</sub></b>	<b>-4042.826265</b>	<b>19.897</b>	<b>1.750</b>
310	16	b	C <sub>1</sub>	-4042.799855	20.616	2.469
311	16	c	C <sub>1</sub>	-4042.792447	20.817	2.670
312	16	d	C <sub>1</sub>	-4042.799995	20.612	2.465
<b>313</b>	<b>17</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4041.559101</b>	<b>22.376</b>	<b>2.478</b>
314	17	b	C <sub>s</sub>	-4041.557839	22.410	2.513
315	18	a	C <sub>1</sub>	-4040.285964	25.017	2.641
316	18	b	C <sub>2v</sub>	-4040.303314	24.544	2.169
<b>317</b>	<b>18</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4040.379735</b>	<b>22.465</b>	<b>0.089</b>
318	19	a	C <sub>1</sub>	-4039.108986	25.041	2.576
<b>319</b>	<b>19</b>	<b>b</b>	<b>C<sub>s</sub></b>	<b>-4039.120834</b>	<b>24.719</b>	<b>2.254</b>
320	19	c	C <sub>1</sub>	-4039.108959	25.042	2.577
321	20	a	C <sub>1</sub>	-4037.840799	27.547	2.829
<b>322</b>	<b>20</b>	<b>b</b>	<b>C<sub>2v</sub></b>	<b>-4037.938729</b>	<b>24.882</b>	<b>0.164</b>
<b>323</b>	<b>21</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4036.654125</b>	<b>27.836</b>	<b>2.953</b>
<b>324</b>	<b>22</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4035.472228</b>	<b>27.994</b>	<b>0.158</b>
325	22	b	C <sub>2v</sub>	-4035.387772	30.292	2.456
<b>326</b>	<b>23</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4034.20832</b>	<b>30.384</b>	<b>2.390</b>
<b>327</b>	<b>24</b>	<b>--</b>	<b>C<sub>2v</sub></b>	<b>-4033.008872</b>	<b>31.020</b>	<b>0.636</b>

Supplementary Table 7. Thermochemical analysis of the successive cyclodehydrogenation via zipper-mechanism of **1** to FP. Calculated at the DFT M06-2X/def2-TZVP[ $\omega$ B97X-D/6-31G(d)] level of theory; **1**  $\rightarrow$  FP + nH<sub>2</sub> + E.

Entry	Bonds	Isomer	Symmetry	E (hartree)	Rel. E (eV)	$\Delta E$ (eV)
328	--	H <sub>2</sub>	D <sub>ih</sub>	-1.16846	--	--
<b>329</b>	<b>0</b>		<b>C<sub>s</sub></b>	<b>-4062.23</b>	<b>0.000</b>	<b>0</b>
<b>330</b>	<b>1</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4061.04</b>	<b>0.546</b>	<b>0.546</b>
331	1	b	C <sub>1</sub>	-4061.04	0.596	0.596
<b>332</b>	<b>2</b>	<b>a</b>	<b>C<sub>1</sub></b>	<b>-4059.86</b>	<b>0.804</b>	<b>0.258</b>
333	2	b	C <sub>1</sub>	-4059.85	1.106	0.560
334	2	c	C <sub>1</sub>	-4059.85	1.229	0.683

335	2	d	C <sub>1</sub>	-4059.85	1.178	0.632
336	2	e	C <sub>1</sub>	-4059.85	1.087	0.542
337	2	f	C <sub>1</sub>	-4059.85	1.106	0.560
338	2	g = a	C <sub>1</sub>	<b>-4059.86</b>	0.804	0.258
339	2	h	C <sub>1</sub>	-4059.81	2.341	1.795
340	3	a	C <sub>1</sub>	-4058.66	1.605	0.801
341	3	b	C <sub>1</sub>	-4058.67	1.441	0.637
<b>342</b>	<b>3</b>	<b>c</b>	C <sub>1</sub>	<b>-4058.67</b>	<b>1.322</b>	<b>0.518</b>
343	3	d	C <sub>1</sub>	-4058.67	1.330	0.526
344	3	e	C <sub>1</sub>	-4058.67	1.396	0.592
345	3	f	C <sub>1</sub>	-4058.67	1.532	0.728
346	3	g	C <sub>1</sub>	-4058.62	2.711	1.907
347	3	h	C <sub>1</sub>	-4058.62	2.711	1.907
348	4	a	C <sub>1</sub>	-4057.48	2.106	0.784
349	4	b	C <sub>1</sub>	-4057.48	2.052	0.729
<b>350</b>	<b>4</b>	<b>c</b>	C <sub>2</sub>	<b>-4057.5</b>	<b>1.441</b>	<b>0.118</b>
351	4	d	C <sub>1</sub>	-4057.47	2.188	0.866
352	4	e	C <sub>1</sub>	-4057.48	2.095	0.773
353	4	f	C <sub>1</sub>	-4057.44	3.229	1.907
354	4	g	C <sub>1</sub>	-4057.44	3.200	1.878
355	4	h	C <sub>1</sub>	-4057.44	3.132	1.810
356	5	a	C <sub>1</sub>	-4056.3	2.313	0.873
<b>357</b>	<b>5</b>	<b>b</b>	C <sub>1</sub>	<b>-4056.3</b>	<b>2.308</b>	<b>0.868</b>
358	5	c	C <sub>1</sub>	-4056.26	3.357	1.916
359	5	d	C <sub>1</sub>	-4056.26	3.341	1.901
360	6	a	C <sub>1</sub>	-4055.1	3.275	0.967
361	6	b	C <sub>1</sub>	-4055.1	3.294	0.986
<b>362</b>	<b>6</b>	<b>c</b>	C <sub>1</sub>	<b>-4055.1</b>	<b>3.163</b>	<b>0.854</b>
363	6	d	C <sub>1</sub>	-4055.07	4.121	1.812
364	6	e	C <sub>1</sub>	-4055.07	4.128	1.820
365	6	f	C <sub>1</sub>	-4055.06	4.288	1.980
366	6	g	C <sub>1</sub>	-4055.06	4.385	2.077
367	6	h	C <sub>1</sub>	-4055.06	4.181	1.873
368	7	a = b	C <sub>1</sub>	-4053.89	4.222	1.059
<b>369</b>	<b>7</b>	<b>b = a</b>	C <sub>1</sub>	<b>-4053.89</b>	<b>4.219</b>	<b>1.057</b>
370	7	c	C <sub>1</sub>	-4053.85	5.303	2.140
371	7	d	C <sub>1</sub>	-4053.86	5.039	1.877
372	7	e	C <sub>1</sub>	-4053.86	5.219	2.057
373	7	f	C <sub>1</sub>	-4053.85	5.314	2.152
374	7	g	C <sub>1</sub>	-4053.86	5.034	1.871
375	7	h	C <sub>1</sub>	-4053.86	5.206	2.043
<b>376</b>	<b>8</b>	<b>a</b>	C <sub>2v</sub>	<b>-4052.69</b>	<b>5.081</b>	<b>0.862</b>
377	8	b	C <sub>1</sub>	-4052.66	6.111	1.892
378	8	c	C <sub>1</sub>	-4052.66	5.940	1.720
379	8	d	C <sub>1</sub>	-4052.65	6.250	2.030
380	8	e	C <sub>1</sub>	-4052.65	6.260	2.041
381	8	f	C <sub>1</sub>	-4052.65	6.247	2.028
382	8	g	C <sub>1</sub>	-4052.65	6.190	1.971
383	8	h	C <sub>1</sub>	-4052.66	6.040	1.821
<b>384</b>	<b>9</b>	<b>a</b>	C <sub>1</sub>	<b>-4051.46</b>	<b>6.779</b>	<b>1.699</b>
385	9	b	C <sub>1</sub>	-4051.46	6.866	1.785

386	10	a	C <sub>1</sub>	-4050.21	8.969	2.189
387	10	b	C <sub>1</sub>	-4050.22	8.773	1.993
388	10	c	C <sub>1</sub>	-4050.23	8.657	1.878
389	10	d	C <sub>1</sub>	-4050.23	8.445	1.666
390	10	e	C <sub>1</sub>	-4050.23	8.539	1.759
391	10	f	C <sub>1</sub>	-4050.23	8.482	1.703
<b>392</b>	<b>10</b>	<b>g</b>	<b>C<sub>s</sub></b>	<b>-4050.24</b>	<b>8.233</b>	<b>1.454</b>
393	11	a	C <sub>1</sub>	-4048.99	10.353	2.120
394	11	b	C <sub>1</sub>	-4049	10.221	1.988
<b>395</b>	<b>11</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4049.01</b>	<b>10.079</b>	<b>1.846</b>
396	11	d	C <sub>1</sub>	-4048.98	10.826	2.593
397	12	a	C <sub>1</sub>	-4047.76	12.132	2.053
398	12	b	C <sub>1</sub>	-4047.76	12.164	2.085
<b>399</b>	<b>12</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4047.78</b>	<b>11.700</b>	<b>1.621</b>
400	12	d	C <sub>1</sub>	-4047.76	12.065	1.986
401	12	e	C <sub>1</sub>	-4047.76	12.239	2.160
402	12	f	C <sub>1</sub>	-4047.74	12.681	2.602
403	13	a=b=d=e	C <sub>1</sub>	-4046.53	13.782	2.082
404	13	b=a=d=e	C <sub>1</sub>	-4046.53	13.776	2.076
405	13	c=f	C <sub>1</sub>	-4046.51	14.329	2.629
406	13	d=a=b=e	C <sub>1</sub>	-4046.53	13.786	2.086
<b>407</b>	<b>13</b>	<b>e=a=b=d</b>	<b>C<sub>1</sub></b>	<b>-4046.53</b>	<b>13.772</b>	<b>2.073</b>
408	13	f=c	C <sub>1</sub>	-4046.51	14.302	2.602
409	14	a	C <sub>1</sub>	-4045.29	15.803	2.027
410	14	b	C <sub>1</sub>	-4045.28	16.147	2.371
411	14	c	C <sub>s</sub>	-4045.29	15.753	1.977
<b>412</b>	<b>14</b>	<b>d</b>	<b>C<sub>1</sub></b>	<b>-4045.29</b>	<b>15.687</b>	<b>1.911</b>
413	14	e	C <sub>1</sub>	-4045.27	16.379	2.603
414	15	a=c	C <sub>1</sub>	-4044.05	17.626	1.940
415	15	b=d	C <sub>1</sub>	-4044.04	18.111	2.424
<b>416</b>	<b>15</b>	<b>c=a</b>	<b>C<sub>1</sub></b>	<b>-4044.05</b>	<b>17.619</b>	<b>1.933</b>
417	15	d=b	C <sub>1</sub>	-4044.04	18.101	2.414
<b>418</b>	<b>16</b>	<b>a</b>	<b>C<sub>2</sub></b>	<b>-4042.82</b>	<b>19.376</b>	<b>1.757</b>
419	16	b	C <sub>1</sub>	-4042.8	20.086	2.467
420	16	c	C <sub>1</sub>	-4042.79	20.276	2.657
421	16	d	C <sub>1</sub>	-4042.8	20.079	2.460
<b>422</b>	<b>17</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4041.56</b>	<b>21.840</b>	<b>2.464</b>
423	17	b	C <sub>s</sub>	-4041.56	21.894	2.518
424	18	a	C <sub>1</sub>	-4040.3	24.494	2.654
425	18	b	C <sub>2v</sub>	-4040.31	23.984	2.144
<b>426</b>	<b>18</b>	<b>c</b>	<b>C<sub>1</sub></b>	<b>-4040.39</b>	<b>21.847</b>	<b>0.007</b>
427	19	a	C <sub>1</sub>	-4039.13	24.433	2.586
<b>428</b>	<b>19</b>	<b>b</b>	<b>C<sub>s</sub></b>	<b>-4039.14</b>	<b>24.076</b>	<b>2.229</b>
429	19	c	C <sub>1</sub>	-4039.13	24.435	2.588
430	20	a	C <sub>1</sub>	-4037.87	26.943	2.867
<b>431</b>	<b>20</b>	<b>b</b>	<b>C<sub>2v</sub></b>	<b>-4037.97</b>	<b>24.165</b>	<b>0.089</b>
<b>432</b>	<b>21</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4036.69</b>	<b>27.155</b>	<b>2.990</b>
<b>433</b>	<b>22</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4035.52</b>	<b>27.227</b>	<b>0.071</b>
434	22	b	C <sub>2v</sub>	-4035.44	29.532	2.377
<b>435</b>	<b>23</b>	<b>a</b>	<b>C<sub>s</sub></b>	<b>-4034.27</b>	<b>29.569</b>	<b>2.342</b>
<b>436</b>	<b>24</b>	<b>--</b>	<b>C<sub>2v</sub></b>	<b>-4033.08</b>	<b>30.084</b>	<b>0.515</b>

## 4.2 Homolytic bond dissociation analysis

Reference calculations for  $E_{\text{BDE}}$  and  $E_{\text{d}}$  for coronene

To calibrate and verify our energy calculations, we used coronene as a reference molecule, for which the threshold displacement energy  $E_{\text{d}} = 7.7$  eV for the C–H bond is reported in the literature.<sup>4,8</sup> As shown in Supplementary Table 8, only minor fluctuations in the bond dissociation energies  $E_{\text{BDE}}$  (5.12 – 5.16 eV) are obtained for calculations using the  $\omega$ B97X-D and M06-2X functional. At the same time, the usage of the def2-TZVP basis set gave in both cases the best results.

The threshold displacement energies  $E_{\text{d}}$ , deviate significantly dependent on the used functional and basis set from 6.40 – 7.92 eV, as shown in Supplementary Table 9, and Supplementary Fig. 16. In particular, the usage of fast and cheap functionals PBE-D3 and B3LYP underestimate  $E_{\text{d}}$  in the best case by about 1.2 and 0.6 eV, respectively. Hereby, the usage of the double- $\zeta$  basis set 6-31G(d) gave the best results, and with increasing basis set, the error becomes larger. On the other hand, the methods  $\omega$ B97X-D/6-311G(d,p) and M06-2X/def2-TZVP gave both the best results, leading to virtually the same displacement cross-section  $\sigma_{\text{d}} = 66$  barn.

$E_{\text{d}}$  was obtained from the Morse potential calculations for the gradual extension of the respective bond from equilibrium length to 7 Å. The intersection of the slopes for the binding potential (equil. – 2.5 Å) and the non-binding potential (4 – 7 Å) resulted in the determined threshold energies for the homolytic bond scissions. Since the momentum transfer and atom displacement in a knock-on displacement is considered to be faster than the reorganization of the molecular geometry to a new minimum, apart from the investigated atom, the rest of the molecular geometry was frozen.



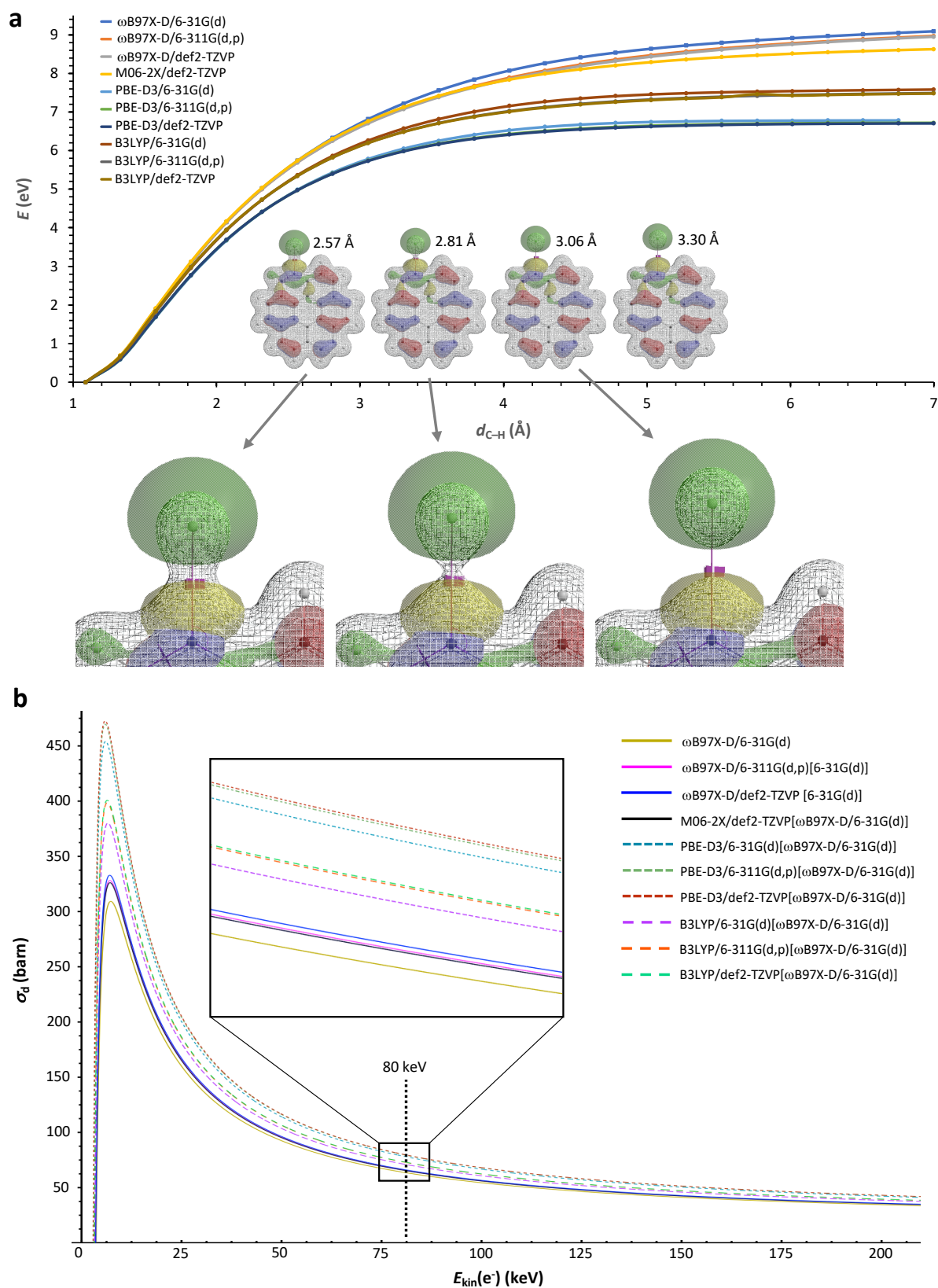
**Supplementary Table 8. Homolytic bond dissociation energies  $E_{\text{BDE}}$  ( $\text{C}_{24}\text{H}_{12} \rightarrow \text{C}_{24}\text{H}_{11}^{\bullet} + \text{H}^{\bullet} + E$ ) for coronene.** Energies are calculated from single point calculations at various levels of theory; geometries are obtained at  $\omega\text{B97X-D/6-31G(d)}$  level of theory.

Entry	Functional, Basis Set	Structure	$E$ (hartree)	$E_{\text{BDE}}$ (eV)
437	$\omega\text{B97X-D/6-31G(d)}$	$\text{H}^{\bullet}$	-0.500608	--
438	$\omega\text{B97X-D/6-31G(d)}$	$\text{C}_{24}\text{H}_{11}^{\bullet}$	-920.891449	--
439	$\omega\text{B97X-D/6-31G(d)}$	$\text{C}_{24}\text{H}_{12}$	-921.581885	5.16548564
440	$\omega\text{B97X-D/6-311G(d,p)}$	$\text{H}^{\bullet}$	-0.502668	--
441	$\omega\text{B97X-D/6-311G(d,p)}$	$\text{C}_{24}\text{H}_{11}^{\bullet}$	-921.07112	--
442	$\omega\text{B97X-D/6-311G(d,p)}$	$\text{C}_{24}\text{H}_{12}$	-921.763175	5.15348541
443	$\omega\text{B97X-D/def-2/TZVP}$	$\text{H}^{\bullet}$	-0.502666	--
444	$\omega\text{B97X-D/def-2/TZVP}$	$\text{C}_{24}\text{H}_{11}^{\bullet}$	-921.18312	--
445	$\omega\text{B97X-D/def-2/TZVP}$	$\text{C}_{24}\text{H}_{12}$	-921.874759	5.14221989
446	M06-2X/def-2/TZVP	$\text{H}^{\bullet}$	-0.498139	--
447	M06-2X/def-2/TZVP	$\text{C}_{24}\text{H}_{11}^{\bullet}$	-921.159302	--
448	M06-2X/def-2/TZVP	$\text{C}_{24}\text{H}_{12}$	-921.845772	5.12475017

**Supplementary Table 9. Summary on the threshold displacement energies  $E_d$ , the resulting displacement cross-section  $\sigma_d$ , and the minimum total electron dose  $TED_d$  for the homolytic C–H bond cleavage in coronene.** Calculated at various levels of theory; geometries are obtained at  $\omega\text{B97X-D/6-31G(d)}$  level of theory.

Entry	Functional, Basis Set	$E_d(\text{C}\cdots\text{H})$ (eV)	$\sigma_d$ (barn)	$TED_d$ [ $10^6 \text{ e}^- \text{ nm}^{-2}$ ] <sup>a</sup>
449	PBE-D3/6-31G(d)	6.5306	78.8054	10.6
450	PBE-D3/6-311G(d,p)	6.4216	80.2218	10.4
451	PBE-D3/def2-TZVP	6.4003	80.5043	10.4
452	B3LYP/6-31G(d)	7.1411	71.6746	11.6
453	B3LYP/6-311G(d,p)	6.9722	73.5219	11.3
454	B3LYP/def2-TZVP	6.9538	73.7286	11.3
455	$\omega\text{B97X-D/6-31G(d)}$	7.9213	64.1681	13.0
456	$\omega\text{B97X-D/6-311G(d,p)}$	7.688	66.2523	12.6
457	$\omega\text{B97X-D/def-2/TZVP}$	7.6332	66.7605	12.5
458	M06-2X/def-2/TZVP	7.7124	66.0284	12.6

<sup>a</sup> assuming an isotropic energy transfer for all H atoms ( $n = 12$ ).



### 4.3 Orbital energies of 1 for ionization cross-section

**Supplementary Table 10. Orbital energies of 1 for the calculation of the ionization cross-section at 80 keV.**

Calculated at the  $\omega$ B97X/6-31G(d) level of theory, using the Gaussian '16 work package.

HOMO- <i>n</i>	<i>B</i> (Hartree)	<i>U</i> (Hartree)	<i>B</i> (eV)	<i>U</i> (eV)	$\sigma_{\text{FRRB}}$ ( $\text{\AA}^2$ )
0	-0.21961	1.293024	-5.976	35.185	0.019129179
1	-0.246209	1.470393	-6.700	40.011	0.016888558
2	-0.275017	1.217286	-7.484	33.124	0.014971365
3	-0.275458	1.215524	-7.496	33.076	0.014945242
4	-0.27551	1.214133	-7.497	33.038	0.014942175
5	-0.276125	1.21025	-7.514	32.933	0.014905914
6	-0.303136	1.237422	-8.249	33.672	0.013462957
7	-0.305436	1.250245	-8.311	34.021	0.013352292
8	-0.306754	1.233055	-8.347	33.553	0.013289793
9	-0.31088	1.272505	-8.459	34.627	0.013097192
10	-0.311151	1.326863	-8.467	36.106	0.013084442
11	-0.318804	1.238818	-8.675	33.710	0.012742441
12	-0.32199	1.195113	-8.762	32.521	0.01260509
13	-0.327357	1.161374	-8.908	31.603	0.012379802
14	-0.329671	1.146942	-8.971	31.210	0.012285024
15	-0.336265	1.277961	-9.150	34.775	0.012021522
16	-0.336941	1.295567	-9.169	35.254	0.011995095
17	-0.350532	1.148131	-9.538	31.242	0.011488713
18	-0.350561	1.149448	-9.539	31.278	0.011487669
19	-0.350598	1.150091	-9.540	31.296	0.011486341
20	-0.350605	1.149549	-9.540	31.281	0.011486093
21	-0.35164	1.131379	-9.569	30.786	0.011449251
22	-0.364133	1.679162	-9.909	45.692	0.01101818
23	-0.36463	1.787365	-9.922	48.637	0.011001267
24	-0.36644	1.15647	-9.971	31.469	0.010944805
25	-0.368775	1.257075	-10.035	34.207	0.010868627
26	-0.369236	1.155694	-10.047	31.448	0.01085426
27	-0.373557	1.071222	-10.165	29.149	0.010717485
28	-0.376564	1.141974	-10.247	31.075	0.010623652
29	-0.385566	1.145196	-10.492	31.162	0.010352773
30	-0.390885	1.228494	-10.637	33.429	0.010198477
31	-0.391682	1.20438	-10.658	32.773	0.010175891
32	-0.3931	1.131751	-10.697	30.797	0.010136069
33	-0.393621	1.206923	-10.711	32.842	0.010121078
34	-0.41369	1.473761	-11.257	40.103	0.009584207
35	-0.415951	1.548396	-11.319	42.134	0.009526926
36	-0.41604	1.544558	-11.321	42.030	0.009524712
37	-0.416138	1.545659	-11.324	42.060	0.009522254
38	-0.421932	1.524114	-11.481	41.473	0.009379366
39	-0.422998	1.450893	-11.510	39.481	0.009353794
40	-0.425065	1.672967	-11.567	45.524	0.009303164

41	-0.425293	1.409515	-11.573	38.355	0.009298739
42	-0.425776	1.460583	-11.586	39.745	0.009286997
43	-0.425973	1.639875	-11.591	44.623	0.009281596
44	-0.427474	1.64932	-11.632	44.880	0.009245901
45	-0.430497	1.426395	-11.714	38.814	0.009175737
46	-0.436117	1.406651	-11.867	38.277	0.009046484
47	-0.440843	1.179084	-11.996	32.085	0.008941246
48	-0.443193	1.523045	-12.060	41.444	0.008888075
49	-0.446343	1.526027	-12.146	41.525	0.008819423
50	-0.447033	1.085501	-12.164	29.538	0.008806157
51	-0.450827	1.597354	-12.268	43.466	0.008723176
52	-0.452042	0.985904	-12.301	26.828	0.008699752
53	-0.452352	0.98406	-12.309	26.778	0.008693232
54	-0.452428	0.979884	-12.311	26.664	0.008691648
55	-0.452898	1.001665	-12.324	27.257	0.008681694
56	-0.454937	1.532039	-12.379	41.689	0.00863717
57	-0.460465	1.176207	-12.530	32.006	0.008524978
58	-0.460494	1.135283	-12.531	30.893	0.008524537
59	-0.461815	1.540629	-12.567	41.923	0.008496388
60	-0.463993	1.496409	-12.626	40.719	0.008452883
61	-0.46592	1.455118	-12.678	39.596	0.008414753
62	-0.466402	1.40423	-12.691	38.211	0.00840541
63	-0.467049	1.418836	-12.709	38.609	0.008392608
64	-0.467082	1.378018	-12.710	37.498	0.008392103
65	-0.467217	1.477389	-12.714	40.202	0.008389096
66	-0.469648	1.516268	-12.780	41.260	0.008341415
67	-0.469904	1.087355	-12.787	29.588	0.008337946
68	-0.474461	1.065897	-12.911	29.005	0.008250352
69	-0.475	1.06043	-12.925	28.856	0.008240118
70	-0.479037	1.056312	-13.035	28.744	0.008164101
71	-0.489734	1.492646	-13.326	40.617	0.007967492
72	-0.493297	1.311329	-13.423	35.683	0.007905068
73	-0.493307	1.311241	-13.424	35.681	0.007904892
74	-0.493342	1.310478	-13.425	35.660	0.00790428
75	-0.49347	1.314582	-13.428	35.772	0.00790202
76	-0.498033	1.467897	-13.552	39.944	0.007822223
77	-0.50014	1.394407	-13.610	37.944	0.007786362
78	-0.501731	1.409941	-13.653	38.366	0.00775926
79	-0.502166	1.40845	-13.665	38.326	0.0077519
80	-0.50226	1.431682	-13.667	38.958	0.007750234
81	-0.502828	1.427056	-13.683	38.832	0.007740656
82	-0.503046	1.430096	-13.689	38.915	0.00773697
83	-0.504853	1.405112	-13.738	38.235	0.007706709
84	-0.505537	1.389776	-13.756	37.818	0.007695333
85	-0.505952	1.419763	-13.768	38.634	0.007688319
86	-0.508973	1.458065	-13.850	39.676	0.007638199
87	-0.509405	1.233427	-13.862	33.563	0.007631823

88	-0.513646	1.435383	-13.977	39.059	0.007562144
89	-0.516224	1.422412	-14.047	38.706	0.007520802
90	-0.517553	1.452571	-14.083	39.526	0.007499541
91	-0.521476	1.308942	-14.190	35.618	0.007438172
92	-0.521924	1.185687	-14.202	32.264	0.007431559
93	-0.52195	1.226901	-14.203	33.386	0.007431024
94	-0.523359	1.433527	-14.241	39.008	0.007408451
95	-0.526264	1.052151	-14.320	28.631	0.007364816
96	-0.526459	1.02998	-14.326	28.027	0.007361895
97	-0.529105	1.305074	-14.398	35.513	0.007320694
98	-0.532591	0.918402	-14.493	24.991	0.007269362
99	-0.533351	1.32188	-14.513	35.970	0.007256771
100	-0.535196	1.35843	-14.563	36.965	0.007229236
101	-0.535898	1.42398	-14.583	38.748	0.007218654
102	-0.537711	1.412677	-14.632	38.441	0.007192006
103	-0.53829	1.430896	-14.648	38.937	0.007183468
104	-0.540238	1.43831	-14.701	39.138	0.007155049
105	-0.540428	1.342418	-14.706	36.529	0.00715258
106	-0.540785	1.199241	-14.716	32.633	0.007147834
107	-0.541212	1.389207	-14.727	37.802	0.007141078
108	-0.541258	1.368212	-14.728	37.231	0.007140476
109	-0.541265	1.369391	-14.729	37.263	0.007140371
110	-0.541305	1.346868	-14.730	36.650	0.00713986
111	-0.541608	1.481925	-14.738	40.325	0.007135074
112	-0.545231	1.485696	-14.836	40.428	0.007083089
113	-0.547053	1.416858	-14.886	38.555	0.007057427
114	-0.550093	1.422748	-14.969	38.715	0.007014649
115	-0.554414	1.41303	-15.086	38.451	0.00695474
116	-0.554981	1.223906	-15.102	33.304	0.006947502
117	-0.555832	1.389945	-15.125	37.822	0.00693535
118	-0.559371	1.183251	-15.221	32.198	0.006887838
119	-0.562988	1.185377	-15.320	32.256	0.006839307
120	-0.567659	1.39717	-15.447	38.019	0.006776992
121	-0.570449	1.295386	-15.523	35.249	0.006740928
122	-0.570513	1.325665	-15.524	36.073	0.006740012
123	-0.574924	1.237438	-15.644	33.672	0.006683549
124	-0.578651	1.414941	-15.746	38.503	0.006635837
125	-0.580023	1.484806	-15.783	40.404	0.006618421
126	-0.580518	1.20659	-15.797	32.833	0.006613005
127	-0.592447	1.329151	-16.121	36.168	0.0064667
128	-0.594406	1.479311	-16.175	40.254	0.006442906
129	-0.600495	1.313938	-16.340	35.754	0.006371684
130	-0.601219	1.312521	-16.360	35.716	0.006363267
131	-0.603823	1.311636	-16.431	35.691	0.006333155
132	-0.605332	1.331993	-16.472	36.245	0.006315774
133	-0.606907	1.232924	-16.515	33.550	0.006298048
134	-0.612969	1.443968	-16.680	39.292	0.006229155

135	-0.613969	1.375596	-16.707	37.432	0.006218197
136	-0.618473	1.280276	-16.830	34.838	0.006168748
137	-0.619681	1.293423	-16.862	35.196	0.006155513
138	-0.620037	1.297184	-16.872	35.298	0.006151623
139	-0.620684	1.306085	-16.890	35.540	0.00614456
140	-0.624326	1.54198	-16.989	41.959	0.00610461
141	-0.626247	1.221226	-17.041	33.231	0.006084875
142	-0.633771	1.429677	-17.246	38.904	0.006005071
143	-0.633818	1.427396	-17.247	38.841	0.006004588
144	-0.63386	1.430187	-17.248	38.917	0.006004144
145	-0.634211	1.408049	-17.258	38.315	0.006000551
146	-0.637265	1.19655	-17.341	32.560	0.005969512
147	-0.639602	1.132401	-17.404	30.814	0.005945723
148	-0.640958	1.140607	-17.441	31.038	0.00593189
149	-0.644322	1.226256	-17.533	33.368	0.005897672
150	-0.645176	1.241167	-17.556	33.774	0.005889062
151	-0.655169	1.53482	-17.828	41.765	0.005789759
152	-0.655954	1.580667	-17.849	43.012	0.005782037
153	-0.66212	1.517865	-18.017	41.303	0.005723065
154	-0.672172	1.381845	-18.291	37.602	0.005629429
155	-0.674001	1.474224	-18.341	40.116	0.005612428
156	-0.685206	1.594704	-18.645	43.394	0.00551138
157	-0.692438	1.511298	-18.842	41.125	0.005448345
158	-0.695944	1.632115	-18.938	44.412	0.00541791
159	-0.703519	1.576405	-19.144	42.896	0.00535395
160	-0.704279	1.382409	-19.164	37.617	0.005348037
161	-0.719827	1.550861	-19.588	42.201	0.005220814
162	-0.728575	1.551609	-19.826	42.221	0.00515193
163	-0.729015	1.540938	-19.838	41.931	0.005148534
164	-0.73145	1.380148	-19.904	37.556	0.005130039
165	-0.731539	1.378808	-19.906	37.519	0.005129355
166	-0.731702	1.374394	-19.911	37.399	0.005128108
167	-0.732246	1.383313	-19.925	37.642	0.0051239
168	-0.739402	1.552967	-20.120	42.258	0.005069032
169	-0.739418	1.545831	-20.121	42.064	0.005068926
170	-0.740128	1.58394	-20.140	43.101	0.005063498
171	-0.746654	1.375355	-20.318	37.425	0.005015287
172	-0.746654	1.375594	-20.318	37.432	0.005015287
173	-0.746666	1.375425	-20.318	37.427	0.005015199
174	-0.746673	1.375625	-20.318	37.433	0.005015146
175	-0.750381	1.579042	-20.419	42.968	0.004987469
176	-0.750553	1.577546	-20.424	42.927	0.004986215
177	-0.750813	1.572111	-20.431	42.779	0.004984327
178	-0.751364	1.566538	-20.446	42.628	0.004980319
179	-0.759318	1.558818	-20.662	42.418	0.004922981
180	-0.759858	1.482092	-20.677	40.330	0.004919291
181	-0.765246	1.474475	-20.823	40.123	0.004881219

182	-0.779454	1.640482	-21.210	44.640	0.004783084
183	-0.784307	1.646418	-21.342	44.801	0.004750518
184	-0.821329	1.711625	-22.350	46.576	0.00451526
185	-0.830975	1.699965	-22.612	46.258	0.004457613
186	-0.838675	1.620781	-22.822	44.104	0.004412721
187	-0.838689	1.620644	-22.822	44.100	0.00441264
188	-0.838723	1.620251	-22.823	44.089	0.004412443
189	-0.838786	1.620118	-22.825	44.086	0.004412079
190	-0.847594	1.683565	-23.064	45.812	0.004361502
191	-0.851615	1.715392	-23.174	46.678	0.004338772
192	-0.856991	1.667897	-23.320	45.386	0.004308893
193	-0.864997	1.701268	-23.538	46.294	0.00426493
194	-0.865052	1.615103	-23.539	43.949	0.004264786
195	-0.865513	1.615635	-23.552	43.964	0.004262283
196	-0.867004	1.657352	-23.592	45.099	0.004254136
197	-0.873281	1.626578	-23.763	44.261	0.004220522
198	-0.876826	1.621361	-23.860	44.120	0.004201739
199	-0.878029	1.624499	-23.892	44.205	0.004195392
200	-0.878249	1.622428	-23.898	44.149	0.004194238
201	-0.878973	1.623387	-23.918	44.175	0.00419043
202	-0.885387	1.591228	-24.093	43.300	0.004157057
203	-0.886442	1.591972	-24.121	43.320	0.004151605
204	-0.892079	1.631555	-24.275	44.397	0.004122644
205	-0.89622	1.625494	-24.387	44.232	0.004101671
206	-0.897829	1.591794	-24.431	43.315	0.004093631
207	-0.897833	1.591229	-24.431	43.300	0.004093612
208	-0.897839	1.59149	-24.431	43.307	0.004093581
209	-0.898063	1.588466	-24.438	43.224	0.004092462
210	-0.908898	1.569871	-24.732	42.718	0.004038768
211	-0.91499	1.579018	-24.898	42.967	0.00400913
212	-0.919844	1.555994	-25.030	42.341	0.003985859
213	-0.943054	1.524238	-25.662	41.477	0.00387792
214	-0.951226	1.524269	-25.884	41.477	0.003841208
215	-0.952975	1.542697	-25.932	41.979	0.003833407
216	-0.9644	1.52224	-26.243	41.422	0.003783398
217	-0.964558	1.494936	-26.247	40.679	0.003782758
218	-0.964562	1.494959	-26.247	40.680	0.003782741
219	-0.964569	1.494861	-26.247	40.677	0.003782711
220	-0.964579	1.495955	-26.248	40.707	0.003782666
221	-0.969316	1.536718	-26.376	41.816	0.003762223
222	-0.970196	1.524123	-26.400	41.474	0.00375848
223	-0.983502	1.520124	-26.762	41.365	0.00370245
224	-0.98389	1.518666	-26.773	41.325	0.003700842
225	-0.991859	1.481397	-26.990	40.311	0.003668119
226	-0.992341	1.479657	-27.003	40.264	0.003666156
227	-0.992974	1.479005	-27.020	40.246	0.00366358
228	-0.996041	1.470377	-27.104	40.011	0.003651152

229	-1.030604	1.441497	-28.044	39.225	0.003516347
230	-1.030673	1.441895	-28.046	39.236	0.003516086
231	-1.030813	1.440299	-28.050	39.193	0.003515562
232	-1.031079	1.43902	-28.057	39.158	0.003514563
233	-1.073001	1.718018	-29.198	46.750	0.003362933
234	-1.076162	1.693992	-29.284	46.096	0.003352065
235	-1.120405	1.774149	-30.488	48.277	0.003206108
236	-1.122179	1.757263	-30.536	47.818	0.003200533
237	-10.26256	15.91486	-279.259	433.066	0.000265811
238	-10.26256	15.914863	-279.259	433.066	0.000265811
239	-10.263024	15.90346	-279.271	432.755	0.000265799
240	-10.263024	15.90346	-279.271	432.755	0.000265799
241	-10.26396	15.90594	-279.297	432.823	0.000265771
242	-10.26396	15.90594	-279.297	432.823	0.000265771
243	-10.263983	15.902618	-279.297	432.732	0.00026577
244	-10.263983	15.902616	-279.297	432.732	0.00026577
245	-10.265464	15.909331	-279.338	432.915	0.000265726
246	-10.265464	15.909339	-279.338	432.915	0.000265726
247	-10.26594	15.898364	-279.351	432.617	0.000265713
248	-10.26594	15.898382	-279.351	432.617	0.000265713
249	-10.270516	15.91461	-279.475	433.059	0.000265576
250	-10.270543	15.914614	-279.476	433.059	0.000265575
251	-10.270963	15.903204	-279.487	432.748	0.000265564
252	-10.27099	15.90321	-279.488	432.749	0.000265563
253	-10.272051	15.90386	-279.517	432.766	0.000265531
254	-10.272058	15.901796	-279.517	432.710	0.000265531
255	-10.272077	15.903857	-279.518	432.766	0.000265531
256	-10.272083	15.901789	-279.518	432.710	0.000265531
257	-10.2746	15.90708	-279.586	432.854	0.000265456
258	-10.274601	15.907185	-279.586	432.857	0.000265456
259	-10.274607	15.907085	-279.586	432.854	0.000265455
260	-10.274607	15.907189	-279.586	432.857	0.000265455
261	-10.275545	15.907668	-279.612	432.870	0.000265428
262	-10.275545	15.90775	-279.612	432.872	0.000265428
263	-10.275547	15.907707	-279.612	432.871	0.000265428
264	-10.275548	15.907782	-279.612	432.873	0.000265428
265	-10.276935	15.91325	-279.650	433.022	0.000265386
266	-10.276935	15.91325	-279.650	433.022	0.000265386
267	-10.27694	15.913208	-279.650	433.021	0.000265386
268	-10.27694	15.913208	-279.650	433.021	0.000265386
269	-10.277124	15.905588	-279.655	432.813	0.000265381
270	-10.277124	15.905588	-279.655	432.813	0.000265381
271	-10.277131	15.905631	-279.655	432.814	0.000265381
272	-10.277131	15.905631	-279.655	432.814	0.000265381
273	-10.277944	15.899044	-279.677	432.635	0.000265358
274	-10.277944	15.899044	-279.677	432.635	0.000265358
275	-10.27795	15.899043	-279.677	432.635	0.000265357



276	-10.27795	15.899043	-279.677	432.635	0.000265357
277	-10.278195	15.912461	-279.684	433.000	0.000265349
278	-10.278195	15.912462	-279.684	433.000	0.000265349
279	-10.278202	15.912471	-279.684	433.001	0.000265349
280	-10.278202	15.912472	-279.684	433.001	0.000265349
281	-10.278719	15.913274	-279.698	433.022	0.000265333
282	-10.278719	15.913275	-279.698	433.022	0.000265333
283	-10.278726	15.913261	-279.699	433.022	0.000265333
284	-10.278726	15.913261	-279.699	433.022	0.000265333
285	-10.279064	15.899375	-279.708	432.644	0.000265325
286	-10.279064	15.899375	-279.708	432.644	0.000265325
287	-10.27907	15.899364	-279.708	432.644	0.000265324
288	-10.27907	15.899364	-279.708	432.644	0.000265324
289	-10.279494	15.898649	-279.719	432.624	0.000265312
290	-10.279494	15.898649	-279.719	432.624	0.000265312
291	-10.279502	15.898663	-279.720	432.625	0.000265312
292	-10.279502	15.898663	-279.720	432.625	0.000265312
293	-10.280857	15.911266	-279.757	432.968	0.00026527
294	-10.280887	15.911266	-279.757	432.968	0.000265269
295	-10.281311	15.899903	-279.769	432.659	0.000265258
296	-10.281342	15.899902	-279.770	432.659	0.000265257
297	-10.283702	15.910861	-279.834	432.957	0.000265186
298	-10.283702	15.910862	-279.834	432.957	0.000265186
299	-10.283709	15.910865	-279.834	432.957	0.000265186
300	-10.283709	15.910865	-279.834	432.957	0.000265186
301	-10.284108	15.909924	-279.845	432.931	0.000265174
302	-10.284109	15.910149	-279.845	432.937	0.000265174
303	-10.284109	15.910226	-279.845	432.940	0.000265174
304	-10.28411	15.910334	-279.845	432.942	0.000265174
305	-10.284839	15.90841	-279.865	432.890	0.000265153
306	-10.284839	15.908415	-279.865	432.890	0.000265153
307	-10.284845	15.908397	-279.865	432.890	0.000265153
308	-10.284845	15.908402	-279.865	432.890	0.000265153
309	-10.285164	15.90776	-279.874	432.872	0.000265143
310	-10.285165	15.907683	-279.874	432.870	0.000265143
311	-10.285202	15.907769	-279.875	432.873	0.000265142
312	-10.285203	15.907688	-279.875	432.870	0.000265142
313	-10.285209	15.904722	-279.875	432.790	0.000265142
314	-10.285209	15.904723	-279.875	432.790	0.000265142
315	-10.285213	15.904704	-279.875	432.789	0.000265142
316	-10.285213	15.904704	-279.875	432.789	0.000265142
317	-10.285306	15.903434	-279.878	432.755	0.00026514
318	-10.285306	15.903434	-279.878	432.755	0.00026514
319	-10.285312	15.903438	-279.878	432.755	0.00026514
320	-10.285312	15.903438	-279.878	432.755	0.00026514
321	-10.285736	15.903393	-279.889	432.754	0.000265127
322	-10.285736	15.903454	-279.889	432.755	0.000265127

323	-10.285747	15.903407	-279.890	432.754	0.000265127
324	-10.285748	15.903468	-279.890	432.756	0.000265127
325	-10.286485	15.904619	-279.910	432.787	0.000265105
326	-10.286485	15.904629	-279.910	432.787	0.000265105
327	-10.286493	15.904626	-279.910	432.787	0.000265105
328	-10.286493	15.904636	-279.910	432.787	0.000265105
329	-10.300163	15.908548	-280.282	432.894	0.000264701
330	-10.300164	15.908644	-280.282	432.896	0.000264701
331	-10.3002	15.909129	-280.283	432.910	0.0002647
332	-10.300201	15.909118	-280.283	432.909	0.0002647
333	-10.319195	15.908304	-280.800	432.887	0.000264143
334	-10.319214	15.908452	-280.800	432.891	0.000264142
335	-10.319235	15.908322	-280.801	432.888	0.000264141
336	-10.319254	15.908466	-280.801	432.892	0.000264141
337	-14.387712	21.985679	-391.510	598.261	0.000179783
338	-14.387713	21.985407	-391.510	598.254	0.000179782
339	-14.455646	21.97864	-393.358	598.070	0.000178807
340	-14.455708	21.978642	-393.360	598.070	0.000178806

---

#### 4.4 Calculated energies for fullerophyrin metal complexes

**Supplementary Table 11. Comparison of orbital energies for FP, Pb@(FP), Pb@(FP-Pb) and (FP-Pb).** Calculated at density functional B3LYP-D3/6-31G(d)/LANL2DZ>Kr level of theory; HLG = HOMO-LUMO gap.

	FP	Pb@(FP)	Pb@(FP-Pb)	(FP-Pb)
<i>E</i> (hartree)	-4033.305437	-4036.810256	-4038.884915	-4035.662244
LUMO+2 (eV)	-3.29	-2.65	-3.19	-3.33
LUMO+1 (eV)	-3.49	-3.38	-3.71	-3.33
<b>LUMO (eV)</b>	<b>-3.71</b>	<b>-3.80</b>	<b>-3.71</b>	<b>-3.65</b>
<b>HOMO (eV)</b>	<b>-4.72</b>	<b>-4.60</b>	<b>-4.45</b>	<b>-4.63</b>
HOMO-1 (eV)	-5.34	-4.72	-4.47	-5.25
HOMO-2 (eV)	-5.71	-5.34	-5.34	-5.60
HOMO-3 (eV)	-5.75	-5.63	-5.69	-5.69
HOMO-4 (eV)	-5.81	-5.86	-5.71	-5.70
HOMO-5 (eV)	-6.05	-5.97	-5.92	-5.97
HOMO-6 (eV)	-6.30	-6.21	-6.09	-6.22
HOMO-7 (eV)	-6.32	-6.23	-6.11	-6.23
HOMO-8 (eV)	-6.42	-6.29	-6.14	-6.34
HOMO-9 (eV)	-6.58	-6.31	-6.27	-6.51
HLG (eV)	1.01	0.80	0.74	0.98

**Supplementary Table 12. Comparison of orbital energies for FP, Pb@(FP), Pb@(FP-Pb) and (FP-Pb).** Calculated at density functional B3LYP/6-31G(d)/LANL2DZ>Kr level of theory; HLG = HOMO-LUMO gap.

	FP	Pb@(FP)	Pb@(FP-Pb)	(FP-Pb)
<i>E</i> (hartree)	-4033.094332	-4036.544549	-4038.881993	-4035.449076
LUMO+2 (eV)	-3.25	-2.71	-3.15	-3.32
LUMO+1 (eV)	-3.45	-3.48	-3.68	-3.32
<b>LUMO (eV)</b>	<b>-3.65</b>	<b>-3.83</b>	<b>-3.69</b>	<b>-3.65</b>
<b>HOMO (eV)</b>	<b>-4.71</b>	<b>-4.53</b>	<b>-4.43</b>	<b>-4.61</b>
HOMO-1 (eV)	-5.34	-4.76	-4.47	-5.25
HOMO-2 (eV)	-5.73	-5.38	-5.31	-5.60
HOMO-3 (eV)	-5.74	-5.70	-5.68	-5.70
HOMO-4 (eV)	-5.83	-5.91	-5.71	-5.70
HOMO-5 (eV)	-6.06	-6.04	-5.90	-5.97
HOMO-6 (eV)	-6.31	-6.27	-6.08	-6.22
HOMO-7 (eV)	-6.33	-6.29	-6.11	-6.22
HOMO-8 (eV)	-6.41	-6.29	-6.13	-6.34
HOMO-9 (eV)	-6.60	-6.37	-6.26	-6.54
HLG (eV)	1.06	0.70	0.74	0.96

**Supplementary Table 13. Comparison of orbital energies for FP, Pb@(FP), Pb@(FP-Pb) and (FP-Pb).** Calculated at density functional B97-D3(BJ)/6-31G(d) level of theory; HLG = HOMO-LUMO gap.

	FP	Pb@(FP)	Pb@(FP-Pb)	(FP-Pb)
<i>E</i> (hartree)	-4031.826859	--	-4037.617615	-4034.179041
LUMO+2 (eV)	-3.35	--	-3.25	-3.40
LUMO+1 (eV)	-3.56	--	-3.70	-3.40
<b>LUMO (eV)</b>	-3.79	--	-3.80	-3.73
<b>HOMO (eV)</b>	-4.73	--	-4.49	-4.65
HOMO-1 (eV)	-5.37	--	-4.54	-5.29
HOMO-2 (eV)	-5.74	--	-5.36	-5.64
HOMO-3 (eV)	-5.78	--	-5.70	-5.73
HOMO-4 (eV)	-5.84	--	-5.74	-5.73
HOMO-5 (eV)	-6.08	--	-5.94	-6.01
HOMO-6 (eV)	-6.31	--	-6.09	-6.25
HOMO-7 (eV)	-6.34	--	-6.14	-6.25
HOMO-8 (eV)	-6.44	--	-6.16	-6.37
HOMO-9 (eV)	-6.62	--	-6.30	-6.56
HLG (eV)	0.94	--	0.69	0.92

**Supplementary Table 14. Comparison of orbital energies for FP, Pb@(FP), Pb@(FP-Pb) and (FP-Pb).** Calculated at density functional PBE0/6-31G(d) level of theory; HLG = HOMO-LUMO gap.

	FP	Pb@(FP)	Pb@(FP-Pb)	(FP-Pb)
<i>E</i> (hartree)	--	-4032.206949	-4034.554926	-4031.106969
LUMO+2 (eV)	--	-2.80	-3.08	-3.43
LUMO+1 (eV)	--	-3.59	-3.81	-3.43
<b>LUMO (eV)</b>	--	<b>-3.96</b>	<b>-3.83</b>	<b>-3.77</b>
<b>HOMO (eV)</b>	--	<b>-4.82</b>	<b>-4.72</b>	<b>-4.90</b>
HOMO-1 (eV)	--	-5.07	-4.74	-5.58
HOMO-2 (eV)	--	-5.72	-5.64	-5.93
HOMO-3 (eV)	--	-6.05	-6.02	-6.04
HOMO-4 (eV)	--	-6.27	-6.05	-6.04
HOMO-5 (eV)	--	-6.4	-6.25	-6.32
HOMO-6 (eV)	--	-6.64	-6.43	-6.60
HOMO-7 (eV)	--	-6.65	-6.47	-6.60
HOMO-8 (eV)	--	-6.67	-6.5	-6.71
HOMO-9 (eV)	--	-6.75	-6.64	-6.92
HLG (eV)	--	0.86	0.89	1.13

**Supplementary Table 15. Comparison of orbital energies and metal atom charges for FP, Zn@(FP), Zn@(FP-Zn) and (FP-Zn).** Calculated at density functional B3LYP-D3/6-311G(2d,p)// $\omega$ B97X-D/6-31G(d). level of theory; HLG = HOMO-LUMO gap.

		<b>FP</b>	<b>Zn@(FP)</b>	<b>Zn@(FP-Zn)</b>	<b>(FP-Zn)</b>
<i>E</i> (hartree)		-4034.189835	-5813.67335	-7591.997162	-5812.513487
Energy (eV)	LUMO+2	-3.49	-3.49	-3.56	-3.55
	LUMO+1	-3.69	-3.69	-3.56	-3.55
	<b>LUMO</b>	<b>-3.89</b>	<b>-3.89</b>	<b>-3.91</b>	<b>-3.89</b>
	<b>HOMO</b>	<b>-4.93</b>	<b>-4.93</b>	<b>-4.91</b>	<b>-4.90</b>
	HOMO-1	-5.55	-5.55	-5.54	-5.52
	HOMO-2	-5.95	-5.95	-5.98	-6.00
	HOMO-3	-5.98	-5.98	-6.01	-6.00
	HOMO-4	-6.05	-6.05	-6.01	-6.03
	HOMO-5	-6.27	-6.26	-6.26	-6.24
	HOMO-6	-6.52	-6.52	-6.53	-6.52
HOMO-7	-6.55	-6.53	-6.53	-6.52	
HOMO-8	-6.62	-6.54	-6.62	-6.60	
HOMO-9	-6.83	-6.61	-6.82	-6.80	
HLG		1.04	1.04	1.00	1.01
Zn(1)	<b>Natural charge</b>	--	--	<b>1.551</b>	<b>1.593</b>
	Mulliken charge	--	--	0.740	0.670
	Electrost. charge	--	--	1.018	1.295
Zn(2)	<b>Natural charge</b>	--	<b>-0.010</b>	<b>0.053</b>	--
	Mulliken charge	--	-0.018	0.061	--
	Electrost. charge	--	0.369	0.363	--

**Supplementary Table 16. Comparison of orbital energies and metal atom charges for FP, Zn@(FP), Zn@(FP-Zn) and (FP-Zn).** Calculated at density functional B3LYP-D3/6-311G(d,p)// $\omega$ B97X-D/6-31G(d). level of theory; HLG = HOMO-LUMO gap.

		<b>FP</b>	<b>Zn@(FP)</b>	<b>Zn@(FP-Zn)</b>	<b>(FP-Zn)</b>
<i>E</i> (hartree)		-4034.056949	-5813.540205	-7591.865589	-5812.381392
Energy (eV)	LUMO+2	-3.66	-3.66	-3.72	-3.71
	LUMO+1	-3.86	-3.86	-3.72	-3.72
	<b>LUMO</b>	<b>-4.06</b>	<b>-4.06</b>	<b>-4.08</b>	<b>-4.06</b>
	<b>HOMO</b>	<b>-5.10</b>	<b>-5.10</b>	<b>-5.08</b>	<b>-5.07</b>
	HOMO-1	-5.73	-5.72	-5.71	-5.70
	HOMO-2	-6.12	-6.12	-6.15	-6.17
	HOMO-3	-6.15	-6.15	-6.19	-6.17
	HOMO-4	-6.22	-6.22	-6.19	-6.20
	HOMO-5	-6.44	-6.43	-6.44	-6.42
	HOMO-6	-6.69	-6.67	-6.70	-6.69
HOMO-7	-6.72	-6.69	-6.70	-6.69	
HOMO-8	-6.79	-6.72	-6.79	-6.77	
HOMO-9	-7.00	-6.79	-6.99	-6.97	
HLG		1.04	1.04	1.00	1.01
Zn(1)	<b>Natural charge</b>	--	--	<b>1.550</b>	<b>1.594</b>
	Mulliken charge	--	--	0.974	0.903
	Electrost. charge	--	--	1.047	1.326
Zn(2)	<b>Natural charge</b>	--	<b>-0.011</b>	<b>0.053</b>	<b>1.594</b>
	Mulliken charge	--	0.002	0.088	0.903
	Electrost. charge	--	0.395	0.389	1.326

**Supplementary Table 17. Comparison of orbital energies and metal atom charges for FP, Zn@(FP), Zn@(FP-Zn) and (FP-Zn).** Calculated at density functional  $\omega$ B97X-D/6-311G(d,p)//6-31G(d). level of theory; HLG = HOMO-LUMO gap.

		<b>FP</b>	<b>Zn@(FP)</b>	<b>Zn@(FP-Zn)</b>	<b>(FP-Zn)</b>
<i>E</i> (hartree)		-4032.513742	-5811.985069	-7590.31525	-5810.843729
Energy (eV)	LUMO+2	-2.51	-2.51	-2.61	-2.60
	LUMO+1	-2.82	-2.82	-2.61	-2.60
	<b>LUMO</b>	<b>-2.84</b>	<b>-2.84</b>	<b>-2.86</b>	<b>-2.85</b>
	<b>HOMO</b>	<b>-6.31</b>	<b>-6.31</b>	<b>-6.29</b>	<b>-6.28</b>
	HOMO-1	-7.35	-7.35	-7.34	-7.33
	HOMO-2	-7.67	-7.68	-7.69	-7.74
	HOMO-3	-7.76	-7.76	-7.83	-7.81
	HOMO-4	-7.87	-7.87	-7.83	-7.81
	HOMO-5	-8.18	-8.17	-8.17	-8.15
	HOMO-6	-8.57	-8.57	-8.58	-8.57
HOMO-7	-8.60	-8.60	-8.58	-8.57	
HOMO-8	-8.71	-8.63	-8.71	-8.69	
HOMO-9	-8.89	-8.70	-8.84	-8.88	
HLG		<b>3.47</b>	<b>3.47</b>	<b>3.43</b>	<b>3.43</b>
Zn(1)	<b>Natural charge</b>	--	--	<b>1.583</b>	<b>1.623</b>
	Mulliken charge	--	--	0.974	0.928
	Electrost. charge	--	--	1.067	1.341
Zn(2)	<b>Natural charge</b>	--	<b>-0.011</b>	<b>0.05</b>	--
	Mulliken charge	--	-0.016	0.077	--
	Electrost. charge	--	0.390	0.380	--

**Supplementary Table 18. Comparison of orbital energies and metal atom charges for FP, Ge@(FP), Ge@(FP-Ge) and (FP-Ge).** Calculated at density functional B3LYP-D3/6-311G(2d,p)// $\omega$ B97X-D/6-31G(d). level of theory; HLG = HOMO-LUMO gap.

		<b>FP</b>	<b>Ge@(FP)</b>	<b>Ge@(FP-Zn)</b>	<b>(FP-Ge)</b>
<i>E</i> (hartree)		-4034.189835	-6111.183316	-8187.04	-6110.026372
<b>Energy (eV)</b>	LUMO+2	-3.49	-2.84	-3.49	-3.58
	LUMO+1	-3.69	-3.54	-3.74	-3.58
	<b>LUMO</b>	<b>-3.89</b>	<b>-3.98</b>	<b>-3.96</b>	<b>-3.89</b>
	<b>HOMO</b>	<b>-4.93</b>	<b>-4.87</b>	<b>-5.01</b>	<b>-4.90</b>
	HOMO-1	-5.55	-4.94	-5.17	-5.53
	HOMO-2	-5.95	-5.53	-5.61	-5.91
	HOMO-3	-5.98	-5.88	-5.95	-6.00
	HOMO-4	-6.05	-6.10	-6.04	-6.00
	HOMO-5	-6.27	-6.18	-6.10	-6.24
	HOMO-6	-6.52	-6.42	-6.29	-6.51
HOMO-7	-6.55	-6.45	-6.55	-6.51	
HOMO-8	-6.62	-6.47	-6.57	-6.60	
HOMO-9	-6.83	-6.51	-6.63	-6.82	
HLG		1.04	0.89	1.05	1.01
<b>Ge(1)</b>	<b>Natural charge</b>	--	--	<b>0.687</b>	<b>1.175</b>
	Mulliken charge	--	--	0.465	0.785
	Electrost. charge	--	--	-0.046	-0.012
<b>Ge(2)</b>	<b>Natural charge</b>	--	<b>1.225</b>	<b>0.757</b>	--
	Mulliken charge	--	0.841	0.621	--
	Electrost. charge	--	0.451	0.124	--



**Supplementary Table 19. Comparison of orbital energies and metal atom charges for FP, Ge@(FP), Ge@(FP-Ge) and (FP-Ge).** Calculated at density functional  $\omega$ B97X-D/6-31G(d). level of theory; HLG = HOMO-LUMO gap.

		<b>FP</b>	<b>Ge@(FP)</b>	<b>Ge@(FP-Zn)</b>	<b>(FP-Ge)</b>
<i>E</i> (hartree)		-4031.804	-6108.589678	-8184.220919	-6107.429824
<b>Energy (eV)</b>	LUMO+2	-2.15	-1.27	-2.22	-2.29
	LUMO+1	-2.47	-2.09	-2.43	-2.29
	<b>LUMO</b>	<b>-2.49</b>	<b>-2.66</b>	<b>-2.59</b>	<b>-2.49</b>
	<b>HOMO</b>	<b>-5.99</b>	<b>-6.13</b>	<b>-6.16</b>	<b>-5.95</b>
	HOMO-1	-7.03	-6.30	-6.54	-7.01
	HOMO-2	-7.33	-7.02	-7.09	-7.32
	HOMO-3	-7.43	-7.34	-7.36	-7.49
	HOMO-4	-7.55	-7.61	-7.54	-7.49
	HOMO-5	-7.86	-7.77	-7.62	-7.83
	HOMO-6	-8.25	-8.12	-7.89	-8.24
	HOMO-7	-8.28	-8.16	-8.30	-8.24
	HOMO-8	-8.40	-8.19	-8.30	-8.38
HOMO-9	-8.56	-8.29	-8.42	-8.51	
HLG		<b>3.50</b>	<b>3.47</b>	<b>3.57</b>	<b>3.46</b>
<b>Ge(1)</b>	<b>Natural charge</b>	--	--	<b>0.745</b>	<b>1.280</b>
	Mulliken charge	--	--	0.363	0.792
	Electrost. charge	--	--	-0.067	0.072
<b>Ge(2)</b>	<b>Natural charge</b>	--	<b>1.301</b>	<b>0.777</b>	--
	Mulliken charge	--	0.796	0.386	--
	Electrost. charge	--	0.431	0.035	--

## 4.5 XYZ Coordinates from thermochemistry

### Precursor 0

C	-2.398961	0.245371	-2.426389	C	-3.416381	0.149153	-3.512171
C	2.398885	0.244799	2.426312	C	-5.449365	0.942375	-4.582711
C	-2.398961	0.245372	2.426389	H	-2.439132	-1.518950	-4.440332
C	-2.811665	-0.108628	1.141250	H	-4.593621	1.797305	-2.801700
C	-4.070101	-0.689961	0.706360	H	-4.593621	1.797305	2.801700
C	-4.070101	-0.689962	-0.706361	C	-4.493943	1.032170	3.567120
C	-2.811665	-0.108628	-1.141250	C	-4.216029	-0.964370	5.519088
N	-2.098715	0.134210	0.000000	C	-5.449365	0.942376	4.582711
C	2.811492	-0.109281	1.141266	C	-3.416381	0.149153	3.512171
C	4.070308	-0.689972	0.706351	C	-3.285686	-0.839297	4.486225
C	4.070308	-0.689972	-0.706351	C	-5.313733	-0.066361	5.572696
C	2.811492	-0.109281	-1.141266	H	-2.439132	-1.518949	4.440332
N	2.098165	0.132518	0.000000	C	1.410494	1.716770	5.176375
C	1.094644	0.631458	-2.787713	H	2.492120	1.751639	5.186941
C	0.701785	1.180588	-4.095255	C	-1.410302	1.717544	5.176177
C	-0.701737	1.180887	-4.095212	H	-2.491912	1.753013	5.186586
C	-1.094778	0.631903	-2.787690	C	-0.699524	2.236281	6.247610
N	-0.000031	0.412067	-2.017034	H	-1.238426	2.658924	7.090398
C	1.094644	0.631458	2.787713	C	0.699843	2.235843	6.247733
C	0.701785	1.180588	4.095255	H	1.238866	2.658106	7.090633
C	-0.701737	1.180887	4.095212	C	-1.410303	1.717544	-5.176177
C	-1.094778	0.631903	2.787690	H	-2.491912	1.753013	-5.186586
N	-0.000031	0.412067	2.017034	C	1.410494	1.716771	-5.176375
C	2.398885	0.244799	-2.426312	H	2.492120	1.751639	-5.186941
H	1.138332	0.460766	0.000000	C	0.699843	2.235843	-6.247733
H	-1.139147	0.463209	0.000000	H	1.238866	2.658107	-7.090633
C	3.416353	0.148712	3.512092	C	-0.699524	2.236281	-6.247610
C	5.313654	-0.066241	5.572711	H	-1.238426	2.658924	-7.090398
C	4.493009	1.032775	3.567710	C	5.139282	-1.268172	1.412484
C	3.286562	-0.840525	4.485477	H	5.143621	-1.310832	2.492964
C	4.216980	-0.965421	5.518316	C	5.139282	-1.268172	-1.412484
C	5.448341	0.943330	4.583414	H	5.143622	-1.310831	-2.492964
H	4.591980	1.798519	2.802804	C	6.188133	-1.816857	-0.702273
H	2.440719	-1.521034	4.438995	H	7.015411	-2.270609	-1.239460
C	4.216980	-0.965421	-5.518316	C	6.188133	-1.816858	0.702273
C	4.493009	1.032775	-3.567710	H	7.015410	-2.270610	1.239460
C	5.313654	-0.066241	-5.572711	C	-5.138659	-1.269007	1.412489
C	3.286562	-0.840524	-4.485478	H	-5.142896	-1.311806	2.492962
C	3.416353	0.148712	-3.512092	C	-6.187090	-1.818438	0.702290
C	5.448341	0.943330	-4.583414	H	-7.014027	-2.272833	1.239460
H	2.440718	-1.521034	-4.438996	C	-5.138658	-1.269008	-1.412489
H	4.591980	1.798519	-2.802804	H	-5.142895	-1.311808	-2.492962
C	-4.216029	-0.964371	-5.519088	C	-6.187090	-1.818439	-0.702290
C	-4.493943	1.032170	-3.567120	H	-7.014027	-2.272833	-1.239460
C	-5.313733	-0.066362	-5.572696	C	-6.278228	-0.179082	-6.618611
C	-3.285686	-0.839298	-4.486225	C	-8.169915	-0.401535	-8.666806

C	-6.137349	-1.187636	-7.608059	H	8.904167	-0.487017	9.462111
C	-7.378197	0.716965	-6.668771	C	-7.491758	1.729040	5.649521
C	-8.312861	0.588083	-7.700846	H	-8.337601	2.410115	5.692740
C	-7.094174	-1.281136	-8.623194	C	-6.575962	1.837496	4.659200
H	-9.156953	1.271541	-7.741701	H	-6.675558	2.605276	3.896701
H	-6.989295	-2.051646	-9.382547	C	-4.097170	-1.976435	6.537148
H	-8.904693	-0.488610	-9.461530	H	-3.250601	-2.655906	6.489922
C	-6.278228	-0.179082	6.618611	C	-5.010016	-2.081579	7.529995
C	-8.169914	-0.401535	8.666806	H	-4.907567	-2.848728	8.292996
C	-7.378197	0.716965	6.668770	C	-6.575962	1.837496	-4.659201
C	-6.137348	-1.187636	7.608059	H	-6.675558	2.605276	-3.896702
C	-7.094174	-1.281136	8.623194	C	-7.491757	1.729040	-5.649522
C	-8.312861	0.588083	7.700846	H	-8.337601	2.410115	-5.692740
H	-6.989294	-2.051646	9.382547	C	-4.097170	-1.976435	-6.537148
H	-9.156953	1.271540	7.741700	H	-3.250601	-2.655907	-6.489922
H	-8.904693	-0.488610	9.461530	C	-5.010016	-2.081580	-7.529995
C	6.278061	-0.178618	-6.618744	H	-4.907567	-2.848729	-8.292995
C	8.169488	-0.400271	-8.667259	C	6.573844	1.839722	-4.660762
C	6.138169	-1.188054	-7.607471	H	6.672763	2.608103	-3.898784
C	7.376920	0.718701	-6.669784	C	7.489507	1.731639	-5.651247
C	8.311485	0.590195	-7.702002	H	8.334560	2.413654	-5.695155
C	7.094837	-1.281139	-8.622771	C	5.011987	-2.083317	-7.528503
H	9.154743	1.274642	-7.743532	H	4.910261	-2.851159	-8.290895
H	6.990692	-2.052297	-9.381562	C	4.099188	-1.978433	-6.535589
H	8.904167	-0.487017	-9.462111	H	3.253421	-2.658862	-6.487689
C	6.278061	-0.178618	6.618745	C	4.099188	-1.978433	6.535589
C	8.169488	-0.400271	8.667260	H	3.253422	-2.658863	6.487688
C	7.376920	0.718702	6.669785	C	5.011988	-2.083318	7.528502
C	6.138170	-1.188054	7.607471	H	4.910261	-2.851160	8.290894
C	7.094838	-1.281139	8.622771	C	7.489507	1.731640	5.651247
C	8.311485	0.590196	7.702003	H	8.334560	2.413655	5.695156
H	6.990692	-2.052297	9.381562	C	6.573844	1.839723	4.660763
H	9.154742	1.274643	7.743533	H	6.672762	2.608103	3.898784

### Intermediate 1a

C	-2.345938	0.234749	-2.622309	C	1.22474	0.370615	-2.79239
C	2.050241	-0.553119	2.498783	C	0.954257	1.131936	-4.017524
C	-2.641929	0.577129	2.25515	C	-0.444627	1.19467	-4.114207
C	-3.006044	0.436242	0.937791	C	-0.954991	0.459201	-2.949128
C	-4.358249	0.349628	0.355533	N	0.028286	0.072356	-2.154449
C	-4.177232	0.281595	-1.032702	C	0.845797	0.02468	2.850299
C	-2.787566	0.27563	-1.323819	C	0.490471	0.547973	4.18128
N	-2.128025	0.367239	-0.12447	C	-0.876584	0.860386	4.112704
C	2.484027	-0.896097	1.185277	C	-1.29091	0.528614	2.735555
C	3.647287	-1.633216	0.780596	N	-0.252324	0.113152	2.009369
C	3.777274	-1.477475	-0.625164	C	2.440596	-0.106751	-2.351939
C	2.684912	-0.666705	-1.067353	H	1.069871	0.12427	0.02357
N	1.932936	-0.40456	0.04104	H	-1.134132	0.22843	0.009363

C	3.05675	-0.804735	3.570934	C	4.820801	-2.129146	-1.320322
C	4.980376	-1.263868	5.562691	H	4.918588	-2.037282	-2.394598
C	4.219405	-0.03777	3.611941	C	5.705672	-2.903523	-0.610323
C	2.852814	-1.803679	4.520816	H	6.510247	-3.412246	-1.132825
C	3.798162	-2.049145	5.520425	C	5.575143	-3.064316	0.78804
C	5.187471	-0.246694	4.59456	H	6.280242	-3.695882	1.319993
H	4.374564	0.732526	2.861298	C	-5.653858	0.265877	0.854846
H	1.940766	-2.393173	4.484379	H	-5.875176	0.292578	1.913305
C	4.694496	-0.782341	-5.320855	C	-6.690502	0.09322	-0.067336
C	4.723616	0.720928	-2.951427	H	-7.701852	-0.033905	0.306945
C	5.827611	0.007552	-4.992854	C	-5.193311	0.21308	-1.986919
C	3.600575	-0.795632	-4.45337	C	-6.484416	0.061017	-1.444211
C	3.609819	-0.053147	-3.273124	H	-7.336289	-0.14091	-2.07997
C	5.835118	0.769577	-3.794978	C	-6.124465	-0.236233	-6.885336
H	2.726755	-1.393738	-4.696783	C	-7.898129	-0.324936	-9.054057
H	4.72742	1.289053	-2.025034	C	-5.681966	-0.714073	-8.14972
C	-3.867967	-0.580223	-5.967381	C	-7.462276	0.206034	-6.732623
C	-4.767793	0.166496	-3.387333	C	-8.333755	0.156979	-7.82906
C	-5.224102	-0.196414	-5.776377	C	-6.583359	-0.756645	-9.21402
C	-2.975489	-0.425687	-4.922195	H	-9.356844	0.503597	-7.708937
C	-3.37346	0.016025	-3.649707	H	-6.246898	-1.128688	-10.178284
C	-5.666444	0.211164	-4.493825	H	-8.583213	-0.361873	-9.895687
H	-1.932186	-0.666594	-5.09319	C	-6.850888	1.197977	6.091212
H	-4.120951	2.78678	2.7249	C	-8.890242	1.503572	7.980704
C	-4.41146	1.958576	3.366058	C	-7.521038	2.443286	6.216598
C	-5.134148	-0.200624	5.004391	C	-7.216194	0.107193	6.923183
C	-5.439262	2.132136	4.296258	C	-8.23841	0.281583	7.861339
C	-3.74316	0.740188	3.247067	C	-8.537389	2.574948	7.167903
C	-4.111448	-0.328786	4.061455	H	-8.520448	-0.551257	8.50015
C	-5.807712	1.042637	5.129147	H	-9.051471	3.527305	7.26776
H	-3.586241	-1.275205	3.96379	H	-9.68116	1.62267	8.715094
C	1.219671	0.833789	5.34069	C	6.958306	0.032846	-5.863422
H	2.281495	0.641279	5.409577	C	9.176124	0.077362	-7.566685
C	-1.529541	1.437428	5.207007	C	6.950044	-0.733349	-7.058763
H	-2.577271	1.701509	5.172666	C	8.091255	0.821892	-5.532452
C	-0.801824	1.697861	6.358989	C	9.189308	0.830357	-6.398101
H	-1.298098	2.14925	7.212859	C	8.069466	-0.696877	-7.895973
C	0.562484	1.402736	6.422118	H	10.058552	1.432761	-6.147546
H	1.122745	1.629894	7.324367	H	8.067359	-1.282784	-8.811395
C	-1.06434	1.956856	-5.107808	H	10.037589	0.093799	-8.227491
H	-2.144401	2.033344	-5.16323	C	5.959617	-1.495326	6.574923
C	1.753119	1.823136	-4.935269	C	7.878022	-1.94773	8.559385
H	2.83414	1.812286	-4.867983	C	7.141077	-0.708731	6.612335
C	1.131271	2.557772	-5.934432	C	5.751652	-2.511677	7.543839
H	1.739713	3.101356	-6.651268	C	6.723299	-2.721189	8.527628
C	-0.265669	2.628868	-6.020033	C	8.087135	-0.951568	7.612458
H	-0.727368	3.227277	-6.79958	H	6.567318	-3.498427	9.271202
C	4.563004	-2.448649	1.484158	H	8.992751	-0.351485	7.643692
H	4.467817	-2.609338	2.54986	H	8.622731	-2.123151	9.329889

C	-7.126875	3.530139	5.356367	C	6.99756	1.562247	-3.485614
H	-7.644751	4.480226	5.45794	H	6.994986	2.141676	-2.566397
C	-6.138832	3.383093	4.443617	C	8.068816	1.58691	-4.311652
H	-5.851541	4.211615	3.801906	H	8.940146	2.187761	-4.064831
C	-5.528288	-1.290605	5.859647	C	5.784958	-1.523365	-7.366475
H	-5.008038	-2.238896	5.756308	H	5.785937	-2.105524	-8.28422
C	-6.517348	-1.14354	6.771183	C	4.712992	-1.547505	-6.54129
H	-6.803636	-1.973967	7.411173	H	3.84035	-2.147067	-6.785548
C	-7.004901	0.73721	-4.401252	C	3.614113	-3.073515	6.51679
H	-7.3169	1.223339	-3.486344	H	2.706113	-3.669234	6.480346
C	-7.85314	0.734696	-5.459144	C	4.542097	-3.29187	7.477376
H	-8.844395	1.169514	-5.360263	H	4.388963	-4.067614	8.223043
C	-3.446141	-1.065021	-7.257929	C	7.323857	0.314849	5.61485
H	-2.408554	-1.36457	-7.377729	H	8.231942	0.910928	5.649468
C	-4.309992	-1.135613	-8.293617	C	6.395593	0.53501	4.655949
H	-3.982153	-1.500448	-9.263431	H	6.545324	1.309007	3.908183

### Intermediate 2a

C	-2.26316	-2.515844	-0.452647	C	4.232383	3.747785	-0.486905
C	2.22451	2.490626	0.314661	C	3.166255	4.446253	1.559227
C	-2.594893	2.360795	-0.258922	C	4.104402	5.467504	1.726363
C	-2.966489	1.029356	-0.235715	C	5.1865	4.759923	-0.363333
C	-4.30663	0.437936	-0.260424	H	4.274033	3.069996	-1.335279
C	-4.106921	-0.937203	-0.446844	H	2.374607	4.316254	2.292045
C	-2.727862	-1.212043	-0.426148	C	4.569957	-5.273933	1.633113
N	-2.078791	-0.025551	-0.288042	C	4.543387	-3.627981	-0.640902
C	2.722939	1.203887	0.589941	C	5.538855	-5.456735	0.611649
C	4.024231	0.842736	1.126933	C	3.61109	-4.270072	1.487469
C	4.134817	-0.566796	1.063309	C	3.592891	-3.44886	0.36154
C	2.895854	-1.072709	0.518838	C	5.521439	-4.621362	-0.536288
N	2.100037	0.017564	0.30437	H	2.860694	-4.125928	2.260085
C	1.260671	-2.838646	-0.109257	H	4.523836	-2.982277	-1.514888
C	0.874349	-4.241229	-0.39864	C	-3.792356	-5.985102	-0.610667
C	-0.51811	-4.19378	-0.451203	C	-4.639145	-3.293091	-0.760766
C	-0.902263	-2.832774	-0.314639	C	-5.136947	-5.676259	-0.946973
N	0.154983	-2.024764	-0.129972	C	-2.819405	-4.962529	-0.653896
C	0.930473	2.872592	-0.070508	C	-3.248382	-3.597348	-0.626328
C	0.539265	4.241376	-0.4642	C	-5.535826	-4.327881	-1.121665
C	-0.862	4.219587	-0.565744	H	-4.112227	2.967732	-2.394678
C	-1.256739	2.83335	-0.27832	C	-4.415612	3.524558	-1.512112
N	-0.171867	2.06558	-0.038043	C	-5.177302	4.935629	0.7892
C	2.537427	-2.402837	0.23265	C	-5.494092	4.407338	-1.589386
H	1.1485	-0.072106	-0.039053	C	-3.720825	3.337391	-0.317793
H	-1.076189	0.108915	-0.201461	C	-4.10323	4.041486	0.821303
C	3.227628	3.587222	0.464524	C	-5.885446	5.122755	-0.426925
C	5.128753	5.630655	0.756653	H	-3.554685	3.892364	1.747498

C	1.243514	5.409015	-0.789771	C	8.460999	-8.484497	0.987612
H	2.322674	5.451175	-0.771141	C	6.538625	-7.31525	1.886585
C	-1.566231	5.368342	-0.949164	C	7.49525	-6.661301	-0.28261
H	-2.642976	5.37587	-1.037607	C	8.453852	-7.669287	-0.138296
C	-0.858381	6.523055	-1.240382	C	7.514081	-8.311456	1.990797
H	-1.396581	7.417465	-1.539893	H	9.197275	-7.810849	-0.918416
C	0.537406	6.53899	-1.170798	H	7.526189	-8.952988	2.868029
H	1.081621	7.443989	-1.42443	H	9.212137	-9.262568	1.084578
C	-1.377499	-5.256216	-0.700061	C	6.100192	6.665588	0.908927
C	1.49066	-5.458433	-0.68707	C	8.007108	8.689609	1.210378
H	2.565848	-5.587195	-0.69324	C	7.123745	6.826345	-0.061714
C	0.666791	-6.532941	-1.034683	C	6.043202	7.532473	2.031688
H	1.131665	-7.472997	-1.31704	C	7.006737	8.53723	2.163639
C	-0.72825	-6.451863	-1.0523	C	8.066916	7.844597	0.108101
H	-1.288651	-7.315483	-1.389145	H	6.967088	9.20172	3.022775
C	5.067035	1.594831	1.70616	H	8.851676	7.970779	-0.633196
H	5.000013	2.666809	1.815445	H	8.74797	9.474687	1.328076
C	5.290414	-1.213091	1.544814	C	-7.279972	5.465491	-2.860045
H	5.389309	-2.288373	1.515403	H	-7.828135	5.609679	-3.787337
C	6.306187	-0.453841	2.082266	C	-6.23129	4.612366	-2.810092
H	7.198874	-0.944777	2.457712	H	-5.924891	4.060199	-3.694309
C	6.189813	0.944104	2.16949	C	-5.59442	5.675347	1.952835
H	6.991096	1.523464	2.618071	H	-5.045468	5.529122	2.879073
C	-5.618411	0.882081	-0.078254	C	-6.641305	6.531183	1.901283
H	-5.862761	1.922051	0.096441	H	-6.944315	7.082991	2.787197
C	-6.627528	-0.080094	-0.067777	C	-6.834673	-4.084255	-1.696007
H	-7.646295	0.240508	0.12842	H	-7.08429	-3.079792	-2.014249
C	-5.096311	-1.916694	-0.530493	C	-7.714452	-5.087741	-1.924943
C	-6.392616	-1.443954	-0.278859	H	-8.67417	-4.87745	-2.38954
H	-7.229105	-2.126587	-0.193928	C	-3.499365	-7.33985	-0.21098
C	-6.091701	-6.730553	-1.113649	H	-2.534538	-7.554545	0.230628
C	-7.964661	-8.796717	-1.438261	C	-4.423372	-8.324929	-0.294149
C	-5.741125	-8.070576	-0.804806	H	-4.183084	-9.328953	0.045565
C	-7.398061	-6.445854	-1.588211	C	6.517308	-4.82872	-1.55669
C	-8.314768	-7.490136	-1.753059	H	6.498943	-4.184711	-2.431718
C	-6.690278	-9.084614	-0.963458	C	7.454403	-5.797402	-1.434999
H	-9.309154	-7.266408	-2.130345	H	8.199924	-5.941522	-2.212601
H	-6.419653	-10.106591	-0.711287	C	5.541398	-7.106595	2.905741
H	-8.688657	-9.596107	-1.56356	H	5.557052	-7.751184	3.780617
C	-6.991306	6.024048	-0.480393	C	4.606135	-6.136482	2.786236
C	-9.161359	7.785753	-0.584288	H	3.85896	-5.989819	3.561355
C	-7.700844	6.2048	-1.696856	C	4.069845	6.3637	2.853879
C	-7.381835	6.737956	0.682816	H	3.281388	6.233215	3.590026
C	-8.469515	7.613976	0.609031	C	4.991443	7.34374	2.99843
C	-8.783096	7.089405	-1.726635	H	4.953713	8.012198	3.854533
H	-8.770829	8.162349	1.497685	C	7.154254	5.930165	-1.189728
H	-9.328757	7.229593	-2.656059	H	7.939986	6.06049	-1.929221
H	-10.004287	8.469033	-0.62436	C	6.234531	4.948366	-1.333641
C	6.526447	-6.479605	0.738929	H	6.270159	4.278397	-2.188334

### Intermediate 3d

C	-2.431228	-2.26788	-0.671405	C	-4.009554	4.158832	-0.95166
C	2.36174	2.291957	0.487926	C	-4.956796	5.136657	1.501444
C	-2.509983	2.537192	0.216393	C	-4.95836	5.183248	-0.955632
C	-2.946125	1.255901	-0.031386	C	-3.5311	3.622572	0.243521
C	-4.308086	0.773459	-0.310462	C	-4.008393	4.11054	1.458041
C	-4.164293	-0.57375	-0.66908	C	-5.439982	5.682991	0.283247
C	-2.813527	-0.954469	-0.523056	H	-3.629398	3.689547	2.385616
N	-2.118256	0.157528	-0.139435	C	1.716011	5.138	0.397327
C	2.774805	0.953855	0.80416	C	-1.123442	5.562218	0.283369
C	3.909463	0.511635	1.555703	H	-2.184746	5.772898	0.263575
C	3.877902	-0.9074	1.583391	C	-0.209749	6.618871	0.204334
C	2.708034	-1.316576	0.86753	H	-0.589899	7.629983	0.093325
N	2.075639	-0.164696	0.480246	C	1.168898	6.42748	0.244053
C	1.0122	-2.93357	0.032418	H	1.803604	7.292179	0.102815
C	0.555702	-4.261653	-0.427576	C	-1.704508	-5.042123	-1.110441
C	-0.810196	-4.086418	-0.644737	C	1.114209	-5.495439	-0.765818
C	-1.105698	-2.711701	-0.41825	H	2.169379	-5.711654	-0.650158
N	-0.032897	-2.020006	-0.044137	C	0.266836	-6.45295	-1.325581
C	1.043685	2.707849	0.425624	H	0.692294	-7.398435	-1.649236
C	0.777597	4.108524	0.389096	C	-1.105356	-6.247971	-1.507722
C	-0.609794	4.27182	0.353344	H	-1.67749	-7.021758	-2.004763
C	-1.133201	2.886169	0.354447	C	4.891565	1.2168	2.286966
N	-0.134798	1.992043	0.411915	H	4.892135	2.299917	2.311254
C	2.264039	-2.618754	0.522947	C	4.863345	-1.617474	2.307967
H	1.173606	-0.184465	0.012543	H	4.854042	-2.698691	2.355237
H	-1.125079	0.215585	0.07262	C	5.828264	-0.909751	2.982783
C	3.389271	3.330051	0.262928	H	6.586419	-1.445897	3.54573
C	5.507001	5.186253	0.042567	C	5.838245	0.505401	2.98106
C	4.661817	2.935188	-0.17896	H	6.597894	1.034324	3.548516
C	3.1198	4.723456	0.399658	C	-5.594294	1.297763	-0.243255
C	4.223029	5.624321	0.450647	H	-5.792387	2.323762	0.040394
C	5.702833	3.83179	-0.342536	C	-6.657472	0.426445	-0.507003
H	4.836743	1.890842	-0.411866	H	-7.671431	0.801581	-0.40555
C	4.000037	-5.710103	1.871962	C	-5.187966	-1.451239	-1.012779
C	4.362484	-3.791206	-0.142704	C	-6.479584	-0.908461	-0.870831
C	5.132066	-5.7798	1.017827	H	-7.359619	-1.52773	-0.992661
C	3.075757	-4.677689	1.694203	C	-6.403963	-6.072271	-2.289771
C	3.251712	-3.720933	0.695854	C	-8.33622	-7.93753	-3.106854
C	5.309351	-4.807226	-0.00097	C	-6.187114	-7.461155	-2.093653
H	2.20364	-4.617581	2.339541	C	-7.607839	-5.636115	-2.900136
H	4.49575	-3.036124	-0.91285	C	-8.555085	-6.58238	-3.310607
C	-4.153043	-5.56916	-1.403687	C	-7.163817	-8.374045	-2.498022
C	-4.791112	-2.81939	-1.356167	H	-9.468484	-6.241843	-3.791135
C	-5.417944	-5.120527	-1.874865	H	-6.997511	-9.435232	-2.33219
C	-3.117801	-4.632265	-1.212889	H	-9.082131	-8.660034	-3.423676
C	-3.452759	-3.243831	-1.088546	C	-6.406138	6.733883	0.303541
C	-5.699452	-3.736413	-1.945486	C	-8.297164	8.794154	0.34326
H	-3.632116	3.771455	-1.894391	C	-6.887681	7.278348	-0.916201

C	-6.884458	7.233875	1.543102	C	-5.460907	5.663123	2.74403
C	-7.829312	8.264747	1.54038	H	-5.085229	5.240354	3.671809
C	-7.832767	8.307764	-0.873525	C	-6.375859	6.659813	2.762803
H	-8.19721	8.650439	2.48754	H	-6.746384	7.048266	3.707774
H	-8.203681	8.726916	-1.805154	C	-6.885521	-3.329434	-2.653247
H	-9.030671	9.594535	0.358628	H	-7.023038	-2.280264	-2.883615
C	6.091256	-6.823672	1.183815	C	-7.786917	-4.229994	-3.113936
C	7.972847	-8.867064	1.511596	H	-8.655939	-3.89527	-3.674164
C	5.911716	-7.796608	2.201973	C	-4.011057	-6.977886	-1.120972
C	7.224871	-6.887757	0.331397	H	-3.136566	-7.313658	-0.578352
C	8.15364	-7.917002	0.512838	C	-4.975765	-7.871061	-1.43811
C	6.864183	-8.809953	2.348417	H	-4.854003	-8.920127	-1.181635
H	9.023375	-7.968152	-0.136894	C	6.468127	-4.89765	-0.851795
H	6.729987	-9.556576	3.126787	H	6.596448	-4.147481	-1.627347
H	8.703811	-9.659771	1.639536	C	7.378429	-5.885796	-0.692679
C	6.610502	6.092992	-0.003925	H	8.249713	-5.940675	-1.339947
C	8.766904	7.878862	-0.108699	C	4.750749	-7.703411	3.050285
C	7.874619	5.656257	-0.487564	H	4.618701	-8.453262	3.825848
C	6.450954	7.431319	0.435226	C	3.842591	-6.71231	2.895016
C	7.541719	8.308943	0.378428	H	2.971521	-6.654518	3.541933
C	8.933234	6.564328	-0.537987	C	4.122991	6.963828	0.972466
H	7.417446	9.332497	0.722054	H	3.206123	7.27065	1.458362
H	9.89745	6.233234	-0.914838	C	5.176438	7.817295	0.966357
H	9.603925	8.569221	-0.152255	H	5.073662	8.809301	1.398396
C	-6.382045	6.749211	-2.1576	C	8.023888	4.284685	-0.908421
H	-6.756189	7.170777	-3.086806	H	8.993657	3.961509	-1.277363
C	-5.465738	5.754119	-2.177332	C	6.992659	3.415618	-0.832541
H	-5.092121	5.365005	-3.120566	H	7.11646	2.378367	-1.131616

#### Intermediate 4c

C	-3.066597	0.022812	1.398204	C	-1.945731	0.09213	2.240016
C	3.066597	0.022812	-1.398204	N	-0.627304	0.065177	1.939671
C	-1.443295	0.015694	-3.237703	C	1.945731	0.09213	-2.240016
C	-2.320742	0.002111	-2.155812	C	2.157093	0.083847	-3.643964
C	-3.775633	0.024701	-2.141322	C	0.906543	0.000297	-4.259373
C	-4.141354	-0.047259	-0.78728	C	-0.044298	0.031429	-3.129263
C	-2.983169	-0.051374	0.009055	N	0.627304	0.065178	-1.939671
N	-1.918591	-0.030016	-0.839103	C	1.443295	0.015694	3.237703
C	2.98317	-0.051374	-0.009055	H	0.931675	-0.005121	0.59309
C	4.141354	-0.047259	0.78728	H	-0.931675	-0.005123	-0.59309
C	3.775633	0.024701	2.141322	C	4.417091	0.020422	-1.999006
C	2.320742	0.002111	2.155812	C	6.99972	0.022704	-3.156976
N	1.918591	-0.030015	0.839103	C	5.581073	-0.104082	-1.175258
C	0.044298	0.031429	3.129263	C	4.576175	0.14471	-3.415929
C	-0.906543	0.000296	4.259374	C	5.869378	0.357599	-3.94484
C	-2.157093	0.083847	3.643964	C	6.838584	-0.313774	-1.789937



C	2.787795	1.203848	6.578747	H	-7.461167	0.382073	-0.966985
C	2.467385	-1.198931	5.164812	C	-8.305225	0.021782	3.744326
C	3.211289	-0.022884	7.154851	C	-10.863908	0.02087	4.894999
C	2.214717	1.194885	5.304447	C	-8.494347	0.497133	5.067973
C	2.05284	0.004743	4.598246	C	-9.420698	-0.454102	3.007975
C	3.046298	-1.235957	6.435553	C	-10.687029	-0.456702	3.602388
H	1.884779	2.128076	4.855847	C	-9.778929	0.498394	5.620607
H	2.337689	-2.121747	4.605652	H	-11.535489	-0.836032	3.039068
C	-5.869378	0.357599	3.94484	H	-9.920802	0.877386	6.629322
C	-5.581072	-0.104082	1.175258	H	-11.853996	0.020509	5.340611
C	-6.99972	0.022704	3.156976	C	-3.801789	-0.037248	-8.454601
C	-4.576175	0.144711	3.415929	C	-4.960228	-0.064796	-10.999905
C	-4.417091	0.020422	1.999006	C	-4.2266	-1.264844	-9.027366
C	-6.838584	-0.313774	1.789937	C	-3.964719	1.176526	-9.172888
H	-2.337689	-2.121746	-4.605652	C	-4.545756	1.140127	-10.444183
C	-2.467385	-1.198931	-5.164812	C	-4.803549	-1.256154	-10.300941
C	-2.787795	1.203848	-6.578747	H	-4.671923	2.067312	-10.99699
C	-3.046298	-1.235957	-6.435553	H	-5.13043	-2.194002	-10.74219
C	-2.05284	0.004744	-4.598246	H	-5.409728	-0.075517	-11.988194
C	-2.214717	1.194886	-5.304447	C	3.801789	-0.037248	8.454601
C	-3.211289	-0.022884	-7.154851	C	4.960228	-0.064796	10.999906
H	-1.88478	2.128076	-4.855847	C	3.964719	1.176526	9.172888
C	3.391634	0.050614	-4.279388	C	4.2266	-1.264844	9.027366
C	0.87115	-0.15953	-5.643906	C	4.803549	-1.256154	10.300941
H	-0.052881	-0.238564	-6.202747	C	4.545756	1.140127	10.444183
C	2.093148	-0.270007	-6.313001	H	5.130431	-2.194002	10.74219
H	2.085115	-0.449927	-7.384023	H	4.671922	2.067312	10.99699
C	3.327033	-0.185149	-5.663791	H	5.409727	-0.075517	11.988195
H	4.225127	-0.35313	-6.245494	C	8.305225	0.021782	-3.744326
C	-3.391634	0.050614	4.279388	C	10.863908	0.02087	-4.894999
C	-0.87115	-0.15953	5.643906	C	9.420698	-0.454102	-3.007975
H	0.052881	-0.238564	6.202747	C	8.494347	0.497133	-5.067973
C	-2.093148	-0.270007	6.313001	C	9.778929	0.498394	-5.620607
H	-2.085115	-0.449927	7.384023	C	10.687029	-0.456702	-3.602388
C	-3.327033	-0.185149	5.663791	H	9.920802	0.877386	-6.629323
H	-4.225127	-0.353129	6.245494	H	11.535489	-0.836032	-3.039068
C	5.44264	-0.013	0.283408	H	11.853996	0.02051	-5.340611
C	4.796407	0.171153	3.086912	C	-4.046401	-2.479266	-8.273248
H	4.599621	0.236435	4.149518	H	-4.373898	-3.414916	-8.718596
C	6.099203	0.284235	2.611585	C	-3.485275	-2.466489	-7.042259
H	6.899797	0.452725	3.325666	H	-3.354509	-3.389955	-6.484849
C	6.429829	0.213317	1.250605	C	-2.964858	2.419468	-7.331283
H	7.461167	0.382073	0.966985	H	-2.636327	3.353615	-6.884091
C	-4.796407	0.171153	-3.086912	C	-3.523613	2.405307	-8.563443
H	-4.59962	0.236435	-4.149517	H	-3.650966	3.330178	-9.119767
C	-6.099203	0.284235	-2.611585	C	-7.970695	-0.885417	1.105209
H	-6.899797	0.452726	-3.325666	H	-7.820301	-1.328266	0.128512
C	-5.44264	-0.013	-0.283408	C	-9.192019	-0.961295	1.685017
C	-6.429829	0.213318	-1.250605	H	-10.018768	-1.429722	1.157611

C	-6.108042	0.926303	5.248028	C	2.964858	2.419468	7.331284
H	-5.276124	1.365268	5.784466	H	2.636327	3.353615	6.884091
C	-7.352026	1.001976	5.77642	C	6.108042	0.926303	-5.248028
H	-7.50596	1.467285	6.74641	H	5.276124	1.365268	-5.784466
C	3.485275	-2.466489	7.042259	C	7.352026	1.001975	-5.77642
H	3.35451	-3.389955	6.484849	H	7.50596	1.467285	-6.74641
C	4.046402	-2.479266	8.273248	C	9.192019	-0.961295	-1.685017
H	4.373899	-3.414916	8.718596	H	10.018768	-1.429722	-1.157611
C	3.523613	2.405307	8.563443	C	7.970695	-0.885417	-1.105209
H	3.650966	3.330178	9.119767	H	7.820301	-1.328267	-0.128512

### Intermediate 5b

C	-2.879292	-0.52503	1.483594	C	3.591817	0.802431	6.85751
C	2.995593	0.049241	-1.689272	C	2.368406	1.720143	4.970472
C	-1.614033	-0.194085	-3.25048	C	2.310122	0.457867	4.384597
C	-2.227522	-0.463372	-2.046746	C	3.529797	-0.484807	6.261238
C	-3.62605	-0.649455	-1.977495	H	1.910711	2.564187	4.461492
C	-3.96778	-0.79445	-0.641444	H	2.838119	-1.614509	4.563295
C	-2.790904	-0.667219	0.117407	C	-5.627329	-0.329827	4.075577
N	-1.745966	-0.52955	-0.756911	C	-5.374568	-0.870847	1.306545
C	2.986002	0.104038	-0.276954	C	-6.754834	-0.765192	3.320171
C	4.173306	0.265739	0.444197	C	-4.335709	-0.44612	3.524282
C	3.875889	0.443585	1.80983	C	-4.20413	-0.629968	2.105659
C	2.447215	0.298558	1.91675	C	-6.609366	-1.119444	1.959369
N	1.975863	0.125335	0.638317	C	-3.948002	-0.29412	-4.317805
C	0.257736	0.081221	3.066761	C	-2.838804	0.853403	-6.660039
C	-0.640952	-0.01271	4.242161	C	-4.708671	-0.253417	-5.523567
C	-1.910224	-0.165235	3.681351	C	-2.541824	0.014222	-4.37672
C	-1.744848	-0.230648	2.272128	C	-2.06228	0.650947	-5.533817
N	-0.475118	-0.083602	1.901252	C	-4.166385	0.343219	-6.685296
C	1.863352	0.022831	-2.498103	H	-1.049921	1.036808	-5.534426
C	2.014691	-0.18913	-3.887924	C	3.22141	-0.353134	-4.554185
C	0.73956	-0.366802	-4.436243	C	0.657139	-0.843572	-5.742636
C	-0.170433	-0.130794	-3.298072	H	-0.291525	-1.057355	-6.222642
N	0.53015	0.047402	-2.16552	C	1.851723	-1.096583	-6.424011
C	1.625979	0.277016	3.072217	H	1.803103	-1.510867	-7.426499
H	0.977605	0.0309	0.473905	C	3.107801	-0.862622	-5.859745
H	-0.791234	-0.288469	-0.532286	H	3.987744	-1.137266	-6.429592
C	4.326914	0.000637	-2.343591	C	-3.113397	-0.343124	4.353553
C	6.864129	-0.124835	-3.603168	C	-0.541116	-0.067574	5.631385
C	5.529587	0.033449	-1.564454	H	0.399818	0.042225	6.157389
C	4.429686	-0.100037	-3.767028	C	-1.713921	-0.327574	6.34753
C	5.696406	0.047043	-4.383063	H	-1.648738	-0.433051	7.426581
C	6.765661	-0.237737	-2.191849	C	-2.967675	-0.479935	5.745186
C	3.002402	1.91438	6.200424	H	-3.807727	-0.747026	6.374571
C	2.888936	-0.63384	5.028777	C	5.44993	0.324092	-0.12667

C	4.939075	0.761843	2.674731	C	10.656655	-0.294838	-5.483532
H	4.793254	0.918794	3.736096	C	9.305451	-0.495644	-3.482772
C	6.195003	0.924583	2.115428	C	8.26613	0.071667	-5.628887
H	7.017851	1.224798	2.757216	C	9.529145	0.020981	-6.230006
C	6.459999	0.726251	0.745032	C	10.546697	-0.556624	-4.122361
H	7.46107	0.928429	0.384139	H	9.618003	0.229822	-7.292851
C	-4.540476	-0.555043	-3.008186	H	11.429613	-0.811441	-3.542074
C	-5.886753	-0.527821	-2.531852	H	11.628804	-0.338765	-5.965075
H	-6.700218	-0.311698	-3.213707	C	-6.73785	-0.778753	-6.782093
C	-5.258409	-0.83437	-0.15178	H	-7.704534	-1.2715	-6.845207
C	-6.226318	-0.655506	-1.183899	C	-6.009931	-0.857911	-5.640423
H	-7.2731	-0.530914	-0.931811	H	-6.386531	-1.456352	-4.820896
C	-8.041452	-0.853794	3.942759	C	-2.322146	1.529959	-7.824175
C	-10.561644	-1.039567	5.167429	H	-1.311282	1.926474	-7.779243
C	-8.232257	-0.378516	5.266519	C	-3.066137	1.658744	-8.944009
C	-9.139714	-1.415	3.241741	H	-2.666379	2.166557	-9.817724
C	-10.386328	-1.509633	3.874152	C	-7.720871	-1.750154	1.299618
C	-9.494456	-0.471318	5.856541	H	-7.571213	-2.172332	0.313534
H	-11.21897	-1.955555	3.336604	C	-8.920508	-1.900395	1.911434
H	-9.63612	-0.09345	6.86571	H	-9.734756	-2.408596	1.401655
H	-11.534775	-1.112971	5.643159	C	-5.884355	0.247474	5.374217
C	-4.94077	0.459428	-7.880028	H	-5.081436	0.767679	5.8801
C	-6.467359	0.694636	-10.218058	C	-7.114816	0.229873	5.934543
C	-6.248423	-0.083928	-7.93614	H	-7.28111	0.700232	6.900085
C	-4.403115	1.120658	-9.018661	C	4.134236	-1.596139	6.950733
C	-5.181712	1.230151	-10.170894	H	4.082374	-2.577863	6.488022
C	-6.995787	0.04114	-9.115584	C	4.750869	-1.429021	8.143335
H	-4.773672	1.740315	-11.039544	H	5.202824	-2.276501	8.65191
H	-7.996295	-0.381253	-9.15661	C	3.698395	3.37561	8.018159
H	-7.056624	0.788244	-11.125175	H	3.749716	4.358621	8.4787
C	4.243248	0.97826	8.115681	C	3.079575	3.209308	6.826592
C	5.520072	1.322657	10.5809	H	2.625664	4.054626	6.316686
C	4.304807	2.266319	8.709302	C	5.860968	0.390601	-5.772252
C	4.830323	-0.135103	8.772426	H	4.991855	0.701742	-6.338663
C	5.462867	0.058959	10.004264	C	7.080275	0.412406	-6.361298
C	4.947451	2.416454	9.942096	H	7.178973	0.707517	-7.402516
H	5.913145	-0.791371	10.509637	C	9.144478	-0.787692	-2.085502
H	4.996347	3.401384	10.398851	H	10.006909	-1.139993	-1.52599
H	6.015238	1.456117	11.537933	C	7.944636	-0.656572	-1.473873
C	8.145872	-0.182126	-4.238247	H	7.846712	-0.939274	-0.433296

### Intermediate 6c

C	-2.899122	-0.005429	1.630835	C	-3.666075	-0.449788	-1.822806
C	2.908914	-0.26164	-1.590968	C	-3.995237	-0.437152	-0.474552
C	-1.656905	-0.249984	-3.175636	C	-2.821489	-0.215419	0.257847
C	-2.275778	-0.270409	-1.9261	N	-1.793797	-0.148041	-0.646816

C	2.833256	-0.087027	-0.212841	C	3.034188	-1.528044	-5.649824
C	4.012668	-0.013455	0.540207	H	3.898096	-1.930298	-6.165857
C	3.671958	0.32569	1.842442	C	-3.133149	0.129772	4.504133
C	2.271545	0.428902	1.905858	C	-0.553634	0.298339	5.764214
N	1.795009	0.158238	0.647386	H	0.397496	0.329774	6.283482
C	0.225951	0.63417	3.209447	C	-1.716839	-0.004273	6.478132
C	-0.66329	0.492998	4.386728	H	-1.634685	-0.201887	7.542821
C	-1.94158	0.36266	3.828167	C	-2.979647	-0.092334	5.883086
C	-1.790695	0.322814	2.423317	H	-3.819357	-0.391941	6.499117
N	-0.499444	0.483335	2.065704	C	5.310949	-0.125024	0.069439
C	1.788129	-0.243117	-2.432389	C	4.591734	0.576681	2.848968
C	1.948913	-0.588	-3.793755	C	5.925365	0.582827	2.366913
C	0.670209	-0.706812	-4.353673	H	6.736663	0.918905	3.000742
C	-0.237221	-0.300398	-3.254615	C	6.266713	0.254601	1.045222
N	0.485554	-0.075404	-2.121636	H	7.3103	0.363643	0.774678
C	1.639885	0.75523	3.105459	C	-4.590924	-0.555477	-2.850056
H	0.809264	0.231344	0.44644	C	-5.92658	-0.509791	-2.375915
H	-0.817367	0.045285	-0.483125	H	-6.752622	-0.420357	-3.070485
C	4.248109	-0.486864	-2.169944	C	-5.28691	-0.507066	0.021195
C	6.802145	-0.863595	-3.336111	C	-6.257458	-0.482004	-1.011988
C	5.429469	-0.489102	-1.346651	H	-7.308868	-0.37678	-0.771586
C	4.373885	-0.704045	-3.5811	C	-8.035538	-0.495719	4.146569
C	5.660106	-0.695089	-4.16368	C	-10.540369	-0.723589	5.392771
C	6.668082	-0.860052	-1.925554	C	-8.227986	-0.002702	5.463402
C	2.820909	2.325974	6.32277	C	-9.121555	-1.104511	3.466368
C	3.992133	0.960921	4.130086	C	-10.360212	-1.218164	4.107769
C	4.176986	1.90892	6.393942	C	-9.48519	-0.1161	6.063847
C	2.05309	1.926894	5.240587	H	-11.183763	-1.699243	3.586733
C	2.570504	1.181036	4.173512	H	-9.629774	0.275412	7.067343
C	4.752495	1.202581	5.309561	H	-11.508704	-0.812426	5.875685
H	1.016634	2.240873	5.200661	C	-5.021067	-0.312312	-7.822678
C	-5.641019	0.097348	4.248278	C	-6.572639	-0.421926	-10.153646
C	-5.393694	-0.472277	1.483452	C	-6.328694	-0.857757	-7.784655
C	-6.756916	-0.382054	3.511601	C	-4.495803	0.17212	-9.051823
C	-4.350771	0.021709	3.679111	C	-5.287616	0.112682	-10.20017
C	-4.225161	-0.154876	2.262248	C	-7.088243	-0.906812	-8.960597
C	-6.607192	-0.760639	2.154658	H	-4.889516	0.489627	-11.138642
C	-4.007032	-0.504303	-4.193457	H	-8.088965	-1.329466	-8.928438
C	-2.912414	0.263995	-6.694258	H	-7.173048	-0.460414	-11.057474
C	-4.771151	-0.657826	-5.385104	C	4.951117	2.234451	7.549558
C	-2.603785	-0.207322	-4.311475	C	6.478075	2.885529	9.806657
C	-2.128893	0.240264	-5.55148	C	4.379968	3.007734	8.597137
C	-4.236215	-0.247241	-6.630636	C	6.292589	1.789078	7.656249
H	-1.116965	0.62331	-5.613319	C	7.039412	2.121708	8.793792
C	3.159639	-0.917852	-4.390008	C	5.160211	3.325337	9.710357
C	0.586193	-1.286897	-5.620061	H	8.066047	1.774464	8.874813
H	-0.360875	-1.465313	-6.116679	H	4.726929	3.922578	10.508351
C	1.77392	-1.697964	-6.232319	H	7.068452	3.141244	10.681321
H	1.715178	-2.191905	-7.19765	C	8.092165	-1.047989	-3.930278

C	10.621302	-1.410946	-5.094634	C	-5.894022	0.672867	5.546368
C	9.216589	-1.353943	-3.121195	H	-5.094091	1.206377	6.044388
C	8.258914	-0.928148	-5.334535	C	-7.120185	0.634403	6.11776
C	9.527431	-1.102578	-5.895259	H	-7.287577	1.105595	7.082645
C	10.467453	-1.540218	-3.720518	C	6.091074	0.700723	5.487759
H	9.650254	-0.99619	-6.96979	H	6.498529	0.021428	4.750452
H	11.321652	-1.788361	-3.096058	C	6.818202	0.976009	6.598549
H	11.599014	-1.551342	-5.545342	H	7.813554	0.555039	6.714123
C	-6.806278	-1.375138	-6.535774	C	3.010742	3.442858	8.474193
H	-7.769861	-1.877492	-6.517374	H	2.584706	4.037045	9.278181
C	-6.07075	-1.279211	-5.400974	C	2.268115	3.11614	7.393293
H	-6.438041	-1.751179	-4.499192	H	1.232912	3.436926	7.3125
C	-2.40547	0.754924	-7.950614	C	5.880395	-0.48728	-5.573752
H	-1.394623	1.153344	-7.975391	H	5.045773	-0.177964	-6.190381
C	-3.159499	0.713395	-9.071492	C	7.111106	-0.588516	-6.127123
H	-2.76738	1.083738	-10.014965	H	7.250991	-0.393906	-7.187146
C	-7.701201	-1.454588	1.526439	C	9.014115	-1.504194	-1.709457
H	-7.542947	-1.910291	0.557443	H	9.848212	-1.836028	-1.096884
C	-8.891421	-1.624502	2.149925	C	7.807447	-1.264234	-1.143197
H	-9.689009	-2.178856	1.662499	H	7.676106	-1.44501	-0.084132

### Intermediate 7b

C	-2.804733	1.0436	1.567377	H	0.983332	1.594172	0.082256
C	2.973782	0.575114	-1.79571	H	-0.798213	1.10058	-0.5517
C	-1.659467	0.407887	-3.207826	C	4.271887	0.095026	-2.310789
C	-2.244693	0.490926	-1.954316	C	6.752051	-0.667988	-3.429049
C	-3.609973	0.173893	-1.776002	C	5.43152	-0.057916	-1.455049
C	-3.897581	0.266699	-0.420421	C	4.361892	-0.245619	-3.697132
C	-2.740082	0.712142	0.225421	C	5.639137	-0.420647	-4.272877
N	-1.751056	0.811845	-0.708866	C	6.611693	-0.60448	-2.017041
C	2.936524	0.900718	-0.448709	C	2.308547	1.296638	6.540476
C	4.056606	0.703905	0.36259	C	3.777058	0.97769	4.096748
C	3.684803	0.974051	1.674246	C	3.665182	0.880511	6.554406
C	2.353308	1.36529	1.649366	C	1.61563	1.37581	5.314067
N	1.920364	1.339779	0.360005	C	2.378253	1.356	4.093929
C	0.328668	1.891537	2.805713	C	4.361789	0.623067	5.336846
C	-0.393354	1.779219	4.01858	C	-5.172871	0.525387	4.473111
C	-1.715946	1.606606	3.643058	C	-5.150844	0.128735	1.643715
C	-1.705924	1.603082	2.219401	C	-6.276228	-0.086877	3.81674
N	-0.4808	1.827471	1.70684	C	-3.977677	0.756117	3.764459
C	1.836115	0.571882	-2.615364	C	-3.995785	0.657338	2.326467
C	1.941614	0.028817	-3.909946	C	-6.226971	-0.365237	2.423887
C	0.640426	-0.132152	-4.411275	C	-4.009643	-0.169663	-4.105217
C	-0.224756	0.424395	-3.345021	C	-3.052705	0.453917	-6.706011
N	0.534753	0.814535	-2.292427	C	-4.788377	-0.496756	-5.252985
C	1.68519	1.631147	2.835903	C	-2.640738	0.239938	-4.302012

C	-2.23851	0.59979	-5.596088	C	3.669406	1.01798	9.028369
C	-4.327093	-0.155296	-6.547808	C	5.636864	0.15052	7.862748
H	-1.260826	1.049682	-5.728078	C	6.26788	-0.026514	9.097594
C	3.124825	-0.434578	-4.478253	C	4.338119	0.840759	10.244774
C	0.508934	-0.867067	-5.591828	H	7.269672	-0.447001	9.12374
H	-0.455226	-1.086569	-6.03603	H	3.832209	1.109144	11.168451
C	1.667653	-1.377237	-6.18292	H	6.129956	0.186427	11.231106
H	1.569045	-1.98013	-7.080734	C	8.016748	-1.009095	-4.009272
C	2.948294	-1.183164	-5.652177	C	10.502028	-1.660495	-5.143981
H	3.784739	-1.677654	-6.132855	C	9.102456	-1.400184	-3.183918
C	-2.701614	1.077875	4.448741	C	8.196255	-0.964989	-5.416715
C	0.135784	1.420864	5.242577	C	9.444759	-1.281804	-5.961975
C	-0.861122	0.893585	6.116139	C	10.331191	-1.726852	-3.766901
H	-0.57725	0.491699	7.083426	H	9.578625	-1.232115	-7.039353
C	-2.206161	0.734276	5.741824	H	11.154276	-2.036334	-3.128232
H	-2.848815	0.2253	6.452567	H	11.463215	-1.909873	-5.582896
C	5.324473	0.30114	-0.02598	C	-6.785133	-1.482981	-6.264346
C	4.494492	0.857603	2.796354	H	-7.700499	-2.060913	-6.167702
C	5.840671	0.64618	2.399188	C	-6.028107	-1.22497	-5.169771
H	6.650423	0.714934	3.11497	H	-6.326655	-1.647354	-4.219816
C	6.231143	0.389873	1.062594	C	-2.624106	0.86692	-8.018746
H	7.297619	0.29377	0.90291	H	-1.651419	1.341953	-8.114469
C	-4.545266	-0.155156	-2.740354	C	-3.403645	0.662706	-9.102918
C	-5.857664	-0.242667	-2.191826	H	-3.072091	0.975888	-10.089325
H	-6.717952	-0.32722	-2.843899	C	-7.270804	-1.191312	1.873608
C	-5.132866	0.051648	0.167726	H	-7.160816	-1.571694	0.867421
C	-6.138046	-0.145234	-0.820113	C	-8.346272	-1.569769	2.603251
H	-7.185284	-0.167172	-0.542663	H	-9.105178	-2.21128	2.163214
C	-7.436237	-0.447296	4.57702	C	-5.332673	0.920282	5.85028
C	-9.719282	-1.143633	6.062661	H	-4.552959	1.511829	6.314354
C	-7.537957	-0.09296	5.947979	C	-6.456981	0.637396	6.546457
C	-8.496502	-1.169255	3.971141	H	-6.563759	0.974053	7.57424
C	-9.622931	-1.511849	4.727553	C	5.641727	-0.032055	5.439383
C	-8.68528	-0.438964	6.667951	H	6.103972	-0.417873	4.542968
H	-10.424843	-2.073625	4.255907	C	6.248031	-0.249604	6.628764
H	-8.758925	-0.152485	7.713707	H	7.205696	-0.762082	6.665997
H	-10.601338	-1.410532	6.63656	C	2.337328	1.545314	8.966508
C	-5.136319	-0.394225	-7.701025	H	1.859471	1.861318	9.889955
C	-6.736165	-0.844909	-9.957669	C	1.68725	1.663645	7.78599
C	-6.390475	-1.04094	-7.569612	H	0.697496	2.103904	7.761074
C	-4.688552	0.018077	-8.986224	C	5.87003	-0.322007	-5.691477
C	-5.503132	-0.212114	-10.095871	H	5.060933	0.020735	-6.325001
C	-7.175273	-1.260403	-8.709518	C	7.086004	-0.564637	-6.233286
H	-5.16433	0.109384	-11.077267	H	7.243073	-0.444967	-7.301894
H	-8.134412	-1.760543	-8.604436	C	8.87361	-1.499416	-1.771251
H	-7.354676	-1.016352	-10.833356	H	9.661219	-1.909394	-1.144611
C	4.324229	0.686748	7.812732	C	7.694814	-1.123919	-1.222134
C	5.62631	0.32386	10.279256	H	7.536766	-1.284473	-0.16502

## Intermediate 8a

C	-2.38325	-2.431106	1.607453	C	4.614078	-2.93169	0.506323
C	2.38325	2.431106	1.607453	C	5.117634	-5.257809	-0.11902
C	2.38325	-2.431106	1.607453	C	4.961319	1.492461	0.627941
C	1.114211	-2.874527	1.952642	C	4.961319	-1.492461	0.627941
C	0.697425	-4.164062	1.601143	C	6.122321	-0.702895	0.356971
C	-0.697425	-4.164062	1.601143	H	7.082878	-1.169389	0.1772
C	-1.114211	-2.874527	1.952642	C	6.122321	0.702895	0.356971
N	0	-2.132047	2.241353	H	7.082878	1.169389	0.1772
C	1.114211	2.874527	1.952642	C	-4.961319	-1.492461	0.627941
C	0.697425	4.164062	1.601142	C	-4.961319	1.492461	0.627941
C	-0.697425	4.164062	1.601142	C	-6.122321	0.702895	0.356971
C	-1.114211	2.874527	1.952642	H	-7.082878	1.169389	0.1772
N	0	2.132047	2.241352	C	-6.122321	-0.702895	0.356971
C	-2.686607	1.07207	1.617296	H	-7.082878	-1.169389	0.1772
C	-3.946887	0.691244	1.105922	C	1.483082	5.098229	0.941922
C	-3.946886	-0.691243	1.105922	C	-1.483082	5.098229	0.941922
C	-2.686607	-1.07207	1.617296	C	-0.704889	6.090224	0.292733
N	-1.924283	0	1.963915	H	-1.187654	6.830592	-0.336508
C	2.686607	1.07207	1.617296	C	0.704889	6.090224	0.292733
C	3.946887	0.691243	1.105922	H	1.187654	6.830592	-0.336508
C	3.946887	-0.691243	1.105922	C	1.483082	-5.098229	0.941922
C	2.686607	-1.07207	1.617296	C	0.704889	-6.090224	0.292733
N	1.924283	0	1.963915	H	1.187654	-6.830593	-0.336508
C	-2.38325	2.431106	1.607453	C	-1.483082	-5.098229	0.941922
H	0	1.118147	2.320111	C	-0.704889	-6.090224	0.292733
H	0	-1.118147	2.320111	H	-1.187654	-6.830593	-0.336508
C	3.323843	3.378042	0.993245	C	-6.041505	-6.225134	-0.634027
C	5.117634	5.25781	-0.11902	C	-7.866415	-8.120754	-1.624333
C	2.909861	4.742422	0.79587	C	-7.232714	-5.807932	-1.28169
C	4.614078	2.93169	0.506323	C	-5.772302	-7.613912	-0.513536
C	5.434647	3.869489	-0.166207	C	-6.698798	-8.542049	-1.002076
C	3.874392	5.695469	0.402175	C	-8.127434	-6.76369	-1.771535
C	-5.434647	3.869489	-0.166207	H	-6.490388	-9.603081	-0.892814
C	-2.909861	4.742422	0.79587	H	-9.031936	-6.432488	-2.274761
C	-5.117634	5.25781	-0.11902	H	-8.57289	-8.852643	-2.003687
C	-4.614078	2.93169	0.506323	C	6.041505	-6.225134	-0.634027
C	-3.323843	3.378042	0.993245	C	7.866415	-8.120754	-1.624333
C	-3.874392	5.695469	0.402175	C	5.772302	-7.613912	-0.513536
C	-5.434647	-3.869489	-0.166207	C	7.232714	-5.807932	-1.28169
C	-2.909861	-4.742422	0.79587	C	8.127434	-6.763691	-1.771535
C	-5.117634	-5.257809	-0.119019	C	6.698798	-8.542049	-1.002076
C	-4.614078	-2.93169	0.506323	H	9.031936	-6.432488	-2.27476
C	-3.323843	-3.378042	0.993245	H	6.490388	-9.603081	-0.892814
C	-3.874392	-5.695469	0.402175	H	8.57289	-8.852643	-2.003687
C	2.909861	-4.742422	0.79587	C	-6.041505	6.225134	-0.634027
C	5.434647	-3.869489	-0.166207	C	-7.866415	8.120754	-1.624333
C	3.874392	-5.695469	0.402175	C	-7.232714	5.807932	-1.28169
C	3.323843	-3.378042	0.993245	C	-5.772303	7.613912	-0.513536

C	-6.698799	8.542049	-1.002076	H	-2.754521	-7.44124	1.062768
C	-8.127434	6.76369	-1.771534	C	-4.555456	-8.021319	0.12675
H	-6.490388	9.603081	-0.892814	H	-4.377784	-9.082432	0.280035
H	-9.031936	6.432488	-2.27476	C	-6.588069	-3.488976	-0.943406
H	-8.57289	8.852643	-2.003686	H	-6.742878	-2.445567	-1.173285
C	6.041505	6.225134	-0.634027	C	-7.441493	-4.400747	-1.463343
C	7.866415	8.120754	-1.624333	H	-8.291139	-4.074493	-2.057334
C	5.772302	7.613912	-0.513536	C	-3.647702	7.109507	0.546483
C	7.232714	5.807932	-1.28169	H	-2.754521	7.44124	1.062767
C	8.127434	6.763691	-1.771534	C	-4.555456	8.021319	0.12675
C	6.698799	8.542049	-1.002076	H	-4.377784	9.082432	0.280035
H	9.031936	6.432488	-2.27476	C	-7.441493	4.400747	-1.463343
H	6.490388	9.603081	-0.892814	H	-8.291139	4.074493	-2.057334
H	8.57289	8.852643	-2.003686	C	-6.588069	3.488976	-0.943406
C	4.555456	-8.021319	0.12675	H	-6.742878	2.445567	-1.173285
H	4.377784	-9.082432	0.280035	C	6.588069	3.488976	-0.943406
C	3.647702	-7.109507	0.546484	H	6.742878	2.445567	-1.173285
H	2.754521	-7.44124	1.062768	C	7.441493	4.400747	-1.463343
C	6.588069	-3.488976	-0.943406	H	8.291139	4.074494	-2.057334
H	6.742878	-2.445567	-1.173285	C	4.555456	8.021319	0.12675
C	7.441493	-4.400747	-1.463343	H	4.377784	9.082432	0.280035
H	8.291139	-4.074493	-2.057334	C	3.647702	7.109507	0.546483
C	-3.647702	-7.109507	0.546484	H	2.754521	7.44124	1.062767

### Intermediate 9a

C	-2.381206	-2.538232	2.015217	C	2.604858	-0.758199	1.77782
C	2.022345	2.705102	1.961788	N	1.790426	0.231149	2.23476
C	2.396686	-2.133128	1.700392	C	-2.711777	2.276376	2.364749
C	1.183099	-2.692057	2.082114	H	-0.119615	1.172831	2.882361
C	0.843392	-3.977751	1.647008	H	-0.046897	-1.074869	2.682609
C	-0.544389	-4.089989	1.710118	C	2.798639	3.742283	1.26412
C	-1.042326	-2.872749	2.201027	C	4.258316	5.779244	-0.053496
N	0.028353	-2.068962	2.490413	C	2.230573	5.054606	1.105781
C	0.786542	3.036604	2.499654	C	4.066519	3.425089	0.636526
C	0.242958	4.30809	2.26345	C	4.71294	4.430461	-0.120972
C	-1.128642	4.169207	2.438909	C	3.038543	6.09415	0.59377
C	-1.44841	2.818851	2.707952	C	-5.418112	3.583214	-0.073942
N	-0.238493	2.181616	2.860501	C	-3.242229	4.451522	1.384813
C	-2.984829	0.904931	2.35148	C	-4.773794	4.814601	-0.405394
C	-4.18629	0.480826	1.695116	C	-4.794778	2.670955	0.847817
C	-4.114908	-0.904246	1.675917	C	-3.658267	3.133377	1.615778
C	-2.856992	-1.241973	2.247113	C	-3.676135	5.211874	0.323982
N	-2.182483	-0.142206	2.682958	C	-5.469268	-4.176506	0.52858
C	2.427925	1.375639	1.869947	C	-2.738913	-4.833915	1.008
C	3.662764	1.123967	1.235458	C	-5.012814	-5.514499	0.375311
C	3.78337	-0.25176	1.185889	C	-4.572526	-3.165318	0.938493



C	-3.239229	-3.524647	1.337774	C	-5.104826	5.618114	-1.525893
C	-3.649611	-5.839516	0.608748	C	-5.752365	7.152558	-3.739138
C	3.051364	-4.341978	0.71706	C	-6.258678	5.300175	-2.269817
C	5.438468	-3.233371	-0.330297	C	-4.237295	6.692825	-1.893075
C	4.06059	-5.200126	0.228773	C	-4.593667	7.443115	-3.017809
C	3.369227	-2.964599	0.972257	C	-6.578876	6.094394	-3.377802
C	4.588413	-2.395686	0.431524	H	-3.953616	8.261351	-3.337817
C	5.236466	-4.644001	-0.330459	H	-7.469937	5.874992	-3.960163
C	4.558646	2.026113	0.702403	H	-6.00493	7.757404	-4.604613
C	4.822767	-0.939335	0.59546	C	5.014519	6.826883	-0.673689
C	5.885674	-0.041483	0.270294	C	6.512392	8.880881	-1.87246
H	6.866996	-0.412498	0.003355	C	4.610969	8.18148	-0.541295
C	5.760637	1.357946	0.319296	C	6.170188	6.52254	-1.43866
H	6.65706	1.917535	0.081794	C	6.901311	7.555911	-2.030878
C	-4.931035	-1.734038	0.931902	C	5.37708	9.191062	-1.135916
C	-5.060996	1.218829	0.901198	H	7.779432	7.310858	-2.622486
C	-5.893326	0.389695	0.099482	H	5.068167	10.226363	-1.018112
H	-6.551418	0.82345	-0.640699	H	7.092958	9.674492	-2.332706
C	-5.84084	-1.008309	0.118838	C	4.900517	-7.451161	-0.187211
H	-6.46162	-1.525932	-0.60397	H	4.811873	-8.528537	-0.076727
C	0.805796	5.277634	1.42204	C	3.946794	-6.632174	0.314327
C	-1.975427	4.975915	1.741263	H	3.10545	-7.054544	0.851494
C	-1.509296	5.959649	0.843463	C	6.511024	-2.729758	-1.152228
C	-0.114235	6.11791	0.713018	H	6.56661	-1.669798	-1.347899
H	0.273019	6.759481	-0.07302	C	7.405474	-3.547588	-1.752708
C	1.665794	-4.807081	0.89791	H	8.191154	-3.129725	-2.376601
C	0.941647	-5.808972	0.20935	C	-3.262707	-7.225109	0.52278
H	1.453124	-6.460281	-0.49181	H	-2.271129	-7.511252	0.847967
C	-1.279646	-5.053522	1.031751	C	-4.127184	-8.187574	0.127467
C	-0.459985	-5.923354	0.270369	H	-3.80935	-9.226247	0.093245
H	-0.91011	-6.647741	-0.398533	C	-6.877261	-3.921371	0.353391
C	-5.927245	-6.536368	-0.042935	H	-7.268056	-2.946756	0.61305
C	-7.710663	-8.531892	-0.907468	C	-7.736288	-4.886004	-0.046789
C	-7.289126	-6.225821	-0.294692	H	-8.795256	-4.664837	-0.150442
C	-5.485912	-7.875313	-0.206881	C	-2.697158	6.209699	-0.060647
C	-6.386135	-8.853747	-0.641571	C	-2.993713	6.94118	-1.168312
C	-8.160561	-7.229784	-0.728452	H	-2.315011	7.690641	-1.568556
H	-6.036266	-9.87523	-0.765317	C	-7.039613	4.172671	-1.822317
H	-9.200615	-6.979753	-0.920379	H	-7.980934	3.971703	-2.327335
H	-8.397821	-9.300955	-1.246625	C	-6.645666	3.359279	-0.802494
C	6.203917	-5.512266	-0.93303	H	-7.30868	2.559707	-0.497709
C	8.119568	-7.21235	-2.088719	C	5.814475	4.156495	-1.010877
C	6.050179	-6.921721	-0.861282	H	6.054973	3.130191	-1.243779
C	7.322422	-4.973396	-1.61918	C	6.508016	5.141081	-1.626246
C	8.263995	-5.833585	-2.190778	H	7.322182	4.892794	-2.301973
C	7.021773	-7.751959	-1.43212	C	3.428636	8.472194	0.216529
H	9.11268	-5.410923	-2.72198	H	3.152012	9.5116	0.371654
H	6.903647	-8.829852	-1.36006	C	2.674004	7.47894	0.741577
H	8.862421	-7.86895	-2.531091	H	1.802656	7.724836	1.337842

## Intermediate 10g

C	-2.42387	-1.852605	-2.358476	C	4.602504	-0.610922	-2.670366
C	2.38898	-2.76775	2.38366	C	5.19883	0.234886	-4.896648
C	2.42387	-1.852605	-2.358475	C	4.693664	-1.030826	1.712405
C	1.120999	-2.049254	-2.826024	C	4.840125	-0.753044	-1.223805
C	0.696533	-1.403472	-3.993845	C	5.628496	0.021203	-0.335609
C	-0.696533	-1.403472	-3.993845	H	6.249741	0.824957	-0.715175
C	-1.120999	-2.049254	-2.826024	C	5.54849	-0.104029	1.056673
N	0	-2.489809	-2.167485	H	6.115373	0.620651	1.624012
C	1.137332	-3.297583	2.756159	C	-4.840125	-0.753044	-1.223805
C	0.694064	-3.241824	4.099054	C	-4.693664	-1.030826	1.712405
C	-0.694063	-3.241823	4.099054	C	-5.54849	-0.104029	1.056673
C	-1.137332	-3.297583	2.756159	H	-6.115373	0.620651	1.624012
N	0	-3.475931	1.981426	C	-5.628495	0.021203	-0.335609
C	-2.771869	-2.569281	1.049167	H	-6.24974	0.824957	-0.715175
C	-3.952088	-1.794438	0.814158	C	1.346952	-2.504759	5.055783
C	-4.001506	-1.629105	-0.561862	C	-1.346952	-2.504759	5.055783
C	-2.818261	-2.228082	-1.073956	C	-0.704984	-1.710002	6.069892
N	-2.086772	-2.83087	-0.087894	C	0.704984	-1.710002	6.069892
C	2.771869	-2.569281	1.049167	C	1.475652	-0.580271	-4.80029
C	3.952088	-1.794438	0.814158	C	0.704318	0.274858	-5.615299
C	4.001506	-1.629105	-0.561862	H	1.186507	1.053259	-6.195839
C	2.818261	-2.228082	-1.073956	C	-1.475652	-0.580271	-4.80029
N	2.086772	-2.83087	-0.087894	C	-0.704318	0.274858	-5.615299
C	-2.38898	-2.76775	2.38366	H	-1.186507	1.053259	-6.195839
H	0	-3.389451	0.97061	C	-6.169825	0.793623	-5.791004
H	0	-2.854911	-1.22163	C	-8.065388	1.921557	-7.534803
C	3.170824	-2.035736	3.400856	C	-7.492507	1.052828	-5.346504
C	3.926457	-0.092134	5.350265	C	-5.824447	1.091541	-7.135255
C	2.602107	-1.964674	4.682145	C	-6.779391	1.655045	-7.987509
C	4.277853	-1.137558	3.128821	C	-8.421091	1.61747	-6.227018
C	4.722334	-0.258948	4.173531	H	-6.504139	1.879379	-9.01461
C	2.864371	-0.938243	5.563388	H	-9.430869	1.812574	-5.875815
C	-4.722334	-0.258948	4.17353	H	-8.796384	2.359986	-8.207234
C	-2.602107	-1.964674	4.682145	C	6.169824	0.793623	-5.791004
C	-3.926457	-0.092134	5.350265	C	8.065388	1.921557	-7.534803
C	-4.277853	-1.137558	3.128821	C	5.824447	1.091541	-7.135255
C	-3.170824	-2.035736	3.400856	C	7.492507	1.052828	-5.346504
C	-2.864371	-0.938243	5.563388	C	8.42109	1.61747	-6.227018
C	-5.555665	-0.051084	-3.551224	C	6.779391	1.655045	-7.987509
C	-2.911282	-0.546894	-4.472996	H	9.430869	1.812574	-5.875815
C	-5.19883	0.234886	-4.896648	H	6.504138	1.879379	-9.014609
C	-4.602504	-0.610922	-2.670366	H	8.796384	2.359986	-8.207234
C	-3.322729	-1.018505	-3.179323	C	-4.081071	0.965208	6.283792
C	-3.874535	-0.003418	-5.352189	C	-4.391787	3.049448	8.084649
C	2.911282	-0.546894	-4.472996	C	-5.195967	1.819227	6.16363
C	5.555665	-0.051084	-3.551224	C	-3.089269	1.154936	7.293605
C	3.874535	-0.003418	-5.352189	C	-3.276216	2.219284	8.182206
C	3.322729	-1.018505	-3.179323	C	-5.344569	2.858961	7.088819

H	-2.536554	2.402077	8.957586	H	-2.629803	-0.084202	-7.139862
H	-6.203128	3.522061	7.022601	C	-4.505107	0.756873	-7.587254
H	-4.513372	3.863024	8.793068	H	-4.264249	0.900009	-8.637283
C	4.081072	0.965208	6.283792	C	-6.928626	0.150684	-3.161629
C	4.391787	3.049448	8.084649	H	-7.250948	-0.192693	-2.187419
C	3.089269	1.154936	7.293605	C	-7.842908	0.681125	-4.006474
C	5.195967	1.819227	6.163631	H	-8.875232	0.799649	-3.688123
C	5.344569	2.858961	7.088819	C	-1.772408	-0.734128	6.489487
C	3.276216	2.219284	8.182206	C	-1.901077	0.31233	7.349204
H	6.203128	3.522061	7.022601	H	-1.134469	0.568434	8.07533
H	2.536554	2.402077	8.957586	C	-6.121879	1.541277	5.09149
H	4.513372	3.863024	8.793067	H	-7.034393	2.129802	5.041776
C	4.505107	0.756873	-7.587254	C	-5.900866	0.579059	4.15318
H	4.264249	0.900009	-8.637283	H	-6.668609	0.402163	3.411157
C	3.5863	0.231935	-6.744393	C	5.900866	0.579059	4.15318
H	2.629803	-0.084202	-7.139861	H	6.668609	0.402163	3.411158
C	6.928626	0.150684	-3.161629	C	6.121879	1.541277	5.09149
H	7.250948	-0.192693	-2.187419	H	7.034393	2.129802	5.041776
C	7.842908	0.681125	-4.006474	C	1.901077	0.31233	7.349204
H	8.875232	0.799649	-3.688123	H	1.134469	0.568434	8.07533
C	-3.5863	0.231934	-6.744393	C	1.772408	-0.734128	6.489487

### Intermediate 11c

C	-2.721194	-2.275985	-2.611873	C	-2.649269	-3.174326	2.134068
C	2.125633	-3.096827	2.036903	H	-0.28872	-3.739781	0.655088
C	2.099477	-2.151698	-2.707177	H	-0.215209	-3.25416	-1.534769
C	0.83066	-2.477178	-3.193497	C	2.908141	-2.372304	3.05972
C	0.378419	-1.909591	-4.39254	C	3.666885	-0.481167	5.060544
C	-1.006036	-2.026383	-4.371395	C	2.372216	-2.362081	4.356387
C	-1.430045	-2.576659	-3.144295	C	3.98045	-1.430096	2.792383
N	-0.271156	-2.942908	-2.49809	C	4.431575	-0.581046	3.85563
C	0.895722	-3.666415	2.418363	C	2.633772	-1.362032	5.269391
C	0.479343	-3.658294	3.770828	C	-4.934487	-0.712919	4.044583
C	-0.909051	-3.681623	3.800449	C	-2.815974	-2.443501	4.464876
C	-1.38043	-3.701071	2.464199	C	-4.135068	-0.600681	5.222809
N	-0.259931	-3.844391	1.663062	C	-4.489516	-1.540492	2.958264
C	-3.060317	-2.946535	0.811425	C	-3.399464	-2.466145	3.187457
C	-4.19402	-2.09115	0.605528	C	-3.067941	-1.452027	5.387435
C	-4.22643	-1.849702	-0.764421	C	-5.177241	0.588982	-3.492758
C	-3.102431	-2.560481	-1.303445	C	-3.044775	-0.810449	-4.548963
N	-2.411112	-3.234855	-0.336797	C	-4.452421	1.114732	-4.601737
C	2.490993	-2.863248	0.700289	C	-4.648604	-0.535049	-2.76197
C	3.63178	-2.031855	0.46736	C	-3.550944	-1.282337	-3.330698
C	3.655552	-1.83424	-0.905073	C	-3.373874	0.409647	-5.088106
C	2.508721	-2.490845	-1.418144	C	2.467333	-0.760737	-4.796594
N	1.811648	-3.140213	-0.434767	C	5.074849	-0.087219	-3.873028

C	3.373672	-0.099997	-5.656768	C	-5.408148	1.265289	6.127158
C	2.927234	-1.238582	-3.518657	C	-3.288631	0.563011	7.211433
C	4.176276	-0.745438	-3.003465	C	-3.474412	1.585194	8.148161
C	4.679321	0.225709	-5.201862	C	-5.555527	2.261085	7.09981
C	4.355402	-1.258113	1.371285	H	-2.729546	1.738934	8.924875
C	4.438468	-0.902017	-1.560926	H	-6.418041	2.921718	7.070184
C	5.192954	-0.104309	-0.664613	H	-4.71697	3.191803	8.8414
H	5.759769	0.744302	-1.031005	C	3.821451	0.545379	6.027617
C	5.144787	-0.269031	0.726192	C	4.130024	2.570652	7.893859
H	5.678816	0.472796	1.303794	C	2.854564	0.672067	7.070779
C	-4.96157	-0.824351	-1.355215	C	4.909966	1.432834	5.906843
C	-4.880898	-1.334482	1.551349	C	5.058399	2.441683	6.8649
C	-5.658146	-0.30126	0.964014	C	3.0396	1.708466	7.992787
H	-6.175153	0.418523	1.583476	H	5.89692	3.129986	6.798906
C	-5.696928	-0.061739	-0.408729	H	2.318015	1.844265	8.794395
H	-6.241489	0.819586	-0.720348	H	4.251408	3.361523	8.627646
C	1.141666	-2.947394	4.741039	C	3.912686	0.808471	-7.860489
C	-1.551354	-2.988712	4.796295	H	3.647762	0.979379	-8.900514
C	-0.899317	-2.227472	5.831594	C	3.050728	0.172049	-7.035058
C	0.508384	-2.203358	5.799391	H	2.115375	-0.198845	-7.434892
C	1.040689	-0.920564	-5.139548	C	6.435144	0.197984	-3.491195
C	0.214984	0.00248	-5.850084	H	6.798001	-0.167813	-2.539744
H	0.673309	0.888652	-6.277473	C	7.294156	0.834546	-4.319719
C	-1.76339	-1.128464	-5.064944	H	8.319807	1.014632	-4.008881
C	-1.193688	-0.078395	-5.806702	C	-2.313319	0.92896	-5.928379
C	-4.675487	2.392374	-5.17402	C	-2.504965	2.177649	-6.430489
C	-5.116303	4.901677	-6.258753	H	-1.759228	2.679155	-7.042773
C	-5.806541	3.127667	-4.766868	C	-6.373277	1.333292	-3.175758
C	-3.725385	2.913	-6.106011	H	-7.089901	0.918533	-2.477055
C	-3.977684	4.18371	-6.629353	C	-6.670496	2.515308	-3.787452
C	-6.022391	4.389155	-5.337864	H	-7.593914	3.027869	-3.530273
H	-3.272513	4.621217	-7.331439	C	-1.966889	-1.279027	6.308431
H	-6.895119	4.96984	-5.05065	C	-2.094315	-0.273419	7.216543
H	-5.288007	5.883483	-6.68909	H	-1.322348	-0.045886	7.946453
C	5.591804	0.898441	-6.079094	C	-6.339148	1.033803	5.048713
C	7.368239	2.254481	-7.786104	H	-7.254983	1.619014	5.03171
C	5.206404	1.228004	-7.405072	C	-6.116732	0.11817	4.064679
C	6.896036	1.241515	-5.636131	H	-6.884062	-0.029451	3.314809
C	7.764765	1.919162	-6.497781	C	5.587462	0.287963	3.831766
C	6.102156	1.905816	-8.238643	H	6.335693	0.158217	3.060314
H	8.76064	2.17775	-6.147792	C	5.81167	1.21991	4.79902
H	5.79637	2.153866	-9.251606	H	6.707084	1.833865	4.746404
H	8.052617	2.781654	-8.443714	C	1.69029	-0.2027	7.126474
C	-4.288034	0.412852	6.202556	H	0.938002	0.005457	7.882232
C	-4.596204	2.411628	8.096168	C	1.563975	-1.219298	6.23064

## Intermediate 12c

C	-2.353478	-2.423829	-3.044117	C	4.240786	-0.55897	-3.052044
C	2.3768	-3.477762	1.729907	C	3.93998	1.159159	-4.808892
C	2.430951	-2.418576	-2.988346	C	4.546826	-1.544553	1.22363
C	1.184809	-2.797728	-3.547392	C	4.576656	-0.894717	-1.657219
C	0.754339	-2.27555	-4.788919	C	5.283775	-0.144142	-0.682278
C	-0.635492	-2.277276	-4.805047	H	5.783983	0.775833	-0.953091
C	-1.093679	-2.800394	-3.573792	C	5.269953	-0.451538	0.679254
N	0.038405	-3.229373	-2.898156	H	5.760374	0.260711	1.329029
C	1.119431	-4.050173	2.047529	C	-4.533656	-0.903799	-1.764827
C	0.659326	-4.101522	3.383873	C	-4.569689	-1.551529	1.116652
C	-0.730241	-4.102792	3.367692	C	-5.282169	-0.460444	0.554694
C	-1.159237	-4.052156	2.021138	H	-5.789629	0.251048	1.192112
N	-0.01077	-4.158684	1.251806	C	-5.264884	-0.154069	-0.807066
C	-2.785552	-3.194093	0.357962	H	-5.760638	0.764641	-1.090046
C	-3.877922	-2.289306	0.158881	C	1.299167	-3.450779	4.413144
C	-3.861149	-1.984377	-1.198539	C	-1.394929	-3.453345	4.381861
C	-2.759816	-2.723181	-1.739711	C	-0.767006	-2.760147	5.472175
N	-2.117861	-3.458421	-0.794964	C	0.644965	-2.758583	5.488586
C	2.783509	-3.189739	0.422766	C	1.412966	-1.251479	-5.429336
C	3.878916	-2.283112	0.249846	C	0.778166	-0.166747	-6.124436
C	3.893592	-1.977188	-1.107364	C	-1.281562	-1.255136	-5.460981
C	2.806896	-2.717662	-1.674842	C	-0.633621	-0.16896	-6.14161
N	2.143962	-3.454533	-0.745925	C	-3.97811	2.457661	-5.42741
C	-2.409617	-3.481491	1.674302	C	-4.278145	5.023438	-6.428122
H	0.000281	-4.018844	0.247945	C	-5.079884	3.232946	-5.012881
H	0.028091	-3.529142	-1.930063	C	-2.991598	2.963088	-6.327891
C	3.118365	-2.801629	2.813256	C	-3.172694	4.26337	-6.809893
C	3.835416	-1.027174	4.933301	C	-5.223268	4.522557	-5.539137
C	2.54861	-2.859104	4.095874	H	-2.437678	4.687884	-7.489084
C	4.180483	-1.836738	2.620239	H	-6.072001	5.134384	-5.244812
C	4.621102	-1.057308	3.742828	H	-4.395833	6.027132	-6.824867
C	2.790868	-1.911796	5.065709	C	4.095604	2.470176	-5.327003
C	-4.703448	-1.063408	3.63399	C	4.408605	5.039651	-6.314851
C	-2.63767	-2.863535	4.035383	C	3.128153	2.974142	-6.248676
C	-3.94609	-1.033353	4.842969	C	5.184759	3.248643	-4.885921
C	-4.235621	-1.842518	2.521904	C	5.335338	4.539987	-5.406028
C	-3.177257	-2.8064	2.739904	C	3.314996	4.276344	-6.72316
C	-2.904036	-1.916999	4.99949	H	6.174989	5.154149	-5.091261
C	-4.611955	0.613039	-3.8365	H	2.59371	4.699759	-7.417604
C	-2.532772	-0.859426	-4.922266	H	4.531348	6.044766	-6.706418
C	-3.8298	1.148194	-4.903419	C	-4.112313	-0.066449	5.866947
C	-4.166306	-0.568581	-3.15174	C	-4.442407	1.84405	7.845286
C	-3.099908	-1.354681	-3.736773	C	-5.210268	0.814719	5.795591
C	-2.782152	0.408036	-5.399054	C	-3.144884	0.010853	6.914495
C	2.650173	-0.852683	-4.861061	C	-3.340483	0.990247	7.893648
C	4.698847	0.624969	-3.724717	C	-5.36957	1.764849	6.811508
C	2.906832	0.416176	-5.330349	H	-2.619207	1.089707	8.700874
C	3.190649	-1.347179	-3.662859	H	-6.215811	2.44635	6.785639

H	-4.571513	2.589833	8.623626	H	-1.046606	2.652501	-7.275604
C	3.976444	-0.059124	5.959878	C	-5.775776	1.405916	-3.513507
C	4.257247	1.854285	7.942644	H	-6.530787	0.997812	-2.852658
C	2.984091	0.018215	6.983872	C	-5.996668	2.626514	-4.077392
C	5.075057	0.822965	5.913425	H	-6.899111	3.174899	-3.819759
C	5.209069	1.774515	6.931542	C	-1.831117	-1.814137	5.963233
C	3.155357	0.999347	7.965955	C	-1.96833	-0.851925	6.915633
H	6.055003	2.456854	6.924946	H	-1.21613	-0.676861	7.679904
H	2.414943	1.099265	8.755632	C	-6.106594	0.661551	4.674614
H	4.367039	2.601257	8.722789	H	-7.007999	1.268654	4.65566
C	1.960166	2.182822	-6.619907	C	-5.866711	-0.207017	3.652731
H	1.206713	2.658488	-7.241547	H	-6.605922	-0.29733	2.866036
C	1.832719	0.907237	-6.164358	C	5.783164	-0.200538	3.78825
C	5.852507	1.421138	-3.374246	H	6.5408	-0.291533	3.019347
H	6.593732	1.014453	-2.697084	C	5.99824	0.669209	4.814531
C	6.08213	2.643353	-3.931076	H	6.899392	1.276977	4.816352
H	6.97679	3.19415	-3.6523	C	1.809056	-0.846549	6.958214
C	-1.690477	0.901432	-6.208486	H	1.038996	-0.671735	7.704553
C	-1.812306	2.17539	-6.67023	C	1.695404	-1.810137	6.003927

### Intermediate 13e

C	-2.818866	-3.39783	2.686235	H	-0.431715	-2.256297	3.74735
C	2.029571	1.510631	3.68788	C	2.824018	2.588669	3.057225
C	2.021144	-3.193392	2.542271	C	3.690652	4.670781	1.300476
C	0.76967	-3.767515	2.855079	C	2.242903	3.868735	3.027662
C	0.352146	-4.978072	2.242267	C	3.963002	2.381771	2.192407
C	-1.034639	-5.047471	2.258429	C	4.47804	3.492571	1.433741
C	-1.516296	-3.877078	2.922102	C	2.564025	4.810203	2.078773
N	-0.388043	-3.198893	3.377442	C	-4.788413	3.148534	0.567765
C	0.725213	1.845716	4.1632	C	-2.922008	3.70563	2.540013
C	0.252021	3.173163	4.118569	C	-4.03484	4.35742	0.527717
C	-1.132425	3.139661	3.996462	C	-4.421449	2.109495	1.490359
C	-1.542758	1.793415	3.984599	C	-3.459723	2.40904	2.532755
N	-0.401078	1.04353	4.191958	C	-3.097772	4.596308	1.507981
C	-3.203473	0.093635	3.237358	C	-4.732078	-3.565734	-0.501767
C	-4.30807	-0.144106	2.356371	C	-2.946953	-5.149116	0.868568
C	-4.385509	-1.520635	2.283807	C	-3.989373	-4.494718	-1.235823
C	-3.259407	-2.064851	3.007477	C	-4.556959	-3.433855	0.873617
N	-2.57439	-1.076519	3.616282	C	-3.542364	-4.097575	1.597769
C	2.438244	0.205889	3.436059	C	-3.126517	-5.316453	-0.515038
C	3.585028	0.015503	2.604584	C	2.288841	-4.980586	0.888244
C	3.574217	-1.3329	2.259879	C	4.462012	-3.858876	-0.394596
C	2.414046	-1.884239	2.909307	C	2.59856	-5.385082	-0.392946
N	1.743151	-0.965554	3.62682	C	2.828433	-3.831719	1.480922
C	-2.76794	1.402397	3.367297	C	3.950324	-3.229967	0.788194
H	-0.361937	0.034269	4.100627	C	3.697342	-4.878389	-1.039344

C	4.329476	0.984252	1.931772	C	-3.228884	7.256022	-1.641738
C	4.313767	-1.867136	1.208721	C	-5.147956	6.085066	-2.556069
C	5.112501	-0.903428	0.541627	H	-2.508003	8.065848	-1.72118
H	5.667758	-1.169032	-0.346995	H	-5.910311	5.99309	-3.325292
C	5.118388	0.446588	0.883524	H	-4.275108	7.841386	-3.422927
H	5.678484	1.09963	0.228015	C	3.910719	5.674076	0.322404
C	-4.957493	-2.112568	1.197875	C	4.346129	7.610587	-1.608898
C	-4.807072	0.696844	1.342927	C	2.916906	6.680102	0.123612
C	-5.3036	0.03803	0.165499	C	5.08683	5.619585	-0.452076
H	-5.469511	0.625006	-0.730555	C	5.297217	6.615879	-1.415081
C	-5.361746	-1.358671	0.070909	C	3.167656	7.639181	-0.861194
C	0.935992	4.19083	3.487779	H	6.202677	6.60311	-2.016164
C	-1.74704	4.112644	3.232598	H	2.430331	8.415177	-1.050801
C	-1.072208	5.168081	2.548364	H	4.515447	8.373376	-2.362676
C	0.339196	5.219705	2.697105	C	1.731732	-6.575714	-2.264527
C	1.033623	-5.544694	1.198004	H	1.00304	-7.177301	-2.801796
C	0.428861	-6.147567	0.038456	C	1.531626	-6.154978	-0.984742
C	-1.659814	-5.645461	1.177613	C	5.6838	-3.528459	-1.094711
C	-0.973296	-6.134119	0.000908	H	6.429193	-2.914238	-0.604677
C	-3.788593	-4.295325	-2.619046	C	5.970295	-4.035078	-2.326488
C	-3.328605	-3.851398	-5.302786	H	6.91407	-3.775342	-2.79901
C	-4.451232	-3.20356	-3.248423	C	-1.962975	-5.93369	-1.115664
C	-2.775432	-5.051778	-3.268123	C	-1.846827	-5.849045	-2.476537
C	-2.588082	-4.825149	-4.639873	H	-0.976882	-6.242394	-2.993964
C	-4.219521	-3.024375	-4.616091	C	-5.23968	-2.331393	-1.081434
H	-1.829434	-5.386327	-5.179366	C	-5.148716	-2.204428	-2.436363
H	-4.706934	-2.207291	-5.141833	H	-5.456379	-1.290014	-2.938883
H	-3.164168	-3.68861	-6.363362	C	-2.029764	5.571029	1.456505
C	3.920606	-5.346042	-2.358872	C	-2.067164	6.444883	0.414735
C	4.373561	-6.241442	-4.939241	H	-1.306303	7.2057	0.263918
C	2.958512	-6.211701	-2.962681	C	-5.992348	4.027766	-1.380654
C	5.077765	-4.91835	-3.04097	H	-6.817364	3.947792	-2.083808
C	5.297095	-5.389432	-4.340002	C	-5.848017	3.081476	-0.410239
C	3.218669	-6.640788	-4.269237	H	-6.582439	2.286698	-0.343541
H	6.188056	-5.084625	-4.882613	C	5.713823	3.528562	0.688678
H	2.50661	-7.293433	-4.768046	H	6.465862	2.769265	0.868207
H	4.551437	-6.596624	-5.949548	C	6.001001	4.536299	-0.184036
C	-4.100325	5.303019	-0.527026	H	6.954969	4.532322	-0.704905
C	-4.226251	7.124056	-2.609422	C	1.662299	6.655653	0.869872
C	-5.091088	5.146319	-1.517456	H	0.903122	7.385203	0.601513
C	-3.13831	6.357689	-0.574657	C	1.468161	5.723626	1.840773

## Intermediate 14d

C	-2.674016	-2.991833	-3.054795	C	3.982169	-0.81627	-2.949186
C	2.484639	-4.062829	1.658943	C	3.585004	1.069694	-4.502057
C	2.168502	-2.691892	-2.979042	C	4.738672	-2.383884	0.940165
C	0.901534	-3.020758	-3.526796	C	4.452226	-1.328743	-1.653251
C	0.435147	-2.395852	-4.70592	C	5.121372	-0.588092	-0.621946
C	-0.949964	-2.481244	-4.752991	H	5.364409	0.452899	-0.799129
C	-1.375206	-3.181397	-3.586951	C	5.248101	-1.090814	0.677251
N	-0.217963	-3.583964	-2.934718	C	-4.84589	-1.600657	-1.728498
C	1.172909	-4.374873	2.091393	C	-4.531384	-1.629707	1.068492
C	0.772164	-4.151119	3.440742	C	-5.151354	-0.518862	0.404087
C	-0.606216	-3.983875	3.44398	H	-5.342996	0.387221	0.966497
C	-1.092136	-4.08849	2.120399	C	-5.290351	-0.481081	-0.987164
N	0.002854	-4.44053	1.346967	C	1.506804	-3.432981	4.372125
C	-2.843543	-3.452374	0.447739	C	-1.175694	-3.147144	4.373409
C	-4.016417	-2.645029	0.2415	C	-0.45531	-2.353331	5.323229
C	-4.174492	-2.629536	-1.131575	C	0.950336	-2.469203	5.285984
C	-3.042542	-3.307258	-1.712121	C	1.05598	-1.298745	-5.253226
N	-2.268714	-3.846901	-0.726143	C	0.386938	-0.167667	-5.821736
C	2.850184	-3.860697	0.293062	C	-1.637379	-1.426347	-5.334267
C	4.021622	-3.071821	0.003376	C	-1.023328	-0.217211	-5.817732
C	3.87742	-2.554768	-1.270341	C	-3.983004	2.248235	-3.992256
C	2.666987	-3.161021	-1.757066	C	-3.697092	4.965236	-3.603555
N	2.060257	-3.94305	-0.815913	C	-4.668685	2.853381	-2.902024
C	-2.334504	-3.511189	1.751743	C	-3.022989	2.948707	-4.771764
H	0.003322	-4.437372	0.332543	C	-2.92441	4.332855	-4.574117
H	-0.2293	-3.967207	-1.995514	C	-4.527969	4.237367	-2.751167
C	3.327148	-3.402428	2.688885	H	-2.209687	4.910234	-5.154881
C	4.091576	-1.011729	4.137102	H	-5.038942	4.744639	-1.936812
C	2.820548	-3.083936	3.969172	H	-3.602783	6.037687	-3.464574
C	4.404786	-2.577645	2.304753	C	3.727756	2.415885	-4.922265
C	4.74066	-1.391495	2.961925	C	4.026113	5.045072	-5.734042
C	3.152204	-1.903762	4.649796	C	2.73149	2.988115	-5.77103
C	-4.405846	-0.713593	3.463049	C	4.842917	3.150422	-4.470763
C	-2.391456	-2.52925	3.995267	C	4.983115	4.475893	-4.90004
C	-3.571845	-0.545668	4.607867	C	2.912624	4.319782	-6.157847
C	-4.049733	-1.674452	2.457334	H	5.840732	5.060529	-4.577589
C	-3.008521	-2.64311	2.743348	H	2.173333	4.795701	-6.797189
C	-2.556183	-1.444182	4.82491	H	4.143451	6.07485	-6.057257
C	-4.776537	0.086231	-3.219194	C	-3.648843	0.545872	5.508529
C	-2.935501	-1.191102	-4.814862	C	-3.814965	2.686516	7.255771
C	-4.097748	0.850946	-4.168304	C	-4.71843	1.454798	5.379613
C	-4.508516	-1.276404	-3.067071	C	-2.632627	0.701697	6.499862
C	-3.470856	-1.946835	-3.747341	C	-2.746558	1.796222	7.363231
C	-3.199927	0.174366	-4.991233	C	-4.792257	2.525693	6.278694
C	2.297589	-0.934062	-4.680298	H	-1.989453	1.955487	8.126989
C	4.397784	0.435532	-3.516356	H	-5.613616	3.234071	6.208837
C	2.526536	0.375325	-5.035003	H	-3.880434	3.523251	7.944457
C	2.895868	-1.547339	-3.572669	C	4.050893	0.351157	4.507624



C	3.912208	3.020966	5.189073	H	-1.217104	2.771059	-5.969186
C	3.120088	0.750035	5.504793	C	-5.28618	0.654543	-1.983451
C	4.7793	1.289604	3.7242	C	-5.286841	2.014252	-1.876273
C	4.713086	2.631614	4.114861	H	-5.606145	2.50778	-0.960977
C	3.096056	2.107901	5.851455	C	-1.435269	-1.279701	5.720547
H	5.258867	3.384039	3.551433	C	-1.496403	-0.212338	6.56391
H	2.405831	2.456971	6.615157	H	-0.721547	-0.000867	7.296106
H	3.875973	4.068591	5.471204	C	-5.681204	1.195311	4.334722
C	1.549584	2.227413	-6.165199	H	-6.560731	1.831951	4.283504
H	0.794443	2.741431	-6.754104	C	-5.535949	0.186685	3.429341
C	1.424635	0.92483	-5.789561	H	-6.321927	0.026037	2.700102
C	5.572331	1.196113	-3.155149	C	5.292106	-0.4223	2.031008
H	6.341723	0.730091	-2.55003	C	5.364262	0.873657	2.450143
C	5.779286	2.463595	-3.61197	H	5.719177	1.661164	1.7889
H	6.690184	2.986305	-3.331717	C	2.100142	-0.187343	5.960346
C	-2.076358	0.838919	-5.620781	H	1.294739	0.222619	6.562009
C	-2.048269	2.204504	-5.560762	C	2.057338	-1.472386	5.495289

### Intermediate 15c

C	-2.882359	-3.141303	-2.661692	C	3.872541	-0.794553	4.257625
C	2.209582	-4.022339	2.031757	C	2.528319	-2.823666	4.231983
C	2.003478	-2.922072	-2.68526	C	4.168695	-2.531908	2.58251
C	0.70507	-3.218989	-3.207605	C	4.539049	-1.311147	3.143946
C	0.223853	-2.573739	-4.362852	C	2.872776	-1.589066	4.801114
C	-1.163597	-2.615336	-4.366954	C	-4.598378	-0.820657	3.134274
C	-1.574942	-3.322759	-3.208371	C	-2.759037	-2.505998	4.268821
N	-0.414041	-3.736082	-2.578438	C	-3.818477	-0.323403	4.178396
C	0.910012	-4.315114	2.488294	C	-4.430304	-2.118016	2.667912
C	0.497561	-3.945371	3.807441	C	-3.385454	-2.967472	3.09434
C	-0.88626	-3.870483	3.830539	C	-2.922456	-1.206988	4.766858
C	-1.380907	-4.217346	2.534765	C	-4.879556	0.000655	-2.666249
N	-0.264607	-4.57763	1.786573	C	-3.112152	-1.26429	-4.345639
C	-3.19753	-3.856854	0.791716	C	-4.185858	0.778574	-3.58545
C	-4.430361	-3.133385	0.534713	C	-4.670451	-1.378609	-2.586546
C	-4.49256	-2.942953	-0.826901	C	-3.657355	-2.047927	-3.303488
C	-3.306312	-3.547643	-1.379201	C	-3.335826	0.108473	-4.465326
N	-2.556343	-4.131133	-0.365146	C	2.145497	-1.18471	-4.417982
C	2.602283	-3.92417	0.640866	C	4.352413	0.098311	-3.357787
C	3.814837	-3.200288	0.320907	C	2.414478	0.111384	-4.784712
C	3.716302	-2.774332	-0.991931	C	2.760075	-1.81896	-3.32889
C	2.494741	-3.362468	-1.460485	C	3.893293	-1.126002	-2.754897
N	1.839329	-4.063199	-0.461339	C	3.526142	0.762363	-4.305871
C	-2.6814	-3.852116	2.138966	C	4.54314	-2.46984	1.215045
H	-0.289195	-4.693315	0.779658	C	4.351705	-1.602593	-1.44815
H	-0.399498	-4.140997	-1.648268	C	5.043611	-0.821348	-0.465892
C	3.050356	-3.282476	3.00457	H	5.333859	0.192436	-0.714907

C	5.126891	-1.228452	0.866182	H	-1.692735	3.313316	5.968555
C	-5.083673	-1.789467	-1.298686	H	-4.722834	4.007512	3.011193
C	-4.948382	-2.154845	1.350046	H	-3.122567	4.848174	4.68153
C	-5.417043	-0.86201	0.913388	C	3.891632	0.591698	4.517744
C	-5.488595	-0.671676	-0.481683	C	3.880509	3.304693	4.991898
C	1.210186	-3.107372	4.640282	C	2.963455	1.109109	5.461393
C	-1.475549	-2.935815	4.660324	C	4.688942	1.424949	3.684834
C	-0.760734	-1.917941	5.397902	C	4.682731	2.793998	3.968902
C	0.639651	-2.026233	5.414031	C	3.007436	2.489619	5.706393
C	0.860533	-1.492756	-4.934031	H	5.278788	3.472917	3.364583
C	0.215086	-0.337525	-5.456046	H	2.326635	2.931382	6.429695
C	-1.834896	-1.523948	-4.912542	H	3.894539	4.371543	5.192439
C	-1.202747	-0.331346	-5.383065	C	1.449424	2.011653	-5.844437
C	-4.019129	2.15982	-3.349277	H	0.679628	2.560951	-6.380823
C	-3.630116	4.837452	-2.833279	C	1.294981	0.711508	-5.473407
C	-4.683923	2.735124	-2.232099	C	5.575208	0.803417	-3.05394
C	-3.040408	2.857959	-4.10741	H	6.350592	0.301801	-2.485059
C	-2.885607	4.223433	-3.840087	C	5.815482	2.062809	-3.519981
C	-4.490498	4.105535	-2.016423	H	6.761084	2.544723	-3.285437
H	-2.152383	4.802236	-4.395861	C	-2.202594	0.757843	-5.097026
H	-4.984725	4.595236	-1.181025	C	-2.112006	2.114416	-4.957667
H	-3.491706	5.89728	-2.64306	H	-1.261938	2.666309	-5.348074
C	3.702016	2.104198	-4.727298	C	-5.384324	0.517969	-1.409984
C	4.055034	4.729201	-5.526497	C	-5.349411	1.875855	-1.254384
C	2.682618	2.722926	-5.513904	H	-5.703379	2.355659	-0.347645
C	4.865918	2.791032	-4.32726	C	-1.740975	-0.770263	5.479322
C	5.033016	4.116174	-4.751874	C	-1.651374	0.572086	5.73874
C	2.892357	4.050509	-5.896221	H	-0.795694	0.99767	6.250638
H	5.927185	4.665549	-4.469051	C	-5.137746	1.373053	2.344029
H	2.137237	4.562483	-6.487445	H	-5.542244	2.088599	1.635597
H	4.192724	5.75793	-5.845111	C	-5.197175	0.026636	2.11702
C	-3.647223	1.065899	4.328569	C	5.16483	-0.44931	2.156694
C	-3.260062	3.776914	4.572401	C	5.286792	0.873316	2.46799
C	-4.382018	1.928198	3.469134	H	5.697913	1.584107	1.754417
C	-2.614709	1.521657	5.19061	C	1.888108	0.261224	5.960591
C	-2.462283	2.910304	5.315072	H	1.126782	0.742761	6.565393
C	-4.182743	3.301964	3.637469	C	1.772426	-1.04448	5.564741

### Intermediate 16a

C	-2.461209	-3.59679	2.420024	N	-2.251995	-4.25678	-0.033933
C	2.461209	-3.59679	-2.420024	C	2.925791	-3.827702	-1.101169
C	-2.38845	-3.597377	-2.49295	C	4.124011	-3.216996	-0.630992
C	-2.892066	-3.827962	-1.188372	C	4.103558	-3.217155	0.753946
C	-4.103558	-3.217155	-0.753946	C	2.892066	-3.827962	1.188372
C	-4.124011	-3.216996	0.630992	N	2.251995	-4.25678	0.033933
C	-2.925791	-3.827702	1.101169	C	1.054454	-3.84326	2.94177

C	0.627114	-3.232538	4.182496	C	-5.279643	-1.006986	-0.785679
C	-0.751285	-3.232167	4.161714	C	-4.779048	-2.180114	1.273559
C	-1.141271	-3.842883	2.908821	C	-5.300067	-1.006551	0.627428
N	-0.03277	-4.244182	2.211591	C	-3.85189	1.543773	3.752707
C	1.141271	-3.842883	-2.908821	C	-3.681672	4.284251	3.589068
C	0.751285	-3.232167	-4.161714	C	-2.885248	2.205438	4.556605
C	-0.627114	-3.232538	-4.182496	C	-4.617194	2.205987	2.756077
C	-1.054454	-3.84326	-2.94177	C	-4.530968	3.604356	2.71832
N	0.03277	-4.244182	-2.211591	C	-2.843901	3.601892	4.472091
C	2.38845	-3.597377	2.49295	H	-5.102843	4.16123	1.98033
H	1.288321	-4.5729	0.019902	H	-2.128016	4.158627	5.0716
H	-1.288321	-4.5729	-0.019902	H	-3.62894	5.367417	3.539838
C	3.262872	-2.608853	-3.184671	C	-3.741692	1.542368	-3.868233
C	3.916738	0.137867	-3.813935	C	-3.579085	4.28313	-3.702345
C	4.336619	-1.914215	-2.588713	C	-4.537268	2.204742	-2.895762
C	2.708405	-1.914648	-4.281012	C	-2.751783	2.204174	-4.643243
C	2.973119	-0.5735	-4.549992	C	-2.714258	3.600768	-4.5589
C	4.61928	-0.571025	-2.846616	C	-4.453635	3.603224	-2.856972
C	2.838009	-0.574547	4.637674	H	-1.980951	4.157527	-5.136935
C	4.25844	-1.915447	2.717319	H	-5.048293	4.160386	-2.13743
C	3.803641	0.13639	3.930322	H	-3.529028	5.366403	-3.652692
C	2.580724	-1.915601	4.360624	C	3.741692	1.542368	3.868233
C	3.167383	-2.609838	3.281144	C	3.579085	4.28313	3.702345
C	4.533935	-0.572589	2.983905	C	2.751783	2.204174	4.643243
C	-2.973119	-0.5735	4.549992	C	4.537268	2.204742	2.895762
C	-4.336619	-1.914215	2.588713	C	4.453635	3.603224	2.856972
C	-3.916738	0.137867	3.813935	C	2.714258	3.600768	4.5589
C	-2.708405	-1.914648	4.281012	H	5.048293	4.160386	2.13743
C	-3.262872	-2.608853	3.184671	H	1.980951	4.157527	5.136935
C	-4.61928	-0.571025	2.846616	H	3.529028	5.366403	3.652692
C	-4.25844	-1.915447	-2.717319	C	3.85189	1.543773	-3.752707
C	-2.838009	-0.574547	-4.637674	C	3.681672	4.284251	-3.589068
C	-4.533935	-0.572589	-2.983905	C	4.617194	2.205987	-2.756077
C	-3.167383	-2.609838	-3.281144	C	2.885248	2.205438	-4.556605
C	-2.580724	-1.915601	-4.360624	C	2.843901	3.601892	-4.472091
C	-3.803641	0.13639	-3.930322	C	4.530968	3.604356	-2.71832
C	1.41035	-2.189452	-4.775579	H	2.128016	4.158627	-5.0716
C	-1.268196	-2.190063	-4.815642	H	5.102843	4.16123	-1.98033
C	-0.625106	-1.009298	-5.33883	H	3.62894	5.367417	-3.539838
C	0.782552	-1.00892	-5.31753	C	-5.230945	1.428176	-1.870646
C	-1.41035	-2.189452	4.775579	H	-5.693302	1.992499	-1.068062
C	1.268196	-2.190063	4.815642	C	-5.171205	0.061046	-1.847744
C	0.625106	-1.009298	5.33883	C	-1.688437	0.060259	-5.252495
C	-0.782552	-1.00892	5.31753	C	-1.710566	1.42583	-5.315184
C	4.779048	-2.180114	-1.273559	H	-0.898661	1.990067	-5.760939
C	4.739808	-2.180778	1.415765	C	-5.222136	0.06207	1.691522
C	5.279643	-1.006986	0.785679	C	-5.280793	1.429279	1.711363
C	5.300067	-1.006551	-0.627428	H	-5.717787	1.993524	0.894659
C	-4.739808	-2.180778	-1.415765	C	-1.842295	0.061125	5.19889

C	-1.865342	1.426734	5.260048	C	1.688437	0.060259	5.252495
H	-1.066555	1.990556	5.72939	C	1.842295	0.061125	-5.19889
C	5.171205	0.061046	1.847744	C	1.865342	1.426734	-5.260048
C	5.230945	1.428176	1.870646	H	1.066555	1.990556	-5.72939
H	5.693302	1.992499	1.068062	C	5.280793	1.429279	-1.711363
C	1.710566	1.42583	5.315184	H	5.717787	1.993524	-0.894659
H	0.898661	1.990067	5.760939	C	5.222136	0.06207	-1.691522

### Intermediate 17a

C	-3.689124	2.409224	2.037218	C	-0.629179	-4.434884	2.752752
C	-3.394595	-2.404976	-2.907903	C	-0.901014	2.860432	4.494645
C	-3.394595	2.404976	-2.907903	C	-1.948627	4.207189	2.3589
C	-3.637756	2.872801	-1.592391	C	-0.068099	3.750914	3.821885
C	-2.964854	4.025562	-1.093319	C	-2.211646	2.628412	4.074193
C	-3.067462	4.034386	0.286111	C	-2.755969	3.181837	2.894976
C	-3.785201	2.876594	0.698469	C	-0.629179	4.434884	2.752752
N	-4.174409	2.242439	-0.472462	C	-1.520155	4.088475	-2.952512
C	-3.637756	-2.872801	-1.592391	C	-0.28265	2.615508	-4.90147
C	-2.964854	-4.025562	-1.093319	C	-0.128025	4.12043	-3.079796
C	-3.067462	-4.034386	0.286112	C	-2.325644	3.147437	-3.627658
C	-3.785201	-2.876594	0.698469	C	-1.687189	2.595174	-4.756212
N	-4.174409	-2.242439	-0.472462	C	0.508854	3.272229	-3.976695
C	-4.009426	-1.096419	2.498353	C	-2.154877	-1.386369	-5.346669
C	-3.543818	-0.691046	3.810806	C	-2.154877	1.386369	-5.346669
C	-3.543818	0.691046	3.810806	C	-1.028327	0.684568	-5.884922
C	-4.009426	1.096419	2.498353	C	-1.028327	-0.684568	-5.884922
N	-4.341083	0	1.749453	C	-2.577748	1.34331	4.546455
C	-3.710139	-1.101617	-3.421503	C	-2.577748	-1.34331	4.546455
C	-3.168565	-0.706378	-4.706475	C	-1.480787	-0.701883	5.23541
C	-3.168565	0.706378	-4.706475	C	-1.480787	0.701883	5.23541
C	-3.710139	1.101617	-3.421503	C	-1.818707	-4.562218	-1.658949
N	-4.076295	0	-2.697372	C	-2.04958	-4.622036	1.014297
C	-3.689124	-2.409224	2.037218	C	-0.780734	-5.028211	0.47865
H	-4.546868	-1.29977	-0.493162	C	-0.642011	-4.931673	-0.921648
H	-4.546868	1.29977	-0.493162	C	-1.818707	4.562218	-1.658949
C	-2.325644	-3.147437	-3.627658	C	-0.642011	4.931673	-0.921648
C	0.508854	-3.272229	-3.976695	C	-2.04958	4.622036	1.014297
C	-1.520155	-4.088475	-2.952512	C	-0.780734	5.028211	0.47865
C	-1.687189	-2.595174	-4.756212	C	1.332156	3.640809	3.93098
C	-0.28265	-2.615508	-4.90147	C	4.06431	3.385584	4.117463
C	-0.128025	-4.12043	-3.079796	C	1.856779	2.698048	4.853628
C	-0.901014	-2.860432	4.494645	C	2.137352	4.336327	2.988697
C	-1.948627	-4.207189	2.3589	C	3.525892	4.208443	3.12968
C	-0.068099	-3.750914	3.821885	C	3.251069	2.612883	4.946943
C	-2.211646	-2.628412	4.074193	H	4.188778	4.72692	2.441598
C	-2.755969	-3.181837	2.894976	H	3.7047	1.91244	5.643724

H	5.142892	3.300582	4.205783	H	4.246251	-0.852333	-4.98192
C	1.822739	2.809212	-3.727212	H	4.479261	-3.645086	-1.761163
C	4.482697	2.262448	-3.409365	H	5.552973	-2.087772	-3.360945
C	2.532421	3.4701	-2.685833	C	1.822769	4.325686	-1.733684
C	2.338361	1.668096	-4.429141	H	2.382299	4.617694	-0.850628
C	3.722116	1.521685	-4.321148	C	0.489477	4.603069	-1.865606
C	3.891642	3.161617	-2.537081	C	0.169801	1.373681	-5.516424
H	4.246251	0.852333	-4.98192	C	1.377257	0.752717	-5.156039
H	4.479261	3.645086	-1.761163	C	0.158386	4.948248	1.652139
H	5.552973	2.087772	-3.360945	C	1.515232	4.966638	1.826224
C	1.332156	-3.640809	3.93098	H	2.181902	5.352568	1.060325
C	4.06431	-3.385584	4.117463	C	-0.383881	1.736142	5.24544
C	1.856779	-2.698048	4.853628	C	0.961866	1.733236	5.490182
C	2.137352	-4.336327	2.988697	H	1.435523	0.948714	6.067967
C	3.525892	-4.208443	3.12968	C	0.158386	-4.948248	1.652139
C	3.251069	-2.612883	4.946943	C	1.515232	-4.966638	1.826224
H	4.188778	-4.72692	2.441598	H	2.181902	-5.352568	1.060325
H	3.7047	-1.91244	5.643724	C	0.961866	-1.733236	5.490182
H	5.142892	-3.300582	4.205783	H	1.435523	-0.948714	6.067967
C	1.822739	-2.809212	-3.727212	C	-0.383881	-1.736142	5.24544
C	4.482697	-2.262448	-3.409365	C	0.169801	-1.373681	-5.516424
C	2.532421	-3.4701	-2.685833	C	1.377257	-0.752717	-5.156039
C	2.338361	-1.668096	-4.429141	C	1.822769	-4.325686	-1.733684
C	3.722116	-1.521685	-4.321148	H	2.382299	-4.617694	-0.850628
C	3.891642	-3.161617	-2.537081	C	0.489477	-4.603069	-1.865606

### Intermediate 18c

C	-3.599557	2.374968	1.866802	C	-3.031695	-0.750915	-4.851448
C	-3.243778	-2.455598	-3.058213	C	-3.048492	0.664165	-4.854041
C	-3.30078	2.369423	-3.066842	C	-3.592161	1.055156	-3.570676
C	-3.558628	2.840818	-1.759427	N	-3.93945	-0.050551	-2.842042
C	-2.910866	4.008913	-1.26589	C	-3.543718	-2.452419	1.87515
C	-3.015179	4.018097	0.114384	H	-4.403222	-1.354333	-0.652856
C	-3.706123	2.843182	0.528355	H	-4.433173	1.248806	-0.657691
N	-4.083518	2.200389	-0.638038	C	-2.172208	-3.198161	-3.779161
C	-3.490732	-2.928628	-1.749431	C	0.685193	-3.303258	-4.119402
C	-2.815439	-4.07946	-1.252032	C	-1.359507	-4.139716	-3.110152
C	-2.920216	-4.086827	0.128201	C	-1.541629	-2.641362	-4.907107
C	-3.638966	-2.927268	0.53832	C	-0.134473	-2.650888	-5.038929
N	-4.031262	-2.297361	-0.630231	C	0.041687	-4.17034	-3.23375
C	-3.869291	-1.138199	2.328334	C	-0.740357	-2.873279	4.318461
C	-3.400222	-0.724222	3.637111	C	-1.799425	-4.245119	2.202452
C	-3.416196	0.65687	3.634652	C	0.088291	-3.772114	3.652498
C	-3.894522	1.055344	2.324506	C	-2.05419	-2.650157	3.904017
N	-4.217882	-0.046735	1.579061	C	-2.604646	-3.21549	2.733445
C	-3.566078	-1.150089	-3.566573	C	-0.478528	-4.467679	2.59331

C	-0.806242	2.868747	4.307699	C	3.722839	2.755596	-2.207498
C	-1.897604	4.209037	2.18774	H	4.298864	3.227329	-1.415582
C	0.001255	3.784119	3.638171	H	4.971315	1.052206	-2.215957
C	-2.114823	2.614058	3.894686	C	1.488663	-3.663147	3.755796
C	-2.67832	3.162609	2.722354	C	4.221399	-3.414926	3.930522
C	-0.581989	4.463311	2.577176	C	2.018359	-2.704373	4.659116
C	-1.45727	4.097669	-3.125014	C	2.288515	-4.381638	2.826418
C	-0.197069	2.631385	-5.04883	C	3.677886	-4.257135	2.961778
C	-0.057367	4.161402	-3.249249	C	3.413245	-2.622057	4.746066
C	-2.24725	3.134655	-3.790768	H	4.33728	-4.794312	2.284655
C	-1.603727	2.588906	-4.916868	H	3.8717	-1.910218	5.427936
C	0.606626	3.306648	-4.13183	H	5.300523	-3.332824	4.015191
C	-2.022148	-1.430154	-5.500486	C	1.940591	-2.727964	-3.744301
C	-2.055373	1.364654	-5.505818	C	4.13212	-1.420229	-2.657294
C	-0.92681	0.670293	-6.045709	C	2.600956	-3.300528	-2.630776
C	-0.910436	-0.711412	-6.043268	C	2.284158	-1.414819	-4.215884
C	-2.452939	1.320834	4.362104	C	3.312268	-0.705089	-3.564061
C	-2.422054	-1.363421	4.366825	C	3.7869	-2.671115	-2.197037
C	-1.323107	-0.709018	5.042279	H	4.373926	-3.125896	-1.403285
C	-1.339131	0.694141	5.039472	H	4.994245	-0.938539	-2.211417
C	-1.668897	-4.61713	-1.819431	C	1.836336	4.320174	-1.800762
C	-1.903546	-4.670629	0.860673	H	2.340005	4.590059	-0.87907
C	-0.636977	-5.084419	0.326195	C	0.525993	4.651589	-2.020246
C	-0.498601	-4.988895	-1.074683	C	0.240898	1.384532	-5.639659
C	-1.777636	4.571877	-1.835657	C	1.364847	0.733043	-5.128954
C	-0.616285	4.973577	-1.092559	C	0.187993	5.009264	1.479923
C	-2.012144	4.627944	0.844605	C	1.543572	5.073026	1.658158
C	-0.756	5.069693	0.308292	H	2.197558	5.500854	0.903711
C	1.403906	3.70713	3.740569	C	-0.26035	1.748483	5.044647
C	4.141739	3.519948	3.912513	C	1.087751	1.768894	5.275232
C	1.955792	2.762985	4.646025	H	1.583046	0.984923	5.835949
C	2.186524	4.440468	2.808177	C	0.304581	-4.998865	1.498129
C	3.578496	4.34707	2.94203	C	1.661075	-5.031341	1.677446
C	3.352254	2.7119	4.731398	H	2.325132	-5.446262	0.92455
H	4.225005	4.896831	2.262567	C	1.127338	-1.727952	5.284046
H	3.827159	2.012285	5.414655	H	1.604246	-0.931455	5.843121
H	5.222535	3.461884	3.995968	C	-0.220647	-1.738362	5.051888
C	1.875333	2.762807	-3.754608	C	0.273857	-1.396251	-5.634583
C	4.097782	1.511533	-2.663169	C	1.381984	-0.716309	-5.126388
C	2.522195	3.354782	-2.643481	C	1.93816	-4.27883	-1.78449
C	2.250065	1.45645	-4.221234	H	2.44793	-4.533363	-0.861739
C	3.294803	0.773708	-3.566949	C	0.636153	-4.6424	-2.002981

**Intermediate 19b**

C	-3.587564	2.395788	2.074494	C	-1.588072	2.605192	-4.778303
C	-3.238893	-2.400883	-2.879082	C	0.673791	3.264679	-4.0857
C	-3.238893	2.400883	-2.879082	C	-2.086478	-1.397399	-5.365713
C	-3.460032	2.86173	-1.559149	C	-2.086478	1.397399	-5.365713
C	-2.731345	3.973444	-1.05181	C	-0.993225	0.691258	-5.963012
C	-2.826103	3.971005	0.326918	C	-0.993225	-0.691258	-5.963012
C	-3.617532	2.855996	0.730708	C	-2.772513	1.387791	4.690855
N	-4.030118	2.248807	-0.446492	C	-2.772513	-1.387791	4.690855
C	-3.460032	-2.86173	-1.559149	C	-1.760917	-0.684743	5.427551
C	-2.731345	-3.973444	-1.05181	C	-1.760917	0.684743	5.427551
C	-2.826103	-3.971005	0.326918	C	-1.574925	-4.475454	-1.626124
C	-3.617532	-2.855996	0.730708	C	-1.75448	-4.460026	1.052916
N	-4.030118	-2.248807	-0.446492	C	-0.458167	-4.749916	0.505835
C	-3.994402	-1.100178	2.536698	C	-0.368021	-4.764293	-0.903256
C	-3.666529	-0.706673	3.894934	C	-1.574925	4.475454	-1.626124
C	-3.666529	0.706673	3.894934	C	-0.368021	4.764293	-0.903256
C	-3.994402	1.100178	2.536698	C	-1.75448	4.460026	1.052916
N	-4.25314	0	1.765703	C	-0.458167	4.749916	0.505835
C	-3.575682	-1.101491	-3.389272	C	1.448576	2.76251	3.797833
C	-3.069039	-0.707845	-4.688244	C	4.121286	2.236484	4.022741
C	-3.069039	0.707845	-4.688244	C	1.822933	1.650192	4.619716
C	-3.575682	1.101491	-3.389272	C	2.342972	3.39988	2.894004
N	-3.928118	0	-2.657673	C	3.706922	3.104779	3.025584
C	-3.587564	-2.395788	2.074494	C	3.201262	1.511899	4.789326
H	-4.442117	-1.323209	-0.476619	H	4.433085	3.573847	2.366864
H	-4.442117	1.323209	-0.476619	H	3.588104	0.864125	5.558275
C	-2.173899	-3.13932	-3.614702	H	5.181418	2.073625	4.189663
C	0.673791	-3.264679	-4.0857	C	1.966659	2.717689	-3.814403
C	-1.324155	-4.04708	-2.945413	C	4.279925	1.4627	-2.943114
C	-1.588072	-2.605192	-4.778303	C	2.689968	3.279308	-2.734585
C	-0.188542	-2.628864	-4.978491	C	2.310028	1.429319	-4.344481
C	0.0689	-4.075668	-3.125822	C	3.404359	0.738361	-3.788797
C	-0.842562	-2.600619	4.569503	C	3.932915	2.688558	-2.422252
C	-1.693686	-4.022681	2.390764	H	4.569656	3.146065	-1.669457
C	0.110711	-3.221313	3.7821	H	5.192492	1.001086	-2.585107
C	-2.200317	-2.587268	4.177752	C	1.448576	-2.76251	3.797833
C	-2.62799	-3.122887	2.94568	C	4.121286	-2.236484	4.022741
C	-0.344843	-4.028984	2.749914	C	1.822933	-1.650192	4.619716
C	-0.842562	2.600619	4.569503	C	2.342972	-3.39988	2.894004
C	-1.693686	4.022681	2.390764	C	3.706922	-3.104779	3.025584
C	0.110711	3.221313	3.7821	C	3.201262	-1.511899	4.789326
C	-2.200317	2.587268	4.177752	H	4.433085	-3.573847	2.366864
C	-2.62799	3.122887	2.94568	H	3.588104	-0.864125	5.558275
C	-0.344843	4.028984	2.749914	H	5.181418	-2.073625	4.189663
C	-1.324155	4.04708	-2.945413	C	1.966659	-2.717689	-3.814403
C	-0.188542	2.628864	-4.978491	C	4.279925	-1.4627	-2.943114
C	0.0689	4.075668	-3.125822	C	2.689968	-3.279308	-2.734585
C	-2.173899	3.13932	-3.614702	C	2.310028	-1.429319	-4.344481

C	3.404359	-0.738361	-3.788797	C	-0.51547	1.372068	5.283064
C	3.932915	-2.688558	-2.422252	C	0.738467	0.749801	5.163724
H	4.569656	-3.146065	-1.669457	C	0.485459	-4.456304	1.646681
H	5.192492	-1.001086	-2.585107	C	1.824202	-4.212654	1.793583
C	2.052074	4.187933	-1.798058	H	2.54911	-4.518768	1.04643
H	2.625255	4.452362	-0.916279	C	0.738467	-0.749801	5.163724
C	0.720793	4.488453	-1.903551	C	-0.51547	-1.372068	5.283064
C	0.202961	1.389902	-5.618165	C	0.202961	-1.389902	-5.618165
C	1.353962	0.724129	-5.19267	C	1.353962	-0.724129	-5.19267
C	0.485459	4.456304	1.646681	C	2.052074	-4.187933	-1.798058
C	1.824202	4.212654	1.793583	H	2.625255	-4.452362	-0.916279
H	2.54911	4.518768	1.04643	C	0.720793	-4.488453	-1.903551

### Intermediate 20b

C	2.402722	2.478283	-3.329218	C	-2.629716	4.77999	-0.43148
C	-2.402722	-2.478283	-3.329218	C	-4.051607	2.67729	-1.426864
C	2.402722	-2.478282	-3.329218	C	-3.267102	3.949012	0.488668
C	2.86615	-1.145987	-3.456823	C	-2.607202	4.486053	-1.814748
C	3.982656	-0.691054	-2.698766	C	-3.141584	3.28566	-2.31946
C	3.982656	0.691054	-2.698766	C	-4.080206	2.951429	-0.050347
C	2.86615	1.145987	-3.456823	C	2.629716	4.77999	-0.43148
N	2.254275	0	-3.947504	C	4.051607	2.67729	-1.426864
C	-2.86615	-1.145987	-3.456823	C	3.267102	3.949012	0.488668
C	-3.982656	-0.691054	-2.698766	C	2.607202	4.486053	-1.814748
C	-3.982656	0.691054	-2.698766	C	3.141584	3.28566	-2.31946
C	-2.86615	1.145987	-3.456823	C	4.080206	2.951429	-0.050347
N	-2.254275	0	-3.947504	C	4.051607	-2.67729	-1.426864
C	-1.101392	2.959619	-3.697625	C	2.629716	-4.77999	-0.43148
C	-0.707676	4.291833	-3.283291	C	4.080206	-2.951429	-0.050347
C	0.707676	4.291833	-3.283291	C	3.141584	-3.28566	-2.31946
C	1.101392	2.959619	-3.697625	C	2.607202	-4.486053	-1.814748
N	0	2.205461	-4.000787	C	3.267102	-3.949012	0.488668
C	-1.101392	-2.959619	-3.697625	C	-1.398058	-5.034986	-2.350819
C	-0.707676	-4.291833	-3.283291	C	1.398058	-5.034986	-2.350819
C	0.707676	-4.291833	-3.283291	C	0.690889	-5.705477	-1.300192
C	1.101392	-2.959619	-3.697625	C	-0.690889	-5.705477	-1.300192
N	0	-2.205461	-4.000787	C	1.398058	5.034986	-2.350819
C	-2.402722	2.478282	-3.329218	C	-1.398058	5.034986	-2.350819
H	-1.325969	0	-4.354862	C	-0.690889	5.705477	-1.300192
H	1.325969	0	-4.354862	C	0.690889	5.705477	-1.300192
C	-3.141584	-3.28566	-2.31946	C	-4.484814	-1.344957	-1.586133
C	-3.267102	-3.949012	0.488668	C	-4.484814	1.344957	-1.586133
C	-4.051607	-2.67729	-1.426864	C	-4.785413	0.707196	-0.3353
C	-2.607202	-4.486053	-1.814748	C	-4.785413	-0.707196	-0.3353
C	-2.629716	-4.77999	-0.43148	C	4.484814	-1.344957	-1.586133
C	-4.080206	-2.951429	-0.050347	C	4.785413	-0.707196	-0.3353



C	4.484814	1.344957	-1.586133	C	-1.464575	-3.043973	4.159633
C	4.785413	0.707196	-0.3353	C	-3.288559	-2.742302	2.59266
C	2.720339	3.765241	1.796667	C	-1.429793	-4.312235	2.102311
C	1.464575	3.043973	4.159633	C	-0.73861	-3.828014	3.229979
C	1.429793	4.312235	2.102311	C	-2.695507	-2.509235	3.851775
C	3.288559	2.742302	2.59266	H	-3.155802	-1.803908	4.539019
C	2.695507	2.509235	3.851775	H	-1.002129	-2.744218	5.09259
C	0.73861	3.828014	3.229979	C	4.209547	-1.773854	2.022179
H	3.155802	1.803908	4.539019	H	4.493658	-0.948028	2.663834
H	1.002129	2.744218	5.09259	C	4.503678	-1.779848	0.684586
C	2.720339	-3.765241	1.796667	C	1.390144	-5.443246	-0.083779
C	1.464575	-3.043973	4.159633	C	0.724131	-5.094639	1.09252
C	3.288559	-2.742302	2.59266	C	4.503678	1.779848	0.684586
C	1.429793	-4.312235	2.102311	C	4.209547	1.773854	2.022179
C	0.73861	-3.828014	3.229979	H	4.493658	0.948028	2.663834
C	2.695507	-2.509235	3.851775	C	1.390144	5.443246	-0.083779
H	3.155802	-1.803909	4.539019	C	0.724131	5.094639	1.09252
H	1.002129	-2.744218	5.09259	C	-4.503678	1.779848	0.684586
C	-2.720339	3.765241	1.796667	C	-4.209547	1.773854	2.022179
C	-1.464575	3.043973	4.159633	H	-4.493658	0.948028	2.663834
C	-1.429793	4.312235	2.102311	C	-0.724131	5.094639	1.09252
C	-3.288559	2.742302	2.59266	C	-1.390144	5.443246	-0.083779
C	-2.695507	2.509235	3.851775	C	-1.390144	-5.443246	-0.083779
C	-0.73861	3.828014	3.229979	C	-0.724131	-5.094639	1.09252
H	-3.155802	1.803908	4.539019	C	-4.209547	-1.773854	2.022179
H	-1.002129	2.744218	5.09259	H	-4.493658	-0.948028	2.663834
C	-2.720339	-3.765241	1.796667	C	-4.503678	-1.779848	0.684586

### Intermediate 21a

C	3.145795	2.456129	-2.770833	N	0.849157	2.201977	-3.783716
C	-1.650552	-2.481402	-3.54755	C	-0.321736	-2.962037	-3.652537
C	3.145795	-2.456129	-2.770833	C	-0.004023	-4.260705	-3.115479
C	3.665267	-1.150841	-2.904383	C	1.388848	-4.252752	-2.869187
C	4.755915	-0.706419	-2.085353	C	1.858605	-2.930078	-3.28129
C	4.755915	0.706419	-2.085353	N	0.849157	-2.201977	-3.783716
C	3.665267	1.150841	-2.904383	C	-1.650552	2.481402	-3.54755
N	3.107244	0	-3.462368	H	-0.398412	0	-4.330471
C	-2.100845	-1.143164	-3.79985	H	2.194049	0	-3.903745
C	-3.361715	-0.694078	-3.332184	C	-2.587072	-3.277319	-2.701396
C	-3.361715	0.694078	-3.332184	C	-3.291573	-3.810655	0.043898
C	-2.100845	1.143164	-3.79985	C	-3.692465	-2.667856	-2.063272
N	-1.390082	0	-4.117898	C	-2.145541	-4.434771	-2.035955
C	-0.321736	2.962037	-3.652537	C	-2.442788	-4.650633	-0.661832
C	-0.004023	4.260705	-3.115479	C	-4.025419	-2.899771	-0.722153
C	1.388848	4.252752	-2.869187	C	-2.442788	4.650633	-0.661832
C	1.858605	2.930078	-3.28129	C	-3.692465	2.667856	-2.063272

C	-3.291573	3.810655	0.043898	C	0.711393	-2.105615	4.248191
C	-2.145541	4.434771	-2.035955	C	2.706283	-1.716311	2.876883
C	-2.587072	3.277319	-2.701396	C	1.071682	-3.559442	2.390328
C	-4.025419	2.899771	-0.722153	C	0.167667	-3.013076	3.315534
C	2.739102	4.424028	0.275091	C	1.931317	-1.49646	4.036687
C	4.543568	2.63082	-0.681106	H	2.297469	-0.834011	4.800248
C	3.193379	3.442949	1.165698	H	0.140436	-1.805164	5.120257
C	3.00763	4.336043	-1.100413	C	-3.013971	3.489506	1.413139
C	3.69801	3.229907	-1.633863	C	-2.210805	2.385307	3.831834
C	4.232311	2.664091	0.716814	C	-1.748232	3.858314	1.971021
C	4.543568	-2.63082	-0.681106	C	-3.805887	2.485005	2.010602
C	2.739102	-4.424028	0.275091	C	-3.442231	2.057367	3.304604
C	4.232311	-2.664091	0.716814	C	-1.284787	3.175417	3.114882
C	3.69801	-3.229907	-1.633863	H	-4.07436	1.346808	3.831063
C	3.00763	-4.336043	-1.100413	H	-1.911619	1.91459	4.76165
C	3.193379	-3.442949	1.165698	C	-3.013971	-3.489506	1.413139
C	-0.851858	-4.976516	-2.291109	C	-2.210805	-2.385308	3.831834
C	1.894817	-4.925115	-1.782906	C	-3.805887	-2.485005	2.010602
C	1.006951	-5.50196	-0.814747	C	-1.748232	-3.858314	1.971021
C	-0.34587	-5.536937	-1.073422	C	-1.284787	-3.175418	3.114882
C	1.894817	4.925115	-1.782906	C	-3.442231	-2.057367	3.304604
C	-0.851858	4.976516	-2.291109	H	-4.074361	-1.346808	3.831063
C	-0.34587	5.536937	-1.073422	H	-1.911619	-1.91459	4.76165
C	1.006951	5.50196	-0.814747	C	3.727244	-0.768972	2.290433
C	-4.123849	-1.352179	-2.369833	C	4.539177	-1.378764	1.314004
C	-4.123849	1.352179	-2.369833	C	1.459267	-5.059253	0.464102
C	-4.741084	0.710997	-1.256405	C	0.591987	-4.560564	1.431221
C	-4.741084	-0.710997	-1.256405	C	4.539177	1.378764	1.314004
C	5.13597	-1.386476	-0.940395	C	3.727244	0.768972	2.290433
C	5.265781	-0.676972	0.300256	C	1.459267	5.059253	0.464102
C	5.13597	1.386476	-0.940395	C	0.591987	4.560564	1.431221
C	5.265781	0.676972	0.300256	C	-4.671929	1.736636	-0.160961
C	2.363599	2.946118	2.219339	C	-4.695273	1.665082	1.205616
C	0.711393	2.105615	4.248191	H	-5.205802	0.869283	1.727844
C	1.071683	3.559442	2.390328	C	-0.831011	4.675455	1.191091
C	2.706283	1.716311	2.876883	C	-1.262729	5.198529	-0.032958
C	1.931317	1.49646	4.036687	C	-1.262729	-5.198529	-0.032958
C	0.167667	3.013076	3.315534	C	-0.831011	-4.675455	1.191091
H	2.29747	0.834011	4.800248	C	-4.695273	-1.665082	1.205616
H	0.140436	1.805164	5.120257	H	-5.205802	-0.869283	1.727844
C	2.363599	-2.946118	2.219339	C	-4.671929	-1.736636	-0.160961

### Intermediate 22a

C	2.455791	-3.332499	-2.482006	C	-1.150707	-3.860625	-2.59984
C	-2.478562	1.426328	-3.477065	C	-0.708058	-4.935855	-1.757844
C	-2.455791	-3.332499	-2.482006	C	0.708058	-4.935855	-1.757844

C	1.150707	-3.860625	-2.59984	C	4.956141	0.682647	-2.149605
N	0	-3.314235	-3.165768	C	5.493086	0.236126	-0.898168
C	-1.143867	1.861569	-3.756199	C	5.450454	-1.099992	-0.570604
C	-0.694223	3.148868	-3.36096	C	-1.353469	3.966338	-2.447809
C	0.694223	3.148868	-3.36096	C	1.353469	3.966338	-2.447809
C	1.143867	1.861569	-3.756199	C	0.709961	4.655321	-1.374685
N	0	1.134957	-4.038552	C	-0.709961	4.655321	-1.374685
C	2.957457	0.088913	-3.50829	C	-1.398032	-5.307045	-0.614154
C	4.252363	-0.203059	-2.942095	C	-0.684069	-5.444062	0.621169
C	4.241974	-1.581054	-2.629281	C	1.398032	-5.307045	-0.614154
C	2.928529	-2.070817	-3.037023	C	0.684069	-5.444062	0.621169
N	2.20219	-1.081209	-3.592792	C	2.804514	-2.320524	2.429363
C	-2.957457	0.088913	-3.50829	C	1.435618	-0.363577	3.824459
C	-4.252363	-0.203059	-2.942096	C	3.378864	-1.01106	2.53725
C	-4.241974	-1.581054	-2.629281	C	1.463411	-2.580106	2.883867
C	-2.928529	-2.070817	-3.037023	C	0.748849	-1.542561	3.532948
N	-2.20219	-1.081209	-3.592792	C	2.686469	-0.035048	3.28702
C	2.478562	1.426328	-3.477065	H	0.895077	0.437683	4.301681
H	0	0.132589	-4.19351	C	-2.804514	-2.320524	2.429363
H	0	-2.41459	-3.634872	C	-1.435618	-0.363577	3.824459
C	-3.271447	2.404613	-2.676203	C	-1.463411	-2.580106	2.883867
C	-3.784103	3.262382	0.027924	C	-3.378864	-1.01106	2.53725
C	-2.665812	3.550121	-2.110794	C	-2.686469	-0.035048	3.28702
C	-4.418792	1.991403	-1.972189	C	-0.748849	-1.542561	3.532948
C	-4.616249	2.358115	-0.615264	H	-0.895077	0.437683	4.301682
C	-2.891141	3.962522	-0.788385	C	3.440903	3.063648	1.403595
C	4.616249	2.358115	-0.615264	C	2.279147	2.405117	3.832555
C	2.665812	3.550121	-2.110794	C	3.750385	1.805026	2.015815
C	3.784103	3.262382	0.027924	C	2.454627	3.912884	1.948352
C	4.418792	1.991403	-1.972189	C	2.020056	3.633018	3.262957
C	3.271447	2.404613	-2.676203	C	2.996504	1.406191	3.132283
C	2.891141	3.962522	-0.788385	H	1.36038	4.3304	3.77287
C	4.374404	-2.794909	0.584958	H	1.829522	2.172614	4.792656
C	2.639152	-4.681904	-0.360376	C	-3.440903	3.063648	1.403595
C	3.388764	-3.239164	1.476451	C	-2.279147	2.405117	3.832555
C	4.310079	-3.118582	-0.787483	C	-2.454626	3.912884	1.948352
C	3.229237	-3.844747	-1.322366	C	-3.750385	1.805026	2.015815
C	2.662634	-4.329565	1.025072	C	-2.996504	1.406191	3.132283
C	-2.639152	-4.681904	-0.360376	C	-2.020056	3.633018	3.262957
C	-4.374404	-2.794909	0.584958	H	-1.36038	4.3304	3.77287
C	-2.662634	-4.329565	1.025072	H	-1.829522	2.172614	4.792656
C	-3.229238	-3.844747	-1.322366	C	-0.731284	-3.760346	2.426857
C	-4.310079	-3.118582	-0.787483	C	-1.387677	-4.672158	1.597844
C	-3.388764	-3.239164	1.476451	C	-4.982859	-1.494327	0.722918
C	-4.956141	0.682647	-2.149605	C	-4.452122	-0.579651	1.629886
C	-4.897365	-2.031853	-1.506507	C	1.387677	-4.672158	1.597844
C	-5.450454	-1.099992	-0.570604	C	0.731284	-3.760346	2.426857
C	-5.493086	0.236126	-0.898168	C	4.982859	-1.494327	0.722918
C	4.897365	-2.031853	-1.506507	C	4.452122	-0.579651	1.629886

C	1.732539	4.653242	-0.274844	C	-5.136566	1.204842	0.086717
C	1.657657	4.767651	1.088692	C	-4.571533	0.832596	1.309268
H	0.871059	5.326757	1.573754	C	-1.657657	4.767651	1.088692
C	4.571533	0.832596	1.309268	H	-0.871059	5.326758	1.573754
C	5.136566	1.204842	0.086717	C	-1.732539	4.653242	-0.274844

### Intermediate 23a

C	-2.783616	-2.475903	-2.829528	C	-4.443853	-2.635581	-0.931047
C	2.076499	2.453883	-3.272001	C	-3.323503	-3.381537	1.110978
C	-2.783616	2.475903	-2.829528	C	-2.831418	-4.31116	-1.104029
C	-3.309223	1.147969	-3.030451	C	-3.473288	-3.24294	-1.750496
C	-4.490779	0.708841	-2.370251	C	-4.340983	-2.666984	0.481873
C	-4.490779	-0.708841	-2.370251	C	-4.443853	2.635581	-0.931047
C	-3.309223	-1.147969	-3.030451	C	-2.723137	4.35726	0.317572
N	-2.664459	0	-3.453137	C	-4.340983	2.666984	0.481873
C	2.539634	1.150939	-3.559334	C	-3.473288	3.24294	-1.750496
C	3.821456	0.706908	-3.094529	C	-2.831418	4.31116	-1.104029
C	3.821456	-0.706908	-3.094529	C	-3.323503	3.381537	1.110978
C	2.539634	-1.150939	-3.559334	C	1.124249	4.870263	-1.906157
N	1.845866	0	-3.935957	C	-1.65197	4.887149	-1.649919
C	0.698503	-2.926096	-3.408576	C	-0.841722	5.370631	-0.575001
C	0.349894	-4.228446	-2.841949	C	0.527267	5.37714	-0.703387
C	-1.056677	-4.23092	-2.713651	C	-1.65197	-4.887149	-1.649919
C	-1.506341	-2.954016	-3.213918	C	1.124249	-4.870263	-1.906157
N	-0.407934	-2.207214	-3.662207	C	0.527267	-5.37714	-0.703387
C	0.698503	2.926096	-3.408576	C	-0.841722	-5.370631	-0.575001
C	0.349894	4.228446	-2.841949	C	4.525557	1.38842	-2.116179
C	-1.056677	4.23092	-2.713651	C	4.525557	-1.38842	-2.116179
C	-1.506341	2.954016	-3.213918	C	5.045092	-0.678373	-0.981677
N	-0.407934	2.207214	-3.662207	C	5.045092	0.678373	-0.981677
C	2.076499	-2.453883	-3.272001	C	-5.045958	1.395625	-1.291534
H	0.847834	0	-4.114957	C	-5.394355	0.691199	-0.114277
H	-1.716302	0	-3.816578	C	-5.045958	-1.395625	-1.291534
C	2.925963	3.219762	-2.326053	C	-5.394355	-0.691199	-0.114277
C	3.283108	3.391372	0.501936	C	-2.595262	-2.78074	2.207678
C	4.027419	2.626878	-1.680072	C	-0.971647	-1.405907	3.973425
C	2.396324	4.298502	-1.586634	C	-1.289261	-3.291403	2.500949
C	2.535103	4.350275	-0.190094	C	-2.974609	-1.45963	2.634434
C	4.167148	2.654709	-0.253312	C	-2.1064	-0.747819	3.493136
C	2.535103	-4.350275	-0.190094	C	-0.473806	-2.577713	3.405834
C	4.027419	-2.626878	-1.680072	H	-0.295116	-0.869971	4.617501
C	3.283108	-3.391372	0.501936	C	-2.595262	2.78074	2.207678
C	2.396324	-4.298502	-1.586634	C	-0.971647	1.405907	3.973425
C	2.925963	-3.219762	-2.326053	C	-2.974609	1.45963	2.634434
C	4.167148	-2.654709	-0.253312	C	-1.289261	3.291403	2.500949
C	-2.723137	-4.35726	0.317572	C	-0.473806	2.577713	3.405834

C	-2.1064	0.747819	3.493136	C	-4.796065	1.392395	0.984477
H	-0.295116	0.869971	4.617501	C	-1.430104	4.900154	0.642751
C	2.829137	-2.860354	1.748553	C	-0.670485	4.30953	1.652849
C	1.874829	-1.925268	4.147442	C	-4.796065	-1.392395	0.984477
C	1.580644	-3.355509	2.267542	C	-4.056961	-0.733783	1.962591
C	3.427465	-1.672958	2.27642	C	-1.430104	-4.900154	0.642751
C	3.053495	-1.441522	3.62135	C	-0.670485	-4.30953	1.652849
C	0.999498	-2.705911	3.360934	C	4.680512	-1.380572	0.211
H	1.591857	-1.621833	5.150984	C	4.241009	-0.764319	1.399072
C	2.829137	2.860354	1.748553	C	0.776722	-4.312865	1.507069
C	1.874829	1.925268	4.147442	C	1.329232	-4.90905	0.377734
C	3.427465	1.672958	2.27642	C	1.329232	4.90905	0.377734
C	1.580644	3.355509	2.267542	C	0.776722	4.312865	1.507069
C	0.999498	2.705911	3.360934	C	4.241009	0.764319	1.399072
C	3.053495	1.441522	3.62135	C	4.680512	1.380572	0.211
H	1.591857	1.621833	5.150984	H	3.700387	-0.865469	4.260494
C	-4.056961	0.733783	1.962591	H	3.700387	0.865469	4.260494

### Product 24

C	-2.43883	-2.463332	-2.960786	C	3.351323	3.352905	0.918324
C	2.43883	2.463332	-2.960786	C	4.275131	2.63418	-1.234537
C	-2.438831	2.463333	-2.960786	C	2.626836	4.284556	-1.228053
C	-2.932241	1.150059	-3.212004	C	2.651295	4.31541	0.18895
C	-4.178774	0.708379	-2.666998	C	4.310746	2.657225	0.189745
C	-4.178774	-0.708379	-2.666998	C	2.651295	-4.31541	0.18895
C	-2.932241	-1.150059	-3.212004	C	4.275131	-2.63418	-1.234537
N	-2.258031	0	-3.602375	C	3.351323	-3.352905	0.918324
C	2.932241	1.150059	-3.212004	C	2.626837	-4.284556	-1.228053
C	4.178774	0.708379	-2.666998	C	3.217817	-3.228211	-1.946082
C	4.178774	-0.708379	-2.666998	C	4.310746	-2.657225	0.189745
C	2.932241	-1.150059	-3.212004	C	-2.651295	-4.31541	0.18895
N	2.258031	0	-3.602375	C	-4.275131	-2.63418	-1.234537
C	1.105362	-2.93784	-3.214092	C	-3.351323	-3.352905	0.918324
C	0.705605	-4.221548	-2.665098	C	-2.626837	-4.284556	-1.228053
C	-0.705605	-4.221548	-2.665098	C	-3.217817	-3.228211	-1.946082
C	-1.105362	-2.93784	-3.214092	C	-4.310746	-2.657225	0.189745
N	0	-2.209109	-3.567709	C	-4.275131	2.63418	-1.234537
C	1.105362	2.93784	-3.214092	C	-2.651295	4.31541	0.18895
C	0.705605	4.221548	-2.665098	C	-4.310746	2.657225	0.189745
C	-0.705605	4.221548	-2.665098	C	-3.217817	3.228211	-1.946082
C	-1.105362	2.93784	-3.214092	C	-2.626837	4.284556	-1.228053
N	0	2.209109	-3.567709	C	-3.351323	3.352905	0.918324
C	2.438831	-2.463333	-2.960786	C	1.391508	4.855958	-1.649973
H	1.278062	0	-3.865552	C	-1.391508	4.855958	-1.649973
H	-1.278062	0	-3.865552	C	-0.686943	5.329578	-0.497956
C	3.217817	3.228211	-1.946082	C	0.686943	5.329578	-0.497956

C	-1.391508	-4.855958	-1.649973	C	1.450343	-3.216243	2.491757
C	1.391508	-4.855958	-1.649973	C	3.21017	-1.451206	2.488209
C	0.686943	-5.329578	-0.497956	C	2.482241	-0.75097	3.475593
C	-0.686943	-5.329578	-0.497956	C	0.750487	-2.488855	3.476036
C	4.831973	1.397765	-1.653196	H	0.888789	-0.890681	4.864316
C	4.831973	-1.397765	-1.653196	C	2.7476	2.749828	2.08424
C	5.302677	-0.687816	-0.510241	C	1.402833	1.403927	4.072108
C	5.302677	0.687816	-0.510241	C	3.21017	1.451206	2.488209
C	-4.831973	1.397765	-1.653196	C	1.450343	3.216243	2.491757
C	-5.302677	0.687816	-0.510241	C	0.750487	2.488855	3.476036
C	-4.831973	-1.397765	-1.653196	C	2.482241	0.75097	3.475593
C	-5.302677	-0.687816	-0.510241	H	0.888789	0.890681	4.864316
C	-2.7476	-2.749828	2.08424	C	-4.213042	0.732122	1.704995
C	-1.402833	-1.403927	4.072108	C	-4.829548	1.390989	0.643983
C	-1.450343	-3.216243	2.491757	C	-1.38822	4.84185	0.648963
C	-3.21017	-1.451206	2.488209	C	-0.729725	4.222688	1.709614
C	-2.482241	-0.75097	3.475593	C	-4.829548	-1.390989	0.643983
C	-0.750487	-2.488855	3.476036	C	-4.213042	-0.732122	1.704995
H	-0.888789	-0.890681	4.864316	C	-1.38822	-4.84185	0.648963
C	-2.7476	2.749828	2.08424	C	-0.729725	-4.222688	1.709614
C	-1.402833	1.403927	4.072108	C	4.829548	-1.390989	0.643983
C	-3.21017	1.451206	2.488209	C	4.213042	-0.732122	1.704995
C	-1.450343	3.216243	2.491757	C	0.729725	-4.222688	1.709614
C	-0.750487	2.488855	3.476036	C	1.38822	-4.84185	0.648963
C	-2.482241	0.75097	3.475593	C	1.38822	4.84185	0.648963
H	-0.888789	0.890681	4.864316	C	0.729725	4.222688	1.709614
C	2.7476	-2.749828	2.08424	C	4.213042	0.732122	1.704995
C	1.402833	-1.403927	4.072108	C	4.829548	1.390989	0.643983

**(FP-Pb)**

C	-2.441342	2.470475	-2.993220	C	-4.186998	0.723075	-2.680381
C	2.475737	-2.442080	-2.987477	C	-2.923964	1.143631	-3.237404
C	2.476321	2.476960	-3.015321	N	-2.213075	0.008918	-3.622306
C	1.147756	2.958825	-3.270332	C	2.950061	-1.106887	-3.252033
C	0.727991	4.224833	-2.714592	C	4.216394	-0.691353	-2.705354
C	-0.688942	4.219117	-2.706452	C	4.217494	0.724742	-2.713476
C	-1.102926	2.950795	-3.253559	C	2.950397	1.142495	-3.268399
N	0.016742	2.234021	-3.646701	N	2.226736	0.011126	-3.644638
C	1.149001	-2.914865	-3.226543	C	-2.444368	-2.442577	-2.971013
C	0.727324	-4.176928	-2.673666	C	3.240838	-3.229251	-1.973178
C	-0.685827	-4.173434	-2.665887	C	3.364619	-3.369012	0.899723
C	-1.105576	-2.910553	-3.211437	C	2.650137	-4.297845	-1.254082
N	0.015145	-2.197127	-3.605131	C	4.300772	-2.633741	-1.262784
C	-2.924794	-1.111841	-3.222822	C	4.330970	-2.663407	0.165997
C	-4.186557	-0.691184	-2.673720	C	2.668253	-4.340765	0.174489

C	-4.334448	-2.664357	0.177235	H	-0.896757	0.893728	4.848350
C	-2.628834	-4.287371	-1.250506	C	2.743895	2.746006	2.037037
C	-3.371451	-3.373324	0.908720	C	1.402916	1.404680	4.047128
C	-4.287222	-2.629549	-1.249853	C	1.439978	3.207713	2.443202
C	-3.219750	-3.219825	-1.961164	C	3.202694	1.440326	2.441094
C	-2.664428	-4.337862	0.176069	C	2.473687	0.740168	3.435041
C	-4.334093	2.665052	0.174728	C	0.741504	2.480346	3.439412
C	-2.631428	4.295400	-1.264795	H	0.897534	0.899557	4.850291
C	-3.364465	3.363515	0.900335	C	-2.771040	-2.772764	2.070761
C	-4.293261	2.644496	-1.254446	C	-1.415585	-1.417384	4.055745
C	-3.225581	3.233939	-1.975472	C	-3.238507	-1.464756	2.473466
C	-2.660677	4.328350	0.163951	C	-1.465044	-3.243711	2.474044
C	2.652801	4.310130	-1.270418	C	-0.759359	-2.503584	3.455964
C	4.330850	2.665837	0.160034	C	-2.497916	-0.757467	3.456017
C	2.666250	4.334532	0.160621	H	-0.899788	-0.902425	4.845739
C	3.247608	3.248613	-1.990648	C	2.744601	-2.767324	2.051757
C	4.306513	2.651493	-1.270595	C	1.392753	-1.414872	4.042855
C	3.360111	3.361862	0.888732	C	1.440139	-3.239454	2.461362
C	4.856761	-1.394668	-1.686689	C	3.202459	-1.459842	2.448610
C	4.862717	1.412790	-1.691016	C	2.469380	-0.754977	3.435766
C	5.322579	0.692305	-0.541872	C	0.737019	-2.502220	3.448143
C	5.324091	-0.686949	-0.537995	H	0.879907	-0.900712	4.834888
C	-4.854650	1.409050	-1.671072	C	0.722784	4.207388	1.665961
C	-4.849057	-1.393650	-1.669518	C	1.392285	4.837951	0.607216
C	-5.339359	-0.689949	-0.524198	C	4.833292	1.391781	0.606414
C	-5.337507	0.691935	-0.526392	C	4.200963	0.722059	1.663615
C	1.412977	-4.855635	-1.671976	C	-1.397241	4.842465	0.610449
C	-1.390844	-4.845258	-1.669925	C	-0.739590	4.210175	1.672090
C	-0.688519	-5.341503	-0.526499	C	-4.860436	1.396003	0.626098
C	0.693956	-5.341389	-0.529549	C	-4.240423	0.723977	1.691685
C	1.414740	4.868198	-1.690543	C	-1.404621	-4.873532	0.627402
C	0.692432	5.326190	-0.541532	C	-0.744652	-4.251486	1.695786
C	-1.394330	4.855624	-1.688299	C	-4.245296	-0.744446	1.696188
C	-0.687033	5.325221	-0.539085	C	-4.869119	-1.405128	0.628720
C	-2.763093	2.749178	2.056286	C	4.840757	-1.398006	0.611390
C	-1.411361	1.402158	4.053076	C	4.203544	-0.740583	1.669567
C	-3.231768	1.443344	2.465267	C	0.723413	-4.248624	1.689209
C	-1.457479	3.211755	2.456018	C	1.397434	-4.867010	0.623578
C	-0.752857	2.480781	3.445173	Pb	-0.062513	-0.062098	-4.715962
C	-2.494252	0.741460	3.453437				

### **Pb@(FP)**

C	2.461404	-2.468263	-2.928826	C	0.729120	-4.203510	-2.622481
C	-2.457880	2.516971	-2.912330	C	1.200105	-3.010635	-3.235614
C	-2.441933	-2.463149	-2.907558	N	0.003375	-2.267366	-3.718146
C	-1.176907	-3.006724	-3.216395	C	-1.179754	3.035002	-3.205130
C	-0.700530	-4.199141	-2.611048	C	-0.707000	4.240632	-2.618743

C	0.721423	4.240880	-2.629302	C	-0.687506	5.335717	-0.441186
C	1.185174	3.032579	-3.223383	C	-1.396560	-4.869830	-1.605747
N	-0.006207	2.269869	-3.649358	C	-0.682338	-5.336281	-0.444401
C	2.930420	1.151576	-3.192933	C	1.415803	-4.881434	-1.617397
C	4.193385	0.733300	-2.660756	C	0.693900	-5.335817	-0.451699
C	4.193430	-0.690767	-2.659505	C	2.753329	-2.772090	2.117767
C	2.939634	-1.107021	-3.193282	C	1.421068	-1.417469	4.122709
N	2.181731	0.022299	-3.519108	C	3.212438	-1.461800	2.507546
C	-2.936832	1.160136	-3.175587	C	1.452244	-3.243412	2.538878
C	-4.181460	0.732414	-2.617086	C	0.755694	-2.501039	3.529316
C	-4.177118	-0.689817	-2.616645	C	2.491624	-0.757831	3.503713
C	-2.938630	-1.108433	-3.177851	H	0.919439	-0.905377	4.924369
N	-2.204992	0.028715	-3.541814	C	-2.753852	-2.776517	2.145167
C	2.458377	2.511013	-2.932802	C	-1.399834	-1.412399	4.125369
C	-3.236694	3.270835	-1.890080	C	-1.448090	-3.247454	2.554452
C	-3.358755	3.372992	0.980457	C	-3.222676	-1.467534	2.541041
C	-2.635418	4.329048	-1.179828	C	-2.487834	-0.760453	3.525735
C	-4.287549	2.654859	-1.167393	C	-0.740641	-2.500462	3.533769
C	-4.332175	2.675283	0.252660	H	-0.882446	-0.892696	4.911236
C	-2.658467	4.348027	0.258922	C	2.744383	2.750501	2.105141
C	4.328329	2.677415	0.221183	C	1.410868	1.395253	4.109917
C	2.644292	4.337337	-1.197693	C	3.205373	1.440444	2.497684
C	3.356863	3.372116	0.956291	C	1.443946	3.210767	2.521619
C	4.290196	2.660447	-1.200821	C	0.746597	2.472522	3.513007
C	3.239077	3.277246	-1.917063	C	2.486400	0.738336	3.495346
C	2.662149	4.352476	0.242971	H	0.905647	0.881674	4.907547
C	4.331574	-2.670617	0.221966	C	-2.756898	2.751499	2.132642
C	2.639292	-4.311447	-1.196709	C	-1.409692	1.395883	4.123173
C	3.363388	-3.373446	0.957392	C	-1.452574	3.211287	2.535529
C	4.282409	-2.629259	-1.201222	C	-3.224912	1.441482	2.531972
C	3.231689	-3.243770	-1.911352	C	-2.492388	0.738079	3.520019
C	2.663910	-4.349838	0.243124	C	-0.747751	2.471818	3.519783
C	-2.615325	-4.296040	-1.179683	H	-0.898648	0.883329	4.917781
C	-4.325755	-2.672194	0.251371	C	-0.726635	-4.259390	1.788340
C	-2.647557	-4.344051	0.258154	C	-1.393986	-4.873706	0.706497
C	-3.212379	-3.229458	-1.885132	C	-4.854910	-1.406479	0.693199
C	-4.267653	-2.623254	-1.169877	C	-4.229991	-0.746996	1.757522
C	-3.354769	-3.376433	0.980930	C	1.401255	-4.866973	0.695334
C	-4.851125	1.414332	-1.596338	C	0.728071	-4.255642	1.778910
C	-4.844361	-1.391800	-1.600349	C	4.836640	-1.397741	0.655211
C	-5.329888	-0.693564	-0.464322	C	4.203513	-0.740554	1.714109
C	-5.333233	0.697991	-0.462804	C	1.392075	4.847912	0.693942
C	4.849427	-1.393611	-1.637547	C	0.721903	4.217263	1.760792
C	4.849528	1.418322	-1.635300	C	4.199228	0.722813	1.708648
C	5.317760	0.699409	-0.499158	C	4.830221	1.392929	0.652960
C	5.317753	-0.689344	-0.499805	C	-4.854823	1.395729	0.692536
C	-1.407750	4.892284	-1.602386	C	-4.229737	0.722699	1.752134
C	1.413664	4.898468	-1.613656	C	-0.732704	4.218709	1.768889
C	0.687607	5.333670	-0.448512	C	-1.396135	4.853684	0.704134



Pb	-0.087005	-0.127670	-2.513212	H	-0.015011	-2.121752	-4.730911
H	-0.024459	1.991476	-4.633540				

### Pb@(FP-Pb)

---

C	-2.403836	2.471590	-2.949670	C	4.335510	2.671976	0.184633
C	2.477134	-2.405321	-2.944088	C	2.669410	4.342593	0.185031
C	2.508653	2.512874	-2.994424	C	3.277699	3.282321	-1.968892
C	1.180509	2.979697	-3.249919	C	4.328077	2.673290	-1.248771
C	0.745602	4.245108	-2.701706	C	3.361784	3.366621	0.911979
C	-0.666641	4.231710	-2.701240	C	4.864580	-1.380086	-1.670465
C	-1.068357	2.961607	-3.225284	C	4.868694	1.430055	-1.667700
N	0.057594	2.232569	-3.616186	C	5.320155	0.701309	-0.517000
C	1.151026	-2.872419	-3.183039	C	5.323459	-0.676364	-0.520867
C	0.731758	-4.137976	-2.678179	C	-4.826053	1.426824	-1.676374
C	-0.689716	-4.184701	-2.702469	C	-4.870624	-1.411027	-1.686296
C	-1.152946	-2.982359	-3.277864	C	-5.292866	-0.683936	-0.526658
N	-0.002919	-2.113996	-3.562967	C	-5.291057	0.696448	-0.520003
C	-2.990487	-1.159380	-3.285229	C	1.435470	-4.828635	-1.677787
C	-4.192565	-0.697730	-2.708915	C	-1.404382	-4.870815	-1.687675
C	-4.144611	0.724176	-2.683625	C	-0.677287	-5.295674	-0.527471
C	-2.877223	1.143374	-3.191406	C	0.702823	-5.294000	-0.521877
N	-2.124676	-0.009905	-3.572648	C	1.428530	4.878682	-1.667008
C	2.960101	-1.071630	-3.223831	C	0.698067	5.328122	-0.516617
C	4.225789	-0.666641	-2.700549	C	-1.382232	4.864764	-1.672305
C	4.232635	0.745208	-2.700254	C	-0.679918	5.327581	-0.521855
C	2.966432	1.177750	-3.247564	C	-2.756580	2.751389	2.073088
N	2.221943	0.053035	-3.613450	C	-1.408295	1.414247	4.085244
C	-2.496905	-2.498238	-2.984663	C	-3.227940	1.444082	2.487667
C	3.249362	-3.204600	-1.956310	C	-1.453738	3.214718	2.474881
C	3.365560	-3.357787	0.913331	C	-0.749093	2.487200	3.472962
C	2.656489	-4.285126	-1.255395	C	-2.486558	0.744614	3.482116
C	4.313273	-2.611937	-1.248851	H	-0.897630	0.910276	4.886471
C	4.344274	-2.654877	0.188305	C	2.743863	2.748972	2.058885
C	2.664978	-4.328358	0.191009	C	1.404861	1.408922	4.071713
C	-4.338821	-2.655939	0.199741	C	1.441431	3.213243	2.466376
C	-2.629141	-4.319619	-1.251942	C	3.205937	1.444535	2.464788
C	-3.351963	-3.357330	0.913084	C	2.475541	0.743189	3.460090
C	-4.315458	-2.634035	-1.250337	C	0.742051	2.484209	3.464011
C	-3.267800	-3.271936	-1.955015	H	0.899025	0.903010	4.874055
C	-2.650732	-4.344838	0.198554	C	-2.750017	-2.754633	2.076821
C	-4.322493	2.659350	0.189214	C	-1.402837	-1.404706	4.080928
C	-2.612639	4.307489	-1.251407	C	-3.223104	-1.448405	2.489290
C	-3.355404	3.362650	0.912573	C	-1.445856	-3.230408	2.491236
C	-4.281109	2.648788	-1.256101	C	-0.744472	-2.492441	3.486938
C	-3.202460	3.241720	-1.959621	C	-2.486367	-0.744304	3.486067
C	-2.654735	4.340170	0.184411	H	-0.891523	-0.893131	4.876860
C	2.671177	4.335377	-1.248376	C	2.747851	-2.758811	2.069731

C	1.405073	-1.409641	4.076543	C	-4.847173	1.402164	0.636121
C	1.442670	-3.234845	2.485619	C	-4.229802	0.725236	1.720529
C	3.205033	-1.453136	2.468368	C	-1.396516	-4.844071	0.634553
C	2.474941	-0.748468	3.464836	C	-0.727744	-4.235475	1.724938
C	0.741305	-2.493604	3.478612	C	-4.227539	-0.731538	1.722865
H	0.896547	-0.899424	4.874551	C	-4.838382	-1.401653	0.635258
C	0.726634	4.211843	1.690295	C	4.844109	-1.395025	0.633971
C	1.397433	4.848128	0.633947	C	4.205722	-0.736032	1.693263
C	4.840513	1.400431	0.633228	C	0.727455	-4.238341	1.720946
C	4.203385	0.729025	1.688813	C	1.407792	-4.852731	0.635205
C	-1.397189	4.846949	0.632238	Pb	0.047162	0.026942	-4.853394
C	-0.738340	4.213424	1.694511	Pb	-1.020130	-1.013539	-1.649748

**(FP-Zn)**

---

C	-2.439522	2.439702	-2.967508	C	-4.286254	-2.635461	-1.275129
C	2.439522	-2.439702	-2.967508	C	-3.228351	-3.228380	-1.984026
C	2.439522	2.439702	-2.967508	C	-2.659081	-4.320569	0.145210
C	1.113952	2.889076	-3.206454	C	-4.320427	2.659014	0.144958
C	0.704004	4.173102	-2.701780	C	-2.635500	4.286416	-1.274867
C	-0.704004	4.173102	-2.701780	C	-3.357709	3.357732	0.872945
C	-1.113952	2.889076	-3.206454	C	-4.286254	2.635461	-1.275129
N	-0.000000	2.125938	-3.518093	C	-3.228350	3.228379	-1.984026
C	1.113952	-2.889076	-3.206454	C	-2.659081	4.320569	0.145211
C	0.704004	-4.173102	-2.701780	C	2.635500	4.286417	-1.274868
C	-0.704004	-4.173102	-2.701780	C	4.320427	2.659014	0.144958
C	-1.113952	-2.889076	-3.206454	C	2.659081	4.320569	0.145210
N	-0.000000	-2.125938	-3.518093	C	3.228351	3.228380	-1.984026
C	-2.888802	-1.114001	-3.207056	C	4.286254	2.635461	-1.275129
C	-4.173020	-0.704026	-2.702606	C	3.357709	3.357732	0.872945
C	-4.173020	0.704025	-2.702606	C	4.837280	-1.394993	-1.699909
C	-2.888802	1.114001	-3.207056	C	4.837280	1.394993	-1.699909
N	-2.126118	-0.000000	-3.521360	C	5.314764	0.687542	-0.555656
C	2.888802	-1.114001	-3.207056	C	5.314764	-0.687542	-0.555656
C	4.173020	-0.704026	-2.702606	C	-4.837280	1.394993	-1.699909
C	4.173020	0.704025	-2.702606	C	-4.837280	-1.394993	-1.699909
C	2.888802	1.114001	-3.207056	C	-5.314764	-0.687542	-0.555657
N	2.126117	-0.000000	-3.521359	C	-5.314764	0.687542	-0.555657
C	-2.439522	-2.439702	-2.967508	C	1.394977	-4.837492	-1.699434
C	3.228351	-3.228380	-1.984026	C	-1.394977	-4.837492	-1.699434
C	3.357709	-3.357732	0.872945	C	-0.687574	-5.315025	-0.555187
C	2.635500	-4.286417	-1.274868	C	0.687574	-5.315025	-0.555187
C	4.286254	-2.635461	-1.275129	C	1.394977	4.837492	-1.699434
C	4.320427	-2.659014	0.144958	C	0.687574	5.315025	-0.555187
C	2.659081	-4.320569	0.145210	C	-1.394977	4.837491	-1.699434
C	-4.320427	-2.659014	0.144958	C	-0.687574	5.315025	-0.555187
C	-2.635500	-4.286417	-1.274868	C	-2.750736	2.750638	2.035303
C	-3.357709	-3.357732	0.872945	C	-1.403261	1.403270	4.020264

C	-3.214339	1.451584	2.439560	C	3.214339	-1.451584	2.439561
C	-1.451598	3.214253	2.439755	C	2.485727	-0.750886	3.424054
C	-0.750853	2.485688	3.424224	C	0.750854	-2.485687	3.424223
C	-2.485726	0.750886	3.424054	H	0.889535	-0.889504	4.812308
H	-0.889535	0.889504	4.812308	C	0.731446	4.219318	1.657272
C	2.750736	2.750638	2.035303	C	1.390647	4.838764	0.598389
C	1.403261	1.403270	4.020264	C	4.838625	1.390596	0.598012
C	1.451598	3.214253	2.439755	C	4.219285	0.731432	1.656973
C	3.214339	1.451584	2.439561	C	-1.390647	4.838764	0.598389
C	2.485727	0.750886	3.424054	C	-0.731446	4.219318	1.657272
C	0.750853	2.485688	3.424224	C	-4.838626	1.390596	0.598012
H	0.889535	0.889504	4.812308	C	-4.219285	0.731432	1.656973
C	-2.750736	-2.750638	2.035303	C	-1.390647	-4.838764	0.598389
C	-1.403261	-1.403270	4.020263	C	-0.731446	-4.219318	1.657272
C	-3.214339	-1.451584	2.439560	C	-4.219285	-0.731432	1.656973
C	-1.451598	-3.214253	2.439755	C	-4.838625	-1.390596	0.598012
C	-0.750853	-2.485687	3.424223	C	4.838625	-1.390596	0.598012
C	-2.485726	-0.750886	3.424054	C	4.219285	-0.731432	1.656974
H	-0.889534	-0.889503	4.812307	C	0.731446	-4.219318	1.657272
C	2.750736	-2.750638	2.035303	C	1.390647	-4.838764	0.598389
C	1.403262	-1.403270	4.020264	Zn	-0.000000	-0.000000	-3.679554
C	1.451598	-3.214253	2.439755				

### Zn@(FP)

C	2.438896	2.461628	-2.953517	C	-2.438910	2.461628	-2.953513
C	-2.438910	-2.461628	-2.953513	C	-3.218827	-3.228156	-1.941207
C	2.438896	-2.461629	-2.953517	C	-3.351523	-3.352788	0.921306
C	2.932431	-1.149555	-3.205795	C	-4.276438	-2.634304	-1.230315
C	4.179029	-0.708183	-2.662007	C	-2.627354	-4.284620	-1.224242
C	4.179029	0.708183	-2.662007	C	-2.651700	-4.315696	0.192420
C	2.932431	1.149555	-3.205795	C	-4.311799	-2.657452	0.193583
N	2.257562	0.000000	-3.596146	C	-2.651700	4.315696	0.192420
C	-2.932453	-1.149558	-3.205793	C	-4.276438	2.634304	-1.230315
C	-4.179054	-0.708184	-2.662012	C	-3.351523	3.352788	0.921306
C	-4.179054	0.708184	-2.662012	C	-2.627354	4.284620	-1.224242
C	-2.932453	1.149558	-3.205793	C	-3.218827	3.228156	-1.941207
N	-2.257571	0.000000	-3.596107	C	-4.311799	2.657452	0.193583
C	-1.105173	2.933631	-3.204916	C	2.651685	4.315695	0.192417
C	-0.705389	4.218215	-2.660053	C	4.276424	2.634305	-1.230317
C	0.705375	4.218217	-2.660055	C	3.351508	3.352787	0.921304
C	1.105160	2.933635	-3.204921	C	2.627339	4.284621	-1.224244
N	-0.000003	2.202371	-3.555248	C	3.218813	3.228156	-1.941210
C	-1.105173	-2.933631	-3.204916	C	4.311784	2.657452	0.193581
C	-0.705389	-4.218215	-2.660053	C	4.276424	-2.634305	-1.230317
C	0.705375	-4.218217	-2.660055	C	2.651685	-4.315695	0.192417
C	1.105160	-2.933635	-3.204921	C	4.311784	-2.657452	0.193581
N	-0.000003	-2.202371	-3.555248	C	3.218813	-3.228156	-1.941210

C	2.627339	-4.284621	-1.224244	C	-1.402372	1.403512	4.074048
C	3.351508	-3.352787	0.921304	C	-1.449799	3.214797	2.493124
C	-1.391746	-4.854807	-1.646400	C	-3.209230	1.450647	2.489911
C	1.391731	-4.854807	-1.646401	C	-2.481208	0.750626	3.476888
C	0.686939	-5.328977	-0.495110	C	-0.750130	2.487731	3.477350
C	-0.686953	-5.328976	-0.495110	H	-0.888712	0.890588	4.866661
C	1.391731	4.854807	-1.646401	C	-2.746871	-2.748841	2.085933
C	-1.391746	4.854807	-1.646400	C	-1.402372	-1.403512	4.074049
C	-0.686953	5.328976	-0.495110	C	-3.209230	-1.450648	2.489911
C	0.686939	5.328977	-0.495110	C	-1.449799	-3.214798	2.493124
C	-4.832916	-1.397816	-1.648864	C	-0.750130	-2.487731	3.477350
C	-4.832916	1.397816	-1.648864	C	-2.481208	-0.750626	3.476888
C	-5.303670	0.687841	-0.506274	H	-0.888713	-0.890589	4.866662
C	-5.303670	-0.687841	-0.506274	C	4.212294	-0.731994	1.707397
C	4.832898	-1.397815	-1.648865	C	4.830157	-1.391090	0.647666
C	5.303653	-0.687840	-0.506275	C	1.388295	-4.841489	0.651839
C	4.832898	1.397815	-1.648865	C	0.729596	-4.221139	1.711248
C	5.303653	0.687840	-0.506275	C	4.830157	1.391090	0.647665
C	2.746857	2.748840	2.085932	C	4.212294	0.731994	1.707397
C	1.402359	1.403512	4.074048	C	1.388295	4.841489	0.651839
C	1.449785	3.214797	2.493124	C	0.729596	4.221139	1.711248
C	3.209217	1.450648	2.489911	C	-4.830174	1.391091	0.647667
C	2.481196	0.750626	3.476888	C	-4.212310	0.731994	1.707399
C	0.750117	2.487731	3.477349	C	-0.729609	4.221140	1.711249
H	0.888698	0.890589	4.866661	C	-1.388309	4.841490	0.651840
C	2.746856	-2.748840	2.085932	C	-1.388309	-4.841490	0.651840
C	1.402359	-1.403511	4.074048	C	-0.729609	-4.221140	1.711249
C	3.209217	-1.450648	2.489911	C	-4.212310	-0.731994	1.707398
C	1.449785	-3.214797	2.493124	C	-4.830173	-1.391091	0.647667
C	0.750117	-2.487731	3.477349	Zn	0.000787	-0.000001	-0.412254
C	2.481195	-0.750626	3.476888	H	-1.278918	0.000000	-3.863757
H	0.888697	-0.890588	4.866660	H	1.278934	0.000000	-3.863897
C	-2.746870	2.748841	2.085933				

### Zn@(FP-Zn)

C	-2.438469	2.438388	-2.961200	N	0.000027	-2.129564	-3.516574
C	2.438473	-2.438389	-2.961200	C	-2.890134	-1.113237	-3.201785
C	2.438383	2.438465	-2.961191	C	-4.175202	-0.704304	-2.698058
C	1.113158	2.890168	-3.201801	C	-4.175215	0.704188	-2.698061
C	0.704194	4.175227	-2.698071	C	-2.890155	1.113154	-3.201787
C	-0.704302	4.175212	-2.698075	N	-2.129577	-0.000039	-3.516596
C	-1.113236	2.890144	-3.201805	C	2.890170	-1.113161	-3.201801
N	-0.000034	2.129616	-3.516663	C	4.175226	-0.704194	-2.698071
C	1.113229	-2.890124	-3.201781	C	4.175205	0.704300	-2.698065
C	0.704296	-4.175194	-2.698056	C	2.890135	1.113232	-3.201794
C	-0.704194	-4.175214	-2.698054	N	2.129605	0.000027	-3.516642
C	-1.113160	-2.890157	-3.201780	C	-2.438394	-2.438475	-2.961194

C	3.227736	-3.227644	-1.978959	C	-1.451007	3.213210	2.441573
C	3.357425	-3.357331	0.875758	C	-0.750615	2.484759	3.425987
C	2.635747	-4.286828	-1.271228	C	-2.484782	0.750548	3.425987
C	4.286896	-2.635640	-1.271228	H	-0.889116	0.889089	4.814554
C	4.320698	-2.659000	0.148545	C	2.749614	2.749684	2.037127
C	2.659109	-4.320631	0.148544	C	1.402446	1.402485	4.022210
C	-4.320607	-2.659090	0.148566	C	1.450857	3.213198	2.441567
C	-2.635633	-4.286889	-1.271209	C	3.213161	1.450938	2.441566
C	-3.357299	-3.357396	0.875781	C	2.484692	0.750505	3.425940
C	-4.286819	-2.635743	-1.271209	C	0.750442	2.484711	3.425942
C	-3.227642	-3.227735	-1.978944	H	0.888816	0.888837	4.814265
C	-2.658980	-4.320678	0.148568	C	-2.749616	-2.749688	2.037125
C	-4.320701	2.658997	0.148546	C	-1.402448	-1.402490	4.022210
C	-2.635747	4.286823	-1.271228	C	-3.213163	-1.450942	2.441564
C	-3.357427	3.357326	0.875759	C	-1.450860	-3.213203	2.441566
C	-4.286895	2.635635	-1.271228	C	-0.750445	-2.484714	3.425940
C	-3.227734	3.227639	-1.978957	C	-2.484694	-0.750511	3.425940
C	-2.659109	4.320626	0.148544	H	-0.888819	-0.888843	4.814266
C	2.635625	4.286877	-1.271207	C	2.749740	-2.749672	2.037123
C	4.320601	2.659084	0.148567	C	1.402671	-1.402634	4.022371
C	2.658975	4.320671	0.148568	C	1.451004	-3.213214	2.441572
C	3.227629	3.227722	-1.978938	C	3.213250	-1.450926	2.441573
C	4.286809	2.635734	-1.271206	C	2.484779	-0.750552	3.425987
C	3.357295	3.357391	0.875781	C	0.750613	-2.484762	3.425986
C	4.839084	-1.395414	-1.695976	H	0.889114	-0.889095	4.814554
C	4.839038	1.395533	-1.695965	C	0.731050	4.218459	1.659563
C	5.315920	0.687697	-0.551608	C	1.390430	4.838602	0.601368
C	5.315948	-0.687571	-0.551617	C	4.838565	1.390553	0.601368
C	-4.839080	1.395409	-1.695975	C	4.218441	0.731156	1.659563
C	-4.839044	-1.395538	-1.695965	C	-1.390576	4.838580	0.601353
C	-5.315927	-0.687702	-0.551608	C	-0.731194	4.218454	1.659556
C	-5.315949	0.687567	-0.551616	C	-4.838625	1.390450	0.601356
C	1.395535	-4.839044	-1.695974	C	-4.218480	0.731084	1.659558
C	-1.395413	-4.839080	-1.695964	C	-1.390434	-4.838608	0.601370
C	-0.687565	-5.315946	-0.551607	C	-0.731053	-4.218466	1.659565
C	0.687704	-5.315930	-0.551616	C	-4.218443	-0.731161	1.659562
C	1.395409	4.839076	-1.695967	C	-4.838568	-1.390557	0.601368
C	0.687562	5.315940	-0.551610	C	4.838621	-1.390454	0.601355
C	-1.395538	4.839046	-1.695977	C	4.218477	-0.731088	1.659558
C	-0.687706	5.315926	-0.551617	C	0.731192	-4.218460	1.659557
C	-2.749743	2.749668	2.037124	C	1.390575	-4.838587	0.601355
C	-1.402672	1.402629	4.022371	Zn	-0.000006	-0.000012	-3.526459
C	-3.213253	1.450921	2.441574	Zn	0.000102	0.000165	-0.511700

**(FP-Ge)**

C	-2.444169	2.444171	-2.979822	C	2.444170	2.444381	-2.979838
C	2.444492	-2.444443	-2.980066	C	1.118144	2.903548	-3.220655

C	0.704336	4.177314	-2.692311	C	-4.836192	-1.393883	-1.686796
C	-0.704410	4.177201	-2.692303	C	-5.314340	-0.687589	-0.542539
C	-1.118027	2.903304	-3.220577	C	-5.314422	0.687353	-0.542541
N	0.000124	2.168353	-3.575004	C	1.393753	-4.836083	-1.686855
C	1.118212	-2.903246	-3.220731	C	-1.393598	-4.835972	-1.686799
C	0.704352	-4.176846	-2.692174	C	-0.687419	-5.314352	-0.542642
C	-0.704241	-4.176750	-2.692142	C	0.687558	-5.314359	-0.542659
C	-1.117978	-2.903033	-3.220614	C	1.393706	4.836244	-1.686860
N	0.000162	-2.167415	-3.574362	C	0.687394	5.314378	-0.542569
C	-2.903427	-1.118324	-3.220668	C	-1.393783	4.836094	-1.686861
C	-4.177104	-0.704512	-2.692157	C	-0.687530	5.314366	-0.542591
C	-4.177031	0.704165	-2.692142	C	-2.750205	2.750162	2.048018
C	-2.903148	1.117808	-3.220485	C	-1.403593	1.403593	4.033978
N	-2.167896	-0.000283	-3.574503	C	-3.214116	1.451460	2.452673
C	2.903193	-1.118272	-3.220583	C	-1.451530	3.214121	2.452685
C	4.176765	-0.704354	-2.692055	C	-0.751020	2.485811	3.437577
C	4.176641	0.704237	-2.692017	C	-2.485791	0.750975	3.437562
C	2.902836	1.117929	-3.220361	H	-0.889946	0.889951	4.826209
N	2.167162	-0.000213	-3.573906	C	2.750009	2.750118	2.047983
C	-2.444351	-2.444338	-2.979976	C	1.403156	1.403195	4.033574
C	3.224977	-3.224923	-1.977730	C	1.451305	3.214048	2.452652
C	3.355782	-3.355711	0.884122	C	3.213961	1.451398	2.452611
C	2.632947	-4.281322	-1.265042	C	2.485633	0.750793	3.437414
C	4.281392	-2.632917	-1.265031	C	0.750730	2.485676	3.437454
C	4.317059	-2.657313	0.155331	H	0.889314	0.889322	4.825503
C	2.657368	-4.316996	0.155275	C	-2.750044	-2.750112	2.048031
C	-4.316913	-2.657351	0.155405	C	-1.403120	-1.403175	4.033580
C	-2.632793	-4.281244	-1.264952	C	-3.213971	-1.451397	2.452674
C	-3.355642	-3.355714	0.884235	C	-1.451310	-3.214016	2.452627
C	-4.281293	-2.632981	-1.264970	C	-0.750714	-2.485653	3.437418
C	-3.224773	-3.224840	-1.977634	C	-2.485613	-0.750782	3.437463
C	-2.657210	-4.316954	0.155356	H	-0.889257	-0.889312	4.825500
C	-4.316934	2.657179	0.155255	C	2.750232	-2.750179	2.047976
C	-2.632947	4.281306	-1.265046	C	1.403611	-1.403565	4.033929
C	-3.355722	3.355669	0.884149	C	1.451543	-3.214103	2.452621
C	-4.281321	2.632821	-1.265027	C	3.214121	-1.451475	2.452639
C	-3.224743	3.224680	-1.977637	C	2.485805	-0.750970	3.437530
C	-2.657306	4.316910	0.155279	C	0.751040	-2.485793	3.437511
C	2.632853	4.281445	-1.265029	H	0.889963	-0.889933	4.826166
C	4.316852	2.657274	0.155299	C	0.731369	4.218962	1.669794
C	2.657170	4.316986	0.155316	C	1.390474	4.837571	0.610249
C	3.224740	3.224876	-1.977634	C	4.837493	1.390569	0.610242
C	4.281221	2.632932	-1.264983	C	4.218896	0.731469	1.669757
C	3.355564	3.355700	0.884151	C	-1.390618	4.837540	0.610210
C	4.836112	-1.393738	-1.686811	C	-0.731546	4.218967	1.669783
C	4.835876	1.393671	-1.686746	C	-4.837561	1.390473	0.610216
C	5.314339	0.687491	-0.542569	C	-4.218940	0.731428	1.669773
C	5.314320	-0.687475	-0.542607	C	-1.390469	-4.837526	0.610215
C	-4.836055	1.393568	-1.686787	C	-0.731371	-4.218929	1.669730

C	-4.218893	-0.731486	1.669807	C	0.731556	-4.218950	1.669705
C	-4.837473	-1.390635	0.610286	C	1.390642	-4.837555	0.610179
C	4.837542	-1.390570	0.610237	Ge	0.000901	0.000381	-4.385265
C	4.218948	-0.731471	1.669754				

### Ge@(FP)

C	2.488411	2.424184	-2.896541	C	-1.394164	-4.814124	-1.627151
C	-2.487726	-2.423602	-2.896449	C	1.394360	-4.815012	-1.626930
C	2.489495	-2.426027	-2.897003	C	0.694417	-5.297012	-0.502190
C	3.005923	-1.172025	-3.191284	C	-0.694355	-5.296567	-0.502303
C	4.219191	-0.711803	-2.610412	C	1.394089	4.814416	-1.626606
C	4.218531	0.711779	-2.610436	C	-1.395016	4.814394	-1.626378
C	3.004639	1.171526	-3.191115	C	-0.694848	5.297329	-0.501614
N	2.232814	-0.000343	-3.634125	C	0.694093	5.297022	-0.501770
C	-3.003689	-1.169695	-3.190072	C	-4.880423	-1.400765	-1.608295
C	-4.218246	-0.710446	-2.609749	C	-4.881923	1.402285	-1.608758
C	-4.219326	0.712883	-2.610844	C	-5.331689	0.684919	-0.441891
C	-3.006097	1.172943	-3.192275	C	-5.330944	-0.683845	-0.441863
N	-2.231586	0.002400	-3.633568	C	4.881377	-1.401674	-1.608699
C	-1.123788	2.873363	-3.148490	C	5.331511	-0.684446	-0.442148
C	-0.707712	4.129969	-2.636292	C	4.881102	1.401714	-1.608941
C	0.706312	4.129945	-2.636332	C	5.331335	0.684477	-0.442247
C	1.122039	2.873389	-3.148514	C	2.758946	2.740814	2.120159
N	-0.000923	2.110227	-3.450995	C	1.401660	1.403687	4.104123
C	-1.121855	-2.874466	-3.150324	C	1.453776	3.202783	2.510205
C	-0.706822	-4.133373	-2.639684	C	3.225366	1.447289	2.537552
C	0.707375	-4.134081	-2.639684	C	2.487891	0.749391	3.520395
C	1.122967	-2.876349	-3.150708	C	0.751033	2.483634	3.497976
N	0.000994	-2.110300	-3.450636	H	0.884716	0.893217	4.896447
C	-2.490631	2.425162	-2.897117	C	2.759577	-2.741637	2.120085
C	-3.255478	-3.211028	-1.900341	C	1.403469	-1.405822	4.105111
C	-3.368497	-3.341359	0.955128	C	3.226098	-1.448284	2.537738
C	-4.315969	-2.625153	-1.190310	C	1.454798	-3.204081	2.510337
C	-2.634603	-4.253075	-1.188198	C	0.752291	-2.484894	3.498168
C	-2.667195	-4.304921	0.220305	C	2.488556	-0.750738	3.520667
C	-4.340881	-2.650156	0.244306	H	0.886344	-0.895432	4.897370
C	-2.668117	4.305994	0.221243	C	-2.759762	2.741539	2.120563
C	-4.317421	2.626159	-1.189788	C	-1.403421	1.405463	4.105529
C	-3.369444	3.342322	0.955847	C	-1.454859	3.203675	2.510713
C	-2.635893	4.254147	-1.187242	C	-3.226183	1.448309	2.538179
C	-3.257188	3.212062	-1.899647	C	-2.488536	0.750599	3.521013
C	-4.342051	2.651122	0.244828	C	-0.752258	2.484386	3.498495
C	2.667326	4.305545	0.221095	H	-0.886262	0.894910	4.897666
C	4.316173	2.625454	-1.190006	C	-2.758832	-2.740790	2.119878
C	3.368708	3.341838	0.955591	C	-1.401585	-1.404047	4.103911
C	2.634731	4.253655	-1.187467	C	-3.225176	-1.447260	2.537425
C	3.255675	3.211344	-1.899711	C	-1.453832	-3.203143	2.509947
C	4.341267	2.650607	0.244538	C	-0.751039	-2.484128	3.497711
C	4.316798	-2.626081	-1.190156	C	-2.487727	-0.749547	3.520324
C	2.667684	-4.305955	0.220665	H	-0.884572	-0.893738	4.896286
C	4.341680	-2.650965	0.244393	C	4.238258	-0.726181	1.772904
C	3.256459	-3.212558	-1.899967	C	4.853462	-1.387940	0.701051
C	2.635043	-4.254214	-1.187762	C	1.392683	-4.823481	0.660409
C	3.369119	-3.342203	0.955273	C	0.733502	-4.203224	1.714657

C	4.853189	1.387688	0.701227	C	-1.392372	-4.822755	0.660214
C	4.237992	0.725636	1.772929	C	-0.732954	-4.202719	1.714471
C	1.392127	4.822613	0.660748	C	-4.237749	-0.725467	1.772969
C	0.732758	4.202276	1.714784	C	-4.852743	-1.387284	0.701206
C	-4.853737	1.388195	0.701602	Ge	-0.001584	0.002140	-2.622467
C	-4.238336	0.726361	1.773291	H	-2.032908	0.003757	-4.635335
C	-0.733607	4.202702	1.714963	H	2.037266	-0.002621	-4.636662
C	-1.392862	4.823201	0.660886				

### Ge@(FP-Ge)

C	-2.335191	2.330490	-2.964658	C	3.342198	3.342549	-1.914681
C	2.331040	-2.334865	-2.964375	C	4.372250	2.703385	-1.197514
C	2.592870	2.593000	-2.937217	C	3.377046	3.377457	0.942378
C	1.261204	3.036702	-3.178415	C	4.826699	-1.352019	-1.669027
C	0.777390	4.277669	-2.665751	C	4.912639	1.451074	-1.629920
C	-0.643281	4.191648	-2.673058	C	5.346485	0.714675	-0.483918
C	-1.015499	2.896365	-3.196398	C	5.307815	-0.661531	-0.512907
N	0.175061	2.229675	-3.461574	C	-4.791590	1.347513	-1.668913
C	1.015614	-2.888331	-3.264613	C	-4.879120	-1.436530	-1.636576
C	0.642374	-4.153572	-2.672235	C	-5.328299	-0.709724	-0.491651
C	-0.769995	-4.249559	-2.674242	C	-5.286394	0.662582	-0.517667
C	-1.261118	-3.052883	-3.284066	C	1.348305	-4.791436	-1.669168
N	-0.189678	-2.316959	-3.736819	C	-1.435716	-4.878632	-1.636874
C	-3.054268	-1.261853	-3.284099	C	-0.709013	-5.328241	-0.492012
C	-4.250905	-0.770869	-2.674390	C	0.663345	-5.286224	-0.517984
C	-4.154833	0.641747	-2.672635	C	1.450714	4.912794	-1.630223
C	-2.889429	1.015078	-3.265189	C	0.714069	5.346233	-0.484049
N	-2.319514	-0.190435	-3.737839	C	-1.352383	4.825901	-1.669184
C	2.896917	-1.015326	-3.196006	C	-0.662010	5.307361	-0.512999
C	4.191801	-0.642936	-2.672678	C	-2.735851	2.735611	2.075792
C	4.277531	0.777685	-2.665409	C	-1.396284	1.395277	4.067946
C	3.036711	1.261257	-3.178165	C	-3.206079	1.441297	2.486424
N	2.229828	0.175031	-3.460206	C	-1.441076	3.204987	2.485474
C	-2.593434	-2.593338	-3.025724	C	-0.744678	2.481286	3.475237
C	3.123755	-3.122713	-1.962114	C	-2.481820	0.744069	3.476319
C	3.326614	-3.324306	0.897465	H	-0.880813	0.880256	4.857982
C	2.565678	-4.200455	-1.253890	C	2.759587	2.759937	2.096069
C	4.207753	-2.561057	-1.253806	C	1.410436	1.410560	4.081807
C	4.276599	-2.620218	0.163708	C	1.459256	3.218831	2.498119
C	2.626352	-4.275992	0.166474	C	3.218683	1.459620	2.498134
C	-4.337267	-2.676962	0.204975	C	2.488748	0.756939	3.480798
C	-2.687198	-4.343129	-1.217674	C	0.756666	2.488775	3.480832
C	-3.368463	-3.368748	0.931127	H	0.899064	0.899072	4.877136
C	-4.343076	-2.687728	-1.217475	C	-2.757507	-2.757831	2.091734
C	-3.316229	-3.316468	-1.947094	C	-1.412094	-1.412286	4.082485
C	-2.676363	-4.337389	0.204648	C	-3.218458	-1.459252	2.496305
C	-4.276118	2.625549	0.166569	C	-1.458842	-3.218605	2.496134
C	-2.561248	4.206905	-1.253783	C	-0.757188	-2.489494	3.480601
C	-3.324644	3.326044	0.897469	C	-2.489390	-0.757509	3.480790
C	-4.200396	2.564692	-1.253603	H	-0.900948	-0.901115	4.878235
C	-3.122590	3.122694	-1.961867	C	2.736013	-2.735604	2.075725
C	-2.620501	4.275924	0.163591	C	1.395461	-1.396087	4.067791
C	2.702926	4.372573	-1.197739	C	1.441745	-3.205890	2.486206
C	4.354735	2.686259	0.222515	C	3.205187	-1.440731	2.485432
C	2.685792	4.355013	0.222480	C	2.481399	-0.744387	3.475161

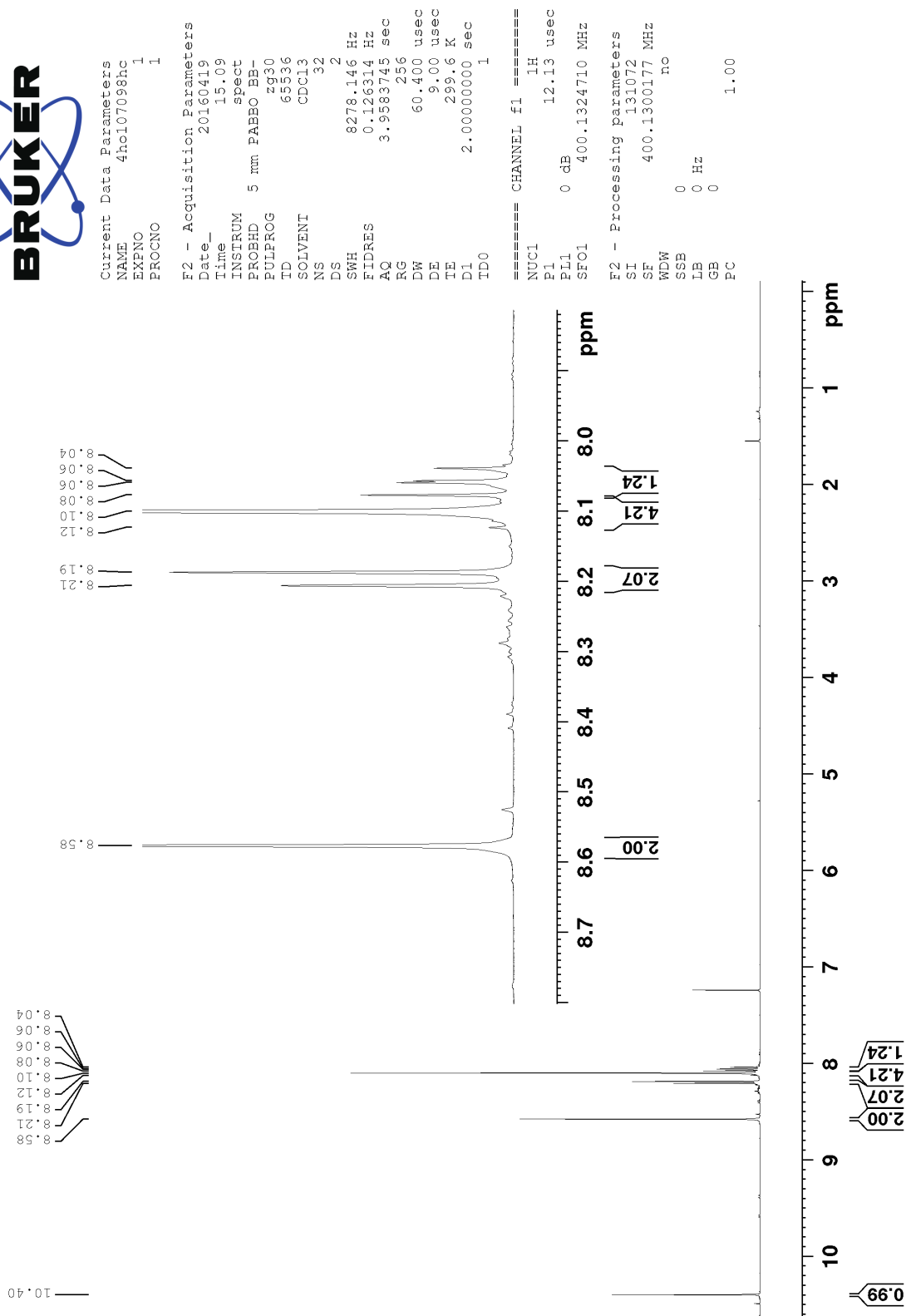


C	0.744405	-2.481686	3.476094	C	-1.403623	-4.849751	0.659465
H	0.880393	-0.880681	4.857833	C	-0.740255	-4.221115	1.712499
C	0.740445	4.222460	1.715403	C	-4.221142	-0.740828	1.712823
C	1.405162	4.858029	0.667914	C	-4.849717	-1.404299	0.659766
C	4.858037	1.405677	0.668017	C	4.815706	-1.369868	0.629979
C	4.222480	0.740918	1.715428	C	4.210902	-0.718372	1.703077
C	-1.370320	4.815383	0.629860	C	0.720310	-4.210852	1.704109
C	-0.718820	4.210704	1.703056	C	1.374582	-4.810977	0.629965
C	-4.811265	1.373880	0.630198	Ge	-0.595729	-0.593997	-4.803091
C	-4.211041	0.719742	1.704398	Ge	0.373930	0.374808	-2.734782

# 5 Spectral Appendix (NMR, MS)



107098/Hoelzel/HH46HPLC/10mg/CDCl3/1H/RT/Maid



Supplementary Fig. 17. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, rt) of 3.

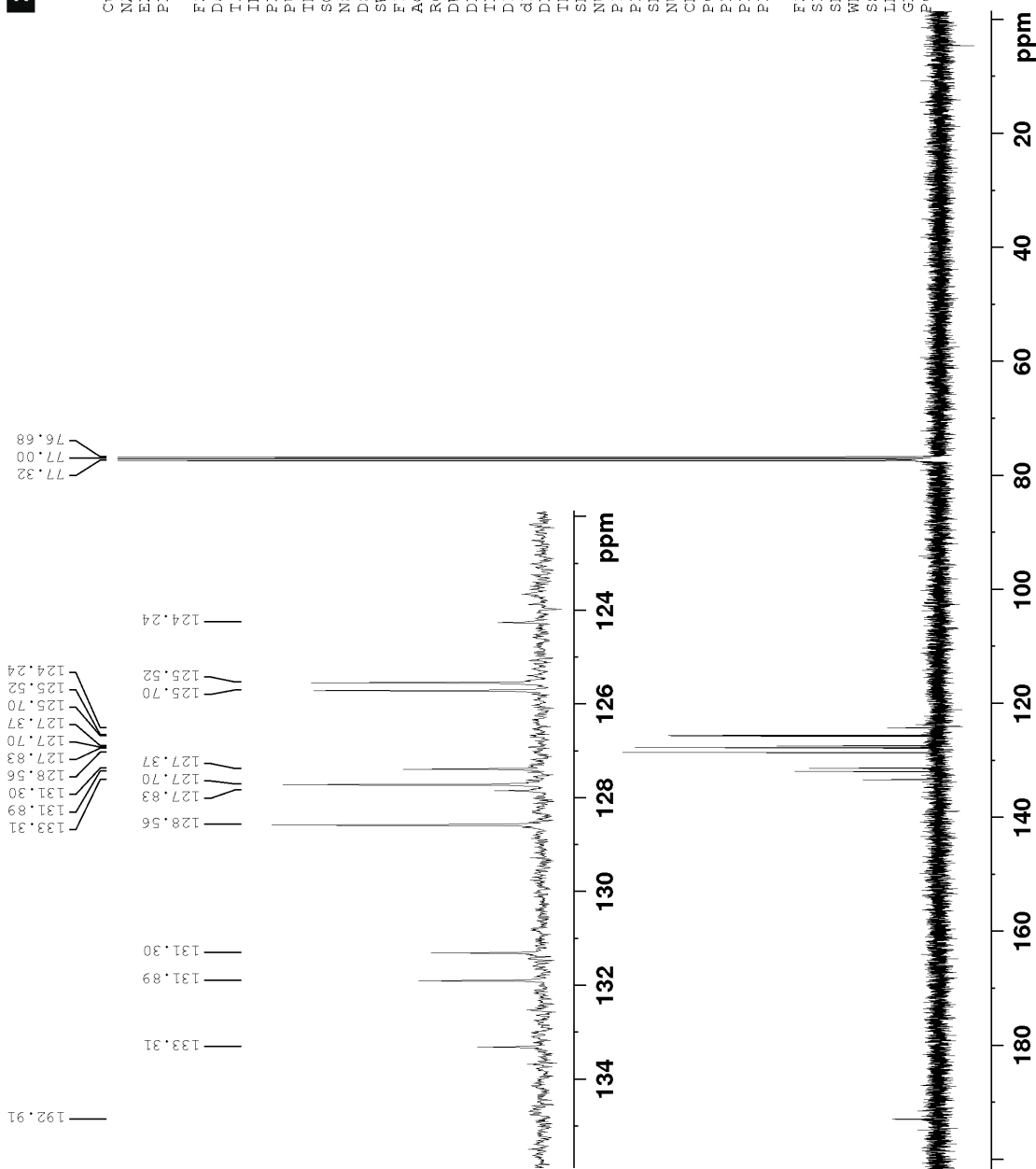


Current Data Parameters  
 NAME 4ho107098hc  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160419  
 Time 15.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO EB-  
 PULPROG zgpg30  
 ID 65536  
 SOLVENT CDCl3  
 NS 546  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664256 sec  
 RG 46341  
 DW 20.850 usec  
 DE 9.00 usec  
 TE 299.7 K  
 D1 4.0000000 sec  
 d11 0.0300000 sec  
 DELTA 3.90000010 sec  
 TD0 1  
 SFO1 100.6227898 MHz  
 NUC1 13C  
 P1 7.00 usec  
 PLW1 -1.0000000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 116.00 usec  
 PLW2 -1.0000000 W  
 PLW12 -1.0000000 W  
 PLW13 -1.0000000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127713 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

107098/Hoelzel/HH46HPLC/10mg/CDCl3/13C/RT/Maid

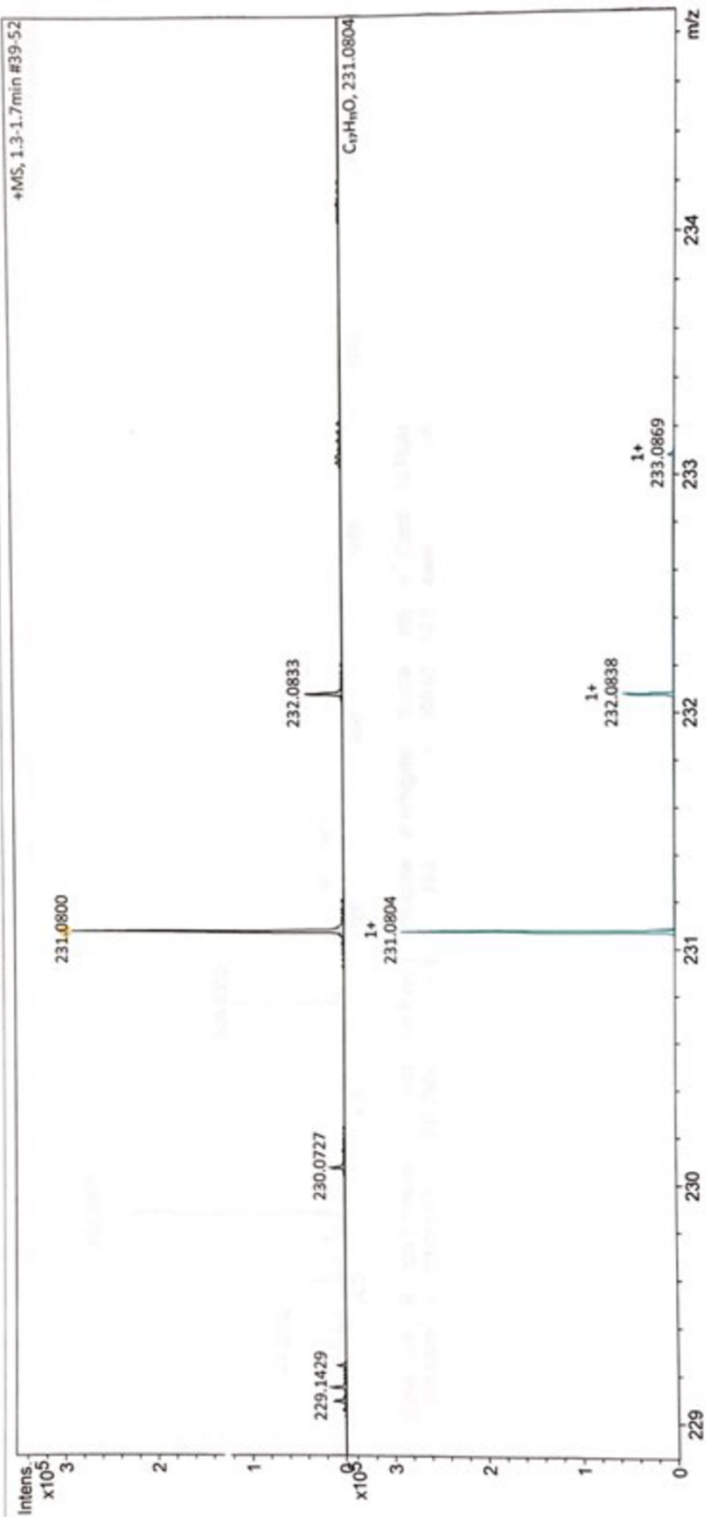


Supplementary Fig. 18. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, rt) of **3**.

# Display Report

**Analysis Info**  
 Analysis Name: D:\Data\2019\Jux-2019\HoelzeltHH-46-appi-.d  
 Method: tune\_low-APPI.m  
 Sample Name: CH2Cl2 THF  
 Acquisition Date: 8/15/2019 10:59:59 AM  
 Operator: MD  
 Instrument: maXis  
 288882.20183

**Acquisition Parameter**  
 Source Type: APPI  
 Focus: Not active  
 Scan Begin: 50 m/z  
 Scan End: 1550 m/z  
 Ion Polarity: Positive  
 Set Capillary: 700 V  
 Set End Plate Offset: -500 V  
 Set Charging Voltage: 0 V  
 Set Corona: 0 nA  
 Set Nebulizer: 2.0 Bar  
 Set Dry Heater: 220 °C  
 Set Dry Gas: 1.0 l/min  
 Set Divert Valve: Waste  
 Set APPI Heater: 250 °C



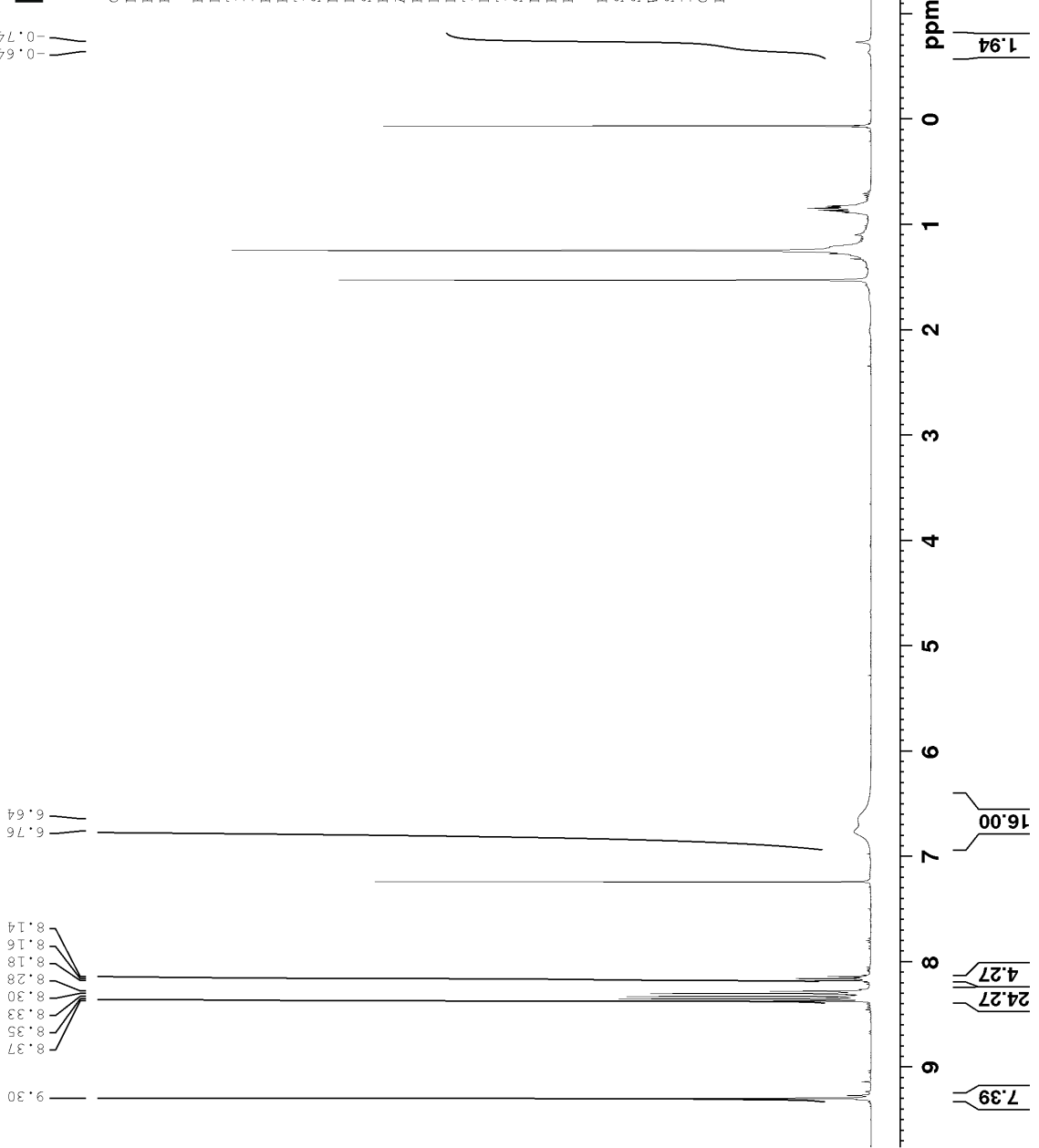
Supplementary Fig. 19. HRMS (APPI; CH<sub>2</sub>Cl<sub>2</sub>, THF) of 3.



0.74  
0.64

hh50neu

Current Data Parameters  
NAME 4ho012954  
EXPNO 10  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20190809  
Time 11.47 h  
INSTRUM CAB AV4 400 MHZ BASIC  
PROBHD Z108618\_0982 (z930)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 64  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 12.31 usec  
TE 298.8 K  
D1 2.00000000 sec  
TD0 1  
SF01 400.3524021 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 12.09300041 W  
F2 - Processing parameters  
SI 32768  
SF 400.3500172 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Supplementary Fig. 20. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, rt) of 1.



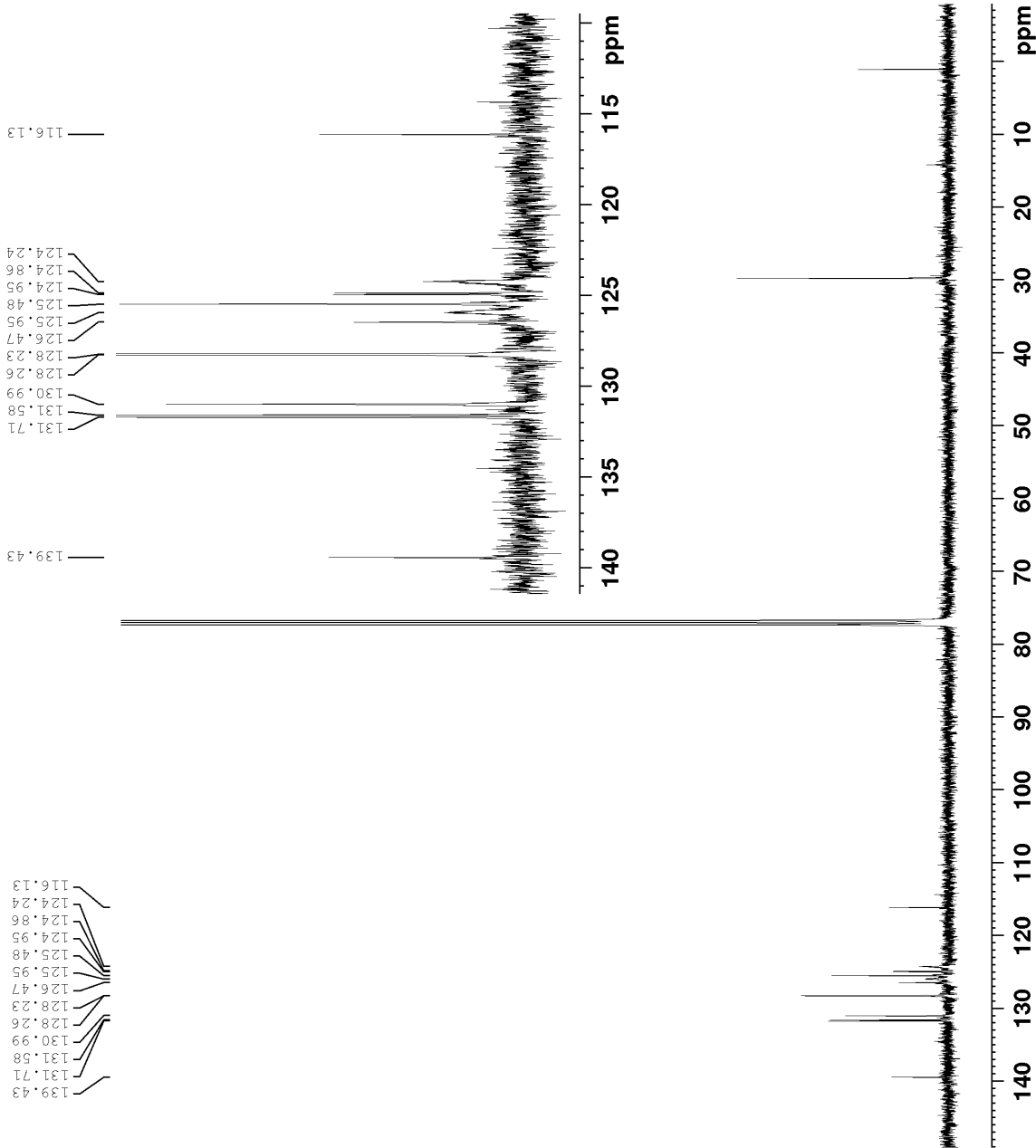
Current Data Parameters  
NAME 4ho012954  
EXNO 11  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20190810  
Time\_ 4.29 h  
INSTRUM CAB AV4 400 MHz BASIC  
PROBHD Z108618\_0982 ( zpgp30  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 4096  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 23.4375  
DW 21.000 usec  
DE 6.50 usec  
TE 299.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 100.6781544 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 58.38000107 W  
SF02 400.3516014 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.09300041 W  
PLW12 0.29260999 W  
PLW13 0.14718001 W  
F2 - Processing parameters  
SI 32768  
SF 100.6680905 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

hh50neu

139.43  
131.71  
131.58  
130.99  
128.26  
128.23  
126.47  
125.95  
125.48  
124.95  
124.86  
124.24  
116.13



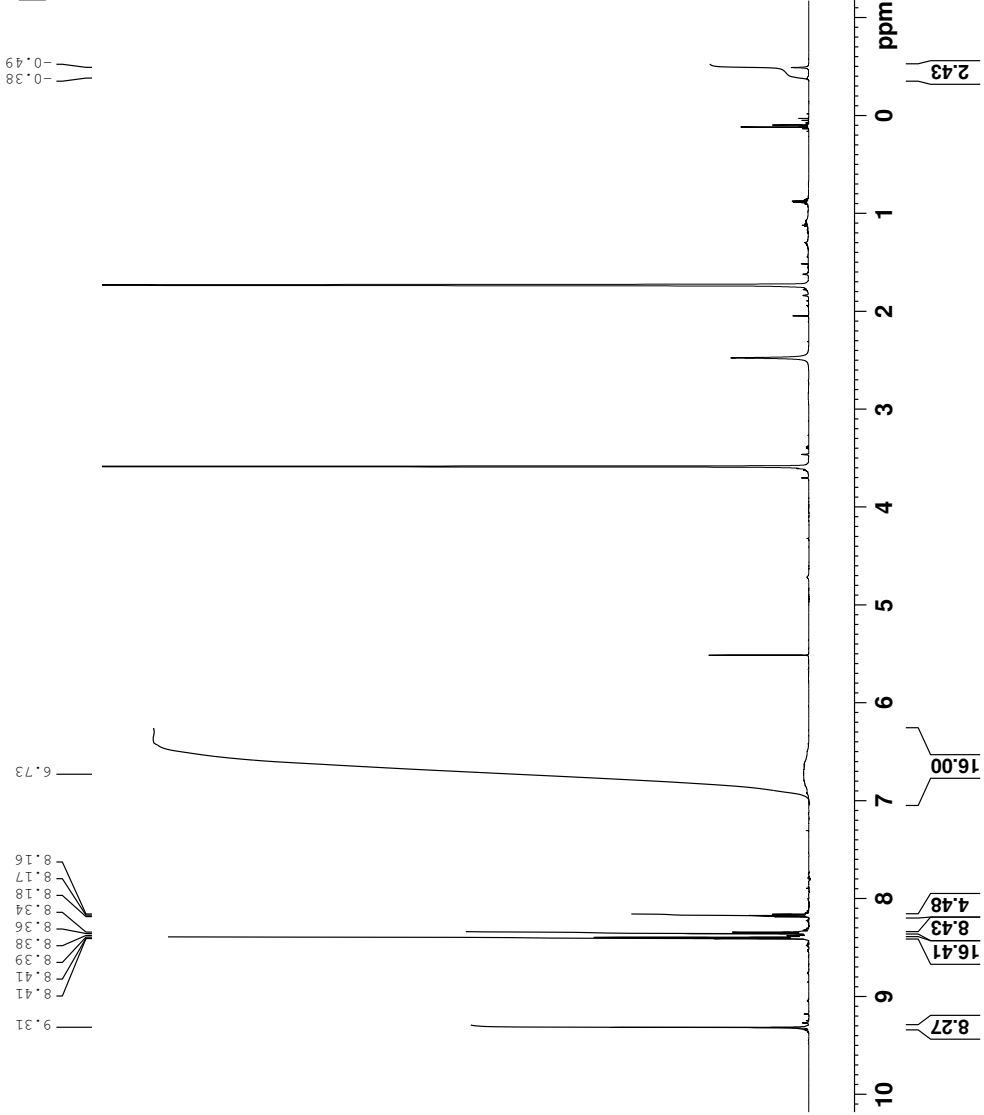
Supplementary Fig. 21. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, rt) of 1.



001370/Hörlzel/HH50/5mg/THF/1H/25°C/Maid

9.31  
8.41  
8.41  
8.39  
8.38  
8.36  
8.34  
8.18  
8.17  
8.16  
6.73  
4.48  
4.48  
4.48  
2.43  
0.49  
0.48  
0.47

Current Data Parameters  
NAME 56h001370  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220628  
Time 16.06 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290-0003 (z950)  
PULPROG zg30  
TD 131072  
SOLVENT THF  
NS 32  
DS 2  
SWH 12500.000 Hz  
FIDRES 0.190735 Hz  
AQ 5.2428799 sec  
RG 36  
DW 40.000 usec  
DE 18.29 usec  
TE 298.1 K  
D1 2.0000000 sec  
TD0 4  
SFO1 600.7036042 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 18.79999924 W  
F2 - Processing parameters  
SI 131072  
SF 600.7000197 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Supplementary Fig. 22. <sup>1</sup>H NMR (600 MHz, THF-D<sub>8</sub>, rt) of 1.

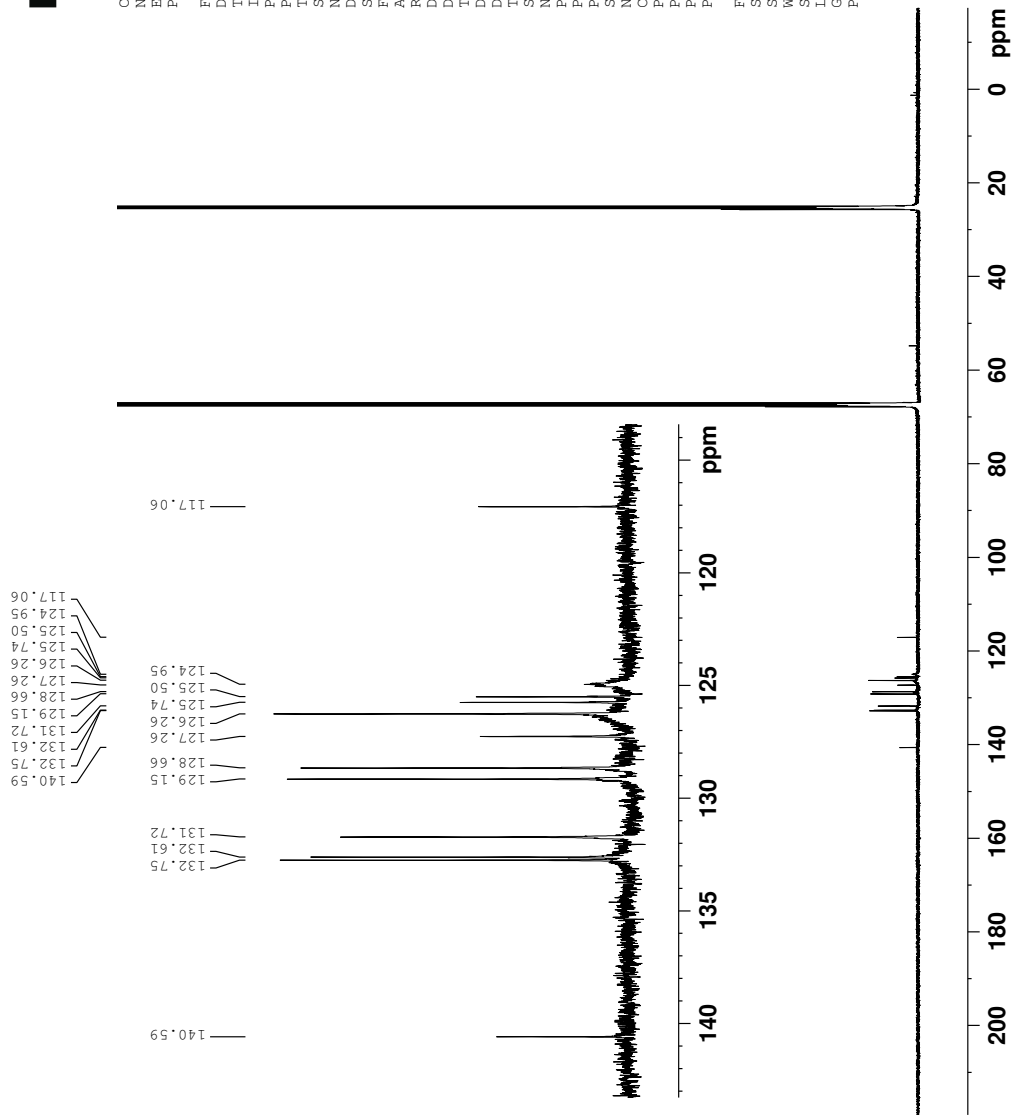


Current Data Parameters  
NAME S6hc001370  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220628  
Time\_ 16:29 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003  
PULPROG zgpg30  
TD 65536  
SOLVENT THF  
NS 264  
DS 4  
SWH 35714.285 Hz  
FIDRES 1.089913 Hz  
AQ 0.9175040 sec  
RG 101  
DW 14.000 usec  
DE 25.00 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D0 128  
SFO1 151.0612398 MHz  
NUC1 13C  
P0 3.53 usec  
P1 10.60 usec  
PLW1 19.89299985 W  
SFO2 600.7024028 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 18.79999924 W  
PLW12 0.38367000 W  
PLW13 0.19298001 W

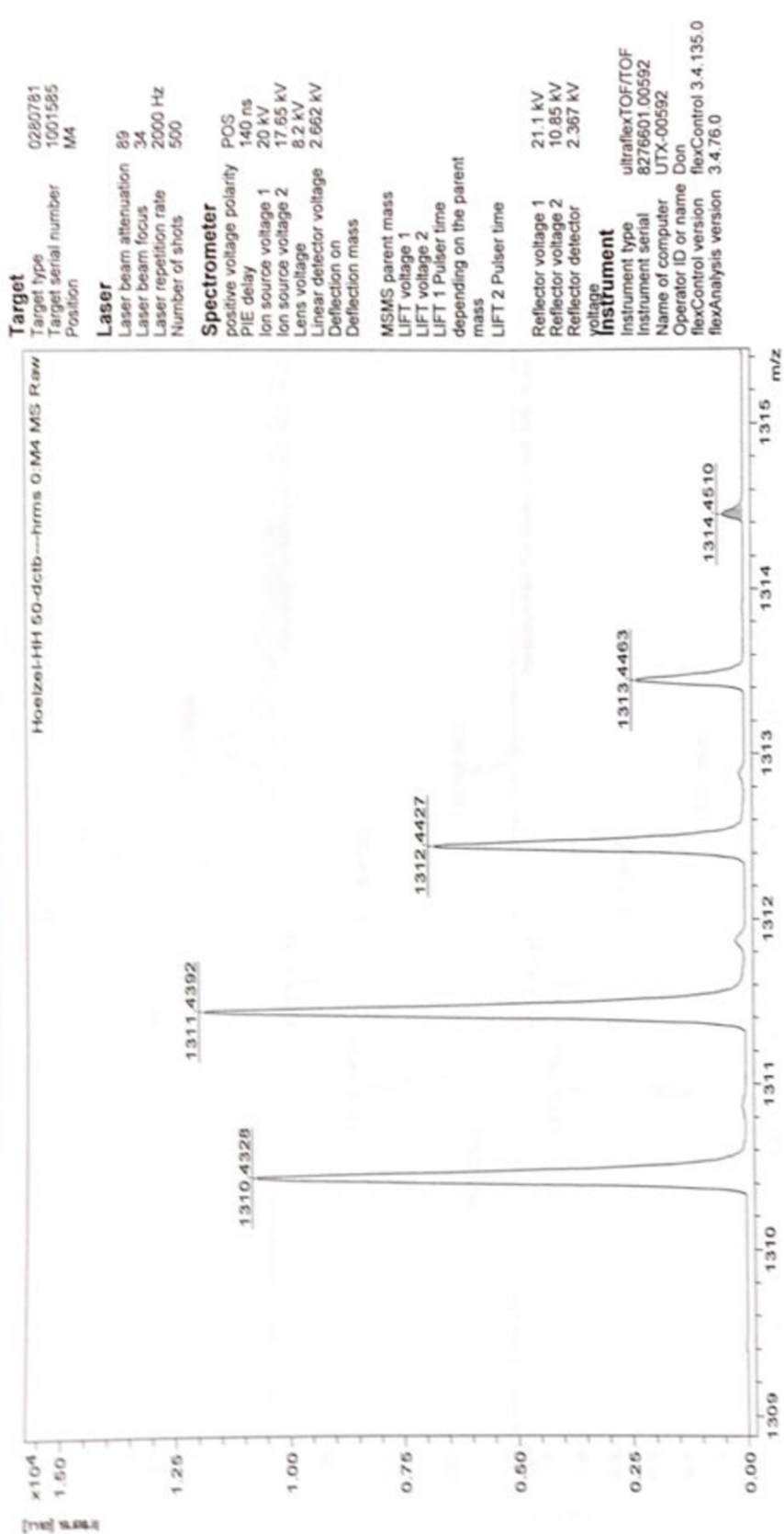
F2 - Processing parameters  
SI 131072  
SF 151.0460054 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

001370/Hölzel/HH50/5mg/THF/13C{1H}/25°C/Maid



Supplementary Fig. 23.  $^{13}\text{C}$  NMR (150 MHz, THF- $\text{D}_8$ , rt) of **1**.





Date of Acquisition 2019-07-11T15:31:00.156+02:00 printed: 7/11/2019 3:32:29 PM  
 Acquisition method D:\Methods\flexControlMethods\Don-70-2100.par  
 Processing method  
 File Name D:\Data\2019\Jux-2019\Hoelzel-HH 50-dctb---hrms\0\_M411

Viewed by	Date / Sign
Performed by	Date / Sign

**Bruker Daltonics**

Supplementary Fig. 24. HRMS (MALDI, DCTB) of 1.

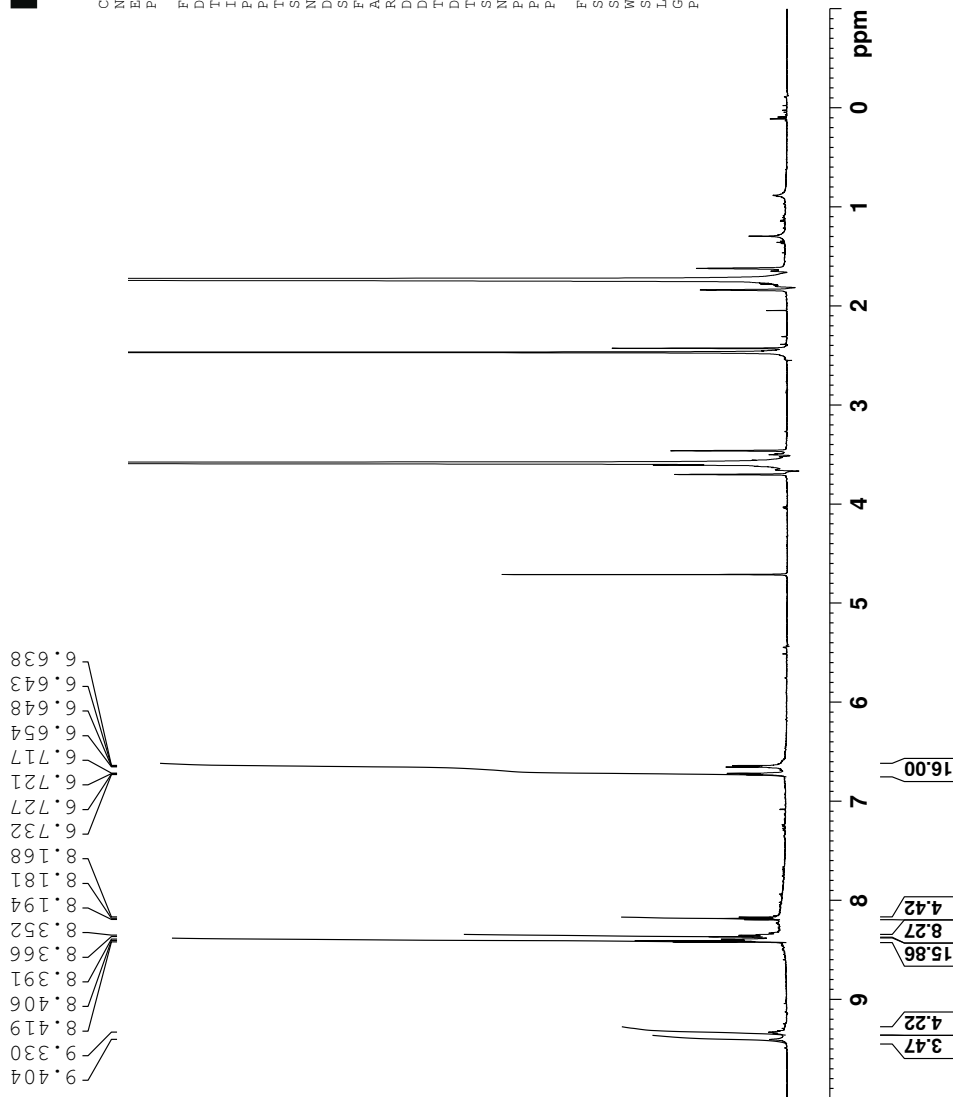


Current Data Parameters  
NAME S6ho001371  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220628  
Time 16.40 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003 (4g30  
PULPROG zg30  
TD 131072  
SOLVENT THF  
NS 32  
DS 2  
SWH 12500.000 Hz  
FIDRES 0.190735 Hz  
AQ 5.2428799 sec  
RG 36  
DW 40.000 usec  
DE 18.29 usec  
TE 298.1 K  
D1 2.00000000 sec  
TD0 4  
SF01 600.7036042 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 18.79999924 W

F2 - Processing parameters  
SI 131072  
SF 600.7000201 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

001371/HöLzel/HH50Pb/1mg/THF/1H/25°C/Maid



Supplementary Fig. 25.  $^1\text{H}$  NMR (600 MHz, THF- $\text{D}_8$ , rt) of **1Pb**.

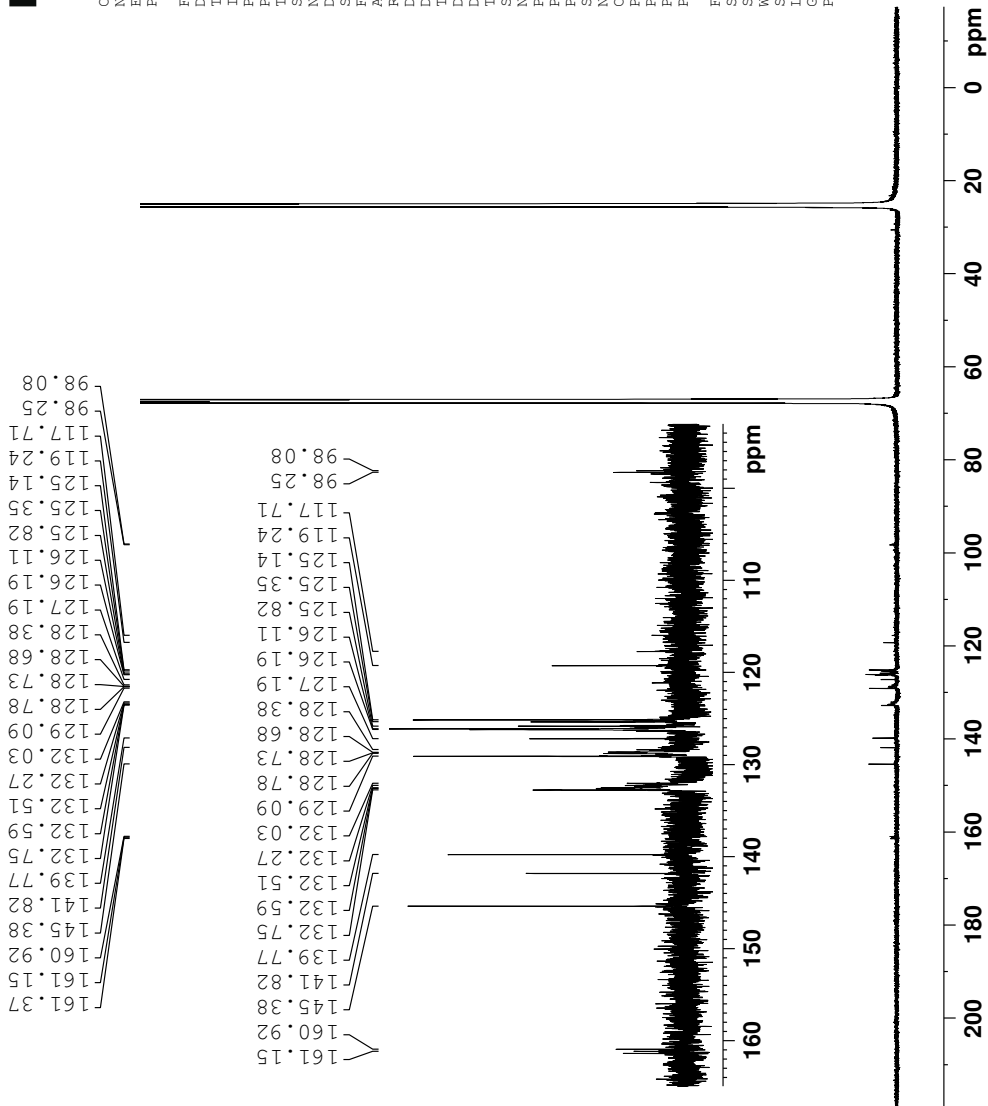


Current Data Parameters  
 NAME S6ho001371  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220629  
 Time\_ 9.16 h  
 INSTRUM CAB AV4 600 MHz BASIC  
 PROBDH Z150290\_0003 ( 20030  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT THF  
 NS 17312  
 DS 4  
 SWH 35714.285 Hz  
 FIDRES 1.089913 Hz  
 AQ 0.9175040 sec  
 RG 11  
 DC 141000 usec  
 DE 2500 usec  
 TE 298.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 15280  
 SF01 151.0612398 MHz  
 NUC1 <sup>13</sup>C  
 F0 3.55 usec  
 F1 10.60 usec  
 PLW1 19.89299965 W  
 SF02 600.7024028 MHz  
 NUC2 <sup>1</sup>H  
 CPDPRG[2] walzr16  
 FCFD2 70.00 usec  
 PLW2 18.79999924 W  
 PLW12 0.38367000 W  
 PLW13 0.19298001 W

F2 - Processing Parameters  
 SI 131072  
 SF 151.0460051 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

001371/Hö1ze1/HH50Pb/1mg/THF/<sup>13</sup>C{<sup>1</sup>H}/25°C/Maid



Supplementary Fig. 26. <sup>13</sup>C NMR (150 MHz, THF-D<sub>8</sub>, rt) of 1Pb.



**Target**  
Target type 0280781  
Target serial number 1001585  
Position N2

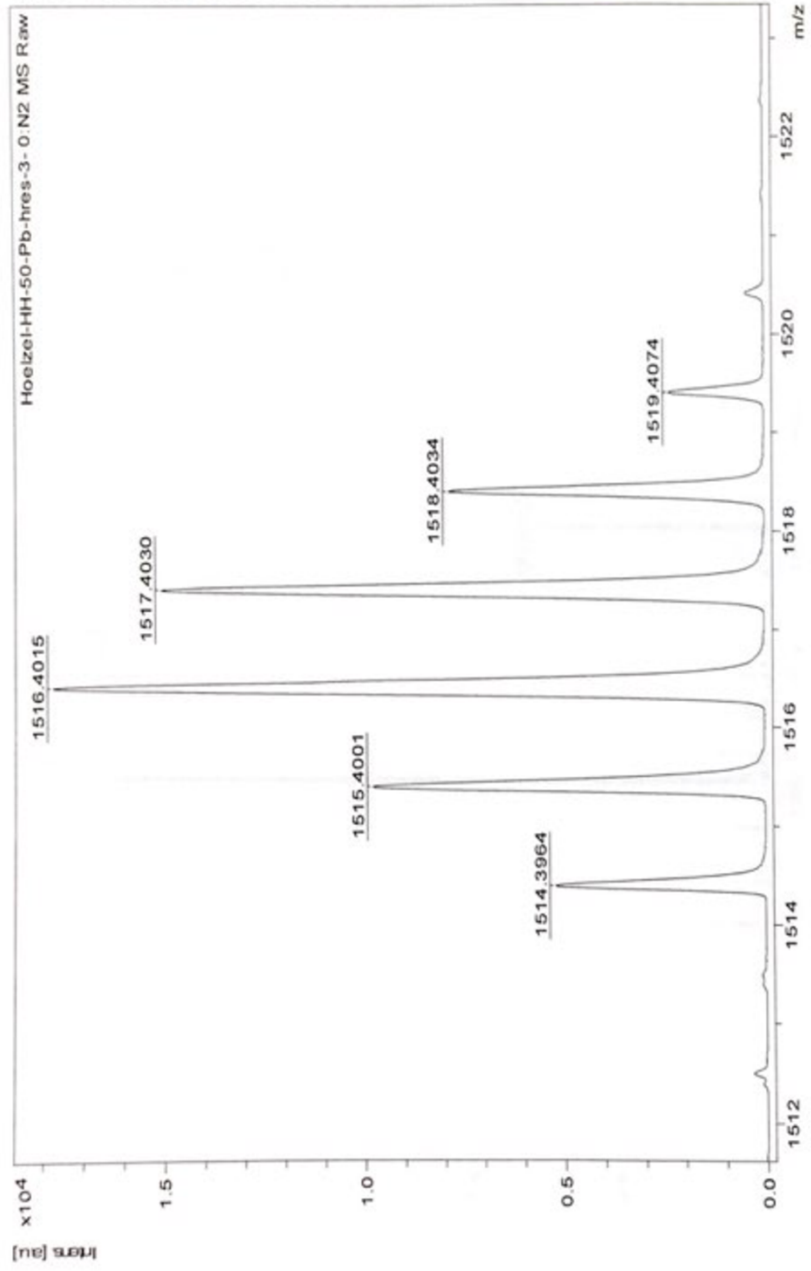
**Laser**  
Laser beam attenuation 68  
Laser beam focus 34  
Laser repetition rate 2000 Hz  
Number of shots 500

**Spectrometer**  
positive voltage polarity POS  
PIE delay 140 ns  
Ion source voltage 1 20 kV  
Ion source voltage 2 17.65 kV  
Lens voltage 8.2 kV  
Linear detector voltage 2.95 kV  
Deflection on  
Deflection mass

MSMS parent mass  
LIFT voltage 1  
LIFT voltage 2  
LIFT 1 Pulser time  
depending on the parent  
mass  
LIFT 2 Pulser time

Reflector voltage 1 21.1 kV  
Reflector voltage 2 10.85 kV  
Reflector detector  
voltage 2.367 kV

**Instrument**  
Instrument type ultraflexTOF/TOF  
Instrument serial 8276601.00592  
Name of computer UTX-00592  
Operator ID or name Don  
flexControl version flexControl 3.4.135.0  
flexAnalysis version 3.4.76.0



Performed by	Viewed by
Date / Sign	Date / Sign

Date of Acquisition 2019-08-08T14:15:16.270+02:00  
Acquisition method D:\Methods\flexControl\Methods\Don-70-2100.par  
Processing method  
File Name D:\Data\2019\lux-2019\Hoelzel-HH-50-Pb-hres-3-0\_N21

printed: 8/8/2019 2:16:17 PM

**Bruker Daltonics**

Supplementary Fig. 27. HRMS (MALDI, DCTB) of 1Pb.

#001374/HÖLZEL/HH50Pt/1mg/THF/1H/25 °C/CHP

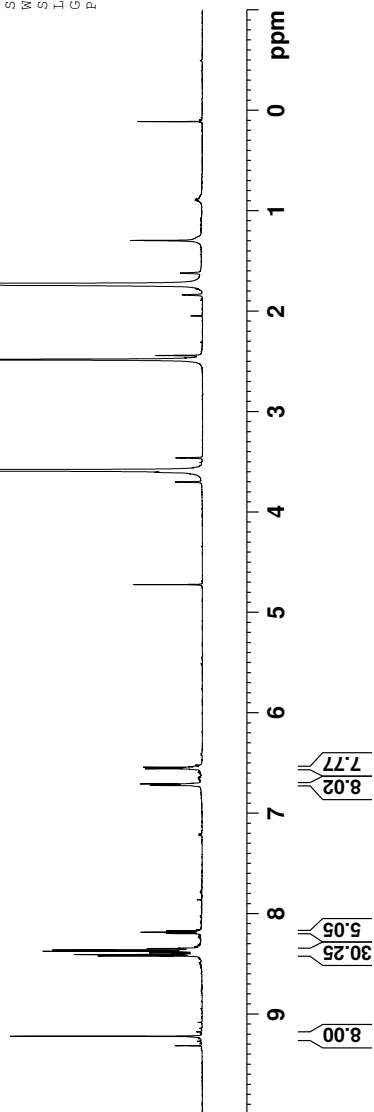


Current Data Parameters  
NAME S6h001374  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220630  
Time\_ 11.09 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003 (1  
PULPROG 131072  
TD 131072  
SOLVENT THF  
NS 24  
DS 2  
SWH 12500.000 Hz  
FIDRES 0.190735 Hz  
AQ 5.2428799 sec  
RG 36  
DW 40.000 usec  
DE 18.29 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 4  
TD0 4  
SFOL 600.7036042 MHz  
NUCL 1H  
P0 3.33 usec  
F1 10.00 usec  
PLW1 18.79999924 W

F2 - Processing parameters  
SI 131072  
SF 600.7000199 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

9.220  
8.420  
8.406  
8.389  
8.374  
8.361  
8.347  
8.197  
8.184  
8.171  
6.722  
6.717  
6.711  
6.706  
6.556  
6.551  
6.546  
6.540



Supplementary Fig. 28. <sup>1</sup>H NMR (600 MHz, THF-D<sub>8</sub>, rt) of 1Pt.

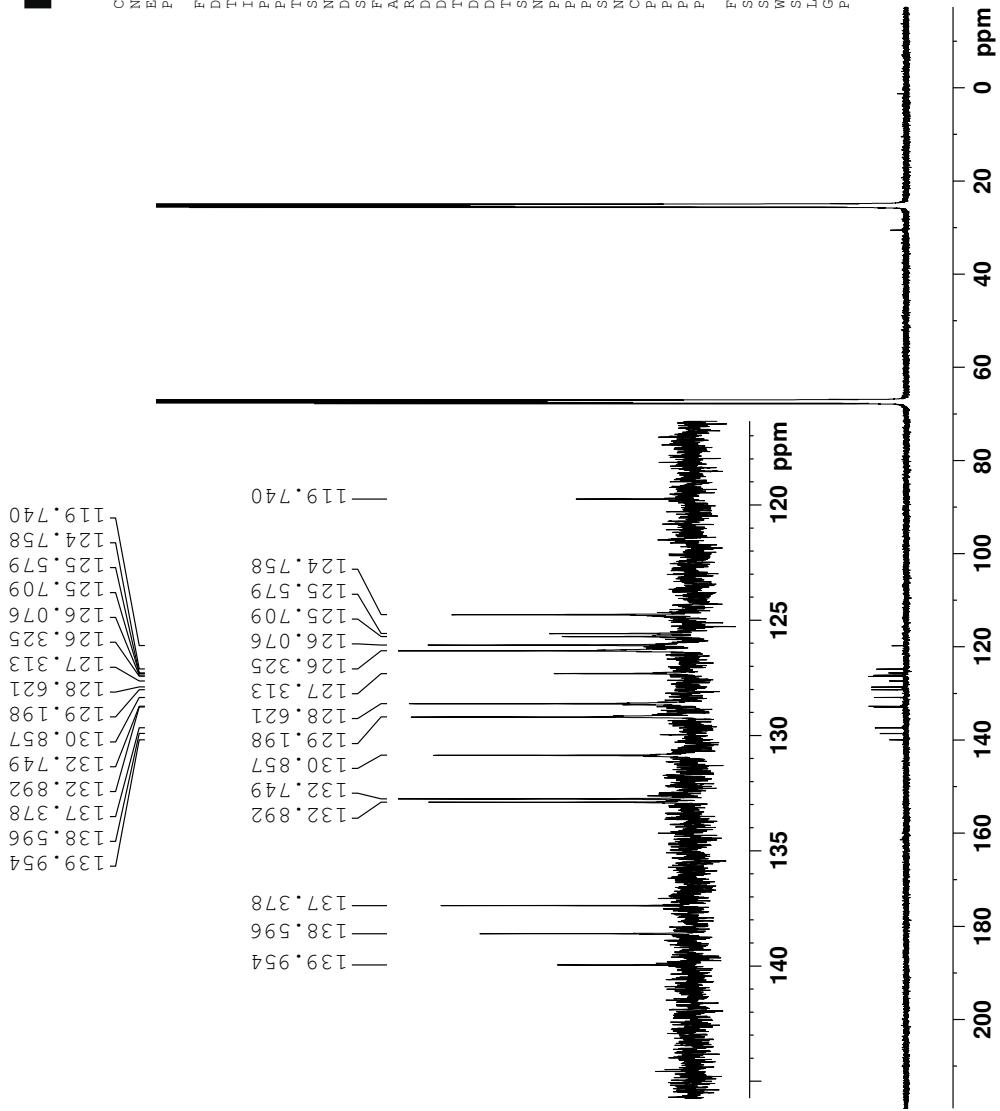
#001374/HÖLZEL/HH50Pt/1mg/THF/13C{1H}/25°C/CHP



Current Data Parameters  
NAME S6h001374  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220630  
Time\_ 12.25 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003 (4)  
PULPROG zgpg30  
TD 98304  
SOLVENT THF  
NS 768  
DS 4  
SWH 35714.285 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762360 sec  
RG 101  
DW 14.000 usec  
DE 25.00 usec  
TE 298.1 K  
D1 4.00000000 sec  
D11 0.03000000 sec  
D0 6  
SFO1 151.0612398 MHz  
NUC1 13C  
P0 3.53 usec  
PL1 10.60 usec  
SFO2 19.89299965 W  
SFO2 600.7024028 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 18.79999824 W  
PLW1 0.38367000 W  
PLW13 0.19298001 W

F2 - Processing parameters  
SI 131072  
SF 151.0460052 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Supplementary Fig. 29. <sup>13</sup>C NMR (150 MHz, THF-D<sub>8</sub>, rt) of 1Pt.



**Target**  
 Target type 0280781  
 Target serial number 1001585  
 Position K6

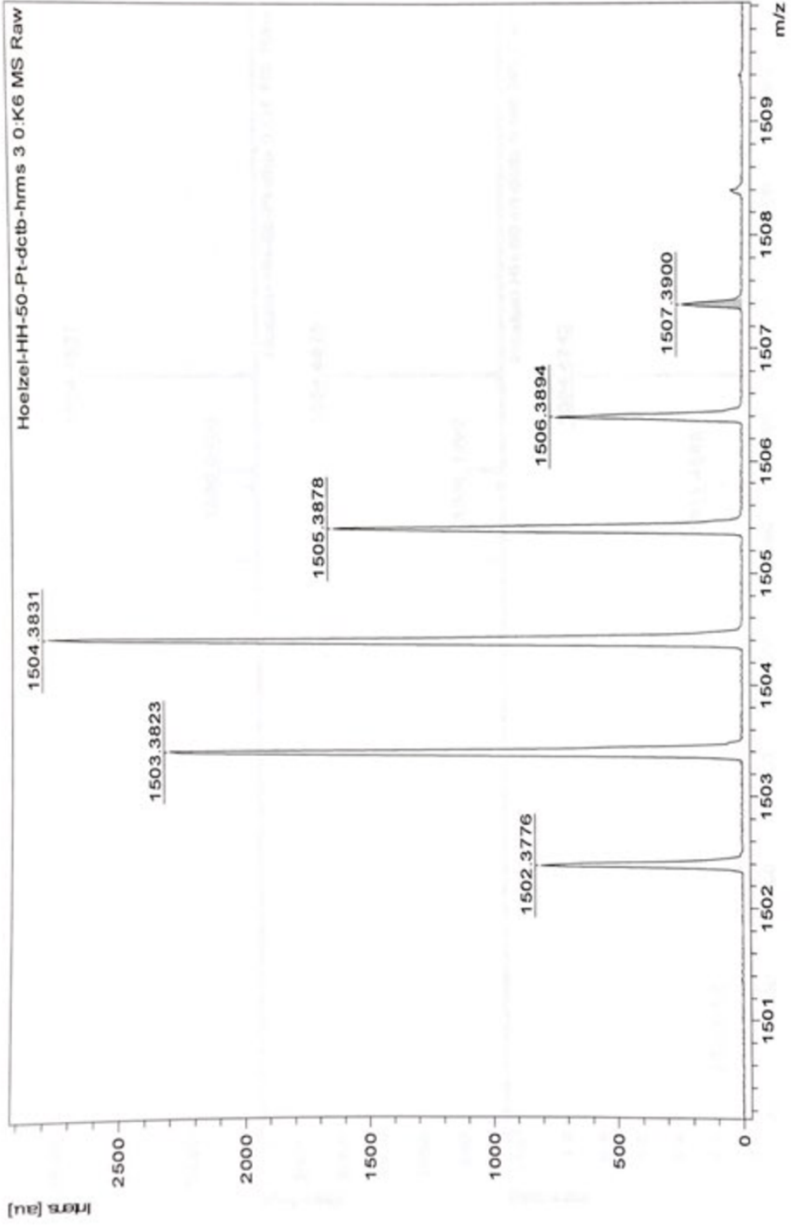
**Laser**  
 Laser beam attenuation 91  
 Laser beam focus 34  
 Laser repetition rate 2000 Hz  
 Number of shots 500

**Spectrometer**  
 positive voltage polarity POS  
 P/E delay 140 ns  
 Ion source voltage 1 20 kV  
 Ion source voltage 2 17.65 kV  
 Lens voltage 8.2 kV  
 Linear detector voltage 2.95 kV  
 Deflection on Deflection mass

**MSMS parent mass**  
 LIFT voltage 1  
 LIFT voltage 2  
 LIFT 1 Pulser time depending on the parent mass  
 LIFT 2 Pulser time

**Reflector voltage 1** 21.1 kV  
**Reflector voltage 2** 10.85 kV  
**Reflector detector voltage** 2.367 kV

**Instrument**  
 ultraflexTOF/TOF  
 Instrument type 8276601.00592  
 Instrument serial UTX-00592  
 Name of computer Operator ID or name Don  
 flexControl version flexControl 3.4.135.0  
 flexAnalysis version 3.4.76.0

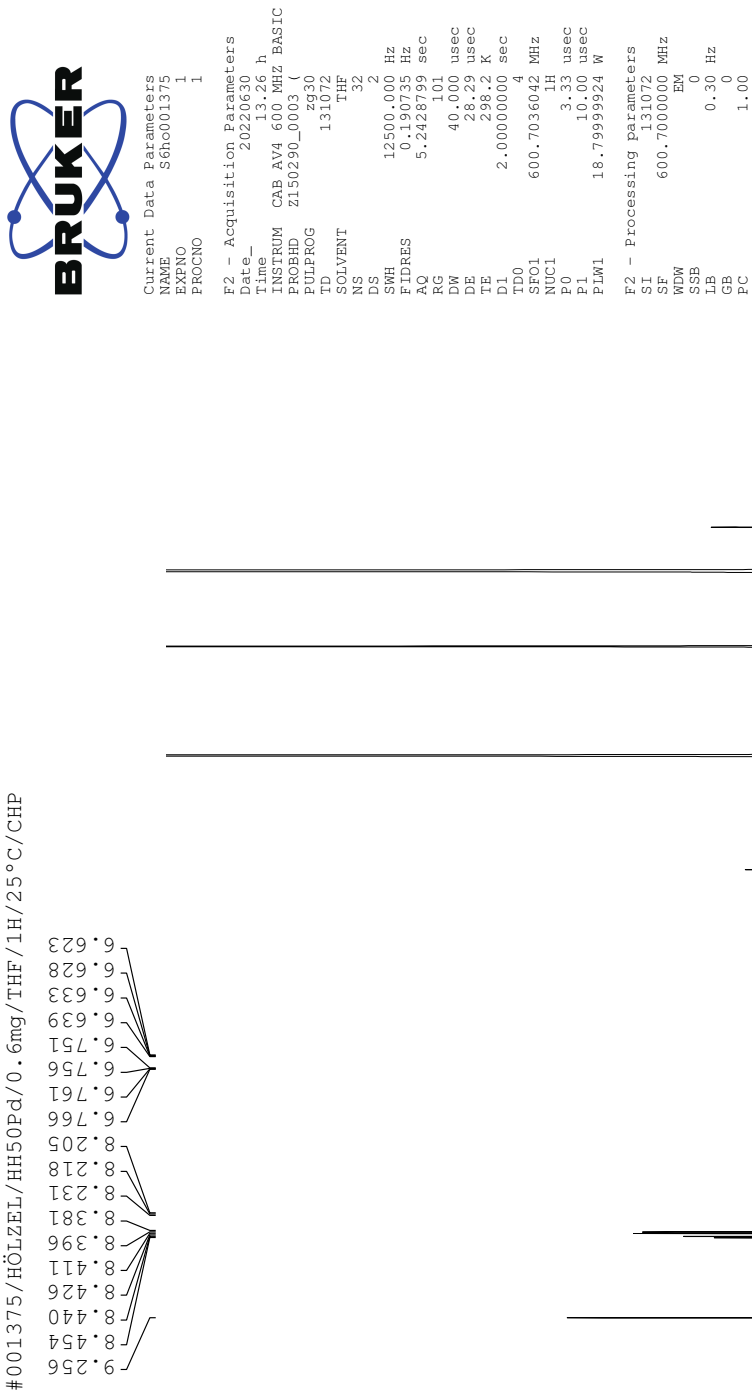


Date of Acquisition 2019-08-08T15:50:27.088+02:00 printed: 8/8/2019 3:50:54 PM  
 Acquisition method D:\Methods\flexControlMethods\Don-70-2100.par  
 Processing method  
 File Name D:\Data\2019\Jux-2019\Hoelzel-HH-50-Pt-dctb-hrms310\_K61

Performed by	Viewed by
Date / Sign	Date / Sign

**Bruker Daltonics**

Supplementary Fig. 30. HRMS (MALDI, DCTB) of 1Pt.



Supplementary Fig. 31. <sup>1</sup>H NMR (600 MHz, THF-D<sub>8</sub>, rt) of 1Pd.

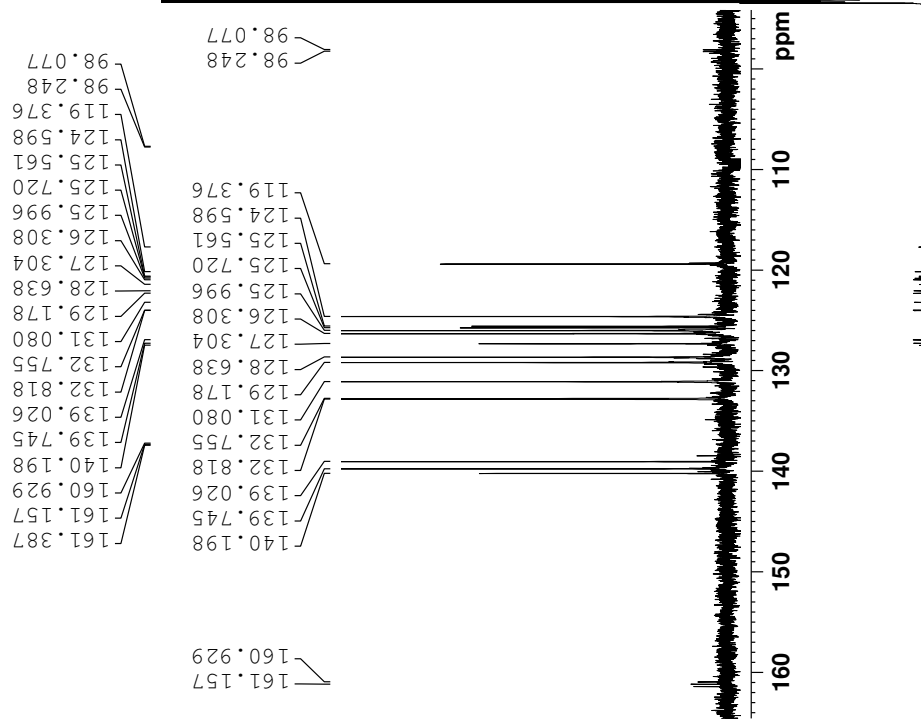




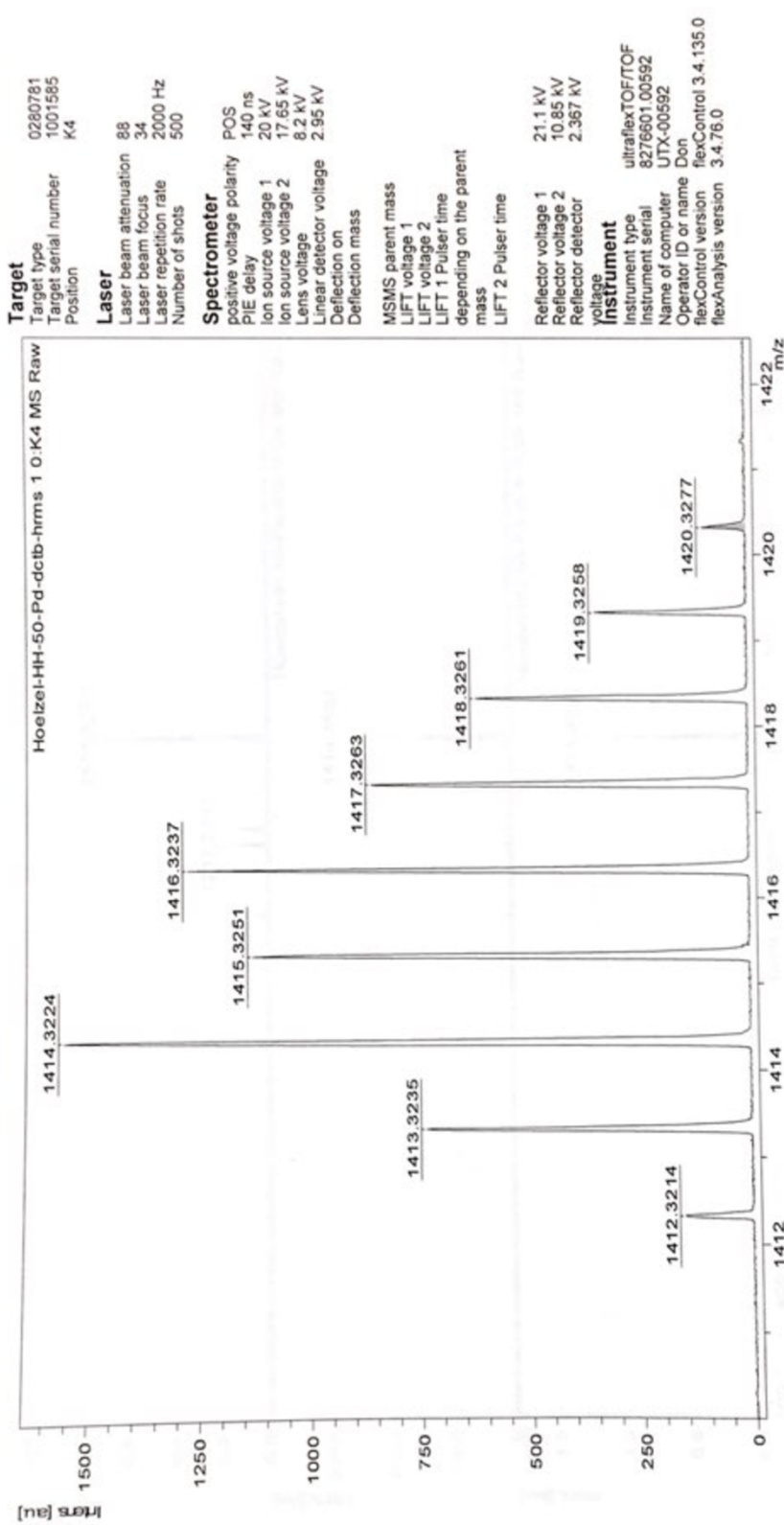
Current Data Parameters  
NAME S6hc001375  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220701  
Time 10.11 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003 (zgpg30)  
PULPROG 98304  
TD 98304  
SOLVENT THF  
NS 13704  
DS 4  
SWH 35714.285 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 101  
DW 14.000 usec  
DE 25.00 usec  
TE 298.2 K  
D1 4.0000000 sec  
D11 0.0300000 sec  
TD0 128  
SF01 151.0612398 MHz  
NUC1 13C  
P0 3.53 usec  
P1 10.60 usec  
PLW1 19.89299965 W  
SFO2 600.7024028 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLM2 18.79999924 W  
PLW2 0.38367000 W  
PLM3 0.00000000 W  
PLW3 0.19298001 W  
F2 - Processing Parameters  
SI 131072  
SF 151.0460049 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

#001375/HÖLZEL/HH50Pd/0.6mg/THF/13C{1H}/25°C/CHP



Supplementary Fig. 32. <sup>13</sup>C NMR (150 MHz, THF-D<sub>8</sub>, rt) of 1Pd.



Performed by	Viewed by
Date / Sign	Date / Sign

printed: 8/8/2019 3:39:38 PM

Date of Acquisition 2019-08-08T15:38:36.119+02:00  
 Acquisition method D:\Methods\flexControl\Methods\Don-70-2100.par  
 Processing method  
 File Name D:\Data\2019\Jux-2019\Hoelzel-HH-50-Pd-dctb-hrms 1\0\_K41

**Bruker Daltonics**

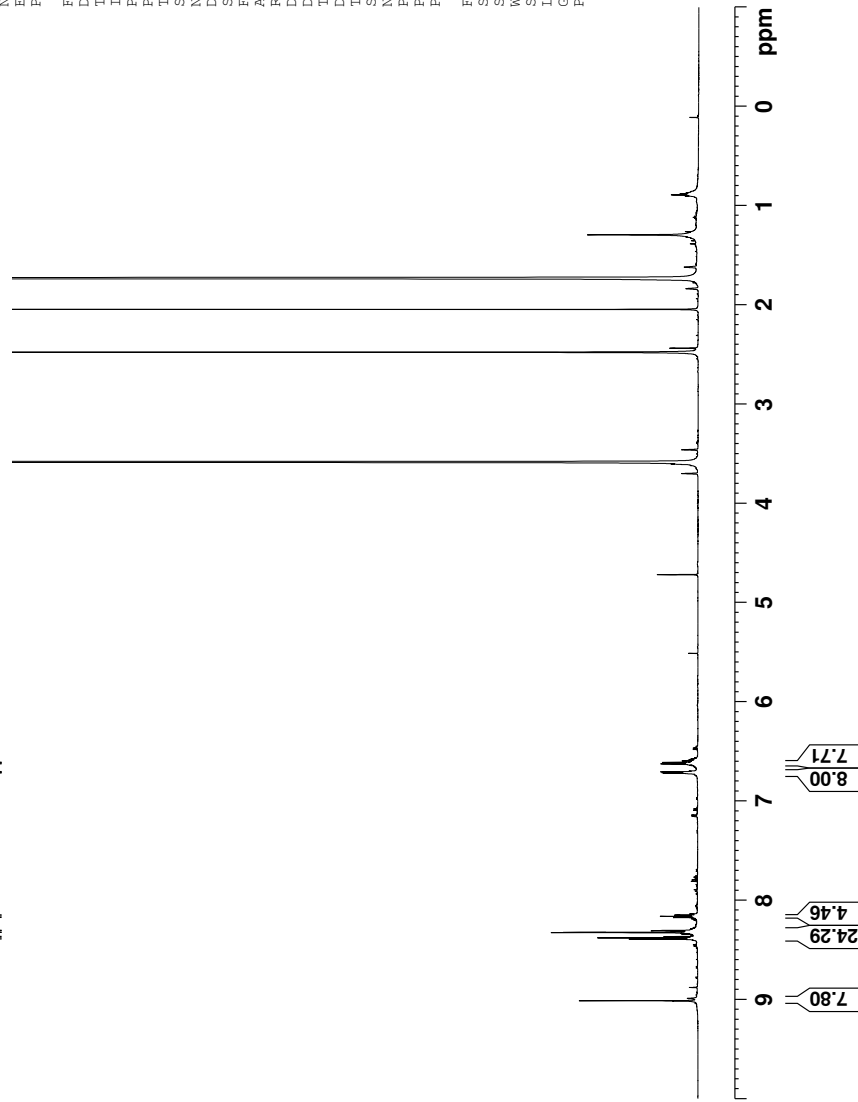
Supplementary Fig. 33. HRMS (MALDI, DCTB) of 1Pd.

001372/Hörlzel/HH50Ni/1mg/THF/1H/25 °C/Maid



Current Data Parameters  
NAME S6ho001372  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220629  
Time 9.27 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290\_0003 (Z150290)  
PULPROG zg30  
TD 131072  
SOLVENT THF  
NS 32  
DS 2  
SWH 12500.000 Hz  
FIDRES 0.190735 Hz  
AQ 5.2428799 sec  
RG 36  
DW 40.000 usec  
DE 18.29 usec  
TE 298.1 K  
D1 2.00000000 sec  
TD0 4  
SFO1 600.7036042 MHz  
NUC1 1H  
P1 3.33 usec  
P2 10.00 usec  
PLW1 18.79999924 W  
F2 - Processing parameters  
SI 131072  
SF 600.7000201 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.392  
8.379  
8.366  
8.326  
8.323  
8.307  
8.304  
8.174  
8.161  
8.148  
6.720  
6.715  
6.709  
6.704  
6.626  
6.621  
6.616  
6.610



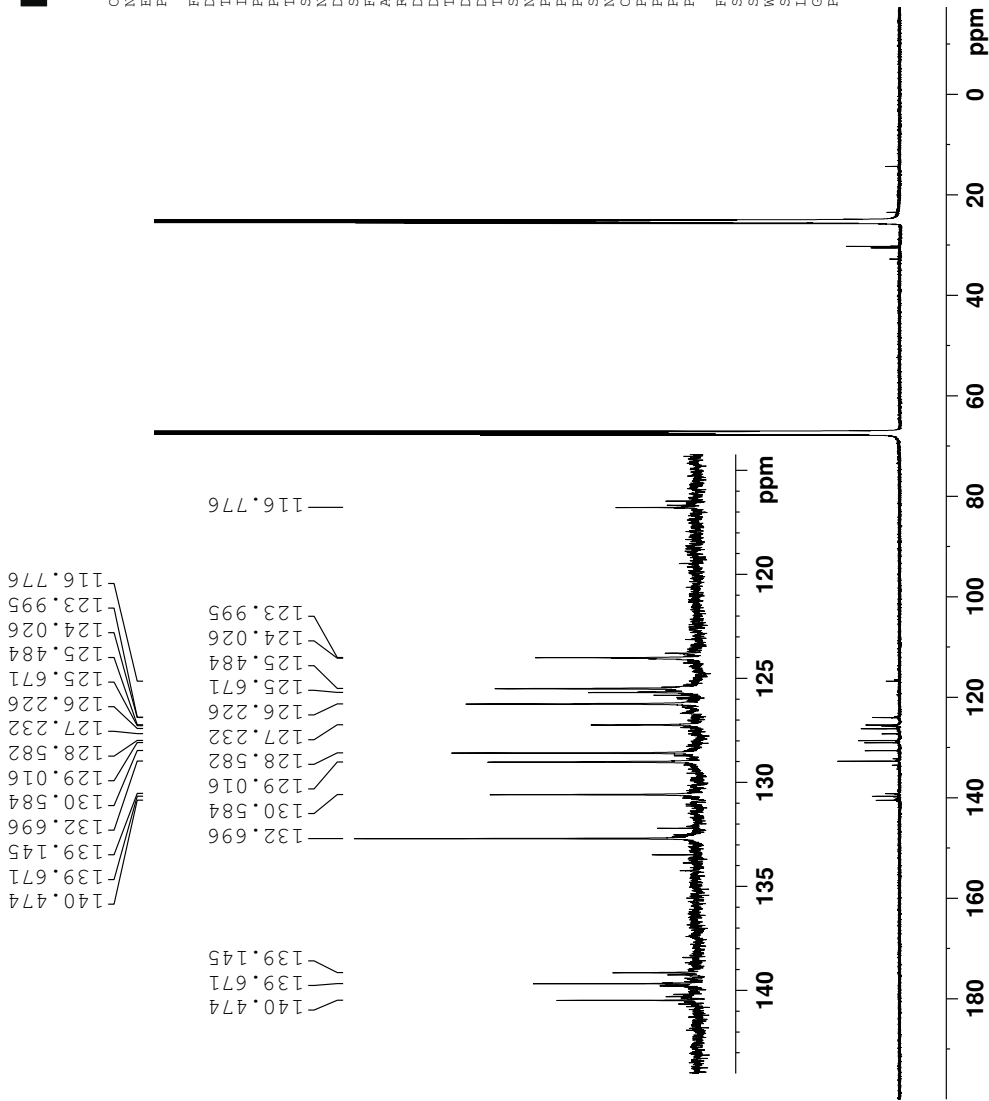
Supplementary Fig. 34. <sup>1</sup>H NMR (600 MHz, THF-D<sub>8</sub>, rt) of 1Ni.

001372/Hölzel/HH50Ni/1mg/THF/13C{1H}/25°C/Maid

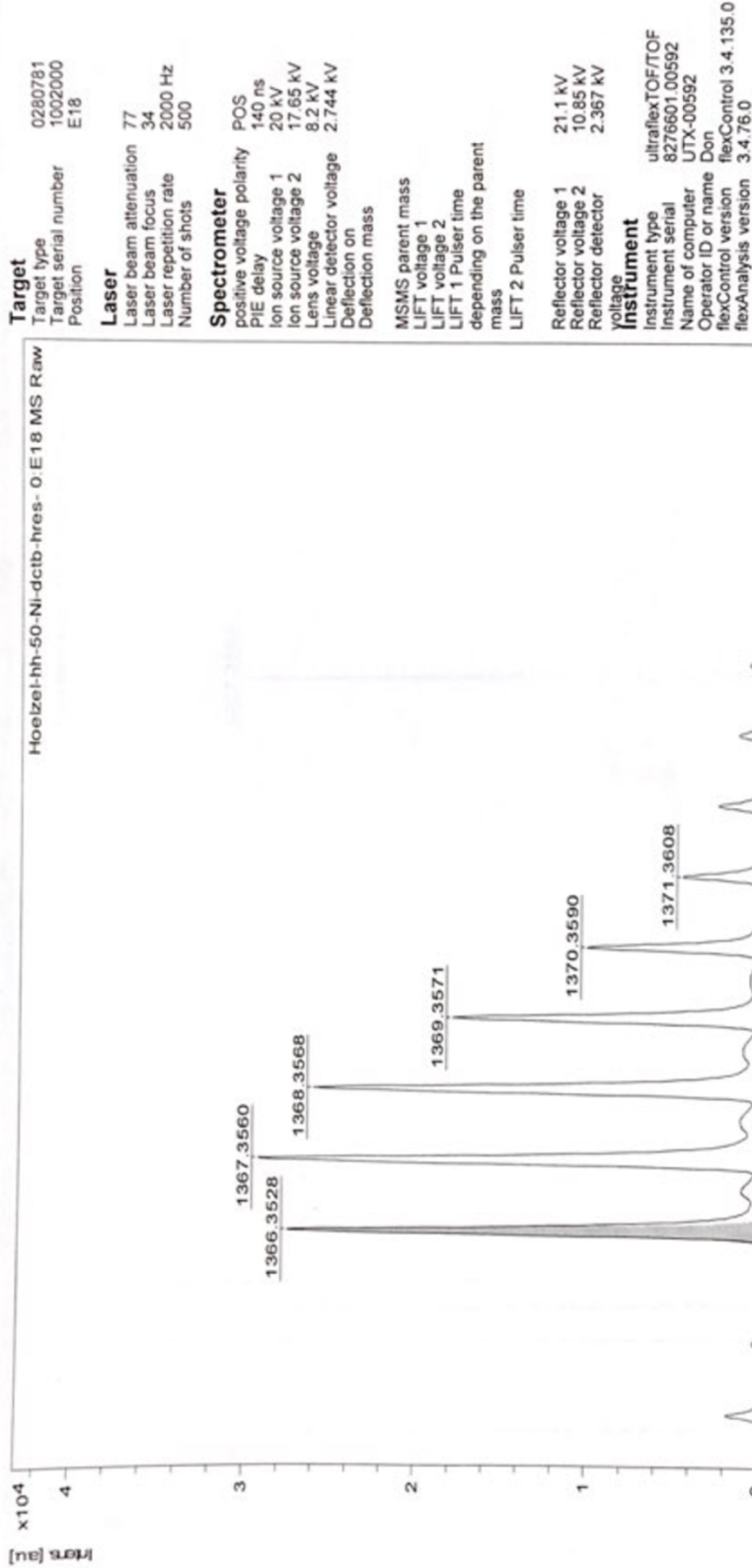


Current Data Parameters  
NAME 56hc001372  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220629  
Time 11.46 h  
INSTRUM CAB AV4 600 MHz BASIC  
PROBHD Z150290.0003 (zggp30  
PULPROG zgpg30  
TD 65536  
SOLVENT THF  
NS 2336  
DS 4  
SWH 35714.285 Hz  
FIDRES 1.089913 Hz  
AQ 0.9175040 sec  
RG 101  
DW 14.000 usec  
DE 25.00 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 12800  
SFO1 151.0612398 MHz  
NUC1 13C  
P0 3.53 usec  
P1 10.60 usec  
PLW1 19.89299965 W  
SFO2 600.7024028 MHz  
NUC2 1H  
waltz16  
CPDPRG2  
PCPD2 70.00 usec  
PLW2 18.79999924 W  
PLW12 0.38367000 W  
PLW13 0.19298001 W  
F2 - Processing parameters  
SI 131072  
SF 151.0460051 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Supplementary Fig. 35. <sup>13</sup>C NMR (150 MHz, THF-D<sub>8</sub>, rt) of 1Ni.



Broker Daltonics

Supplementary Fig. 36. HRMS (MALDI, DCTB) of 1Ni.

## 6 Supplementary References

1. Jablonski, A., Salvat, F., Powell, C. J. & Lee, A. Y. *NIST Electron Elastic-Scattering Cross-Section Database Version 4.0, NIST Standard Reference Database Number 64, National Institute of Standards and Technology.* (2016).
2. Egerton, R. F., Li, P. & Malac, M. Radiation damage in the TEM and SEM. *Micron* **35**, 399–409 (2004).
3. Susi, T., Meyer, J. C. & Kotakoski, J. Quantifying transmission electron microscopy irradiation effects using two-dimensional materials. *Nat. Rev. Phys.* **1**, 397–405 (2019).
4. Chamberlain, T. W. *et al.* Isotope Substitution Extends the Lifetime of Organic Molecules in Transmission Electron Microscopy. *Small* **11**, 622–629 (2015).
5. Brydson, R. *Electron Energy Loss Spectroscopy.* (Taylor & Francis, 2001). doi:10.1201/9781003076858-1.
6. Kim, Y.-K., Santos, J. P. & Parente, F. Extension of the binary-encounter-dipole model to relativistic incident electrons. *Phys. Rev. A* **62**, 052710 (2000).
7. Avillez, M. A. de *et al.* Relativistic electron impact ionization cross sections of carbon ions and application to an optically thin plasma. *Astron. Astrophys.* **631**, A42 (2019).
8. Chamberlain, T. W. *et al.* Isotope Substitution Extends the Lifetime of Organic Molecules in Transmission Electron Microscopy. *Small* **13**, 1–1 (2017).