Supplementary information

# Whole-Electrolyte Design Enables Concentrated Two-Electron Storage of Viologens

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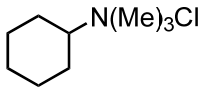
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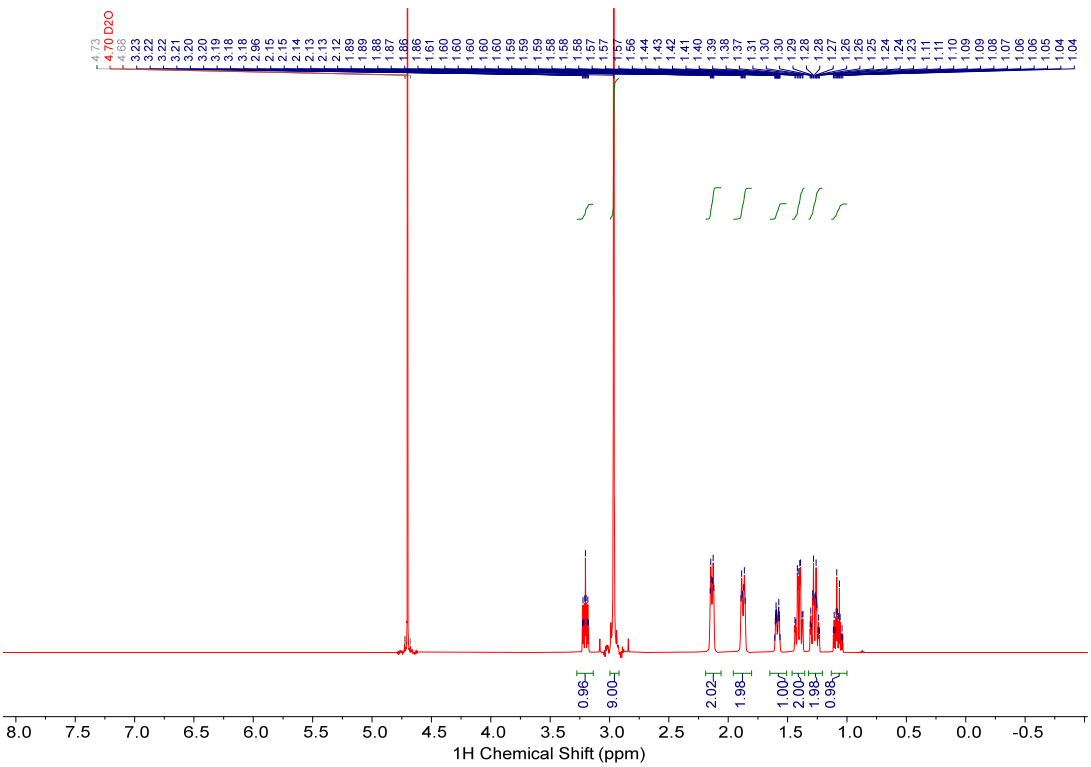
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**Methods**

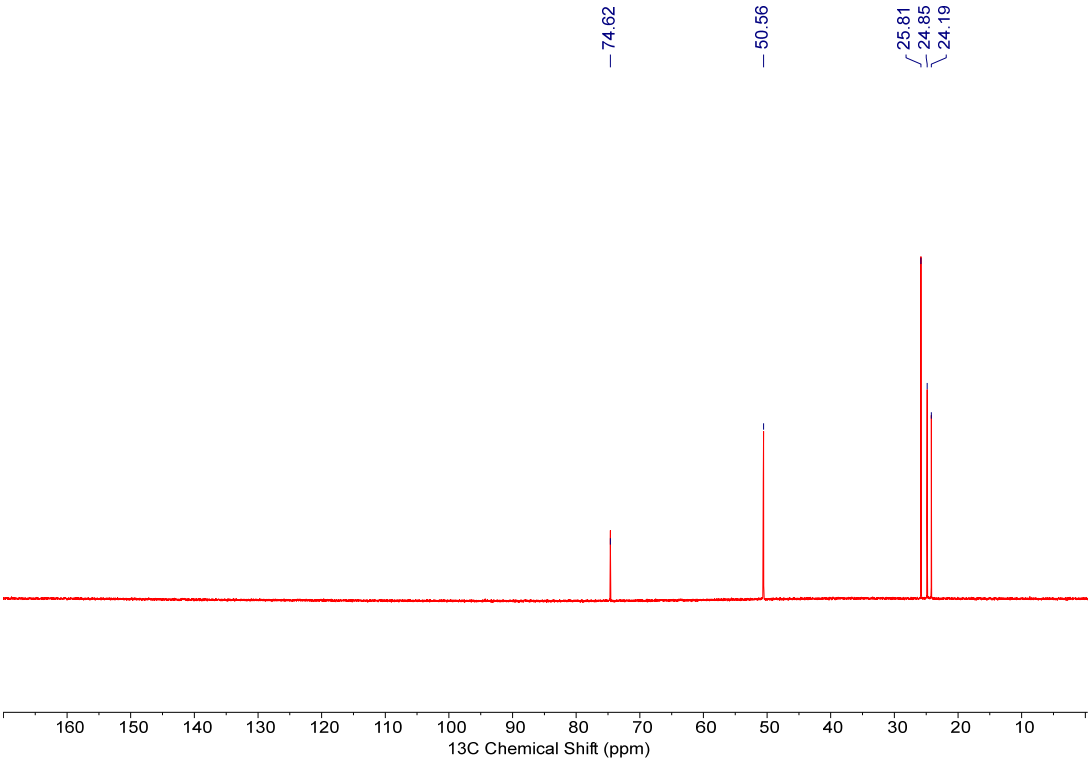
Synthesis of cyclohexyltrimethylammonium chloride ($CyN(Me)_3Cl$)




N,N-dimethylcyclohexylamine (9.4 mL, 62.7 mmol) was added to a solution of $CH_3I$ (1.5 equiv.) in $CH_2Cl_2$ (50 mL). The reaction mixture was stirred at room temperature overnight. The resulting precipitate was collected by filtration, washed with $Et_2O$, and dried under vacuum to afford $CyN(Me)_3I$. The iodide salt was dissolved in $H_2O$, and $NH_4PF_6$ (2.5 equiv.) dissolved in $H_2O$ was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration and dried to afford $CyN(Me)_3PF_6$. $CyN(Me)_3PF_6$ was dissolved in a small amount of acetone, and $Bu_4NCl$ (1.2 equiv.) dissolved in acetone was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration, washed with cold acetone, and dried under reduced pressure to afford $CyN(Me)_3Cl$. $^1H$ NMR (600 MHz, $D_2O$) δ 3.20 (tt, $J$ = 12.0, 3.4 Hz, 1H), 2.96 (s, 9H), 2.14 (dt, $J$ = 12.0, 3.1 Hz, 2H), 1.88 (dt, $J$ = 14.2, 3.9 Hz, 2H), 1.65–1.51 (m, 1H), 1.40 (qd, $J$ = 12.1, 3.5 Hz, 2H), 1.32–1.21 (m, 2H), 1.07 (qt, $J$ = 13.2, 3.8 Hz, 1H). $^{13}C$ NMR (151 MHz, $D_2O$) δ 74.62, 50.56, 25.81, 24.85, 24.19. HRMS (ESI) m/z: $[M]^+$ calcd for $C_9H_{20}N^+$ 142.1596; found 142.1596.

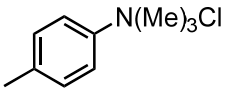



**Supplementary Fig. 1. $^{1}$H NMR of CyN(Me)$_3$Cl in D$_2$O.**

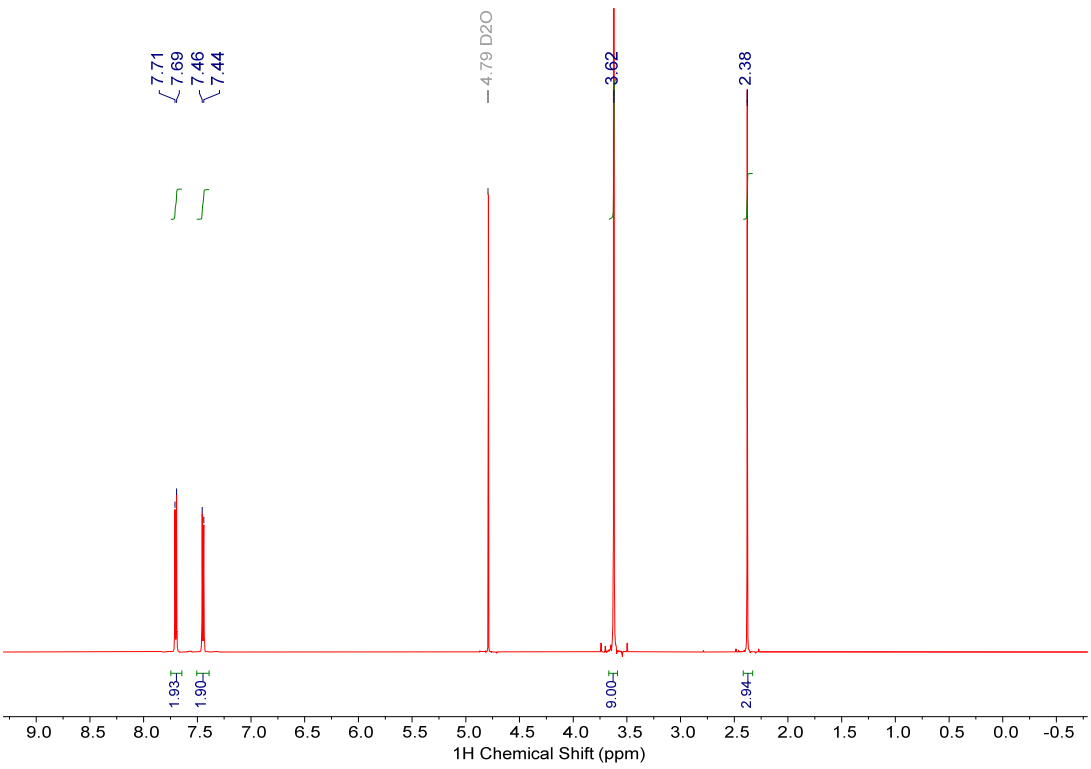



**Supplementary Fig. 2. $^{13}$C NMR of CyN(Me)$_3$Cl in D$_2$O.**

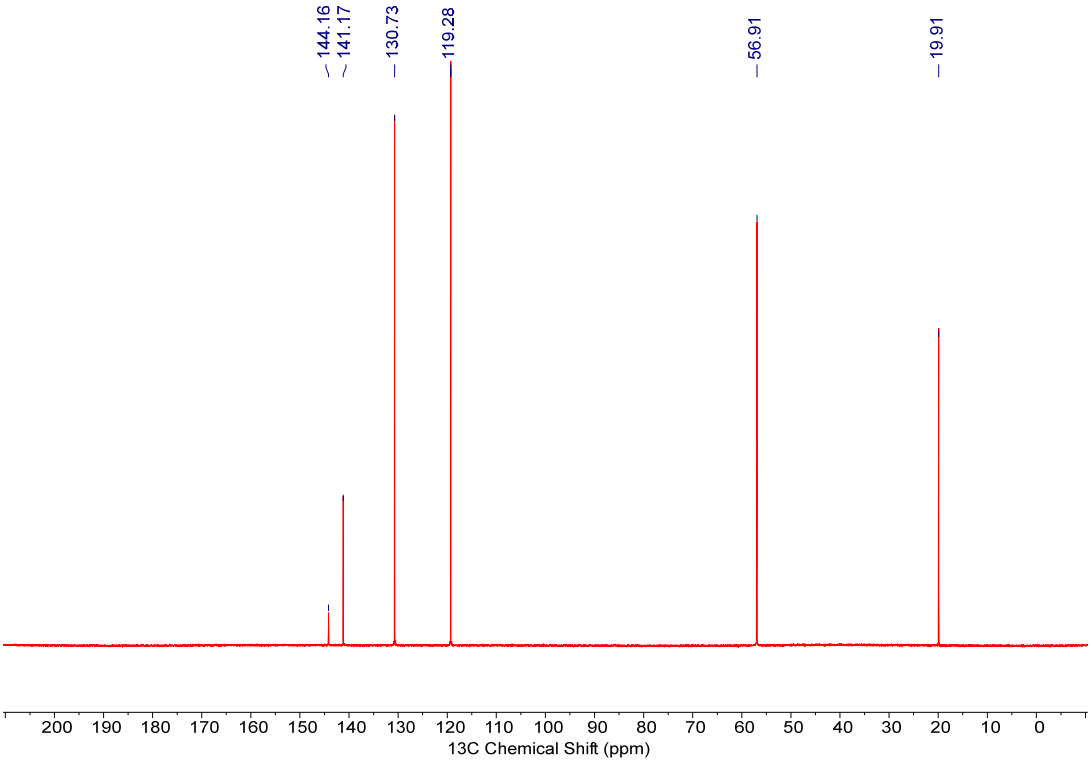
Synthesis of *N,N,N,*4-tetramethylbenzenaminium chloride ($Ph^{Me}N(Me)_3Cl$)




*N,N,*4-trimethylaniline (2.0 mL, 13.9 mmol) was added to a solution of $CH_3I$ (1.5 equiv.) in $CH_2Cl_2$ (15 mL). The reaction mixture was stirred at room temperature overnight. The resulting precipitate was collected by filtration, washed with $Et_2O$, and dried under vacuum to afford $Ph^{Me}N(Me)_3I$. The iodide salt was dissolved in $H_2O$, and $NH_4PF_6$ (2.5 equiv.) dissolved in $H_2O$ was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration and dried to afford $Ph^{Me}N(Me)_3PF_6$. $Ph^{Me}N(Me)_3PF_6$ was dissolved in a small amount of acetone, and $Bu_4NCl$ (1.2 equiv.) dissolved in acetone was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration, washed with cold acetone, and dried under reduced pressure to afford $Ph^{Me}N(Me)_3Cl$. $^1H$ NMR (600 MHz, $D_2O$) δ 7.70 (d, $J$ = 9.1 Hz, 2H), 7.45 (d, $J$ = 9.1 Hz, 2H), 3.62 (s, 9H), 2.38 (s, 3H). $^{13}C$ NMR (151 MHz, $D_2O$) δ 144.16, 141.17, 130.73, 119.28, 56.91, 19.91. HRMS (ESI) m/z: $[M]^+$ calcd for $C_9H_{16}N^+$ 150.1283; found 150.1284.

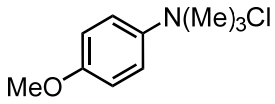



**Supplementary Fig. 3. $^{1}$H NMR of Ph$^{Me}$N(Me)$_3$Cl in D$_2$O.**

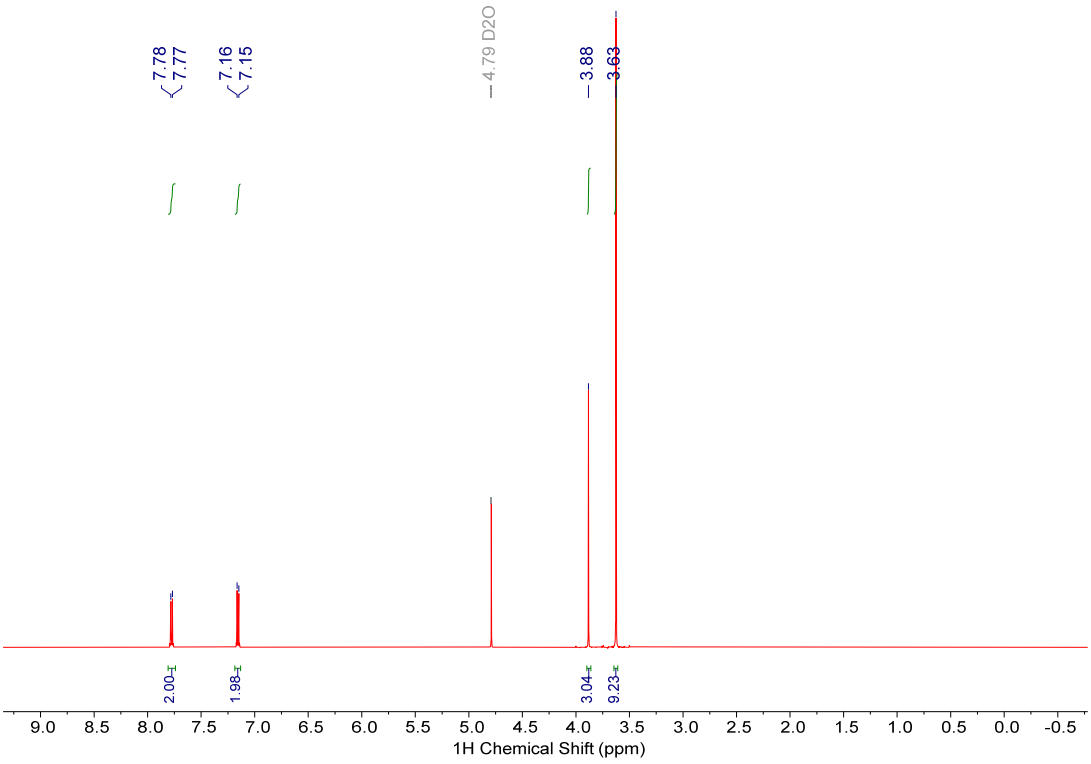



**Supplementary Fig. 4. $^{13}$C NMR of Ph$^{Me}$N(Me)$_3$Cl in D$_2$O.**

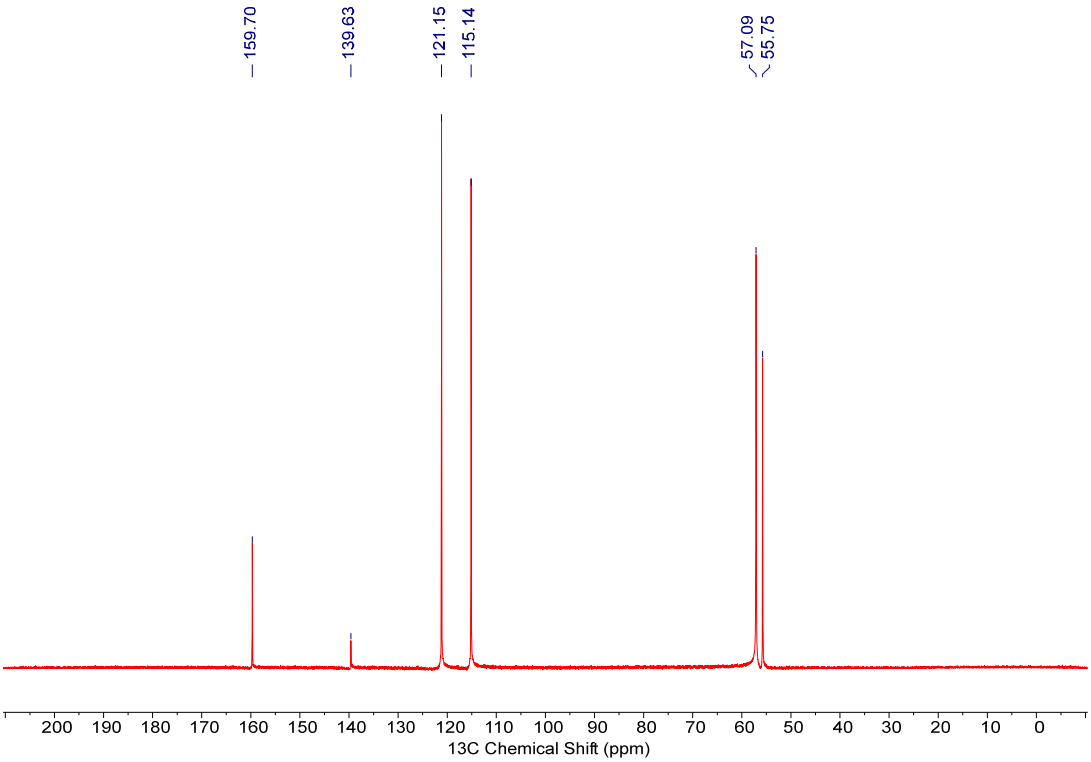
Synthesis of 4-methoxy-*N,N,N*-trimethylbenzenaminium chloride ($Ph^{OMe}N(Me)_3Cl$)




*p*-anisidine (4.0 g, 32.5 mmol) was added to a solution of $CH_3I$ (1.5 equiv.) in DMF (15 mL). The reaction mixture was stirred at 80 °C overnight. After the reaction, the solvent was removed under reduced pressure, and the residue was washed with $Et_2O$ and dried under vacuum to afford $Ph^{OMe}N(Me)_3I$. The iodide salt was dissolved in $H_2O$, and $NH_4PF_6$ (2.5 equiv.) dissolved in $H_2O$ was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration and dried to afford $Ph^{OMe}N(Me)_3PF_6$. $Ph^{OMe}N(Me)_3PF_6$ was dissolved in a small amount of acetone, and $Bu_4NCl$ (1.2 equiv.) dissolved in acetone was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration, washed with cold acetone, and dried under reduced pressure to afford $Ph^{OMe}N(Me)_3Cl$. $^1H$ NMR (600 MHz, $D_2O$) δ 7.78 (d, $J$ = 9.5 Hz, 2H), 7.16 (d, $J$ = 9.5 Hz, 2H), 3.88 (s, 3H), 3.63 (s, 9H). $^{13}C$ NMR (151 MHz, $D_2O$) δ 159.70, 139.63, 121.15, 115.14, 57.09, 55.75. HRMS (ESI) m/z: $[M]^+$ calcd for $C_9H_{16}NO^+$ 166.1232; found 166.1240.

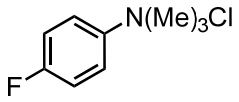



**Supplementary Fig. 5. $^{1}$H NMR of Ph$^{OMe}$N(Me)$_3$Cl in D$_2$O.**

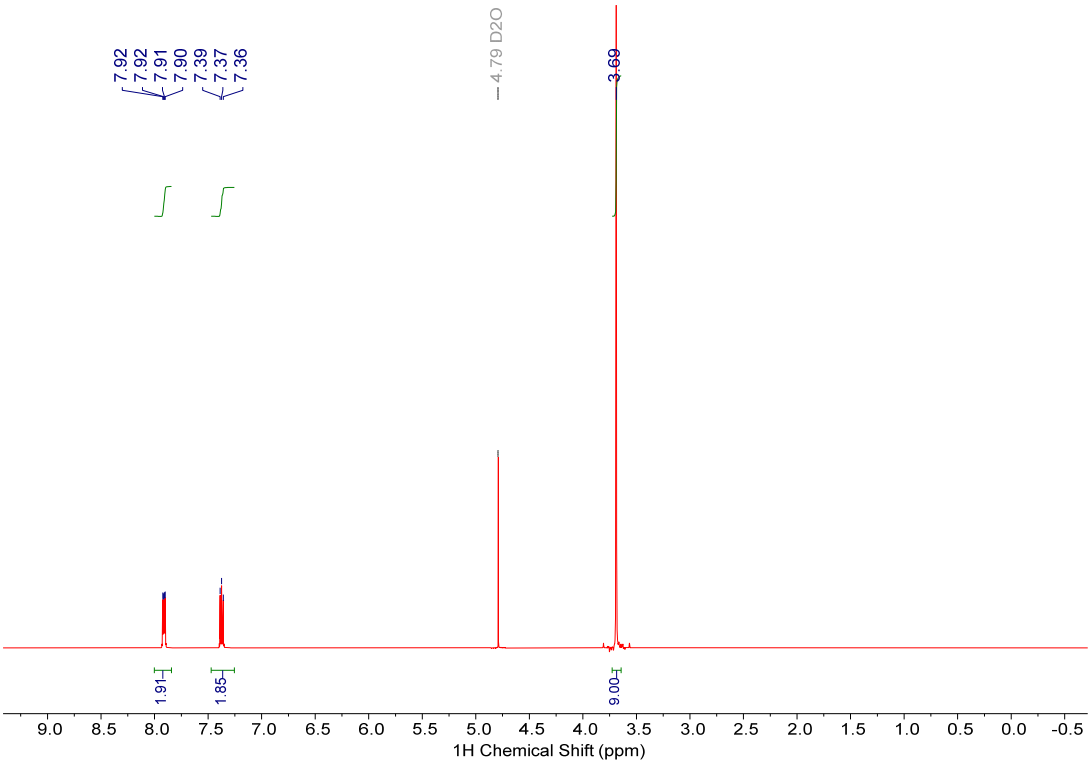



**Supplementary Fig. 6. $^{13}$C NMR of Ph$^{OMe}$N(Me)$_3$Cl in D$_2$O.**

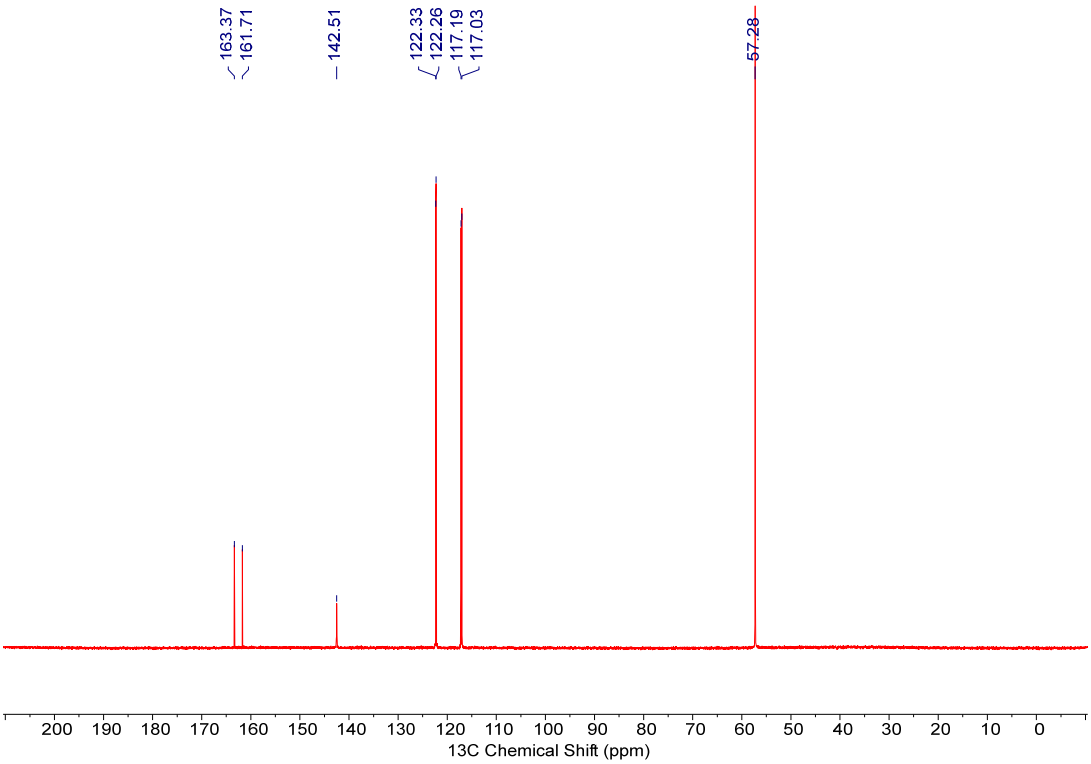
Synthesis of 4-fluoro-*N,N,N*-trimethylbenzenaminium chloride ($Ph^FN(Me)_3Cl$)




4-fluoro-*N,N*-dimethylaniline (2.0 g, 14.4 mmol) was added to a solution of $CH_3I$ (1.5 equiv.) in $CH_3CN$ (8.0 mL). The reaction mixture was stirred at 60 °C overnight. The resulting precipitate was collected by filtration, washed with $Et_2O$, and dried under vacuum to afford $Ph^FN(Me)_3I$. The iodide salt was dissolved in $H_2O$, and $NH_4PF_6$ (2.5 equiv.) dissolved in $H_2O$ was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration and dried to afford $Ph^FN(Me)_3PF_6$. $Ph^FN(Me)_3PF_6$ was dissolved in a small amount of acetone, and $Bu_4NCl$ (1.2 equiv.) dissolved in acetone was added. The mixture was stirred at room temperature for 1 h. The resulting precipitate was collected by filtration, washed with cold acetone, and dried under reduced pressure to afford $Ph^FN(Me)_3Cl$. $^1H$ NMR (600 MHz, $D_2O$) δ 7.91 (dd, $J$ = 9.5, 4.2 Hz, 2H), 7.47–7.25 (m, 2H), 3.69 (s, 9H). $^{13}C$ NMR (151 MHz, $D_2O$) δ 162.54, 142.51, 122.30, 117.11, 57.28. HRMS (ESI) m/z: $[M]^+$ calcd for $C_9H_{13}FN^+$ 154.1032; found 154.1032.




**Supplementary Fig. 7. $^{1}$H NMR of Ph$^{F}$N(Me)$_3$Cl in D$_2$O.**




**Supplementary Fig. 8. $^{13}$C NMR of Ph$^{F}$N(Me)$_3$Cl in D$_2$O.**

**Density functional theory calculations**

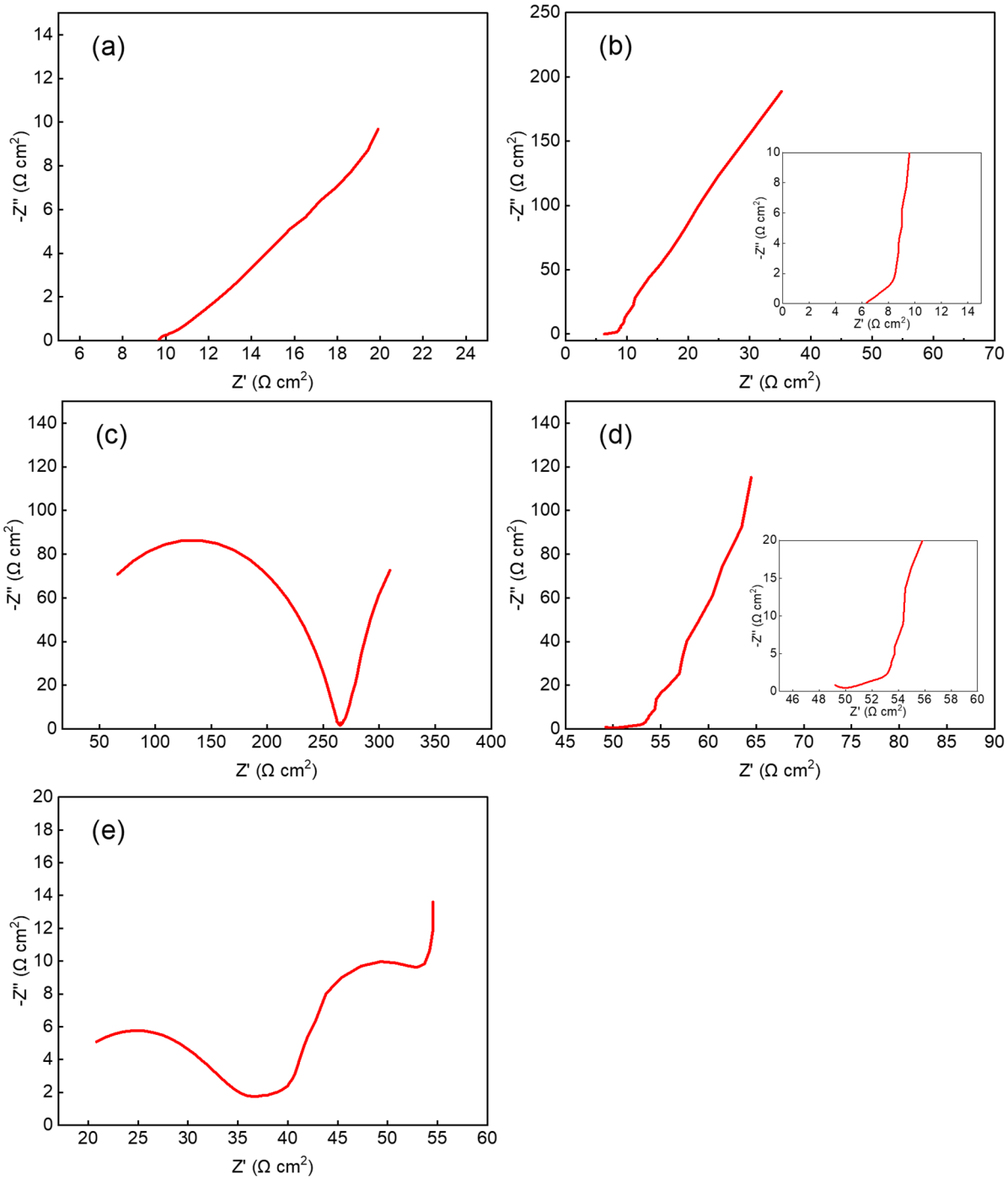
All density functional theory (DFT) calculations were performed using PySCF (version 2.13.1)[1] with GPU4PySCF (version 1.7.4).[2] The B3LYP exchange–correlation functional[3,4] was used with Grimme's D3 dispersion correction with Becke–Johnson damping (D3BJ).[5] The def2-SVP basis set[6] was used for all atoms, and Coulomb and exchange integrals were evaluated using density fitting with the def2-universal-JKFIT auxiliary basis set.[7] Solvation in water was treated with the conductor-like polarizable continuum model (C-PCM, $\varepsilon = 78.36$).[8] Geometry optimizations were performed using geomeTRIC[9] with translation–rotation internal coordinates. Initial structures were generated from SMILES strings using the ETKDG version 3 algorithm in RDKit and pre-optimized with the MMFF94s force field. The optimized structures used for the energy analysis are summarized in Supplementary Table 4. Association energies were calculated from the electronic energies of the optimized complexes and the corresponding isolated neutral components:

$\Delta E_{dimer} = E(\{[(NPr)_2V]^{2+}2Cl^-\}_2) - 2E([(NPr)_2V]^{2+}2Cl^-)$

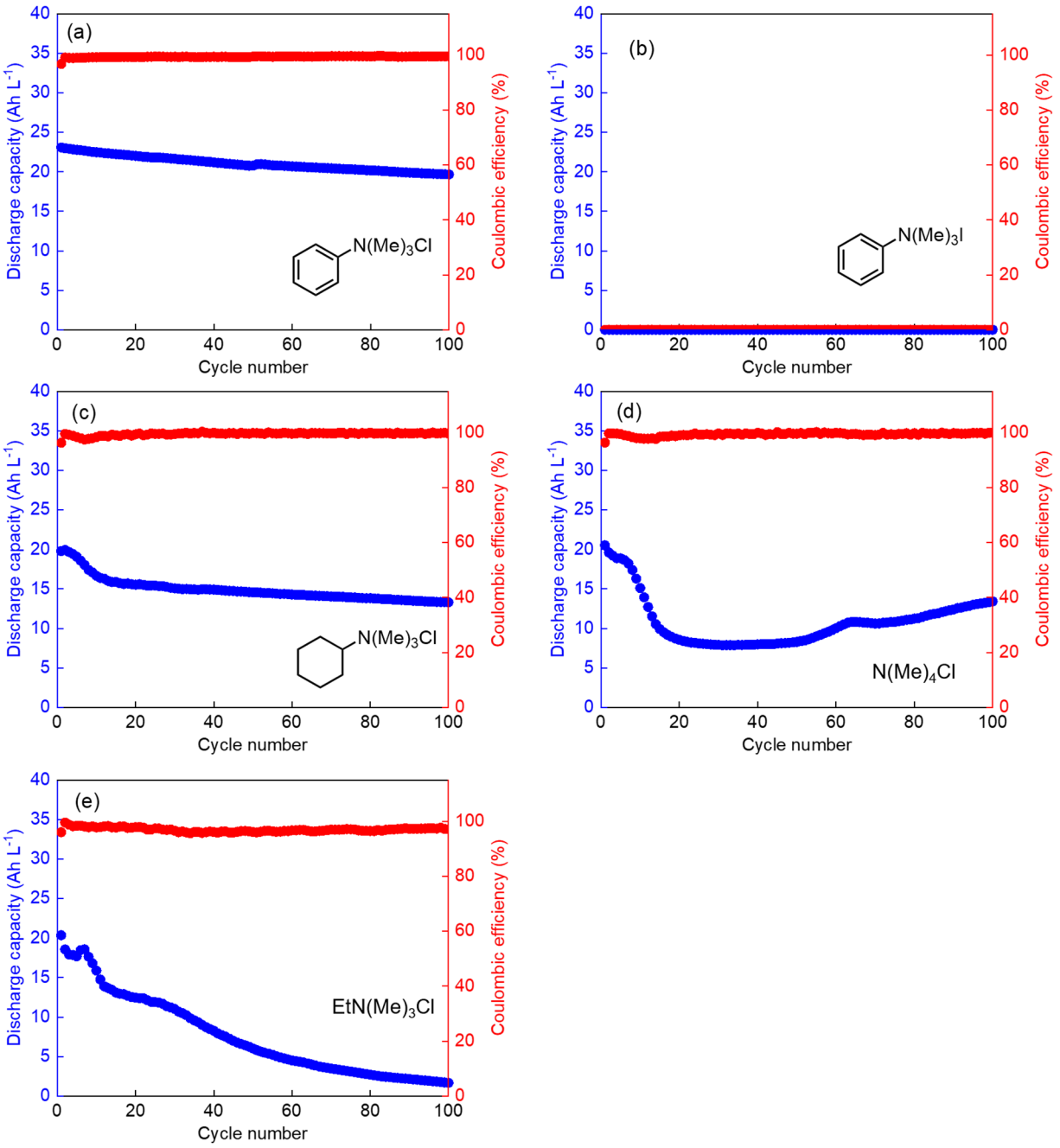
$\Delta E_{1:1} = E([(NPr)_2V]^{2+}2Cl^-\cdot additive) - E([(NPr)_2V]^{2+}2Cl^-) - E(additive)$

$\Delta E_{trimer} = E(\{[(NPr)_2V]^{2+}2Cl^-\}_2\cdot additive) - E(\{[(NPr)_2V]^{2+}2Cl^-\}_2) - E(additive)$

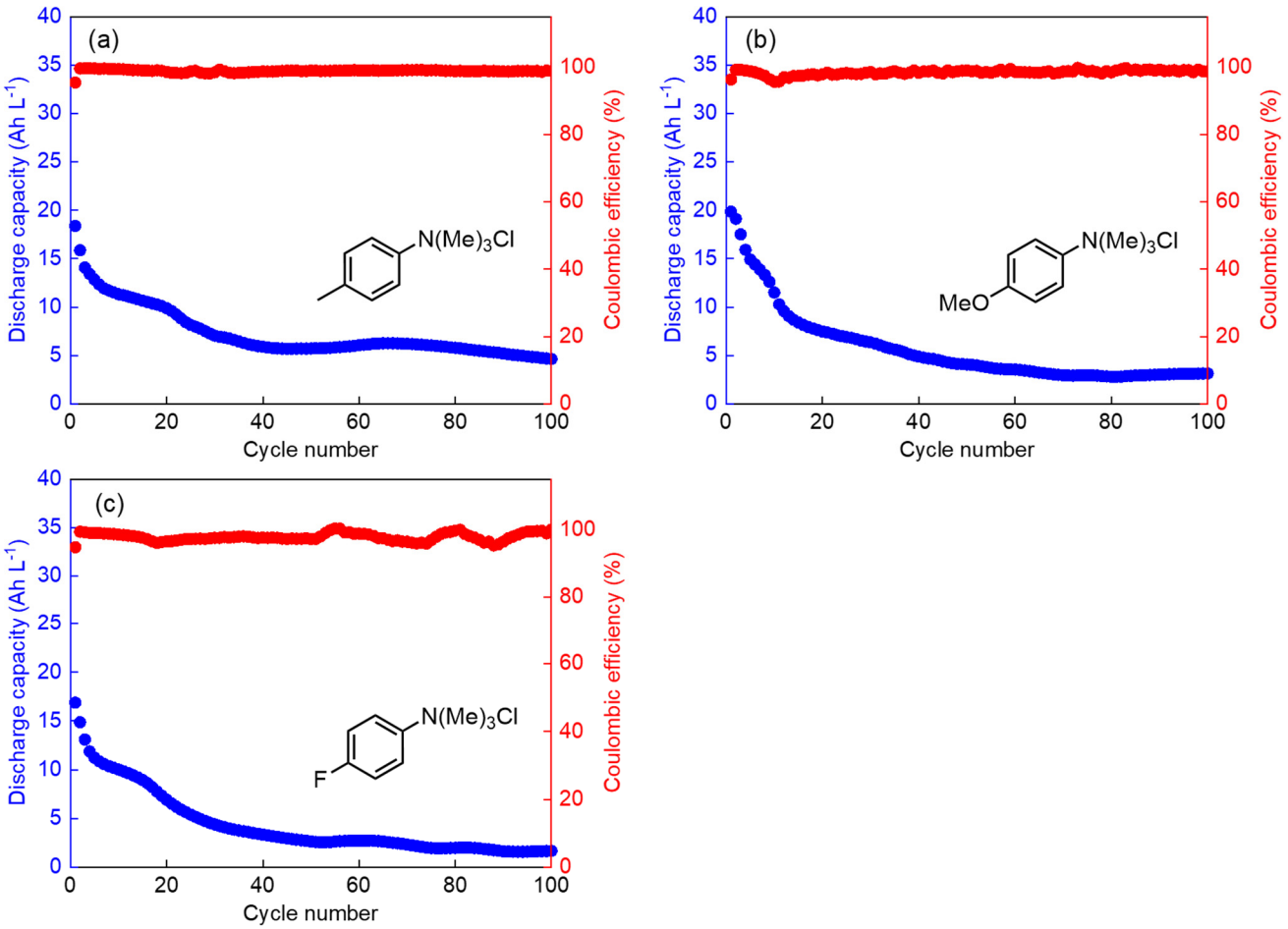
Here, "additive" denotes $Na^+Cl^-$ or $PhN(Me)_3^+Cl^-$. Energies were converted from Hartree to kcal $mol^{-1}$ using 1 Hartree = 627.5095 kcal $mol^{-1}$. Zero-point, thermal, and entropic corrections were not included; therefore, the reported values are electronic association energies at the B3LYP-D3BJ/def2-SVP/C-PCM(water) level.



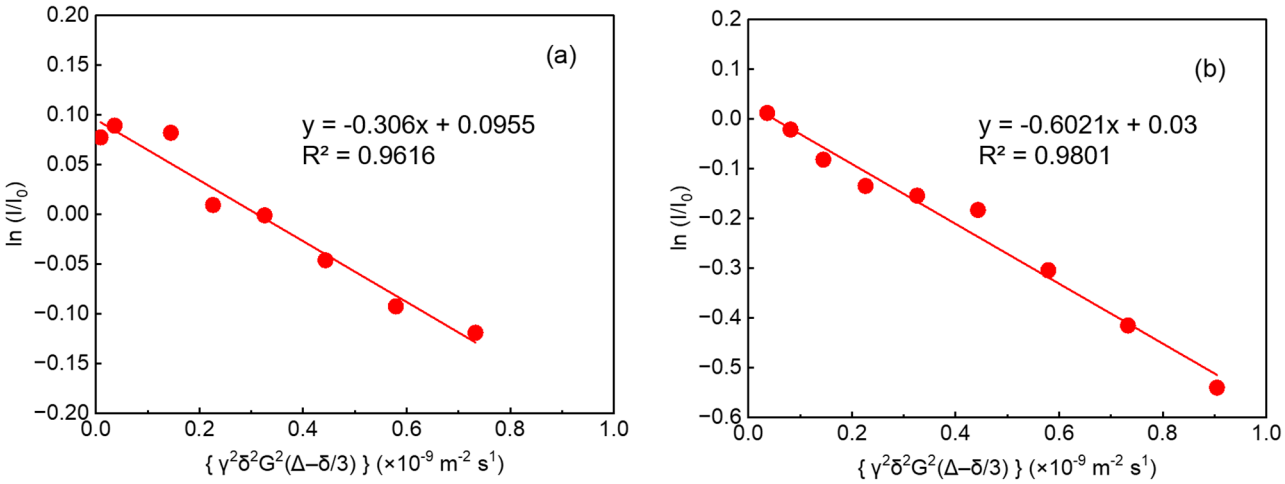

**Supplementary Fig. 9. Electrochemical impedance spectra of flow cells with charge-matched and charge-mismatched electrolyte combinations recorded before charge–discharge testing.** (a) 0.5 M $[(SPr)_2V]$/0.5 M $K_4[Fe(CN)_6]$ containing 0.84 M $PhSO_3Na$ with E620K; (b) 0.5 M $[(NPr)_2V]Cl_4$/0.5 M FcNCl containing 0.84 M $PhN(Me)_3Cl$ with FAA-3-PK-75; (c) 0.5 M $[(SPr)_2V]$/0.5 M $K_4[Fe(CN)_6]$ containing 0.84 M $PhN(Me)_3Cl$ with E620K; (d) 0.5 M $[(NPr)_2V]Cl_4$/0.5 M FcNCl containing 0.84 M $PhSO_3Na$ with FAA-3-PK-75; (e) 0.5 M $[(NPr)_2V]Cl_4$/0.5 M FcNCl containing 0.84 M $PhSO_3Na$ with E620K.



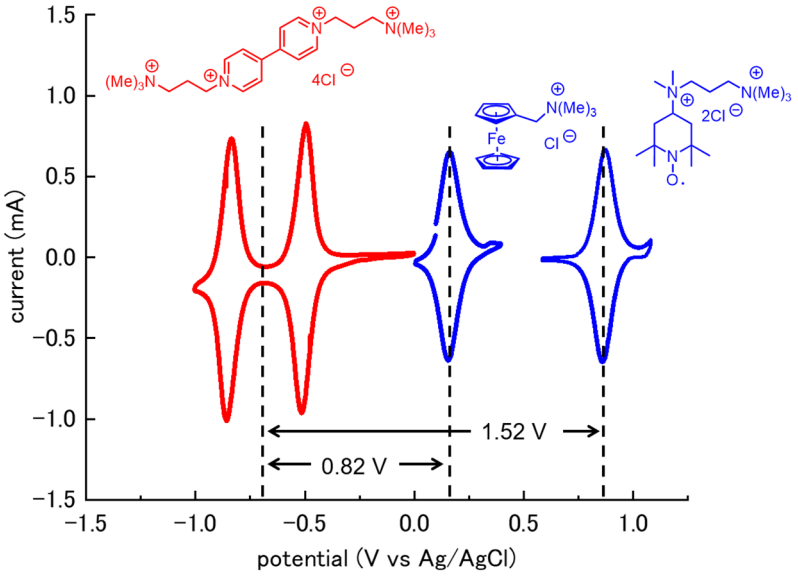

**Supplementary Fig. 10. Effect of electrolyte composition on cycling performance, showing the volumetric discharge capacity and coulombic efficiency for the electrolyte systems corresponding to Entries 1–6 in Table 2**. (a) $PhN(Me)_3Cl$, (b) $PhN(Me)_3I$, (c) $CyN(Me)_3Cl$, (d) $N(Me)_4Cl$, and (e) $EtN(Me)_3Cl$.



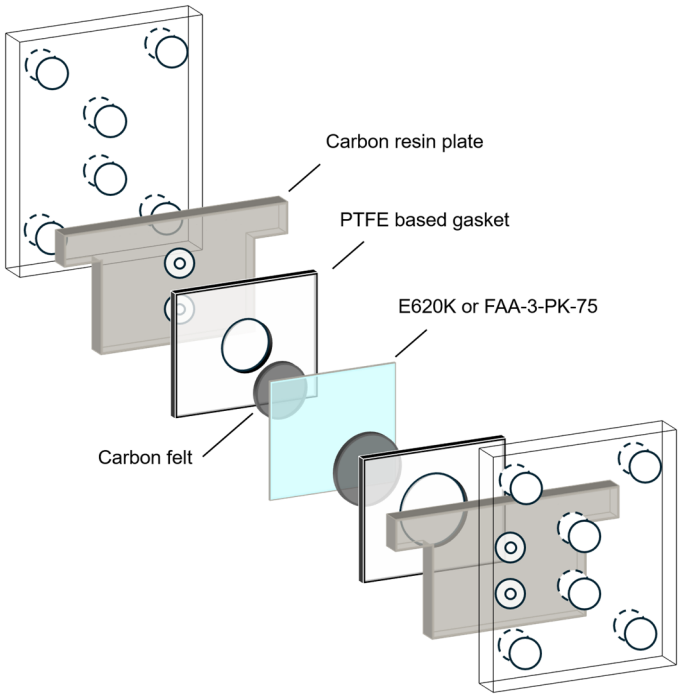

**Supplementary Fig. 11. Effect of electrolyte composition on cycling performance, showing the volumetric discharge capacity and coulombic efficiency for the electrolyte systems corresponding to Entries 7–9 in Table 2**. (a) Ph$^{Me}$N(Me)$_3$Cl, (b) Ph$^{OMe}$N(Me)$_3$Cl, (c) Ph$^{F}$N(Me)$_3$Cl.



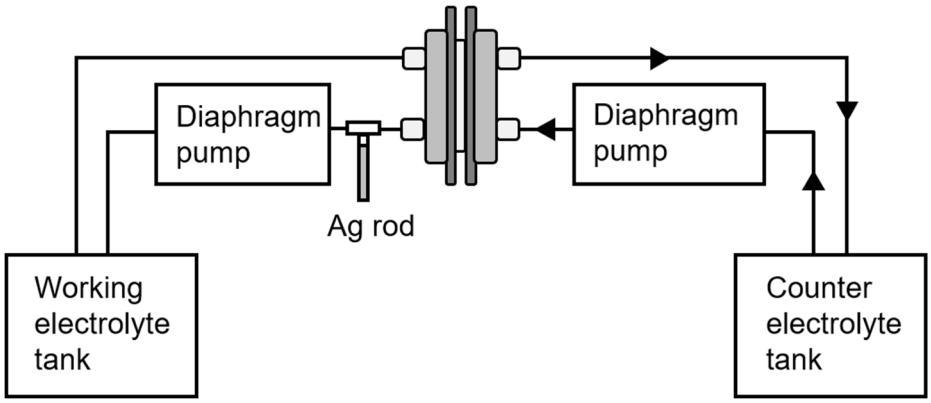

**Supplementary Fig. 12. PGSE-NMR diffusion analysis of reduced $[(NPr)_2V]Cl_4$ species in different electrolytes.** Stejskal–Tanner plots of $\ln(I/I_0)$ against $\gamma^2\delta^2G^2(\Delta-\delta/3)$ for the two-electron-reduced species in electrolytes containing (a) NaCl or (b) $PhN(Me)_3Cl$.



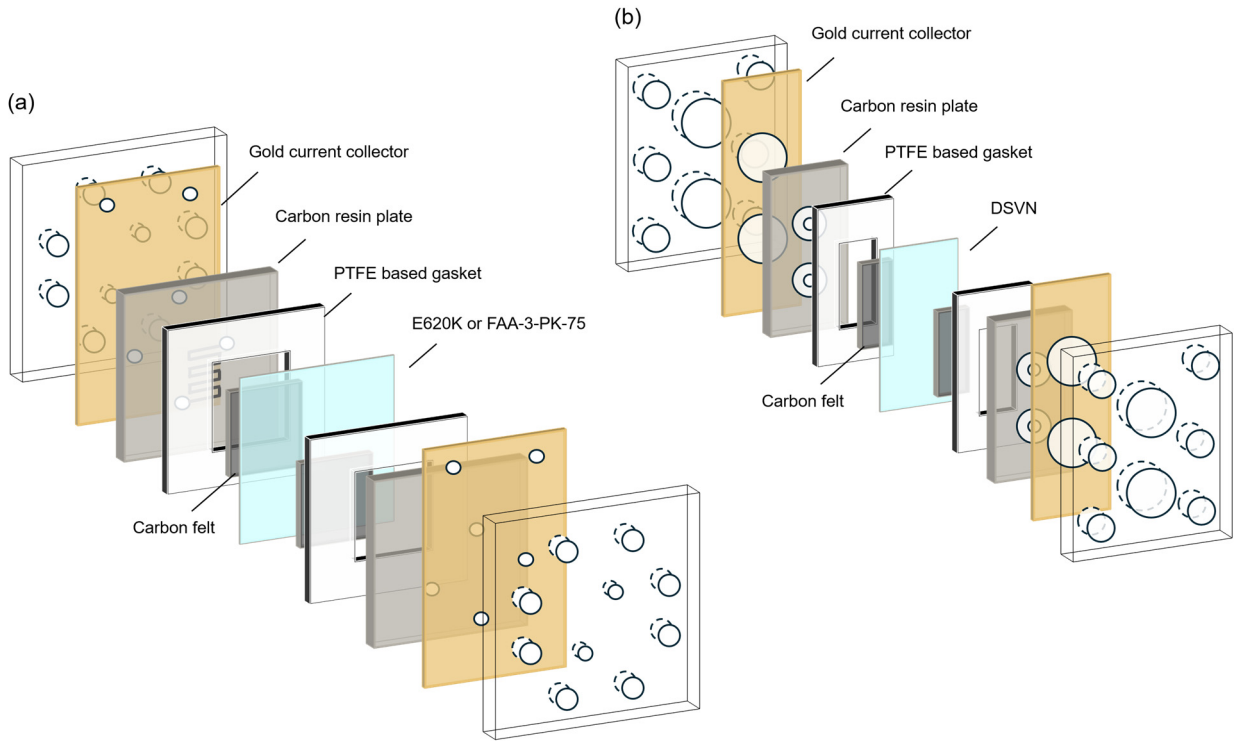

**Supplementary Fig. 13. Cyclic voltammograms of $[(NPr)_2V]Cl_4$, $[N_2\text{-TEMPO}]Cl_2$, and FcNCl.**



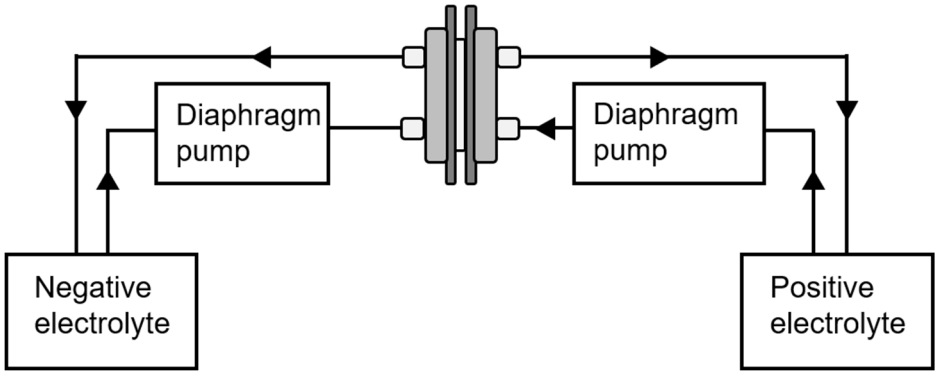

**Supplementary Fig. 14. Schematic of experimental cell for the cyclic voltammetry.**




**Supplementary Fig. 15. Schematic of set up for the cyclic voltammetry.**

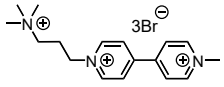
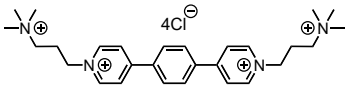
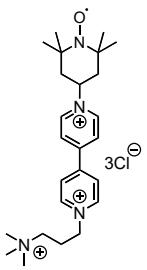
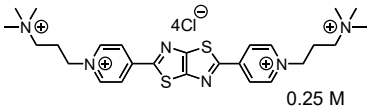
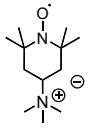
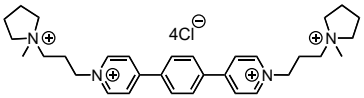
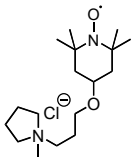
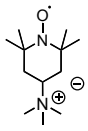
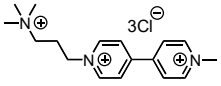
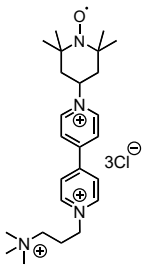
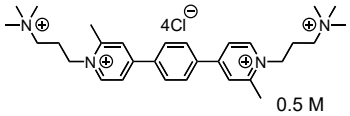
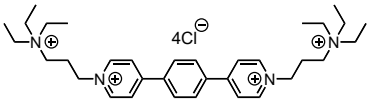
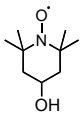
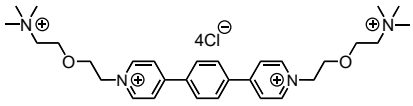
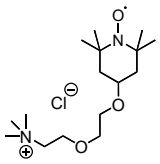



**Supplementary Fig. 16. Schematic of the electrochemical flow cells used for charge–discharge tests.** (a) For testing 0.5 M active material solutions. (b) For testing 1 M active material solutions.




**Supplementary Fig. 17. Schematic of set up for charge–discharge tests.**

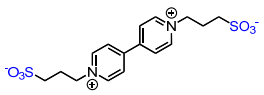
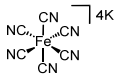
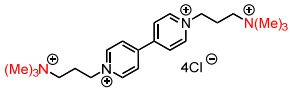
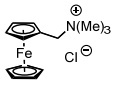
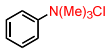
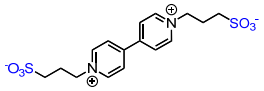
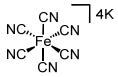
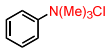
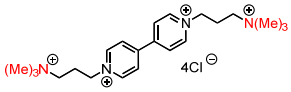
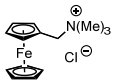
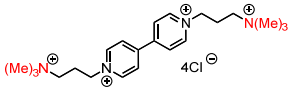
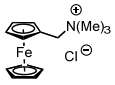
**Supplementary Table 1 Comparison of two-electron storage performance among viologen derivatives.**

| Negative electrolyte | Positive electrolyte | Discharge capacity (Ah $L^{-1}$) | Capacity fade rate (% per cycle) | Cycle | Current density (mA $cm^{-2}$) | Ref. |
|---|---|---|---|---|---|---|
|  0.25 M | FcNCl | 12.0 | 0.01 | 100 | 60 | 10 |
|  0.50 M |  | 20.0 | 0.04 | 100 | 60 | 11 |
|  0.25 M |  | 9.1 | 0.06 | 50 | 60 | 12 |
|  0.50 M |  | 23.9 | 0.2 | 250 | 40 | 13 |
| $[(NPr)_2V]Cl_4I$ 0.1 M |  | ≈5.0 | 0.06 | 300 | 20 | 14 |
|  with HE-β-CD[b] 0.30 M |  | ≈15.0 | ≈0.2 | 100 | 40 | 15 |
|  0.5 M | FcNCl | ≈18.0 | 0.17 | 100 | 80 | 16 |
|  0.1 M |  | ≈3.6 | 0.04 | 300 | 100 | 17 |
|  0.5 M |  | ≈22.0 | ≈0.19 | 400 | 40 | 18 |
| **$[(NPr)_2V]Cl_4$ with $PhN(Me)_3Cl$ 1.0 M** | **$[N2\text{-}TEMPO]Cl_2$** | **39.3** | **0.19** | **100** | **60** | **This work** |

[a]The data from the long-term charge-discharge cycle test with two electron storage were used.[10-18]

[b]hydroxyethyl-β-cyclodextrin.

**Supplementary Table 2 Effect of charge matching between viologen active materials and aromatic electrolyte components on initial cell resistance and charge–discharge behavior.**

| Negative active material | Positive active material | Negative electrolyte | Membrane | ReZ@1 Hz (Ω cm²) | Charge–discharge |
|---|---|---|---|---|---|
|  |  |  | CEM | 19.0 | Yes |
|  |  |  | AEM | 9.0 | Yes |
|  |  |  | CEM | 274.3 | Limited[a] |
|  |  |  | AEM | 53.7 | Limited[a] |
|  |  |  | CEM | 40.2 | Limited[a] |

[a]Charge–discharge could not be evaluated under the applied current density, as the high initial cell resistance caused the voltage to reach the cutoff limits.

**Supplementary Table 3. Summary of diffusion coefficients and viscosities.**

| Electrolyte | D (m $s^{-1}$) | η (mPa·s) |
|---|---|---|
| 1.0 M $[(NPr)_2V]Cl_2$+1.68 M NaCl | $3.06\times10^{-10}$ | 2.16 |
| 1.0 M $[(NPr)_2V]Cl_2$+1.68 M $PhN(Me)_3Cl$ | $6.02\times10^{-10}$ | 2.24 |

Diffusion coefficients and viscosities were measured using an Oxford X-Pulse and a DMA 4100 M (Anton Paar), respectively.

**Supplementary Table 4 Optimized Cartesian coordinates and electronic energies of DFT-calculated structures.**

S1. $[(NPr)_2V]^{4+}$ (oxidized, 4+)

Charge = +4, Multiplicity = 1, N = 64, E = (see manuscript)

| | | | |
|---|---|---|---|
| C | -2.70066400 | 1.87301500 | 6.65783300 |
| N | -1.34037700 | 1.78174000 | 7.28522800 |
| C | -1.49941300 | 1.71065700 | 8.77818600 |
| C | -0.54563200 | 3.00811600 | 6.94280600 |
| C | -0.61860800 | 0.52394300 | 6.84577000 |
| C | -0.39196400 | 0.39371600 | 5.34600400 |
| C | 0.37657900 | -0.90094700 | 5.07661300 |
| N | 0.60170600 | -1.08698600 | 3.62506900 |
| C | 1.71709600 | -0.58394200 | 3.05216700 |
| C | 1.92966800 | -0.70687600 | 1.69061000 |
| C | 0.98000100 | -1.36604500 | 0.89334200 |
| C | 1.18302300 | -1.52190200 | -0.56557900 |
| C | 1.85789000 | -0.54198900 | -1.31162300 |
| C | 2.02634200 | -0.71135100 | -2.67424000 |
| N | 1.55581300 | -1.81449500 | -3.29672700 |
| C | 1.70349400 | -1.94300100 | -4.76472500 |
| C | 0.50723000 | -1.31772100 | -5.48442000 |
| C | 0.69825400 | -1.47000700 | -6.98674600 |
| N | -0.42331100 | -0.90822800 | -7.83752000 |
| C | -0.05095700 | -1.12432900 | -9.27752100 |
| C | -1.71668200 | -1.61814700 | -7.56156400 |
| C | -0.59822300 | 0.56360800 | -7.60002300 |
| C | 0.90677100 | -2.77737300 | -2.60587700 |
| C | 0.70522700 | -2.65557500 | -1.24277600 |
| C | -0.16884400 | -1.87622200 | 1.51963600 |
| C | -0.33426600 | -1.71963400 | 2.88397500 |
| H | -3.21617500 | 2.73962000 | 7.08704800 |
| H | -2.59387200 | 2.00416500 | 5.57638000 |

| | | | |
|---|---|---|---|
| H | -3.25136500 | 0.95183300 | 6.88163600 |
| H | -2.01357700 | 2.61746200 | 9.11574800 |
| H | -2.09125800 | 0.82184000 | 9.02447300 |
| H | -0.50420100 | 1.64493600 | 9.23242300 |
| H | -1.06356000 | 3.87825100 | 7.36171500 |
| H | -0.47816200 | 3.10647600 | 5.85478700 |
| H | 0.45359300 | 2.91069000 | 7.38306200 |
| H | -1.22120800 | -0.31589500 | 7.21747300 |
| H | 0.33909400 | 0.52311500 | 7.38384300 |
| H | -1.34772800 | 0.35915000 | 4.80304700 |
| H | 0.19153100 | 1.24024600 | 4.95552200 |
| H | 1.36077400 | -0.89107800 | 5.56147500 |
| H | -0.17716800 | -1.77796400 | 5.43531100 |
| H | 2.42835800 | -0.08999600 | 3.71479200 |
| H | 2.85240300 | -0.30579900 | 1.27189200 |
| H | 2.24062100 | 0.36885200 | -0.85155000 |
| H | 2.53452300 | 0.02438800 | -3.29840900 |
| H | 2.64277400 | -1.44873000 | -5.04310100 |
| H | 1.79460400 | -3.01274200 | -4.99147200 |
| H | 0.43732500 | -0.25778200 | -5.19981900 |
| H | -0.41101700 | -1.82114800 | -5.14851200 |
| H | 1.61269900 | -0.95656700 | -7.31354000 |
| H | 0.78327700 | -2.53025500 | -7.26117800 |
| H | 0.88484800 | -0.59117400 | -9.48023900 |
| H | 0.07684000 | -2.19933200 | -9.44814100 |
| H | -0.85809700 | -0.73170400 | -9.90597300 |
| H | -2.47091600 | -1.23698300 | -8.25920500 |
| H | -2.02957500 | -1.41600500 | -6.53236400 |
| H | -1.56504100 | -2.69313000 | -7.71365300 |
| H | -0.95537000 | 0.72658300 | -6.57821200 |
| H | -1.33940700 | 0.93800400 | -8.31509200 |
| H | 0.36658600 | 1.06043300 | -7.75546500 |
| H | 0.56172300 | -3.64128000 | -3.17473300 |

| | | | |
|---|---|---|---|
| H | 0.19453300 | -3.46386900 | -0.71980200 |
| H | -0.95316100 | -2.38232600 | 0.95707800 |
| H | -1.21121500 | -2.09166000 | 3.41461700 |

S2. $[(NPr)_2V]^{2+}$ (2e-reduced, 2+)

Charge = +2, Multiplicity = 1, N = 64, E = (see manuscript)

| | | | |
|---|---|---|---|
| C | -2.76108600 | 1.57629800 | 6.49768000 |
| N | -1.40797900 | 1.81350700 | 7.09916400 |
| C | -1.54827000 | 1.90555200 | 8.59133600 |
| C | -0.85151000 | 3.10892400 | 6.58684200 |
| C | -0.46735900 | 0.66076800 | 6.79422200 |
| C | -0.24895200 | 0.35782200 | 5.32143400 |
| C | 0.80028400 | -0.75521800 | 5.16997700 |
| N | 1.04319100 | -1.11357800 | 3.78641800 |
| C | 1.90092800 | -0.35306300 | 3.00027200 |
| C | 2.00493800 | -0.52624200 | 1.65916400 |
| C | 1.20971100 | -1.51602800 | 0.93303400 |
| C | 1.30940700 | -1.72875800 | -0.43514600 |
| C | 2.21404800 | -0.98107800 | -1.30827300 |
| C | 2.30165000 | -1.22083800 | -2.64036400 |
| N | 1.55458100 | -2.20861300 | -3.27079700 |
| C | 1.51365200 | -2.29791500 | -4.71714000 |
| C | 0.45443900 | -1.37532100 | -5.34165300 |
| C | 0.46325500 | -1.53580900 | -6.85241000 |
| N | -0.55704500 | -0.70640800 | -7.61277300 |
| C | -0.39267100 | -1.00957200 | -9.07433200 |
| C | -1.95479900 | -1.06245100 | -7.20081900 |
| C | -0.32742100 | 0.75951300 | -7.39347900 |
| C | 0.65559500 | -2.92903700 | -2.49318700 |
| C | 0.52548000 | -2.72985100 | -1.15804300 |
| C | 0.30236600 | -2.26177800 | 1.80496200 |
| C | 0.23744900 | -2.04473900 | 3.14213200 |
| H | -3.42955900 | 2.37860400 | 6.83049000 |

| | | | |
|---|---|---|---|
| H | -2.67904700 | 1.58935300 | 5.40629000 |
| H | -3.13175800 | 0.60387500 | 6.84281200 |
| H | -2.21100300 | 2.74562100 | 8.82813500 |
| H | -1.97541200 | 0.96650400 | 8.96118800 |
| H | -0.55555000 | 2.06909800 | 9.02610700 |
| H | -1.52591600 | 3.91678700 | 6.89285700 |
| H | -0.78985000 | 3.07077500 | 5.49482500 |
| H | 0.14363000 | 3.25804900 | 7.02181100 |
| H | -0.89053600 | -0.21310900 | 7.30853200 |
| H | 0.48241300 | 0.91705500 | 7.28391300 |
| H | -1.18299800 | 0.02605300 | 4.84372000 |
| H | 0.10713200 | 1.24705100 | 4.77966200 |
| H | 1.75241000 | -0.43429200 | 5.62111100 |
| H | 0.47311600 | -1.65700600 | 5.71045400 |
| H | 2.49800200 | 0.38427900 | 3.54040600 |
| H | 2.72312100 | 0.10115100 | 1.13080400 |
| H | 2.85771400 | -0.20159800 | -0.90002900 |
| H | 2.97705100 | -0.66060900 | -3.28983600 |
| H | 2.51075500 | -2.04591800 | -5.11041000 |
| H | 1.30945200 | -3.34351100 | -4.99659300 |
| H | 0.67747700 | -0.33783900 | -5.05039300 |
| H | -0.52738600 | -1.63864300 | -4.92042400 |
| H | 1.44168700 | -1.25475000 | -7.26621400 |
| H | 0.26317000 | -2.57977900 | -7.13096800 |
| H | 0.62704300 | -0.74267100 | -9.37445700 |
| H | -0.56773200 | -2.08008400 | -9.23107800 |
| H | -1.12281900 | -0.41767600 | -9.63769000 |
| H | -2.65164100 | -0.50722100 | -7.83916800 |
| H | -2.10671500 | -0.78250800 | -6.15378500 |
| H | -2.09389500 | -2.14180500 | -7.33327700 |
| H | -0.50671700 | 1.00090600 | -6.34109000 |
| H | -1.02827000 | 1.31478800 | -8.02734400 |
| H | 0.70649700 | 0.99673300 | -7.67021400 |

| | | | |
|---|---|---|---|
| H | 0.07167100 | -3.67940200 | -3.02973900 |
| H | -0.18850700 | -3.36091000 | -0.62842600 |
| H | -0.35271200 | -3.03007600 | 1.39375700 |
| H | -0.44143100 | -2.60222600 | 3.79031500 |

S3. $PhN(Me)_3^+$ (bare cation)

Charge = +1, Multiplicity = 1, N = 24, E = (see manuscript)

| | | | |
|---|---|---|---|
| C | 3.09924600 | 0.65900900 | 0.20181800 |
| C | 2.17638200 | 1.47019400 | 0.86214200 |
| C | 0.80511100 | 1.20125700 | 0.78265100 |
| C | 0.36634300 | 0.10971000 | 0.03325700 |
| C | 1.28250500 | -0.71033700 | -0.63443800 |
| C | 2.64679000 | -0.43185700 | -0.54678500 |
| N | -1.09430500 | -0.22005100 | -0.07812800 |
| C | -1.51505200 | -0.16562000 | -1.52686500 |
| C | -1.34085200 | -1.60363400 | 0.47337800 |
| C | -1.96744400 | 0.73583000 | 0.68558600 |
| H | 4.16780700 | 0.87417700 | 0.26881000 |
| H | 2.51454000 | 2.32588000 | 1.45018200 |
| H | 0.11393300 | 1.85364300 | 1.31025800 |
| H | 0.95542900 | -1.56629700 | -1.22473200 |
| H | 3.35647500 | -1.07622500 | -1.06960600 |
| H | -1.32179600 | 0.84654900 | -1.89919000 |
| H | -2.58442100 | -0.40024500 | -1.57893100 |
| H | -0.94147200 | -0.90016500 | -2.09931200 |
| H | -2.41439600 | -1.81198100 | 0.39978300 |
| H | -0.77596700 | -2.33410200 | -0.11280100 |
| H | -1.01490400 | -1.61566200 | 1.51934500 |
| H | -1.83111000 | 1.74594500 | 0.28693700 |
| H | -3.00438200 | 0.41426100 | 0.54287400 |
| H | -1.70532100 | 0.69315400 | 1.74739600 |

S4. $Na^+Cl^-$ (neutral pair)

Charge = 0, Multiplicity = 1, N = 2, E = (see manuscript)

| | | | |
|---|---|---|---|
| Na | -0.00680500 | -0.00000000 | -0.00000000 |
| Cl | 2.40741900 | 0.00000000 | 0.00000000 |

S5. $PhN(Me)_3^+Cl^-$ (neutral pair)

Charge = 0, Multiplicity = 1, N = 25, E = -865.96737722 Hartree

| | | | |
|---|---|---|---|
| C | 3.10889300 | 0.86174000 | 0.07350800 |
| C | 2.17194500 | 1.59970300 | 0.79695100 |
| C | 0.80862500 | 1.29193100 | 0.72022400 |
| C | 0.38981100 | 0.23580000 | -0.08937800 |
| C | 1.32169400 | -0.51081000 | -0.81937300 |
| C | 2.67803900 | -0.19489400 | -0.73501400 |
| N | -1.05711100 | -0.12754600 | -0.20422100 |
| C | -1.51263700 | 0.00926900 | -1.63895000 |
| C | -1.27270200 | -1.55406500 | 0.24655700 |
| C | -1.95671800 | 0.74205900 | 0.63211400 |
| H | 4.17115400 | 1.10711800 | 0.13768200 |
| H | 2.49320400 | 2.42758200 | 1.43247400 |
| H | 0.10394900 | 1.88608000 | 1.29659000 |
| H | 1.00880200 | -1.33785100 | -1.45684300 |
| H | 3.39902500 | -0.78198200 | -1.30774100 |
| H | -1.35664000 | 1.04996100 | -1.94556600 |
| H | -2.57729700 | -0.26645800 | -1.66140900 |
| H | -0.92349100 | -0.66510600 | -2.26796000 |
| H | -2.34803300 | -1.76083400 | 0.14002600 |
| H | -0.68405100 | -2.22406900 | -0.38752500 |
| H | -0.94620000 | -1.63206000 | 1.28993900 |
| H | -1.85445200 | 1.78139000 | 0.30311300 |
| H | -2.97994400 | 0.37741900 | 0.46134100 |
| H | -1.67585800 | 0.63630500 | 1.68517700 |
| Cl | -4.69054700 | -1.13174300 | -0.56069600 |

S6. $[(NPr)_2V]^{2+}2Cl^-$ (neutral monomer)

Charge = 0, Multiplicity = 1, N = 66, E = -1999.71584873 Hartree

| | | | |
|---|---|---|---|
| C | -2.51936300 | 1.90064000 | 6.62202500 |
| N | -1.15052300 | 2.12259100 | 7.19739300 |
| C | -1.27959500 | 2.25071500 | 8.68983400 |
| C | -0.60023600 | 3.41318100 | 6.66182800 |
| C | -0.22752900 | 0.96091100 | 6.90049100 |
| C | -0.01544100 | 0.64345100 | 5.42939900 |
| C | 1.01053900 | -0.49049900 | 5.28104600 |
| N | 1.24599900 | -0.85857500 | 3.89806600 |
| C | 2.11618000 | -0.11578700 | 3.10893400 |
| C | 2.21046300 | -0.28907500 | 1.76706800 |
| C | 1.38998600 | -1.25957000 | 1.04294000 |
| C | 1.47454700 | -1.46780100 | -0.32697800 |
| C | 2.38606900 | -0.73315600 | -1.20405000 |
| C | 2.45237000 | -0.96262400 | -2.53914500 |
| N | 1.67765200 | -1.92881400 | -3.16970100 |
| C | 1.59837200 | -1.98481200 | -4.61688200 |
| C | 0.53900900 | -1.03223600 | -5.19190400 |
| C | 0.52021600 | -1.13145800 | -6.70812000 |
| N | -0.53546900 | -0.30410000 | -7.40856500 |
| C | -0.37203700 | -0.48987900 | -8.89133900 |
| C | -1.92031300 | -0.74541700 | -7.03031000 |
| C | -0.38663300 | 1.15705600 | -7.09695300 |
| C | 0.77364100 | -2.63761700 | -2.38710500 |
| C | 0.66349200 | -2.44790600 | -1.04874800 |
| C | 0.47263400 | -1.98872100 | 1.91849300 |
| C | 0.41853800 | -1.77197300 | 3.25627800 |
| H | -3.14374000 | 2.74619600 | 6.94505100 |
| H | -2.44881000 | 1.87146500 | 5.52965300 |
| H | -2.90682100 | 0.94841200 | 7.00433100 |
| H | -1.94844900 | 3.10035300 | 8.88936600 |
| H | -1.69798500 | 1.31623900 | 9.08230200 |
| H | -0.28152400 | 2.42335600 | 9.10989000 |

| | | | |
|---|---|---|---|
| H | -1.28943900 | 4.21004400 | 6.97665800 |
| H | -0.55055300 | 3.35769600 | 5.56944200 |
| H | 0.40185600 | 3.56350000 | 7.08138500 |
| H | -0.65723400 | 0.09418300 | 7.42220100 |
| H | 0.72793400 | 1.20793100 | 7.38466300 |
| H | -0.95681100 | 0.32885900 | 4.95418500 |
| H | 0.35646500 | 1.52333000 | 4.88290000 |
| H | 1.96965500 | -0.18808500 | 5.73031900 |
| H | 0.66584700 | -1.38413400 | 5.82428200 |
| H | 2.73120200 | 0.60801000 | 3.64727300 |
| H | 2.93950600 | 0.32359800 | 1.23630900 |
| H | 3.05145300 | 0.02837500 | -0.79669300 |
| H | 3.13146500 | -0.41059500 | -3.19180200 |
| H | 2.58965500 | -1.73976500 | -5.02897500 |
| H | 1.37067800 | -3.02068000 | -4.91405200 |
| H | 0.77468700 | -0.00793200 | -4.86604800 |
| H | -0.43898900 | -1.30136900 | -4.76504900 |
| H | 1.48346600 | -0.80738700 | -7.12673100 |
| H | 0.34522800 | -2.16926300 | -7.02547800 |
| H | 0.63184600 | -0.15165300 | -9.17432700 |
| H | -0.49035800 | -1.55543500 | -9.12169800 |
| H | -1.14853800 | 0.11296500 | -9.38372700 |
| H | -2.62214000 | -0.14605800 | -7.62824400 |
| H | -2.07584200 | -0.56638900 | -5.96137300 |
| H | -2.01683900 | -1.81444500 | -7.25542900 |
| H | -0.56968600 | 1.31685500 | -6.02922600 |
| H | -1.13491100 | 1.69143600 | -7.70006400 |
| H | 0.63265800 | 1.46583700 | -7.35904300 |
| H | 0.16815700 | -3.37118400 | -2.92305200 |
| H | -0.05618900 | -3.06968000 | -0.51579600 |
| H | -0.20021600 | -2.74267100 | 1.50934900 |
| H | -0.26905700 | -2.31583200 | 3.90686600 |
| Cl | -3.42693800 | 5.00233300 | 8.10253600 |

| | | | |
|---|---|---|---|
| Cl | -3.11614300 | 1.70658100 | -9.30402400 |

S7. ([(NPr)$_2$V]$^{2+}$2Cl$^-$)2 (dimer)

Charge = 0, Multiplicity = 1, N = 132, E = -3999.47733307 Hartree

| | | | |
|---|---|---|---|
| C | 0.75980400 | 7.22924300 | -0.34924700 |
| N | 1.23703600 | 7.49549500 | -1.74924100 |
| C | 1.77069800 | 8.90181500 | -1.79671000 |
| C | 0.07882100 | 7.39249400 | -2.69521400 |
| C | 2.36218100 | 6.55770800 | -2.13532500 |
| C | 2.01354400 | 5.07717400 | -2.12462300 |
| C | 3.19923100 | 4.24540900 | -2.63740000 |
| N | 2.88948400 | 2.83114000 | -2.75292400 |
| C | 2.25113700 | 2.34505400 | -3.88748000 |
| C | 1.77595500 | 1.07746500 | -3.97009800 |
| C | 1.88229100 | 0.12719000 | -2.86377900 |
| C | 1.43402100 | -1.18477800 | -2.93303700 |
| C | 0.79721500 | -1.76455800 | -4.11513600 |
| C | 0.38145600 | -3.05465700 | -4.15547600 |
| N | 0.54868600 | -3.92788500 | -3.08630800 |
| C | -0.11823600 | -5.21594500 | -3.08027800 |
| C | -1.57307900 | -5.12493100 | -2.59638800 |
| C | -2.21931500 | -6.50047500 | -2.61478800 |
| N | -3.65272000 | -6.55038900 | -2.12988200 |
| C | -4.11386100 | -7.98008700 | -2.15398400 |
| C | -3.76254400 | -6.04478500 | -0.72256100 |
| C | -4.55937000 | -5.74642600 | -3.01604500 |
| C | 1.12118400 | -3.42004900 | -1.92599200 |
| C | 1.55613800 | -2.13840000 | -1.83210500 |
| C | 2.51845800 | 0.70610000 | -1.68083600 |
| C | 2.97769500 | 1.98264400 | -1.65636700 |
| H | -0.01492800 | 7.97745500 | -0.12964700 |
| H | 0.34071800 | 6.21844300 | -0.30036200 |
| H | 1.62355600 | 7.33287000 | 0.32046300 |

| | | | |
|---|---|---|---|
| H | 0.94485600 | 9.57212200 | -1.51973000 |
| H | 2.60142500 | 8.96780400 | -1.08218400 |
| H | 2.11710100 | 9.10420100 | -2.81762100 |
| H | -0.65204700 | 8.15733500 | -2.39488500 |
| H | -0.36215900 | 6.39293000 | -2.61911400 |
| H | 0.44417000 | 7.56955400 | -3.71435000 |
| H | 3.18036100 | 6.78115700 | -1.43483200 |
| H | 2.67227300 | 6.86868800 | -3.14333600 |
| H | 1.75662900 | 4.73792200 | -1.10949800 |
| H | 1.14846300 | 4.87137500 | -2.77304500 |
| H | 3.50938400 | 4.61004600 | -3.62909700 |
| H | 4.06575000 | 4.36340600 | -1.96935800 |
| H | 2.17180400 | 3.05088600 | -4.71647500 |
| H | 1.31141400 | 0.78102600 | -4.91073600 |
| H | 0.64545300 | -1.16458800 | -5.01266900 |
| H | -0.09400100 | -3.48560900 | -5.03871000 |
| H | -0.08468100 | -5.63046000 | -4.10002200 |
| H | 0.45130800 | -5.90035900 | -2.43233100 |
| H | -2.11601600 | -4.42418300 | -3.24852300 |
| H | -1.57262300 | -4.70232300 | -1.58043800 |
| H | -2.22945200 | -6.91370500 | -3.63323600 |
| H | -1.66203200 | -7.19578000 | -1.97127200 |
| H | -4.04601500 | -8.35156000 | -3.18319500 |
| H | -3.46238600 | -8.56610900 | -1.49516900 |
| H | -5.15039700 | -8.00034000 | -1.79353000 |
| H | -4.79665600 | -6.21247300 | -0.39285300 |
| H | -3.53723100 | -4.97410500 | -0.70728000 |
| H | -3.04859700 | -6.59614900 | -0.09921900 |
| H | -4.27468500 | -4.69073500 | -2.95850500 |
| H | -5.58353700 | -5.88321900 | -2.64506600 |
| H | -4.45623800 | -6.11485200 | -4.04367200 |
| H | -2.00161400 | -4.56449200 | 0.95461700 |
| H | 0.03199000 | -3.24064900 | 0.98596600 |

| | | | |
|---|---|---|---|
| H | 1.80401200 | -2.21316800 | 1.15297100 |
| H | 3.82292100 | -0.86676800 | 1.37786600 |
| Cl | -1.48699600 | 9.98849700 | -0.82478500 |
| Cl | -7.19757300 | -6.61677400 | -0.68814900 |
| C | 3.87762100 | 5.19000600 | 3.18774700 |
| N | 4.89754500 | 4.50008000 | 2.32929400 |
| C | 6.16445300 | 5.30711200 | 2.36019500 |
| C | 4.40049400 | 4.45607800 | 0.91546600 |
| C | 5.20384900 | 3.10840400 | 2.84116800 |
| C | 4.03991600 | 2.13198400 | 2.81101100 |
| C | 4.48718300 | 0.75786200 | 3.33093900 |
| N | 3.40917400 | -0.21250500 | 3.33511900 |
| C | 3.08855900 | -0.92225100 | 2.18391900 |
| C | 1.95318900 | -1.65718600 | 2.07719200 |
| C | 0.96460200 | -1.73555500 | 3.15096400 |
| C | -0.20654800 | -2.47515800 | 3.06207600 |
| C | -0.59089000 | -3.24653700 | 1.88069300 |
| C | -1.72501300 | -3.98983400 | 1.83769800 |
| N | -2.59867800 | -4.08523400 | 2.91406600 |
| C | -3.90492100 | -4.70333600 | 2.76760100 |
| C | -4.95582200 | -3.74561400 | 2.18577100 |
| C | -6.32589500 | -4.40613300 | 2.17170800 |
| N | -7.46442800 | -3.53242000 | 1.68738600 |
| C | -8.72921600 | -4.34638100 | 1.74070400 |
| C | -7.64083700 | -2.31997000 | 2.55089900 |
| C | -7.25262100 | -3.10209600 | 0.26302900 |
| C | -2.30681700 | -3.32843700 | 4.04256600 |
| C | -1.18691900 | -2.57017100 | 4.14268400 |
| C | 1.34485600 | -0.95577900 | 4.32818100 |
| C | 2.49502900 | -0.23987400 | 4.38276800 |
| H | 3.75405600 | 6.20698400 | 2.79294900 |
| H | 2.93010000 | 4.64444500 | 3.13040500 |
| H | 4.24630900 | 5.20734200 | 4.22024100 |

| | | | |
|---|---|---|---|
| H | 5.92983400 | 6.30768200 | 1.97476700 |
| H | 6.52135400 | 5.35591900 | 3.39563300 |
| H | 6.90778000 | 4.81087800 | 1.72523400 |
| H | 4.29781100 | 5.49380300 | 0.57069400 |
| H | 3.42614500 | 3.95843100 | 0.89347300 |
| H | 5.12811700 | 3.90314600 | 0.30947300 |
| H | 5.57887600 | 3.23865500 | 3.86613800 |
| H | 6.03170500 | 2.73775100 | 2.22043900 |
| H | 3.20780400 | 2.48910700 | 3.43660900 |
| H | 3.65676300 | 2.00497300 | 1.78734600 |
| H | 5.30580800 | 0.36724500 | 2.70655100 |
| H | 4.87660200 | 0.85110800 | 4.35692300 |
| H | 3.45564200 | 2.40388800 | -0.77284400 |
| H | 2.64234000 | 0.11766600 | -0.77127900 |
| H | 2.02065500 | -1.83672900 | -0.89482400 |
| H | 1.21601500 | -4.12807100 | -1.10025900 |
| H | -3.80482800 | -5.59478400 | 2.13022000 |
| H | -4.22928200 | -5.05543400 | 3.75917800 |
| H | -4.64503800 | -3.45493100 | 1.17067200 |
| H | -4.96428200 | -2.83540400 | 2.80427500 |
| H | -6.33882000 | -5.28964200 | 1.51653200 |
| H | -6.60629500 | -4.72182600 | 3.18685000 |
| H | -8.59630100 | -5.21366300 | 1.08088800 |
| H | -8.88912800 | -4.66585700 | 2.77779300 |
| H | -9.54701700 | -3.69705600 | 1.39722500 |
| H | -8.52996000 | -1.78807700 | 2.18224700 |
| H | -6.75372100 | -1.68340100 | 2.46616600 |
| H | -7.77488100 | -2.64826900 | 3.58905900 |
| H | -6.35356200 | -2.47896100 | 0.20747600 |
| H | -8.13994000 | -2.52285200 | -0.02919200 |
| H | -7.14415800 | -4.01034800 | -0.34416300 |
| H | -3.03603300 | -3.39831600 | 4.85190700 |
| H | -1.03380500 | -2.03000200 | 5.07716700 |

| | | | |
|---|---|---|---|
| H | 0.70438500 | -0.93685700 | 5.21021500 |
| H | 2.77666700 | 0.34335800 | 5.26165000 |
| Cl | 4.13248700 | 7.93212100 | 0.83035100 |
| Cl | -10.42568700 | -1.45775200 | 0.50898200 |

S8. $[(NPr)_2V]^{2+}2Cl^-+Na^+Cl^-$ (1:1)

Charge = 0, Multiplicity = 1, N = 68, E = -2622.16564356 Hartree

| | | | |
|---|---|---|---|
| C | -3.29295900 | 1.58910300 | 6.34575400 |
| N | -1.91062800 | 2.07627000 | 6.66534800 |
| C | -1.87429900 | 2.47712200 | 8.11294300 |
| C | -1.57242600 | 3.26190200 | 5.81739300 |
| C | -0.90217600 | 0.95625000 | 6.47403900 |
| C | -0.65091800 | 0.53090200 | 5.03808400 |
| C | 0.22737000 | -0.73074600 | 5.01483500 |
| N | 0.55669900 | -1.14979300 | 3.66528000 |
| C | 1.56825600 | -0.50518000 | 2.96626200 |
| C | 1.75976900 | -0.68443200 | 1.63548200 |
| C | 0.90516300 | -1.55283900 | 0.82841800 |
| C | 1.07740800 | -1.75243500 | -0.53442200 |
| C | 2.14059000 | -1.11798100 | -1.31371000 |
| C | 2.28266200 | -1.31797100 | -2.64695800 |
| N | 1.44467100 | -2.16318600 | -3.36971200 |
| C | 1.43452500 | -2.11977000 | -4.81840800 |
| C | 0.55863500 | -0.98310200 | -5.37085700 |
| C | 0.59744700 | -0.99078000 | -6.88911100 |
| N | -0.23217800 | 0.08043600 | -7.57606800 |
| C | -0.05635800 | -0.08504100 | -9.05810900 |
| C | -1.68630700 | -0.07167200 | -7.24179200 |
| C | 0.23169700 | 1.45219500 | -7.18481800 |
| C | 0.40332200 | -2.77682300 | -2.67892900 |
| C | 0.21595600 | -2.61181500 | -1.34638800 |
| C | -0.15885300 | -2.18026900 | 1.61134700 |
| C | -0.30633400 | -1.96181100 | 2.94300100 |

| | | | |
|---|---|---|---|
| H | -3.99912500 | 2.40732000 | 6.52913600 |
| H | -3.33710900 | 1.28894500 | 5.29377700 |
| H | -3.50909400 | 0.73672200 | 7.00156000 |
| H | -2.61510000 | 3.26966800 | 8.27107800 |
| H | -2.11705900 | 1.59260200 | 8.71609000 |
| H | -0.86818500 | 2.84338000 | 8.34777700 |
| H | -2.25636800 | 4.07830700 | 6.07698000 |
| H | -1.69140200 | 2.99895200 | 4.76132800 |
| H | -0.53574000 | 3.55383300 | 6.02391000 |
| H | -1.30189700 | 0.12215400 | 7.06741100 |
| H | 0.03144500 | 1.29058800 | 6.94501500 |
| H | -1.59294900 | 0.31106700 | 4.51186200 |
| H | -0.13412800 | 1.32468400 | 4.47726600 |
| H | 1.15750700 | -0.55153800 | 5.57488800 |
| H | -0.29371900 | -1.55971100 | 5.51936900 |
| H | 2.21921900 | 0.16700600 | 3.53310700 |
| H | 2.59181100 | -0.13081200 | 1.19882800 |
| H | 2.86168800 | -0.46243300 | -0.82499400 |
| H | 3.07540300 | -0.84127800 | -3.22706700 |
| H | 2.47071000 | -2.00043100 | -5.17210900 |
| H | 1.07223800 | -3.08936300 | -5.19484800 |
| H | 0.93382000 | -0.02969100 | -4.96945300 |
| H | -0.46763300 | -1.12254600 | -4.99896300 |
| H | 1.62522900 | -0.84802300 | -7.25074100 |
| H | 0.22874800 | -1.94876400 | -7.28133400 |
| H | 1.00531200 | 0.04004800 | -9.29988500 |
| H | -0.39562900 | -1.08808400 | -9.34083600 |
| H | -0.65581200 | 0.67787900 | -9.56767800 |
| H | -2.25071600 | 0.66682700 | -7.82254200 |
| H | -1.83282000 | 0.10654900 | -6.17190400 |
| H | -2.00165200 | -1.08739800 | -7.50779800 |
| H | 0.04045800 | 1.60967000 | -6.11876900 |
| H | -0.32987500 | 2.18507100 | -7.77539400 |

| | | | |
|---|---|---|---|
| H | 1.30405700 | 1.53263000 | -7.39794900 |
| H | -0.24270600 | -3.41651600 | -3.28362500 |
| H | -0.60995100 | -3.15691700 | -0.88840300 |
| H | -0.87142300 | -2.85475600 | 1.13566200 |
| H | -1.10517200 | -2.42788000 | 3.52350200 |
| Cl | -2.52887300 | -0.98090300 | 9.08391200 |
| Cl | 4.13615600 | 1.89630100 | 3.06781500 |
| Na | -0.04405800 | -1.12838000 | 9.23842900 |
| Cl | 2.02023800 | -0.16672200 | 8.27625600 |

S9. $[(NPr)_2V]^{2+}2Cl^-+PhN(Me)_3^+Cl^-$ (1:1)

Charge = 0, Multiplicity = 1, N = 91, E = -2865.71655752 Hartree

| | | | |
|---|---|---|---|
| C | 2.40170800 | 6.08653100 | 2.24805700 |
| N | 3.86448800 | 6.15395800 | 1.91674400 |
| C | 4.49081300 | 7.23738300 | 2.74747900 |
| C | 4.04159500 | 6.47753900 | 0.46660400 |
| C | 4.56567300 | 4.84869200 | 2.25939000 |
| C | 3.88762600 | 3.59303700 | 1.72701400 |
| C | 4.90629000 | 2.44821900 | 1.60347600 |
| N | 4.26568100 | 1.15780400 | 1.40775400 |
| C | 3.66259500 | 0.84065300 | 0.19969500 |
| C | 2.81908600 | -0.21469200 | 0.06091500 |
| C | 2.46572000 | -1.08185100 | 1.18281000 |
| C | 1.56412500 | -2.13375100 | 1.09548000 |
| C | 0.82527600 | -2.48556200 | -0.11739400 |
| C | -0.14836700 | -3.42955100 | -0.12399800 |
| N | -0.48916500 | -4.16458500 | 1.01121700 |
| C | -1.80463400 | -4.77078700 | 1.11231800 |
| C | -2.93099900 | -3.72819700 | 1.23648300 |
| C | -4.18206500 | -4.37465900 | 1.80928300 |
| N | -5.46971000 | -3.58811900 | 1.61379200 |
| C | -6.50377700 | -4.18368300 | 2.52547100 |
| C | -5.28757500 | -2.14369400 | 1.98093300 |

| | | | |
|---|---|---|---|
| C | -5.93708800 | -3.69462500 | 0.19572300 |
| C | 0.24050600 | -3.91768200 | 2.17104700 |
| C | 1.22668100 | -2.99160900 | 2.23029800 |
| C | 3.13995900 | -0.70583400 | 2.42406900 |
| C | 3.96974000 | 0.36422400 | 2.50753700 |
| H | 1.96668300 | 7.07393100 | 2.05216700 |
| H | 1.92235300 | 5.33845100 | 1.60856400 |
| H | 2.31621700 | 5.82409100 | 3.31221800 |
| H | 4.03776700 | 8.19544400 | 2.46596800 |
| H | 4.29165400 | 7.00078500 | 3.80150700 |
| H | 5.56792700 | 7.25298900 | 2.54242700 |
| H | 3.52884800 | 7.42354800 | 0.25707100 |
| H | 3.60498100 | 5.67671600 | -0.13967100 |
| H | 5.11324500 | 6.57150400 | 0.25553600 |
| H | 4.61222500 | 4.80961900 | 3.35648800 |
| H | 5.58407000 | 4.95550000 | 1.85967800 |
| H | 3.08819100 | 3.28534900 | 2.41863400 |
| H | 3.42238800 | 3.75940900 | 0.74338900 |
| H | 5.58699600 | 2.64804300 | 0.75957500 |
| H | 5.50551700 | 2.38536700 | 2.52495500 |
| H | 3.92185500 | 1.49154400 | -0.63815600 |
| H | 2.40856800 | -0.40117300 | -0.93212700 |
| H | 1.04349200 | -1.98474500 | -1.06166500 |
| H | -0.71177600 | -3.67948200 | -1.02586600 |
| H | -1.98439200 | -5.40871600 | 0.23148500 |
| H | -1.79902400 | -5.42920200 | 1.99419400 |
| H | -3.11054200 | -3.28147300 | 0.24671800 |
| H | -2.59157100 | -2.92203900 | 1.90425300 |
| H | -4.37102500 | -5.35932800 | 1.35918400 |
| H | -4.06640200 | -4.48699600 | 2.89598200 |
| H | -6.60251900 | -5.25011100 | 2.29043300 |
| H | -6.15855000 | -4.04251300 | 3.55741200 |
| H | -7.45642700 | -3.66783300 | 2.35711400 |

| | | | |
|---|---|---|---|
| H | -6.26643700 | -1.65392900 | 1.91666300 |
| H | -4.59386900 | -1.67778200 | 1.27381100 |
| H | -4.89640500 | -2.10745700 | 3.00634100 |
| H | -5.16560900 | -3.29089400 | -0.46886700 |
| H | -6.86143800 | -3.11478800 | 0.08989800 |
| H | -6.12206000 | -4.75032900 | -0.03470900 |
| H | -0.02613700 | -4.53858400 | 3.02882000 |
| H | 1.77166300 | -2.90267900 | 3.17016300 |
| H | 2.97196700 | -1.27367900 | 3.33864100 |
| H | 4.46351100 | 0.66875000 | 3.43516200 |
| Cl | -4.08220200 | -3.14334000 | 5.16058900 |
| Cl | 3.21354100 | 5.41449800 | 5.56921600 |
| C | 2.33717400 | 1.85440200 | 5.84249100 |
| C | 1.07006600 | 2.42725300 | 5.73985900 |
| C | -0.07427700 | 1.62272900 | 5.67677000 |
| C | 0.06436600 | 0.23468400 | 5.72086300 |
| C | 1.33120800 | -0.35094900 | 5.83493800 |
| C | 2.46194900 | 0.46325800 | 5.89281700 |
| N | -1.12679200 | -0.66920000 | 5.62332400 |
| C | -0.98018200 | -1.56145300 | 4.41295300 |
| C | -1.23240100 | -1.53036600 | 6.85850500 |
| C | -2.42665900 | 0.07160400 | 5.48345500 |
| H | 3.22904900 | 2.48321600 | 5.85590500 |
| H | 0.98496400 | 3.51525500 | 5.70186200 |
| H | -1.04834400 | 2.09815900 | 5.58913500 |
| H | 1.45330100 | -1.43375700 | 5.86490500 |
| H | 3.45516200 | 0.01534000 | 5.96327100 |
| H | -0.89266100 | -0.92389700 | 3.52648300 |
| H | -1.87196100 | -2.20099500 | 4.36476200 |
| H | -0.08005000 | -2.16781300 | 4.52428500 |
| H | -2.10470200 | -2.18391600 | 6.72541700 |
| H | -0.32057600 | -2.12637800 | 6.96025700 |
| H | -1.35545500 | -0.87037400 | 7.72471300 |

| | | | |
|---|---|---|---|
| H | -2.40081500 | 0.66936700 | 4.56652000 |
| H | -3.21419200 | -0.69034900 | 5.42292500 |
| H | -2.57302100 | 0.70947500 | 6.36115000 |
| Cl | 5.87583100 | 2.08922700 | 5.08129400 |

S10. $([(NPr)_2V]^{2+}2Cl^-)2+Na^+Cl^-$ (trimer)

Charge = 0, Multiplicity = 1, N = 134, E = -4621.98001438 Hartree

| | | | |
|---|---|---|---|
| C | 0.66118000 | 5.02236800 | 0.57099700 |
| N | 0.48629200 | 5.32302100 | -0.89006800 |
| C | 0.22197700 | 6.79379000 | -1.03334000 |
| C | -0.67344300 | 4.54825200 | -1.43538500 |
| C | 1.76202300 | 5.01223900 | -1.65604200 |
| C | 2.10978100 | 3.53694000 | -1.73283800 |
| C | 3.45878100 | 3.32554300 | -2.43271700 |
| N | 3.68560600 | 1.92227000 | -2.74840300 |
| C | 3.19589500 | 1.40788700 | -3.94473600 |
| C | 3.03129200 | 0.08063600 | -4.15566300 |
| C | 3.30608000 | -0.91307100 | -3.12073400 |
| C | 3.02010700 | -2.26102100 | -3.27265600 |
| C | 2.46103500 | -2.82832400 | -4.49793800 |
| C | 2.01471700 | -4.10449500 | -4.56180700 |
| N | 2.08403900 | -4.98432900 | -3.48028900 |
| C | 1.04080100 | -5.99644000 | -3.36789000 |
| C | -0.28183500 | -5.34619000 | -2.94035200 |
| C | -1.44620800 | -6.31943500 | -2.91890100 |
| N | -2.79241900 | -5.65699900 | -2.69209400 |
| C | -3.83696800 | -6.72093500 | -2.52482400 |
| C | -2.77267500 | -4.81671100 | -1.45005800 |
| C | -3.18092500 | -4.79971300 | -3.86302500 |
| C | 2.70229500 | -4.51474600 | -2.32311200 |
| C | 3.18696500 | -3.25291300 | -2.21283300 |
| C | 3.85799700 | -0.32530100 | -1.89922600 |
| C | 4.01014900 | 1.01854100 | -1.74879100 |

| | | | |
|---|---|---|---|
| H | -0.27358500 | 5.28247200 | 1.08208900 |
| H | 0.88842800 | 3.96016900 | 0.71530900 |
| H | 1.49225100 | 5.64066200 | 0.93566800 |
| H | -0.68208700 | 7.04072200 | -0.46442300 |
| H | 1.09100100 | 7.33018600 | -0.63084200 |
| H | 0.07702600 | 7.02413600 | -2.09531200 |
| H | -1.58122600 | 4.87945400 | -0.91755600 |
| H | -0.51554000 | 3.47641900 | -1.26634700 |
| H | -0.75673700 | 4.75224300 | -2.51002300 |
| H | 2.54724800 | 5.59729300 | -1.15400300 |
| H | 1.61103700 | 5.42403600 | -2.66407600 |
| H | 2.15994800 | 3.08732200 | -0.72945900 |
| H | 1.34537200 | 2.98086400 | -2.29401000 |
| H | 3.49912700 | 3.89135600 | -3.37581500 |
| H | 4.28527500 | 3.68848800 | -1.80534700 |
| H | 2.96292300 | 2.15206000 | -4.70842300 |
| H | 2.66315900 | -0.22681800 | -5.13421700 |
| H | 2.39806600 | -2.22971500 | -5.40703300 |
| H | 1.58005400 | -4.52436400 | -5.47186100 |
| H | 0.92836800 | -6.49390900 | -4.34419800 |
| H | 1.36060300 | -6.75758400 | -2.63998200 |
| H | -0.48473400 | -4.52375100 | -3.64270900 |
| H | -0.13374600 | -4.89601300 | -1.94777300 |
| H | -1.53161100 | -6.86064500 | -3.87185700 |
| H | -1.32964700 | -7.05753900 | -2.11319700 |
| H | -3.85408800 | -7.34191300 | -3.42820700 |
| H | -3.57983300 | -7.32917000 | -1.64972600 |
| H | -4.80124100 | -6.21908200 | -2.37679400 |
| H | -3.79546300 | -4.45383100 | -1.28111800 |
| H | -2.10531300 | -3.96368800 | -1.60644300 |
| H | -2.41547600 | -5.43425200 | -0.61725900 |
| H | -2.44995900 | -3.99307400 | -3.97821500 |
| H | -4.17099300 | -4.37697300 | -3.64585600 |

| | | | |
|---|---|---|---|
| H | -3.20079300 | -5.42864800 | -4.76091000 |
| H | -0.30668900 | -3.31216100 | -0.07520300 |
| H | 2.05206100 | -2.99830600 | 0.39318400 |
| H | 4.06700500 | -2.47981400 | 0.82706600 |
| H | 6.19016600 | -1.33178500 | 1.18571100 |
| Cl | -0.26847900 | 0.59327500 | -1.60346900 |
| Cl | -5.95310500 | -3.54601300 | -1.99238600 |
| C | 4.63508100 | 4.56217900 | 2.97880600 |
| N | 5.76461000 | 4.29134500 | 2.02435600 |
| C | 6.66385700 | 5.49132800 | 2.00131700 |
| C | 5.19412000 | 4.08995600 | 0.65116900 |
| C | 6.57569200 | 3.08399400 | 2.45637100 |
| C | 5.81186500 | 1.77582100 | 2.38161900 |
| C | 6.57236100 | 0.59086100 | 2.99152400 |
| N | 5.69359100 | -0.57063000 | 3.08471600 |
| C | 5.38856000 | -1.28174100 | 1.92657200 |
| C | 4.19145800 | -1.89038900 | 1.73515800 |
| C | 3.09680000 | -1.75885000 | 2.69518500 |
| C | 1.78159300 | -2.10116700 | 2.42010900 |
| C | 1.33559600 | -2.69091100 | 1.15523800 |
| C | 0.01850600 | -2.88927200 | 0.87608300 |
| N | -0.98891600 | -2.59000500 | 1.77720400 |
| C | -2.37360400 | -2.51222200 | 1.33509000 |
| C | -2.63600700 | -1.25141200 | 0.50594200 |
| C | -4.10672700 | -1.12583400 | 0.14663700 |
| N | -4.41434200 | -0.06794400 | -0.89177900 |
| C | -5.90835800 | 0.04184400 | -1.01472500 |
| C | -3.85229100 | 1.26814600 | -0.50546500 |
| C | -3.86549400 | -0.45921700 | -2.23699100 |
| C | -0.61701600 | -2.04388800 | 3.00060900 |
| C | 0.67683200 | -1.82426600 | 3.33776600 |
| C | 3.51373900 | -1.13741200 | 3.95018000 |
| C | 4.73202000 | -0.56797600 | 4.09669900 |

| | | | |
|---|---|---|---|
| H | 4.15871000 | 5.49760100 | 2.65761500 |
| H | 3.91008200 | 3.74257000 | 2.91894900 |
| H | 5.04859300 | 4.65451200 | 3.99010200 |
| H | 6.06157700 | 6.35381300 | 1.68919000 |
| H | 7.07249700 | 5.64276100 | 3.00757300 |
| H | 7.47444500 | 5.30753600 | 1.28623500 |
| H | 4.73583900 | 5.03991500 | 0.34512800 |
| H | 4.42472300 | 3.31191500 | 0.70402700 |
| H | 6.00677500 | 3.79858200 | -0.02516200 |
| H | 6.90602800 | 3.29471100 | 3.48359300 |
| H | 7.46297000 | 3.06563200 | 1.80813400 |
| H | 4.84988600 | 1.86229800 | 2.90560500 |
| H | 5.57153900 | 1.52624900 | 1.33824100 |
| H | 7.45152800 | 0.32684000 | 2.38352100 |
| H | 6.92872600 | 0.83627900 | 4.00434000 |
| H | 4.41178400 | 1.45163100 | -0.83200400 |
| H | 4.18921700 | -0.95727900 | -1.07397800 |
| H | 3.70920800 | -2.99427300 | -1.29264400 |
| H | 2.78657300 | -5.24233300 | -1.51260100 |
| H | -2.61019000 | -3.41112900 | 0.74872800 |
| H | -3.01579000 | -2.53341900 | 2.22798700 |
| H | -2.00642800 | -1.28329000 | -0.39441100 |
| H | -2.30166500 | -0.37823600 | 1.08668000 |
| H | -4.51279400 | -2.06173800 | -0.26578400 |
| H | -4.69720100 | -0.85962500 | 1.03488500 |
| H | -6.29451300 | -0.94487000 | -1.30273800 |
| H | -6.31250500 | 0.34741100 | -0.04170400 |
| H | -6.11764400 | 0.80046900 | -1.78202600 |
| H | -4.21107200 | 1.99372500 | -1.24977400 |
| H | -2.75769300 | 1.21093500 | -0.53073600 |
| H | -4.21011200 | 1.51967500 | 0.50087700 |
| H | -2.77091600 | -0.47912000 | -2.18370700 |
| H | -4.19161600 | 0.31392300 | -2.94691200 |

| | | | |
|---|---|---|---|
| H | -4.28211000 | -1.44223900 | -2.49103000 |
| H | -1.44180300 | -1.81341000 | 3.67704000 |
| H | 0.87086100 | -1.40648000 | 4.32520700 |
| H | 2.84281500 | -1.11912700 | 4.80957700 |
| H | 5.03786500 | -0.07575100 | 5.02288100 |
| Cl | 3.53206500 | 7.19629900 | 0.69716100 |
| Cl | -5.34982400 | 2.58901900 | -3.46015700 |
| Na | 1.56898300 | 0.06920500 | 0.09628900 |
| Cl | 2.22671800 | 1.95579800 | 1.69368800 |

S11. $([(NPr)_2V]^{2+}2Cl^-)2+PhN(Me)_3^+Cl^-$ (trimer)

Charge = 0, Multiplicity = 1, N = 157, E = -4865.49026915 Hartree

| | | | |
|---|---|---|---|
| C | 1.20462600 | 5.15091000 | 2.89198700 |
| N | 2.52426000 | 5.59749500 | 2.33267700 |
| C | 2.84121600 | 6.95383100 | 2.89816800 |
| C | 2.41071300 | 5.72007300 | 0.84403000 |
| C | 3.63397300 | 4.64212500 | 2.73197500 |
| C | 3.33175500 | 3.18326700 | 2.42475500 |
| C | 4.59400900 | 2.31169400 | 2.35832500 |
| N | 4.24971800 | 0.93296300 | 2.03584500 |
| C | 3.77483800 | 0.63222700 | 0.76276000 |
| C | 2.98838000 | -0.44453200 | 0.51027400 |
| C | 2.55222100 | -1.35286600 | 1.56705700 |
| C | 1.64941100 | -2.38910900 | 1.37837400 |
| C | 0.97406100 | -2.67441300 | 0.11363800 |
| C | -0.02847800 | -3.58316000 | 0.01927500 |
| N | -0.45161400 | -4.35221400 | 1.10313300 |
| C | -1.81622300 | -4.85199900 | 1.14029700 |
| C | -2.83747800 | -3.72861900 | 1.39551700 |
| C | -4.14970500 | -4.30642400 | 1.89709600 |
| N | -5.32152900 | -3.33557300 | 1.90816500 |
| C | -6.41226800 | -3.95512700 | 2.73413100 |
| C | -4.93580500 | -2.02716200 | 2.53601800 |

| | | | |
|---|---|---|---|
| C | -5.82365800 | -3.10148700 | 0.51759700 |
| C | 0.22481200 | -4.17604100 | 2.30775800 |
| C | 1.23140100 | -3.28340500 | 2.45537700 |
| C | 3.13104600 | -1.02631700 | 2.86761400 |
| C | 3.90451700 | 0.06781800 | 3.06818300 |
| H | 0.47194200 | 5.92152000 | 2.62197800 |
| H | 0.92925300 | 4.19097300 | 2.44364900 |
| H | 1.31714800 | 5.06805900 | 3.98096700 |
| H | 2.05143000 | 7.64162800 | 2.57007900 |
| H | 2.85512800 | 6.86490700 | 3.99252400 |
| H | 3.81953200 | 7.26787600 | 2.51435100 |
| H | 1.59589200 | 6.42468300 | 0.63401600 |
| H | 2.17901800 | 4.74038900 | 0.41299000 |
| H | 3.36245800 | 6.09387100 | 0.44789200 |
| H | 3.77941600 | 4.79467600 | 3.81024500 |
| H | 4.53189600 | 4.98819900 | 2.20014300 |
| H | 2.65579000 | 2.76540200 | 3.18630900 |
| H | 2.82151400 | 3.08946800 | 1.45427100 |
| H | 5.28124700 | 2.70070700 | 1.58939200 |
| H | 5.12720200 | 2.31296600 | 3.32116800 |
| H | 4.08949400 | 1.31896100 | -0.02646400 |
| H | 2.69063600 | -0.61750800 | -0.52486600 |
| H | 1.25759400 | -2.14331400 | -0.79628700 |
| H | -0.55409700 | -3.77575600 | -0.91881400 |
| H | -2.04279400 | -5.36325000 | 0.19131200 |
| H | -1.87455700 | -5.60615200 | 1.94035100 |
| H | -2.96564400 | -3.14682800 | 0.46981900 |
| H | -2.41879900 | -3.05112800 | 2.15443000 |
| H | -4.47882000 | -5.15825300 | 1.28553400 |
| H | -4.02743500 | -4.63122600 | 2.93976400 |
| H | -6.66190300 | -4.93261600 | 2.30456500 |
| H | -6.03297100 | -4.06409100 | 3.75815800 |
| H | -7.28710100 | -3.29487000 | 2.70834800 |

| | | | |
|---|---|---|---|
| H | -5.84021800 | -1.41291400 | 2.61792600 |
| H | -4.20319300 | -1.52301400 | 1.89781800 |
| H | -4.51773800 | -2.24504800 | 3.52754200 |
| H | -5.01857800 | -2.67298200 | -0.08890400 |
| H | -6.66672200 | -2.40240000 | 0.56604600 |
| H | -6.14867500 | -4.05972400 | 0.09574100 |
| H | -0.10520000 | -4.82056500 | 3.12525100 |
| H | 1.72598300 | -3.24744700 | 3.42412100 |
| H | 2.93159200 | -1.65191500 | 3.73451000 |
| H | 4.32140900 | 0.32278700 | 4.04709200 |
| Cl | -3.86869400 | -3.79832600 | 5.42153100 |
| Cl | 2.33020800 | 5.58418100 | 6.21065100 |
| C | 1.88138500 | 1.95370000 | 6.04907000 |
| C | 0.56285100 | 2.35722200 | 5.84623700 |
| C | -0.46721100 | 1.41266800 | 5.78158200 |
| C | -0.15850000 | 0.05921500 | 5.92428400 |
| C | 1.16354200 | -0.35422400 | 6.12216600 |
| C | 2.17989800 | 0.59604400 | 6.18459000 |
| N | -1.22239800 | -0.99314500 | 5.85425500 |
| C | -0.94053400 | -1.90649400 | 4.68455900 |
| C | -1.23470200 | -1.80675000 | 7.12502900 |
| C | -2.60404400 | -0.43119200 | 5.67555500 |
| H | 2.66908700 | 2.70607000 | 6.11628900 |
| H | 0.33427400 | 3.41967900 | 5.75678600 |
| H | -1.48748000 | 1.75718500 | 5.63175300 |
| H | 1.41863400 | -1.40809300 | 6.23133300 |
| H | 3.21838800 | 0.29482200 | 6.33554500 |
| H | -0.92974100 | -1.29959300 | 3.77277000 |
| H | -1.73653300 | -2.66270300 | 4.65490600 |
| H | 0.03423600 | -2.37618000 | 4.82982800 |
| H | -2.01139600 | -2.57420900 | 7.01194800 |
| H | -0.25424900 | -2.27002500 | 7.26825200 |
| H | -1.45570500 | -1.13092700 | 7.95876300 |

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|---|---|---|---|
| H | -2.65149200 | 0.11017500 | 4.72516600 |
| H | -3.29041000 | -1.28757000 | 5.66267800 |
| H | -2.82869000 | 0.23505700 | 6.51507100 |
| Cl | 5.70143300 | 0.82770600 | 6.11565100 |
| C | -1.95234500 | 5.82051900 | 4.25375100 |
| N | -1.96731400 | 6.98259200 | 5.20190400 |
| C | -2.94389700 | 7.99826500 | 4.68565900 |
| C | -0.60718500 | 7.62385300 | 5.24379100 |
| C | -2.39965300 | 6.54598600 | 6.58660800 |
| C | -1.58925200 | 5.39481300 | 7.16181600 |
| C | -1.79509300 | 5.26771600 | 8.67824200 |
| N | -0.96923800 | 4.21800800 | 9.24942600 |
| C | 0.40670100 | 4.41212300 | 9.32030400 |
| C | 1.27946000 | 3.39193700 | 9.49307200 |
| C | 0.84695800 | 2.00142800 | 9.59117200 |
| C | 1.73070900 | 0.93711800 | 9.68431200 |
| C | 3.18253400 | 1.09490900 | 9.65408500 |
| C | 4.02716500 | 0.03612000 | 9.64647000 |
| N | 3.58039800 | -1.27987300 | 9.72120400 |
| C | 4.44436600 | -2.35472100 | 9.26147100 |
| C | 4.45770400 | -2.44852700 | 7.72956700 |
| C | 5.23252500 | -3.66619700 | 7.25798800 |
| N | 5.22247200 | -3.87923300 | 5.75945700 |
| C | 5.96331100 | -5.14731000 | 5.44607300 |
| C | 3.81996100 | -4.02116000 | 5.24536400 |
| C | 5.90435400 | -2.74666900 | 5.04547200 |
| C | 2.20289500 | -1.48241200 | 9.75836500 |
| C | 1.31324400 | -0.45939600 | 9.76066000 |
| C | -0.60547100 | 1.85275700 | 9.52582300 |
| C | -1.43441200 | 2.91068200 | 9.33816000 |
| H | -1.72929600 | 6.21523800 | 3.25431000 |
| H | -1.17801200 | 5.11284600 | 4.56429000 |
| H | -2.93756100 | 5.33948000 | 4.27866400 |

| | | | |
|---|---|---|---|
| H | -2.59225400 | 8.32625500 | 3.69932100 |
| H | -3.93236100 | 7.53013900 | 4.60990800 |
| H | -2.97535100 | 8.84102400 | 5.38619300 |
| H | -0.37146100 | 7.94832400 | 4.22109800 |
| H | 0.14376800 | 6.90517400 | 5.59635800 |
| H | -0.66045000 | 8.48175500 | 5.92504400 |
| H | -3.46329500 | 6.28129800 | 6.50894900 |
| H | -2.31608400 | 7.44173800 | 7.21834200 |
| H | -1.86982200 | 4.44349300 | 6.68484300 |
| H | -0.51426300 | 5.54442700 | 6.97793400 |
| H | -1.53902300 | 6.22184300 | 9.16757800 |
| H | -2.84781400 | 5.05108200 | 8.91436500 |
| H | 0.74096600 | 5.44414400 | 9.20517900 |
| H | 2.33812200 | 3.64772200 | 9.52699600 |
| H | 3.63029800 | 2.08709300 | 9.60133900 |
| H | 5.10883400 | 0.15779300 | 9.56705200 |
| H | 5.46097200 | -2.17964900 | 9.64713900 |
| H | 4.08484800 | -3.29854200 | 9.70093700 |
| H | 4.88917000 | -1.52064200 | 7.32134400 |
| H | 3.41137800 | -2.50331500 | 7.39402600 |
| H | 6.29057400 | -3.59933900 | 7.54883800 |
| H | 4.81665900 | -4.58602500 | 7.69349200 |
| H | 6.98960700 | -5.05179200 | 5.82000300 |
| H | 5.45462300 | -5.98064200 | 5.94540100 |
| H | 5.94714200 | -5.27378000 | 4.35440000 |
| H | 3.89004400 | -4.25540100 | 4.17371000 |
| H | 3.28505700 | -3.07918100 | 5.39690500 |
| H | 3.32584000 | -4.82780800 | 5.80027500 |
| H | 5.40860500 | -1.79834200 | 5.27981800 |
| H | 5.85408100 | -2.96766600 | 3.97044300 |
| H | 6.94435900 | -2.70415300 | 5.39162400 |
| H | 1.88804200 | -2.52716400 | 9.80026400 |
| H | 0.25586200 | -0.71722900 | 9.81933200 |

| | | | |
|---|---|---|---|
| H | -1.06461600 | 0.86679900 | 9.60415500 |
| H | -2.51730000 | 2.79541200 | 9.25962400 |
| Cl | -0.53441600 | 8.00131500 | 1.70565000 |
| Cl | 5.11937000 | -4.48148600 | 2.01113000 |

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