Supporting Information for

Reductive Benzylation of C₆₀ Imidazoline with a Bulky Addend

Hui-Lei Hou, Zong-Jun Li and Xiang Gao*

State Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry,
University of the Chinese Academy of Sciences, Chinese Academy of Sciences, 5625 Renmin
Street, Changchun, Jilin 130022, China

xgao@ciac.ac.cn

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Experimental

General Methods. All reactions were carried out under an atmosphere of Ar. All reagents were obtained commercially and used without further purification, unless otherwise noted. Benzonitrile (PhCN) was distilled over P₂O₅ under vacuum at 305 K prior to use. Tetra-*n*-butylammonium perchlorate (TBAP) was recrystallized from absolute ethanol and dried under vacuum at 313 K prior to use.

Controlled-potential bulk electrolysis (CPE) was carried out on a Potentiostat/Galvanostat using an “H” type cell. Two platinum gauze electrodes (working and counter electrodes) were separated by a sintered glass frit. A three-electrode cell was used for CV measurements and a glassy carbon, a platinum wire were used as working electrode and counter electrode. In both controlled-potential bulk electrolysis and CV measurements, a saturated calomel electrode (SCE) was used as reference electrode. A fritted-glass bridge of low porosity which contained the solvent/supporting electrolyte mixture was used to separate the SCE from the bulk of the solution.

Preparation of Compounds 2a, 3a and 4a. Typically, 70 mg (74 μmol) of compound **1** in 50 mL of freshly distilled PhCN solution containing 0.1 M TBAP was electrolyzed at –1.00 V vs SCE under Ar atmosphere. The potentiostat was switched off once the theoretical number of electrons required for reducing **1** to **1**^{2–} was achieved. Sixty-fold PhCH₂Br (530 μL, 4.4 mmol) was added to the solution. The benzylation reaction was allowed to proceed for 3 h under Ar. The solvent was removed under reduced pressure, and the residue was washed with methanol to remove TBAP. The crude product was put into toluene, and the soluble part was purified with HPLC by eluting a 70:30 v/v mixture of toluene/hexane over a semi-preparative YMC-pack silica column (10 mm × 250 mm) at a flow rate of 3.7 mL/min with the detector wavelength set at 380 nm. Compounds **2a**, **3a** and **4a**

were obtained with an isolated yield of 34% (28 mg), 7% (6 mg) and 3% (2.6 mg), along with 3.5 mg of unreacted **1** and 2.7 mg of C₆₀ produced by decomposition of **1** during the reaction.

Spectral Characterization of 2a: Positive ESI FT-ICR MS, m/z calcd for C₈₈H₂₅N₂O⁺ [M + H]⁺ 1125.19614, found 1125.19734; ¹H NMR (600 MHz, DMSO-*d*₆) δ 7.52 (d, 2H), 7.45-7.43 (m, 2H), 7.18 (d, 2H), 7.06 (t, 1H), 7.00 (t, 2H), 6.95-6.83 (m, 11H), 4.40 (AB_q, 2H, $\Delta\nu_{AB}$ = 594 Hz, J_{AB} = 12.2 Hz), 4.11 (AB_q, 2H, $\Delta\nu_{AB}$ = 444 Hz, J_{AB} = 12.2 Hz); ¹³C NMR (150 MHz, DMSO-*d*₆) δ 168.86 (1C, C=O), 160.14 (1C, C=N), 158.48 (1C), 157.95 (1C), 152.69 (1C), 152.07 (1C), 151.20 (1C), 149.55 (1C), 148.78 (1C), 148.38 (1C), 148.33 (1C), 148.17 (1C), 147.63 (1C), 147.55 (1C), 147.49 (1C), 147.42 (1C), 147.32 (1C), 146.95 (1C), 146.69 (1C), 146.54 (1C), 146.25 (1C), 146.14 (1C), 145.86 (1C), 145.75 (1C), 145.73 (1C), 145.54 (1C), 145.35 (1C), 145.32 (1C), 145.24 (1C), 145.12 (1C), 144.86 (1C), 144.81 (1C), 144.76 (1C), 144.63 (1C), 144.42 (2C), 144.15 (1C), 144.03 (1C), 143.98 (1C), 143.91 (1C), 143.19 (1C), 142.87 (1C), 142.73 (1C), 141.90 (1C), 141.84 (1C), 141.70 (1C), 141.36 (1C), 141.17 (1C), 141.11 (1C), 140.83 (1C), 140.80 (1C), 139.77 (1C), 138.88 (1C), 138.37 (1C), 136.84 (1C, Ph), 136.45 (1C), 136.19 (1C), 136.08 (1C, Ph), 135.77 (1C), 134.66 (1C), 132.02 (1C, Ph), 131.74 (1C, Ph), 131.52 (2C, Ph), 130.94 (2C, Ph), 130.36 (1C, Ph), 129.22 (2C, Ph), 128.57 (2C, Ph), 128.16 (2C, Ph), 128.11 (2C, Ph), 127.95 (2C, Ph), 127.77 (2C, Ph), 127.65 (1C, Ph), 126.96 (1C, Ph), 126.73 (1C, Ph), 91.09 (1C, sp³, C₆₀-N=), 75.61 (1C, sp³, C₆₀-N-), 62.94 (1C, C-CH₂Ph), 60.16 (1C, C-CH₂Ph), 47.24 (1C, CH₂), 43.66 (1C, CH₂); UV-vis (toluene): λ_{max} 323, 415, 456, 525, 704 nm.

Spectral Characterization of 3a: Positive ESI FT-ICR MS, m/z calcd for C₈₈H₂₅N₂O⁺ [M + H]⁺ 1125.19614, found 1125.19130; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.53-7.52 (m, 2H), 7.11 (d, 2H), 7.08-7.06 (m, 2H), 7.03-7.01 (m, 5H), 6.98 (t, 2H), 6.91 (t, 1H), 6.87 (t, 4H), 6.79 (t, 2H), 4.37

(AB_q, 2H, $\Delta\nu_{AB}$ = 78 Hz, J_{AB} = 13.8 Hz), 4.29 (AB_q, 2H, $\Delta\nu_{AB}$ = 766 Hz, J_{AB} = 13.8 Hz); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 171.02 (1C, C=O), 159.80 (1C, C=N), 153.32 (1C), 151.88 (1C), 149.11 (1C), 148.98 (1C), 148.73 (1C), 148.62 (1C), 147.97 (1C), 147.03 (2C), 146.91 (2C), 146.79 (1C), 146.05 (1C), 145.86 (1C), 145.82 (1C), 145.69 (1C), 145.49 (1C), 145.32 (2C), 145.29 (1C), 144.76 (2C), 144.73 (1C), 144.57 (1C), 144.51 (1C), 144.31 (2C), 144.15 (1C), 144.13 (2C), 144.11 (1C), 144.01 (1C), 143.80 (1C), 143.61 (2C), 143.43 (1C), 143.37 (1C), 143.17 (1C), 142.89 (1C), 142.79 (1C), 142.53 (1C), 142.23 (1C), 142.16 (1C), 141.98 (1C), 141.82 (1C), 141.80 (1C), 141.43 (1C), 140.71 (1C), 140.12 (1C), 139.84 (1C), 139.25 (1C), 138.71 (1C), 137.71 (1C, Ph), 137.63 (1C), 136.89 (1C), 136.78 (1C, Ph), 136.68 (1C), 136.23 (1C), 134.32 (1C, Ph), 132.40 (1C, Ph), 132.21 (2C, Ph), 132.12 (2C, Ph), 131.28 (1C, Ph), 130.46 (1C, Ph), 128.74 (2C, Ph), 128.36 (2C, Ph), 128.17 (2C, Ph), 127.95 (2C, Ph), 127.85 (2C, Ph), 127.83 (2C, Ph), 126.87 (1C, Ph), 126.78 (1C, Ph), 91.39 (1C, sp³, C₆₀-N=), 87.27 (1C, sp³, C₆₀-N-), 63.98 (1C, C-CH₂Ph), 62.53 (1C, C-CH₂Ph), 48.03 (1C, CH₂), 44.94 (1C, CH₂). UV-vis (toluene): $\lambda_{\max}$ 338, 431, 640, 703 nm.

Spectral Characterization of 4a: Positive MALDI MS, m/z calcd for C₈₈H₂₅N₂O⁺ [M + H]⁺ 1125.2, found 1125.2; ¹H NMR (600 MHz, DMSO-*d*₆) δ 7.54 (d, 2H), 7.22 (d, 2H), 7.18 (d, 2H), 7.05-6.97 (m, 6H), 6.94 (d, 3H), 6.89-6.84 (m, 5H), 4.38 (AB_q, 2H, $\Delta\nu_{AB}$ = 654 Hz, J_{AB} = 12 Hz), 3.93 (AB_q, 2H, $\Delta\nu_{AB}$ = 84 Hz, J_{AB} = 12 Hz); ¹³C NMR (150 MHz, DMSO-*d*₆) δ 168.94 (1C, C=O), 161.12 (1C, C=O), 157.66 (1C), 154.79 (1C), 150.60 (1C), 150.55 (1C), 149.17 (2C), 148.15 (1C), 147.66 (1C), 147.64 (1C), 147.47 (1C), 147.31 (1C), 147.28 (1C), 146.63 (1C), 146.30 (2C), 146.09 (1C), 146.01 (1C), 145.77 (1C), 145.70 (1C), 145.47 (1C), 145.35 (1C), 145.31 (1C), 145.22 (1C), 145.02 (1C), 144.86 (1C), 144.53 (1C), 144.43 (1C), 144.30 (1C), 144.12 (1C), 144.01 (1C), 143.80 (1C), 143.78 (1C), 143.67 (1C), 143.65 (1C), 143.16 (1C), 143.09 (1C), 142.55 (1C), 142.24 (1C),

142.16 (1C), 141.69 (1C), 141.43 (1C), 141.05 (2C), 140.61 (1C), 140.38 (1C), 140.37 (1C), 140.28 (1C), 140.02 (1C), 138.38 (1C), 138.01 (1C), 137.78 (1C), 137.53 (1C), 135.75 (1C), 135.50 (1C), 135.40 (1C), 135.29 (1C), 131.97 (1C, Ph), 131.32 (2C, Ph), 131.03 (1C, Ph), 131.00 (1C, Ph), 130.19 (1C, Ph), 129.96 (2C, Ph), 129.85 (1C, Ph), 128.18 (4C, Ph), 127.68 (2C, Ph), 127.64 (2C, Ph), 127.43 (2C, Ph), 127.37 (2C, Ph), 126.86 (1C, Ph), 126.61 (1C, Ph), 126.41 (1C, Ph), 86.73 (1C, sp^3 , $\text{C}_{60}\text{-N-}$), 83.22 (1C, sp^3 , $\text{C}_{60}\text{-N=}$), 61.87 (1C, $\text{C-CH}_2\text{Ph}$), 58.84 (1C, $\text{C-CH}_2\text{Ph}$), 46.91 (1C, CH_2), 45.15 (1C, CH_2); UV-vis (toluene): λ_{max} 323, 409, 453, 521, 705 nm.

Deuterium Isotope Experiments. Compounds **2aI** and **3aI**: The procedures were similar to those for preparation of **2a** and **3a**, except PhCD_2Br (30-fold, 265 μL , 2.2 mmol) and PhCH_2Br (30-fold, 265 μL , 2.2 mmol) were added simultaneously into the mixture. The reaction was allowed to react for 3 h. Compounds **2aII** and **3aII**: The procedures were similar to those for preparation of **2a** and **3a**, except PhCD_2Br (30-fold, 265 μL , 2.2 mmol) was added first, followed by adding PhCH_2Br (30-fold, 265 μL , 2.2 mmol) with a time interval of 3 min. The reaction was allowed to react for 3 h.

Preparation of Compounds 2b, 3b and 4b. The procedures were similar to those for preparation of **2a**, **3a** and **4a**, except $o\text{-BrPhCH}_2\text{Br}$ was used instead of PhCH_2Br . Compounds **2b**, **3b** and **4b** were obtained with an isolated yield of 46% (44 mg), 5% (4.7 mg) and 5% (4.8 mg), along with 2.6 mg of unreacted **1** and 1.8 mg of C_{60} produced by decomposition of **1** during the reaction.

Spectral Characterization of 2b: Positive ESI FT-ICR MS, m/z calcd for $\text{C}_{88}\text{H}_{23}\text{Br}_2\text{N}_2\text{O}^+ [\text{M} + \text{H}]^+$ 1281.01716, found 1281.01891; ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.66 (d, 2H), 7.9 (d, 1H), 7.48-7.46 (m, 2H), 7.20 (d, 1H), 7.16 (d, 1H), 7.07 (d, 1H), 7.02 (t, 3H), 6.97-6.92 (m, 4H), 6.87 (d,

1H), 6.81-6.77 (m, 2H), 4.72 (AB_q, 2H, $\Delta\nu_{AB}$ = 413 Hz, J_{AB} = 13 Hz), 4.37 (AB_q, 2H, $\Delta\nu_{AB}$ = 134 Hz, J_{AB} = 13 Hz); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 168.96 (1C, C=O), 159.98 (1C, C=N), 158.43 (1C), 158.20 (1C), 152.02 (1C), 151.62 (1C), 151.27 (1C), 149.55 (1C), 148.82 (1C), 148.35 (1C), 148.23 (1C), 147.93 (1C), 147.63 (1C), 147.60 (1C), 147.43 (1C), 147.27 (1C), 147.19 (1C), 146.77 (1C), 146.69 (1C), 146.65 (1C), 146.35 (1C), 145.92 (1C), 145.82 (1C), 145.67 (1C), 145.55 (1C), 145.43 (1C), 145.31 (3C), 145.17 (1C), 144.90 (1C), 144.89 (1C), 144.87 (1C), 144.68 (1C), 144.47 (1C), 144.12 (2C), 144.08 (1C), 143.93 (1C), 143.91 (1C), 143.26 (1C), 142.88 (1C), 142.70 (1C), 142.13 (1C), 141.90 (1C), 141.75 (1C), 141.70 (1C), 141.39 (1C), 140.93 (1C), 140.85 (1C), 140.77 (1C), 140.00 (1C), 139.26 (1C), 138.25 (1C), 136.80 (1C, Ph), 136.43 (1C), 136.15 (1C, Ph), 135.70 (1C), 135.67 (1C), 134.68 (1C), 133.75 (1C, Ph), 133.15 (1C, Ph), 133.05 (1C, Ph), 132.91 (1C, Ph), 132.02 (1C, Ph), 131.77 (1C, Ph), 130.42 (1C, Ph), 129.43 (2C, Ph), 128.70 (1C, Ph), 128.62 (2C, Ph), 128.28 (1C, Ph), 128.16 (2C, Ph), 128.13 (2C, Ph), 127.89 (1C, Ph), 127.06 (1C, Ph), 126.81 (1C, Ph), 126.80 (1C, Ph), 126.54 (1C, Ph), 91.09 (1C, sp³, C₆₀-N=), 75.53 (1C, sp³, C₆₀-N-), 62.79 (1C, C-CH₂Ph), 59.66 (1C, C-CH₂Ph), 45.77 (1C, CH₂), 41.99 (1C, CH₂); UV-vis (toluene): λ_{max} 324, 409, 449, 521, 706 nm.

X-Ray Single Crystal Diffractions of 2b. Black crystals of **2b** suitable for X-ray diffractions were obtained by slowly diffusing hexane into a CS₂ solution of **2b** at room temperature. Single crystal X-ray diffraction data were collected on an instrument equipped with a CCD area detector using graphite-monochromated Mo K α radiation (λ = 0.71073 Å) in the scan range $1.55^\circ < \theta < 25.06^\circ$. The structure was solved with the direct method of SHELXS-97 and refined with full-matrix least-squares techniques using the SHELXL-97 program within WINGX. Crystal data of **2b**•2CS₂; C₉₀H₂₂Br₂N₂OS₄, M_w = 1435.16, monoclinic, space group P2(1)/n, a = 19.6200(11) Å, b =

12.7399(7) Å, $c = 24.5552(14)$ Å, $\alpha = 90^\circ$, $\beta = 105.702(1)$, $\gamma = 90^\circ$, $V = 5908.7(6)$ Å³, $Z = 4$, $D_{\text{calcd}} = 1.613$ Mg•m⁻³, $\mu = 1.574$ mm⁻¹, $T = 188$ (2) K, crystal size $0.35 \times 0.20 \times 0.18$ mm; reflections collected 33529, independent reflections 10428; 6295 with $I > 2\sigma(I)$; $R1 = 0.0797$ [$I > 2\sigma(I)$], $wR2 = 0.2196$ [$I > 2\sigma(I)$]; $R1 = 0.1212$ (all data), $wR2 = 0.2436$ (all data), GOF (on F^2) = 1.008.

Spectral Characterization of 3b: Positive ESI FT-ICR MS, m/z calcd for C₈₈H₂₃Br₂N₂O⁺ [M + H]⁺ 1281.01716, found 1281.01984; ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.60-7.58 (m, 2H), 7.44-7.39 (m, 2H), 7.28 (d, 1H), 7.16 (d, 1H), 7.06 (d, 2H), 7.01-6.99 (m, 4H), 6.90-6.86 (m, 3H), 6.82-6.76 (m, 3H), 4.67 (AB_q, $\Delta\nu_{AB} = 759$ Hz, $J_{AB} = 12.5$ Hz), 4.84 (AB_q, $\Delta\nu_{AB} = 332$ Hz, $J_{AB} = 12.5$ Hz); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 171.15 (1C, C=O), 159.67 (1C, C=N), 151.62 (1C), 151.58 (1C), 149.10 (1C), 148.96 (1C), 148.68 (1C), 148.56 (1C), 147.48 (1C), 147.07 (1C), 147.02 (1C), 146.95 (1C), 146.90 (1C), 146.61 (1C), 146.03 (1C), 145.99 (1C), 145.81 (1C), 145.66 (1C), 145.54 (1C), 145.26 (1C), 145.25 (1C), 144.73 (2C), 144.59 (1C), 144.51 (1C), 144.34 (1C), 144.32 (2C), 144.20 (1C), 144.18 (2C), 144.15 (1C), 143.97 (1C), 143.81 (1C), 143.61 (1C), 143.57 (1C), 143.40 (1C), 143.38 (1C), 142.94 (1C), 142.64 (1C), 142.51 (1C), 142.49 (1C), 142.47 (1C), 142.29 (1C), 142.20 (1C), 141.61 (1C), 141.19 (1C), 141.16 (1C), 141.13 (1C), 139.61 (1C), 139.49 (1C), 139.17 (1C), 138.87 (1C), 137.46 (1C), 137.22 (2C), 136.68 (1C, Ph), 136.64 (1C, Ph), 136.61 (1C), 136.54 (1C), 135.08 (1C, Ph), 134.56 (1C, Ph), 134.03 (2C, Ph), 133.29 (1C, Ph), 133.19 (1C, Ph), 132.08 (1C, Ph), 131.34 (1C, Ph), 130.51 (1C, Ph), 128.72 (1C, Ph), 128.56 (2C, Ph), 128.39 (1C, Ph), 128.32 (1C, Ph), 128.26 (2C, Ph), 127.87 (2C, Ph), 127.21 (1C, Ph), 127.13 (1C, Ph), 126.74 (1C, Ph), 126.36 (1C, Ph), 91.69 (1C, sp³, C₆₀-N=), 87.37 (1C, sp³, C₆₀-N-), 63.61 (1C, C-CH₂Ph), 62.16 (1C, C-CH₂Ph), 45.66 (1C, CH₂), 44.04 (1C, CH₂); UV-vis (toluene): λ_{max} 339, 432, 645, 704 nm.

Spectral Characterization of 4b: Positive MALDI MS, m/z calcd for $C_{88}H_{23}Br_2N_2O^+$ [$M + H$] $^+$ 1281.0, found 1281.0; 1H NMR (600 MHz, DMSO- d_6), δ 7.50 (d, 2H), 7.34 (d, 1H), 7.29 (d, 1H), 7.20 (d, 2H), 7.13 (d, 1H), 7.06-7.02 (m, 2H), 7.01-6.93 (m, 4H), 6.91-6.84 (m, 4H), 6.74 (t, 1H), 4.62 (AB_q, 2H, $\Delta\nu_{AB}$ = 448 Hz, J_{AB} = 12 Hz), 4.15 (AB_q, 2H, $\Delta\nu_{AB}$ = 33.6 Hz, J_{AB} = 12 Hz); ^{13}C NMR (150 MHz, DMSO- d_6), δ 168.95 (1C, C=O), 161.00 (1C, C=N), 157.17 (1C), 154.84 (1C), 150.52 (1C), 150.01 (1C), 149.20 (2C), 148.18 (1C), 147.66 (1C), 147.51 (1C), 147.45 (1C), 147.35 (1C), 147.31 (1C), 146.34 (1C), 146.24 (1C), 146.15 (1C), 146.04 (1C), 145.92 (2C), 145.85 (1C), 145.74 (1C), 145.45 (1C), 145.37 (1C), 145.25 (1C), 145.25 (1C), 144.83 (1C), 144.52 (1C), 144.44 (2C), 144.31 (1C), 144.17 (1C), 144.04 (1C), 143.86 (1C), 143.77 (1C), 143.65 (1C), 143.63 (1C), 143.15 (1C), 143.13 (1C), 142.62 (1C), 142.17 (1C), 141.98 (1C), 141.83 (1C), 141.46 (1C), 141.03 (1C), 141.00 (1C), 140.90 (1C), 140.49 (1C), 140.39 (1C), 140.34 (1C), 140.24 (1C), 138.57 (1C), 138.41 (1C), 137.99 (1C), 137.90 (1C), 137.10 (1C), 135.72 (1C), 135.57 (1C, Ph), 135.17 (1C, Ph), 135.10 (1C), 133.45 (1C, Ph), 132.73 (1C, Ph), 132.64 (1C, Ph), 132.31 (1C, Ph), 132.11 (1C, Ph), 131.04 (1C, Ph), 131.00 (1C, Ph), 130.17 (1C, Ph), 128.21 (1C, Ph), 128.16 (4C, Ph), 128.08 (1C, Ph), 127.65 (2C, Ph), 127.43 (2C, Ph), 126.81 (1C, Ph), 126.56 (1C, Ph), 126.17 (1C, Ph), 125.74 (1C, Ph), 86.60 (1C, sp^3 , C₆₀-N-), 83.29 (1C, sp^3 , C₆₀-N=), 61.53 (1C, C-CH₂Ph), 58.15 (1C, C-CH₂Ph), 45.45 (1C, CH₂), 43.70 (1C, CH₂) ; UV-vis (toluene): λ_{max} 325, 410, 454, 524, 710 nm.

Generation of $1^{\cdot-}$ and 1^{2-} via Controlled-Potential Bulk Electrolysis and vis-NIR Characterization of 1^{2-} . Reduced species of $1^{\cdot-}$ and 1^{2-} (20 mg, 21 μ mol) were generated by controlled-potential bulk electrolysis at potentials of -0.60 and -1.00 V vs SCE respectively in 16 mL of PhCN containing 0.1 M TBAP under Ar. The potentiostat was switched off after the theoretical number of electrons required for the reduction was achieved.

The solution of 1^{2-} was transferred to a 1-mm cuvette under argon, and the cuvette was sealed with a rubber septum and Parafilm for the vis-NIR measurement.

Quantum Computational Methods. The structures of **A**, **B**, **C**, **2a**, **3a**, **4a**, $2a^{2-}$ and $3a^{2-}$ were optimized with Gaussian09 at the HF/6-31G level, followed by harmonic frequency calculations at the same level to confirm them as the energy minima. The NBO charge distributions of intermediates **A**, **B** and **C** were calculated with Gaussian09 at the HF/6-311G(d) level. The energies of **2a**, **3a** and **4a** were obtained at the HF/6-311G(d) level.

Figure S1. Vis-NIR spectrum of 1^{2-} (1.3×10^{-3} M) in PhCN containing 0.1 M TBAP, recorded in 1-mm cuvette.

Figure S2. HPLC trace of the crude product obtained from the reaction of $\mathbf{1}^{2-}$ with PhCH_2Br . The mixture was eluted with a 70:30 v/v mixture of toluene/hexane over a semi-preparative YMC-pack silica column (10 mm $\times$ 250 mm) at a flow rate of 3.7 mL/min with the detector wavelength set at 380 nm. Peaks marked with the number sign and asterisk are likely due to 1,2-HBnC₆₀ and 1,4-Bn₂C₆₀ respectively according to the HPLC retention time (see Zheng, M.; Li, F.; Shi, Z.; Gao, X.; Kadish, K. M. *J. Org. Chem.* **2007**, 72, 2538).

Figure S3. UV-vis spectrum of compound **2a** in toluene.

Figure S4. Positive ESI FT-ICR MS of compound **2a**.

Figure S6. ¹³C NMR (DEPTQGPSP) spectrum (150 MHz) of compound **2a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S7. HMBC NMR spectrum of **2a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S8. ¹H NMR spectrum (400 MHz) of compound **2aI** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO.

Figure S10. UV-vis spectrum of compound **3a** in toluene.

Figure S11. Positive ESI FT-ICR MS of compound **3a**.

Figure S12. ¹H NMR spectrum (500 MHz) of compound **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO.

Figure S13. ¹³C NMR (DEPTQGPSP) spectrum (125 MHz) of compound **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S14. HMBC NMR spectrum of **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S15. ¹H NMR spectrum (400 MHz) of compound **3aI** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO.

Figure S17. UV-vis spectrum of compound **4a** in toluene.

Figure S18. MALDI MS of compound **4a**.

Figure S20. ^{13}C NMR spectrum (150 MHz) of compound **4a** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The resonance at around 109 ppm is due to the artifact from the instrument.

Figure S21. HMBC NMR spectrum of **4a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 109 ppm is due to the artifact from the instrument.

Figure S22. ¹H NMR spectrum (600 MHz) of compound **4aII** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO.

Figure S23. HPLC trace of the crude product obtained from the reaction of $\mathbf{1}^{2-}$ with *o*-BrPhCH₂Br. The mixture was eluted with a 70:30 v/v mixture of toluene/hexane over a semi-preparative YMC-pack silica column (10 mm × 250 mm) at a flow rate of 3.7 mL/min with the detector wavelength set at 380 nm. The peak marked with asterisks has not been identified.

Figure S24. UV-vis spectrum of compound **2b** in toluene.

Figure S25. Positive ESI FT-ICR MS of compound **2b**.

Figure S26. ^1H NMR spectrum (500 MHz) of compound **2b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H_2O residue in DMSO.

Figure S27. ^{13}C NMR (DEPTQGPSP) spectrum (125 MHz) of compound **2b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock.

Figure S28. UV-vis spectrum of compound **3b** in toluene.

Figure S29. Positive ESI FT-ICR MS of compound **3b**.

Figure S30. ¹H NMR spectrum (500 MHz) of compound **3b** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO.

Figure S31. ^{13}C NMR (DEPTQGPSP) spectrum (125 MHz) of compound **3b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock.

Figure S32. UV-vis spectrum of compound **4b** in toluene.

Figure S33. MALDI MS of compound **4b**.

Figure S34. ¹H NMR spectrum (600 MHz) of compound **4b** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 2.1 and 3.3 ppm is due to the toluene and H₂O residue in DMSO.

Figure S35. ¹³C NMR spectrum (125 MHz) of compound **4b** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S36. Optimized structure of 1^{2-} obtained using Gaussian09 at HF/6-31G level.

Figure S37. Calculated NBO charge distributions of 1^{2-} obtained using Gaussian09 at HF/6-311G(d) level.

Figure S38. Optimized structure of intermediate **B** obtained using Gaussian09 at HF/6-31G level.

Figure S39. Calculated NBO charge distributions of intermediate **B** obtained using Gaussian09 at HF/6-311G(d) level.

Figure S40. Optimized structure of intermediate **C** obtained using Gaussian09 at HF/6-31G level.

Figure S41. Calculated NBO charge distributions of intermediate **C** obtained using Gaussian09 at HF/6-311G(d) level.

Figure S42. Cyclic voltammograms of (a) **2b** (1,2,3,16-adduct) and (b) **3b** (1,2,3,4-adduct) in benzonitrile containing 0.1 M TBAP at rt. Scan rate = 0.1 V/s. The arrows indicate the starting potentials and the scan direction for the cyclic voltammetric measurements. The dianion of **2b** exhibits a less stability than that of **2a** as evidenced by the appearance of a new cathodic peak (labeled with an asterisk) at -1.22 V.

Cartesian coordinates and the lowest frequencies of **A**, **B**, **C**, **2a**, **3a**, **4a**, **2a²⁻** and **3a²⁻** obtained with Gaussian09 at HF/6-31G level. Total energies of **2a**, **3a**, and **4a** obtained with Gaussian09 at HF/6-311G(d) level.

Geometry of A

Charge = -2 Multiplicity = 1

C	-4.20672100	0.97389300	-0.35756800
C	-5.51467200	1.69479200	-0.12427600
C	-5.70961800	2.43312400	1.04205700
H	-4.91014300	2.46803900	1.75308100
C	-6.89742900	3.11161600	1.25976100
H	-7.03397700	3.66871400	2.16886400
C	-7.90844800	3.07803000	0.30644500
H	-8.82970500	3.60653800	0.47425100
C	-7.71672200	2.36094700	-0.86371000
H	-8.48656700	2.33525700	-1.61316300
C	-6.52867600	1.67233900	-1.07697600
H	-6.38323400	1.12770200	-1.98836100
C	-5.01517500	-1.02534300	-1.48909500
C	-5.75487800	-1.69070600	-0.33907100
C	-5.30400600	-1.64312000	0.97526900
H	-4.40352700	-1.11438300	1.21140100
C	-6.00195300	-2.29364000	1.98559900
H	-5.63468400	-2.25258100	2.99401900
C	-7.16141600	-2.99488300	1.69384600
H	-7.70280400	-3.49418700	2.47709500
C	-7.61509000	-3.05428300	0.38173200
H	-8.51012500	-3.60111000	0.14573700
C	-6.91026000	-2.41467700	-0.62477600
H	-7.22912200	-2.46877300	-1.64577800
N	-4.16336400	-0.03196700	-1.25298700
N	-3.20645700	1.49960600	0.26560800
O	-5.22169000	-1.51761100	-2.62007400
C	3.01261800	-0.92571300	3.23614200
C	1.71286600	-0.37827800	3.54524200
C	0.56446900	-1.02877300	3.08680700
C	0.70588500	-2.29323800	2.36796700
C	1.95387200	-2.81995400	2.11879200
C	3.14820800	-2.12792400	2.57025000
C	3.91619400	0.17528500	2.92804700
C	3.15442000	1.40704700	3.01712400
C	1.78994200	1.05464100	3.37936700
C	0.74457100	1.75603100	2.82347300

C	-0.55692100	-0.32529400	2.56230300
C	-0.31970000	-2.33615600	1.35173300
C	-0.05830600	-2.91606300	0.12758800
C	1.25664400	-3.46298300	-0.14200400
C	2.23699500	-3.41780900	0.82487800
C	3.59969100	-3.07838000	0.46353600
C	4.15501400	-2.26812800	1.53630600
C	5.01048700	-1.22900900	1.24151000
C	4.87859100	0.02903500	1.95623400
C	3.39171900	2.42879500	2.12703600
C	4.40402600	2.27440800	1.09867500
C	5.12919000	1.10867100	1.01525800
C	5.41476400	0.51682700	-0.28065600
C	5.33026200	-0.92523000	-0.14104200
C	4.80991600	-1.69319600	-1.16059600
C	3.91602800	-2.79316400	-0.84680800
C	2.88560600	-2.84204500	-1.86926200
C	1.59084500	-3.16270300	-1.52433200
C	-1.09425200	-1.11537300	1.43996000
C	-0.05213900	-0.17769900	-2.90183500
C	-0.99874900	-0.01985300	-1.90831000
C	-1.17223500	1.22908400	-1.22400000
C	-0.31274400	2.25639600	-1.50140400
C	0.70706700	2.09955200	-2.51467200
C	2.14652900	0.37603500	-3.48931300
C	2.07629500	-1.06905800	-3.35033500
C	0.71435900	-1.41308200	-2.98929500
C	0.47842900	-2.43110000	-2.09993100
C	-0.53902000	-2.27831700	-1.06964700
C	-1.24617500	-1.09802000	-0.96695800
C	-1.83233900	1.01129200	0.17023400
C	-0.96170500	1.70842000	1.20940500
C	-0.05951800	2.74466400	0.87688600
C	0.24355200	3.11135300	-0.43603300
C	1.59451200	3.40674500	-0.77964300
C	1.88894300	2.80938000	-2.07971700
C	3.14162700	2.30513100	-2.34908100
C	3.27260400	1.04992800	-3.07053500
C	3.13561300	-1.76455000	-2.80901100
C	4.31997800	-1.05031000	-2.36644900
C	4.38733800	0.31964700	-2.49907900
C	4.94180500	1.12523400	-1.42269900
C	4.18852100	2.36214400	-1.34402600
C	3.90475800	2.91460400	-0.11124700

C	2.60948500	3.48636400	0.17592900
C	2.27979200	3.16328400	1.54353100
C	0.99222300	2.82288100	1.89360300
C	-1.58259800	-0.52391000	0.30617800
C	-0.45259000	1.05457000	2.34767200
C	0.82882900	0.91514100	-3.21380000

Lowest frequency = 7.46 cm⁻¹

Geometry of **B**

Charge = -1 Multiplicity = 1

C	3.76349500	-0.58429100	1.09416700
C	5.11010100	-0.87220600	1.63812700
C	5.87127000	0.16635000	2.16477600
H	5.48321400	1.16431300	2.13220700
C	7.10809300	-0.09151900	2.73244400
H	7.69087500	0.71727600	3.12966400
C	7.58956700	-1.39221000	2.79230900
H	8.54689000	-1.59236100	3.23470900
C	6.82675400	-2.43322400	2.28488500
H	7.18659300	-3.44254000	2.33994300
C	5.59278200	-2.17522000	1.70736600
H	5.00164600	-2.98813500	1.33288100
C	3.84799800	-2.03166400	-0.95199900
C	5.12702500	-1.53477600	-1.53808900
C	5.39384700	-0.17760300	-1.66738400
H	4.68601900	0.54189800	-1.30812900
C	6.55841100	0.24929100	-2.28831500
H	6.75262300	1.29922400	-2.39284600
C	7.46453800	-0.67969800	-2.77672400
H	8.36834800	-0.34919800	-3.25246300
C	7.19762900	-2.03779300	-2.65861100
H	7.89287200	-2.75869400	-3.04378000
C	6.02870200	-2.46229800	-2.05068000
H	5.79793100	-3.50597600	-1.97420900
N	3.21091000	-1.27162300	0.01884900
N	2.98762900	0.25177600	1.65590400
O	3.35553100	-3.06950900	-1.36377000
C	-2.61103700	0.88434800	-3.28006300
C	-1.27292800	1.35966500	-2.98316100
C	-0.24684600	0.44928200	-2.84491700
C	-0.48436400	-0.95299000	-3.02443000
C	-1.74983500	-1.41389800	-3.30981300
C	-2.84332900	-0.46321800	-3.43494200
C	-3.54686500	1.69959900	-2.52547600

C	-2.77498300	2.67296800	-1.77120800
C	-1.37093300	2.46308300	-2.07361400
C	-0.42614000	2.56653800	-1.06472800
C	0.37809000	-1.65761400	-2.07659900
C	-0.08672000	-2.85427000	-1.51477300
C	-1.42949200	-3.26739500	-1.77062400
C	-2.25275400	-2.61628000	-2.68574500
C	-3.64294300	-2.39222200	-2.36578400
C	-4.02059600	-1.06866500	-2.84632100
C	-4.90730300	-0.29861700	-2.12910800
C	-4.66388400	1.12436800	-1.96418700
C	-3.17353500	3.03871700	-0.50825300
C	-4.34722800	2.42714500	0.08385400
C	-5.07936300	1.49898400	-0.62400900
C	-5.57086500	0.30599400	0.03990900
C	-5.47613400	-0.80278100	-0.89179900
C	-5.11627900	-2.05264800	-0.43949300
C	-4.19833700	-2.87864400	-1.20017400
C	-3.34778900	-3.57983300	-0.25699600
C	-2.01355700	-3.77391500	-0.53201700
C	1.20497900	-0.73104100	-1.41122800
C	-0.66250200	-2.28827800	2.52070300
C	0.43769900	-1.69358600	1.91656600
C	0.69709900	-0.29848000	2.09964000
C	-0.16179300	0.45942400	2.82417400
C	-1.33699000	-0.13080800	3.41807400
C	-2.92563600	-1.95149700	3.01318000
C	-2.82524000	-3.06302900	2.08400000
C	-1.41816900	-3.26763800	1.78858700
C	-1.02674800	-3.60374100	0.51158700
C	0.15106300	-3.00785000	-0.08306100
C	0.89656400	-2.10251500	0.62701300
C	1.64602000	0.23458400	1.03208600
C	1.23561500	1.69440300	0.48316800
C	0.01482700	2.29984400	1.21075500
C	-0.52570200	1.81699600	2.35955100
C	-1.92631400	2.00840000	2.65140300
C	-2.42882000	0.81619400	3.30866500
C	-3.70767300	0.37163100	3.06348800
C	-3.96093900	-1.05058200	2.90322500
C	-3.76348500	-3.21073000	1.08847300
C	-4.85572400	-2.26508200	0.97469400
C	-4.95229900	-1.21148900	1.85808600
C	-5.32494100	0.10944700	1.38118000

C	-4.55310700	1.08751700	2.12241300
C	-4.08234600	2.22027000	1.49766700
C	-2.73706700	2.69343500	1.77013400
C	-2.17493900	3.18638200	0.54016700
C	-0.84013100	2.96391100	0.26867500
C	1.72832300	-1.00006700	-0.03494000
C	0.67943400	1.67217000	-0.95120300
C	-1.57986500	-1.47881100	3.27888400
C	2.47708500	2.64717500	0.60538800
H	2.79514400	2.64041800	1.63708200
H	3.28037900	2.20480100	0.03050300
C	0.74217600	0.58298000	-1.78363300
C	2.28861000	4.07848300	0.14994500
C	2.51911300	4.45144400	-1.17249600
C	1.93116700	5.07128800	1.05983700
C	2.38644000	5.77190400	-1.57641200
H	2.79189900	3.70173200	-1.89041100
C	1.79675800	6.39318800	0.66115200
H	1.75146800	4.80522300	2.08451700
C	2.02388000	6.74853200	-0.66030900
H	2.56224600	6.03485900	-2.60243500
H	1.51500900	7.14027200	1.37907500
H	1.91869800	7.77058500	-0.97188200

Lowest frequency = 21.13 cm⁻¹

Geometry of C

Charge = -1 Multiplicity = 1

N	-3.07446500	1.29835500	-0.73759300
N	-3.51784000	-0.90033400	-0.50242000
C	-1.00203600	1.31163700	0.65411600
C	0.32535500	1.19675700	2.55729700
C	-0.82963600	0.62406100	1.93413200
C	-2.01769100	-0.90094400	-0.36502400
C	3.57000700	-3.10562900	1.83542700
C	-0.71635600	-0.45847900	-2.37953900
C	-4.26126900	-2.01853600	-0.13520000
C	-0.86752200	0.81513100	-1.74070500
C	-0.08434600	-1.56564600	2.76928500
C	-0.81415400	-2.76215500	0.91036600
O	-3.97404900	-3.12566400	-0.55971700
C	2.63047200	0.66042800	3.15635500
C	1.23629100	1.51554000	-2.70414300
C	4.46632200	1.47628000	-0.98068800
C	2.16319500	2.46192900	1.57498100

C	4.88528000	0.18312700	1.50028100
C	-0.61456700	-2.70348900	-1.50251400
C	1.69936400	-4.11089400	0.82160700
C	-1.25877900	-1.49601900	-1.55364100
C	-1.53633700	-1.53487900	0.91351300
C	2.74429700	2.72193500	0.23495000
C	0.07853300	1.77385800	-1.89598200
C	1.46579900	-3.78012300	-1.60000100
C	1.95269900	2.78407100	-0.87326400
C	-3.96902600	0.39341600	-0.75686800
C	3.76094800	0.24155500	-2.84198500
C	3.30465100	-0.63166500	3.18604900
C	2.41457900	-2.85858100	2.68005800
C	1.22141500	0.43907900	3.30083700
C	0.04524000	-2.82370500	2.08883400
C	0.87439500	-4.03861900	-0.29188400
C	-0.06008700	2.27575600	0.51077800
C	4.69067700	-2.60065700	-0.70683700
C	4.47835000	-1.93657700	-1.98059400
C	-5.93010900	1.90802000	-0.74389200
C	0.40536200	2.82917800	-0.82253800
C	4.02612700	2.06257100	0.18751700
C	3.62396800	1.51229300	-2.14695000
C	0.81862000	2.23390800	1.67905100
C	3.09698900	1.65948100	2.31507400
C	2.28760500	-1.65852600	3.33956400
C	1.37195100	0.31934700	-3.37308500
C	-1.75181100	0.69662800	-0.50091600
C	0.54056700	-2.95109200	-2.33916400
C	-1.01251900	-0.75133800	1.97532500
C	5.13557100	0.18749500	-0.94205700
C	0.99935100	-0.99008800	3.38780500
C	-5.33048900	-0.89795300	1.84386700
H	-4.49660400	-0.22753700	1.90706700
C	3.68160700	-3.63161000	-0.55676000
C	2.82248100	-3.58247400	-1.72592100
C	1.26150200	-3.46736200	2.03922500
C	-5.37709800	-1.85821800	0.84004500
C	0.36415700	-0.69369900	-3.21792700
C	5.11377100	-1.87346400	0.38502600
C	2.38994000	2.13233900	-2.07540600
C	2.44140400	-1.76503900	-3.32690500
C	-7.37525000	0.18159200	-2.36210100
H	-7.92614500	-0.48473100	-2.99761700

C	-6.34564700	-0.82771100	2.78668100
H	-6.29796400	-0.09182800	3.56575300
C	-0.42167900	-3.42766800	-0.24335000
C	-6.43821900	-2.75699000	0.79679300
H	-6.44694600	-3.51327700	0.03745400
C	-7.21367200	2.24280600	-1.14196000
H	-7.64350400	3.17388500	-0.82583600
C	4.24457900	1.39816800	1.46065900
C	-5.36550400	0.69956000	-1.13987600
C	4.53132500	-2.13282400	1.68929700
C	3.11950400	-3.86548000	0.68015700
C	-7.45851200	-2.67761200	1.72886100
H	-8.27915800	-3.36759500	1.68480500
C	4.39536400	-0.86282300	2.38450400
C	1.01245600	-1.97683700	-3.19122100
C	3.32336100	-2.54378500	-2.61108500
C	4.69215200	-0.57841600	-2.09250400
C	2.66645000	-0.33627600	-3.44097400
C	5.32690300	-0.44478100	0.26520900
C	-6.09345600	-0.15931700	-1.95702700
H	-5.65737400	-1.07974300	-2.29340100
C	-7.94018200	1.37931900	-1.95084100
H	-8.93429100	1.64003400	-2.26083100
C	-7.41320200	-1.71048200	2.72504800
H	-8.20085300	-1.65147500	3.45214500
H	-5.35350400	2.57492300	-0.13530900
C	-0.20233400	4.21420900	-1.20000100
H	0.15311000	4.47415000	-2.19174500
H	-1.27449100	4.07399600	-1.26994400
C	0.10617500	5.34125300	-0.24018300
C	1.21249100	6.16468000	-0.43421500
C	-0.71921100	5.58975100	0.85469300
C	1.49177200	7.20360700	0.44220300
H	1.86055600	5.98870200	-1.27212000
C	-0.44333600	6.62686900	1.73313100
H	-1.57328600	4.96160900	1.02112400
C	0.66382200	7.43831300	1.52980900
H	2.35210300	7.82429600	0.27625000
H	-1.08891800	6.79833900	2.57369700
H	0.87885300	8.24051900	2.21023900

Lowest frequency = 19.00 cm⁻¹

Geometry of **2a**

Charge = 0 Multiplicity = 1

N	-2.78071800	-1.72086800	1.52533700
N	-3.15057500	0.38572800	0.83343500
C	-1.06483800	-2.24819500	-0.27965200
C	0.55341000	-2.13479100	-2.10372200
C	-0.55974100	-1.45140800	-1.48874200
C	-1.66930300	0.29191800	0.70401700
C	3.94493300	2.05828900	-1.79052800
C	-0.30430500	-0.07579600	2.69490300
C	-3.90663100	1.42562200	0.31330000
C	-0.50643000	-1.36643500	2.12109700
C	0.22749400	0.59684000	-2.51861300
C	-0.44104800	1.97225100	-0.73338200
O	-3.48161200	2.57145500	0.35197500
C	2.86701300	-1.74746000	-2.81610400
C	1.57840500	-2.11155100	3.10977600
C	4.76461000	-2.33740800	1.30148400
C	2.37648200	-3.41254700	-1.09073700
C	5.17409800	-1.23155800	-1.26712600
C	-0.16517000	2.11547900	1.69850000
C	2.15532000	3.18680500	-0.77517500
C	-0.83927600	0.93825500	1.83146700
C	-1.11054300	0.80751300	-0.59695300
C	2.97729900	-3.60506300	0.20340100
C	0.39684900	-2.35488300	2.32309300
C	1.98734700	3.06529500	1.62571000
C	2.18908400	-3.51043800	1.32866600
C	-3.62387200	-0.77606500	1.47114800
C	-0.94086900	5.09645200	-0.79280000
C	4.15176300	-0.94775800	3.09793400
C	3.57227500	-0.48643900	-2.96497700
C	2.76012000	1.79853800	-2.58724300
C	-2.07180700	-4.11219500	-1.83246600
C	1.44420000	-1.46880400	-2.91281600
C	0.41699400	1.89374900	-1.93544500
C	-2.21834000	-4.60619300	-4.19587900
H	-2.45472800	-4.28779200	-5.19305500
C	1.38881400	3.27100700	0.34458500
C	-2.37507600	-3.72538300	-3.13568700
C	0.19665100	-3.09357300	-0.00666500
C	5.14243400	1.69764100	0.74984900
C	4.93715600	1.13120200	2.07059300
C	-5.62624300	-2.06386900	2.15080200

C	0.77324000	-3.25303100	1.21029300
C	4.29574900	-2.99476900	0.18735300
C	3.94103600	-2.25299900	2.49652800
C	1.02662000	-3.13912300	-1.17784700
C	3.31942800	-2.68889100	-1.92550300
C	2.57941500	0.55684000	-3.16356900
C	1.77868300	-0.88144100	3.69437700
C	-1.48302100	-1.31329000	0.96024500
C	1.04070700	2.33926100	2.45215600
C	-0.70291300	-0.11767200	-1.67608300
C	5.47175300	-1.08065000	1.16013400
C	1.27514300	-0.05505600	-3.13334900
C	-1.46336400	-6.29676900	-2.67299600
H	-1.11372800	-7.29385400	-2.48566300
C	-5.44065900	-0.04169400	-1.04297900
H	-4.69284400	-0.80791900	-1.07258500
C	4.15586400	2.74638300	0.55647100
C	3.34333700	2.82226400	1.74092500
C	1.64675100	2.47932000	-1.97147400
C	-5.20575200	1.14053600	-0.35054800
C	0.80997300	0.16145600	3.48340800
C	0.00047300	6.10557900	-0.97932400
C	5.49655200	0.88481500	-0.30104800
C	-1.89392800	4.88423900	-1.78793800
H	-2.63980900	4.12650500	-1.64578500
C	2.68758000	-2.81806800	2.50366400
C	2.93092000	1.14345800	3.47189100
C	-6.65549900	0.11999900	3.51723300
H	-7.04373300	0.96221100	4.05577000
C	-0.95685300	4.26135500	0.46963000
H	-1.96706700	3.99503400	0.71935600
H	-0.54900500	4.83744000	1.29304100
C	-6.63446500	-0.22685400	-1.72193800
H	-6.80565700	-1.13743100	-2.26176400
C	-0.11777800	2.94109700	0.39525700
C	-6.17206800	2.14277400	-0.35444900
H	-5.97329000	3.06183400	0.15913900
C	-6.82834700	-2.17518600	2.82914700
H	-7.35544800	-3.10917100	2.82916300
C	4.50714900	-2.42776500	-1.13111200
C	-2.27921000	-3.16479100	-0.67013600
H	-2.55093600	-3.72624000	0.21067100
H	-3.11462700	-2.51615900	-0.89623600
C	-4.93989200	-0.85395100	2.13795700

C	4.88602300	1.07390600	-1.60799500
C	3.56359100	2.91156100	-0.67724500
C	-7.37039000	1.95233100	-1.02006700
H	-8.11535000	2.72350900	-1.01079300
C	0.00223300	6.87408600	-2.13501200
H	0.73583500	7.64756800	-2.26000600
C	4.69188300	-0.23465300	-2.20757500
C	-1.62180200	-5.41251400	-1.61608400
H	-1.39446400	-5.73478300	-0.61732700
C	1.50610100	1.40879700	3.35469300
C	-1.75958500	-5.89515700	-3.96739400
H	-1.63842300	-6.57824700	-4.78588100
C	3.82539600	1.82886700	2.68586800
C	-1.89345600	5.64985400	-2.94442200
H	-2.63485000	5.47292700	-3.70026800
C	5.09445900	-0.22321700	2.26954800
C	3.09820700	-0.28171700	3.68422700
C	5.66802800	-0.53937600	-0.09186400
C	-5.45730700	0.23646500	2.83052500
H	-4.92174600	1.16571900	2.85650700
C	-7.34586700	-1.08303000	3.51208300
H	-8.27535400	-1.17085600	4.04043600
C	-7.60273900	0.76626800	-1.70418600
H	-8.52941700	0.62001500	-2.22453900
C	-0.94360400	6.64581600	-3.12310200
H	-0.94445300	7.23942500	-4.01722600
H	-2.73322800	-2.73041900	-3.32416800
H	0.73350700	6.29489800	-0.21784800
H	-5.21157300	-2.90812700	1.63793700

Lowest frequency = 21.43 cm⁻¹

Total energy = -3530.4825 hartree (1 hartree = 627.51 kcal/mol)

Geometry of **3a**

Charge = 0 Multiplicity = 1

N	-2.64175600	0.11664900	-2.13723800
N	-3.12271100	-1.02447900	-0.25348000
C	-0.78589800	1.62561500	-1.31139000
C	0.96844300	2.72488100	-0.03046500
C	-0.23128900	1.92956200	0.07956400
C	-1.66168800	-0.72903000	-0.04886100
C	4.07826500	-0.54895000	2.94946800
C	-0.36829800	-2.08319000	-1.61842000
C	-3.83412700	-1.84956400	0.61500400
C	-0.45811900	-0.79625100	-2.22188900

C	0.50775200	1.27834500	2.27925000
C	-0.37784000	-0.87467200	2.25332900
O	-3.23560400	-2.66452800	1.30511000
C	3.29514800	2.79762500	0.73198500
C	1.59103900	-1.27025700	-3.43245800
C	4.91372200	-0.08166600	-2.41684400
C	2.78576400	2.64828400	-1.65794300
C	5.44988200	1.08634200	0.10229200
C	-0.26838400	-2.75172800	0.68321700
C	2.13669700	-1.85553800	3.15719800
C	-0.86565400	-2.01524300	-0.28471000
C	-1.33117900	-0.02853600	1.36666400
C	3.30134900	1.74674700	-2.65493100
C	0.48973200	-0.39954400	-3.10480100
C	1.78230400	-3.57756900	1.46004600
C	2.42521300	0.91974500	-3.32342600
C	-3.51542900	-0.56885800	-1.53014400
C	-2.46378000	1.16543100	3.42666100
C	4.07854300	-2.27674100	-2.54168200
C	3.93258900	2.02169800	1.78015600
C	2.97160700	0.33004400	3.26968200
C	-1.53037700	4.11215800	-1.70381100
C	1.86990200	2.81477000	1.00052900
C	0.56604500	-0.01466300	2.91402400
C	-1.42174100	6.23997300	-0.55742300
H	-1.58382200	6.81943400	0.33125300
C	1.26523800	-2.66511900	2.46221500
C	-1.73345600	4.88813400	-0.56587900
C	0.50852000	1.84636300	-2.13495100
C	5.07291500	-2.33440500	0.99745300
C	4.79936800	-2.93584900	-0.29577100
C	-5.52318800	0.04202200	-2.85102200
C	1.00581800	0.98367700	-3.05576300
C	4.57400100	1.23020800	-2.18388900
C	3.99859800	-0.95162900	-3.13505100
C	1.43079600	2.66245100	-1.39526800
C	3.74108500	2.70770400	-0.56427200
C	2.90043300	1.57725900	2.69866100
C	1.67017400	-2.53124000	-2.88578800
C	-1.36168800	0.13732000	-1.41809300
C	0.83168300	-3.62224900	0.36649400
C	-0.45042400	1.21765100	1.20338700
C	5.54764600	-0.86555800	-1.37321400
C	1.62874900	2.06573500	2.20148700

C	-0.70694800	6.08298200	-2.83978700
H	-0.31359500	6.54061800	-3.72714000
C	-5.94208000	-0.45336200	0.67078900
H	-5.39364300	0.41523200	0.36799000
C	4.04482600	-2.77110500	1.92371300
C	3.13084200	-3.63746200	1.20028400
C	1.77305800	-0.48313300	3.39190100
C	-5.30218100	-1.68145400	0.79521400
C	0.65823900	-2.95315600	-1.95585200
C	-2.32819600	0.50211800	4.64418200
C	5.56524700	-1.05146500	1.06931200
C	-2.50254600	2.55677900	3.43183200
H	-2.62236400	3.08714000	2.50614100
C	2.78799500	-0.46321900	-3.56813000
C	2.70232500	-3.80272800	-1.20865400
C	-6.27807500	-2.61684200	-3.07062800
H	-6.55829000	-3.64764300	-3.16521500
C	-2.63838500	0.37810100	2.14267100
H	-3.24573800	0.95811000	1.46070700
H	-3.17796600	-0.51630200	2.39554800
C	-7.29386900	-0.33995300	0.95237100
H	-7.77903100	0.61192800	0.86149400
C	-0.01349300	-2.16002700	2.01208400
C	-6.02645200	-2.79200400	1.21989300
H	-5.51973400	-3.72758100	1.34531300
C	-6.65446400	-0.29941500	-3.57465500
H	-7.22951500	0.46694900	-4.05666200
C	4.84767400	1.82962400	-0.88832400
C	-1.90395200	2.64528000	-1.73095300
H	-2.22688400	2.37532600	-2.72413000
H	-2.75101800	2.48389700	-1.07482300
C	-4.77634800	-0.94267500	-2.21521700
C	5.05524000	-0.13405400	2.07184400
C	3.56061400	-1.90502000	2.87556000
C	-7.38037000	-2.68232200	1.48613400
H	-7.93401000	-3.54425300	1.80294900
C	-2.21224400	1.21017600	5.83112100
H	-2.10575900	0.68102000	6.75847900
C	4.98320400	1.18639200	1.47323900
C	-1.02070800	4.73210900	-2.84285800
H	-0.86873500	4.15531400	-3.73571600
C	1.27903500	-3.74290500	-0.93055000
C	-0.90475800	6.84153200	-1.69504000
H	-0.66351700	7.88700300	-1.69125700

C	3.60370400	-3.74479900	-0.17153900
C	-2.38843700	3.26932600	4.61639500
H	-2.41819200	4.34191900	4.59894300
C	5.03053600	-2.22037800	-1.45067600
C	2.94542000	-3.04808700	-2.42541700
C	5.80882500	-0.29775900	-0.14727500
C	-5.15258200	-2.27586000	-2.33794800
H	-4.56494000	-3.04924300	-1.88185400
C	-7.03542500	-1.62905800	-3.68334400
H	-7.90880200	-1.89405300	-4.24699500
C	-8.01561500	-1.45524100	1.35213200
H	-9.06352900	-1.36719600	1.56441500
C	-2.23937200	2.59714300	5.82042700
H	-2.15112100	3.14614900	6.73801900
H	-2.13757900	4.43439600	0.31929800
H	-2.31457700	-0.57134400	4.66356300
H	-5.21200000	1.06557700	-2.78531400

Lowest frequency = 20.51 cm⁻¹

Total energy = -3530.4729 hartree (1 hartree = 627.51 kcal/mol)

Geometry of **4a**

Charge = 0 Multiplicity = 1

N	-2.53890600	2.10361200	-0.23161500
N	-3.33706800	0.04799600	-0.72854900
C	-0.45008200	1.47110000	0.95219800
C	0.97356800	0.72127400	2.65923500
C	-0.27170100	0.44100900	1.98490400
C	-1.88247200	-0.25575400	-0.48248200
C	3.51357300	-3.64069700	0.68350900
C	-0.56951300	0.48188200	-2.40546900
C	-4.20703100	-0.93894500	-1.18060400
C	-0.50830900	1.56573900	-1.47983100
C	0.17122900	-1.91164900	2.24709500
C	-0.85636700	-2.58699900	0.26012100
O	-3.75107500	-1.93558700	-1.72785600
C	3.20249400	-0.22784100	2.92421100
C	1.61677200	2.20947900	-2.43019500
C	4.89469000	1.34297300	-1.04917800
C	2.89615500	1.95282700	1.84882200
C	5.25961000	-0.56164200	1.01280200
C	-0.74252100	-1.89191700	-2.09014200
C	1.46596400	-4.10043100	-0.36805400
C	-1.18887400	-0.64842100	-1.78958500
C	-1.64453700	-1.33425500	0.71501300

C	3.43909200	2.46262800	0.56712900
C	0.55292800	2.40859600	-1.48788900
C	1.14909400	-3.17606900	-2.60919300
C	2.60303700	2.88760800	-0.42164200
C	-3.55870400	1.44033200	-0.58778200
C	3.92239400	0.69860800	-3.08004000
C	3.68034500	-1.56075100	2.59537600
C	2.45202700	-3.46264000	1.65867400
C	1.77591700	-0.30113000	3.11361200
C	0.07276900	-2.98448500	1.28579400
C	0.60880200	-3.67178000	-1.35635100
C	0.61244200	2.29817100	0.95961400
C	4.55429300	-2.67333000	-1.76030000
C	4.36597900	-1.69618500	-2.81745800
C	-5.33698900	3.07127100	-0.02711000
C	1.08269700	3.11460200	-0.22896400
C	4.60490400	1.67513100	0.25658300
C	4.00340100	1.76667100	-2.09542800
C	1.54769800	1.87038800	2.01866600
C	3.74732700	0.87578100	2.29592100
C	2.53518300	-2.45548700	2.58741900
C	1.54667600	1.20701600	-3.37206500
C	-1.34466500	1.25961100	-0.23310900
C	0.31222000	-2.08113600	-3.05136500
C	-0.67292900	-0.83431800	1.79521800
C	5.36873600	0.00700600	-1.36908800
C	1.35821400	-1.66402300	2.89679500
C	-6.22007700	-0.35466500	0.23951500
H	-5.59071000	0.08800100	0.98387100
C	3.41084500	-3.56373100	-1.76013700
C	2.50806500	-3.13004900	-2.81310900
C	1.18858300	-3.74410400	0.99837000
C	-5.67390800	-0.86895100	-0.93071200
C	0.41796500	0.31945300	-3.36425700
C	5.13037300	-2.29373900	-0.56757200
C	2.87853000	2.50488100	-1.77678900
C	2.30792900	-0.94519500	-3.90599300
C	-6.50304400	2.77736600	-2.52530800
H	-6.94254500	2.67082600	-3.49769300
C	-7.58646700	-0.42169700	0.45902000
H	-7.99929000	-0.02941400	1.36751400
C	-0.57305300	-2.90580200	-1.02823100
C	-6.50776400	-1.46904700	-1.87020000
H	-6.07616800	-1.89839000	-2.75188500

C	-6.45329200	3.82063400	-0.36315500
H	-6.85611100	4.52124500	0.34204100
C	4.80153200	0.69846600	1.31577000
C	-4.81311200	2.15410200	-0.93050600
C	4.59706200	-2.79144300	0.68594400
C	2.90351600	-4.03579500	-0.57169500
C	-7.87499400	-1.51961500	-1.65943100
H	-8.51204800	-1.97285900	-2.39334500
C	4.68046100	-1.72216300	1.66637000
C	0.87410200	-1.00113600	-3.69547000
C	3.10484100	-1.98020600	-3.47148800
C	4.76490600	-0.39023900	-2.62771100
C	2.72775400	0.42871200	-3.70315600
C	5.54425100	-0.91859600	-0.36802200
C	-5.39307800	2.02037800	-2.18712500
H	-4.97749200	1.34085300	-2.90570000
C	-7.04030000	3.67245600	-1.61132100
H	-7.90222500	4.25493100	-1.87317800
C	-8.41591600	-0.99508600	-0.49362500
H	-9.47445800	-1.04008800	-0.32504000
H	-4.86419200	3.20126700	0.92606700
C	0.65585100	4.61441500	-0.18584900
H	1.00814900	5.08131600	-1.09882300
H	-0.42690800	4.63198300	-0.21374100
C	1.15430100	5.38880000	1.01396100
C	2.37942400	6.04996500	0.98102200
C	0.38739100	5.46774600	2.17425800
C	2.83307400	6.76215200	2.08194500
H	2.98033000	6.01013000	0.09200800
C	0.83785800	6.17855300	3.27677200
H	-0.56447800	4.97227500	2.21276300
C	2.06369100	6.82705600	3.23424600
H	3.77991700	7.26542100	2.03798000
H	0.23363600	6.22828900	4.16236200
H	2.41258700	7.37877500	4.08590100
C	-2.99915400	-1.72138900	1.41590600
H	-3.48527200	-0.79632500	1.69297700
H	-3.61804500	-2.22876100	0.69694100
C	-2.91538300	-2.60671300	2.64357700
C	-2.96980000	-3.99269200	2.51820800
C	-2.84803500	-2.05797400	3.92172800
C	-2.93751800	-4.80978200	3.63876300
H	-3.03932300	-4.43400100	1.54177500
C	-2.81668400	-2.87136900	5.04477700

H	-2.81721600	-0.99108100	4.04063700
C	-2.85840900	-4.25102600	4.90593300
H	-2.97810500	-5.87565500	3.52193500
H	-2.76202800	-2.42997700	6.02137500
H	-2.83469600	-4.88179500	5.77357900

Lowest frequency = 17.92 cm⁻¹

Total energy = -3530.4718 hartree (1 hartree = 627.51 kcal/mol)

Geometry of **2a²⁻**

Charge = -2 Multiplicity = 1

N	-2.84507900	-1.57801900	1.60842700
N	-3.12666200	0.56809500	0.99108600
C	-1.18035900	-2.20736700	-0.21469800
C	0.36380200	-2.14191600	-2.07090700
C	-0.69331100	-1.45563200	-1.46528400
C	-1.63380400	0.38388200	0.73819100
C	4.01257100	1.92557800	-1.87943200
C	-0.25207200	-0.02342400	2.70701500
C	-3.88455900	1.59701000	0.44747300
C	-0.52855100	-1.31280100	2.16245900
C	0.18274700	0.61423400	-2.46245800
C	-0.36311700	2.03813300	-0.77204400
O	-3.64921800	2.77212400	0.67841800
C	2.69370900	-1.82118500	-2.82986000
C	1.55734300	-2.13322600	3.09906700
C	4.68851900	-2.50326400	1.22193400
C	2.18980600	-3.48444900	-1.10505800
C	5.08959800	-1.41499400	-1.37756900
C	-0.02695500	2.14254600	1.66914400
C	2.28251600	3.11967900	-0.87312200
C	-0.75057900	0.99840600	1.83273000
C	-1.15556400	0.85347800	-0.59407400
C	2.81379100	-3.69020600	0.16967900
C	0.34048300	-2.33949400	2.35233200
C	2.15511700	3.00827300	1.53543100
C	2.06451300	-3.57310700	1.32868600
C	-3.63785100	-0.59068100	1.56603700
C	-0.80015300	5.20831700	-0.67755400
C	4.18232900	-1.08280200	3.02083700
C	3.45824000	-0.58810400	-3.01024400
C	2.76543000	1.73205300	-2.62741300
C	-2.29966200	-4.14063200	-1.61075100
C	1.28454400	-1.50495800	-2.93789100
C	0.41812900	1.91987500	-1.91714200

C	-2.48783100	-4.77872500	-3.93818100
H	-2.67595200	-4.50114300	-4.95859700
C	1.54031500	3.26617600	0.28878900
C	-2.55450300	-3.81625700	-2.94203600
C	0.05705000	-3.09111900	0.03743500
C	5.23665400	1.51341900	0.63545200
C	5.03276700	0.96187900	1.96298000
C	-5.71480700	-1.82066000	2.14582600
C	0.65267000	-3.26957000	1.24399000
C	4.15338500	-3.12866300	0.11365500
C	3.89893900	-2.37576000	2.42966500
C	0.84754300	-3.16090900	-1.15968500
C	3.15052800	-2.79297200	-1.96916100
C	2.53457300	0.47369200	-3.20789100
C	1.82264900	-0.90542400	3.66701500
C	-1.52956900	-1.22923000	1.01976400
C	1.19965100	2.32257700	2.39622200
C	-0.77234100	-0.06279800	-1.60142800
C	5.45413800	-1.27918200	1.05401900
C	1.18850500	-0.10086400	-3.09523900
C	-1.90717000	-6.42885600	-2.30246600
H	-1.64635200	-7.43884400	-2.04521800
C	-4.90308600	0.19853800	-1.36444300
H	-3.99148100	-0.36152900	-1.41050000
C	4.29377900	2.60791700	0.45812500
C	3.51928000	2.73553400	1.66051100
C	1.73897100	2.51971200	-2.05788600
C	-5.02012300	1.24207000	-0.45542800
C	0.89614000	0.17464100	3.46323800
C	0.11219000	6.25705500	-0.76826700
C	5.53268200	0.68062800	-0.41818800
C	-1.72369900	5.04933600	-1.71024700
H	-2.42521800	4.24039800	-1.65842800
C	2.61875000	-2.90013600	2.47865800
C	3.06173200	1.06754100	3.41589000
C	-6.72187400	0.36611700	3.51963700
H	-7.10142200	1.21258100	4.05985600
C	-0.81640300	4.28257300	0.51708700
H	-1.83352100	4.00388700	0.73942800
H	-0.42228300	4.81257100	1.38014000
C	-5.94031200	-0.07641100	-2.24495700
H	-5.83731400	-0.87529600	-2.95365000
C	0.02093100	2.97125700	0.36596800
C	-6.17107500	2.02327000	-0.44734300

H	-6.23659400	2.84607900	0.23651900
C	-6.94929400	-1.90191900	2.76868900
H	-7.51123400	-2.81536900	2.71957800
C	4.36455700	-2.58986700	-1.21607200
C	-2.43147000	-3.11216000	-0.50795600
H	-2.69260400	-3.61897800	0.40920600
H	-3.26228900	-2.46128000	-0.74676700
C	-4.97889400	-0.64042800	2.19340500
C	4.90366200	0.88663100	-1.71650400
C	3.69786600	2.79380200	-0.77258900
C	-7.21230200	1.73914300	-1.31424800
H	-8.10379500	2.33699800	-1.29523600
C	0.10447800	7.12324700	-1.85271700
H	0.82438000	7.91968000	-1.90418800
C	4.65695400	-0.40974800	-2.30861100
C	-1.97681600	-5.46184200	-1.30957900
H	-1.76585600	-5.72930200	-0.29127100
C	1.64299700	1.38732600	3.30455300
C	-2.16506200	-6.09097200	-3.62238400
H	-2.10670100	-6.83568700	-4.39456400
C	3.95720500	1.70939000	2.58566200
C	-1.73420300	5.91207700	-2.79580600
H	-2.44900300	5.76467300	-3.58442300
C	5.13193000	-0.40004700	2.16383600
C	3.16814000	-0.35826100	3.61938300
C	5.63839400	-0.75097800	-0.20555200
C	-5.48879600	0.45159800	2.88943800
H	-4.91770200	1.35707100	2.95460600
C	-7.45730300	-0.80766600	3.45634000
H	-8.41385800	-0.87156600	3.94054600
C	-7.09803600	0.68557500	-2.21324000
H	-7.90281300	0.46785700	-2.89033600
C	-0.82150800	6.95524000	-2.87127600
H	-0.82648900	7.62062200	-3.71541000
H	-2.78187700	-2.79997100	-3.19892900
H	0.84131700	6.38401000	0.00945400
H	-5.30648100	-2.66352300	1.62604900

Lowest frequency = 19.81 cm⁻¹

Geometry of **3a²⁻**

Charge = -2 Multiplicity = 1

N	-2.63842400	-0.24190700	-2.10261600
N	-3.10152500	-1.10935300	-0.07087900
C	-0.81173300	1.40874100	-1.50357100

C	0.92090300	2.71362800	-0.41927300
C	-0.27333000	1.93327700	-0.17253300
C	-1.62568400	-0.76253800	0.08172100
C	4.13052800	-0.06512800	2.97555400
C	-0.33885100	-2.29758100	-1.29149300
C	-3.83632200	-1.79421000	0.87553800
C	-0.43736500	-1.12146300	-2.05970200
C	0.49904800	1.59207800	2.09281100
C	-0.32981800	-0.54402900	2.37653400
O	-3.31475800	-2.53615900	1.69711700
C	3.26097400	2.91372700	0.32246500
C	1.63727500	-1.70485700	-3.21228400
C	4.93270800	-0.35240800	-2.40996600
C	2.75108000	2.44000700	-2.03220700
C	5.46043200	1.18706700	-0.06918200
C	-0.19520800	-2.63145200	1.09608800
C	2.21391500	-1.34236100	3.36679700
C	-0.81046400	-2.05506500	0.01589000
C	-1.30829700	0.14114700	1.38046600
C	3.26821900	1.40545100	-2.86660900
C	0.49953500	-0.81596700	-3.01150600
C	1.87990500	-3.32208500	1.95857800
C	2.40905900	0.46137100	-3.41479500
C	-3.48875300	-0.85620300	-1.40435600
C	-2.50970100	1.58566400	3.24126700
C	4.15224900	-2.53187700	-2.21927600
C	3.91879900	2.33028700	1.46132700
C	2.99266600	0.82617800	3.16951800
C	-1.67853600	3.79231000	-2.21849300
C	1.82840400	2.95530000	0.59270000
C	0.57559600	0.40944700	2.89707500
C	-1.78596600	6.05937100	-1.37346000
H	-2.03029500	6.73581800	-0.57550300
C	1.35838400	-2.27589100	2.79837600
C	-1.99872600	4.69757800	-1.21081800
C	0.47714600	1.54493200	-2.35750300
C	5.16702300	-2.08107800	1.29452200
C	4.90115500	-2.86645900	0.09992800
C	-5.50759700	-0.57280400	-2.83071900
C	0.98017400	0.54286600	-3.15606900
C	4.57078600	0.98790500	-2.35170300
C	4.06034300	-1.33072300	-2.99520500
C	1.36346600	2.46820300	-1.75971000
C	3.69351000	2.64798400	-0.96458000

C	2.90543200	1.98780200	2.42251400
C	1.73055600	-2.87889700	-2.47446000
C	-1.34991300	-0.09286600	-1.39416500
C	0.94432000	-3.51408200	0.89450100
C	-0.47110800	1.38288500	1.04111800
C	5.59822100	-0.95437900	-1.26343700
C	1.61038900	2.38239200	1.88073900
C	-0.92950100	5.65351200	-3.57271100
H	-0.50451400	6.01475900	-4.49059700
C	-5.90919900	-0.34008700	0.68593600
H	-5.31998800	0.45993900	0.28710900
C	4.14276000	-2.41418500	2.27313700
C	3.26632500	-3.39700100	1.69658100
C	1.82543800	0.02893000	3.43643300
C	-5.31444000	-1.55871100	0.98707300
C	0.72832000	-3.21263400	-1.51874600
C	-2.34223700	1.12877400	4.54716700
C	5.63031800	-0.79224100	1.18053000
C	-2.63823900	2.95612000	3.03683500
H	-2.75987600	3.32859900	2.03787800
C	2.79859500	-0.92163200	-3.49165100
C	2.80824500	-3.88264000	-0.66744600
C	-6.08951900	-3.27623900	-2.66968600
H	-6.29901100	-4.32750800	-2.61675500
C	-2.62998500	0.60438000	2.09189500
H	-3.26486800	1.05106600	1.33740400
H	-3.13042700	-0.26478400	2.48162800
C	-7.26376700	-0.14634800	0.91308600
H	-7.71056600	0.80186400	0.68368200
C	0.05521900	-1.86423800	2.29797000
C	-6.08974200	-2.57743200	1.53259300
H	-5.61523200	-3.50156800	1.79426300
C	-6.59633000	-1.08930000	-3.51530200
H	-7.20413200	-0.43951000	-4.11607500
C	4.83258300	1.76046400	-1.16928400
C	-1.96451000	2.31386500	-2.06433700
H	-2.25124900	1.91037700	-3.02364400
H	-2.82226800	2.19878900	-1.41052600
C	-4.71451700	-1.39995200	-2.04430300
C	5.10234100	0.25799400	2.03813400
C	3.64831300	-1.41465500	3.09913200
C	-7.44492500	-2.39091200	1.74601900
H	-8.03524700	-3.18676800	2.15856600
C	-2.29545700	2.01464700	5.61251000

H	-2.15320100	1.64015700	6.60893900
C	5.01495800	1.47004600	1.26738300
C	-1.14287300	4.29434700	-3.40360500
H	-0.87581100	3.61132100	-4.18678900
C	1.38121800	-3.79589200	-0.39260400
C	-1.25127600	6.54348700	-2.55728200
H	-1.07972000	7.59629300	-2.68448800
C	3.71742500	-3.67231200	0.36470000
C	-2.59139900	3.84746800	4.09924900
H	-2.68021300	4.90184400	3.91430800
C	5.11124700	-2.31855500	-1.14278000
C	3.02696100	-3.30905600	-1.96685800
C	5.85196600	-0.21251900	-0.13444300
C	-5.00496500	-2.75861200	-1.97864300
H	-4.37278800	-3.41352500	-1.41040100
C	-6.89297900	-2.44229900	-3.43331800
H	-7.73399100	-2.84398900	-3.96663000
C	-8.03493900	-1.17284700	1.43600800
H	-9.08451600	-1.02348500	1.60694400
C	-2.42022600	3.37925000	5.39289500
H	-2.37706600	4.06696400	6.21699200
H	-2.40454500	4.33171300	-0.28710800
H	-2.23123100	0.07626500	4.72281200
H	-5.25776200	0.46637800	-2.91177600

Lowest frequency = 20.00 cm⁻¹