Supporting Information

Site-Specific Reduction-Induced Hydrogenation of a Helical Bilayer Nanographene with K and Rb Metals: Electron Multiaddition and Selective Rb⁺ Complexation

Z. Zhou, J. M. Fernández-García, Y. Zhu, P. J. Evans, R. Rodríguez, J. Crassous, Z. Wei, I. Fernández*, M. A. Petrukhina*, N. Martín*
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I. Materials and Methods

All manipulations were carried out using break-and-seal and glove-box techniques under an atmosphere of argon.[1] THF and hexanes (Sigma Aldrich) were dried over Na/benzophenone and distilled prior to use. Tetrahydrofuran-d$_8$ (≥ 99.5 atom %D, Sigma Aldrich) was dried over NaK alloy and vacuum-transferred. 18-Crown-6 ether (99%, Sigma Aldrich) was dried over P$_2$O$_5$ in vacuo for 24 hours prior to use. Potassium (99%) and rubidium (99.5%) metals were purchased from Sigma Aldrich and used as received. The sample of C$_{138}$H$_{120}$ (1) was prepared as described previously.[2] The $^1$H NMR spectra were recorded on a Bruker Ascend-500 spectrometer (500 MHz for $^1$H). Chemical shifts (δ) are reported in parts per million (ppm) and referenced to the resonances of the corresponding solvent used. The extreme air- and moisture sensitivity of crystals 2·10C$_6$H$_{14}$ and 3·4THF coupled with the presence of loosely bound interstitial solvent molecules prevented us from obtaining the elemental analysis data and carrying out spectroscopic characterization.

$$[\text{K}^+ (18\text{-crown-6})(\text{THF})_2][[\text{K}^+(18\text{-crown-6})]_2(\text{THF})_{0.5}] [\text{C}_{138}\text{H}_{122}^{3-}] \cdot 10\text{C}_6\text{H}_{14} (2 \cdot 10\text{C}_6\text{H}_{14})$$

THF (1.5 mL) was added to a customized glass system containing excess K (4.0 mg, 0.103 mmol), I (5.0 mg, 0.006 mmol), and 18-crown-6 (5.5 mg, 0.021 mmol). The mixture was allowed to stir under argon at 25 °C for 30 minutes in a closed system. The initial yellow color of the suspension (neutral ligand) has changed to yellow-brown after 8 minutes, deepened to dark brown after 15 minutes and remained the same color until the reaction was stopped. The suspension was filtered, and the dark brown filtrate was layered with 1.5 mL of hexanes. The ampule was sealed and stored at 5 °C. After 3 weeks, small black plates were present in moderate yield (9.4 mg, 45%).

$$[\text{Rb}^+(18\text{-crown-6})_2][[\text{Rb}^+(18\text{-crown-6})]_2(\text{C}_{138}\text{H}_{122}^{3-})] \cdot 4\text{THF} (3 \cdot 4\text{THF})$$

THF (1.5 mL) was added to a customized glass system containing excess Rb (5.0 mg, 0.063 mmol), I (5.0 mg, 0.006 mmol), and 18-crown-6 (5.5 mg, 0.021 mmol). The mixture was allowed to stir under argon at 25 °C for 20 minutes in a closed system. The initial yellow color of the suspension (neutral ligand) has changed to yellow-brown after 5 minutes, deepened to dark brown after 10 minutes and remained the same color until the reaction was stopped. The suspension was filtered, and the dark brown filtrate was layered with 1.4 mL of hexanes. The ampule was sealed and stored at 5 °C. After 2 weeks, black blocks were present in moderate yield (8.2 mg, 40%).
II. Crystal Structure Solution and Refinement

Data collection of 2 was performed at 100(2) K on a Huber Kappa system with a Pilatus 3×2M CdTe pixel array detector using φ scans (synchrotron radiation at λ = 0.49594 Å) located at the Advanced Photon Source, Argonne National Laboratory (ChemMatCARS, Sector 15). Data collection of 3 was performed on a Bruker D8 VENTURE X-ray diffractometer equipped with a PHOTON 100 CMOS shutterless mode detector and a Mo-target X-ray tube (λ = 0.71073 Å) at 100(2) K. The data reduction and integration were performed with SAINT (version 8.38A).\(^3\) Data were corrected for absorption effects using the empirical methods as implemented in SADABS (version 2016/2).\(^4\) The structures were solved by SHELXT (version 2018/2)\(^5\) and refined by full-matrix least-squares procedures using the SHELXL program (version 2018/3)\(^6\) through the OLEX2\(^7\) graphical interface. All non-hydrogen atoms, including those in disordered parts, were refined anisotropically. H-atoms on C39 and C59 in both structures were localized in the difference Fourier map; and their coordinates were refined while \(U_{\text{iso}}(H)\) were constrained to 1.2 \(U_{\text{eq}}(C)\). Other H-atoms were included at calculated positions and refined as riders, with \(U_{\text{iso}}(H) = 1.2 \ U_{\text{eq}}(C)\) and \(U_{\text{iso}}(H) = 1.5 \ U_{\text{eq}}(C)\) for methyl groups. In 2, two tert-butyl groups, two 18-crown-6 molecules, two THF molecules, and two K\(^+\) ions were found to be disordered. In 3, one side six-membered ring, two tert-butyl groups, as well as the crown ether moieties were found to be disordered. All disordered molecules were modeled with two orientations with their relative occupancies refined. The geometries of the disordered parts were restrained to be similar. The anisotropic displacement parameters of the disordered molecules in the direction of the bonds were restrained to be equal with a standard uncertainty of 0.004 Å\(^2\). They were also restrained to have the same \(U_{ij}\) components, with a standard uncertainty of 0.01 Å\(^2\). In each unit cell of 2, twenty \(n\)-hexane solvent molecules were found to be severely disordered and removed by the solvent mask subroutine in OLEX2.\(^5\) The total void volume was 2849.9 Å\(^3\) indicated by the program, which is equivalent to 27.91 % of the unit cell’s total volume. In each unit cell of 3, eight THF solvent molecules were found to be severely disordered and removed by the solvent mask subroutine in OLEX2.\(^5\) The total void volume was 1502.8 Å\(^3\) indicated by the program, which is equivalent to 17.09 % of the unit cell’s total volume.
Table S1. Crystallographic data of 2 and 3.

| Compound | 2 | 3 |
|----------|---|---|
| **Empirical formula** | C<sub>244</sub>H<sub>354</sub>K<sub>3</sub>O<sub>20.50</sub> | C<sub>218</sub>H<sub>282</sub>Rb<sub>3</sub>O<sub>32</sub> |
| **Formula weight** | 3732.55 | 3670.83 |
| **Temperature (K)** | 100 | 100 |
| **Wavelength (Å)** | 0.49594 | 0.71073 |
| **Crystal system** | Triclinic | Triclinic |
| **Space group** | P-1 | P-1 |
| **a (Å)** | 16.057(3) | 18.705(5) |
| **b (Å)** | 21.550(4) | 21.825(6) |
| **c (Å)** | 29.920(5) | 25.716(7) |
| **α (°)** | 90.293(3) | 72.537(3) |
| **β (°)** | 90.604(3) | 70.132(3) |
| **γ (°)** | 99.530(3) | 64.962(3) |
| **V (Å<sup>3</sup>)** | 10210(3) | 8794(4) |
| **Z** | 2 | 2 |
| **ρ<sub>calcd</sub> (g·cm<sup>-3</sup>)** | 1.214 | 1.386 |
| **μ (mm<sup>-1</sup>)** | 0.061 | 0.910 |
| **F(000)** | 4078 | 3914 |
| **Crystal size (mm)** | 0.004×0.007×0.103 | 0.02×0.12×0.18 |
| **θ range for data collection (°)** | 0.950-12.245 | 2.79-25.16 |
| **Reflections collected** | 85474 | 165674 |
| **Independent reflections** | 12528 | 31255 |
| **[R<sub>int</sub> = 0.1545]** | [R<sub>int</sub> = 0.2260] | |
| **Transmission factors (min/max)** | 0.5157/0.7182 | 0.4375/0.6086 |
| **Data/restraints/params.** | 12528/4726/2405 | 31255/5309/2562 |
| **R<sub>1</sub>,<sup>a</sup> wR<sub>2</sub><sup>b</sup> (I > 2σ(I))** | 0.1070, 0.3004 | 0.1191, 0.2642 |
| **R<sub>1</sub>,<sup>a</sup> wR<sub>2</sub><sup>b</sup> (all data)** | 0.1577, 0.3491 | 0.2293, 0.3336 |
| **Quality-of-fit<sup>c</sup>** | 1.163 | 1.011 |

<sup>a</sup>R1 = Σ||Fo||Fc||/Σ||Fo||.  
<sup>b</sup>wR2 = Σ[w(Fo<sup>-2</sup>-Fc<sup>-2</sup>)<sup>2</sup>]/Σ[w(Fo<sup>-2</sup>)<sup>2</sup>].  
<sup>c</sup>Quality-of-fit = [Σ[w(Fo<sup>-2</sup>-Fc<sup>-2</sup>)<sup>2</sup>]/(N<sub>obs</sub>-N<sub>params</sub>)]<sup>1/2</sup>, based on all data.
**Figure S1.** ORTEP drawing of the asymmetric unit of 2, drawn with thermal ellipsoids at the 35% probability level. The color scheme used: C grey, O red, and K purple.

**Figure S2.** ORTEP drawing of the asymmetric unit of 3, drawn with thermal ellipsoids at the 40% probability level. The color scheme used: C grey, O red, and Rb orange.
Figure S3. C–H···π (blue) interactions in the solid-state structure of 2.

Figure S4. C–H···π (blue) interactions in the solid-state structure of 3.
Table S2. Least-square-plane calculations (Å) in **2–3** along with a C-atom labeling scheme.

|   | 2       | 3    |   | 2       | 3    |
|---|---------|------|---|---------|------|
| C1| 0.037   | 0.010|   | C7      | 0.013| 0.014|
| C2| −0.004  | 0.011|   | C8      | 0.008| −0.009|
| C3| −0.025  | −0.024|   | C9      | −0.033| −0.002|
| C4| 0.020   | 0.016|   | C10     | 0.037| 0.007|
| C5| 0.013   | 0.004|   | C11     | −0.015| −0.002|
| C6| −0.042  | −0.017|   | C12     | −0.010| −0.009|
|   | −0.785x−0.537y−0.309z−17.045=0 |   |   | −0.643x−0.750y−0.155z−14.109=0 |   |
|   | 0.524x+0.640y+0.562z+2.958=0 |   |   | 0.428x+0.750y+0.505z+6.393=0 |   |
| RMSD/A | 0.027 | 0.015 | RMSD/A | 0.023 | 0.008 |
| C1| 0.026   | −0.007|   | C13     | 0.020| −0.023|
| C2| 0.009   | 0.014|   | C14     | −0.005| 0.004 |
| C7| −0.046  | −0.012|   | C15     | −0.015| 0.012 |
| C12| 0.029 | 0.023|   | C16     | 0.020| −0.008|
| C13| −0.025 | −0.003|   | C17     | −0.006| −0.012|
| C14| 0.006  | −0.015|   | C18     | −0.014| 0.027 |
|   | −0.705x−0.682y−0.195z−14.891=0 |   |   | −0.690x−0.710y−0.143z−14.057=0 |   |
|   | 0.480x+0.706y+0.522z+4.745=0 |   |   | 0.483x+0.674y+0.560z+4.583=0 |   |
| RMSD/A | 0.027 | 0.014 | RMSD/A | 0.015 | 0.017 |
| Column 1 | Column 2 | Column 3 | Column 4 | Column 5 | Column 6 | Column 7 |
|---------|---------|---------|---------|---------|---------|---------|
| C2      | -0.079  | -0.016  | C19     | -0.066  | -0.030  |          |
| C3      | 0.054   | -0.002  | C20     | 0.048   | 0.018   |          |
| C13     | 0.025   | 0.012   | C21     | 0.001   | 0.016   |          |
| C18     | 0.053   | 0.010   | C22     | -0.032  | -0.038  |          |
| C19     | 0.026   | 0.025   | C23     | 0.015   | 0.026   |          |
| C20     | -0.079  | -0.029  | C24     | 0.034   | 0.008   |          |
|         | -0.730x–0.626y– | 0.511x+0.671y+ | -0.682x–0.589y– | 0.433z–18.185=0 | 0.528x+0.616y+ | 0.585z+2.721=0 |
|         | 0.275z–16.233=0 | 0.537z+3.594=0 |          |          |          |          |
| RMSD/A  | 0.18    | 0.018   | RMSD/A  | 0.39    | 0.024   |          |
| C1      | -0.038  | -0.029  | C25     | -0.005  | 0.002   |          |
| C6      | 0.049   | 0.043   | C26     | -0.002  | -0.009  |          |
| C7      | -0.012  | -0.010  | C27     | 0.005   | 0.010   |          |
| C8      | 0.050   | 0.035   | C28     | -0.002  | -0.004  |          |
| C37     | -0.010  | -0.018  | C29     | -0.004  | -0.003  |          |
| C38     | -0.039  | -0.021  | C30     | 0.008   | 0.004   |          |
|         | -0.744x–0.629y– |          | -0.815x–0.388y– |          | 0.587x+0.533y+ |          |
|         | 0.226z–15.508=0 |          | 0.429z–9.300=0 |          | 0.609z–0.210=0 |          |
|         | 0.518z+4.212=0 |          |          |          |          |          |
| RMSD/A  | 0.037   | 0.028   | RMSD/A  | 0.005   | 0.006   |          |
| C3      | 0.041   | 0.009   | C31     | 0.043   | 0.051   |          |
| C4      | -0.057  | -0.022  | C32     | -0.008  | -0.017  |          |
| C19     | 0.020   | 0.012   | C33     | -0.025  | -0.029  |          |
| C24     | -0.069  | -0.020  | C34     | 0.022   | 0.039   |          |
| C25     | 0.010   | 0.013   | C35     | 0.014   | -0.004  |          |
| C26     | 0.053   | 0.007   | C36     | -0.045  | -0.040  |          |
|         | -0.781x–0.483y– |          | -0.799x–0.282y– |          | 0.565x+0.399y+ |          |
|         | 0.385z–18.411=0 |          | 0.531z–21.075=0 |          | 0.722z–1.624=0 |          |
|         | 0.583z+1.107=0 |          |          |          |          |          |
| RMSD/A  | 0.047   | 0.015   | RMSD/A  | 0.029   | 0.034   |          |
| C4      | 0.035   | 0.017   | C37     | -0.030  | -0.016  |          |
| C5      | 0.006   | 0.004   | C38     | -0.077  | -0.088  |          |
| C25     | -0.034  | -0.007  | C39     | 0.092   | 0.087   |          |
| C30     | -0.008  | -0.026  | C40     | -0.004  | 0.014   |          |
Table S3. Selected C–C bond length distances (Å) in 2–3.

| Bond   | 2       | 3       | Bond   | 2       | 3       |
|--------|---------|---------|--------|---------|---------|
| C1–C2  | 1.426(12)| 1.418(11)| C23–C24| 1.394(12)| 1.432(12)|
| C1–C6  | 1.441(12)| 1.432(10)| C24–C26| 1.437(13)| 1.457(11)|
| C1–C7  | 1.417(12)| 1.407(11)| C25–C26| 1.423(12)| 1.393(12)|
| C2–C3  | 1.412(11)| 1.405(11)| C25–C30| 1.429(13)| 1.442(11)|
| C2–C13 | 1.440(12)| 1.429(11)| C26–C27| 1.366(12)| 1.414(12)|
| C3–C4  | 1.413(12)| 1.399(10)| C27–C28| 1.400(13)| 1.399(12)|
| C3–C19 | 1.462(12)| 1.428(11)| C28–C29| 1.441(13)| 1.379(12)|
| C4–C5  | 1.453(12)| 1.419(11)| C29–C30| 1.375(12)| 1.405(12)|
| C4–C25 | 1.435(12)| 1.419(11)| C30–C32| 1.460(13)| 1.422(12)|
| C5–C6  | 1.426(12)| 1.406(11)| C31–C32| 1.405(12)| 1.413(11)|
| C5–C31 | 1.424(12)| 1.451(10)| C31–C36| 1.459(12)| 1.415(11)|
| C6–C37 | 1.449(12)| 1.428(11)| C32–C33| 1.414(13)| 1.394(11)|
| C7–C8  | 1.404(12)| 1.405(11)| C33–C34| 1.379(13)| 1.387(12)|
Table S4. Selected dihedral angles (°)* in 1 and C138H122 3− in 2 and 3, along with a labelling scheme ( tert-butyl groups and H-atoms are omitted for clarity).

|      | 1  | 2   | 3   |
|------|----|-----|-----|
| ∠A/B | 19.8 | 11.5 | 9.2 |
| ∠A/CD | 12.1 | 12.9 | 12.6 |
| ∠A/E | 2.0  | 7.4  | 2.1  |
| ∠A/FG | 6.3  | 11.1 | 7.2  |

* Values are averaged.
III. NMR Spectroscopic Investigation

*Sample preparation for NMR study:* THF-\(d_8\) (0.60 mL) was added to an NMR tube containing 1 (1.0 mg, 0.001 mmol) and K (1.2 mg, 0.030 mmol). The tube was sealed under argon. The \(^1\)H NMR spectrum of neutral ligand was collected immediately, the spectra of *in situ* generated monoanion and dianion were collected after 10 and 13 minutes, respectively, followed by the spectrum of *in situ* generated trianion (collected after 40 minutes). The solution was then exposed to air by opening the tube. The resulting yellow solution was checked as the spectrum of a quenched product.

![Figure S5](image.png)

**Figure S5.** \(^1\)H NMR spectra of neutral ligand, *in situ* generated products and air-quenched product at different time, 25 °C in THF-\(d_8\).

*Sample preparation for NMR study:* THF-\(d_8\) (0.70 mL) was added to an NMR tube containing 1 (1.0 mg, 0.001 mmol) and K (1.5 mg, 0.038 mmol). The tube was sealed under argon. The \(^1\)H NMR spectrum of neutral ligand was collected immediately, the spectra of *in situ* generated monoanion and dianion were collected after 10 and 15 minutes, respectively, followed by the spectrum of *in situ* generated trianion (collected after 25 minutes). The solution was then exposed
to pure oxygen gas by opening the tube. The resulting yellow solution was checked as the spectrum of a quenched product.

**Figure S6.** $^1$H NMR spectra of neutral ligand, *in situ* generated products and oxygen-quenched product at different time, 25 °C in THF-$d_8$. 
IV. Electrochemical study

Electrochemical measurements were performed using a standard one-compartment, three-electrode electrochemical cell connected to an electrochemical analyzer (Metrohm Autolab). The working electrode was a glassy carbon electrode (3 mm diameter) that was freshly polished with a suspension of Al₂O₃ in distilled water and sonically rinsed with acetone before each measurement. Silver (Ag/0.1 M AgNO₃ in CH₃CN) and platinum wires were used as reference and counter electrodes, respectively. Electrochemical grade (Aldrich) tetrabutylammonium hexafluorophosphate 0.1 M in Toluene/acetonitrile (4:1) was used as supporting electrolyte. All measurements were conducted under dry argon. Solutions were saturated with argon for deaeration and to maintain an argon blanket for at least 15 minutes prior to each measurement.
Figure S7. Oxidation (up) and reduction (down) cyclic voltammetry of bilayer 1 referenced to Fc/Fc⁺.
V. Computational Details
All the calculations reported in this paper were obtained with the GAUSSIAN 09 suite of programs. Electron correlation was partially taken into account using the (u)B3LYP functional in conjunction with the D3 dispersion correction suggested by Grimme et al. and the double- quality plus polarization functions def2-SVP basis set for all atoms. All species were characterized by frequency calculations, and have positive definite Hessian matrices. This level is denoted B3LYP-D3/def2-SVP.
Cartesian coordinates (in Å) and total energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the B3LYP-D3/def2-SVP level.

1M:  
\[E = -4148.112174\]

|          | X     | Y     | Z     |
|----------|-------|-------|-------|
| C        | -1.320147000 | 1.314830000 | 1.448433000 |
| C        | -1.547651000 | -2.929253000 | 1.797275000 |
| C        | -3.781882000 | -0.015048000 | 0.947453000 |
| C        | 0.265053000 | -2.301805000 | -1.599026000 |
| C        | -1.058623000 | -0.235155000 | -1.914086000 |
| C        | -0.080693000 | 1.990911000 | 1.755301000 |
| C        | -0.188569000 | -0.882442000 | 1.694832000 |
| C        | -1.390680000 | -0.102902000 | 1.510158000 |
| C        | -5.033456000 | -0.699234000 | 0.730693000 |
| C        | 1.307341000 | 1.319782000 | -1.450684000 |
| C        | -3.692034000 | 1.394085000 | 0.791358000 |
| C        | -4.836837000 | 2.137788000 | 0.327042000 |
| C        | 1.093253000 | 1.240705000 | 2.045935000 |
| C        | -2.471304000 | 2.063496000 | 1.083962000 |
| C        | 1.390673000 | -0.097404000 | -1.511769000 |
| C        | 0.196608000 | -0.888119000 | 1.695548000 |
| H        | 0.790703000 | -4.782821000 | 2.596528000 |
| C        | -2.231130000 | -0.758405000 | 1.308407000 |
| C        | -3.987465000 | -2.827026000 | 1.526235000 |
| C        | -1.682078000 | -4.234199000 | 2.293348000 |
| H        | -0.790703000 | -4.782821000 | 2.596528000 |
| C        | -2.774262000 | 1.896570000 | -2.432033000 |
| H        | -3.176875000 | 1.319951000 | -2.664739000 |
| C        | -2.394040000 | 3.501446000 | 0.884236000 |
| C        | -1.006960000 | -4.397805000 | 0.804204000 |
| C        | 0.061641000 | 1.983816000 | -1.757705000 |
| C        | -6.371565000 | -2.735582000 | 0.770303000 |
| H        | -6.468520000 | -3.805917000 | 0.957552000 |
| C        | -3.513237000 | 4.250067000 | 0.519338000 |
| C        | 3.781968000 | 0.013480000 | -0.951025000 |
| C        | -2.929501000 | -4.853854000 | 2.404207000 |
| C        | 1.060461000 | 0.217356000 | 1.912011000 |
| C        | -2.336682000 | 3.281026000 | -2.534748000 |
| C        | -2.192987000 | -1.026592000 | -2.009137000 |
| H        | -3.161973000 | -0.585933000 | -2.239628000 |
C    1.047521000  -4.384108000   0.811371000
C   -5.150782000  -2.094240000  1.019313000
C   -1.111717000  -7.210268000  -0.432917000
H   -1.088404000  -8.301244000  -0.370354000
C   -0.937024000  -3.050244000  -1.367000000
C    5.170478000  -2.052739000  -1.022513000
C   -2.210567000   6.317659000   0.704796000
C   -0.243849000  -2.296892000   1.600741000
C    2.973177000  -4.227938000   2.288573000
C    1.720356000  -4.227938000  -2.288573000
C    4.013563000  -2.796963000  -1.527923000
C    2.637796000  -0.741048000  -1.310257000
C   -3.380101000  -3.156409000   1.806781000
H   -4.300799000  -2.639891000  -2.086693000
C   -1.188369000   4.181744000   1.330002000
C   -3.389384000   5.643828000   0.385919000
H   -4.229464000   6.233482000   0.019762000
C    3.678895000   1.421572000  -0.795387000
C   -0.022006000   3.413228000   1.772871000
C   -2.724213000  -2.176043000  -1.531053000
C    0.023280000  -5.046152000   0.005089000
C    2.451329000  -2.079241000  -1.086660000
C   -1.130170000   5.573820000   1.185576000
H   -0.208327000   6.104021000   1.419998000
C   -2.191949000  -5.144000000  -1.076741000
C   -4.062197000  -4.154851000   1.975965000
H   -5.027847000  -4.659980000   2.020718000
C    6.397021000  -2.682620000  -0.773348000
H    6.503673000  -3.752277000  -0.959380000
C    1.148114000   4.184608000  -1.331511000
C    2.188273000  -2.376471000   1.725042000
C   -7.120665000   2.204188000  -0.524208000
H   -8.047423000   1.702050000  -0.801272000
C    7.013999000   3.645573000   0.696469000
C    6.036941000   1.510759000  -0.006983000
C   -2.227674000  -6.553537000  -0.863810000
H   -3.142002000  -7.098491000  -1.111266000
C   -7.480700000  -2.050769000   0.262994000
C    6.162124000   0.067513000  -0.243311000
C    2.359890000   3.516260000  -0.986053000
C    4.817125000   2.176382000  -0.332535000
C    1.179682000  -7.197325000   0.450685000
H    1.167072000  -8.288699000   0.392392000
C   -0.010615000   3.405529000  -1.775023000
C    4.100333000  -4.123139000  -1.977837000
H    5.071089000  -4.618335000  -2.025764000
C    3.409524000  -3.116363000   1.807872000
C    4.325365000  -2.589976000   2.085352000
C    7.101202000   2.264865000   0.516191000
H    8.033024000   1.771705000   0.792220000

S16
C -7.406044000  1.924566000  -0.141226000
C  6.073261000  -0.131599000  0.239758000
C  2.237167000  -3.526256000  1.082680000
C  4.714327000  -2.230638000  0.427117000
C  1.140091000  7.296106000  -0.445586000
H  1.117395000  8.387239000  -0.373990000
C -0.151680000  -3.368792000  1.801210000
C  4.075337000  4.118973000  1.887341000
H  5.052556000  4.603575000  1.903740000
C  3.422827000  3.255648000  -1.819494000
H  4.344620000  2.747417000  -2.111916000
C  7.011877000  -2.371097000  -0.381060000
H  7.952317000  -1.896993000  -0.664521000
C  7.270682000  0.543565000  -0.040683000
H  8.135054000  -0.007814000  -0.412921000
C  5.732079000  -4.380846000  -0.115268000
H  5.674208000  -5.466185000  -0.195793000
C  0.926666000  -5.570287000  -1.309166000
H  0.011755000  -6.075479000  -1.532945000
C  2.255999000  6.641795000  -0.888822000
H  3.169833000  7.189477000  -1.135802000
C  2.497633000  6.641795000  -0.888822000
H  3.169833000  7.189477000  -1.135802000
C  2.408147000  -1.807131000  -2.381583000
C  3.304923000  -1.220546000  -2.581312000
C  7.405984000  1.924900000  0.143111000
C  4.615323000  -3.651273000  0.329213000
C  1.368777000  -3.958106000  -2.178281000
H  1.459911000  -5.043232000  -2.219762000
C  3.401996000  4.600208000  -1.584126000
C  4.299142000  5.207491000  1.731346000
C -6.924698000  -3.763888000  0.484853000
C  2.497633000  -3.197391000  -2.485021000
C  2.004513000  -6.346851000  0.882043000
C  3.206169000  -5.707325000  0.576085000
H  4.042838000  -6.324033000  0.247698000
C -3.096574000  6.271715000  -2.797561000
C -2.521019000  6.441141000  -3.722468000
H -4.145501000  6.545229000  -2.991681000
H -2.698333000  6.963007000  -2.035730000
C -8.704151000  3.666998000  -0.984930000
H -9.565118000  2.115652000  -0.260160000
H -8.880586000  2.588237000  1.305123000
1M-H^-: E = -4148.749572
C  1.024377000  -2.998569000  -1.772056000
C  -0.848848000  1.556252000  -1.970773000
C  -5.719405000  2.419595000  0.085228000
C  2.310764000  -2.466936000  -1.478592000
C  -6.087975000  1.014369000  0.309131000
C  4.844112000  -1.423200000  -0.677573000
C  0.393046000  -3.305843000  -1.380703000
C  -4.052438000  4.234528000  0.228086000
C  -2.447328000  -2.210459000  2.196321000
C  -1.672988000  -4.773160000  2.466213000
C  -1.877706000  2.427712000  -2.357799000
C  -2.873407000  2.034377000  -2.561290000
C  -1.732006000  3.738940000  1.001781000
C  -1.802853000  -4.053891000  -0.887125000
C  0.442779000  -2.090405000  0.788835000
C  -6.785804000  -1.662129000  0.754231000
C  2.698744000  -2.701665000  0.553717000
C  3.776595000  -4.448315000  -2.492251000
C  0.946660000  -0.538298000  -1.922597000
C  -3.206868000  0.163638000  -2.136601000
C  0.234614000  -0.529642000  -0.887888000
C  -3.776595000  -4.448315000  2.241668000
C  0.946660000  -0.538298000  2.004469000
C  -1.672988000  3.738940000  1.001781000
C  -2.447328000  -2.210459000  2.196321000
H  -1.023917000  6.469898000  0.698986000
C  -0.687330000  -2.364366000  1.640412000
C  2.076352000  -5.086123000  -2.496786000
C  -7.391640000  0.549008000  0.079697000
H  -8.160783000  1.232844000  -0.282163000
C  0.947232000  -4.276994000  -2.344397000
H  -0.020736000  -4.653074000  -2.673983000
C  3.446743000  -3.320672000  -1.504878000
C  2.463617000  -1.061333000  -1.225561000
C  -3.899251000  -2.316569000  -1.777009000
H  -4.703360000  -1.615513000  -2.010494000
C  -0.408967000  4.179749000  1.320040000
C  -2.316892000  6.033951000  0.410564000
H  -3.038199000  6.771542000  0.057799000
C  3.898525000  0.874107000  -0.755302000
C  0.600050000  3.208852000  1.755573000
C  -3.095842000  -1.786892000  1.569820000
C  -0.912244000  -4.951512000  -0.149485000
C  2.812639000  1.744823000  -1.047294000
C  -0.994588000  5.536104000  1.164271000
H  0.915198000  5.881564000  1.381597000
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | -6.31621200 | 4.70043300 | -0.58973600 |
| C       | 2.86268600  | 2.65994100 | 2.51763600  |
| C       | 3.32397500  | 5.98148400 | -0.74998700 |
| C       | 4.36570700  | 5.11412900 | -0.42382100 |
| H       | 5.29956800  | 5.54942100 | -0.06799300 |
| C       | -4.15462000 | -5.85951200 | 2.62236000  |
| H       | -3.30661500 | 6.39885200 | 3.07088300  |
| H       | -4.99415300 | -5.74998700 | 3.33799900  |
| H       | -4.46878200 | -6.42782500 | 1.72966700  |
| C       | -9.15511300 | 1.25611500 | -0.00456800 |
| H       | -9.38910700 | 2.19902900 | 0.51367300  |
| H       | -9.09505000 | -0.50916100 | 0.29264100  |
| H       | -9.28782400 | -1.43438500 | -1.08689400 |
| C       | -7.34438200 | 5.66358000 | -1.13446600 |
| H       | -8.25727300 | 6.69464000 | -0.51472900 |
| H       | -6.95792800 | 6.93500000 | -1.17361500 |
| H       | -7.65366800 | 5.38264500 | 2.15610200  |
| C       | -0.61101100 | 7.90368800 | 0.46694400  |
| H       | -1.47773300 | 8.58274500 | 0.44559100  |
| H       | 0.08100700  | 8.25736300 | 1.24845600  |
| H       | -0.08438500 | 8.01412100 | -0.49877400 |
| C       | 4.21877000  | 3.12410300 | 2.99387900  |
| H       | 4.52979800  | 4.04402400 | 2.47573700  |
| H       | 4.20292400  | 3.34281900 | 4.07706200  |
| H       | 4.99335100  | 2.36305000 | 2.81508400  |
| C       | 3.46058600  | 7.47749000 | -0.59786600 |
| H       | 3.34410000  | 7.99200100 | -1.56718600 |
| H       | 2.67975400  | 7.87902600 | 0.07031900  |
| H       | 4.43962200  | 7.76018000 | -0.18194700 |
| C       | 8.87450600  | 2.99826000 | 1.28855700  |
| H       | 9.02679700  | 4.05572800 | 1.02212100  |
| H       | 8.85636000  | 2.93683100 | 2.39131000  |
| H       | 9.75567600  | 2.43110600 | 0.94757800  |
| C       | 8.12935700  | -4.14155200 | 0.14207000  |
| H       | 9.11135600  | -3.69285300 | -0.07881000 |
| H       | 8.12707800  | -4.40383900 | 1.21510100  |
| H       | 8.04959200  | -5.08223200 | -0.42453800 |
| C       | 1.93738700  | -6.46803200 | -3.08692100 |
| H       | 1.43809600  | -7.13990500 | -2.36859400 |
| H       | 1.32194900  | -6.45404800 | -4.00133200 |
| H       | 2.91562600  | -6.90603300 | -3.33962000 |
| C       | -2.77896300 | 4.70822500 | -2.97291300 |
| H       | -3.76997800 | 4.27184400 | -2.78214500 |
| H       | -2.74119500 | 5.68242700 | -2.46162500 |
| H       | -2.69313900 | 4.89688000 | -4.05809600 |
| H       | 2.07111500  | -1.63852200 | 3.46870000  |

$1M-2H^2-$: $E = -4149.306439$

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 1.95987800 | 1.40900600 | -1.24431100 |
| C       | 1.79058400 | -2.82999400 | -1.69356500 |
| C       | 4.29958400 | -0.14481000 | -0.76747700 |
| C                  | X            | Y            | Z            |
|--------------------|--------------|--------------|--------------|
| -0.571425000       | -2.105748000 | 1.541029000  |
| 0.518194000        | 0.101649000  | 1.803285000  |
| 0.791998000        | 2.186876000  | -1.521823000 |
| 0.627756000        | -0.673165000 | -1.555784000 |
| 1.894558000        | -0.012507000 | -1.316228000 |
| 5.474052000        | -0.938665000 | -0.532400000 |
| -1.959828000       | 1.409025000  | 1.244415000  |
| 4.346512000        | 1.268617000  | -0.624334000 |
| 5.565778000        | 1.906187000  | -0.189887000 |
| -0.446935000       | 1.516040000  | -1.823679000 |
| 3.192839000        | 2.050379000  | -0.899470000 |
| -1.894581000       | -0.012491000 | 1.316317000  |
| 1.879687000        | -2.055434000 | 1.858723000  |
| -0.627812000       | -0.673219000 | 1.555853000  |
| -1.790748000       | -2.829993000 | 1.693595000  |
| 0.447002000        | 1.515925000  | -1.823734000 |
| 6.713456000        | 1.120840000  | 0.142466000  |
| -3.042816000       | -2.195691000 | 1.381829000  |
| 6.672927000        | -0.332403000 | -0.047875000 |
| -5.474115000       | -0.938460000 | 0.532443000  |
| -0.738227000       | -2.753541000 | -1.426185000 |
| 5.630709000        | 3.329880000  | -0.073089000 |
| 3.078827000        | -0.785370000 | -1.137323000 |
| 4.235741000        | -2.976227000 | -1.315711000 |
| 1.842673000        | -4.173551000 | -2.163912000 |
| 0.922924000        | -4.637238000 | -2.518310000 |
| 1.577968000        | 2.319028000  | 2.151406000  |
| 2.528951000        | 1.839221000  | 2.381106000  |
| 3.259116000        | 3.483460000  | -0.841519000 |
| 0.939684000        | -4.081671000 | 0.880951000  |
| -0.791899000       | 2.186831000  | 1.521902000  |
| 6.588709000        | -3.106201000 | -0.471867000 |
| 6.564679000        | -4.188553000 | -0.609115000 |
| 4.473974000        | 4.137559000  | -0.470318000 |
| -4.299612000       | -0.144666000 | 0.767555000  |
| 3.017014000        | 4.137559000  | 2.909620000  |
| 0.512025000        | 0.101766000  | -1.803231000 |
| 1.515887000        | 3.703030000  | 2.167031000  |
| 0.738066000        | -0.580531000 | 2.176670000  |
| 2.021285000        | -0.419282000 | 3.257220000  |
| 2.658485000        | -0.100806000 | 1.652664000  |
| 0.939916000        | -4.081569000 | -0.880977000 |
| 5.448889000        | -2.350255000 | -0.779589000 |
| 1.124914000        | -6.886237000 | 0.535141000  |
| 1.131925000        | -7.972270000 | 0.472158000  |
| 0.738066000        | -2.753659000 | 1.426214000  |
| -5.449021000       | -2.350056000 | 0.779609000  |
| 3.417527000        | 6.319806000  | -0.809328000 |
| 0.571298000        | -2.105693000 | -1.540986000 |
| 3.017292000        | -4.906341000 | 2.190979000  |
| 7.788302000        | -1.146692000 | 0.223867000  |
| 8.710136000        | -0.701227000 | 0.600477000  |
| -1.842908000       | -4.173551000 | 2.163925000  |
1M-2H·3+: E= -4149.198670

C  2.011669000  1.407745000 -1.122469200
C  1.828006000 -2.832222000 -1.678464000
C  4.348459000 -0.011113000 -0.747878000
C -0.608102000 -2.101934000  1.536757000
C  0.467765000  0.113306000  1.803031000
C  0.389348000  1.529417000  1.823919000
C  6.779928000  1.104047000  0.135723000
C -3.082079000 -2.199902000  1.360386000
C  6.729129000 -0.337530000 -0.046752000
C -5.521036000 -0.950671000  0.517830000
C -0.703999000 -2.741979000 -1.435143000
C  5.695580000  3.323238000 -0.059562000
C  3.121796000 -0.789215000 -1.116774000
C  4.274320000 -2.981523000 -1.290291000
C  1.879810000 -4.173868000 -2.148104000
H  0.960312000 -4.638217000 -2.503329000
C  1.509728000  2.337020000  2.169707000
H  2.462294000  1.862894000  2.405278000
C  3.317409000  3.479212000 -0.809065000
C  0.922087000 -4.071243000  0.895987000
C -0.850624000  2.199000000  1.508779000
C  6.632689000 -3.126015000 -0.458458000
H  6.603168000 -4.209590000 -0.585170000
C  4.540975000  4.125122000 -0.430034000
C -4.348411000 -0.153876000  0.747721000
C  3.055155000 -4.911032000 -2.168845000
C -0.467772000  0.113180000 -1.803079000
C  1.435925000  3.722292000  2.199758000
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.943071 | -2.11032  | -2.36025  |
| C    | -7.950752 | 1.75694   | -0.60445  |
| H    | -8.83396  | 1.17142   | -0.86310  |
| C    | -7.84792  | -1.16396  | -0.21942  |
| H    | -8.77449  | -0.72068  | -0.58759  |
| C    | -6.89318  | 3.91228   | -0.42128  |
| H    | -6.95171  | 4.99322   | -0.55569  |
| C    | 0.00029   | -6.17159  | -0.00000  |
| C    | -2.11353  | -4.77290  | -1.26758  |
| H    | -1.76631  | -0.55982  | -2.17953  |
| H    | -1.97505  | -0.39205  | -3.25985  |
| H    | -2.60978  | -0.07709  | -1.65341  |
| C    | 0.22793   | 4.35318   | 1.86290   |
| H    | 0.20519   | 5.44345   | 1.86691   |
| C    | -4.54132  | 4.12487   | 0.43011   |
| C    | 6.89292   | 3.91269   | 0.42116   |
| H    | 6.95138   | 4.99364   | 0.55560   |
| C    | -2.27261  | 5.67276   | 1.05240   |
| H    | -1.39775  | 6.28983   | 1.25977   |
| C    | -2.18115  | -6.19059  | -1.07584  |
| H    | -3.08699  | -6.71588  | -1.39606  |
| C    | 3.19681   | -4.05622  | 1.82820   |
| H    | 4.13056   | -4.58041  | 2.05083   |
| C    | -1.50997  | 2.33681   | -2.16951  |
| H    | -2.46250  | 1.86212   | -2.40505  |
| C    | -7.80782  | -2.54258  | -0.03367  |
| C    | -5.69579  | 3.32289   | 0.05949   |
| C    | -0.22838  | 4.35308   | -1.86256  |
| H    | -0.20575  | 5.44336   | -1.86645  |
| C    | -3.19644  | -4.05660  | -1.82826  |
| H    | -4.13013  | -4.58087  | -2.05088  |
| C    | 8.00768   | 3.14154   | 0.75705   |
| C    | -1.43632  | 3.72205   | -2.19939  |
| C    | -3.47216  | 6.31481   | 0.71418   |
| C    | -4.58750  | 5.53873   | 0.41553   |
| H    | -5.51762  | 6.04840   | 0.15948   |
| C    | 3.04218   | -6.35507  | -2.61329  |
| H    | 2.20181   | -6.56031  | -3.29623  |
| H    | 3.97997   | -6.63710  | -3.12422  |
| H    | 2.91965   | -7.02272  | -1.74174  |
| C    | 8.99982   | -3.41254  | 0.36247   |
| H    | 9.31351   | -4.01924  | -0.50663  |
| H    | 9.86736   | -2.81302  | 0.68390   |
| H    | 8.76721   | -4.12541  | 1.17483   |
| C    | 9.24585   | 3.80375   | 1.32051   |
| H    | 10.13778  | 3.16559   | 1.20427   |
| H    | 9.45218   | 4.76741   | 0.82293   |
| H    | 9.13515   | 4.01893   | 2.40000   |
| C    | 3.52352   | 7.82386   | -0.64338  |
| H    | 4.55005   | 8.18960   | -0.47639  |
| H    | 3.14570   | 8.28865   | -1.57179  |
| H    | 2.89460   | 8.20930   | 0.18014   |
| C    | -2.64029  | 4.55956   | -2.55661  |
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H    | -2.914700000| 5.222900000  | -1.721444000 |
| H    | -2.437182000| 5.200874000  | -3.434469000 |
| H    | -3.519004000| 3.936103000  | -2.780383000 |
| C    | -3.524321000| 7.823708000  | 0.644208000  |
| H    | -3.148045000| 8.288290000  | 1.573354000  |
| H    | -2.894181000| 8.209521000  | -0.178210000 |
| H    | -4.550658000| 8.189315000  | 0.475742000  |
| C    | -9.246003000| 3.803008000  | -1.321079000 |
| H    | -9.450981000| 4.768019000  | -0.825595000 |
| H    | -9.136424000| 4.015390000  | -2.401245000 |
| H    | -10.138339000| 3.165867000   | -1.202272000 |
| C    | -8.999626000| -3.413069000 | -0.362455000 |
| H    | -9.867443000| -2.813553000 | -0.683139000 |
| H    | -8.767261000| -4.125428000 | -1.175339000 |
| C    | -9.312776000| -4.020345000 | 0.506444000  |
| H    | -3.041718000| -6.355207000 | 2.613221000  |
| H    | -2.919014000| -7.022863000 | 1.741706000  |
| H    | -2.201399000| -6.560345000 | 3.296266000  |
| H    | -3.979535000| -6.637320000 | 3.123948000  |
| C    | 2.639803000| 4.559866000  | 2.557010000  |
| H    | 3.518279000| 3.936457000  | 2.781852000  |
| H    | 2.914829000| 5.221859000  | 1.721455000  |
| H    | 2.436240000| 5.201956000  | 3.434185000  |
VI. References

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