Supporting Information

for

Reactions of 2-carbonyl- and 2-hydroxy(or methoxy)alkyl-substituted benzimidazoles with arenes in the superacid CF$_3$SO$_3$H. NMR and DFT studies of dicationic electrophilic species

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Experimental details, compound characterization data, copies of $^1$H and $^{13}$C NMR spectra, and details of DFT calculations
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1. Experimental part

General

NMR spectra of solutions of compounds in CDCl$_3$, MeOD-d$_4$, (CD$_3$)$_2$CO were recorded on Bruker AVANCE 500 spectrometer (at 500 and 125 MHz for $^1$H and $^{13}$C NMR spectra respectively) at 25 °C. The solvent residual signals CDCl$_3$ (δ 7.26 ppm), MeOD-d$_4$ (δ 3.31 ppm), (CD$_3$)$_2$CO (δ 2.05 ppm) for $^1$H NMR spectra and the carbon signal of CDCl$_3$ (δ 77.0 ppm), MeOD-d$_4$ (δ 49.0 ppm), (CD$_3$)$_2$CO (δ 29.8 ppm) for $^{13}$C NMR spectra were used as references. NMR spectra in TfOH were recorded on a Bruker AVANCE III 400 spectrometer (at 400 and 100 MHz for $^1$H and $^{13}$C NMR spectra, respectively) using CH$_2$Cl$_2$ as internal standard. HRMS was carried out with a Bruker maXis HRMS-ESI-QTOF instrument or by matrix-assisted laser desorption ionization (MALDI–MS) using Fourier Transform (Ion Cyclotron Resonance). The preparative reactions were monitored by thin-layer chromatography carried out on silica gel plates (Silufol UV-254), using UV light for detection. Column chromatography was performed on silica gel Merck-60 with petroleum ether/diethyl ether or DCM/MeOH mixtures as eluents.

DFT calculations. All computations were carried out at the DFT/HF hybrid level of theory using hybrid exchange functional M06 by using GAUSSIAN 2009 program packages [1]. The geometry optimizations were performed using the 6-311+G(2d,2p) basis set (standard 6-311 basis set added with polarization (d, p) and diffuse functions). Optimizations were performed on all degrees of freedom and solvent-phase optimized structures were verified as true minima with no imaginary frequencies. The Hessian matrix was calculated analytically for the optimized structures in order to prove the location of correct minima and to estimate the thermodynamic parameters. Solvent-phase calculations used the Polarizable Continuum Model (PCM).

Procedures for the synthesis of 2-carbonylbenzimidazoles 1-2. Analogous as described in [2].

Dess–Martin reagent (1.1 mmol) was added to a solution of benzimidazol-2-ylmethanol 4 or 7 (1 mmol) in methylene chloride (10 mL). The reaction mixture was stirred at 4 °C for 1 h prior to being quenched with saturated aqueous sodium thiosulfate solution (3 mL). The subsequent mixture was extracted with methylene chloride (3 × 10 mL). The combined organic extracts were dried over anhydrous magnesium sulfate and concentrated in vacuo to provide a crude product, which was crystallized from methanol to give corresponding product.

1-Methyl-1H-benzimidazole-2-carboxaldehyde (1) [3] was obtained as beige solid in 30% yield. M.p. 134-136°C from methanol. $^1$H NMR (500 MHz, CDCl$_3$) δ 4.12 (s, NMe), 7.35-7.39 (m, 1H$_{arom}$.), 7.43-7.48 (m, 2H$_{arom}$.), 7.90 (d, 1H$_{arom}$, J = 10.3 Hz), 10.09 (s, 1H, CHO). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 31.2, 110.5, 122.3, 124.0, 126.8, 136.9, 142.7, 146.1, 185.0.
2-Acetyl-1H-benzimidazole (2) [4] was obtained as beige solid in 30% yield. M.p. 134-136°C from methanol. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 2.81 (s, 3H, Me), 7.38 (br.s, 2H$_{arom}$), 7.68 38 (br.s, 2H$_{arom}$), 10.16 (br.s, 1H, NH). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 25.9, 141.7, 147.7, 191.8.

**Procedures for synthesis of substituted benzimidazol-2-methanols 3a–c and 4.**

Mixture of phenylenediamine 10 g (92.6 mmol), glycolic/lactic acid (166.7 mmol), 135 ml 4M HCl was refluxed for 6 hours. Then reaction mixture was alkalinized to pH 7 with aqueous solution of KOH. Precipitate was filtered and crystallized from water.

**(Benzimidazol-2-yl)methanol (3a) [5]** was obtained as beige solid in 74% yield. M.p. 159-161°C from H$_2$O. $^1$H NMR (500 MHz, (CD$_3$)$_2$CO) $\delta$ 4.86 (s, 2H), 7.23 – 7.11 (m, 2H$_{arom}$), 7.64 – 7.46 (m, 2H$_{arom}$), 11.47 (brs, 1H). $^{13}$C NMR (125 MHz, (CD$_3$)$_2$CO) $\delta$ 59.2, 122.4, 155.8. HRMS, m/z calculated for C$_8$H$_8$N$_2$O [M+Na]: 171.0534. Found: 171.0537.

**(5,7-Dimethylbenzimidazol-2-yl)methanol (3b)** was obtained as beige solid in 54% yield. M.p. 173-175°C. $^1$H NMR (500 MHz, MeOD-d$_4$) $\delta$ 2.39 (s, 3H), 2.50 (s, 3H), 4.80 (s, 2H), 6.84 (s, 1H$_{arom}$), 7.14 (s, 1H$_{arom}$). $^{13}$C NMR (125 MHz, MeOD-d$_4$) $\delta$ 17.0, 21.6, 58.9, 125.5, 133.3, 155.1. HRMS, m/z calculated for C$_{10}$H$_{13}$N$_2$O [M+Na]: 177.1022. Found: 177.1029.

**(5-Chlorobenzimidazol-2-yl)methanol (3c) [6]** was obtained as beige solid in 54% yield. M.p. 186-188°C. $^1$H NMR (500 MHz, MeOD-d$_4$) $\delta$ 4.82 (s, 2H), 7.20 (dd, 1H$_{arom}$, $J = 2.0, 8.6$ Hz), 7.50 (d, 1H$_{arom}$, $J = 8.6$ Hz), 7.53 (s, 1H$_{arom}$). $^{13}$C NMR (125 MHz, MeOD-d$_4$) $\delta$ 58.9, 123.8, 129.0, 157.8.

**1-(1H-benzimidazol-2-yl)ethan-1-ol 4 [4]** was obtained as beige solid in 93% yield. M.p. 172-174°C from ethanol. $^1$H NMR (500 MHz, MeOD-d$_4$) $\delta$ 1.61 (d, 3H, $J = 6.5$ Hz), 5.06 (q, 1H, $J = 6.5$ Hz), 7.35 – 6.98 (m, 2H), 7.67-7.34 (m, 2H). $^{13}$C NMR (125 MHz, MeOD-d$_4$) $\delta$ 23.1, 65.5, 111.1, 115.8, 123.3, 139.3, 159.8.

**Procedures for synthesis of substituted 2-(methoxymethyl)-1H-benzimidazole 5a–c and 6.**

NaOH (9.5 mmol) was added to a stirring solution of benzimidazole (6.7 mmol) in 10 mL of EtOH/H$_2$O 3:1 (v/v). Dimethyl sulfate (9.5 mmol) was added dropwise over 5 min and the mixture was stirred for additional 2 h. Solvents were evaporated to give colorless solid, which was crystallized from methanol to give corresponding product.

**2-(Methoxymethyl)-1H-benzimidazole (5a) [7]** was obtained as beige solid in 95% yield. M.p. 137-139°C from methanol.$^1$H NMR (500 MHz, MeOD-d$_4$) $\delta$ 3.67 (s, 3H, OMe), 5.10 (s, 2H), 7.55 (dd, 2H$_{arom}$, $J = 3.1, 6.2$ Hz), 7.76 (dd, 2H$_{arom}$, $J = 3.1, 6.2$ Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) $\delta$ 55.1, 56.7, 114.9, 127.2, 132.5, 156.0. HRMS, m/z calculated for C$_9$H$_{11}$N$_2$O [M+H]$^+$: 163.0866. Found: 163.0873.
5,7-Dimethyl-2-(methoxymethyl)-1H-benzimidazole (5b) was obtained as beige solid in 94% yield. M.p. 110-112°C from methanol. $^1$H NMR (500 MHz, MeOD-d$_4$) δ 3.68 (s, 3H, OMe), 4.99 (s, 2H), 7.13 (s, 2H$_{arom}$), 7.30 (s, 2H$_{arom}$). $^{13}$C NMR (125 MHz, MeOD-d$_4$) δ 16.6, 21.5, 55.1, 57.1, 111.9, 125.5, 128.5, 132.0, 133.9, 137.1, 155.0. HRMS, m/z calculated for C$_{11}$H$_{15}$N$_2$O [M+H]$^+$: 191.1179. Found: 191.0981.

5-Chloro-2-(methoxymethyl)-1H-benzimidazole (5c) was obtained as purple solid in 86% yield. M.p. 127-129°C from methanol. $^1$H NMR (500 MHz, MeOD-d$_4$) δ 3.67 (s, 3H, OMe), 5.06 (s, 2H), 7.52 (dd, 1H$_{arom}$, J = 1.8, 8.8 Hz), 7.72 (d, 1H$_{arom}$, J = 8.8 Hz), 7.77 (d, 1H$_{arom}$, J = 1.8 Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) δ 55.1, 57.0, 115.0, 116.3, 127.4, 131.9, 132.6, 134.0, 157.5. HRMS, m/z calculated for C$_9$H$_{10}$ClN$_2$O [M+H]$^+$: 197.0476. Found: 197.0482.

2-(1-Methoxyethyl)-1H-benzimidazole (6) was obtained as beige solid in 89% yield. M.p. 109-111°C from methanol. $^1$H NMR (500 MHz, MeOD-d$_4$) δ 1.71 (d, J = 6.8 Hz, 3H), 3.67 (s, 3H), 5.34 (q, J = 6.8 Hz, 1H), 7.57 (dd, 2H$_{arom}$, J = 3.1, 6.2 Hz), 7.77 (dd, 2H$_{arom}$, J = 3.1, 6.2 Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) δ 22.5, 55.1, 63.6, 115.0, 127.4, 131.9, 132.6, 134.0, 157.5. HRMS, m/z calculated for C$_{10}$H$_{13}$N$_2$O [M+H]$^+$: 177.1022. Found: 177.1029.

Procedures for the synthesis of substituted (1-methylbenzimidazol-2-yl)methanol 7 and 8. Analogously as described in [2].

Potassium carbonate (5 mmol) was added to a stirring solution of benzimidazole-2-methanol (1 mmol) in DMF (2 mL). The reaction mixture was stirred at room temperature for 24 h prior to being diluted with methylene chloride (8 mL) and sodium chloride (8 mL). The organic layer was separated, and the aqueous layer was extracted with methylene chloride (8 mL × 2). The combined organic layers were dried over anhydrous sodium sulfate and concentrated in vacuo to provide a crude product, which was subjected to column purification using DCM/MeOH 100:5 (v/v) as eluent to yield the title compounds.

(1-Methylbenzimidazol-2-yl)methanol (7) [8] was obtained as beige solid in 30% yield. M.p. 134-136°C from methanol. $^1$H NMR (500 MHz, MeOD-d$_4$) δ 3.89 (s, 3H, NMe), 4.85 (s, 2H), 7.25 (t, 1H$_{arom}$, J = 7.6 Hz), 7.31 (t, 1H$_{arom}$, J = 7.6 Hz), 7.49 (d, 1H$_{arom}$, J = 8.0 Hz), 7.61 (d, 1H$_{arom}$, J = 8.0 Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) δ 30.5, 57.7, 110.9, 119.7, 123.4, 124.2, 137.3, 142.5, 154.8. HRMS, m/z calculated for C$_9$H$_{11}$N$_2$O [M+H]$^+$: 163.0866. Found: 163.0865.

2-(1-Hydroxyethyl)-1-methylbenzimidazole (8) [9] was obtained as beige solid in 87% yield. M.p. 197-199°C from methanol. $^1$H NMR (500 MHz, MeOD-d$_4$) δ 1.73 (d, J = 6.9 Hz, 3H), 4.20 (s, 3H), 5.70 (q, J = 6.9 Hz, 1H), 7.71 (dd, 2H$_{arom}$, J = 3.1, 6.2 Hz), 7.94 (dd, 2H$_{arom}$, J = 3.1, 6.2 Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) δ 20.8, 33.0, 62.8, 113.9, 128.1, 133.5, 154.7. HRMS, m/z calculated for C$_{10}$H$_{13}$N$_2$O [M+H]$^+$: 177.1022. Found: 177.1029.
General procedure for the reaction of benzimidazoles 1,2 with arenes in TfOH and H$_2$SO$_4$. Synthesis of compounds 9–11 (Table 3 and Scheme 2). Benzimidazole 1 or 2 (1 mmol) was added to the mixture of TfOH (1 mL) or H$_2$SO$_4$ (2 mL) and arene (2–18 mmol). Reaction mixture was stirred at room temperature for the time as indicated in Table 3 or Scheme 2. The mixture was poured into ice water (30 mL). After extraction with CH$_2$Cl$_2$ (3 × 30 mL), the combined extracts were consequently washed with water (50 mL), saturated aqueous solution of Na$_2$CO$_3$ (30 mL), water (50 mL), dried with anhydrous Na$_2$SO$_4$ and evaporated in vacuo to give crude products, which was subjected to chromatographic separation on silica gel using petroleum ether/diethyl ether as an eluent.

General procedure for the reaction of benzimidazole 1 with benzene under the action of strong Lewis acids AlCl$_3$ or AlBr$_3$. Synthesis of compound 9a (Table 3). Benzimidazole 1 (1 mmol) was added to the mixture of AlCl$_3$ or AlBr$_3$ (5.0 mmol) in benzene (3 mL). The reaction mixture was stirred at room temperature for the time as indicated in Table 1. The mixture was quenched with ice water (50 mL), extracted and worked-up as described above.

General procedures for the reaction of benzimidazoles 3–8 with arenes in TfOH in high pressure tube. Synthesis of compounds 12–14 (Tables 4, 5, Scheme 3). Solution of benzimidazole (0.1 mmol) in TfOH (1 mL) and arene (0.1 mL) was magnetically stirred at 140 °C in glass high pressure tube for 2.5 h, then poured into water (50 mL). After extraction with CH$_2$Cl$_2$ (3 × 30 mL), the combined extracts were consequently washed with water (50 mL), saturated aqueous solution of Na$_2$CO$_3$ (30 mL), water (50 mL), dried with anhydrous Na$_2$SO$_4$ and evaporated in vacuo to give crude products, which were subjected to chromatographic separation on silica gel using petroleum ether/diethyl ether as an eluent.

2-Diphenylmethyl-1-methyl-1H-benzimidazole (9a). White solid. M.p. 135-137°C. $^1$H NMR (500 MHz, CDCl$_3$) δ 3.61 (s, 3H, Me), 5.80 (s, 1H, CH), 7.25 (s, 3H arom.), 7.27–7.35 (m, 10H arom.), 7.81 (d, 1H arom., $J=7.9$). $^{13}$C NMR (125 MHz, CDCl$_3$) δ 30.1, 50.1, 108.9, 120.1, 121.8, 122.4, 127.1, 128.7, 129.1, 135.9, 140.0, 142.4, 155.2. HRMS, m/z calculated for C$_{21}$H$_{19}$N$_2$ [M+H]$^+$: 299.1543. Found: 299.1548.

1-Methyl-2-[bis(4-methylphenyl)methyl]-1H-benzimidazole (9b) and 1-methyl-2-[α-(4-methylphenyl)-α-(2-methylphenyl)methyl]-1H-benzimidazole (9c) were obtained as an oily mixture with the ratio of 6:1. Compound 9b: $^1$H NMR (500 MHz, CDCl$_3$, from the spectrum of the mixture) δ 2.38 (s, 6H, 2Me), 3.61 (s, 3H, NMe), 5.72 (s, 1H, CH), 7.18–7.32 (m, 11H arom.), 7.87–7.89 (m, 1H arom.). Compound 9c: $^1$H NMR (500 MHz, CDCl$_3$, from the spectrum of the mixture) δ 2.33 (s, 3H, Me), 2.40 (s, 3H, Me), 3.58 (s, 3H, NMe), 7.18–7.32 (m, 11H arom.), 7.87–7.89 (m, 1H arom.). For the mixture of compounds 9b,c: $^{13}$C NMR (125 MHz, CDCl$_3$) δ 20.9, 29.9, 46.6, 49.3,
108.8, 119.9, 121.5, 122.1, 128.72, 128.74, 129.1, 129.24, 129.28, 135.8, 136.5, 137.1, 155.5. HRMS, m/z calculated for C_{23}H_{23}N_{2} [M+H]^+: 327.1856. Found: 327.1860.

1-Methyl-2-[bis(4-methoxyphenyl)methyl]-1H-benzimidazole (9d) and 1-methyl-2-[a-(4-methoxyphenyl)-a-(2-methoxyphenyl)methyl]-1H-benzimidazole (9e) were obtained as an oily mixture with the ratio of 5:1. Compound 9d: \(^1\)H NMR (500 MHz, CDCl\(_3\), from the spectrum of the mixture) \(\delta\) 3.60 (s, 3H, NMe), 3.78 (s, 6H, 2MeO), 5.66 (s, 1H, CH), 6.85–7.29 (m, 11H\textsubscript{arom.}), 7.80–7.81 (m, 1H\textsubscript{arom.}). Compound 9e: \(^1\)H NMR (500 MHz, CDCl\(_3\), from the spectrum of the mixture) \(\delta\) 3.63 (s, 3H, NMe), 3.75 (s, 3H, MeO), 3.78 (s, 3H, MeO), 6.12 (s, 1H, CH), 6.85–7.29 (m, 11H\textsubscript{arom.}), 7.80–7.81 (m, 1H\textsubscript{arom.}). For the mixture of compounds 9d,e: \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 30.1, 41.7, 48.5, 55.2, 55.7, 108.9, 110.5, 114.0, 114.07, 114.09, 120.0, 121.0, 121.8, 122.4, 128.3, 130.0, 130.3, 134.4, 135.9, 155.8, 158.6. HRMS, m/z calculated for C_{23}H_{23}N_{2}O_{2} [M+H]^+: 359.1754. Found: 359.1751.

1-Methyl-2-[bis(4-chlorophenyl)methyl]-1H-benzimidazole (9f) and 1-methyl-2-[a-(4-chlorophenyl)-a-(2-chlorophenyl)methyl]-1H-benzimidazole (9g) were obtained as an oily mixture with the ratio 3:1. Compound 9f: \(^1\)H NMR (500 MHz, CDCl\(_3\), from the spectrum of the mixture) \(\delta\) 3.62 (s, 3H, NMe), 5.67 (s, 1H, CH), 7.17–7.33 (m, 11H\textsubscript{arom.}), 7.80–7.82 (m, 1H\textsubscript{arom.}). Compound 9g: \(^1\)H NMR (500 MHz, CDCl\(_3\), from the spectrum of the mixture) \(\delta\) 3.66 (s, 3H, NMe), 6.16 (s, 1H, CH), 7.17–7.33 (m, 11H\textsubscript{arom.}), 7.80–7.82 (m, 1H\textsubscript{arom.}). For the mixture of compounds 9f,g: \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 30.1, 45.7, 48.6, 109.1, 120.0, 122.2, 122.8, 127.4, 128.9, 129.0, 129.6, 130.3, 130.6, 130.7, 133.3, 138.0, 154.1. HRMS, m/z calculated for C_{21}H_{17}Cl_{2}N_{2} [M+H]^+: 367.0763. Found: 367.0766.

1-Methyl-2-[bis(3,4-dimethylphenyl)methyl]-1H-benzimidazole (9h). Oily compound. \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.21 (s, 6H, 2Me), 2.23 (s, 6H, 2Me), 3.60 (s, 3H, Me), 5.64 (s, 1H, CH), 6.97 (dd, 2H\textsubscript{arom.}, \(J = 7.8\) Hz), 7.03 (s, 2H\textsubscript{arom.}), 7.08 (d, 2H\textsubscript{arom.}, \(J = 7.8\) Hz), 7.22–7.26 (m, 1H\textsubscript{arom.}), 7.26–7.31 (m, 2H\textsubscript{arom.}), 7.82 (d, 1H, \(J = 7.3\) Hz). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 19.4, 19.8, 30.1, 49.4, 108.9, 120.1, 121.7, 122.2, 126.4, 129.86, 129.88, 130.2, 135.3, 135.9, 136.7, 137.5, 155.8. HRMS, m/z calculated for C_{23}H_{27}N_{2} [M+H]^+: 355.2169. Found: 355.2174.

1-Methyl-2-[bis(2,4-dimethylphenyl)methyl]-1H-benzimidazole (9i). White solid. M.p. 224–226°C. \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.16 (s, 6H, 2Me), 2.30 (s, 6H, 2Me), 3.52 (s, 3H, Me), 5.77 (s, 1H, CH), 6.71 (d, 2H\textsubscript{arom.}, \(J = 7.8\) Hz), 6.91 (d, 2H\textsubscript{arom.}, \(J = 7.1\) Hz), 7.02 (s, 2H\textsubscript{arom.}), 7.20–7.24 (m, 2H\textsubscript{arom.}), 7.27–7.30 (m, 1H\textsubscript{arom.}), 7.78 (d, 1H\textsubscript{arom.}, \(J = 7.8\) Hz). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 19.4, 21.0, 29.7, 43.3, 108.8, 120.2, 121.6, 122.1, 127.1, 128.9, 131.3, 134.9, 135.7, 135.9, 136.6, 142.6, 155.6. HRMS, m/z calculated for C_{25}H_{27}N_{2} [M+H]^+: 355.2169. Found: 355.2173.

1-Methyl-2-[bis(2,5-dimethylphenyl)methyl]-1H-benzimidazole (9j). White solid. M.p. 205–207°C. \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.13 (s, 6H, 2Me), 2.19 (s, 6H, 2Me), 3.55 (s, 3H, NMe),
5.79 (s, 1H, CH), 6.66 (s, 2H\text{arom.}); 7.0 (d, 2H\text{arom.}, \textit{J} = 7.6 Hz), 7.09 (d, 2H\text{arom.}, \textit{J} = 7.6 Hz), 7.21-7.24 (m, 1H\text{arom.}), 7.27-7.33 (m, 2H\text{arom.}), 7.78 (d, 1H\text{arom.}, \textit{J} = 7.6 Hz). $^{13}$C NMR (125 MHz, CDCl$_3$) \textit{δ} 19.0, 21.1, 29.6, 43.8, 108.7, 120.2, 121.4, 122.0, 127.8, 129.5, 130.2, 132.8, 135.7, 135.8, 137.4, 142.7, 155.4. HRMS, m/z calculated for C$_{25}$H$_{27}$N$_2$ [M+H]$^+$: 355.2169. Found: 355.2168.

1-Methyl-2-[bis(3,4-dichlorophenyl)methyl]-1H-benzimidazole (9k). White solid. M.p. 147-149°C. $^1$H NMR (500 MHz, CDCl$_3$) \textit{δ} 3.65 (s, 3H, Me), 5.62 (s, 1H, CH), 7.09 (dd, 2H\text{arom.}, \textit{J} = 8.4 Hz), 7.28-7.32 (m, 2H\text{arom.}), 7.33-7.34 (m, 3H\text{arom.}), 7.41 (s, 1H\text{arom.}), 7.42 (s, 1H\text{arom.}), 7.80 (d, 1H\text{arom.}, \textit{J} = 7.8 Hz). $^{13}$C NMR (125 MHz, CDCl$_3$) \textit{δ} 30.1, 48.0, 109.2, 120.2, 122.4, 123.1, 128.3, 130.8, 130.9, 132.0, 133.1, 135.7, 139.2, 152.8. HRMS, m/z calculated for C$_{25}$H$_{15}$Cl$_4$N$_2$ [M+H]$^+$: 434.9984. Found: 434.9991.

1-Methyl-2-[bis(2,4,5-trimethylphenyl)methyl]-1H-benzimidazole (9l). White solid. M.p. 239-241°C. $^1$H NMR (500 MHz, CDCl$_3$) \textit{δ} 2.08 (s, 6H, 2Me), 2.10 (s, 6H, 2Me), 2.20 (s, 6H, 2Me), 3.53 (s, 3H, NMe), 5.72 (s, 1H, CH), 6.60 (s, 2H\text{arom.}), 6.96 (s, 2H\text{arom.}), 7.20-7.24 (m, 1H\text{arom.}), 7.27-7.31 (m, 2H\text{arom.}), 7.78 (d, 1H, \textit{J} = 7.6 Hz). $^{13}$C NMR (125 MHz, CDCl$_3$) \textit{δ} 18.9, 19.3, 19.5, 29.7, 43.3, 108.7, 120.3, 121.4, 122.0, 130.2, 131.9, 133.0, 134.2, 135.0, 135.1, 136.0, 156.0. HRMS, m/z calculated for C$_{22}$H$_{31}$N$_2$ [M+H]$^+$: 383.2482. Found: 383.2479.

2-(1,1-Diphenylethyl)-1H-benzimidazole (10). White solid. M.p. 228-230°C. $^1$H NMR (500 MHz, CDCl$_3$) \textit{δ} 2.30 (s, 3H, Me), 7.12-7.28 (m, 12H\text{arom.}), 7.53 (br.s, 2H\text{arom.}). $^{13}$C NMR (125 MHz, CDCl$_3$) \textit{δ} 28.8, 50.9, 115.1, 122.9, 127.2, 128.0, 128.6, 145.7, 158.6. HRMS, m/z calculated for C$_{21}$H$_{19}$N$_2$ [M+H]$^+$: 299.1543. Found: 299.1549.

2-(1-Phenylethenyl)-1H-benzimidazole (11). White solid. M.p. 221-223°C. $^1$H NMR (500 MHz, CDCl$_3$) \textit{δ} 5.70 (s, 1H, =CH$_2$), 6.40 (s, 1H, =CH$_2$), 7.26 (dd, 2H\text{arom.}, \textit{J} = 6.0, 3.1 Hz), 7.28-7.29 (m, 3H\text{arom.}), 7.36-7.37 (m, 2H\text{arom.}), 7.58 (dd, 2H\text{arom.}, \textit{J} = 6.0, 3.1 Hz). HRMS, m/z calculated for C$_{15}$H$_{13}$N$_2$ [M+H]$^+$: 221.1073. Found: 221.1076.

2-Benzyl-1H-benzimidazole (12a) [10]. M.p. 184-186°C. $^1$H NMR (500 MHz, (CD$_3$)$_2$CO) \textit{δ} 4.25 (s, 2H), 7.14 (td, 2H\text{arom.}, \textit{J} = 9.0, 3.0 Hz), 7.22 (t, 1H\text{arom.}, \textit{J} = 7.5 Hz), 7.29 (t, 2H\text{arom.}, \textit{J} = 7.5 Hz), 7.35 (d, 2H\text{arom.}, \textit{J} = 7.5 Hz), 7.48 (td, 2H\text{arom.}, \textit{J} = 9.0, 3.0 Hz). $^{13}$C NMR (125 MHz, (CD$_3$)$_2$CO) \textit{δ} 36.3, 115.7, 122.5, 127.6, 129.5, 129.9, 138.7, 154.5. HRMS, m/z calculated for C$_{14}$H$_{13}$N$_2$ [M+H]$^+$: 209.1073. Found: 209.1066.

2-(3,4-Dichlorobenzyl)-1H-benzimidazole (12b) and 2-(2,3-dichlorobenzyl)-1H-benzimidazole (12c). Compound 12b and 12c were obtained as a mixture with M.p. 165-167°C (for the ratio of 1:0.5). Compound 12b: $^1$H NMR (500 MHz, (CD$_3$)$_2$CO, from the spectrum of the mixture) \textit{δ} 4.28 (s, 2H), 7.14-7.16 (m, 2H\text{arom.}), 7.36-7.33 (m, 1H\text{arom.}), 7.47-7.51 (m, 3H\text{arom.}), 7.60 (m, 1H\text{arom.}). Compound 12c: $^1$H NMR (500 MHz, (CD$_3$)$_2$CO, from the spectrum of the mixture) \textit{δ} 4.45 (s, 2H), 7.14-7.16 (m, 2H\text{arom.}), 7.31 (t, 1H\text{arom.}, \textit{J} = 8.0 Hz), 7.39 (d, 1H\text{arom.}, \textit{J} = 7.5 Hz), 7.47-
7.51 (m, 3H). For the mixture of compounds 12b,c: $^{13}$C NMR (125 MHz, (CD$_3$)$_2$CO) $\delta$ 34.8, 35.1, 122.5, 122.6, 128.8, 129.3, 130.1, 130.2, 130.8, 130.9, 131.4, 131.9, 132.6, 138.9, 139.6, 152.5, 153.2. HRMS (for mixture of isomers), m/z calculated for C$_{14}$H$_{11}$Cl$_2$N$_2$ [M+H]$^+$: 277.0294. Found: 277.0298.

2-(2,4-Dibromobenzyl)-1H-benzimidazole (12d) and 2-(3,5-dibromobenzyl)-1H-benzimidazole (12e). Compound 12d and 12e were obtained as a mixture with M.p. 204-206°C (for the ratio of 1:0.25). Compound 12d: $^1$H NMR (500 MHz, (CD$_3$)$_2$CO, from the spectrum of the mixture) $\delta$ 4.37 (s, 2H), 7.17–7.12 (m, 2H$_{arom}$), 7.37 (d, 1H$_{arom}$, $J$ = 8.5 Hz), 7.48–7.49 (m, 2H$_{arom}$), 7.54 (dd, 1H$_{arom}$, $J$ = 8.0, 2.0 Hz), 7.81 (d, 1H$_{arom}$, $J$ = 2.0 Hz). Compound 12e: $^1$H NMR (500 MHz, (CD$_3$)$_2$CO, from the spectrum of the mixture) $\delta$ 4.69 (s, 2H), 7.11–7.13 (m, 2H$_{arom}$), 7.19 (t, 1H$_{arom}$, $J$ = 8.0Hz), 7.44–7.46 (m, 2H$_{arom}$), 7.69 (d, 2H$_{arom}$, $J$ = 8.0Hz). HRMS (for mixture of isomers), m/z calculated for C$_{14}$H$_{11}$Br$_2$N$_2$ [M+H]$^+$: 364.9283. Found: 364.9278.

2-Benzyl-5,7-dimethylbenzimidazole (12f). M.p. 186-188°C.$^1$H NMR (500 MHz, (CD$_3$)$_2$CO) $\delta$ 2.35 (s, 3H, Me), 2.46 (s, 3H, Me), 4.19 (s, 2H), 6.78 (s, 1H$_{arom}$), 7.08 (s, 1H$_{arom}$), 7.20 (t, 1H$_{arom}$, $J$ = 7.0 Hz), 7.27 (t, 2H$_{arom}$, $J$ = 7.5 Hz), 7.32 (d, 2H$_{arom}$, $J$ = 7.0 Hz). $^{13}$C NMR (125 MHz, (CD$_3$)$_2$CO) $\delta$ 17.1, 21.8, 36.4, 124.5, 127.5, 129.5, 129.8, 131.9, 139.1.

2-Benzyl-5-chloro-1H-benzimidazole (12g) [11]. M.p. 153-155°C.$^1$H NMR (500 MHz, MeOD-d$_4$) $\delta$ 4.19 (s, 2H), 7.15 (dd, 1H$_{arom}$, $J$ = 8.6, 1.8 Hz), 7.19–7.24 (m, 1H$_{arom}$), 7.27–7.29 (m, 4H$_{arom}$), 7.42 (d, 1H$_{arom}$, $J$ = 8.6 Hz), 7.47 (d, 1H$_{arom}$, $J$ = 1.8 Hz). $^{13}$C NMR (125 MHz, MeOD-d$_4$) $\delta$ 36.1, 115.5, 116.4, 123.7, 128.1, 128.9, 129.76, 129.8, 137.9, 156.7.

2-(1-Phenylethyl)-1H-benzimidazole (12h) [12]. M.p. 206-208°C.$^1$H NMR (500 MHz, (CD$_3$)$_2$CO) $\delta$ 1.77 (d, 3H, $J$ = 7.5 Hz), 4.43 (q, 1H, $J$ = 7.0 Hz), 7.11-7.14 (m, 2H$_{arom}$), 7.21 (t, 1H$_{arom}$, $J$ = 7.5 Hz), 7.30 (t, 2H$_{arom}$, $J$ = 7.5 Hz), 7.38-7.33 (m, 2H$_{arom}$), 7.47-7.49 (m, 2H$_{arom}$). $^{13}$C NMR (125 MHz, (CD$_3$)$_2$CO) $\delta$ 21.2, 41.1, 122.5, 127.7, 128.5, 129.6.

2-Benzyl-1-methyl-1H-benzimidazole (13). Oily compound. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 3.55 (s, 3H, NMe), 4.30 (s, 2H, CH$_2$), 7.19-7.28 (m, 8H$_{arom}$), 7.74-7.76 (m, 1H$_{arom}$). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 30.1, 34.3, 109.1, 119.3, 122.1, 122.4, 127.0, 128.5, 128.9, 136.0, 142.2, 153.2. HRMS, m/z calculated for C$_{15}$H$_{15}$N$_2$ [M+H]: 223.1230. Found: 223.1237.

1-Methyl-2-(1-phenylethyl)-1H-benzimidazole (14). Oily compound. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 2.00 (d, 3H, $J$ = 7.2 Hz), 3.94 (s, 3H, NMe), 5.20 (q, 1H, $J$ = 7.2 Hz), 7.21 (d, 2H$_{arom}$, $J$ = 7.6 Hz), 7.35 (t, 1H$_{arom}$, $J$ = 7.6 Hz), 7.41 (t, 2H$_{arom}$, $J$ = 7.6 Hz), 7.62 (dd, 2H$_{arom}$, $J$ = 6.2, 3.0 Hz), 7.71 (dd, 2H$_{arom}$, $J$ = 6.2, 3.0 Hz). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 15.9, 32.7, 35.0, 112.7, 126.8, 127.3, 128.6, 129.8, 131.8, 135.9, 154.3. HRMS, m/z calculated for C$_{16}$H$_{17}$N$_2$ [M+H]: 237.1386. Found: 237.1395.
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3. $^1$H and $^{13}$C NMR Spectra of compounds 1–14

Figure S1. $^1$H NMR spectrum of compound 1 (500 MHz, CDCl$_3$).

Figure S2. $^{13}$C NMR spectrum of compound 1 (125 MHz, CDCl$_3$).
Figure S3. $^1$H NMR spectrum of compound 2 (500 MHz, CDCl$_3$).

Figure S4. $^{13}$C NMR spectrum of compound 2 (125 MHz, CDCl$_3$).
Figure S5. $^1$H NMR spectrum of compound 3a (500 MHz, (CD$_3$)$_2$CO).

Figure S6. $^{13}$C NMR spectrum of compound 3a (125 MHz, (CD$_3$)$_2$CO).
Figure S7. $^1$H NMR spectrum of compound 3b (500 MHz, MeOD-$d_4$).

Figure S8. $^{13}$C NMR spectrum of compound 3b (125 MHz, MeOD-$d_4$).
Figure S9. $^1$H NMR spectrum of compound 3c (500 MHz, MeOD-$d_4$).

Figure S10. $^{13}$C NMR spectrum of compound 3c (125 MHz, MeOD-$d_4$).
Figure S11. $^1$H NMR spectrum of compound 4 (500 MHz, MeOD-$d_4$).

Figure S12. $^{13}$C NMR spectrum of compound 4 (125 MHz, MeOD-$d_4$).
Figure S13. $^1$H NMR spectrum of compound 5a (500 MHz, MeOD-$d_4$).

Figure S14. $^{13}$C NMR spectrum of compound 5a (125 MHz, MeOD-$d_4$).
Figure S15. $^1$H NMR spectrum of compound 5b (500 MHz, MeOD-$d_4$).

Figure S16. $^{13}$C NMR spectrum of compound 5b (125 MHz, MeOD-$d_4$).
Figure S17. $^1$H NMR spectrum of compound 5c (500 MHz, MeOD-$d_4$).

Figure S18. $^{13}$C NMR spectrum of compound 5c (125 MHz, MeOD-$d_4$).
Figure S19. $^1$H NMR spectrum of compound 6 (500 MHz, MeOD-$d_4$).

Figure S20. $^{13}$C NMR spectrum of compound 6 (125 MHz, MeOD-$d_4$).
Figure S21. $^1$H NMR spectrum of compound 7 (500 MHz, MeOD-$d_4$).

Figure S22. $^{13}$C NMR spectrum of compound 7 (125 MHz, MeOD-$d_4$).
Figure S23. $^1$H NMR spectrum of compound 8 (500 MHz, MeOD-d$_4$).

Figure S24. $^{13}$C NMR spectrum of compound 8 (125 MHz, MeOD-d$_4$).
Figure S25. $^1$H NMR spectrum of compound 9a (500 MHz, CDCl$_3$).

Figure S26. $^{13}$C NMR spectrum of compound 9a (125 MHz, CDCl$_3$).
Figure S27. $^1$H NMR spectrum of mixture of compounds 9b and 9c (500 MHz, CDCl$_3$).

Figure S28. $^{13}$C NMR spectrum of mixture of compounds 9b and 9c (125 MHz, CDCl$_3$).
Figure S29. $^1$H NMR spectrum of mixture of compounds 9d and 9e (500 MHz, CDCl$_3$).

Figure S30. $^{13}$C NMR spectrum of mixture of compounds 9d and 9e (125 MHz, CDCl$_3$).
Figure S31. $^1$H NMR spectrum of mixture of compounds 9f and 9g (500 MHz, CDCl$_3$).

Figure S32. $^{13}$C NMR spectrum of mixture of compounds 9f and 9g (125 MHz, CDCl$_3$).
Figure S33. $^1$H NMR spectrum of compound 9h (500 MHz, CDCl$_3$).

Figure S34. $^{13}$C NMR spectrum of compound 9h (125 MHz, CDCl$_3$).
Figure S35. $^{1}$H NMR spectrum of compound 9i (500 MHz, CDCl$_3$).

Figure S36. $^{13}$C NMR spectrum of compound 9i (125 MHz, CDCl$_3$).
Figure S37. $^1$H NMR spectrum of compound $9j$ (500 MHz, CDCl$_3$).

Figure S38. $^{13}$C NMR spectrum of compound $9j$ (125 MHz, CDCl$_3$).
Figure S39. $^1$H NMR spectrum of compound 9k (500 MHz, CDCl$_3$).

Figure S40. $^{13}$C NMR spectrum of compound 9k (125 MHz, CDCl$_3$).
Figure S41. $^1$H NMR spectrum of compound 91 (500 MHz, CDCl$_3$).

Figure S42. $^{13}$C NMR spectrum of compound 91 (125 MHz, CDCl$_3$).
Figure S43. $^1$H NMR spectrum of compound 10 (500 MHz, CDCl$_3$).

Figure S44. $^{13}$C NMR spectrum of compound 10 (125 MHz, CDCl$_3$).
Figure S45. $^1$H NMR spectrum of compound 11 (500 MHz, CDCl$_3$).

Figure S46. $^1$H NMR spectrum of compound 12a (500 MHz, (CD$_3$)$_2$CO).
Figure S47. $^{13}$C NMR spectrum of compound 12a (125 MHz, (CD$_3$)$_2$CO).

Figure S48. $^1$H NMR spectrum of mixture of compounds 12b and 12c (500 MHz, (CD$_3$)$_2$CO).
Figure S49. $^{13}$C NMR spectrum of mixture of compounds 12b and 12c (125 MHz, (CD$_3$)$_2$CO).

Figure S50. $^1$H NMR spectrum of mixture of compounds 12d and 12e (500 MHz, (CD$_3$)$_2$CO).
Figure S51. $^1$H NMR spectrum of compound 12f (500 MHz, (CD$_3$)$_2$CO).

Figure S52. $^{13}$C NMR spectrum of compound 12f (125 MHz, (CD$_3$)$_2$CO).
Figure S53. $^1$H NMR spectrum of compound 12g (500 MHz, (D$_3$)$_2$CO).

Figure S54. $^{13}$C NMR spectrum of compound 12g (125 MHz, (D$_3$)$_2$CO).
Figure S55. $^1$H NMR spectrum of compound **12h** (500 MHz, (CD$_3$)$_2$CO).

Figure S56. $^{13}$C NMR spectrum of compound **12h** (125 MHz, (CD$_3$)$_2$CO).
Figure S57. $^1$H NMR spectrum of compound 13 (500 MHz, CDCl$_3$).

Figure S58. $^{13}$C NMR spectrum of compound 13 (125 MHz, CDCl$_3$).
Figure S59. $^1$H NMR spectrum of compound 14 (500 MHz, CDCl$_3$).

Figure S60. $^{13}$C NMR spectrum of compound 14 (125 MHz, CDCl$_3$).
4. $^1$H, $^{15}$N and $^{13}$C NMR spectra of cations I, III, VIII in TfOH.

Figure S61. $^1$H NMR spectrum of cations I (400 MHz, TfOH).

Figure S62. $^{13}$C NMR spectrum of cations I (100 MHz, TfOH).
Figure S63. HSQC $^1$H-$^{15}$N NMR spectrum of cations I (400 MHz, TfOH).

Figure S64. HMBC $^1$H-$^{15}$N NMR spectrum of cations I (400 MHz, TfOH).
Figure S65. $^1$H NMR spectra of cations I (400 MHz, TfOH) and neutral initial compounds I (400 MHz, CDCl$_3$).

Figure S66. $^1$H NMR spectra of cations I (400 MHz, TfOH) and neutral initial compounds I (400 MHz, CDCl$_3$).
Figure S67. $^1$H NMR spectrum of cations III (400 MHz, TfOH).

Figure S68. $^{13}$C NMR spectrum of cations III (100 MHz, TfOH).
Figure S69. HSQC $^1$H-$^{15}$N NMR spectrum of cations III (400 MHz, TfOH).

Figure S70. $^1$H NMR spectrum of cations VIII (400 MHz, TfOH).
Figure S71. $^{13}$C NMR spectrum of cations VIII (100 MHz, TfOH).

Figure S72. HSQC $^1$H-$^{15}$N NMR spectrum of cations VIII (400 MHz, TfOH).
Figure S73. HMBC $^1$H-$^{15}$N NMR spectrum of cations VIII (400 MHz, TfOH).
5. Details of DFT-calculation of cations I–IX

**I q=0**

Energy $E = -494.369025175 \text{ h}$, $G^{298} = -494.250859 \text{ h}$, $\mu = 4.6 \text{ D}$

Cartesian coordinates, Å

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | -1.958250 | -1.339476 | -0.000028 |
| 2 | C    | -0.681328 | -0.776506 | 0.000018  |
| 3 | C    | -0.531873 | 0.621836  | 0.000070  |
| 4 | C    | -1.618320 | 1.491038  | 0.000051  |
| 5 | C    | -2.876726 | 0.913415  | -0.000050 |
| 6 | C    | -3.044340 | -0.481707 | -0.000088 |
| 7 | C    | 1.419549  | -0.398245 | 0.000068  |
| 8 | N    | 0.830898  | 0.827314  | 0.000114  |
| 9 | H    | -2.087499 | -2.412924 | -0.000072 |
|10 | H    | -1.486799 | 2.563543  | 0.000108  |
|11 | H    | -3.750540 | 1.549831  | -0.000103 |
|12 | H    | -4.045399 | -0.889595 | -0.000154 |
|13 | H    | 1.330352  | 1.701637  | 0.000357  |
|14 | N    | 0.565012  | -1.387048 | 0.000015  |
|15 | C    | 2.907023  | -0.544551 | 0.000102  |
|16 | H    | 3.204894  | -1.110633 | 0.885102  |
|17 | H    | 3.204778  | -1.111181 | -0.884595 |
|18 | O    | 3.467522  | 0.754168  | -0.000306 |
|19 | H    | 4.424270  | 0.679284  | 0.000045  |
## Summary of Natural Population Analysis:

| Natural Population |
|--------------------|

| Atom | No | Charge | Core | Valence | Rydberg | Total |
|------|----|--------|------|---------|---------|-------|
| C 1  | -0.21368 | 1.99902 | 4.19479 | 0.01987  | 6.21368  |
| C 2  | 0.11387  | 1.99888 | 3.86176 | 0.02549  | 5.88613  |
| C 3  | 0.12704  | 1.99890 | 3.85388 | 0.02017  | 5.87296  |
| C 4  | -0.23088 | 1.99903 | 4.21323 | 0.01862  | 6.23088  |
| C 5  | -0.21665 | 1.99916 | 4.19750 | 0.01998  | 6.21665  |
| C 6  | -0.22671 | 1.99916 | 4.20741 | 0.02014  | 6.22671  |
| C 7  | 0.44094  | 1.99924 | 3.53022 | 0.02961  | 5.55906  |
| N 8  | -0.56754 | 1.99920 | 5.55162 | 0.01672  | 7.56754  |
| H 9  | 0.21538  | 0.00000 | 0.78242 | 0.00220  | 0.78462  |
| H 10 | 0.22017  | 0.00000 | 0.77786 | 0.00197  | 0.77983  |
| H 11 | 0.21013  | 0.00000 | 0.78827 | 0.00160  | 0.78987  |
| H 12 | 0.20931  | 0.00000 | 0.78907 | 0.00161  | 0.79069  |
| H 13 | 0.44682  | 0.00000 | 0.55006 | 0.00312  | 0.55318  |
| N 14 | -0.58403 | 1.99934 | 5.54665 | 0.03804  | 7.58403  |
| C 15 | -0.05263 | 1.99909 | 4.03147 | 0.02207  | 6.05263  |
| H 16 | 0.19303  | 0.00000 | 0.80453 | 0.00243  | 0.80697  |
| H 17 | 0.19302  | 0.00000 | 0.80454 | 0.00243  | 0.80698  |
| O 18 | -0.77736 | 1.99978 | 6.76571 | 0.01187  | 8.77736  |
| H 19 | 0.49977  | 0.00000 | 0.49575 | 0.00448  | 0.50023  |

* Total * 0.00000  21.99080  55.74676  0.26244  78.00000
\( q = 2 \)

Energy \( E = -495.183537902 \ \text{h}, \quad G^{298} = -495.036881 \ \text{h}, \quad \mu = 18.8 \ \text{D} \)

Cartesian coordinates, Å

| N | atom | x          | y          | z          |
|---|------|------------|------------|------------|
| 1 | C    | 1.825647   | 1.454948   | -0.017676  |
| 2 | C    | 0.671538   | 0.684549   | 0.104551   |
| 3 | C    | 0.707708   | -0.711133  | 0.073487   |
| 4 | C    | 1.900445   | -1.414630  | -0.083083  |
| 5 | C    | 3.039736   | -0.651432  | -0.207366  |
| 6 | C    | 3.003136   | 0.758335   | -0.174231  |
| 7 | C    | -1.393834  | -0.071609  | 0.339654   |
| 8 | N    | -0.601180  | -1.131603  | 0.222848   |
| 9 | H    | 1.791176   | 2.533051   | 0.009506   |
|10 | H    | 1.923391   | -2.493274  | -0.107824  |
|11 | H    | 3.992160   | -1.144660  | -0.334656  |
|12 | H    | 3.928995   | 1.305217   | -0.275071  |
|13 | H    | -0.917699  | -2.093116  | 0.241177   |
|14 | N    | -0.655960  | 1.031539   | 0.275049   |
|15 | C    | -2.868296  | -0.115574  | 0.509080   |
|16 | H    | -3.218302  | -1.086731  | 0.840082   |
|17 | H    | -3.216943  | 0.672245   | 1.167605   |
|18 | O    | -3.487505  | 0.183489   | -0.808531  |
|19 | H    | -4.396514  | 0.533099   | -0.731289  |
|20 | H    | -3.483267  | -0.567699  | -1.433674  |
|21 | H    | -1.019461  | 1.973681   | 0.340625   |
**Summary of Natural Population Analysis:**

### Natural Population

| Atom No | Charge | Core     | Valence | Rydberg | Total       |
|---------|--------|----------|---------|---------|-------------|
| C 1     | -0.19950 | 1.99902  | 4.18238 | 0.01810 | 6.19950     |
| C 2     | 0.15815  | 1.99890  | 3.82308 | 0.01987 | 5.84185     |
| C 3     | 0.15473  | 1.99890  | 3.82639 | 0.01998 | 5.84527     |
| C 4     | -0.19796 | 1.99902  | 4.18088 | 0.01805 | 6.19796     |
| C 5     | -0.16938 | 1.99916  | 4.18038 | 0.01894 | 6.16938     |
| C 6     | -0.16766 | 1.99916  | 4.14958 | 0.01892 | 6.16766     |
| C 7     | 0.46045  | 1.99926  | 3.51624 | 0.02404 | 5.53955     |
| N 8     | -0.47236 | 1.99918  | 5.45761 | 0.01556 | 7.47236     |
| H 9     | 0.24228  | 0.00000  | 0.75599 | 0.00173 | 0.75772     |
| H 10    | 0.24235  | 0.00000  | 0.75593 | 0.00173 | 0.75765     |
| H 11    | 0.22744  | 0.00000  | 0.77109 | 0.00146 | 0.77256     |
| H 12    | 0.22745  | 0.00000  | 0.77108 | 0.00146 | 0.77255     |
| H 13    | 0.47681  | 0.00000  | 0.52076 | 0.00243 | 0.52319     |
| N 14    | -0.47602 | 1.99918  | 5.46103 | 0.01580 | 7.47602     |
| C 15    | -0.05970 | 1.99901  | 4.04144 | 0.01924 | 6.05970     |
| H 16    | 0.26203  | 0.00000  | 0.73646 | 0.00151 | 0.73797     |
| H 17    | 0.26943  | 0.00000  | 0.72892 | 0.00164 | 0.73057     |
| O 18    | -0.63686 | 1.99972  | 6.62783 | 0.00931 | 8.63686     |
| H 19    | 0.59256  | 0.00000  | 0.40464 | 0.00280 | 0.40744     |
| H 20    | 0.58930  | 0.00000  | 0.40784 | 0.00286 | 0.41070     |
| H 21    | 0.47645  | 0.00000  | 0.52110 | 0.00245 | 0.52355     |

* Total * | 2.00000 | 21.99053 | 55.79156 | 0.21791 | 78.00000
II q=2
Energy $E= -418.701138027 \text{ h}$, $G^{298} = -418.584651 \text{ h}$, $\mu = 7.3 \text{ D}$

Cartesian coordinates, Å

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | 1.355268 | 1.469278 | 0.000036 |
| 2 | C    | 0.151153  | 0.731472  | 0.000005  |
| 3 | C    | 0.151170  | -0.731480 | 0.000034  |
| 4 | C    | 1.355269  | -1.469268 | -0.000002 |
| 5 | C    | 2.488444  | -0.727421 | -0.000008 |
| 6 | C    | 2.488437  | 0.727432  | 0.000009  |
| 7 | C    | -1.946900 | -0.000012 | -0.000046 |
| 8 | N    | -1.111479 | -1.103515 | -0.000015 |
| 9 | H    | 1.352524  | 2.547545  | 0.000026  |
|10 | H    | 1.352513  | -2.547535 | -0.000027 |
|11 | H    | 3.447755  | -1.224138 | -0.000046 |
|12 | H    | 3.447744  | 1.224156  | -0.000006 |
|13 | H    | -1.450666 | -2.062259 | -0.000006 |
|14 | N    | -1.111510 | 1.103500  | -0.000039 |
|15 | C    | -3.288768 | 0.000000  | 0.000033  |
|16 | H    | -3.831398 | -0.934475 | 0.000141  |
|17 | H    | -3.831294 | 0.934547  | 0.000012  |
|18 | H    | -1.450688 | 2.062254  | -0.000086 |
### Summary of Natural Population Analysis:

| Atom | No | Charge | Core   | Valence | Rydberg | Total   |
|------|----|--------|--------|---------|---------|---------|
| C    | 1  | -0.22355 | 1.99901 | 4.20554 | 0.01900 | 6.22355 |
| C    | 2  | 0.31791  | 1.99908 | 3.66215 | 0.02086 | 5.68209 |
| C    | 3  | 0.31790  | 1.99908 | 3.66216 | 0.02086 | 5.68210 |
| C    | 4  | -0.22356 | 1.99901 | 4.20555 | 0.01900 | 6.22356 |
| C    | 5  | -0.05983 | 1.99915 | 4.04228 | 0.01840 | 5.68210 |
| C    | 6  | -0.05981 | 1.99915 | 4.04230 | 0.01840 | 5.68210 |
| C    | 7  | 0.31324  | 1.99919 | 3.66570 | 0.01218 | 5.68676 |
| N    | 8  | -0.42428 | 1.99916 | 5.40868 | 0.01645 | 7.42428 |
| H    | 9  | 0.26656  | 0.00000 | 0.73179 | 0.00166 | 0.73344 |
| H    | 10 | 0.26656  | 0.00000 | 0.73179 | 0.00166 | 0.73344 |
| H    | 11 | 0.24729  | 0.00000 | 0.75137 | 0.00135 | 0.75271 |
| H    | 12 | 0.24729  | 0.00000 | 0.75137 | 0.00135 | 0.75271 |
| H    | 13 | 0.49449  | 0.00000 | 0.50311 | 0.00239 | 0.50551 |
| N    | 14 | -0.42429 | 1.99916 | 5.40868 | 0.01645 | 7.42429 |
| C    | 15 | -0.06389 | 1.99910 | 4.05280 | 0.01199 | 6.06389 |
| H    | 16 | 0.25677  | 0.00000 | 0.74198 | 0.00125 | 0.74323 |
| H    | 17 | 0.25676  | 0.00000 | 0.74198 | 0.00125 | 0.74324 |
| H    | 18 | 0.49450  | 0.00000 | 0.50311 | 0.00239 | 0.50550 |

* Total *  2.00000  19.99108  47.81233  0.19658  68.00000
### III q=0

Energy $E = -533.66804816 \ h, \quad G^{298} = -533.523079 \ h, \quad \mu = 5.6 \ D$

Cartesian coordinates, Å

| N | atom | x       | y       | z       |
|---|------|---------|---------|---------|
| 1 | C    | -2.119462 | -1.457640 | -0.035984 |
| 2 | C    | -0.838698  | -0.910902 | 0.060796  |
| 3 | C    | -0.669609  | 0.483778  | 0.047751  |
| 4 | C    | -1.738993  | 1.369605  | -0.059872 |
| 5 | C    | -3.000855  | 0.807893  | -0.153016 |
| 6 | C    | -3.188517  | -0.585649 | -0.142323 |
| 7 | C    | 1.261281   | -0.548340 | 0.228043  |
| 8 | N    | 0.685842   | 0.689206  | 0.161574  |
| 9 | H    | -2.264470  | -2.529096 | -0.028059 |
|10 | H    | -1.593814  | 2.440782  | -0.070223 |
|11 | H    | -3.862666  | 1.455169  | -0.235878 |
|12 | H    | -4.191969  | -0.980084 | -0.219658 |
|13 | N    | 0.394478   | -1.530051 | 0.171987  |
|14 | C    | 2.736028   | -0.733890 | 0.355648  |
|15 | H    | 3.099085   | -0.223493 | 1.251908  |
|16 | H    | 2.924205   | -1.801581 | 0.462218  |
|17 | O    | 3.355538   | -0.204587 | -0.809078 |
|18 | H    | 4.307914   | -0.234962 | -0.685150 |
|19 | C    | 1.336752   | 1.985437  | 0.202564  |
|20 | H    | 0.879507   | 2.597646  | 0.977424  |
|21 | H    | 2.390064   | 1.850817  | 0.422837  |
|22 | H    | 1.238043   | 2.485660  | -0.759366 |

![Diagram of the molecule with distances labeled]
Summary of Natural Population Analysis:

Natural Population

| Atom No | Charge | Core   | Valence | Rydberg   | Total   |
|---------|--------|--------|---------|-----------|---------|
| C 1     | -0.20609 | 1.99902 | 4.18757 | 0.01950   | 6.20609 |
| C 2     | 0.11085  | 1.99888 | 3.86518 | 0.02509   | 5.88915 |
| C 3     | 0.14671  | 1.99891 | 3.83620 | 0.01819   | 5.85329 |
| C 4     | -0.23849 | 1.99904 | 4.22166 | 0.01779   | 6.23849 |
| C 5     | -0.20929 | 1.99917 | 4.19017 | 0.01995   | 6.20929 |
| C 6     | -0.22827 | 1.99916 | 4.20895 | 0.02016   | 6.22827 |
| C 7     | 0.44381  | 1.99918 | 3.52699 | 0.03002   | 5.55619 |
| N 8     | -0.43043 | 1.99912 | 5.41157 | 0.01975   | 7.43043 |
| H 9     | 0.21580  | 0.00000 | 0.78208 | 0.00211   | 0.78420 |
| H 10    | 0.22077  | 0.00000 | 0.77728 | 0.00195   | 0.77923 |
| H 11    | 0.21051  | 0.00000 | 0.78788 | 0.00161   | 0.78949 |
| H 12    | 0.20993  | 0.00000 | 0.78846 | 0.00161   | 0.79007 |
| N 13    | -0.56652 | 1.99936 | 5.52928 | 0.03788   | 7.56652 |
| C 14    | -0.06138 | 1.99906 | 4.04030 | 0.02202   | 6.06138 |
| H 15    | 0.18662  | 0.00000 | 0.81150 | 0.00188   | 0.81338 |
| H 16    | 0.19107  | 0.00000 | 0.80649 | 0.00244   | 0.80893 |
| O 17    | -0.77183 | 1.99978 | 6.75974 | 0.01231   | 8.77183 |
| H 18    | 0.49241  | 0.00000 | 0.50290 | 0.00468   | 0.50759 |
| C 19    | -0.35649 | 1.99931 | 4.34348 | 0.01370   | 6.35649 |
| H 20    | 0.20873  | 0.00000 | 0.78950 | 0.00177   | 0.79127 |
| H 21    | 0.22199  | 0.00000 | 0.77646 | 0.00155   | 0.77801 |
| H 22    | 0.20957  | 0.00000 | 0.78871 | 0.00172   | 0.79043 |

* Total *  0.00000  23.98998  61.73236  0.27766  86.00000
III q=2
Energy $E = -534.48468214 \text{ h}$, $G^{298} = -534.312749 \text{ h}$, $\mu = 18.2 \text{ D}$
Cartesian coordinates, Å

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | -2.010449 | -1.586263 |  0.033017 |
| 2 | C    | -0.812582  | -0.879379  |  0.113139 |
| 3 | C    | -0.770460  |  0.511850  |  0.025760 |
| 4 | C    | -1.922675  |  1.277065  | -0.143397 |
| 5 | C    | -3.107068  |  0.577616  | -0.221655 |
| 6 | C    | -3.149047  | -0.829338  | -0.135353 |
| 7 | C    |  1.288950  | -0.214712  |  0.302751 |
| 8 | N    |  0.559162  |  0.887024  |  0.142825 |
| 9 | H    | -2.039260  | -2.663049  |  0.100228 |
|10 | H    | -1.888837  |  2.354150  | -0.208128 |
|11 | H    | -4.032072  |  1.119269  | -0.352822 |
|12 | H    | -4.105398  | -1.326800  | -0.203850 |
|13 | N    |  0.493485  | -1.284957  |  0.288758 |
|14 | C    |  2.759562  | -0.289713  |  0.492497 |
|15 | H    |  3.205169  |  0.651478  |  0.787700 |
|16 | H    |  3.019223  | -1.068994  |  1.200112 |
|17 | O    |  3.374521  | -0.723134  | -0.789408 |
|18 | H    |  4.208723  | -1.215045  | -0.662530 |
|19 | H    |  3.517513  | -0.004729  | -1.435708 |
|20 | H    |  0.810340  | -2.239660  |  0.394177 |
|21 | C    |  0.997832  |  2.282637  |  0.101530 |
|22 | H    |  0.567137  |  2.805121  |  0.950662 |
|23 | H    |  2.078247  |  2.339220  |  0.143642 |
|24 | H    |  0.650141  |  2.721060  | -0.829040 |
Summary of Natural Population Analysis:

Natural Population

| Atom | No | Charge | Core   | Valence | Rydberg | Total   |
|------|----|--------|--------|---------|---------|---------|
| C    | 1  | -0.19821 | 1.99902 | 4.18128 | 0.01791 | 6.19821 |
| C    | 2  | 0.16170  | 1.99890 | 3.81929 | 0.02011 | 5.83830 |
| C    | 3  | 0.16590  | 1.99889 | 3.81704 | 0.01816 | 5.83410 |
| C    | 4  | -0.20505 | 1.99903 | 4.18789 | 0.01723 | 6.20505 |
| C    | 5  | -0.16882 | 1.99917 | 4.15061 | 0.01905 | 6.16882 |
| C    | 6  | -0.16781 | 1.99916 | 4.14968 | 0.01897 | 6.16781 |
| C    | 7  | 0.46685  | 1.99918 | 3.51095 | 0.02302 | 5.53315 |
| N    | 8  | -0.33843 | 1.99911 | 5.32334 | 0.01598 | 7.33843 |
| H    | 9  | 0.24168  | 0.00000 | 0.75659 | 0.00172 | 0.75832 |
| H    | 10 | 0.24109  | 0.00000 | 0.75724 | 0.00167 | 0.75891 |
| H    | 11 | 0.22727  | 0.00000 | 0.77126 | 0.00148 | 0.77273 |
| H    | 12 | 0.22712  | 0.00000 | 0.77142 | 0.00146 | 0.77288 |
| N    | 13 | -0.48089 | 1.99919 | 5.46573 | 0.01597 | 7.48089 |
| C    | 14 | -0.06105 | 1.99900 | 4.04295 | 0.01910 | 6.06105 |
| H    | 15 | 0.25811  | 0.00000 | 0.74041 | 0.00148 | 0.74189 |
| H    | 16 | 0.26973  | 0.00000 | 0.72861 | 0.00166 | 0.73027 |
| O    | 17 | -0.63773 | 1.99972 | 6.62860 | 0.00941 | 8.63773 |
| H    | 18 | 0.59238  | 0.00000 | 0.40484 | 0.00278 | 0.40762 |
| H    | 19 | 0.58971  | 0.00000 | 0.40748 | 0.00281 | 0.41029 |
| H    | 20 | 0.47404  | 0.00000 | 0.52353 | 0.00243 | 0.52596 |
| C    | 21 | -0.35841 | 1.99928 | 4.34623 | 0.01291 | 6.35841 |
| H    | 22 | 0.23672  | 0.00000 | 0.76194 | 0.00134 | 0.76328 |
| H    | 23 | 0.22742  | 0.00000 | 0.77133 | 0.00124 | 0.77258 |
| H    | 24 | 0.23666  | 0.00000 | 0.76199 | 0.00134 | 0.76334 |

* Total * 2.00000 23.98965 61.78111 0.22925 86.00000
IV  q=2  

Energy  $E= -458.006787024 \, \text{h}$,  $G^{298}= -457.863021 \, \text{h}$,  $\mu=5.3 \, \text{D}$

Cartesian coordinates, \( \text{Å} \)

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | -1.840493 | -1.405874 | -0.000218 |
| 2 | C    | -0.514482  | -0.921929  | -0.000158  |
| 3 | C    | -0.220276  | 0.511022   | 0.000081   |
| 4 | C    | -1.261962  | 1.471405   | 0.000347   |
| 5 | C    | -2.518512  | 0.970467   | 0.000232   |
| 6 | C    | -2.805693  | -0.455731  | -0.000095  |
| 7 | C    | 1.683779   | -0.621673  | -0.000093  |
| 8 | N    | 1.089773   | 0.640421   | -0.000005  |
| 9 | H    | -2.050752  | -2.463020  | -0.000214  |
|10 | H    | -1.060078  | 2.530137   | 0.000721   |
|11 | H    | -3.359817  | 1.647429   | 0.000441   |
|12 | H    | -3.844148  | -0.754107  | -0.000087  |
|13 | N    | 0.644404   | -1.540648  | -0.000118  |
|14 | C    | 2.996113   | -0.886136  | 0.000479   |
|15 | H    | 3.717488   | -0.081615  | 0.000689   |
|16 | H    | 3.349050   | -1.907327  | 0.000840   |
|17 | H    | 0.781997   | -2.547351  | -0.000237  |
|18 | C    | 1.854219   | 1.891421   | -0.000537  |
|19 | H    | 2.467437   | 1.921149   | 0.894837   |
|20 | H    | 2.467479   | 1.920418   | -0.895824  |
|21 | H    | 1.155966   | 2.718051   | -0.000530  |
### Summary of Natural Population Analysis:

#### Natural Population

| Atom No | Charge | Core      | Valence   | Rydberg   | Total     |
|--------|--------|-----------|-----------|-----------|-----------|
| C 1    | -0.22610 | 1.99901   | 4.20823   | 0.01886   | 6.22610   |
| C 2    | 0.32413   | 1.99908   | 3.65568   | 0.02111   | 5.67587   |
| C 3    | 0.32410   | 1.99902   | 3.65724   | 0.01964   | 5.67590   |
| C 4    | -0.22456  | 1.99901   | 4.20749   | 0.01806   | 6.22456   |
| C 5    | -0.06840  | 1.99915   | 4.05076   | 0.01849   | 6.06840   |
| C 6    | -0.05574  | 1.99915   | 4.03819   | 0.01840   | 6.05574   |
| C 7    | 0.32538   | 1.99912   | 3.65460   | 0.02090   | 5.67462   |
| N 8    | -0.28631  | 1.99909   | 5.27061   | 0.01661   | 7.28631   |
| H 9    | 0.26548   | 0.00000   | 0.73287   | 0.00166   | 0.73452   |
| H 10   | 0.26088   | 0.00000   | 0.73745   | 0.00167   | 0.73912   |
| H 11   | 0.24699   | 0.00000   | 0.75165   | 0.00136   | 0.75301   |
| H 12   | 0.24661   | 0.00000   | 0.75204   | 0.00135   | 0.75339   |
| N 13   | -0.43040  | 1.99915   | 5.41463   | 0.01662   | 7.43040   |
| C 14   | -0.08334  | 1.99909   | 4.07263   | 0.01162   | 6.08334   |
| H 15   | 0.25277   | 0.00000   | 0.74607   | 0.00116   | 0.74723   |
| H 16   | 0.25941   | 0.00000   | 0.73930   | 0.00129   | 0.74059   |
| H 17   | 0.49275   | 0.00000   | 0.50490   | 0.00235   | 0.50725   |
| C 18   | -0.36824  | 1.99927   | 4.35512   | 0.01385   | 6.36824   |
| H 19   | 0.25091   | 0.00000   | 0.74794   | 0.00115   | 0.74909   |
| H 20   | 0.25091   | 0.00000   | 0.74794   | 0.00115   | 0.74909   |
| H 21   | 0.24278   | 0.00000   | 0.75595   | 0.00127   | 0.75722   |

* Total * 2.00000 21.99015 53.80127 0.20858 76.00000
\[ \text{Energy} \quad E = -572.977907965 \text{ h}, \quad G^{298} = -572.806501 \text{ h}, \quad \mu = 5.4 \text{ D} \]

Cartesian coordinates, Å

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| 1    | 2.383886 | -1.481565 | -0.045499 |
| 2    | 1.111077 | -0.909491 | -0.056933 |
| 3    | 0.969061 | 0.486197  | -0.002088 |
| 4    | 2.059332 | 1.349853  | 0.066892 |
| 5    | 3.313911 | 0.763745  | 0.078681 |
| 6    | 3.474107 | -0.631690 | 0.023176 |
| 7    | -0.989695 | -0.504737 | -0.108382 |
| 8    | -0.387371 | 0.721397  | -0.037002 |
| 9    | 2.507538 | -2.554926 | -0.088881 |
| 10   | 1.936105 | 2.422898  | 0.112489 |
| 11   | 4.191198 | 1.393209  | 0.131488 |
| 12   | 4.472707 | -1.045324 | 0.034817 |
| 13   | -0.138059 | -1.501380 | -0.126253 |
| 14   | -2.476009 | -0.708196 | -0.104869 |
| 15   | -2.624151 | -1.768159 | -0.317815 |
| 16   | -3.030979 | 0.081448  | -1.151938 |
| 17   | -3.983707 | -0.048363 | -1.152183 |
| 18   | -0.989214 | 2.042801  | 0.028886 |
| 19   | -0.503648 | 2.692020  | -0.697370 |
| 20   | -2.041985 | 1.969895  | -0.214672 |
| 21   | -0.863339 | 2.463263  | 1.025636 |
| 22   | -3.092428 | -0.376088 | 1.248822 |
| 23   | -4.166199 | -0.560248 | 1.218931 |
| 24   | -2.658266 | -1.008237 | 2.022212 |
| 25   | -2.924580 | 0.667297  | 1.511528 |
### Summary of Natural Population Analysis:

#### Natural Population Analysis

| Atom | No  | Charge  | Core    | Valence | Rydberg | Total   |
|------|-----|---------|---------|---------|---------|---------|
| C    | 1   | -0.20704| 1.99902 | 4.18853 | 0.01949 | 6.20704 |
| C    | 2   | 0.11161 | 1.99887 | 3.86434 | 0.02517 | 5.88839 |
| C    | 3   | 0.14648 | 1.99890 | 3.83640 | 0.01822 | 5.85352 |
| C    | 4   | -0.23873| 1.99904 | 4.22196 | 0.01774 | 6.23873 |
| C    | 5   | -0.21069| 1.99917 | 4.19153 | 0.02000 | 6.21069 |
| C    | 6   | -0.22842| 1.99916 | 4.20909 | 0.02018 | 6.22842 |
| C    | 7   | 0.45514 | 1.99911 | 3.51267 | 0.03307 | 5.54486 |
| N    | 8   | -0.43316| 1.99911 | 5.41473 | 0.01931 | 7.43316 |
| H    | 9   | 0.21549 | 0.00000 | 0.78239 | 0.00213 | 0.78451 |
| H    | 10  | 0.22043 | 0.00000 | 0.77761 | 0.00196 | 0.77957 |
| H    | 11  | 0.21031 | 0.00000 | 0.78808 | 0.00161 | 0.78969 |
| H    | 12  | 0.20968 | 0.00000 | 0.78872 | 0.00161 | 0.79032 |
| N    | 13  | -0.56992| 1.99936 | 5.53293 | 0.03763 | 7.56992 |
| C    | 14  | 0.09492 | 1.99901 | 3.88059 | 0.02548 | 5.90508 |
| H    | 15  | 0.18955 | 0.00000 | 0.80759 | 0.00286 | 0.81045 |
| O    | 16  | -0.77781| 1.99977 | 6.76488 | 0.01316 | 8.77781 |
| H    | 17  | 0.49059 | 0.00000 | 0.50481 | 0.00460 | 0.50941 |
| C    | 18  | -0.36572| 1.99931 | 4.35286 | 0.01355 | 6.36572 |
| H    | 19  | 0.21024 | 0.00000 | 0.78800 | 0.00177 | 0.78976 |
| H    | 20  | 0.23197 | 0.00000 | 0.76638 | 0.00165 | 0.76803 |
| H    | 21  | 0.20617 | 0.00000 | 0.79221 | 0.00162 | 0.79383 |
| C    | 22  | -0.59641| 1.99928 | 4.58593 | 0.01120 | 6.59641 |
| H    | 23  | 0.21142 | 0.00000 | 0.78693 | 0.00165 | 0.78858 |
| H    | 24  | 0.21825 | 0.00000 | 0.78010 | 0.00165 | 0.78175 |
| H    | 25  | 0.20566 | 0.00000 | 0.79278 | 0.00156 | 0.79434 |

* Total *  0.00000  25.98911  67.71203  0.29886  94.00000
V \ q=2 
Energy \ E= -573.797055441 \ h, \ G^{298}= -573.59919 \ h, \ \mu=15.7 \ D

Cartesian coordinates, \ A

| N | atom | x       | y       | z       |
|---|------|---------|---------|---------|
| 1 | C    | -2.116991 | -1.683796 | -0.050505 |
| 2 | C    | -0.995716 | -0.859491 | -0.006556 |
| 3 | C    | -1.100821 | 0.530025  | 0.028462  |
| 4 | C    | -2.335553 | 1.175467  | 0.035345  |
| 5 | C    | -3.445979 | 0.359621  | -0.004754 |
| 6 | C    | -3.338181 | -1.044733 | -0.049102 |
| 7 | C    | 1.038926  | 0.007676  | 0.042057  |
| 8 | N    | 0.192766  | 1.034045  | 0.044122  |
| 9 | H    | -2.027851 | -2.758584 | -0.083558 |
| 10| H    | -2.419304 | 2.251028  | 0.073566  |
| 11| H    | -4.428472 | 0.807911  | -0.002012 |
| 12| H    | -4.241206 | -1.636466 | -0.080763 |
| 13| N    | 0.356394  | -1.137126 | 0.011903  |
| 14| C    | 2.529154  | 0.087912  | 0.095216  |
| 15| H    | 2.864311  | 1.117085  | 0.147753  |
| 16| O    | 3.002348  | -0.452504 | -1.230470 |
| 17| H    | 3.941300  | -0.722791 | -1.214958 |
| 18| H    | 2.852935  | 0.144024  | -1.990279 |
| 19| H    | 0.769932  | -2.059233 | -0.015295 |
| 20| C    | 0.495936  | 2.465696  | 0.075815  |
| 21| H    | 0.362791  | 2.838586  | 1.086898  |
| 22| H    | 1.509413  | 2.641930  | -0.262485 |
| 23| H    | -0.189358 | 2.962675  | -0.603413 |
| 24| C    | 3.145931  | -0.765771 | 1.173654  |
| 25| H    | 4.227366  | -0.651633 | 1.170737  |
| 26| H    | 2.769679  | -0.413293 | 2.131899  |
| 27| H    | 2.885328  | -1.815283 | 1.055706  |
**Summary of Natural Population Analysis:**

**Natural Population**

| Atom | No | Charge | Core | Valence | Rydberg | Total |
|------|----|--------|------|---------|---------|-------|
| C    |  1 | -0.19836 | 1.99902 | 4.18150 | 0.01784 | 6.19836 |
| C    |  2 |  0.16089 | 1.99889 | 3.81996 | 0.02025 | 5.83911 |
| C    |  3 |  0.16524 | 1.99889 | 3.81776 | 0.01811 | 5.83476 |
| C    |  4 | -0.20452 | 1.99903 | 4.18825 | 0.01725 | 6.20452 |
| C    |  5 | -0.17089 | 1.99917 | 4.15268 | 0.01904 | 6.17089 |
| C    |  6 | -0.16893 | 1.99916 | 4.15079 | 0.01898 | 6.16893 |
| C    |  7 |  0.47616 | 1.99912 | 3.49895 | 0.02577 | 5.52384 |
| N    |  8 | -0.34047 | 1.99910 | 5.32518 | 0.01618 | 7.34047 |
| H    |  9 |  0.24121 | 0.00000 | 0.75706 | 0.00173 | 0.75879 |
| H   | 10 |  0.24043 | 0.00000 | 0.75788 | 0.00169 | 0.75957 |
| H   | 11 |  0.22701 | 0.00000 | 0.77151 | 0.00148 | 0.77299 |
| H   | 12 |  0.22702 | 0.00000 | 0.77151 | 0.00147 | 0.77298 |
| N   | 13 | -0.48831 | 1.99918 | 5.47347 | 0.01565 | 7.48831 |
| C   | 14 |  0.11310 | 1.99897 | 3.86893 | 0.01900 | 5.88690 |
| H   | 15 |  0.25504 | 0.00000 | 0.74304 | 0.00192 | 0.74496 |
| O   | 16 | -0.65310 | 1.99973 | 6.64271 | 0.01066 | 8.65310 |
| H   | 17 |  0.58662 | 0.00000 | 0.41060 | 0.00278 | 0.41338 |
| H   | 18 |  0.58879 | 0.00000 | 0.40853 | 0.00268 | 0.41121 |
| H   | 19 |  0.47124 | 0.00000 | 0.52610 | 0.00266 | 0.52876 |
| C   | 20 | -0.35873 | 1.99928 | 4.34668 | 0.01277 | 6.35873 |
| H   | 21 |  0.23725 | 0.00000 | 0.76150 | 0.00124 | 0.76275 |
| H   | 22 |  0.22778 | 0.00000 | 0.77093 | 0.00129 | 0.77222 |
| H   | 23 |  0.23593 | 0.00000 | 0.76270 | 0.00137 | 0.76407 |
| C   | 24 | -0.61687 | 1.99926 | 4.60270 | 0.01492 | 6.61687 |
| H   | 25 |  0.24669 | 0.00000 | 0.75186 | 0.00146 | 0.75331 |
| H   | 26 |  0.26494 | 0.00000 | 0.73388 | 0.00118 | 0.73506 |
| H   | 27 |  0.23482 | 0.00000 | 0.76361 | 0.00156 | 0.76518 |

* Total * 2.00000 25.98879 67.76029 0.25093 94.00000
VI q=2
Energy $E = -497.328171971 \; \text{h}$, $G^{298} = -497.159717 \; \text{h}$, $\mu = 5.3 \; \text{D}$

Cartesian coordinates, Å

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | 1.820935 | -1.693335 | 0.004030 |
| 2 | C    | 0.663620 | -0.888949 | 0.003595 |
| 3 | C    | 0.736576 | 0.555123  | 0.000649 |
| 4 | C    | 1.983855 | 1.222709  | -0.005671 |
| 5 | C    | 3.079522 | 0.422860  | -0.006593 |
| 6 | C    | 3.000145 | -1.020367 | -0.001233 |
| 7 | C    | -1.387187 | -0.057718 | 0.004968 |
| 8 | N    | -0.511630 | 1.010218  | 0.004286 |
| 9 | H    | 1.754111 | -2.769300 | 0.007200 |
|10 | H    | 2.056717 | 2.298087  | -0.010075 |
|11 | H    | 4.061789 | 0.871669  | -0.011734 |
|12 | H    | 3.926947 | -1.575028 | -0.002166 |
|13 | N    | -0.624184 | -1.199418 | 0.004928 |
|14 | C    | -2.747644 | 0.029836  | 0.001819 |
|15 | H    | -3.163749 | 1.030882  | 0.010364 |
|16 | H    | -1.000728 | -2.141202 | 0.013485 |
|17 | C    | -0.925861 | 2.418549  | 0.002854 |
|18 | H    | -1.498649 | 2.615237  | -0.898329 |
|19 | H    | -1.514505 | 2.611960  | 0.894431 |
|20 | H    | -0.034303 | 3.031693  | 0.012315 |
|21 | C    | -3.680334 | -1.091378 | -0.011863 |
|22 | H    | -4.315180 | -1.008726 | 0.877565 |
|23 | H    | -4.361019 | -0.952741 | -0.857965 |
|24 | H    | -3.222498 | -2.072102 | -0.054915 |
Summary of Natural Population Analysis:

| Atom | No | Charge | Core   | Valence | Rydberg | Total   |
|------|----|--------|--------|---------|---------|---------|
| C    | 1  | -0.21894| 1.99902| 4.20140 | 0.01853 | 6.21894 |
| C    | 2  | 0.28990 | 1.99906| 3.69022 | 0.02082 | 5.71010 |
| C    | 3  | 0.28883 | 1.99900| 3.69299 | 0.01918 | 5.71117 |
| C    | 4  | -0.21781| 1.99902| 4.20100 | 0.01779 | 6.21781 |
| C    | 5  | -0.09083| 1.99916| 4.07311 | 0.01857 | 6.09083 |
| C    | 6  | -0.07882| 1.99916| 4.06116 | 0.01850 | 6.07882 |
| C    | 7  | 0.32883 | 1.99904| 3.65037 | 0.02175 | 5.67117 |
| N    | 8  | -0.28140| 1.99910| 5.26644 | 0.01586 | 7.28140 |
| H    | 9  | 0.26040 | 0.00000| 0.73794 | 0.00166 | 0.73960 |
| H    | 10 | 0.25594 | 0.00000| 0.74238 | 0.00168 | 0.74406 |
| H    | 11 | 0.24292 | 0.00000| 0.75570 | 0.00138 | 0.75708 |
| H    | 12 | 0.24268 | 0.00000| 0.75595 | 0.00137 | 0.75732 |
| N    | 13 | -0.43190| 1.99916| 5.41722 | 0.01551 | 7.43190 |
| C    | 14 | 0.14082 | 1.99910| 3.84718 | 0.01290 | 5.85918 |
| H    | 15 | 0.25321 | 0.00000| 0.74514 | 0.00165 | 0.74679 |
| H    | 16 | 0.48537 | 0.00000| 0.51199 | 0.00264 | 0.51463 |
| C    | 17 | -0.36918| 1.99927| 4.35608 | 0.01383 | 6.36918 |
| H    | 18 | 0.24871 | 0.00000| 0.75013 | 0.00116 | 0.75129 |
| H    | 19 | 0.24841 | 0.00000| 0.75042 | 0.00116 | 0.75159 |
| H    | 20 | 0.24169 | 0.00000| 0.75702 | 0.00129 | 0.75831 |
| C    | 21 | -0.65066| 1.99925| 4.63835 | 0.01306 | 6.65066 |
| H    | 22 | 0.29071 | 0.00000| 0.70791 | 0.00137 | 0.70929 |
| H    | 23 | 0.28810 | 0.00000| 0.71054 | 0.00136 | 0.71190 |
| H    | 24 | 0.23301 | 0.00000| 0.76553 | 0.00146 | 0.76699 |

* Total * 2.00000 23.98932 59.78618 0.22449 84.00000
VII  q=0
Energy  $E = -533.659161533 \, \text{h}$,  $G^{298} = -533.514487 \, \text{h}$,  $\mu = 4.7 \, \text{D}$

Cartesian coordinates, Å

| N | atom | x           | y           | z           |
|---|------|-------------|-------------|-------------|
| 1 | C    | -2.501009   | -1.276892   | 0.000307    |
| 2 | C    | -1.196917   | -0.779874   | 0.000043    |
| 3 | C    | -0.976298   | 0.609044    | -0.000223   |
| 4 | C    | -2.016719   | 1.532544    | -0.000186   |
| 5 | C    | -3.302877   | 1.020118    | 0.000081    |
| 6 | C    | -3.541658   | -0.364814   | 0.000310    |
| 7 | C    | 0.920382    | -0.509137   | -0.000346   |
| 8 | N    | 0.395332    | 0.744893    | -0.000403   |
| 9 | H    | -2.684450   | -2.342405   | 0.000517    |
|10 | H    | -1.831136   | 2.596994    | -0.000351   |
|11 | H    | -4.143042   | 1.700135    | 0.000119    |
|12 | H    | -4.562154   | -0.721462   | 0.000524    |
|13 | H    | 0.940073    | 1.592008    | -0.000518   |
|14 | N    | 0.016806    | -1.453104   | 0.000062    |
|15 | C    | 2.398468    | -0.729503   | -0.000753   |
|16 | H    | 2.678352    | -1.311783   | 0.883481    |
|17 | H    | 2.678198    | -1.309451   | -0.886602   |
|18 | O    | 3.032680    | 0.524704    | 0.000751    |
|19 | C    | 4.442628    | 0.401252    | 0.000425    |
|20 | H    | 4.783378    | -0.134534   | 0.889885    |
|21 | H    | 4.783320    | -0.131868   | -0.890650   |
|22 | H    | 4.855057    | 1.405781    | 0.002020    |
### Summary of Natural Population Analysis:

#### Natural Population

| Atom | No | Charge  | Core      | Valence  | Rydberg  | Total    |
|------|----|---------|-----------|----------|----------|----------|
| C    |  1 | -0.21319| 1.99902   | 4.19442  | 0.01975  | 6.21319  |
| C    |  2 |  0.11461| 1.99888   | 3.86153  | 0.02499  | 5.88539  |
| C    |  3 |  0.12821| 1.99890   | 3.85364  | 0.01925  | 5.87179  |
| C    |  4 | -0.23038| 1.99903   | 4.21317  | 0.01819  | 6.23038  |
| C    |  5 | -0.21574| 1.99916   | 4.19683  | 0.01975  | 6.21574  |
| C    |  6 | -0.22658| 1.99916   | 4.20732  | 0.02010  | 6.22658  |
| C    |  7 |  0.44192| 1.99923   | 3.52989  | 0.02896  | 5.55808  |
| N    |  8 | -0.57162| 1.99920   | 5.55235  | 0.02007  | 7.57162  |
| H    |  9 |  0.21548| 0.00000   | 0.78236  | 0.00217  | 0.78452  |
| H    | 10 |  0.22032| 0.00000   | 0.77778  | 0.00189  | 0.77968  |
| H    | 11 |  0.21009| 0.00000   | 0.78830  | 0.00161  | 0.78991  |
| H    | 12 |  0.20937| 0.00000   | 0.78902  | 0.00161  | 0.79063  |
| H    | 13 |  0.44693| 0.00000   | 0.55037  | 0.00271  | 0.55307  |
| N    | 14 | -0.58202| 1.99934   | 5.54547  | 0.03720  | 7.58202  |
| C    | 15 | -0.04886| 1.99908   | 4.02897  | 0.02082  | 6.04886  |
| H    | 16 |  0.19470| 0.00000   | 0.80284  | 0.00246  | 0.80530  |
| H    | 17 |  0.19470| 0.00000   | 0.80285  | 0.00246  | 0.80530  |
| O    | 18 | -0.62303| 1.99976   | 6.60459  | 0.01868  | 8.62303  |
| C    | 19 | -0.19123| 1.99925   | 4.17656  | 0.01542  | 6.19123  |
| H    | 20 |  0.16796| 0.00000   | 0.82973  | 0.00231  | 0.83204  |
| H    | 21 |  0.16797| 0.00000   | 0.82972  | 0.00231  | 0.83203  |
| H    | 22 |  0.19040| 0.00000   | 0.80829  | 0.00131  | 0.80960  |

* Total * 0.00000 23.99001 61.72597 0.28401 86.00000
VII q=1

Energy $E = -534.10265871 \text{ h}$, $G_{298} = -533.944512 \text{ h}$, $\mu = 4.3 \text{ D}$

Cartesian coordinates, \AA

| N | atom | x       | y       | z       |
|---|------|---------|---------|---------|
| 1 | C    | -1.994322 | -1.557197 | 0.000073 |
| 2 | C    | -0.978950 | -0.609604 | 0.000043 |
| 3 | C    | -1.247277 | 0.758728  | -0.000063|
| 4 | C    | -2.546023 | 1.250847  | -0.000162|
| 5 | C    | -3.557728 | 0.309119  | -0.000147|
| 6 | C    | -3.287356 | -1.069459 | -0.000021|
| 7 | C    | 0.953576  | 0.478376  | 0.000146 |
| 8 | N    | -0.008937 | 1.394119  | 0.000045 |
| 9 | H    | -1.780259 | -2.615157 | 0.000179 |
| 10| H    | -2.750379 | 2.310511  | -0.000257|
| 11| H    | -4.585278 | 0.642342  | -0.000210|
| 12| H    | -4.112976 | -1.765778 | 0.000021 |
| 13| H    | 0.150281  | 2.390974  | -0.000246|
| 14| N    | 0.406170  | -0.727669 | 0.000163 |
| 15| C    | 2.423798  | 0.717704  | 0.000387 |
| 16| H    | 2.690848  | 1.301897  | -0.886711|
| 17| H    | 2.690672  | 1.301118  | 0.888055 |
| 18| O    | 3.030891  | -0.540978 | -0.000066|
| 19| C    | 4.448741  | -0.448119 | -0.000361|
| 20| H    | 4.796750  | 0.076558  | -0.892110|
| 21| H    | 4.797139  | 0.076646  | 0.891186 |
| 22| H    | 4.830552  | -1.463688 | -0.000381|
| 23| H    | 0.958134  | -1.575114 | 0.000176 |
### Summary of Natural Population Analysis:

| Atom No | Charge | Core     | Valence | Rydberg | Total    |
|---------|--------|----------|---------|---------|----------|
| C 1     | -0.20276 | 1.99902  | 4.18572 | 0.01802 | 6.20276  |
| C 2     | 0.14340  | 1.99888  | 3.83784 | 0.01988 | 5.85660  |
| C 3     | 0.14803  | 1.99888  | 3.83324 | 0.01985 | 5.85197  |
| C 4     | -0.20592 | 1.99902  | 4.18872 | 0.01817 | 6.20592  |
| C 5     | -0.18496 | 1.99916  | 3.83324 | 0.01985 | 5.85197  |
| C 6     | -0.18716 | 1.99916  | 3.83324 | 0.01985 | 5.85197  |
| C 7     | 0.53940  | 1.99926  | 3.43718 | 0.02416 | 5.46060  |
| N 8     | -0.51169 | 1.99918  | 5.49739 | 0.01512 | 7.51169  |
| H 9     | 0.23636  | 0.00000  | 0.76188 | 0.00176 | 0.76364  |
| H 10    | 0.23635  | 0.00000  | 0.76188 | 0.00177 | 0.76365  |
| H 11    | 0.22251  | 0.00000  | 0.77600 | 0.00149 | 0.77749  |
| H 12    | 0.22251  | 0.00000  | 0.77599 | 0.00150 | 0.77749  |
| H 13    | 0.46631  | 0.00000  | 0.53133 | 0.00236 | 0.53369  |
| N 14    | -0.50684 | 1.99917  | 5.49124 | 0.01644 | 7.50684  |
| C 15    | -0.05934 | 1.99908  | 4.03922 | 0.02104 | 6.05934  |
| H 16    | 0.21788  | 0.00000  | 0.77974 | 0.00238 | 0.78212  |
| H 17    | 0.21789  | 0.00000  | 0.77973 | 0.00238 | 0.78211  |
| O 18    | -0.61680 | 1.99976  | 6.59833 | 0.01870 | 8.61680  |
| C 19    | -0.19242 | 1.99924  | 4.17799 | 0.01519 | 6.19242  |
| H 20    | 0.17413  | 0.00000  | 0.82378 | 0.00209 | 0.82587  |
| H 21    | 0.17413  | 0.00000  | 0.82378 | 0.00209 | 0.82587  |
| H 22    | 0.19680  | 0.00000  | 0.80198 | 0.00121 | 0.80320  |
| H 23    | 0.47219  | 0.00000  | 0.52506 | 0.00275 | 0.52781  |

* Total * 1.00000 23.98983 61.76358 0.24659 86.00000
VII q=2
Energy E = -534.47886956 h, G^298 = -534.307497 h, μ = 15.7 D

Cartesian coordinates, Å

| N | atom | x     | y     | z     |
|---|------|-------|-------|-------|
| 1 | C    | -2.469728 | -1.330548 | -0.183826 |
| 2 | C    | -1.231910 | -0.728133 | 0.029489  |
| 3 | C    | -1.093980 | 0.656919  | 0.138074  |
| 4 | C    | -2.184340 | 1.517356  | 0.035301  |
| 5 | C    | -3.407431 | 0.920374  | -0.178085 |
| 6 | C    | -3.547548 | -0.478601 | -0.285283 |
| 7 | C    | 0.903819  | -0.263184 | 0.373763  |
| 8 | N    | 0.251462  | 0.893792  | 0.357506  |
| 9 | H    | -2.571974 | -2.401814 | -0.264142 |
|10 | H    | -2.070041 | 2.587058  | 0.121214  |
|11 | H    | -4.287465 | 1.540750  | -0.262987 |
|12 | H    | -4.531046 | -0.893430 | -0.450162 |
|13 | H    | 0.680508  | 1.801180  | 0.484350  |
|14 | N    | 0.040115  | -1.252460 | 0.177173  |
|15 | C    | 2.363200  | -0.433122 | 0.597192  |
|16 | H    | 2.702536  | 0.160851  | 1.439959  |
|17 | H    | 2.635131  | -1.476160 | 0.726640  |
|18 | O    | 3.078211  | 0.112268  | -0.565191 |
|19 | C    | 4.520335  | 0.397089  | -0.342403 |
|20 | H    | 4.540075  | 1.189401  | 0.395006  |
|21 | H    | 4.996472  | -0.514240 | 0.000349  |
|22 | H    | 4.893951  | 0.730762  | -1.301501 |
|23 | H    | 0.287766  | -2.233525 | 0.150620  |
|24 | H    | 2.942858  | -0.427193 | -1.365896 |
Summary of Natural Population Analysis:

| Atom | No | Charge  | Core    | Valence | Rydberg | Total   |
|------|----|---------|---------|---------|---------|---------|
| C    |  1 | -0.19754| 1.99902 | 4.18049 | 0.01803 | 6.19754 |
| C    |  2 |  0.15306| 1.99889 | 3.82809 | 0.01996 | 5.84694 |
| C    |  3 |  0.15773| 1.99890 | 3.82353 | 0.01984 | 5.84227 |
| C    |  4 | -0.19999| 1.99902 | 4.18288 | 0.01809 | 6.19999 |
| C    |  5 | -0.16875| 1.99916 | 4.15068 | 0.01891 | 6.16875 |
| C    |  6 | -0.17133| 1.99916 | 4.15323 | 0.01894 | 6.17133 |
| C    |  7 |  0.46618| 1.99926 | 3.50995 | 0.02460 | 5.53382 |
| N    |  8 | -0.47981| 1.99918 | 5.46430 | 0.01633 | 7.47981 |
| H    |  9 |  0.24186| 0.00000 | 0.75642 | 0.00173 | 0.75814 |
| H   | 10 |  0.24181| 0.00000 | 0.75646 | 0.00173 | 0.75819 |
| H   | 11 |  0.22719| 0.00000 | 0.77134 | 0.00146 | 0.77281 |
| H   | 12 |  0.22718| 0.00000 | 0.77135 | 0.00147 | 0.77282 |
| H   | 13 |  0.47545| 0.00000 | 0.52196 | 0.00259 | 0.52455 |
| N   | 14 | -0.47304| 1.99918 | 5.45826 | 0.01560 | 7.47304 |
| C   | 15 | -0.06018| 1.99902 | 4.04234 | 0.01882 | 6.06018 |
| H   | 16 |  0.26457| 0.00000 | 0.73365 | 0.00178 | 0.73543 |
| H   | 17 |  0.25838| 0.00000 | 0.74006 | 0.00156 | 0.74162 |
| O   | 18 | -0.51446| 1.99974 | 6.50356 | 0.01117 | 8.51446 |
| C   | 19 | -0.18455| 1.99921 | 4.17501 | 0.01034 | 6.18455 |
| H   | 20 |  0.22595| 0.00000 | 0.77294 | 0.00112 | 0.77405 |
| H   | 21 |  0.22006| 0.00000 | 0.77883 | 0.00110 | 0.77994 |
| H   | 22 |  0.23612| 0.00000 | 0.76282 | 0.00106 | 0.76388 |
| H   | 23 |  0.47602| 0.00000 | 0.52157 | 0.00241 | 0.52398 |
| H   | 24 |  0.57810| 0.00000 | 0.41888 | 0.00302 | 0.42190 |

* Total * 2.00000 23.98976 61.77859 0.23166 86.00000
VIII \( q=0 \)
Energy \( E= -532.452416636 \) h, \( G^{298}= -532.331442 \) h, \( \mu=8.3 \) D

Cartesian coordinates, Å

| N | atom | x      | y      | z      |
|---|------|--------|--------|--------|
| 1 | C    | -1.824239 | -1.606975 | 0.000002 |
| 2 | C    | -0.625538  | -0.879619  | -0.000019 |
| 3 | C    | -0.652233  | 0.529619   | -0.000032 |
| 4 | C    | -1.849850  | 1.251989   | 0.000000 |
| 5 | C    | -3.014376  | 0.514778   | 0.000023 |
| 6 | C    | -3.004088  | -0.897889  | 0.000017 |
| 7 | C    | 1.400240   | -0.232574  | -0.000039 |
| 8 | N    | 0.661104   | 0.920616   | -0.000038 |
| 9 | H    | -1.809721  | -2.687695  | 0.000011 |
|10 | H    | -1.871253  | 2.331903   | 0.000042 |
|11 | H    | -3.963869  | 1.031158   | 0.000054 |
|12 | H    | -3.946495  | -1.426784  | 0.000029 |
|13 | N    | 0.671562   | -1.325539  | -0.000022 |
|14 | C    | 2.876019   | -0.209435  | 0.000000 |
|15 | O    | 3.544967   | -1.212102  | 0.000049 |
|16 | H    | 3.343515   | 0.785971   | -0.000026 |
|17 | C    | 1.154691   | 2.291823   | 0.000026 |
|18 | H    | 1.747386   | 2.483151   | 0.890901 |
|19 | H    | 1.747730   | 2.483077   | -0.890633 |
|20 | H    | 0.300558   | 2.960202   | -0.000220 |
### Summary of Natural Population Analysis:

| Atom No | Charge   | Core        | Valence | Rydberg | Total     |
|---------|----------|-------------|---------|---------|-----------|
| C 1     | -0.19542 | 1.99902     | 4.17700 | 0.01940 | 6.19542   |
| C 2     | 0.11351  | 1.99890     | 3.86247 | 0.02512 | 5.88649   |
| C 3     | 0.16494  | 1.99891     | 3.81744 | 0.01871 | 5.83506   |
| C 4     | -0.23625 | 1.99903     | 4.21926 | 0.01796 | 6.23625   |
| C 5     | -0.18913 | 1.99917     | 4.17036 | 0.01961 | 6.18913   |
| C 6     | -0.21797 | 1.99916     | 4.19886 | 0.01995 | 6.21797   |
| C 7     | 0.31025  | 1.99915     | 3.66320 | 0.02740 | 5.68975   |
| N 8     | -0.40132 | 1.99914     | 5.38531 | 0.01687 | 7.40132   |
| H 9     | 0.22055  | 0.00000     | 0.77739 | 0.00206 | 0.77945   |
| H 10    | 0.22314  | 0.00000     | 0.77486 | 0.00200 | 0.77686   |
| H 11    | 0.21426  | 0.00000     | 0.78419 | 0.00156 | 0.78574   |
| H 12    | 0.21381  | 0.00000     | 0.78461 | 0.00158 | 0.78619   |
| N 13    | -0.50346 | 1.99936     | 5.46727 | 0.03682 | 7.50346   |
| C 14    | 0.43133  | 1.99938     | 3.53856 | 0.03073 | 5.56867   |
| O 15    | -0.57115 | 1.99976     | 6.54369 | 0.02770 | 8.57115   |
| H 16    | 0.12962  | 0.00000     | 0.86848 | 0.00190 | 0.87038   |
| C 17    | -0.36302 | 1.99930     | 4.34990 | 0.01382 | 6.36302   |
| H 18    | 0.21771  | 0.00000     | 0.78089 | 0.00140 | 0.78229   |
| H 19    | 0.21771  | 0.00000     | 0.78089 | 0.00140 | 0.78229   |
| H 20    | 0.22089  | 0.00000     | 0.77763 | 0.00148 | 0.77911   |

* Total * | 0.00000 | 23.99029 | 59.72224 | 0.28747 | 84.00000
VIII $q=2$
Energy $E = -533.261671252 \text{ h, } \ G^{298} = -533.113079 \text{ h, } \mu = 10.7 \text{ D}$

Cartesian coordinates, Å

| N | atom | x             | y             | z             |
|---|------|---------------|---------------|---------------|
| 1 | C    | -1.816222     | -1.663875     | -0.006540     |
| 2 | C    | -0.653213     | -0.878650     | -0.006052     |
| 3 | C    | -0.706333     | 0.541687      | -0.002900     |
| 4 | C    | -1.930752     | 1.233197      | 0.011137      |
| 5 | C    | -3.051111     | 0.454491      | 0.013755      |
| 6 | C    | -2.994608     | -0.974921     | 0.002071      |
| 7 | C    | 1.394800      | -0.079231     | -0.012353     |
| 8 | N    | 0.568816      | 0.991347      | -0.015220     |
| 9 | H    | -1.766524     | -2.741012     | -0.013688     |
|10 | H    | -1.977049     | 2.310653      | 0.025776      |
|11 | H    | -4.022269     | 0.926621      | 0.026244      |
|12 | H    | -3.925625     | -1.522298     | 0.001435      |
|13 | N    | 0.653060      | -1.207371     | -0.010179     |
|14 | C    | 2.800063      | -0.049740     | 0.006411      |
|15 | O    | 3.406452      | -1.160878     | 0.016457      |
|16 | H    | 3.349836      | 0.884953      | 0.016583      |
|17 | C    | 0.956649      | 2.406812      | -0.004646     |
|18 | H    | 0.949614      | 2.763113      | 1.021184      |
|19 | H    | 1.938583      | 2.520506      | -0.447269     |
|20 | H    | 0.235596      | 2.950730      | -0.605122     |
|21 | H    | 1.040100      | -2.145300     | -0.013614     |
|22 | H    | 4.377351      | -1.087383     | 0.029301      |
Summary of Natural Population Analysis:

| Atom | No | Charge | Core   | Valence | Rydberg | Total   |
|------|----|--------|--------|---------|---------|---------|
| C    | 1  | -0.20835 | 1.99902 | 4.19108 | 0.01825 | 6.20835 |
| C    | 2  | 0.23986  | 1.99900 | 3.74072 | 0.02041 | 5.76014 |
| C    | 3  | 0.23676  | 1.99897 | 3.74541 | 0.01886 | 5.76324 |
| C    | 4  | -0.21018 | 1.99902 | 4.19370 | 0.01745 | 6.21018 |
| C    | 5  | -0.11796 | 1.99916 | 4.10005 | 0.01875 | 6.11796 |
| C    | 6  | -0.10939 | 1.99916 | 4.09161 | 0.01861 | 6.10939 |
| C    | 7  | 0.32529  | 1.99918 | 3.65231 | 0.02322 | 5.67471 |
| N    | 8  | -0.28903 | 1.99912 | 5.27400 | 0.01592 | 7.28903 |
| H    | 9  | 0.25465  | 0.00000 | 0.74368 | 0.00167 | 0.74535 |
| H    | 10 | 0.25265  | 0.00000 | 0.74570 | 0.00165 | 0.74735 |
| H    | 11 | 0.23809  | 0.00000 | 0.76050 | 0.00141 | 0.76191 |
| H    | 12 | 0.23797  | 0.00000 | 0.76063 | 0.00140 | 0.76203 |
| N    | 13 | -0.44039 | 1.99918 | 5.42517 | 0.01604 | 7.44039 |
| C    | 14 | 0.46513  | 1.99919 | 3.51389 | 0.02179 | 5.53487 |
| O    | 15 | -0.54461 | 1.99969 | 6.52146 | 0.02346 | 8.54611 |
| H    | 16 | 0.24736  | 0.00000 | 0.75136 | 0.00128 | 0.75264 |
| C    | 17 | -0.36320 | 1.99927 | 4.35071 | 0.01321 | 6.36320 |
| H    | 18 | 0.24945  | 0.00000 | 0.74942 | 0.00113 | 0.75055 |
| H    | 19 | 0.23578  | 0.00000 | 0.76293 | 0.00129 | 0.76422 |
| H    | 20 | 0.24430  | 0.00000 | 0.75442 | 0.00128 | 0.75570 |
| H    | 21 | 0.48783  | 0.00000 | 0.50958 | 0.00258 | 0.51217 |
| H    | 22 | 0.56797  | 0.00000 | 0.42961 | 0.00242 | 0.43203 |

* Total *

2.00000  23.98998  59.76795  0.24208  84.00000
**IX q=0**

Energy $E = -571.774355517 \ h$, $G^{298} = -571.627163 \ h$, $\mu = 2.5 \ D$

Cartesian coordinates, Å

| N | atom | x      | y      | z      |
|---|------|--------|--------|--------|
| 1 | C    | 2.126345 | -1.614131 | -0.002087 |
| 2 | C    | 0.933311 | -0.879894 | -0.000702 |
| 3 | C    | 0.965193 | 0.527392  | 0.001001  |
| 4 | C    | 2.166966 | 1.241857  | 0.000881  |
| 5 | C    | 3.329108 | 0.498749  | -0.000505 |
| 6 | C    | 3.311917 | -0.912385 | -0.001873 |
| 7 | C    | -1.093181 | -0.218652 | 0.000478  |
| 8 | N    | -0.347516 | 0.929636  | 0.002255  |
| 9 | H    | 2.105467 | -2.694863 | -0.003313 |
|10 | H    | 2.195607 | 2.321566  | 0.000910  |
|11 | H    | 4.280767 | 1.011285  | -0.000932 |
|12 | H    | 4.251069 | -1.447081 | -0.002998 |
|13 | N    | -0.369070 | -1.315758 | -0.000686 |
|14 | C    | -2.578999 | -0.232221 | -0.002434 |
|15 | O    | -3.205059 | 0.805744  | -0.013828 |
|16 | C    | -0.809302 | 2.311627  | 0.006061  |
|17 | H    | -1.379309 | 2.521928  | -0.893811 |
|18 | H    | -1.433563 | 2.497225  | 0.874377  |
|19 | H    | 0.063460  | 2.955394  | 0.041267  |
|20 | C    | -3.232550 | -1.582196 | 0.008049  |
|21 | H    | -2.913707 | -2.140680 | 0.887342  |
|22 | H    | -4.310386 | -1.456142 | 0.007960  |
|23 | H    | -2.915680 | -2.152602 | -0.864375 |
Summary of Natural Population Analysis:

| Atom No | Charge   | Core      | Valence | Rydberg | Total   |
|---------|----------|-----------|---------|---------|---------|
| C 1     | -0.19626 | 1.99902   | 4.17789 | 0.01934 | 6.19626 |
| C 2     | 0.10871  | 1.99890   | 3.86706 | 0.02533 | 5.89129 |
| C 3     | 0.16365  | 1.99890   | 3.81919 | 0.01825 | 5.83635 |
| C 4     | -0.23705 | 1.99903   | 4.22027 | 0.01775 | 6.23705 |
| C 5     | -0.19336 | 1.99917   | 4.17452 | 0.01968 | 6.19336 |
| C 6     | -0.22244 | 1.99915   | 4.20329 | 0.01999 | 6.22244 |
| C 7     | 0.33261  | 1.99907   | 3.64016 | 0.02816 | 5.66739 |
| N 8     | -0.40250 | 1.99913   | 5.38532 | 0.01805 | 7.40250 |
| H 9     | 0.21909  | 0.00000   | 0.77884 | 0.00207 | 0.78091 |
| H 10    | 0.22161  | 0.00000   | 0.77639 | 0.00200 | 0.77839 |
| H 11    | 0.21308  | 0.00000   | 0.78536 | 0.00156 | 0.78692 |
| H 12    | 0.21269  | 0.00000   | 0.78572 | 0.00158 | 0.78731 |
| N 13    | -0.51708 | 1.99937   | 5.48374 | 0.03397 | 7.51708 |
| C 14    | 0.58144  | 1.99926   | 3.38864 | 0.03065 | 5.41856 |
| O 15    | -0.61153 | 1.99975   | 6.58328 | 0.02849 | 8.61153 |
| C 16    | -0.34685 | 1.99930   | 4.33398 | 0.01356 | 6.34685 |
| H 17    | 0.21694  | 0.00000   | 0.78151 | 0.00155 | 0.78306 |
| H 18    | 0.21845  | 0.00000   | 0.78001 | 0.00154 | 0.78155 |
| H 19    | 0.20711  | 0.00000   | 0.79135 | 0.00154 | 0.79289 |
| C 20    | -0.67010 | 1.99924   | 4.65889 | 0.01197 | 6.67010 |
| H 21    | 0.23988  | 0.00000   | 0.75841 | 0.00171 | 0.76012 |
| H 22    | 0.22172  | 0.00000   | 0.77618 | 0.00210 | 0.77828 |
| H 23    | 0.24019  | 0.00000   | 0.75810 | 0.00171 | 0.75981 |

* Total * 0.00000 25.98932 65.70811 0.30257 92.00000
IX q=2
Energy $E = -572.586361722 \text{ h}$, $G^{298} = -572.41236 \text{ h}$, $\mu = 10.7 \text{ D}$

Cartesian coordinates, Å

| N | atom | x        | y        | z        |
|---|------|----------|----------|----------|
| 1 | C    | -2.215999| -1.606015| 0.000046 |
| 2 | C    | -1.019142| -0.876566| -0.000157|
| 3 | C    | -0.996784| 0.534877 | -0.000140|
| 4 | C    | -2.186162| 1.281601 | -0.000048|
| 5 | C    | -3.347958| 0.559966 | 0.000157 |
| 6 | C    | -3.364235| -0.864126| 0.000232 |
| 7 | C    | 1.075244 | -0.192718| -0.000274|
| 8 | N    | 0.312819 | 0.918664 | -0.000092|
| 9 | H    | -2.217699| -2.684887| 0.000037 |
|10 | H    | -2.190719| 2.359594 | -0.000162|
|11 | H    | -4.291776| 1.084735 | 0.000279 |
|12 | H    | -4.319330| -1.368267| 0.000431 |
|13 | N    | 0.275715 | -1.274519| -0.000263|
|14 | C    | 2.506845 | -0.279148| 0.000032 |
|15 | O    | 3.122778 | 0.830108 | 0.000125 |
|16 | C    | 0.778008 | 2.312842 | 0.000014 |
|17 | H    | 1.368170 | 2.493032 | 0.892328 |
|18 | H    | 1.366649 | 2.493666 | -0.893179|
|19 | H    | -0.097293| 2.948725 | 0.000961 |
|20 | H    | 0.592674 | -2.236631| -0.000816|
|21 | H    | 4.093590 | 0.741852 | 0.000355 |
|22 | C    | 3.193154 | -1.578109| 0.000236 |
|23 | H    | 2.893445 | -2.144942| -0.884934|
|24 | H    | 4.270230 | -1.447066| 0.000831 |
|25 | H    | 2.892281 | -2.145310| 0.884762 |
Summary of Natural Population Analysis:

| Natural Population |
|---------------------|
| Atom   | No | Charge | Core       | Valence | Rydberg | Total   |
|--------|----|--------|------------|---------|---------|---------|
| C      | 1  | -0.20283 | 1.99902    | 4.18579 | 0.01802 | 6.20283 |
| C      | 2  | 0.21251  | 1.99897    | 3.76808 | 0.02043 | 5.78749 |
| C      | 3  | 0.22062  | 1.99894    | 3.76203 | 0.01841 | 5.77938 |
| C      | 4  | -0.20876 | 1.99902    | 4.19226 | 0.01748 | 6.20876 |
| C      | 5  | -0.13120 | 1.99916    | 4.11330 | 0.01873 | 6.13120 |
| C      | 6  | -0.12970 | 1.99916    | 4.11179 | 0.01875 | 6.12970 |
| C      | 7  | 0.35218  | 1.99907    | 3.62508 | 0.02368 | 5.64782 |
| N      | 8  | -0.29692 | 1.99912    | 5.28228 | 0.01552 | 7.29692 |
| H      | 9  | 0.25100  | 0.00000    | 0.74732 | 0.00168 | 0.74900 |
| H      | 10 | 0.24678  | 0.00000    | 0.75152 | 0.00170 | 0.75322 |
| H      | 11 | 0.23507  | 0.00000    | 0.76351 | 0.00142 | 0.76493 |
| H      | 12 | 0.23500  | 0.00000    | 0.76359 | 0.00141 | 0.76500 |
| N      | 13 | -0.44369 | 1.99912    | 5.43029 | 0.01421 | 7.44369 |
| C      | 14 | 0.65378  | 1.99912    | 3.32552 | 0.02159 | 5.34622 |
| O      | 15 | -0.55274 | 1.99966    | 6.52681 | 0.02627 | 8.55274 |
| C      | 16 | -0.35859 | 1.99927    | 4.34506 | 0.01427 | 6.35859 |
| H      | 17 | 0.24458  | 0.00000    | 0.75419 | 0.00124 | 0.75542 |
| H      | 18 | 0.24458  | 0.00000    | 0.75418 | 0.00124 | 0.75542 |
| H      | 19 | 0.23294  | 0.00000    | 0.76574 | 0.00132 | 0.76706 |
| H      | 20 | 0.48090  | 0.00000    | 0.51667 | 0.00243 | 0.51910 |
| H      | 21 | 0.56071  | 0.00000    | 0.43676 | 0.00253 | 0.43929 |
| C      | 22 | -0.69081 | 1.99920    | 4.67786 | 0.01375 | 6.69081 |
| H      | 23 | 0.29035  | 0.00000    | 0.70829 | 0.00136 | 0.70965 |
| H      | 24 | 0.26394  | 0.00000    | 0.73420 | 0.00186 | 0.73606 |
| H      | 25 | 0.29030  | 0.00000    | 0.70833 | 0.00136 | 0.70970 |

* Total * 2.00000  25.98890  65.75044  0.26066  92.00000