Supporting Information

for

# Direct Access to 2-Aryl Substituted Pyrrolinium Salts for Carbon Centre Based Radicals *without* Pyrrolidine-2-Ylidene *alias* cyclic(Alkyl)(Amino)Carbenes (CAAC) as a Precursor

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**General Considerations**

All experiments were carried out under an argon atmosphere using standard Schlenk techniques or in a PL-HE-2GB Innovative Technology GloveBox. *n*Hexane, diethyl ether and THF were dried by PS-MD-5 Innovative Technology solvent purification system. Benzoyl chloride (synthesis grade) was purchased from SD fine chemicals. $PCl_5$ (97%) was purchased from AVRA. Isopropyl amine (≥99.5%), isopropylmagnesium chloride solution (2.0 M in THF), *p*-Toluoyl chloride (98%), and 4-*tert*-butylbenzoyl chloride (98%) were purchased from Merck (Sigma-Aldrich). 4-Ethylbenzoyl chloride (≥98%) was purchased from Alpha-Aesar. All the chemicals were used without further purifications. Dichloromethane and acetonitrile were dried and distilled over $CaH_2$. Benzene-$d_6$ was dried and distilled over potassium under argon. Chloroform-$d_1$ and acetonitrile-$d_3$ were dried and distilled over $CaH_2$ under argon.

**NMR spectroscopy**

NMR spectra were recorded on a BrukerNanoBay 300 MHz NMR spectrometer. $^{1}H$ and $^{13}C\{^{1}H\}$ NMR spectra were referenced to the peaks of residual protons of the deuterated solvent ($^{1}H$) or the deuterated solvent itself ($^{13}C\{^{1}H\}$). $^{19}F\{^{1}H\}$ NMR spectra were referenced to external tol-$CF_3$.

**Crystallographic Details**

Single crystal X-ray data of all the compounds were collected at 120 K on a Rigaku Xtalab Pro using graphite-monochromated Mo K$\alpha$ radiation ($\lambda_\alpha$ = 0.71069 Å). Data integration and reduction were processed with CrysAlis Pro software. The structure was solved by direct methods using ShelXT[S1] and programs and refined by full matrix least-squares method based on $F^2$ using SHELXL[S2] in the Olex-2[S3] software. Hydrogens were fixed in their ideal geometries and their contributions included in the refinement. Crystal data and structure refinement of all these compounds are formulated in Tables S30-S34.

**Electrochemistry**

Cyclic voltammograms were recorded with a PAR VersaStat 4 potentiostat (Ametek) by working in anhydrous and degassed DMF (99.8 % extra dry, Acros Organics) or anhydrous and degassed acetonitrile ($H_2O$ ≤ 0.005%, puriss., Sigma Aldrich) distilled from $P_2O_5$ with 0.1 M $NBu_4PF_6$ (dried, > 99.0 %, electrochemical grade, Fluka) as electrolyte. Concentrations of the complexes were about $1x10^{-4}$m. A three-electrode setup was used with a glassy carbon, gold or platinum working electrode, a coiled platinum wire as counter electrode, and a coiled silver wire as a pseudoreference electrode. The ferrocene/ferrocenium couple was used as internal reference.

**UV/Vis/NIR spectroscopy and spectroelectrochemistry**

UV/Vis/NIR spectra were recorded with an Avantes spectrometer consisting of a light source (AvaLight-DH-S-Bal), a UV/Vis detector (AvaSpec-ULS2048), and an NIR detector (AvaSpec-NIR256-TEC). Spectroelectrochemical measurements were carried out in an optically transparent thin-layer electrochemical (OTTLE) cell ($CaF_2$ windows) with a platinum-mesh or a gold-mesh working electrode, a platinum-mesh counter electrode, and a silver-foil pseudoreference electrode. The OTTLE cell with the gold working electrode was build analogous to the one with the platinum working electrode (100 mesh woven from 0.064 mm

diameter wire; 99.99% (metals basis)). Anhydrous and degassed DMF (99.8 % extra dry, Acros Organics) or anhydrous and degassed acetonitrile ($H_2O \leq 0.005\%$, puriss., Sigma Aldrich) distilled from $P_2O_5$ with 0.1 M $NBu_4PF_6$ as electrolyte was used as the solvent.

**Electron paramagnetic resonance spectroelectrochemistry**

EPR spectra at X-band frequency (ca. 9.5 GHz) were obtained with a Magnettech MS-5000 bench top EPR spectrometer equipped with a rectangular TE 102 cavity. The measurements were carried out in synthetic quarz glass tubes. For EPR spectroelectrochemistry a three-electrode setup was employed using two teflon-coated platinum wires (0.005" bare, 0.008" coated) as working (or a teflon-coated gold wire (0.003" bare, 0.0055" coated) as working electrode) and counter electrode and a Teflon-coated silver wire (0.005" bare, 0.007" coated) as pseudoreference electrode.

**Computational Details**

The program package ORCA 4.0.1.2 was used for all DFT calculations.[S4] Starting from the molecular structure obtained from X-ray diffraction geometry optimizations were carried out using the PBEh-3c method as developed by Grimme and co-workers[S5] and no symmetry restrictions were imposed during the optimization. Subsequent single-point calculations were performed on the optimized geometries using the B3LYP, TPSSh, PBE0 and M06L functionals. [S6] All calculations were run with empirical Van der Waals correction (D3).[S7] The restricted and unrestricted DFT methods were employed for closed and open shell molecules respectively unless otherwise stated. Convergence criteria were set to default for geometry-optimization (OPT), and tight for SCF calculations (TIGHTSCF). Relativistic effects were included with the zeroth-order regular approximation (ZORA).[S8] Triple- ζ – valence basis sets (TZVP-ZORA)[S9] were employed for all atoms. Calculations were performed using resolution of the identity approximation[S10] with matching auxiliary basis sets[S11] for geometry optimizations and numerical frequency calculations and the RIJCOSX (combination of the resolution of the identity and chain of spheres algorithms) approximation for single point calculations using the B3LYP functional, where applicable.[S10] Low-lying excitation energies were calculated with time-dependent DFT (TD-DFT). Solvent effects were taken into account with the conductor-like polarizable continuum model (CPCM).[S12] For all calculations. Spin densities were calculated according to the Löwdin population analysis.[S13] The absence of imaginary frequency confirmed that the optimized geometries represent local minima. Spin densities and difference densities were visualized with the modified Avogadro 1.2.0 program with extended ORCA support.[S14] Calculations of EPR parameters and spin density evaluations were carried out with the PBE0 functional[S15] and the IGLO-III basis set.[S16] NPA charge analysis were performed with JANPA programme.[S17]

**Experimental Details and Analytical Data**

**Synthesis of $3^H$.** a) Benzoyl chloride, $1^H$ (42.1g, 300.0 mmol) and triethylamine (30.3 g, 300.0 mmol) were taken in a 2-Lit round bottom flask which contain 1200 mL of DCM. The resultant mixture was kept in ice bath and isopropylamine (17.8 g, 300.0 mmol) was added drop wise into this ice-cooled reaction mixture for an over of 1hr period of time. On complete addition of isopropylamine, the ice bath was removed and the reaction mixture was stirred for overnight followed by reflux for 3hrs. Then the reaction mixture was extracted with 1 M aqueous HCl solution and with 1 M aqueous NaOH solution, sequentially followed by washed with brine solution. The resulting organic layer was passed through anhydrous $Na_2SO_4$. On evaporation of all volatiles followed by washing with cold diethyl ether white color crystalline solid was obtained as desired *N*-isopropylbenzamide.

**Yield:** 35.14 g (215 mmol, 72%)

**$^1$H NMR** (300 MHz, $CDCl_3$, 298 K): $\delta$ = 1.26 (d, 6.6 Hz, 6H, CH(C*H*$_3$)$_2$), 4.36–4.21 (m, 1H, C*H*(CH$_3$)$_2$), 5.97 (br, 1H, N*H*), 7.36–7.50 (m, 3H, *m*- and *p*-Ph*H*), 7.73–7.78 (m, 2H, *o*-Ph*H*) ppm.

b) At room temperature, $PCl_5$ (47.0 g, 225.7 mmol) was added portion-wise into a toluene suspension of *N*-isopropylbenzamide (30.50 g, 186.8 mmol in toluene 100 mL). The resultant turbid solution was stirred for 1h at room temperature followed by refluxed for 3hrs until a faint yellow clear solution was obtained. Then all the volatiles were distilled off under high vacuum and the residue was distilled at 90 °C in 0.1 Torr pressure that gave 28.83 g of *N*-isopropylbenzimidoyl chloride, $1^H$ as a colorless oil.

Yield: 28.83 g (159.2 mmol, 85%)

**$^1$H NMR** (300 MHz, $CDCl_3$, 298 K): $\delta$ = 1.29 (d, 6.3 Hz, 6H, NCH(C*H*$_3$)$_2$), 4.17 (sep, 6.3 Hz, 1H, NC*H*(CH$_3$)$_2$), 7.37–7.46 (m, 3H, *m*- and *p*-Ph*H*), 7.97–8.01 (m, 2H, *o*-Ph*H*) ppm.

c) Isopropyl magnesium bromide (2(M) in THF, 7.9 ml, 15.8 mmol) was added dropwise to a THF solution of chloroimine, $1^H$ (2.88 g, 15.8 mmol in 100 ml THF) at 0 °C. On complete addition, the resultant deep yellow solution was stirred for 1h at room temperature followed by refluxed for 3hrs. After removal of all volatiles, the residue was quenched by water. The reaction mixture was then extracted with DCM and the organic layer was passed through anhydrous $Na_2SO_4$. The residue obtained on evaporation of all the volatiles was distilled at 100 °C at 0.1 Torr pressure to get pure imine, $2^H$ as a colorless liquid.

Yield: 1.1g (36%, 5.81 mmol)

**$^1$H NMR** (300 MHz, $CDCl_3$, 298 K) $\delta$ = 0.98 (d, 6.6 Hz, 6H, CCH(C*H*$_3$)$_2$), 1.01 (d, 6.9 Hz, 6H, NCH(C*H*$_3$)$_2$), 2.68 (sep, 6.9 Hz, 1H, CC*H*(CH$_3$)$_2$), 3.22 (sep, 6.3 Hz, 1H, NC*H*(CH$_3$)$_2$), 6.95 (d, 2H, 7.2 Hz, *o*-Ph*H*), 7.23–7.34 (m, 3H, *m*- and *p*-Ph*H*) ppm.

d) *n*BuLi (1.6 M solution in *n*hexane, 27.7 mL, 44.3 mmol) was added dropwise to a diethylether solution of $2^H$ (8.0 g, 42.2 mmol in 200 mL dry diethyl ether) at –78 °C and during the addition time a color change from colorless to light yellow with slight turbidity was observed. After stirring the reaction mixture at –78 °C for 1h, isobutylene oxide (4 mL, 44.3 mmol) was added. The reaction mixture was allowed to reach room temperature in 1h and then stirring was continued for another 1h at room temperature. The reaction mixture again cooled down to –78 °C and triflic anhydride (7.60 mL, 44.3 mmol) was added to it dropwise at –78 °C. During addition of triflic anhydride, the formation of voluminous white precipitate was observed. On complete addition, the reaction mixture was allowed to reach room temperature in 2hrs and stirring was continued for another 1h at room temperature. The reaction mixture was filtered through a G4 sintered funnel and washed with diethyl ether in a three times (3 × 100 mL). On vacuum drying white solid was obtained as desired product $3^H$. Single crystals of compound $3^H$, suitable for single crystal XRD study were grown by diethyl ether vapor diffusion into concentrated acetonitrile solution of it at room temperature.

**Yield :** 9.0 g (22.8 mmol, 54%). **M. P.:** > 200 °C.

**$^1$H NMR** (300 MHz, $CD_3CN$, 298 K): $\delta$ = 1.23 (d, 6H, CH(C$H_3$)$_2$), 1.28 (s, 6H, CC(C$H_3$)$_2$), 1.69 (s, 6H, NC(C$H_3$)$_2$), 2.29 (s, 1H, C$H_2$), 4.28 (sep, 1H, C*H*Me$_2$), 7.38–7.48 (m, 2H, Ph-C*H*), 7.56–7.74 (m, 3H, Ph-C*H*) ppm.

**$^{13}$C{$^1$H} NMR** (75.4 MHz, $CD_3CN$, 298 K): $\delta$ = 22.93 (2C, CH(*C*H$_3$)$_2$), 26.94 (2C, CC(*C*H$_3$)$_2$), 27.69(2C, NC(*C*H$_3$)$_2$), 48.77 (*C*H$_2$), 51.35 (*C*Me$_2$), 54.81 (*C*HMe$_2$), 79.64 (N*C*Me$_2$), 122.14 ($^1J_{C-F}$ = 320.45 Hz, $CF_3SO_3^-$), 127.44 (HC*C*CH), 127.86 (2C, Ph-*C*H), 129.30 (2C, Ph-*C*H), 132.34 (1C, Ph-*C*H), 194.70 (1C, N*C*CMe$_2$) ppm.

**$^{19}$F{$^1$H} NMR** (169.2 MHz, $CD_3CN$, 298 K): $\delta$ = –79.26 ppm.

**HRMS:** Calcd (m/z) for $[C_{17}H_{26}N]^+$: 244.2060; found: 244.2062.

**Synthesis of $\mathbf{3^{Me}}$.** The amide, chloroimine, $\mathbf{1^{Me}}$ and imine, $\mathbf{2^{Me}}$ were prepared from the corresponding reactants following the similar synthetic procedure as discussed for the synthesis of compound $\mathbf{3^H}$. *n*BuLi (1.6 M in *n*hexane, 10 mL, 16.0 mmol) was added dropwise to a diethylether solution of $\mathbf{2^{Me}}$ (3.1 g, 15.24 mmol in 80 mL dry diethyl ether) at –78 °C and during the addition a color change from colorless to light yellow with slight turbidity was observed. After stirring the reaction mixture at –78 °C for 1h, isobutylene oxide (1.45 mL, 16.0 mmol) was added. The reaction mixture was allowed to reach room temperature in 1h and then stirring was continued for another 1h. The reaction mixture again cooled down to –78 °C and triflic anhydride (2.75 mL, 16.0 mmol) was added to it dropwise at –78 °C. During addition of triflic anhydride, the formation of voluminous white precipitate was observed. On complete addition, the reaction mixture was allowed to reach room temperature in 2h and stirring was continued for another 1h at room temperature. The reaction mixture was filtered through a G4 sintered funnel and washed with diethyl ether in three times (3 × 50 mL). On vacuum drying white solid was obtained as desired product $\mathbf{3^{Me}}$. Single crystals of compound $\mathbf{3^{Me}}$, suitable for single crystal XRD study were grown by diethyl ether vapor diffusion into concentrated acetonitrile solution of it at room temperature.

**Yield :** 1.20 g (2.94 mmol, 19%). **M. P.:** > 200 °C.

**$^1$H NMR** (300 MHz, $CD_3CN$, 298 K): $\delta$ = 1.23 (s, 2H, CH(C$H_3$)$_2$), 1.27 (s, 6H, CC(C$H_3$)$_2$), 1.68 (s, 6H, NC(C$H_3$)$_2$), 2.27 (s, 2H, C$H_2$), 2.44 (s, 3H, *p*-C$H_3$), 4.27 (sep, 1H, C*H*Me$_2$), 7.24–7.35 (m, 2H, Ph-C*H*), 7.38–7.48 (m, 2H, Ph-C*H*) ppm.

**$^{13}$C{$^1$H} NMR** (75.4 MHz, $CD_3CN$, 298 K): $\delta$ = 21.40 (*p*-*C*H$_3$), 22.93 (2C, CH(*C*H$_3$)$_2$), 26.97 (2C, CC(*C*H$_3$)$_2$), 27.70 (2C, NC(*C*H$_3$)$_2$), 48.76 (*C*H$_2$), 51.27 (C*C*Me$_2$), 54.69 (*C*HMe$_2$), 79.39 (N*C*Me$_2$), 122.15 ($^1J_{C-F}$ = 320.45 Hz, $CF_3SO_3^-$), 127.78 (2C, Ph-*C*H), 124.50 (HC*C*CH), 129.82 (2C, Ph-*C*H), 143.04 (*C*Me), 195.14 (N*C*CMe$_2$) ppm.

**$^{19}$F{$^1$H} NMR** (169.2 MHz, $CD_3CN$, 298 K): $\delta$ = –79.25 ppm.

**HRMS:** Calcd (m/z) for $[C_{18}H_{28}N]^+$: 258.2216; found: 258.2209.

**Synthesis of $\mathbf{3^{Et}}$.** The amide, chloroimine, $\mathbf{1^{Et}}$ and imine, $\mathbf{2^{Et}}$ were prepared from the corresponding reactants following a similar synthetic procedure as discussed for the synthesis of compound $\mathbf{3^H}$. *n*BuLi (1.6 M in *n*hexane, 7.67 mL, 12.2 mmol) was added dropwise to a diethyl solution of $\mathbf{2^{Et}}$ (2.54 g 11.68 mmol in 80 mL dry diethyl ether) at –78 °C and during the addition a color change from colorless to light yellow with slight turbidity was observed. After stirring the reaction mixture at –78 °C for 1h, isobutylene oxide (1.11 mL, 12.2 mmol) was added. The reaction mixture was allowed to reach room temperature in 1h and then stirring was continued for another 1h. The reaction mixture again cooled down to –78 °C and triflic anhydride (2.10 mL, 12.2 mmol) was added to it dropwise at –78 °C. During addition of triflic anhydride, the formation of voluminous white precipitate was observed. On complete addition, the reaction mixture was allowed to reach room temperature in 2h and stirring was continued for another 1h at room temperature. The reaction mixture was filtered through a G4 sintered funnel and

washed with diethyl ether in a three times (3 × 50 mL). On vacuum drying white solid was obtained as desired product **3$^{Et}$**. Single crystals of compound **3$^{Et}$**, suitable for single crystal XRD study were grown by diethyl ether vapor diffusion into concentrated acetonitrile solution of it at room temperature.

**Yield :** 2.36 g (5.61 mmol, 48%). **M. P.:** above 200 °C.

**$^{1}$H NMR** (300 MHz, $CD_3CN$, 298 K): $\delta$ = 1.34–1.16 (m, 15H; 6H, CC(C$H_3$)$_2$, 3H, $CH_2CH_3$, 6H, CH(C$H_3$)$_2$), 1.68 (s, 6H, NC(C$H_3$)$_2$), 2.27 (s, 2H, C$H_2$), 2.75 (q, 2H, C$H_2$CH$_3$), 4.27 (sep, 1H, C*H*Me$_2$), 7.26–7.38 (m, 2H, Ph-C*H*), 7.41–7.52 (m, 2H, Ph-C*H*) ppm.

**$^{13}$C{$^{1}$H} NMR** (75.4 MHz, $CD_3CN$, 298 K): $\delta$ = 15.54 ($CH_2CH_3$), 22.94 (2C, CH(*C*H$_3$)$_2$), 26.98 (2C, CC(*C*H$_3$)$_2$), 27.71 (2C, NC(*C*H$_3$)$_2$), 29.20 (*C*H$_2$CH$_3$), 48.78(*C*H$_2$), 51.29 (C*C*Me$_2$), 54.70 (*C*HMe$_2$), 79.41 (N*C*Me$_2$), 122.14 ($^{1}J_{C-F}$ = 320.45 Hz, $CF_3SO_3^-$), 124.72 (HC*C*CH), 127.87 (2C, Ph-*C*H), 128.68 (2C, Ph-*C*H), 149.18 (*C*Et), 195.14 (N*C*CMe$_2$) ppm.

**$^{19}$F{$^{1}$H} NMR** (169.2 MHz, $CD_3CN$, 298 K): $\delta$ = –79.25 ppm.

**HRMS:** Calcd (m/z) for $[C_{19}H_{30}N]^+$: 272.2373; found: 272.2372.

**Synthesis of 3$^{tBu}$.** The amide, chloroimine, **1$^{tBu}$** and imine, **2$^{tBu}$** were prepared from the corresponding reactants following the similar synthetic procedure as discussed for the synthesis of compound **3$^{H}$**. *n*BuLi (1.6 M in *n*hexane, 5 mL, 8.0 mmol) was added dropwise to a diethylether solution of **2$^{tBu}$** (1.87 g, 7.615 mmol in 70 mL dry diethylether) at –78 °C and during the addition time a color change from colorless to light yellow with slight turbidity was observed. After stirring the reaction mixture at –78 °C for 1h, isobutylene oxide (0.73 mL, 8 mmol) was added. The reaction mixture was allowed to reach room temperature in 1h and then stirring was continued for another 1h. The reaction mixture again cooled down to –78 °C and triflic anhydride (1.4 mL, 8 mmol) was added to it dropwise at –78 °C. During addition of triflic anhydride, the formation of voluminous white precipitate was observed. On complete addition, the reaction mixture was allowed to reach room temperature in 2h and stirring was continued for another 1h at room temperature. The reaction mixture was filtered through a G4 sintered funnel and washed with diethylether in a three times (3 × 50 mL). On vacuum drying white solid was obtained as desired product **3$^{tBu}$**. Crystal of compound **3$^{tBu}$**, suitable for single crystal XRD measurement were obtained by *n*-hexane layering on concentrated DCM solution at room temperature.

**Yield :** 1.40 g (3.11 mmol, 40.92%). **M. P.:** above 200 °C.

**$^{1}$H NMR** (300 MHz, $CD_3CN$, 298 K): $\delta$ = 1.22 (d, 6H, CH(C$H_3$)$_2$), 1.27 (s, 6H, CC(C$H_3$)$_2$), 1.36 (s, 9H, C(C$H_3$)$_3$), 1.68 (s, 6H, NC(C$H_3$)$_2$), 2.28 (s, 2H, C$H_2$), 4.27 (sep, 1H, C*H*Me$_2$), 7.29–7.41 (m, 2H, Ph-C*H*), 7.60–7.70 (m, 2H, Ph-C*H*) ppm.

**$^{13}$C{$^{1}$H} NMR** (75.4 MHz, $CD_3CN$, 298 K): $\delta$ = 22.93 (2C, CH(*C*H$_3$)$_2$), 26.98 (2C, CC(*C*H$_3$)$_2$), 27.72 (2C, NC(*C*H$_3$)$_2$), 31.22 (3C, C(*C*H$_3$)$_3$), 35.66 (*C*Me$_3$), 48.79 (*C*H$_2$), 51.30 (C*C*Me$_2$), 54.69 (*C*HMe$_2$), 79.42 (N*C*Me$_2$), 122.14 ($^{1}J_{C-F}$ = 320.45 Hz, $CF_3SO_3^-$), 124.57 (HC*C*CH), 126.22 (2C, Ph-*C*H), 127.63 (2C, Ph-*C*H), 155.95 (*C*CMe$_3$), 195.19 (N*C*CMe$_2$) ppm.

**$^{19}$F{$^{1}$H} NMR** (169.2 MHz, $CD_3CN$, 298 K): $\delta$ = –79.28 ppm.

**HRMS:** Calcd (m/z) for $[C_{21}H_{34}N]^+$: 300.2686; found: 300.2681.

**$KC_8$ reduction of 3$^{H}$.** Dry THF (20 mL) was added to a mixture of **3$^{H}$** (1.080 g, 2.74 mmol) and $KC_8$ (0.408 g, 3.02 mmol) at –78 °C. A dark red color solution was formed on bringing the reaction mixture slowly to room temperature in 1h. The stirring was continued for another 2h at room temperature. After removal of all the volatiles, the solid residue was extracted with *n*hexane. Pale yellow color crystals were isolated after overnight from the concentrated *n*hexane that was kept at –35 °C and which is also suitable for single crystal XRD study.

Isolated yield: 0.170 g (0.348 mmol, 25.40%).

**$KC_8$ Reduction of $\mathbf{3^{Me}}$:** Dry THF (20 mL) was added to a mixture of $\mathbf{3^{Me}}$ (0.341 g, 0.84 mmol) and $KC_8$ (0.124 g, 0.921 mmol) at −78 °C. On bringing the reaction mixture was slowly raise to room temperature in 1 hr, followed by stirring for 0.5 h at room temperature pale brown color suspension formed. The color of that suspension gradually changes to bright yellow color on further stirring for 2hrs. After removals of all the in vacuum the sticky residue was extracted with *n*hexane. After concentrating the *n*hexane solution to about 1 mL, it was kept at −80 °C. No crystal were isolated even keeping this solution at −80 °C for 15 days. On evaporation of the hexane extract yellow color dense oil was obtained and measurement of $^1$H NMR indicate the formation of interactive mixture of unassigned products.

**$KC_8$ Reduction of $\mathbf{3^{Et}}$:** Dry THF (20 mL) was added to a mixture of $\mathbf{3^{Et}}$ (0.527 g, 1.25 mmol) and $KC_8$ (0.186 g, 1.37 mmol) at −78 °C. On bringing the reaction mixture was slowly to room temperature in 1 hr, the reaction mixture become dark red color. After stirring for 2 hrs at room temperature, all the volatiles were removed in vacuum. During drying the intensity of the red color residue started decreasing to orange red color. The solid residue was extracted with *n*hexane. During evaporation of the *n*hexane extract the intensity of the orange-red color solution further decreased to orange color solution. After concentrating the *n*hexane solution to about 1 mL, it was kept at −80 °C. After 1 day the whole solution turned into deep yellow solution. No crystal were isolated even keeping this solution at −80 °C for 15 days. On evaporation of the hexane extract yellow color dense oil was obtained and measurement of $^1$H NMR indicate the formation of interactive mixture of unassigned products.

**$KC_8$ reduction of $\mathbf{3^{tBu}}$:** Dry THF (20 mL) was added to a mixture of $\mathbf{3^{tBu}}$ (1.023 g, 2.27 mmol) and $KC_8$ (0.338 g, 2.50 mmol) at −78 °C. After few minutes of THF addition, the reaction mixture started turning into red color that get intensified on bringing the reaction mixture slowly to room temperature in 1hr. The stirring was continued for another 2 hrs at room temperature. After removal of all the volatiles, the solid residue was extracted with *n*hexane. On keeping the concentrated *n*hexane solution (2 mL) at −80 °C for 3 days, deep red color polycrystalline compound were obtained.
Isolated yield: 0.057 g (0.189 mmol, 8.35 %).

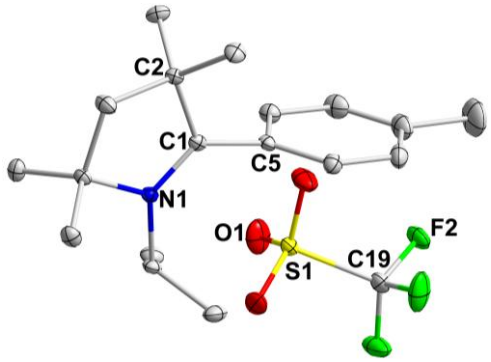



**Figure S1.** Solid state molecular structures of $\mathbf{3}^{Me}$ (thermal ellipsoids at 30% probability level and all H atoms are omitted for clarity). Selected bond lengths (Å) and angles (°): N1–C1 1.2870(19), C1–C2 1.518(2), C1–C5 1.485(2), N1–C1–C2 112.95(13).

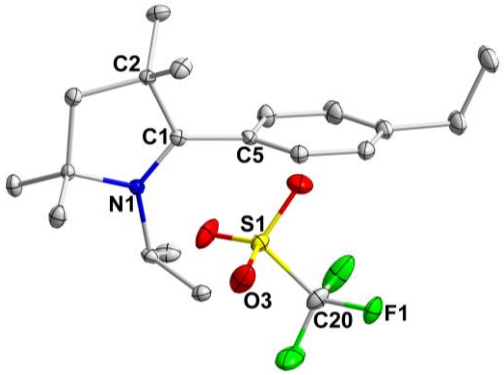



**Figure S2.** Solid state molecular structures of $\mathbf{3}^{Et}$ (thermal ellipsoids at 30% and all H atoms are omitted for clarity). Selected bond lengths (Å) and angles (°): N1–C1 1.287(3), C1–C2 1.516(3), C5–C1 1.478(3), N1–C1–C2 112.8(2).

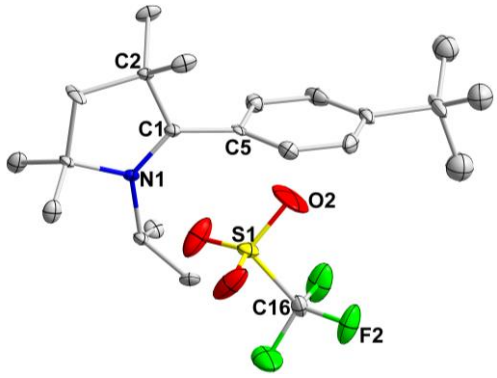



**Figure S3.** Solid state molecular structures of $\mathbf{3}^{tBu}$ (thermal ellipsoids at 30% probability level and all H atoms are omitted for clarity). Selected bond lengths (Å) and angles (°): N1–C1 1.279(10), C1–C2 1.502(10), C5–C1 1.477(11), N1–C1–C2 112.5(7).

**NMR Spectra**

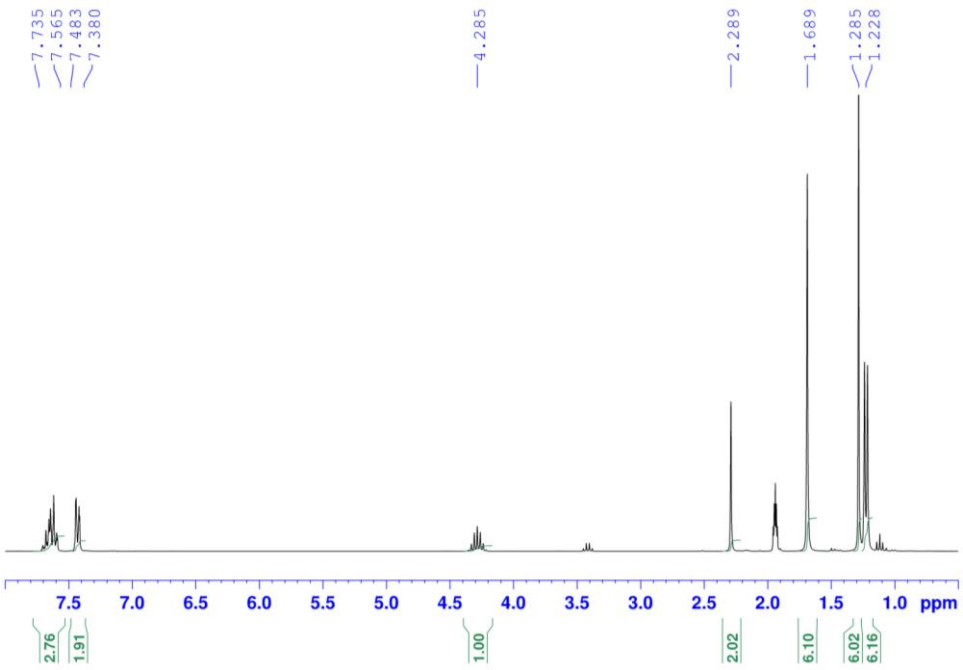



**Figure S4.** $^{1}$H NMR of spectrum compound **3$^{H}$** in $CD_3CN$ at 298 K.

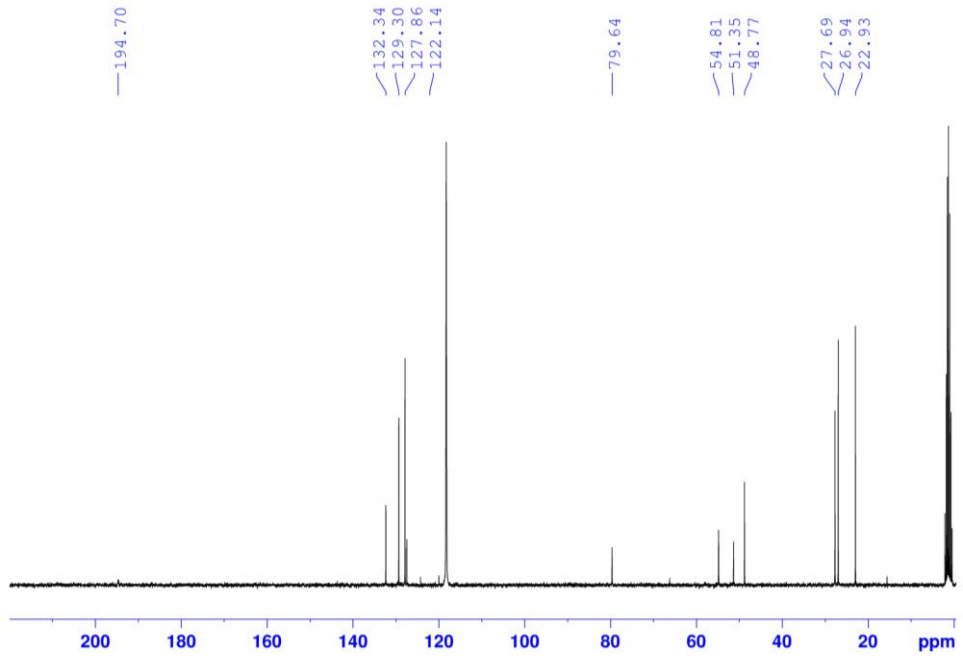



**Figure S5.** $^{13}C\{^{1}H\}$ NMR spectrum of compound **3$^{H}$** in $CD_3CN$ at 298 K.

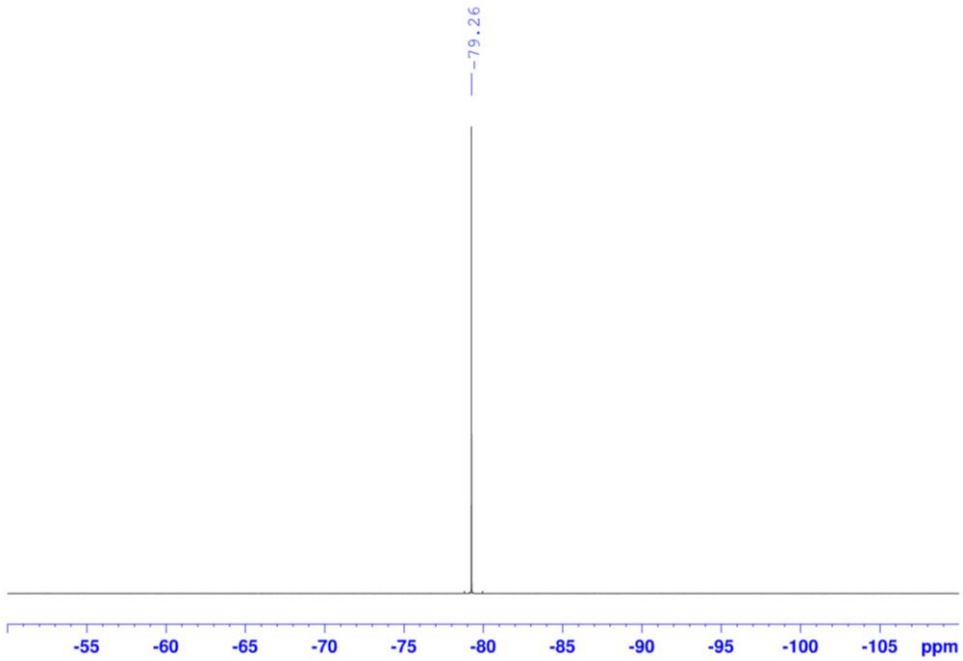



**Figure S6.** $^{19}F\{^{1}H\}$ NMR spectrum of compound $\mathbf{3^{H}}$ in $CD_3CN$ at 298 K.

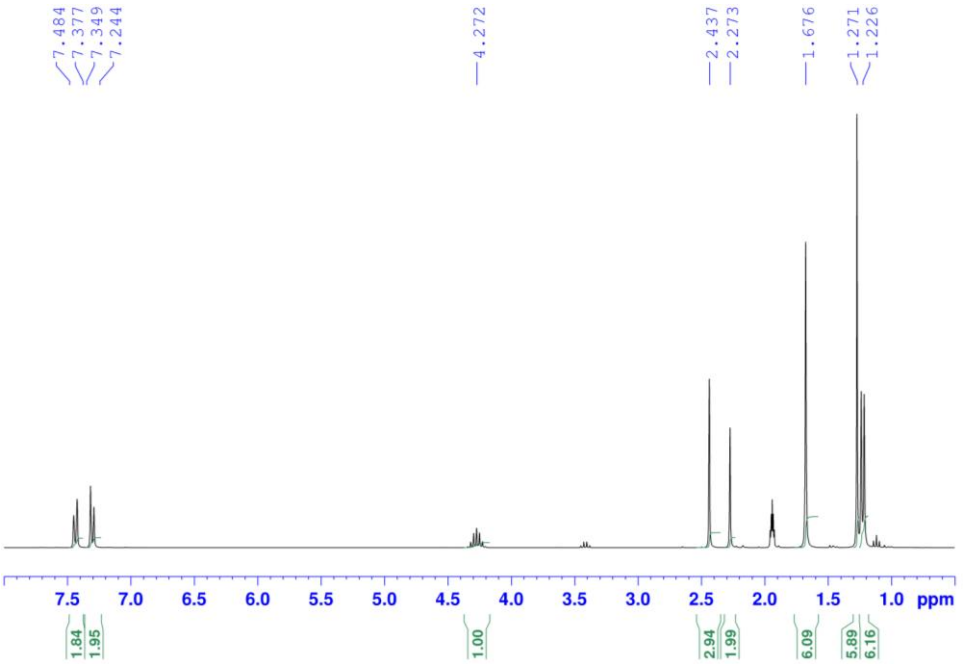



**Figure S7.** $^{1}H$ NMR spectrum of compound $\mathbf{3^{Me}}$ in $CD_3CN$ at 298 K.

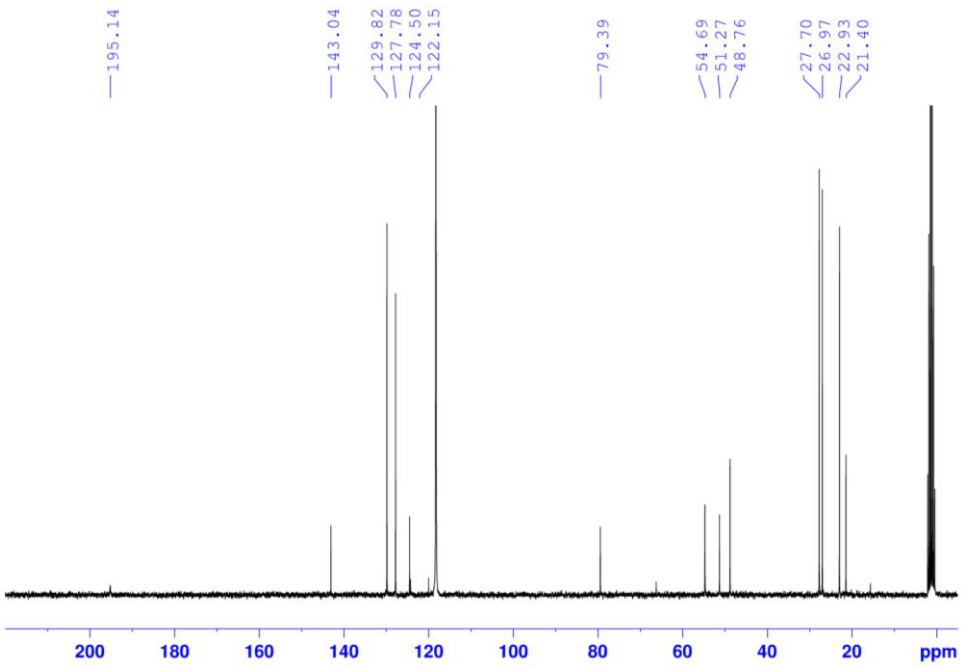



**Figure S8.** $^{13}C\{^{1}H\}$ NMR spectrum of compound **3**$^{Me}$ in $CD_3CN$ at 298 K.

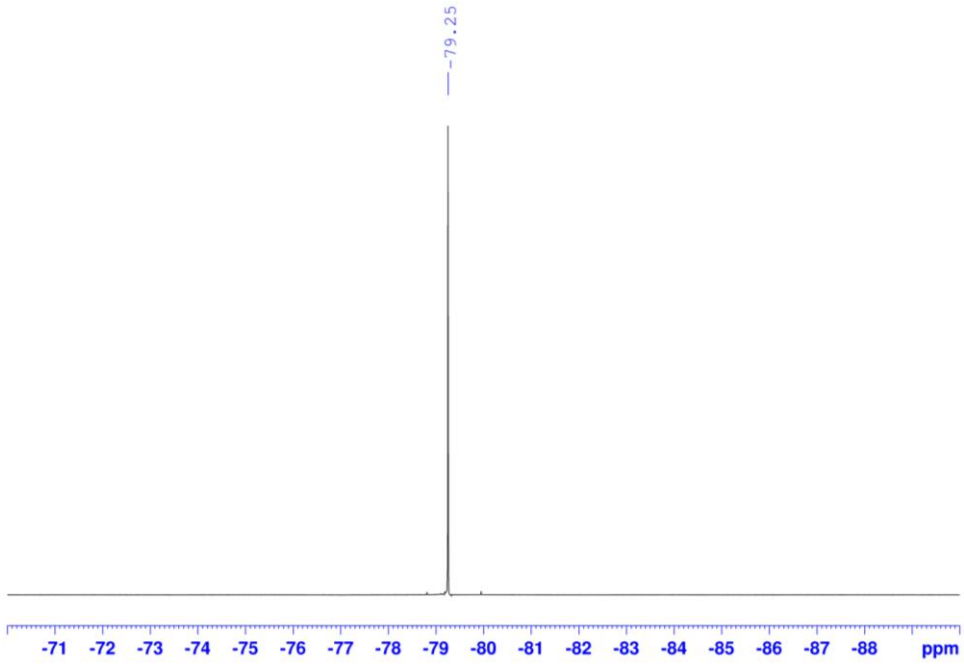



**Figure S9.** $^{19}F\{^{1}H\}$ NMR spectrum of compound **3**$^{Me}$ in $CD_3CN$ at 298 K.

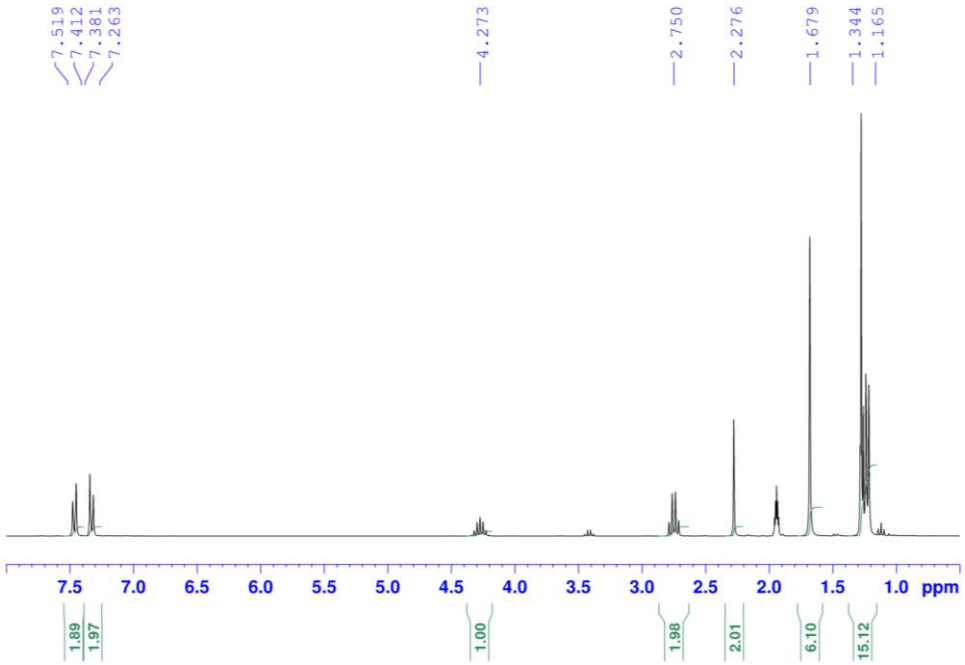



**Figure S10.** $^{1}$H NMR spectrum of compound **3$^{Et}$** in $CD_3CN$ at 298 K.

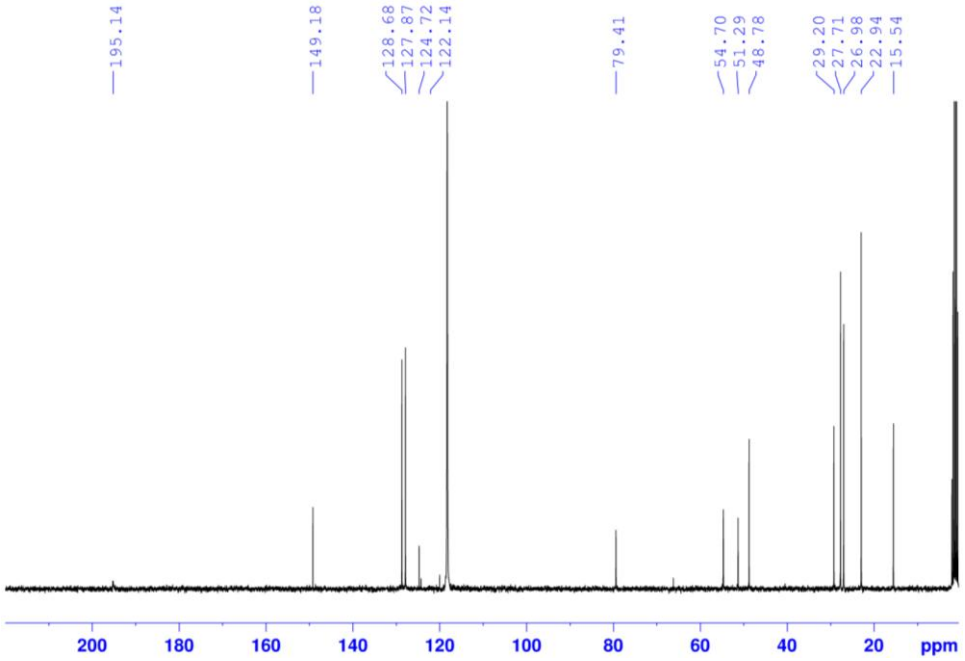



**Figure S11.** $^{13}C\{^{1}H\}$ NMR spectrum of compound **3$^{Et}$** in $CD_3CN$ at 298 K.

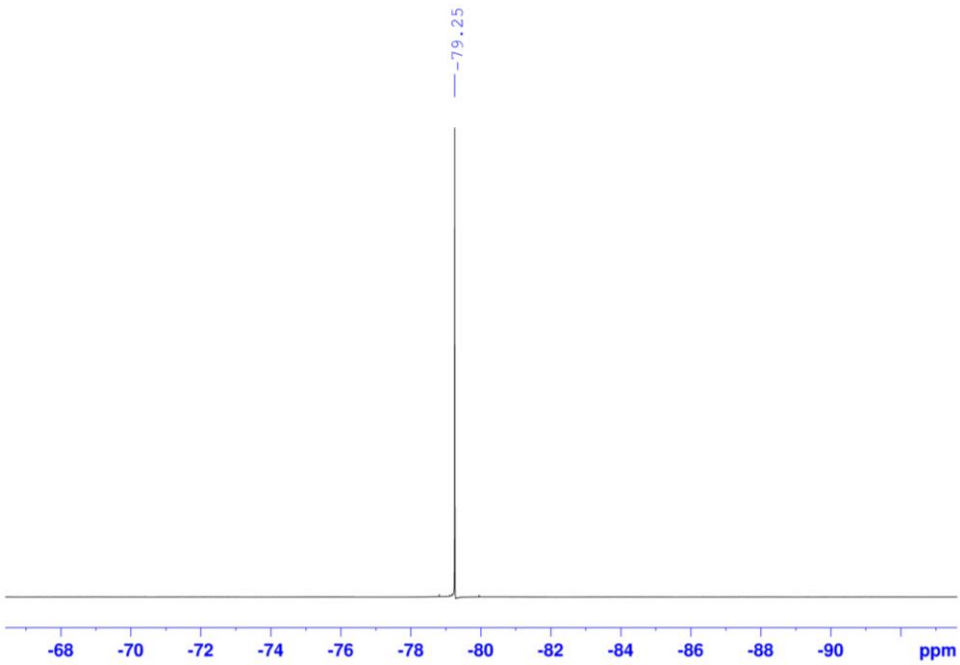



**Figure S12.** $^{19}F\{^{1}H\}$ NMR spectrum of compound $\mathbf{3^{Et}}$ in $CD_3CN$ at 298 K.

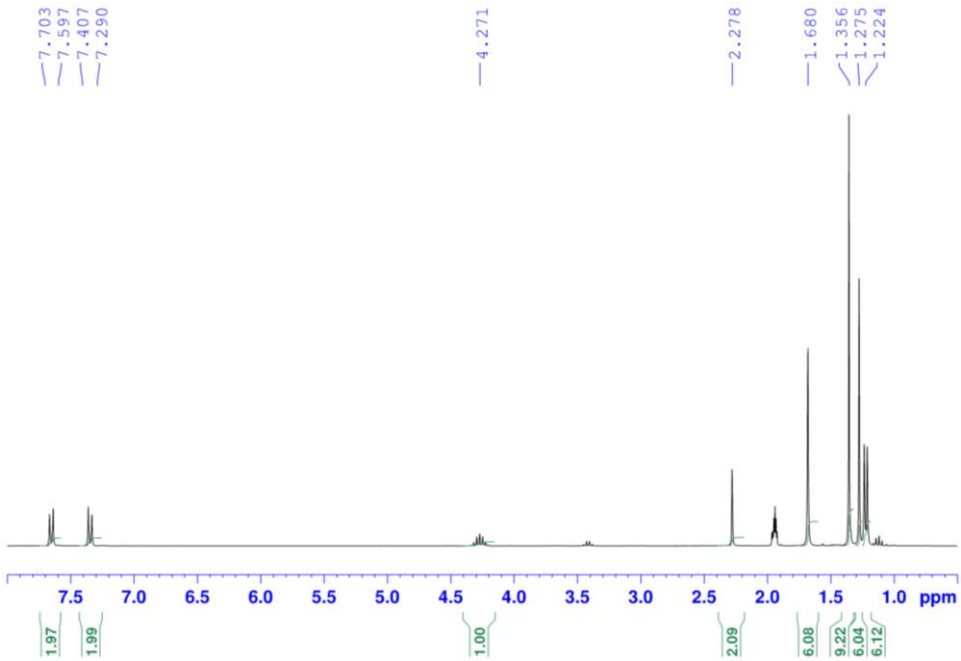



**Figure S13.** $^{1}H$ NMR spectrum of compound $\mathbf{3^{tBu}}$ in $CD_3CN$ at 298 K.

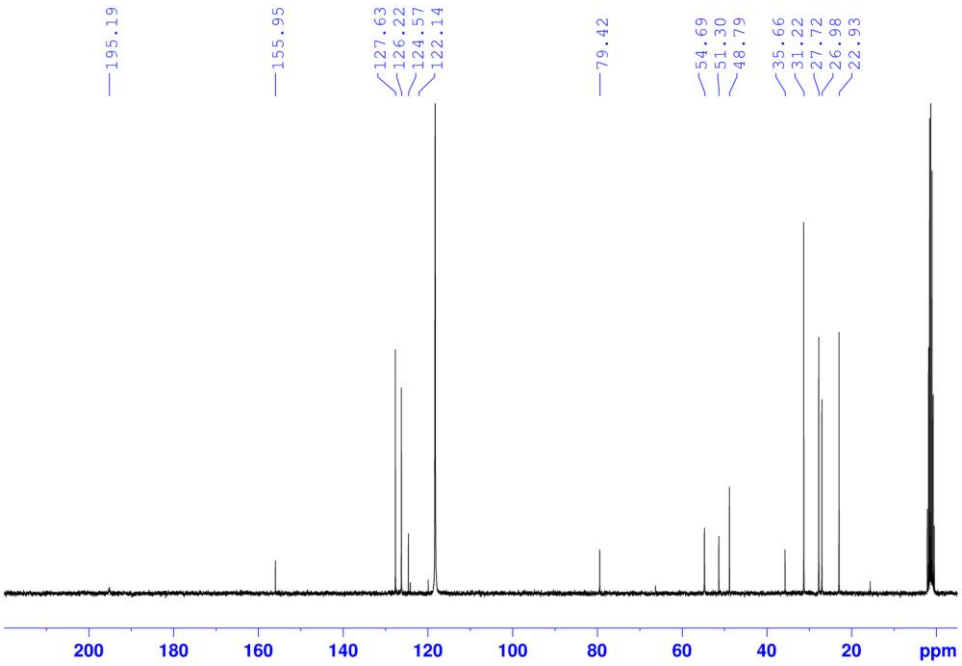



**Figure S14.** $^{13}C\{^{1}H\}$ NMR spectrum of compound **3**$^{tBu}$ in $CD_3CN$ at 298 K.

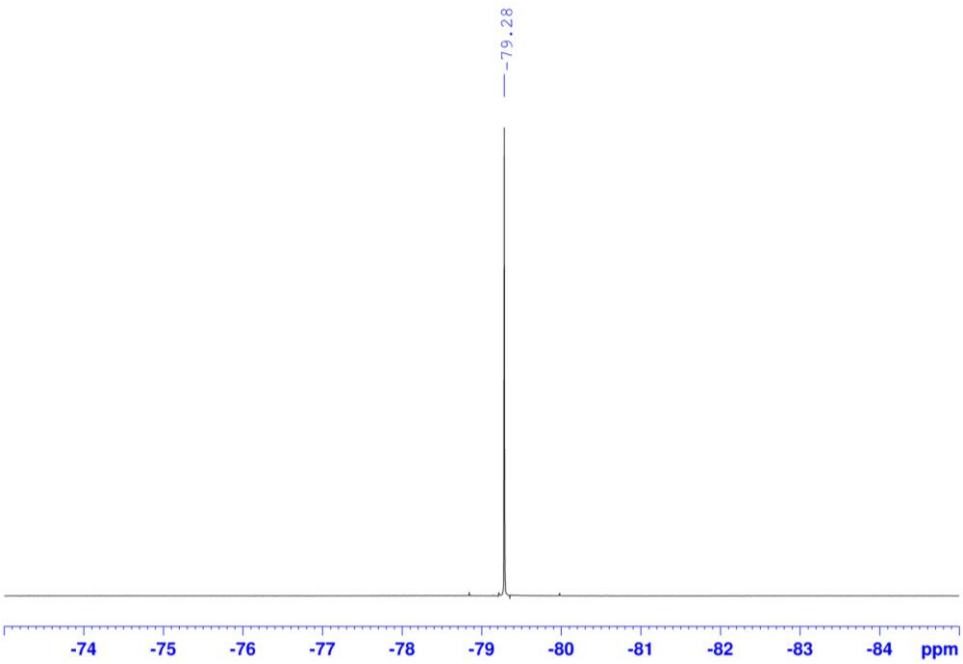



**Figure S15.** $^{19}F\{^{1}H\}$ NMR spectrum of compound **3**$^{tBu}$ in $CD_3CN$ at 298 K.

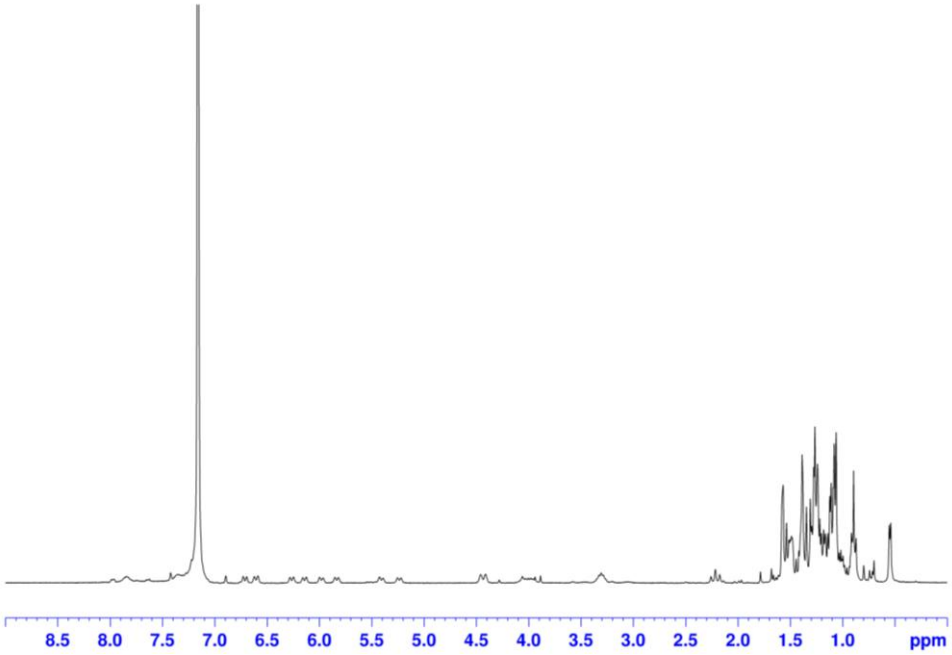



**Figure S16.** $^{1}$H NMR spectrum of compound $\mathbf{3^{H}_{2}}$ in $C_6D_6$ at 298 K.

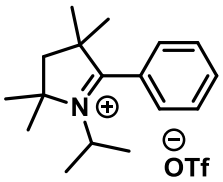
## Cyclic Voltammetry

**Table S1.** Redoxpotentials ($E_{1/2}$) vs $Fc/Fc^+$ measured in $CH_2Cl_2$ at 100 $mVs^{-1}$ with 0.1 M $Bu_4NPF_6$ at room temperature.

| | $E_{1/2}$ ($1^{st}$ Red) | $E_{1/2}$($2^{nd}$ Red) [a] |
|---|---|---|
| 3 | -1.80 | -2.53 |
| $3^{Me}$ | -1.82 | -2.62 |
| $3^{Et}$ | -1.81 | -2.61 |
| $3^{tBu}$ | -1.81 | -2.75 |

All values given were measured with GCWE at 100 $mVs^{-1}$, given in Volts.
[a] No Reoxidation wave observed.

**CV of $3^H$**




$3^H$

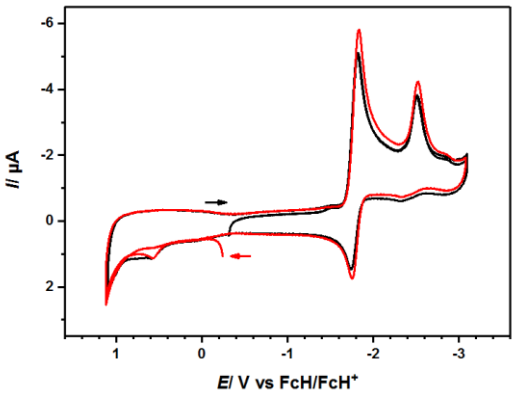



**Figure S17.** CV of $3^H$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

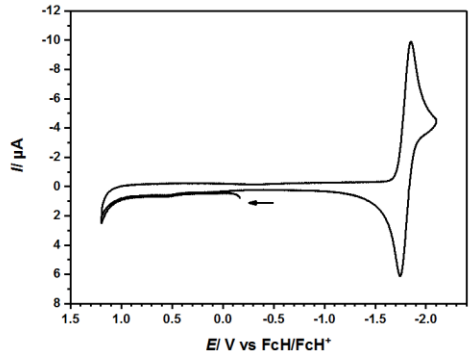



**Figure S18.** CV of $3^H$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

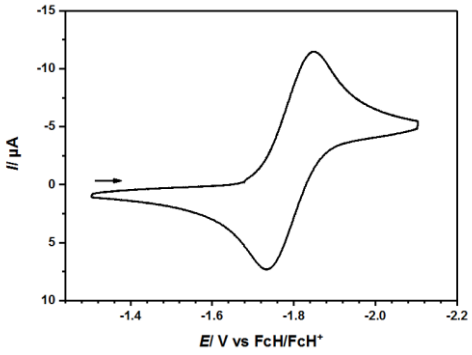



**Figure S19.** CV of $3^H$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

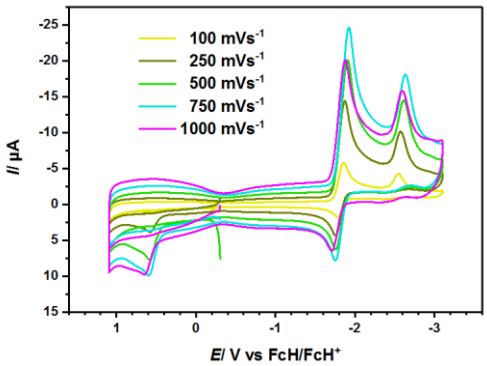



**Figure S20.** CV of $3^H$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode. Comparison of faster scan rates. Note the higher current for 750 $mVs^{-1}$ than 1000 $mVs^{-1}$.

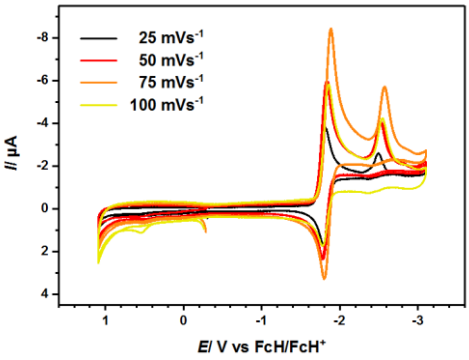
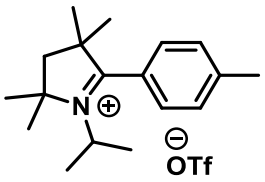



**Figure S21.** CV of $3^H$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode. Comparison of slower scan rates. Note the higher current for 75 $mVs^{-1}$ than 100 $mVs^{-1}$.

**CV of $3^{Me}$ and $3^{Et}$**




$3^{Me}$

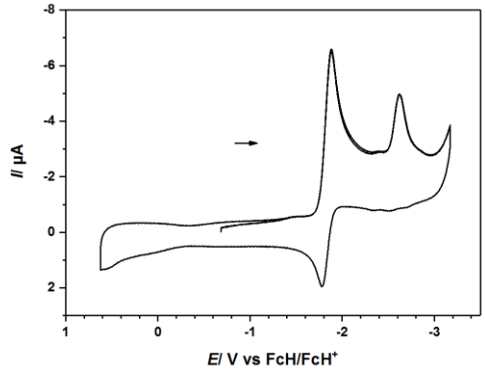



**Figure S22.** CV of $3^{Me}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

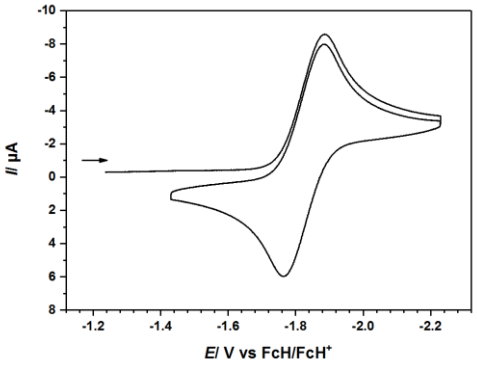
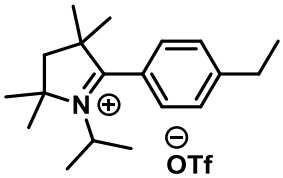



**Figure S23.** CV of $3^{Me}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.




$3^{Et}$

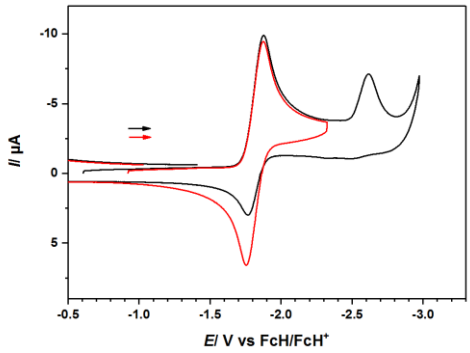



**Figure S24.** CV of $3^{Et}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

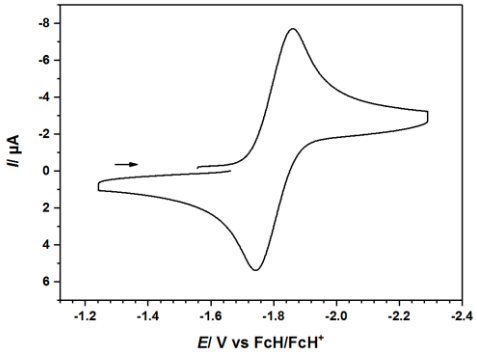
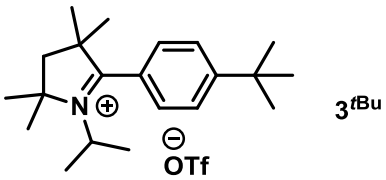



**Figure S25.** CV of $3^{Et}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

**CV of $3^{tBu}$**




$3^{tBu}$

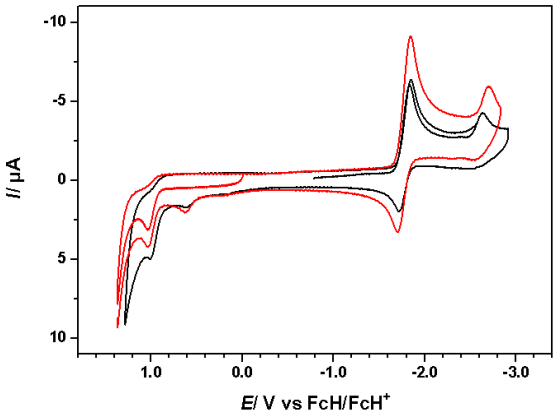



**Figure S26.** CV of $3^{tBu}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

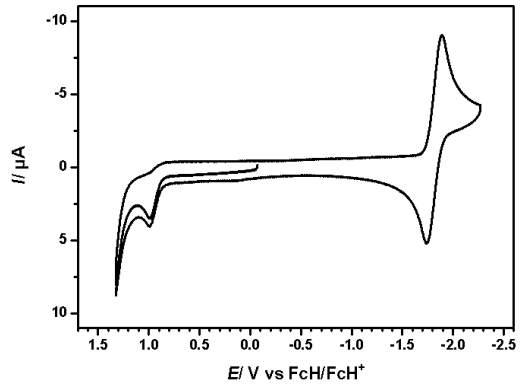



**Figure S27.** CV of $3^{tBu}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

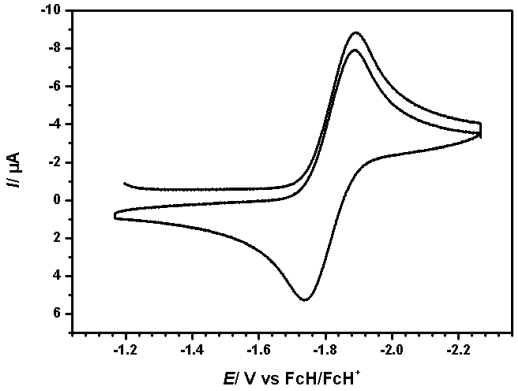



**Figure S28.** CV of $3^{tBu}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode at 100 $mVs^{-1}$.

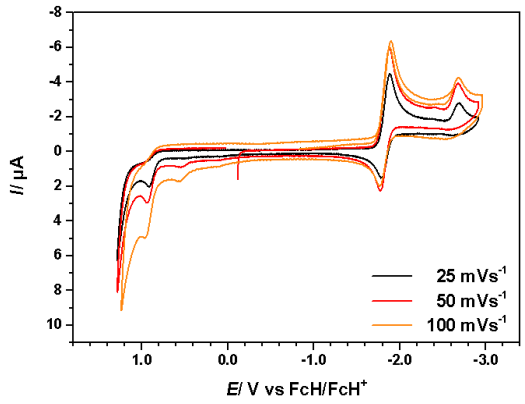



**Figure S29.** CV of $3^{tBu}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode. Comparison of slower scan rates.

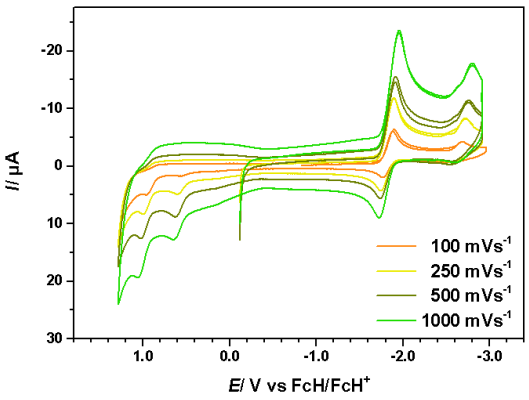



**Figure S30.** CV of $3^{tBu}$ in THF / 0.1 $NBu_4PF_6$ measured at a GC working electrode. Comparison of faster scan rates.

## Ratio of peak currents from the CVs of $3^{H}$, $3^{Me}$, $3^{Et}$ and $3^{tBu}$

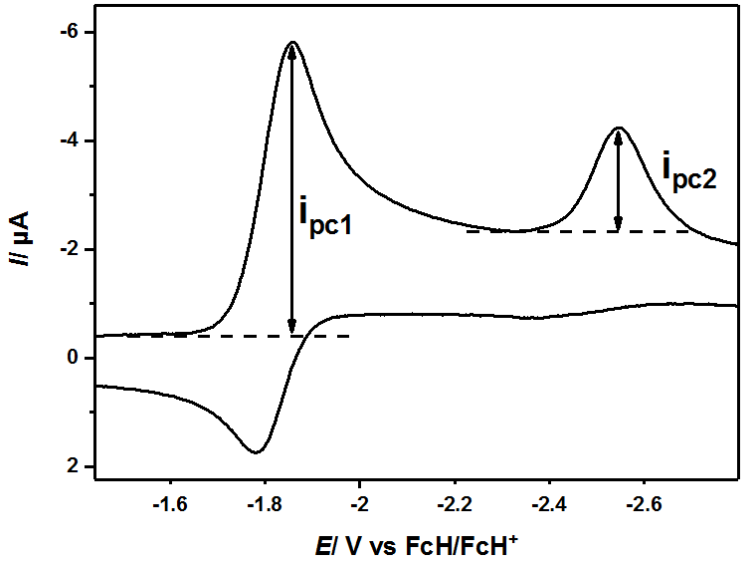



**Figure S31.** Evaluation of peak currents as a measure for dimerisation.

**Table S2.** Overview of peak currents measured at 100 $mVs^{-1}$ at gcwe in 0.1 $NBu_4PF_6$ / THF.

| Compound | $i_{pc1}$ | $i_{pc2}$ | $i_{pc2}/i_{pc1}$ |
|---|---|---|---|
| $\mathbf{3^{H}}$ | −5.4 | −1.9 | 0.35 |
| $\mathbf{3^{Me}}$ | −6.0 | −2.1 | 0.35 |
| $\mathbf{3^{Et}}$ | −9.6 | −3.3 | 0.34 |
| $\mathbf{3^{tBu}}$ | −6.7 | −1.5 | 0.22 |

**Temperature dependent CV of $3^{H}$**

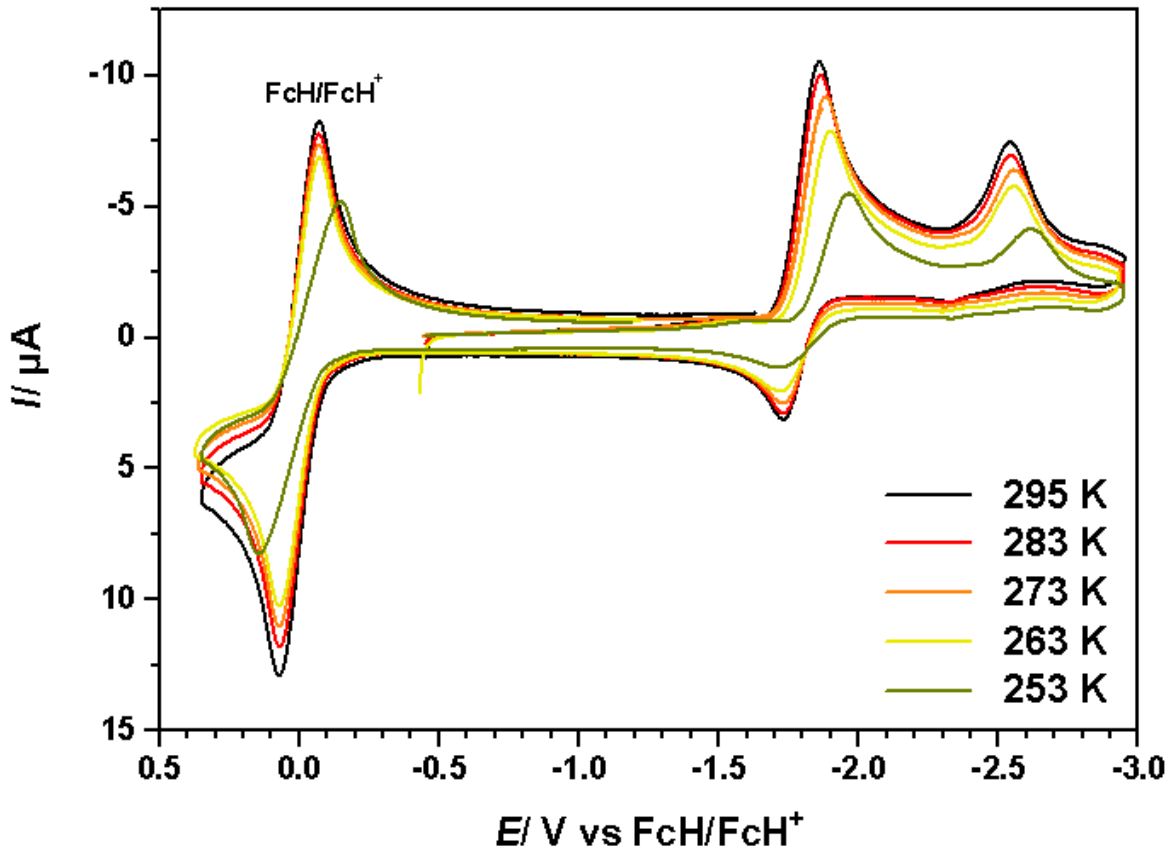



**Figure S32.** Temperature-dependant CV of 3 in presence of ferrocene measured at a GC working electrode at 100 $mVs^{-1}$.[S18]

## CV Simulation for $3^{H}$

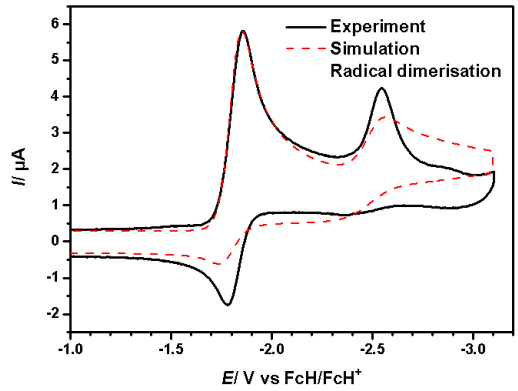



**Figure S33.** Comparison for experiment and simulation for the radical dimerization mechanism.

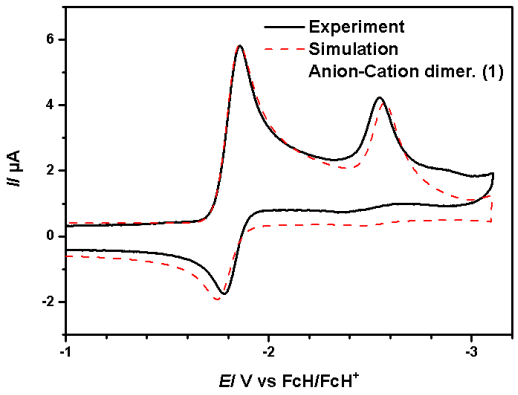



**Figure S34.** Comparison for experiment and simulation for the Anion-Cation dimerization mechanism.

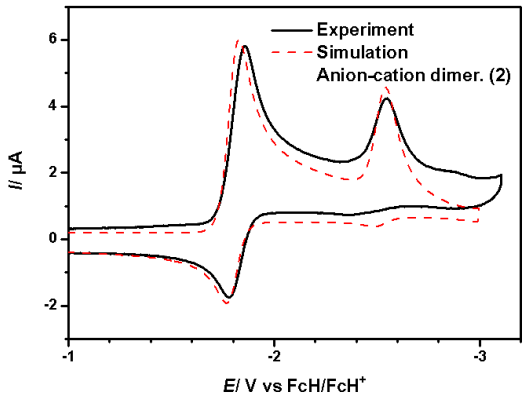



**Figure S35.** Comparison for experiment and simulation for the Anion-Cation dimerization mechanism with a different parameter set.

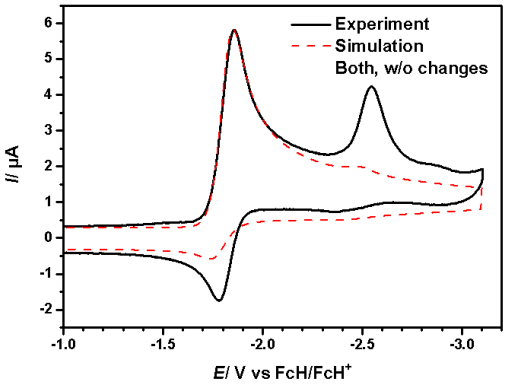



**Figure S36.** Comparison for experiment and simulation for both dimerization mechanisms without changes.

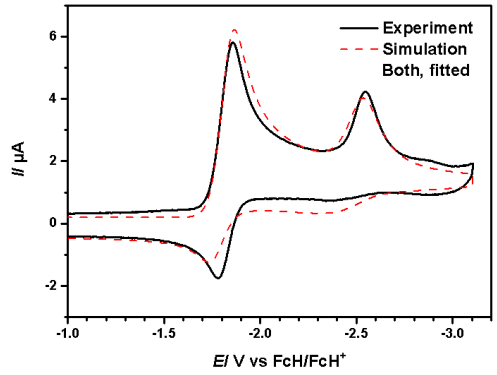



**Figure S37.** Comparison for experiment and simulation for both dimerization mechanisms with parameter fitting.

The cyclic voltammogram was simulated in two segments from 0.00 V to −3.1 V and from −3.1 V to 0.00 V with the software DigiElch Professional[S19] by using the Butler-Volmer equation. The surface area of the working electrode was set to 0.07 $cm^2$ and the starting concentration of 3 was set to 0.3 mM. The charge transfer coefficients α were left at their initial value of 0.5 and the heterogeneous rate constants $k_s$ were calculated from the peak-to-peak separation[S20] and consequently set to 0.005 cm/s. The diffusion coefficients were left at their initial values of 1x10^−5 $cm^2$ $s^{-1}$. The simulated charge-transfer reactions are described by the following equations for the mechanisms (1)-(5), the $E^0$ values for $\mathbf{3}^{\mathbf{H}}$ was set to −1.80 V and for $\mathbf{3}^{\mathbf{H}\bullet}$ to −2.53 V. The electrochemical reactions are denoted with (E) and the coupled chemical reactions with (C), which was assumed to be irreversible for the simulation with $Pyr^+$ = $\mathbf{3}^{\mathbf{H}}$, $Pyr^{0\bullet}$ = $\mathbf{3}^{\mathbf{H}\bullet}$ and Dimer = $\mathbf{3}^{\mathbf{H}}_{\mathbf{2}}$.

| Mechanism | Reaction |
|---|---|
| (1) Radical-radical | $Pyr^+ + e^- \rightleftarrows Pyr^{0\bullet}$ (E) |
| | $Pyr^{0\bullet} + e^- \rightleftarrows Pyr^-$ (E) |
| | $2\ Pyr^{0\bullet} \rightarrow$ Dimer (C) |
| (2) Anion-cation 1 | $Pyr^+ + e^- \rightleftarrows Pyr^{0\bullet}$ (E) |
| | $Pyr^{0\bullet} + e^- \rightleftarrows Pyr^-$ (E) |
| | $Pyr^+ + Pyr^- \rightarrow$ Dimer (C) |
| (3) Anion-cation 2 | $Pyr^+ + e^- \rightleftarrows Pyr^{0\bullet}$ (E) |
| | $Pyr^{0\bullet} + e^- \rightleftarrows Pyr^-$ (E) |
| | $Pyr^+ + Pyr^- \rightarrow$ Dimer (C) |
| (4) Both, w/o changes | $Pyr^+ + e^- \rightleftarrows Pyr^{0\bullet}$ (E) |
| | $Pyr^{0\bullet} + e^- \rightleftarrows Pyr^-$ (E) |
| | $Pyr^+ + Pyr^- \rightarrow$ Dimer (C) |
| | $2\ Pyr^{0\bullet} \rightarrow$ Dimer (C) |
| (5) Both, fitted | $Pyr^+ + e^- \rightleftarrows Pyr^{0\bullet}$ (E) |
| | $Pyr^{0\bullet} + e^- \rightleftarrows Pyr^-$ (E) |
| | $Pyr^+ + Pyr^- \rightarrow$ Dimer (C) |
| | $2\ Pyr^{0\bullet} \rightarrow$ Dimer (C) |

**Table S3.** Overview of kinetic parameters used for the various simulations.

| Mechanism | $K_1$ | $k_{f1}$ | $k_{b1}$ | $K_2$ | $k_{f2}$ | $k_{b2}$ |
|---|---|---|---|---|---|---|
| Radical Radical | 10^8 | 10^4 | 10^−4 | --- | --- | --- |
| Cation-Anion 1 | --- | --- | --- | 1000 | 5*10^6 | 0 (no back reaction) |
| Cation-Anion 2 | --- | --- | --- | 10 | 10^6 | 0 (no back reaction) |
| Both, w/o change | 10^8 | 1.2*10^4 | 1.2*10^−4 | 6.7*10^19 | 5*10^^6 | 7.4*10^−14 |
| Both, fitted | 10^5 | 3080 | 0.0308 | 6.7651*10^16 | 51000 | 7.5387*10^−13 |
| Annotations: $K_1$, $k_{f1}$, $k_{b1}$ refer to the radical-radical dimerization and $K_2$, $k_{f2}$, $k_{b2}$ refer to the cation-anion dimerization. | | | | | | |

## EPR spectroelectrochemistry

**Table S4.** Experimentally measured g-values via EPR-spectroelectrochemistry.

| Compound | g(exp) |
|---|---|
| $\mathbf{3}^{H}$ | 2.003 |
| $\mathbf{3}^{t\mathrm{Bu}}$ | 2.003 |

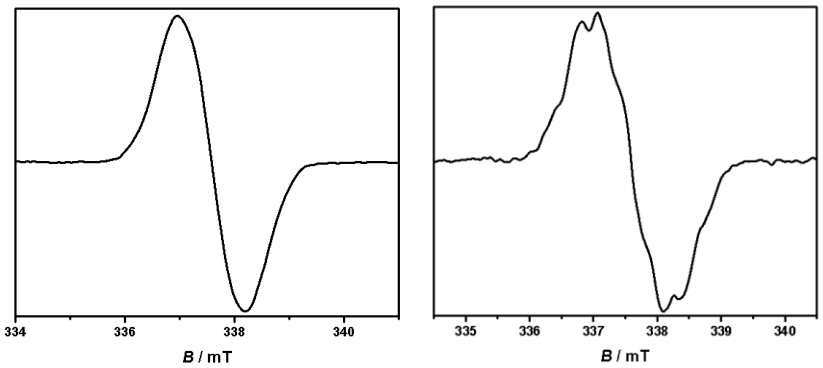



**Figure S38.** EPR spectrum of $\mathbf{3}^{H\bullet}$ in THF. Electrolysis with Au electrode at ca. -2.0 V, signal vanishes at around -2.5 V in 0.1 M $NBu_4PF_6$ in THF. Right: 0.6 mT modulation amplitude, left: 0.01 mT modulation amplitude.

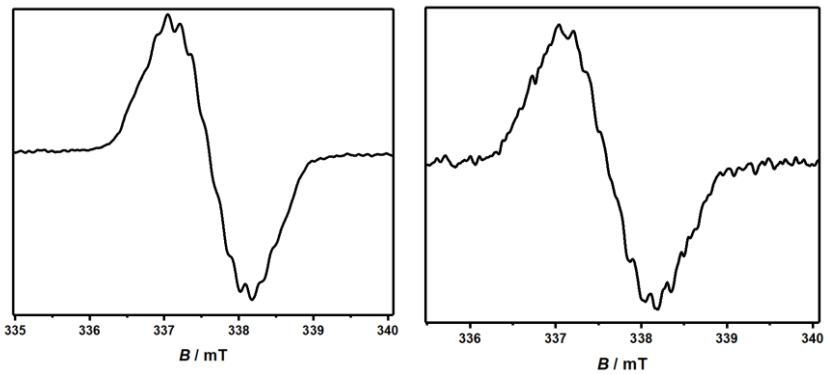



**Figure S39.** EPR spectrum of $\mathbf{3}^{t\mathrm{Bu}\bullet}$ in THF at 262 K. Electrolysis with Au electrode at ca. -2.0 V, signal vanishes at around -2.5 V vs Ag-Pseudoreference in 0.1 M $NBu_4PF_6$ in THF. Right: 0.01 mT modulation amplitude, left: 0.06 mT modulation amplitude.

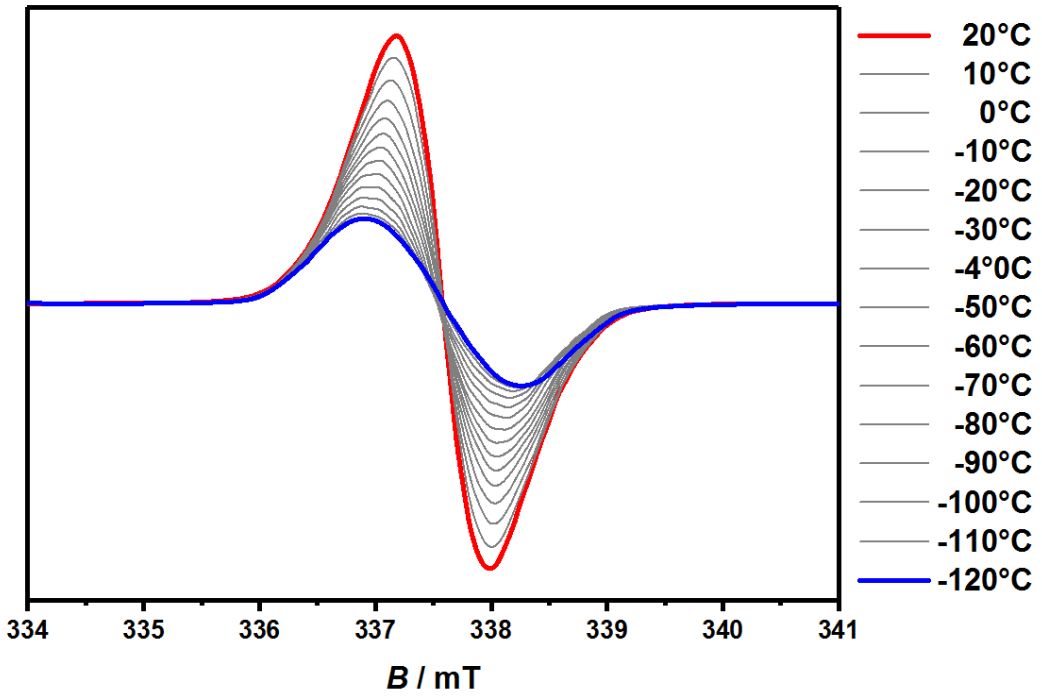



**Figure S40.** Temperature-dependent EPR spectra of the $3^{H\bullet}/3^{H}_{2}$ mixture after chemical reduction with $KC_8$, measured in THF.

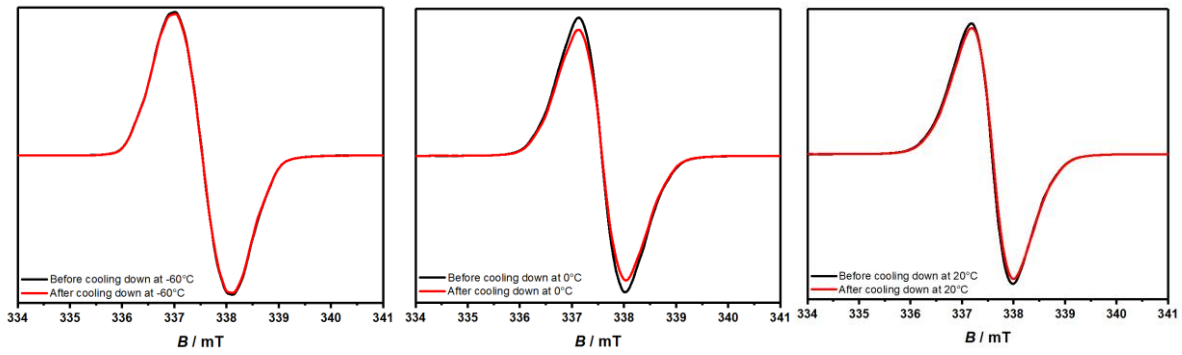



**Figure S41.** Comparison of EPR spectra after cooling down to −120°C and re-heating to 20°C of the $3^{H\bullet}/3^{H}_{2}$ mixture after chemical reduction with $KC_8$ measured in THF.

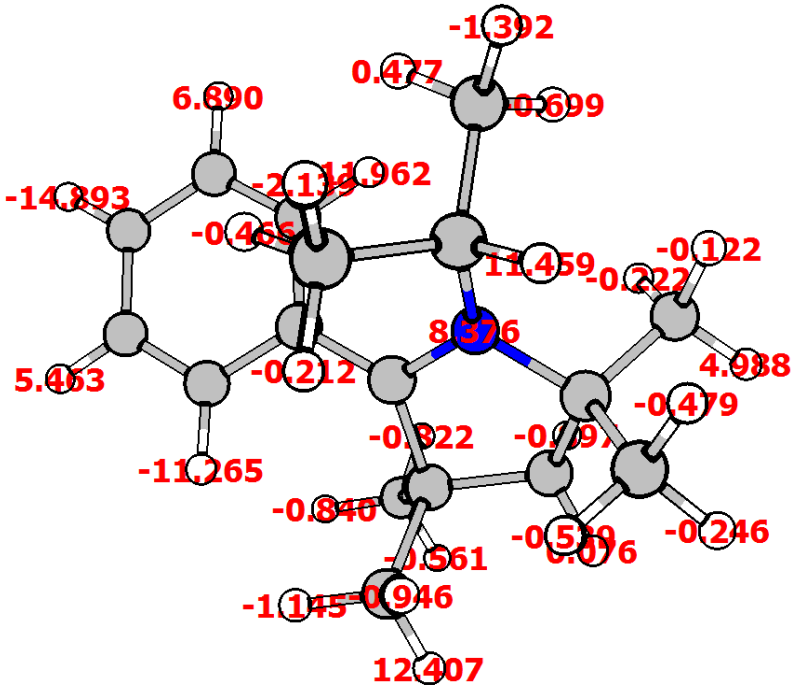



**Figure S42.** Calculated hyperfine coupling constants at PBE0/IGLO-III level for $\mathbf{3}^{H\bullet}$.

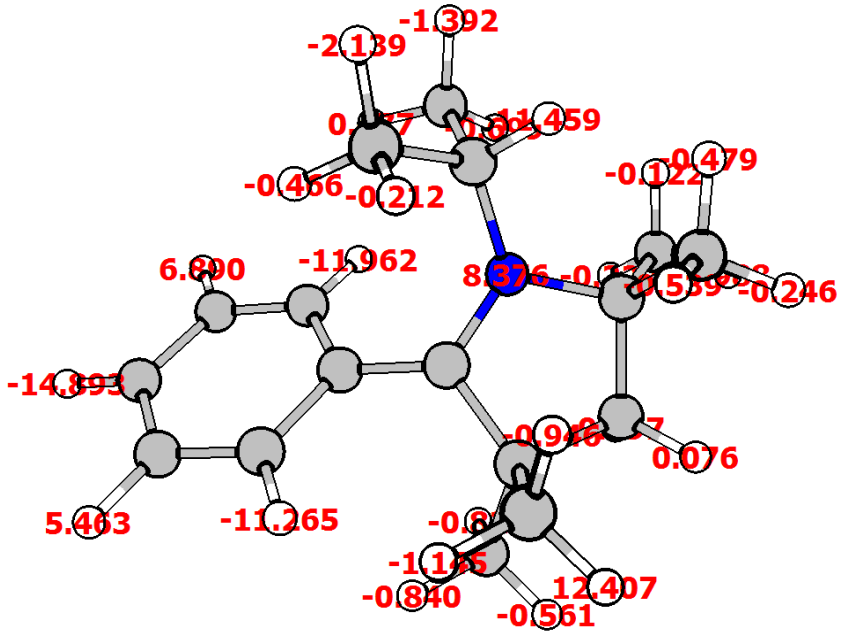



**Figure S43.** Calculated hyperfine coupling constants at PBE0/IGLO-III level for $\mathbf{3}^{H\bullet}$. (different view)

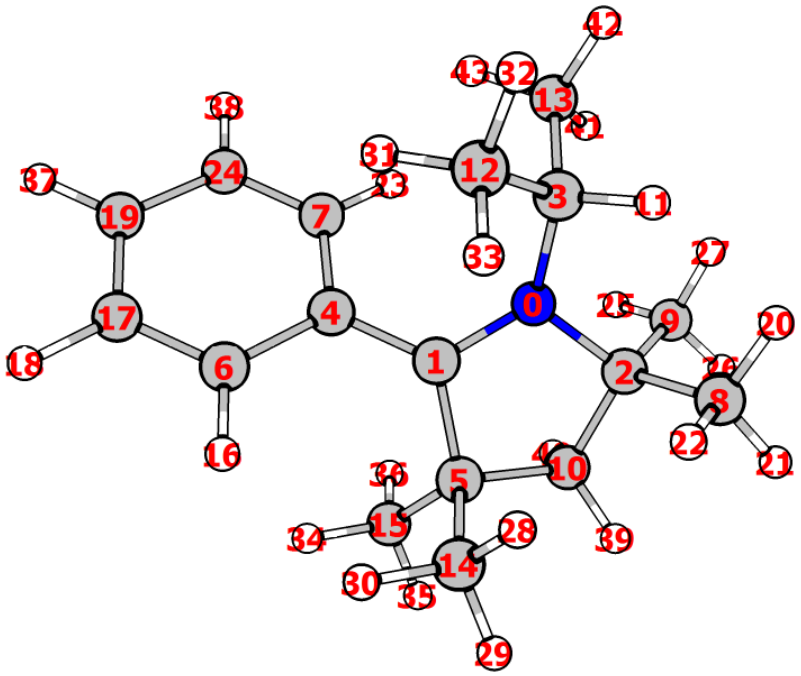



**Figure S44.** Atom numbering for $\mathbf{3}^{H\bullet}$ for hyperfine coupling constants.

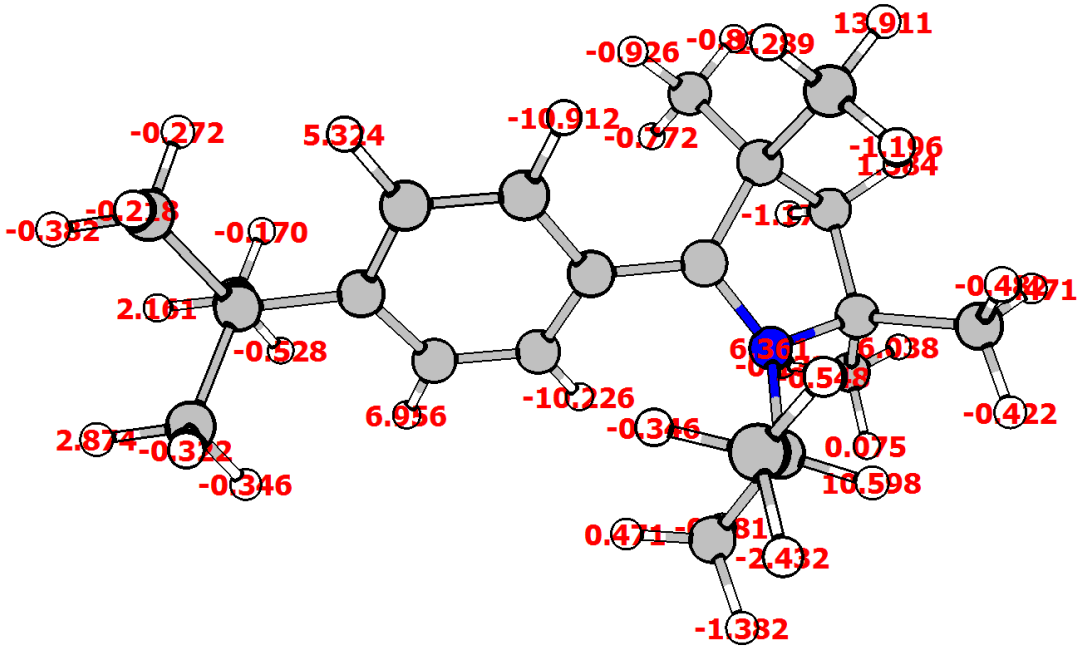



**Figure S45.** Calculated hyperfine coupling constants at PBE0/IGLO-III level for $\mathbf{3}^{tBu\bullet}$.

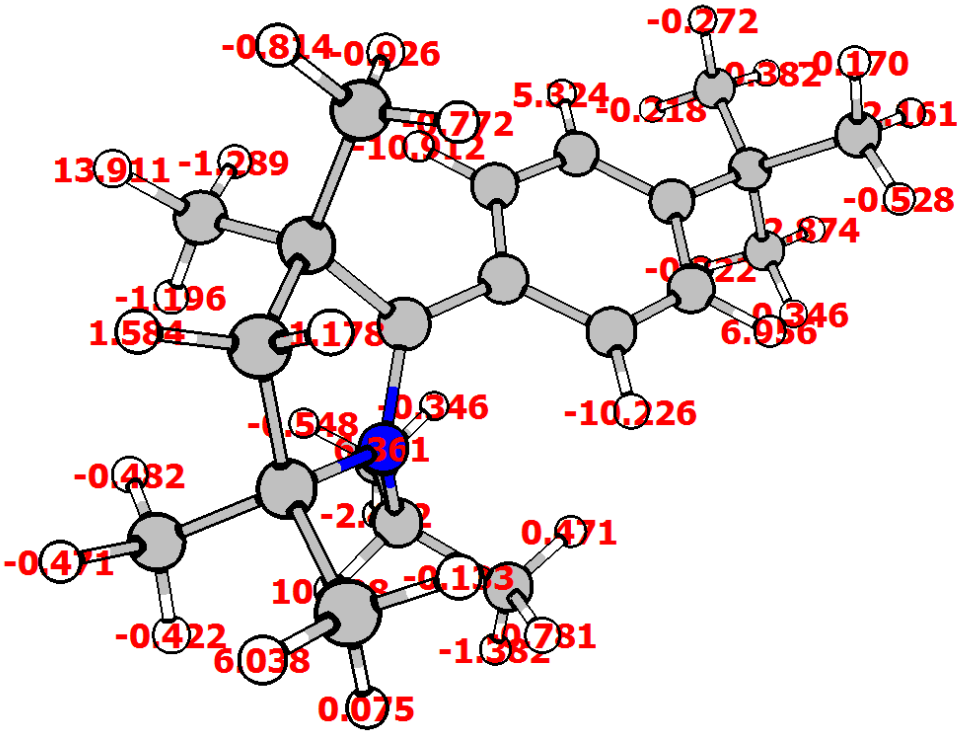



**Figure S46.** Calculated hyperfine coupling constants at PBE0/IGLO-III level for $\mathbf{3}^{tBu\bullet}$. (different view)

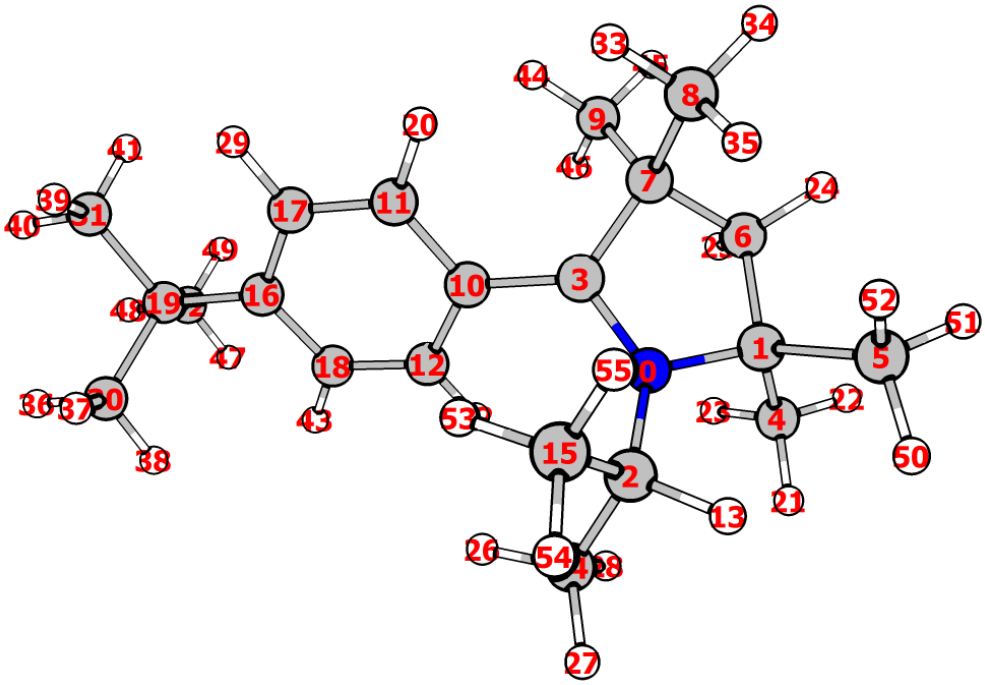



**Figure S47.** Atom numbering for $\mathbf{3}^{tBu\bullet}$ for hyperfine coupling constants.

Calculated g values g($\mathbf{3}^{H\bullet}$) = 2.077 and g($\mathbf{3}^{tBu\bullet}$) = 2.057

**Table S5.** Calculated hyperfine coupling constants at PBE0/IGLO-III level for $\mathbf{3^{H\bullet}}$ and $\mathbf{3^{tBu\bullet}}$.

| Atom ($3^{H\bullet}$) | Hyperfine Coupling Constant / MHz | Atom ($3^{tBu\bullet}$) | Hyperfine Coupling Constant / MHz |
|---|---|---|---|
| 0N | 8.3755 | 0N | 6.3612 |
| 11H | 11.4585 | 13H | 10.5975 |
| 16H | -11.2654 | 20H | -10.9123 |
| 18H | 5.4630 | 21H | 0.0754 |
| 20H | -0.4793 | 22H | 6.0376 |
| 21H | -0.2458 | 23H | -0.1333 |
| 22H | -0.5388 | 24H | 1.5837 |
| 23H | -11.9621 | 25H | -1.1777 |
| 25H | -0.2221 | 26H | 0.4711 |
| 26H | 4.9875 | 27H | -1.3822 |
| 27H | -0.1215 | 28H | -0.7807 |
| 28H | -0.9457 | 29H | 5.3236 |
| 29H | 12.4067 | 33H | -1.2888 |
| 30H | -1.1447 | 34H | 13.9106 |
| 31H | -0.4659 | 35H | -1.1960 |
| 32H | -2.1393 | 36H | 2.8745 |
| 33H | -0.2120 | 37H | -0.3216 |
| 34H | -0.8398 | 38H | -0.3461 |
| 35H | -0.5605 | 39H | -0.2175 |
| 36H | -0.8221 | 40H | -0.3819 |
| 37H | -14.8933 | 41H | -0.2722 |
| 38H | 6.8902 | 42H | -10.2255 |
| 39H | 0.0759 | 43H | 6.9556 |
| 40H | -0.8973 | 44H | -0.9255 |
| 41H | -0.6989 | 45H | -0.8136 |
| 42H | -1.3922 | 46H | -0.7718 |
| 43H | 0.4765 | 47H | -0.5277 |
| | | 48H | 2.1612 |
| | | 49H | -0.1699 |
| | | 50H | -0.4218 |
| | | 51H | -0.4714 |
| | | 52H | -0.4819 |
| | | 53H | -0.3455 |
| | | 54H | -2.4322 |
| | | 55H | -0.5484 |

**Table S6.** Parameters used for EPR simulation. Values for coupling constants are given in MHz.

| | A(N) | A(H) | A(H) | A(H) | A(H) | A(H) | A(H) | g |
|---|---|---|---|---|---|---|---|---|
| $3^{H\bullet}$ | 9 | 11 | 13 | 10 | 10 | 5 | 5 | 2.0027 |
| $3^{tBu\bullet}$ | 7 | 11 | 10 | 12 | 13 | 5 | 7 | 2.0027 |

## Atomic charges and Spin densities

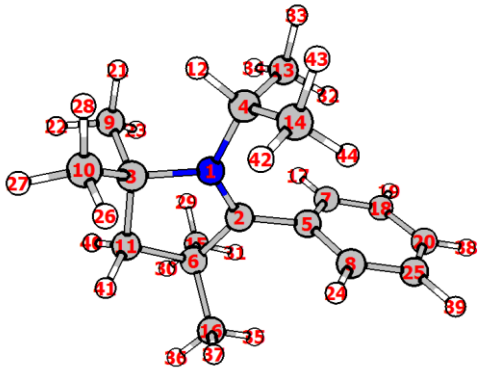


**Figure S48.** Numbering scheme for NPA charge analysis for $\mathbf{3}^{H}$.

**Table S7.** NPA charge analysis with JANPA for $\mathbf{3}^{H+}$ and $\mathbf{3}^{H\bullet}$.

| $\mathbf{3}^{H+}$ | | | | | $\mathbf{3}^{H\bullet}$ | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Center | Nuclear charge | Electron population | NMB population | NPA charge | Center | Nuclear charge | Electron population | NMB population | NPA charge |
| N1 | 7.0 | 7.2561950 | 7.2253634 | -0.2561950255 | N1 | 7.0 | 7.3918449 | 7.3634026 | -0.3918449187 |
| C2 | 6.0 | 5.4816587 | 5.4555046 | 0.5183413188 | C2 | 6.0 | 5.7842297 | 5.7594995 | 0.2157703334 |
| C3 | 6.0 | 5.8443929 | 5.8294499 | 0.1556071499 | C3 | 6.0 | 5.8443000 | 5.8288678 | 0.1557000147 |
| C4 | 6.0 | 6.0440763 | 6.0293409 | -0.0440762508 | C4 | 6.0 | 6.0321026 | 6.0166140 | -0.0321025683 |
| C5 | 6.0 | 6.1499500 | 6.1268268 | -0.1499499727 | C5 | 6.0 | 6.1242795 | 6.1018627 | -0.1242795491 |
| C6 | 6.0 | 6.1077125 | 6.0929115 | -0.1077124663 | C6 | 6.0 | 6.0803717 | 6.0643811 | -0.0803717276 |
| C7 | 6.0 | 6.1852738 | 6.1679988 | -0.1852738311 | C7 | 6.0 | 6.2242496 | 6.2059473 | -0.2242495715 |
| C8 | 6.0 | 6.1851790 | 6.1678933 | -0.1851790237 | C8 | 6.0 | 6.2270720 | 6.2080007 | -0.2270720034 |
| C9 | 6.0 | 6.6155772 | 6.6044373 | -0.6155772308 | C9 | 6.0 | 6.6216289 | 6.6105543 | -0.6216289292 |
| C10 | 6.0 | 6.6167228 | 6.6054982 | -0.6167228449 | C10 | 6.0 | 6.6065954 | 6.5956322 | -0.6065953723 |
| C11 | 6.0 | 6.3986953 | 6.3851383 | -0.3986952546 | C11 | 6.0 | 6.3874637 | 6.3740433 | -0.3874636729 |
| H12 | 1.0 | 0.7743509 | 0.7717820 | 0.2256491479 | H12 | 1.0 | 0.7983874 | 0.7954509 | 0.2016125784 |
| C13 | 6.0 | 6.6077141 | 6.5974852 | -0.6077140702 | C13 | 6.0 | 6.6074437 | 6.5972441 | -0.6074437087 |
| C14 | 6.0 | 6.6045532 | 6.5944166 | -0.6045532305 | C14 | 6.0 | 6.6078963 | 6.5979656 | -0.6078963366 |
| C15 | 6.0 | 6.5877520 | 6.5775324 | -0.5877520310 | C15 | 6.0 | 6.5885424 | 6.5784716 | -0.5885424072 |
| C16 | 6.0 | 6.5883441 | 6.5780369 | -0.5883441240 | C16 | 6.0 | 6.5898476 | 6.5795592 | -0.5898476469 |
| H17 | 1.0 | 0.7687129 | 0.7671253 | 0.2312870824 | H17 | 1.0 | 0.7927020 | 0.7908119 | 0.2072979859 |
| C18 | 6.0 | 6.1979811 | 6.1799705 | -0.1979810747 | C18 | 6.0 | 6.2204062 | 6.2022384 | -0.2204061626 |
| H19 | 1.0 | 0.7702030 | 0.7688771 | 0.2297969940 | H19 | 1.0 | 0.7875335 | 0.7860762 | 0.2124665093 |
| C20 | 6.0 | 6.1899571 | 6.1723455 | -0.1899570864 | C20 | 6.0 | 6.2691124 | 6.2489913 | -0.2691124326 |
| H21 | 1.0 | 0.7806771 | 0.7792856 | 0.2193228778 | H21 | 1.0 | 0.7943168 | 0.7928047 | 0.2056832448 |
| H22 | 1.0 | 0.7644215 | 0.7633125 | 0.2355785347 | H22 | 1.0 | 0.7823632 | 0.7811386 | 0.2176367951 |
| H23 | 1.0 | 0.7836146 | 0.7822567 | 0.2163854009 | H23 | 1.0 | 0.7906032 | 0.7892392 | 0.2093968239 |
| H24 | 1.0 | 0.7688828 | 0.7672793 | 0.2311172428 | H24 | 1.0 | 0.7889493 | 0.7866568 | 0.2110506883 |
| C25 | 6.0 | 6.1979314 | 6.1799304 | -0.1979313510 | C25 | 6.0 | 6.2211000 | 6.2029109 | -0.2211000036 |
| H26 | 1.0 | 0.7795164 | 0.7781654 | 0.2204836422 | H26 | 1.0 | 0.7896698 | 0.7881275 | 0.2103302111 |
| H27 | 1.0 | 0.7625457 | 0.7614717 | 0.2374542877 | H27 | 1.0 | 0.7888290 | 0.7874332 | 0.2111709976 |
| H28 | 1.0 | 0.7804171 | 0.7790187 | 0.2195828574 | H28 | 1.0 | 0.7947421 | 0.7932512 | 0.2052579175 |
| H29 | 1.0 | 0.7871289 | 0.7857652 | 0.2128711184 | H29 | 1.0 | 0.7971476 | 0.7957100 | 0.2028523622 |
| H30 | 1.0 | 0.7688382 | 0.7675972 | 0.2311617994 | H30 | 1.0 | 0.7966790 | 0.7949255 | 0.2033210235 |
| H31 | 1.0 | 0.7779688 | 0.7766094 | 0.2220312194 | H31 | 1.0 | 0.7964041 | 0.7949893 | 0.2035958800 |
| H32 | 1.0 | 0.7820944 | 0.7805504 | 0.2179056304 | H32 | 1.0 | 0.7871726 | 0.7854224 | 0.2128273712 |
| H33 | 1.0 | 0.7675190 | 0.7664096 | 0.2324809555 | H33 | 1.0 | 0.7879428 | 0.7867366 | 0.2120571917 |
| H34 | 1.0 | 0.7802643 | 0.7790425 | 0.2197356775 | H34 | 1.0 | 0.7912973 | 0.7899796 | 0.2087026884 |
| H35 | 1.0 | 0.7789763 | 0.7776187 | 0.2210236507 | H35 | 1.0 | 0.7908382 | 0.7893015 | 0.2091617525 |
| H36 | 1.0 | 0.7714345 | 0.7702469 | 0.2285655168 | H36 | 1.0 | 0.7945024 | 0.7931334 | 0.2054976216 |
| H37 | 1.0 | 0.7842681 | 0.7829511 | 0.2157318758 | H37 | 1.0 | 0.7926226 | 0.7912206 | 0.2073774267 |
| H38 | 1.0 | 0.7719795 | 0.7707326 | 0.2280204906 | H38 | 1.0 | 0.7876097 | 0.7862250 | 0.2123902834 |
| H39 | 1.0 | 0.7701080 | 0.7687832 | 0.2298920115 | H39 | 1.0 | 0.7879390 | 0.7864228 | 0.2120609912 |
| H40 | 1.0 | 0.7619693 | 0.7604470 | 0.2380306776 | H40 | 1.0 | 0.7848306 | 0.7830802 | 0.2151693847 |
| H41 | 1.0 | 0.7724901 | 0.7707309 | 0.2275098851 | H41 | 1.0 | 0.7916334 | 0.7896216 | 0.2083665896 |
| H42 | 1.0 | 0.7807842 | 0.7795509 | 0.2192158004 | H42 | 1.0 | 0.7895713 | 0.7882397 | 0.2104287250 |
| H43 | 1.0 | 0.7681654 | 0.7670580 | 0.2318345605 | H43 | 1.0 | 0.7914128 | 0.7901081 | 0.2085872223 |
| H44 | 1.0 | 0.7830025 | 0.7815073 | 0.2169974671 | H44 | 1.0 | 0.7958136 | 0.7942081 | 0.2041864029 |

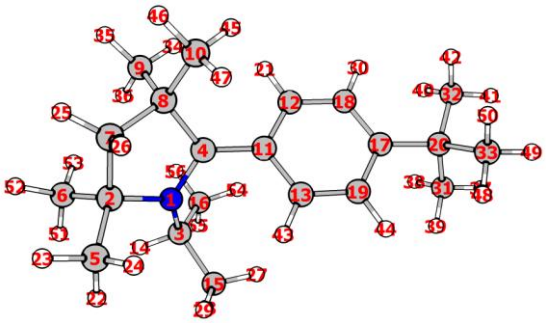


**Figure S49.** Numbering scheme for NPA charge analysis for $\mathbf{3}^{tBu}$.

**Table S8.** NPA charge analysis with JANPA for $\mathbf{3}^{tBu+}$ and $\mathbf{3}^{tBu\bullet}$.

| $\mathbf{3}^{tBu+}$ | | | | | $\mathbf{3}^{tBu\bullet}$ | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Center | Nuclear charge | Electron population | NMB population | NPA charge | Center | Nuclear charge | Electron population | NMB population | NPA charge |
| N1 | 7.0 | 7.2574043 | 7.2266725 | -0.2574043362 | N1 | 7.0 | 7.3978459 | 7.3683006 | -0.3978459017 |
| C2 | 6.0 | 5.8450571 | 5.8301264 | 0.1549429308 | C2 | 6.0 | 5.8524321 | 5.8367451 | 0.1475678916 |
| C3 | 6.0 | 6.0436659 | 6.0289018 | -0.0436659174 | C3 | 6.0 | 6.0328530 | 6.0171716 | -0.0328530190 |
| C4 | 6.0 | 5.4780710 | 5.4520816 | 0.5219289947 | C4 | 6.0 | 5.7851751 | 5.7603861 | 0.2148249007 |
| C5 | 6.0 | 6.6162470 | 6.6050365 | -0.6162469771 | C5 | 6.0 | 6.6011199 | 6.5902903 | -0.6011198502 |
| C6 | 6.0 | 6.6153734 | 6.6042427 | -0.6153734093 | C6 | 6.0 | 6.6182375 | 6.6073068 | -0.6182374584 |
| C7 | 6.0 | 6.3984797 | 6.3849440 | -0.3984796904 | C7 | 6.0 | 6.3809820 | 6.3677722 | -0.3809820438 |
| C8 | 6.0 | 6.1082098 | 6.0934036 | -0.1082098136 | C8 | 6.0 | 6.0914485 | 6.0753310 | -0.0914485112 |
| C9 | 6.0 | 6.5870966 | 6.5768860 | -0.5870966183 | C9 | 6.0 | 6.5850686 | 6.5750036 | -0.5850686429 |
| C10 | 6.0 | 6.5877694 | 6.5774709 | -0.5877693981 | C10 | 6.0 | 6.5857531 | 6.5755097 | -0.5857530885 |
| C11 | 6.0 | 6.1621921 | 6.1395080 | -0.1621920948 | C11 | 6.0 | 6.1250187 | 6.1025164 | -0.1250187152 |
| C12 | 6.0 | 6.1755568 | 6.1587001 | -0.1755567800 | C12 | 6.0 | 6.2146519 | 6.1964079 | -0.2146518508 |
| C13 | 6.0 | 6.1799481 | 6.1628667 | -0.1799481401 | C13 | 6.0 | 6.2108405 | 6.1920287 | -0.2108405321 |
| H14 | 1.0 | 0.7752017 | 0.7726279 | 0.2247983223 | H14 | 1.0 | 0.8001456 | 0.7971967 | 0.1998543525 |
| C15 | 6.0 | 6.6041703 | 6.5940314 | -0.6041702548 | C15 | 6.0 | 6.6033458 | 6.5934607 | -0.6033457561 |
| C16 | 6.0 | 6.6075400 | 6.5973038 | -0.6075399815 | C16 | 6.0 | 6.6034913 | 6.5933368 | -0.6034913235 |
| C17 | 6.0 | 5.9699940 | 5.9481014 | 0.0300059760 | C17 | 6.0 | 6.0367955 | 6.0143888 | -0.0367955269 |
| C18 | 6.0 | 6.2103723 | 6.1930773 | -0.2103723195 | C18 | 6.0 | 6.2228236 | 6.2053346 | -0.2228236380 |
| C19 | 6.0 | 6.2016233 | 6.1846073 | -0.2016233475 | C19 | 6.0 | 6.2186961 | 6.2013461 | -0.2186960585 |
| C20 | 6.0 | 6.0713737 | 6.0568177 | -0.0713736985 | C20 | 6.0 | 6.0635475 | 6.0486230 | -0.0635474653 |
| H21 | 1.0 | 0.7707925 | 0.7692118 | 0.2292074804 | H21 | 1.0 | 0.7948994 | 0.7930168 | 0.2051005917 |
| H22 | 1.0 | 0.7809895 | 0.7795868 | 0.2190105230 | H22 | 1.0 | 0.7968740 | 0.7953876 | 0.2031259690 |
| H23 | 1.0 | 0.7629072 | 0.7618308 | 0.2370927512 | H23 | 1.0 | 0.7919996 | 0.7905758 | 0.2080004335 |
| H24 | 1.0 | 0.7796114 | 0.7782585 | 0.2203886130 | H24 | 1.0 | 0.7925288 | 0.7909951 | 0.2074711799 |
| H25 | 1.0 | 0.7621354 | 0.7606118 | 0.2378646219 | H25 | 1.0 | 0.7874180 | 0.7856787 | 0.2125820349 |
| H26 | 1.0 | 0.7730669 | 0.7713053 | 0.2269330635 | H26 | 1.0 | 0.7937561 | 0.7917687 | 0.2062438688 |
| H27 | 1.0 | 0.7828696 | 0.7813751 | 0.2171304486 | H27 | 1.0 | 0.7947955 | 0.7932012 | 0.2052045416 |
| H28 | 1.0 | 0.7688031 | 0.7676929 | 0.2311969169 | H28 | 1.0 | 0.7950246 | 0.7937059 | 0.2049754162 |
| H29 | 1.0 | 0.7810228 | 0.7797893 | 0.2189771874 | H29 | 1.0 | 0.7930871 | 0.7917490 | 0.2069129084 |
| H30 | 1.0 | 0.7715531 | 0.7700208 | 0.2284468994 | H30 | 1.0 | 0.7885728 | 0.7869300 | 0.2114271723 |
| C31 | 6.0 | 6.5849642 | 6.5749650 | -0.5849642136 | C31 | 6.0 | 6.5850580 | 6.5749784 | -0.5850579894 |
| C32 | 6.0 | 6.5971692 | 6.5865294 | -0.5971692140 | C32 | 6.0 | 6.5941138 | 6.5834588 | -0.5941138215 |
| C33 | 6.0 | 6.5849641 | 6.5749725 | -0.5849640586 | C33 | 6.0 | 6.5851410 | 6.5750709 | -0.5851409502 |
| H34 | 1.0 | 0.7786444 | 0.7772764 | 0.2213556076 | H34 | 1.0 | 0.7976625 | 0.7962296 | 0.2023374571 |
| H35 | 1.0 | 0.7693015 | 0.7680582 | 0.2306985471 | H35 | 1.0 | 0.7993661 | 0.7975899 | 0.2006339465 |
| H36 | 1.0 | 0.7873338 | 0.7859683 | 0.2126661943 | H36 | 1.0 | 0.7986194 | 0.7971808 | 0.2013805783 |
| H37 | 1.0 | 0.7908225 | 0.7894206 | 0.2091775150 | H37 | 1.0 | 0.7989360 | 0.7974000 | 0.2010640349 |
| H38 | 1.0 | 0.7926853 | 0.7913569 | 0.2073146929 | H38 | 1.0 | 0.7959913 | 0.7946106 | 0.2040087147 |
| H39 | 1.0 | 0.7945121 | 0.7932073 | 0.2054879365 | H39 | 1.0 | 0.7968245 | 0.7954820 | 0.2031755493 |
| H40 | 1.0 | 0.7919003 | 0.7905589 | 0.2080996831 | H40 | 1.0 | 0.7949681 | 0.7935648 | 0.2050319150 |
| H41 | 1.0 | 0.7866634 | 0.7853517 | 0.2133365775 | H41 | 1.0 | 0.7937538 | 0.7923627 | 0.2062462326 |
| H42 | 1.0 | 0.7917656 | 0.7904260 | 0.2082343837 | H42 | 1.0 | 0.7949021 | 0.7934944 | 0.2050978743 |
| H43 | 1.0 | 0.7705827 | 0.7689753 | 0.2294173110 | H43 | 1.0 | 0.7890015 | 0.7867081 | 0.2109984651 |
| H44 | 1.0 | 0.7757901 | 0.7741241 | 0.2242099338 | H44 | 1.0 | 0.7933229 | 0.7914916 | 0.2066770565 |
| H45 | 1.0 | 0.7789394 | 0.7775783 | 0.2210606349 | H45 | 1.0 | 0.7929708 | 0.7914261 | 0.2070292083 |
| H46 | 1.0 | 0.7721473 | 0.7709577 | 0.2278527062 | H46 | 1.0 | 0.7961743 | 0.7948099 | 0.2038257256 |
| H47 | 1.0 | 0.7847862 | 0.7834611 | 0.2152138106 | H47 | 1.0 | 0.7942765 | 0.7928773 | 0.2057235220 |
| H48 | 1.0 | 0.7944106 | 0.7931041 | 0.2055893936 | H48 | 1.0 | 0.7969874 | 0.7956313 | 0.2030125947 |
| H49 | 1.0 | 0.7908436 | 0.7894428 | 0.2091564439 | H49 | 1.0 | 0.7988367 | 0.7973072 | 0.2011632804 |
| H50 | 1.0 | 0.7924015 | 0.7910803 | 0.2075984875 | H50 | 1.0 | 0.7959101 | 0.7945356 | 0.2040899169 |
| H51 | 1.0 | 0.7809964 | 0.7796024 | 0.2190036104 | H51 | 1.0 | 0.7958597 | 0.7943398 | 0.2041402525 |
| H52 | 1.0 | 0.7646732 | 0.7635637 | 0.2353268144 | H52 | 1.0 | 0.7843769 | 0.7831700 | 0.2156231217 |
| H53 | 1.0 | 0.7838989 | 0.7825391 | 0.2161011105 | H53 | 1.0 | 0.7923957 | 0.7910373 | 0.2076043126 |
| H54 | 1.0 | 0.7814145 | 0.7798468 | 0.2185855322 | H54 | 1.0 | 0.7910953 | 0.7893394 | 0.2089047411 |
| H55 | 1.0 | 0.7680752 | 0.7669613 | 0.2319248249 | H56 | 1.0 | 0.7937319 | 0.7924128 | 0.2062680963 |
| H56 | 1.0 | 0.7812162 | 0.7799850 | 0.2187837889 | H55 | 1.0 | 0.7904957 | 0.7892919 | 0.2095042914 |

**Table S9.** Loewdin and Mulliken atomic charges and spin densities for $\mathbf{3}^{\mathbf{H}\bullet}$.

| | $Q_{Loewdin}$ | $\rho_{Spin,\ Loewdin}$ | $Q_{Mulliken}$ | $\rho_{Spin,\ Mulliken}$ |
|---|---|---|---|---|
| N | 0.27 | 0.17 | -0.03 | 0.16 |
| C=N | -0.11 | 0.39 | -0.01 | 0.56 |
| $C_{ipso}$ | -0.15 | 0.04 | 0.06 | -0.09 |
| $C_{ortho}$ | -0.12 | 0.09 | -0.26 | 0.15 |
| $C_{meta}$ | -0.16 | -0.01 | -0.16 | -0.07 |
| $C_{para}$ | -0.18 | 0.11 | -0.18 | 0.17 |

**Table S10.** Loewdin and Mulliken atomic charges and spin densities for $\mathbf{3}^{\mathbf{tBu}\bullet}$.

| | $Q_{Loewdin}$ | $\rho_{Spin,Loewdin}$ | $Q_{Mulliken}$ | $\rho_{Spin,Mulliken}$ |
|---|---|---|---|---|
| N | 0.27 | 0.15 | -0.03 | 0.16 |
| C=N | -0.12 | 0.39 | -0.05 | 0.54 |
| $C_{ipso}$ | -0.15 | 0.03 | 0.11 | -0.09 |
| $C_{ortho}$ | -0.12 | 0.09 | -0.29 | 0.18 |
| $C_{meta}$ | -0.13 | -0.02 | -0.22 | -0.08 |
| $C_{para}$ | -0.11 | 0.11 | 0.16 | 0.19 |

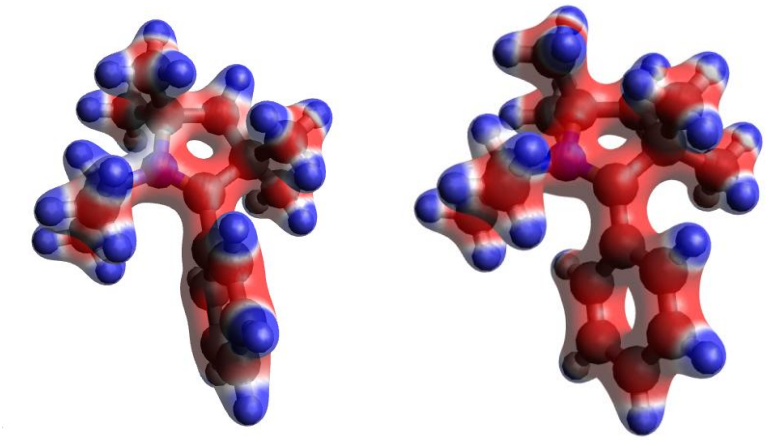


**Figure S50.** Electron densities of $\mathbf{3}^{H}$ (left) and $\mathbf{3}^{H\bullet}$ (right) with an iso-value of 0.08. Taken from a calculation with B3LYP/def2-TZVP.

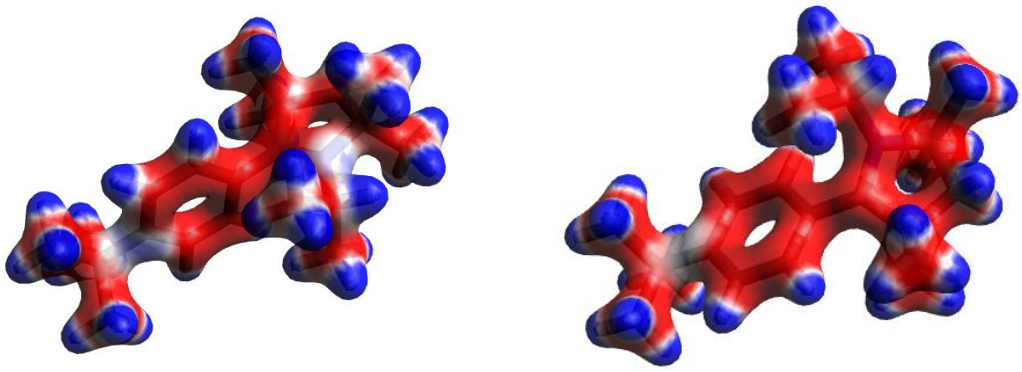


**Figure S51.** Electron densities of $\mathbf{3}^{tBu}$ (left) and $\mathbf{3}^{tBu\bullet}$ (right) with an iso-value of 0.08. Taken from a calculation with B3LYP/def2-TZVP.

## Calculated Energies of various Isomers

**Table S11.** Final Single Point Energies with different functionals for the **H**-substituted monomer, head-to-tail dimer and head-to-head dimer.

| Functional | Monomer Cation | Monomer Radical | Monomer Anion | Head-to-Tail Dimer | Head to Head Dimer |
|---|---|---|---|---|---|
| PBEh-3c (UKS) | ---------- | -716.202811083328 | ---------- | ---------- | ---------- |
| PBEh-3c (RKS) | -716.066514396295 | ---------- | -716.635684430896 | -1432.741051673214 | -1433.088308270493 |
| B3LYP (UKS) | -717.943607688966 | -718.051222983471 | -718.114668869832 | -1436.117066868625 | -1436.085976053292 |
| B3LYP (RKS) | -718.455718594047 | ---------- | -718.114668864621 | -1436.117066991070 | -1436.085976137692 |
| PBE0 (UKS) | -717.511027880874 | -717.622809356041 | -717.689101867494 | -1435.266248227500 | -1435.235811358463 |
| PBE0 (RKS) | -717.511027982316 | ---------- | -717.689101844752 | -1435.266248372699 | -1435.235811574712 |
| M06L (UKS) | -718.239745083561 | -718.350271153059 | -718.416043737010 | -1436.719121627786 | -1436.682717946314 |
| M06L (RKS) | -718.239744814839 | ---------- | -718.416043535408 | -1436.719120988254 | -1436.682717441611 |
| TPSSh (UKS) | -718.455718664650 | -718.565663094356 | -718.630753006319 | -1437.148413125609 | -1437.116438334753 |
| TPSSh (RKS) | -718.455718594047 | ---------- | -718.630752990531 | -1437.148413006569 | -1437.116438226319 |
| PBEh-3c (ZPVE) | 0.40875819 | 0.40570437 | 0.40228668 | 0.81848429 | 0.81736355 |

**Table S12.** Final Single Point Energies with different functionals for the **Me**-substituted monomer, head-to-tail dimer and head-to-head dimer.

| Functional | Monomer Cation | Monomer Radical | Monomer Anion | Head-to-Tail Dimer | Head to Head Dimer |
|---|---|---|---|---|---|
| PBEh-3c(UKS) | ---------- | -755.422989687168 | ---------- | ---------- | ---------- |
| PBEh-3c(RKS) | -755.701200655818 | ---------- | -755.870517640895 | -1511.106220150467 | -1511.715283438797 |
| B3LYP (UKS) | -757.252393044115 | -757.357923608668 | -757.421467020389 | -1514.704992034309 | -1514.697062270741 |
| B3LYP (RKS) | -757.252393034966 | ---------- | -757.421467063258 | -1514.704992125686 | -1514.697062370078 |
| PBE0 (UKS) | -756.797148315578 | -756.906856749703 | -756.973439859882 | -1513.808116616196 | -1513.800633116922 |
| PBE0 (RKS) | -756.797148439144 | ---------- | -756.973439834860 | -1513.808116972019 | -1513.800633492300 |
| M06L (UKS) | -757.566928272065 | -757.675242406129 | -757.740965466836 | -1515.342199369441 | -1515.329490124749 |
| M06L (RKS) | -757.566927944757 | ---------- | -757.740965285829 | -1515.342198748593 | -1515.329489426914 |
| TPSSh (UKS) | -757.794385998556 | -757.902384455203 | -757.968262633683 | -1515.797731385949 | -1515.787827962455 |
| TPSSh (RKS) | -757.794385959906 | ---------- | -757.968262590891 | -1515.797731220895 | -1515.787828106720 |
| PBEh-3c (ZPVE) | 0.43680327 | 0.43389541 | 0.43027147 | 0.87628733 | 0.87185579 |

**Table S13.** Final Single Point Energies with different functionals for the **Et**-substituted monomer, head-to-tail dimer and head-to-head dimer.

| Functional | Monomer Cation | Monomer Radical | Monomer Anion | Head-to-Tail Dimer | Head to Head Dimer |
|---|---|---|---|---|---|
| PBEh-3c(UKS) | ---------- | -794.626085287057 | ---------- | ---------- | ---------- |
| PBEh-3c(RKS) | -794.489467067321 | ---------- | -795.096696547988 | -1590.177291627277 | -1590.171748375601 |
| B3LYP (UKS) | -796.556455113803 | -796.661960586163 | -796.722229936561 | -1593.310876756393 | -1593.304804040221 |
| B3LYP (RKS) | -796.556455134320 | ---------- | -796.722229969571 | -1593.310877049672 | -1593.304804210314 |
| PBE0 (UKS) | -796.077994529353 | -796.187679104837 | -796.250781098403 | -1592.367747372241 | -1592.362425053634 |
| PBE0 (RKS) | -796.077994612652 | ---------- | -796.250781066337 | -1592.367747719263 | -1592.362425439825 |
| M06L (UKS) | -796.887694119479 | -796.996068144811 | -797.058523305611 | -1593.983610325870 | -1593.973888575093 |
| M06L (RKS) | -796.887693766838 | ---------- | -797.058523052491 | -1593.983609532065 | -1593.973887550711 |
| TPSSh (UKS) | -797.128385210458 | -797.236291190233 | -797.298463725356 | -1594.464375523885 | -1594.456444364170 |
| TPSSh (RKS) | -797.128385202101 | ---------- | -797.298463720958 | -1594.464375467018 | -1594.456444374739 |
| PBEh-3c (ZPVE) | 0.46666026 | 0.46357693 | 0.46031778 | 0.93543625 | 0.93054792 |

**Table S14.** Final Single Point Energies with different functionals for the ***t*Bu**-substituted monomer, head-to-tail dimer and head-to-head dimer.

| Functional | Monomer Cation | Monomer Radical | Monomer Anion | Head-to-Tail Dimer | Head to Head Dimer |
|---|---|---|---|---|---|
| PBEh-3c (UKS) | ---------- | -873.037068940899 | ---------- | ---------- | ---------- |
| PBEh-3c (RKS) | -873.389619862228 | ---------- | -872.909194452958 | -1747.064860483502 | -1747.067144273739 |
| B3LYP (UKS) | -875.164268971984 | -875.269230732933 | -875.329833771185 | -1750.498155886293 | -1750.498097261491 |
| B3LYP (RKS) | -875.164268908874 | ---------- | -875.329833820598 | -1751.773934899478 | -1750.498097481124 |
| PBE0 (UKS) | -874.640180023274 | -874.749463297085 | -874.812885051283 | -1749.463096052478 | -1749.463653943646 |
| PBE0 (RKS) | -874.640180125330 | ---------- | -874.812885135408 | -1751.243726013758 | -1749.463654267866 |
| M06L (UKS) | -875.530846000109 | -875.639478879157 | -875.701927307387 | -1751.243728211521 | -1751.243019336171 |
| M06L (RKS) | -875.530845492071 | ---------- | -875.701927042841 | -1751.243726013758 | -1751.243018334281 |
| TPSSh (UKS) | -875.796159553234 | -875.903870501859 | -875.966195677634 | -1751.773934833843 | -1751.772940307912 |
| TPSSh (RKS) | -875.796159438487 | ---------- | -875.966195693313 | -1751.773934899478 | -1751.772940339404 |
| PBEh-3c (ZPVE) | 0.52451290 | 0.52016884 | 0.51809614 | 1.05175211 | 1.04606879 |

**Table S15.** Final Single Point Energies with different functionals for the **H**-substituted monomer and possible reaction products in kcal/mol.

| Functional | ΔG(Cation+Anion) | ΔG(2xRadical) | ΔG(HT-Dimer) | ΔG(TT-Dimer) |
|---|---|---|---|---|
| B3LYP | 32.35 | 4.768 | 0 | 18.88 |
| PBE0 | 36.97 | 8.54 | 0 | 18.47 |
| M06L | 35.21 | 7.25 | 0 | 22.23 |
| TPSSh | 34.34 | 6.31 | 0 | 19.44 |

**Table S16.** Final Single Point Energies with different functionals for the **Me**-substituted monomer and possible reaction products.

| Functional | ΔG(Cation+Anion) | ΔG(2xRadical) | ΔG(HT-Dimer) | ΔG(TT-Dimer) |
|---|---|---|---|---|
| B3LYP | 13.80 | -12.19 | 0 | 2.20 |
| PBE0 | 17.83 | -8.88 | 0 | 1.92 |
| M06L | 15.80 | -10.57 | 0 | 5.22 |
| TPSSh | 16.29 | -9.79 | 0 | 3.45 |

**Table S17.** Final Single Point Energies with different functionals for the **Et**-substituted monomer and possible reaction products.

| Functional | ΔG(Cation+Anion) | ΔG(2xRadical) | ΔG(HT-Dimer) | ΔG(TT-Dimer) |
|---|---|---|---|---|
| B3LYP | 14.951 | -13.44 | 0 | 0.75 |
| PBE0 | 19.22 | -10.02 | 0 | 0.27 |
| M06L | 18.23 | -10.59 | 0 | 3.04 |
| TPSSh | 18.31 | -10.39 | 0 | 1.92 |

**Table S18.** Final Single Point Energies with different functionals for the ***t*Bu**-substituted monomer and possible reaction products.

| Functional | ΔG(Cation+Anion) | ΔG(2xRadical) | ΔG(HT-Dimer) | ΔG(TT-Dimer) |
|---|---|---|---|---|
| B3LYP | -3.20 | -32.58 | 0 | -3.54 |
| PBE0 | 0.56 | -29.76 | 0 | -3.93 |
| M06L | 1.14 | -29.38 | 0 | -3.13 |
| TPSSh | 1.54 | -28.49 | 0 | -2.95 |

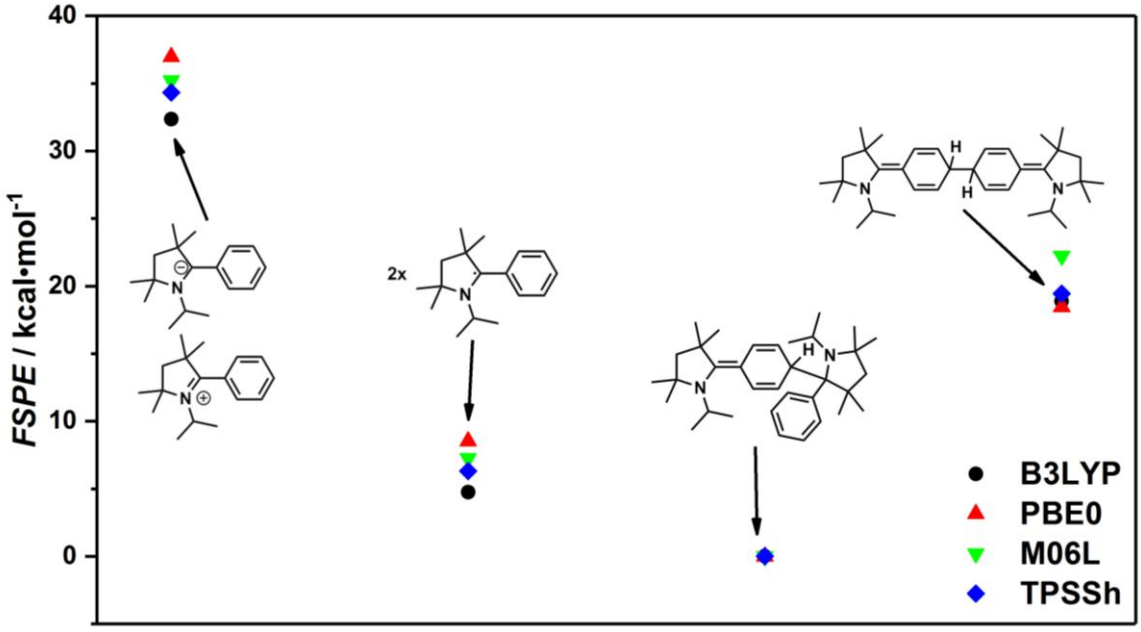



**Figure S52.** Energy differences for **H**-substituted isomers. From left to right: Energy of two monomers, Head-to-tail dimer and head-to-head dimer.

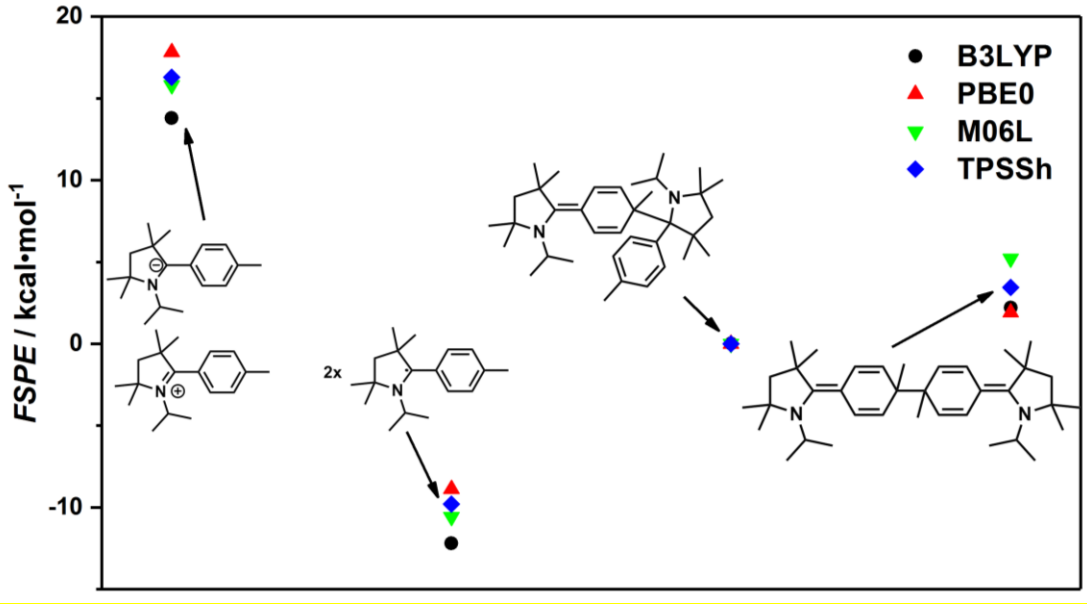



**Figure S53.** Energy differences for **Me**-substituted isomers. From left to right: Energy of two monomers, Head-to-tail dimer and head-to-head dimer.

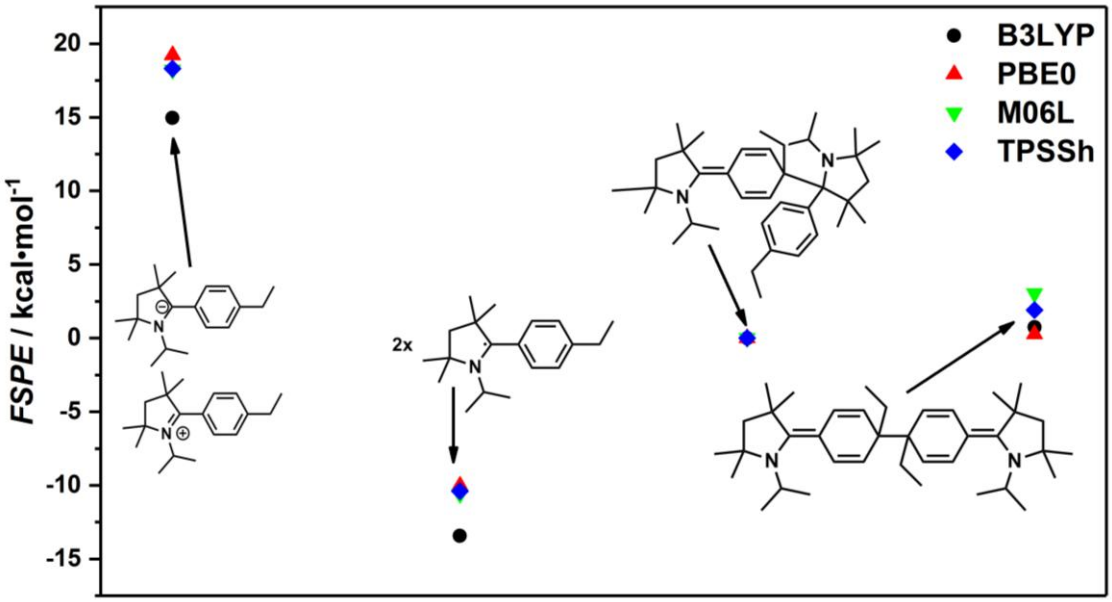



**Figure S54.** Energy differences for **Et**-substituted isomers. From left to right: Energy of two monomers, Head-to-tail dimer and head-to-head dimer.

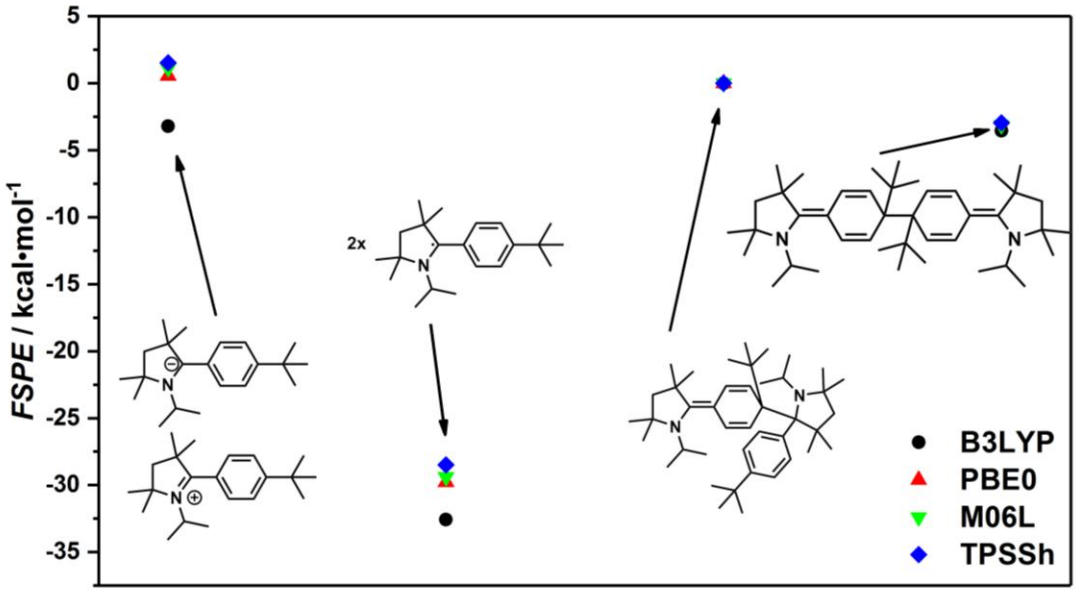



**Figure S55.** Energy differences for ***t*Bu**-substituted isomers. From left to right: Energy of two monomers, Head-to-tail dimer and head-to-head dimer.

## UV-Vis-NIR-Spectroelectrochemistry

**Table S19.** (UV-)Vis-NIR data for compounds $\mathbf{3}^{H}$ and $\mathbf{3}^{tBu}$ from OTTLE-spectroelectrochemistry in DCM with 0.1 $NBu_4PF_6$ measured with a gold mesh working electrode.

| λ [nm] (e [$10^3$ $M^{-1}$ • $cm^{-1}$]) | |
|---|---|
| $\mathbf{3}^{H}$ | 214, 260 |
| $\mathbf{3}^{H\bullet}$ | 214, 246, 271, 353, 487 |
| $\mathbf{3}^{H-}$ | 215, 330 |
| | |
| $\mathbf{3}^{tBu}$ | 216, 270 br |
| $\mathbf{3}^{tBu\bullet}$ | 212, 225 sh, 249, 273, 356, 486 br |
| $\mathbf{3}^{tBu-}$ | 216, 250 sh, 380 br |
| Obtained from spectroelectrochemical measurements using an OTTLE-cell with a gold working electrode in THF/0.1 M $NBu_4PF_6$ at 295K. | |

### *UV/Vis spectrum of radical monomer / dimer-mixture*

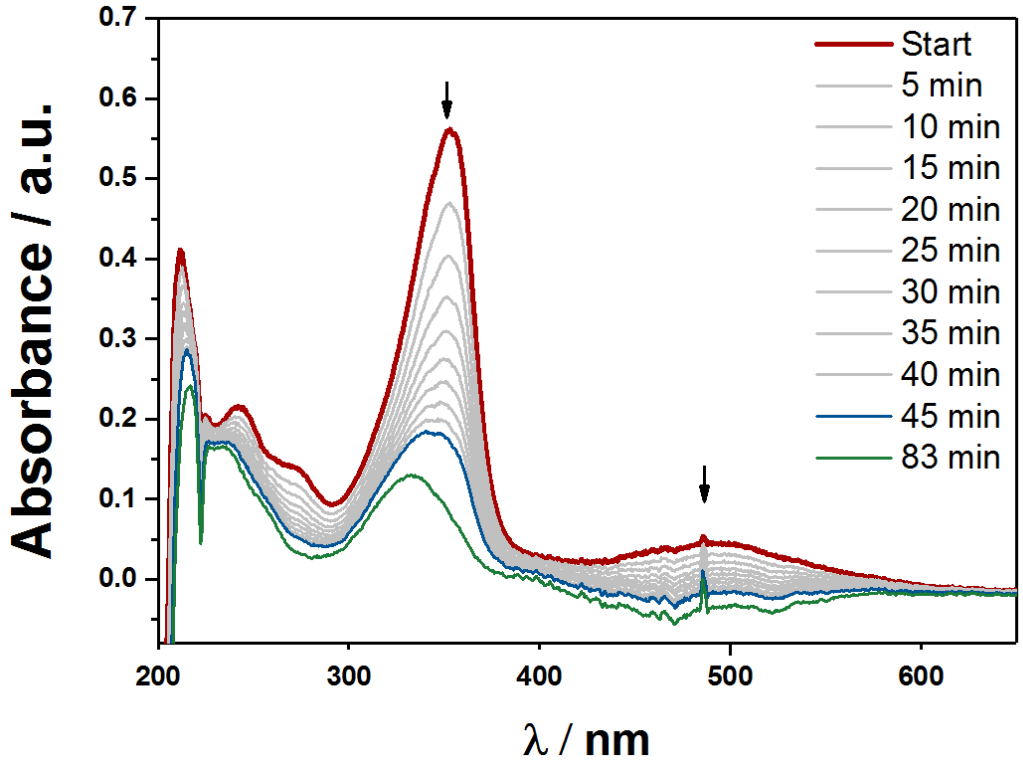



**Figure S56.** UV/vis spectra of the $\mathbf{3}^{H\bullet}/\mathbf{3}^{H}_{2}$ mixture in THF collected over 83 minutes.

## UV-Vis-NIR spectra of $3^{H}$ and $3^{H\bullet}$

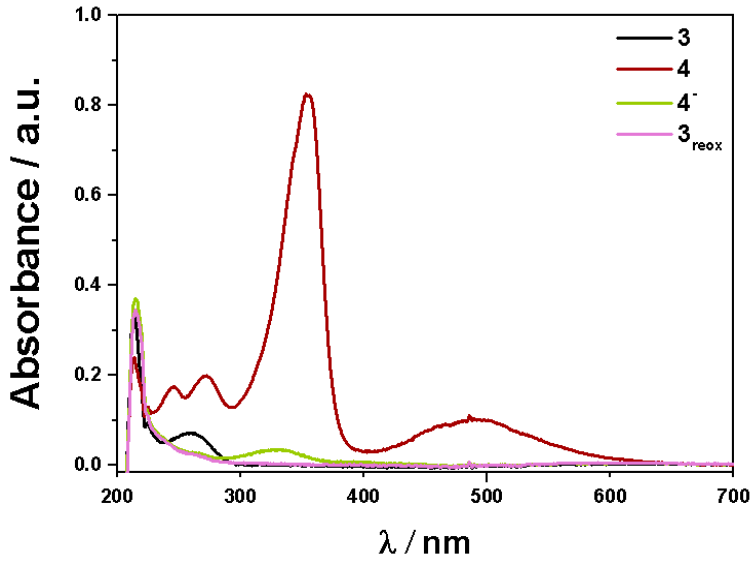



**Figure S57.** Overview of $3^{H}$ in various oxidation states. Re-oxidation took place after second reduction.

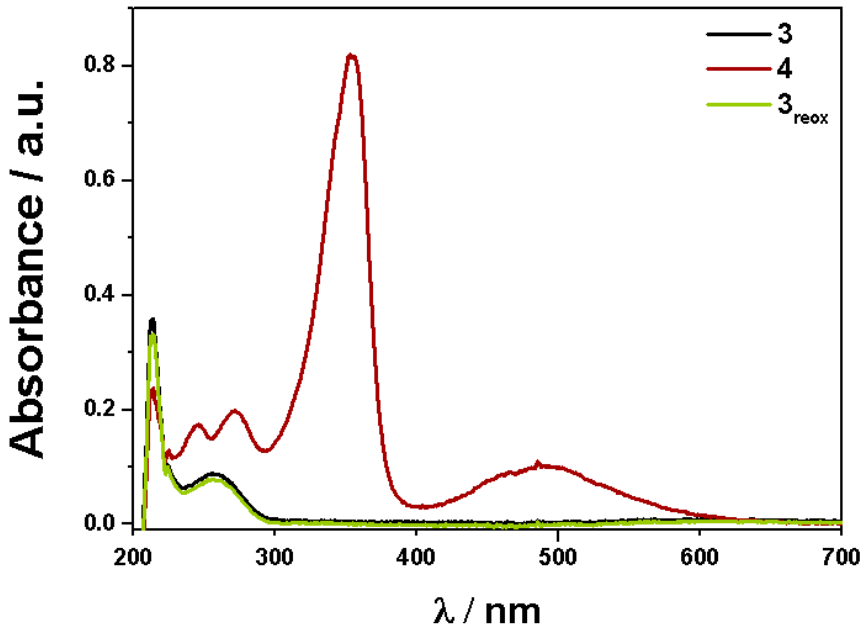



**Figure S58.** Overview of $3^{H}$ in various oxidation states. Re-oxidation took place after first reduction.

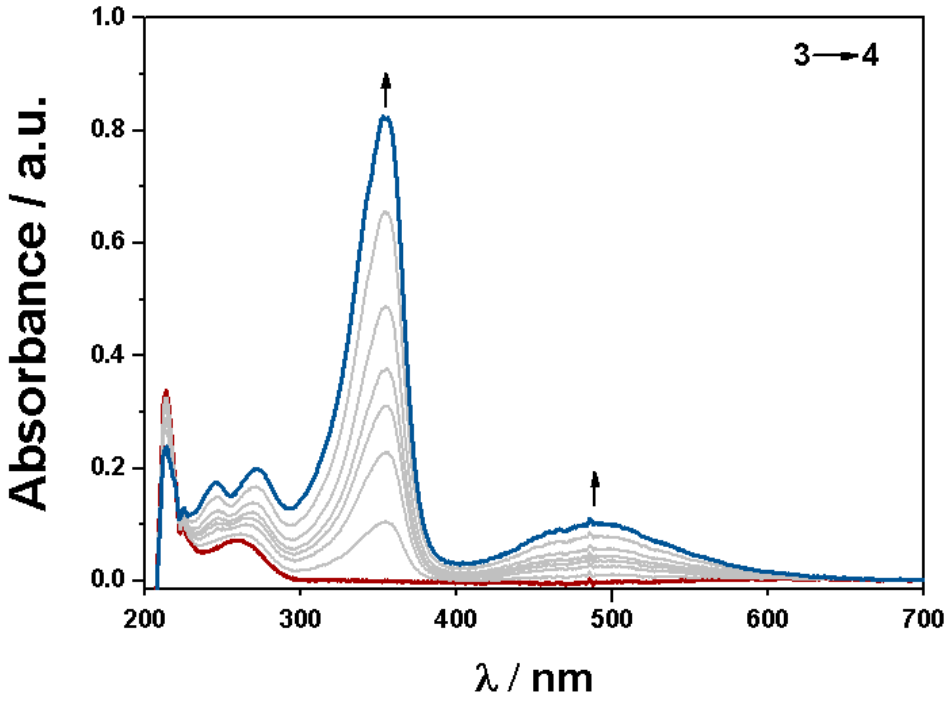



**Figure S59.** Changes in the UV-Vis-NIR spectrum of $\mathbf{3}^{H}$ during OTTLE-spectroelectrochemistry in THF/0.1 M $NBu_4PF_6$.

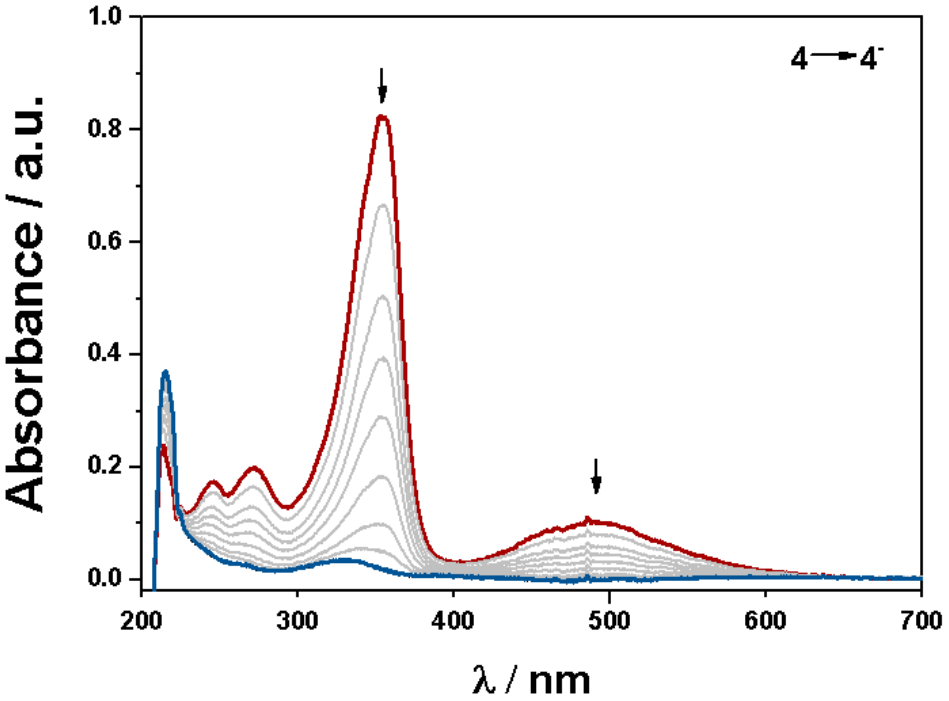



**Figure S60.** Changes in the UV-Vis-NIR spectrum of $\mathbf{3}^{H\bullet}$ during OTTLE-spectroelectrochemistry in THF/0.1 M $NBu_4PF_6$.

## UV-Vis spectra of $3^{tBu}$

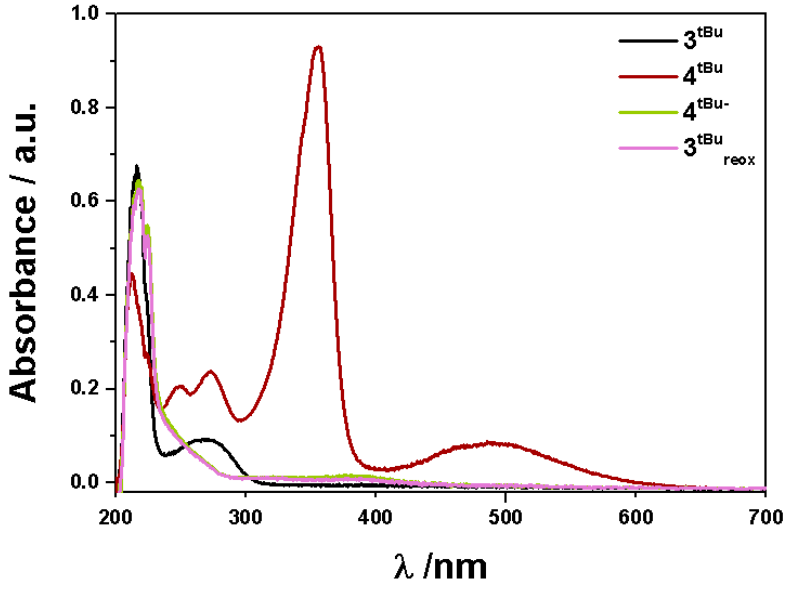



**Figure S61.** Overview of $3^{tBu}$ in various oxidation states. Re-oxidation took place after second reduction.

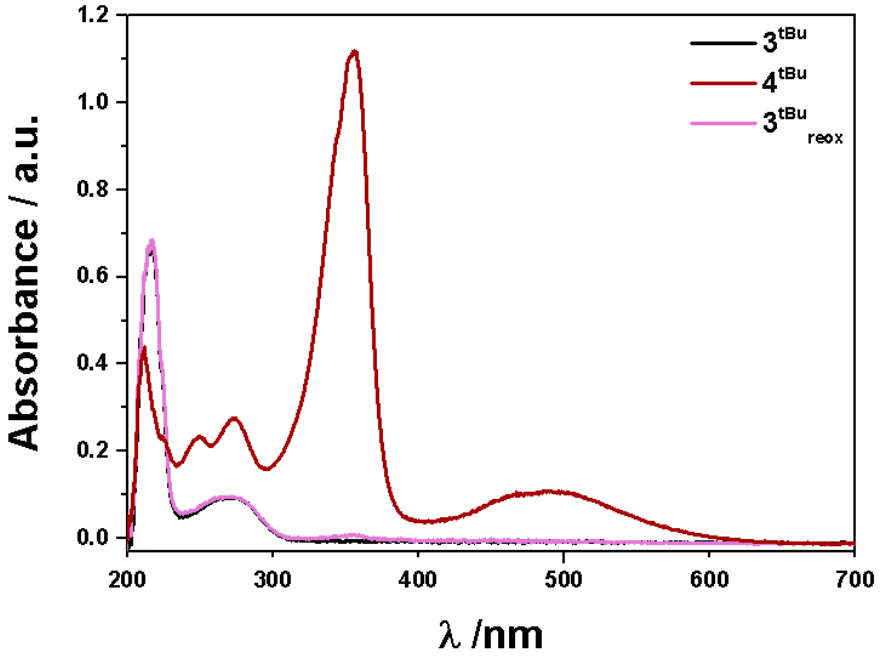



**Figure S62.** Overview of $3^{tBu}$ in various oxidation states. Re-oxidation took place after first reduction.

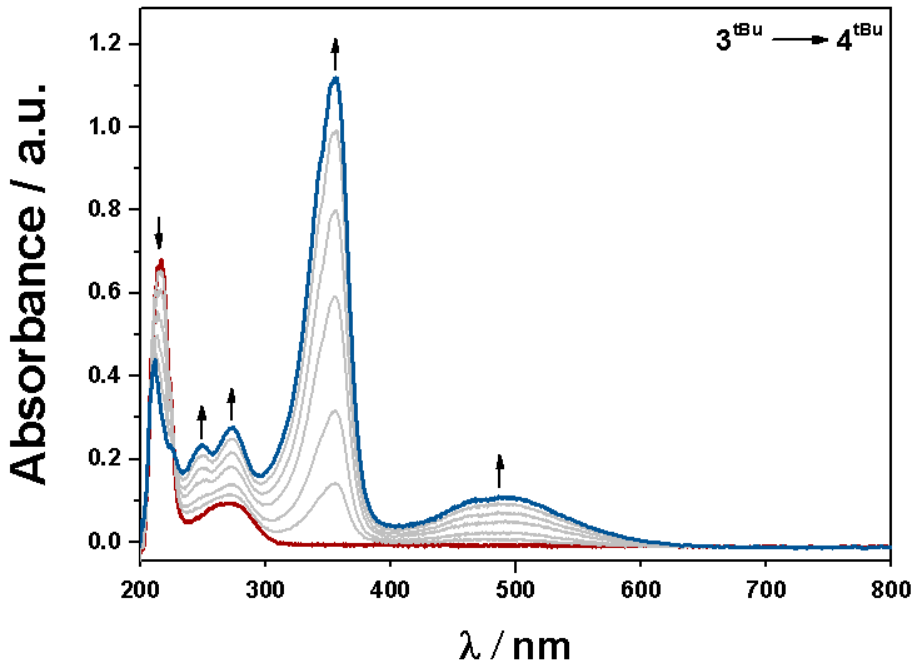



**Figure S63.** Changes in the UV-Vis-NIR spectrum of $\mathbf{3}^{tBu}$ during OTTLE-spectroelectrochemistry in THF/0.1 M $NBu_4PF_6$.

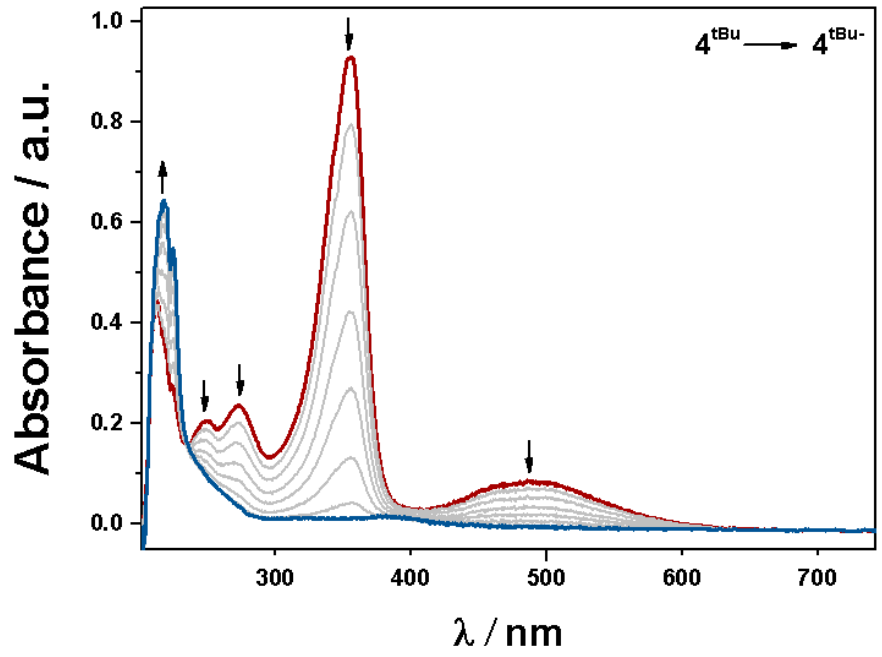



**Figure S64.** Changes in the UV-Vis-NIR spectrum of $\mathbf{3}^{tBu\bullet}$ during OTTLE-spectroelectrochemistry in THF/0.1 M $NBu_4PF_6$.

## (TD-)DFT calculations

### General remarks

A quick comparison of three levels of theory was conducted in order to interpret the absorption spectrum of compound $\mathbf{3}^{\mathbf{H}}$. Various TD-DFT calculations were carried out with B3PLYP Doubles , B3LYP TDA-TD-DFT ex and B3LYP Full TD-DFT. As expected, Full TD-DFT showed the best match with the experimentally obtained absorption spectrum., as depicted below for compound $\mathbf{3}^{\mathbf{H}}$.

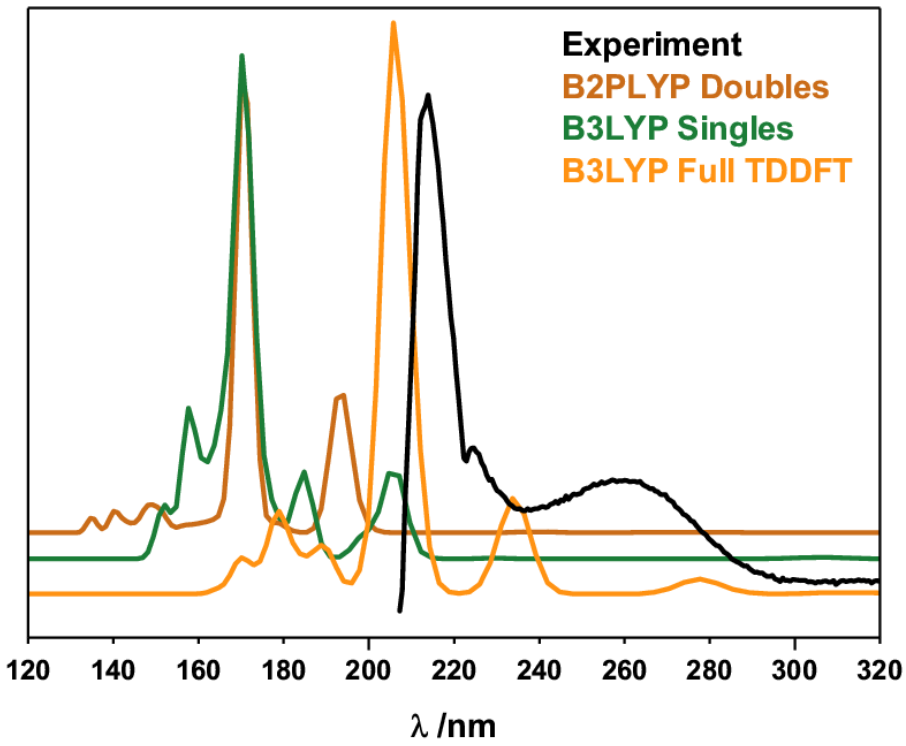
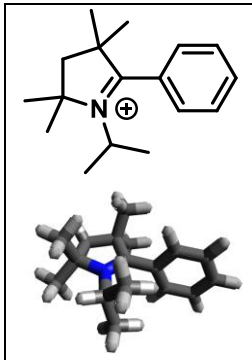



**Figure S65.** Comparison of calculated absorption spectra and experimental spectrum from TD-DFT calculations for $\mathbf{3}^{\mathbf{H}}$.

## *TDA-TD-DFT Calculation 3$^{H}$ (singlet state)*



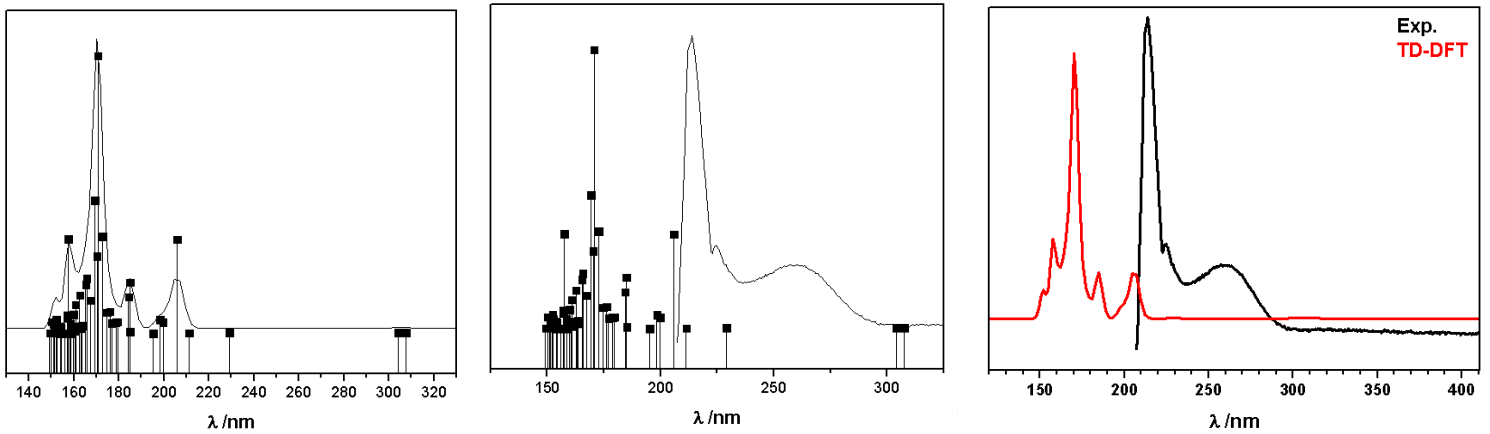



**Figure S66.** Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

**Table S20.** TD-DFT transitions for $\mathbf{3^H}$.

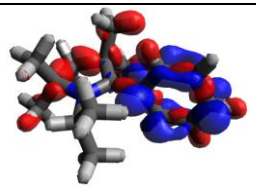
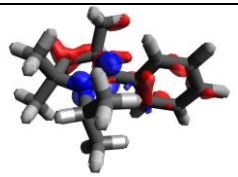
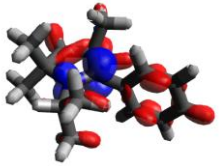
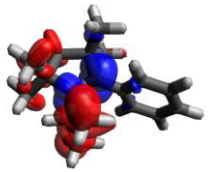
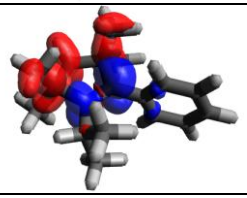
| State | Difference density (iso value 0.002) | Transition | Transition homo lumo | Calculated Transition energy | Oscillator strength | Experimental transition energy |
|---|---|---|---|---|---|---|
| 20 |  | 63a -> 68a (0.49) | HOMO-3 -> LUMO+1 (0.49) | 169.3 | 0.2279 | 216 |
| 15 |  | 56a -> 67a (0.17)<br>65a -> 69a (0.17)<br>66a -> 70a (0.17) | HOMO-10 -> LUMO (0.17)<br>HOMO-1 -> LUMO+2 (0.17)<br>HOMO -> LUMO+3 (0.17) | 170.7 | 0.4759 | |
| 14 |  | 55a -> 67a (0.40)<br>65a -> 68a (0.15)<br>66a -> 69a (0.18) | HOMO-11 -> LUMO (0.40)<br>HOMO-1 -> LUMO+1 (0.15)<br>HOMO -> LUMO+2 (0.18) | 172.7 | 0.1661 | |
| 10 |  | 59a -> 67a (0.67)<br>60a -> 67a (0.21) | HOMO-7 -> LUMO (0.67)<br>HOMO-6 -> LUMO (0.21) | 184.3 | 0.0627 | |
| 5 |  | 64a -> 67a (0.80) | HOMO-2 -> LUMO (0.80) | 205.9 | 0.1614 | 260 |

**Table S21.** Molecular orbitals for $\mathbf{3^H}$.

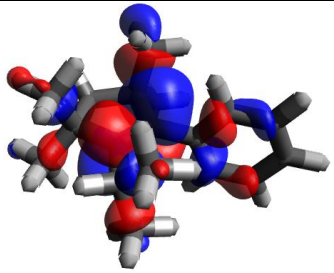
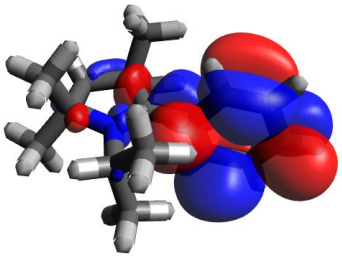
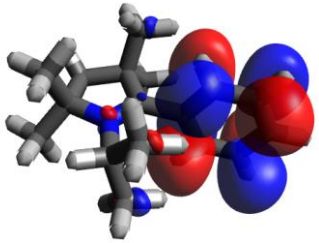
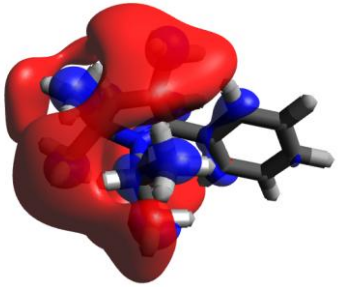
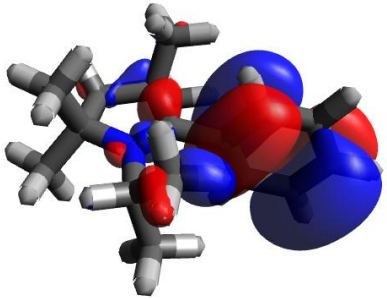
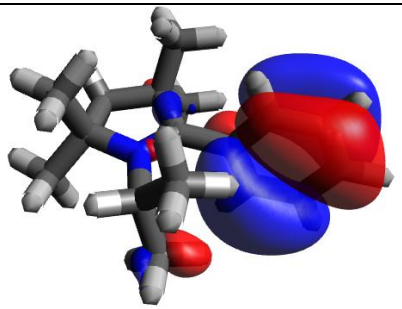
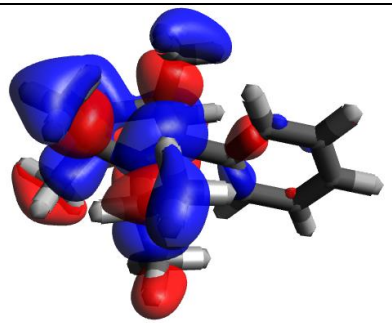
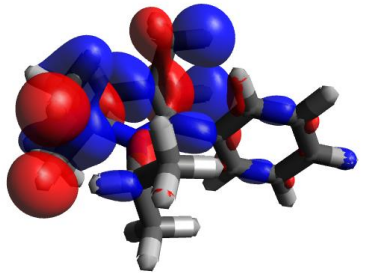
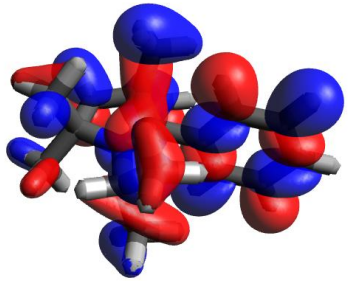
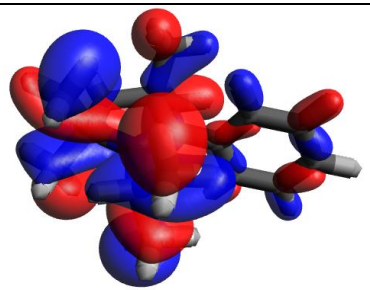
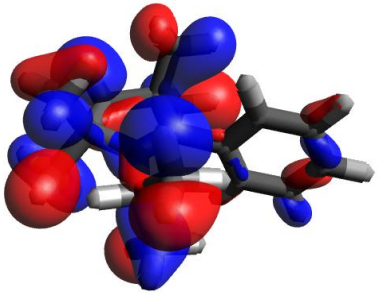
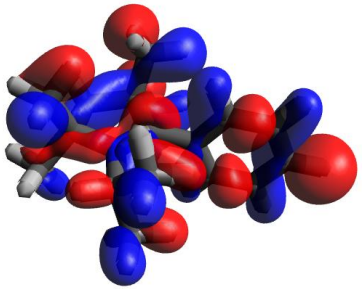
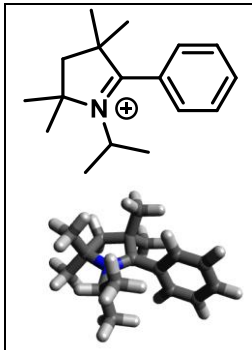
| LUMO | LUMO+1 | LUMO+2 | LUMO+3 |
|---|---|---|---|
|  |  |  |  |
| HOMO | HOMO-1 | HOMO-2 | HOMO-3 |
|  |  |  |  |
| HOMO-6 | HOMO-7 | HOMO-10 | HOMO-11 |
|  |  |  |  |

**Table S22.** Orbital energies for $\mathbf{3}^{H}$.

| Orbital No. | HOMO/LUMO | Energy (Eh) | Energy (eV) |
|---|---|---|---|
| 55 | HOMO-11 | -0.393308 | -10.7025 |
| 56 | HOMO-10 | -0.389973 | -10.6117 |
| 57 | HOMO-9 | -0.386481 | -10.5167 |
| 58 | HOMO-8 | -0.380233 | -10.3467 |
| 59 | HOMO-7 | -0.373473 | -10.1627 |
| 60 | HOMO-6 | -0.368433 | -10.0256 |
| 61 | HOMO-5 | -0.367359 | -9.9963 |
| 62 | HOMO-4 | -0.362142 | -9.8544 |
| 63 | HOMO-3 | -0.348688 | -9.4883 |
| 64 | HOMO-2 | -0.337256 | -9.1772 |
| 65 | HOMO-1 | -0.286633 | -7.7997 |
| 66 | HOMO | -0.286293 | -7.7904 |
| 67 | LUMO | -0.088517 | -2.4087 |
| 68 | LUMO+1 | -0.048959 | -1.3323 |
| 69 | LUMO+2 | -0.040165 | -1.0930 |
| 70 | LUMO+3 | 0.006274 | 0.1707 |

## *Full TD-DFT Calculation $3^H$ (singlet state)*



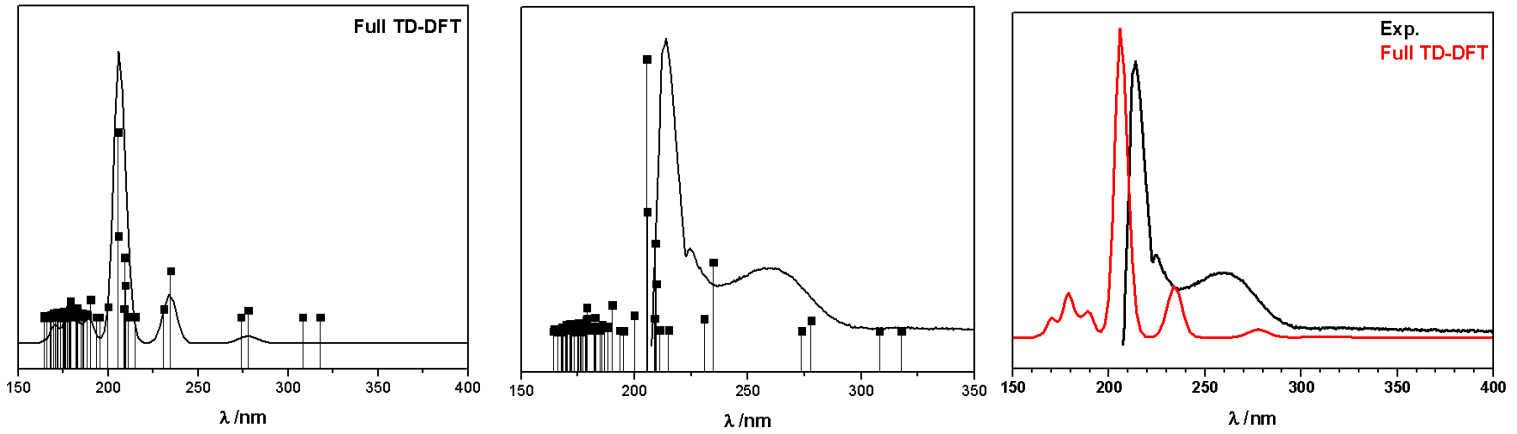



**Figure S67.** Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

**Table S23.** Full TD-DFT transitions for $\mathbf{3^H}$.

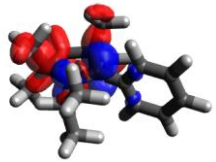
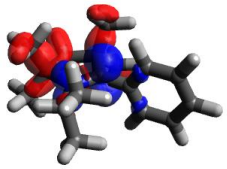
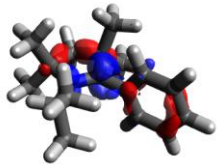
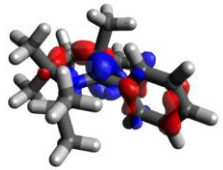
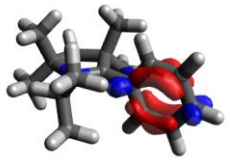
| State | Difference density (iso value 0.002) | Transition | Transition homo lumo | Calculated Transition energy | Oscillator strength | Experimental transition energy |
|---|---|---|---|---|---|---|
| 12 |  | 65a -> 69a (0.37)<br>66a -> 68a (0.17)<br>66a -> 69a (0.12) | HOMO-1 -> LUMO+2 (0.37)<br>HOMO -> LUMO+1 (0.17)<br>HOMO -> LUMO+2 (0.12) | 205.3 | 0.4653 | 214 |
| 11 |  | 59a -> 67a (0.19)<br>65a -> 68a (0.15)<br>65a -> 69a (0.16)<br>66a -> 69a (0.18) | HOMO-7 -> LUMO (0.19)<br>HOMO-1 -> LUMO+1 (0.15)<br>HOMO-1 -> LUMO+2 (0.16)<br>HOMO -> LUMO+2 (0.18) | 205.5 | 0.2048 | |
| 9 |  | 60a -> 67a (0.80) | HOMO-6 -> LUMO (0.80) | 209.3 | 0.1509 | |
| 10 |  | 59a -> 67a (0.66)<br>66a -> 69a (0.13) | HOMO-7 -> LUMO (0.66)<br>HOMO -> LUMO+2 (0.13) | 209.5 | 0.0817 | |
| 6 |  | 64a -> 67a (0.84) | HOMO-2 -> LUMO (0.84) | 234.6 | 0.1181 | 260 |

**Table S24.** Molecular orbitals for $\mathbf{3^H}$.

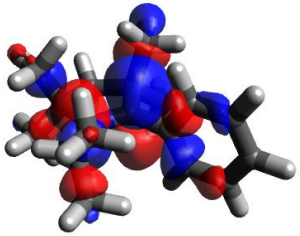
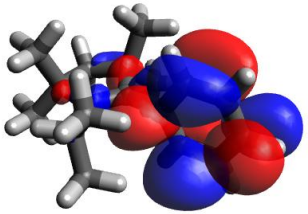
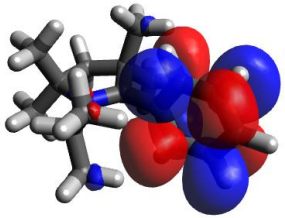
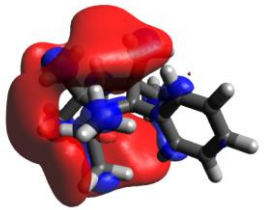
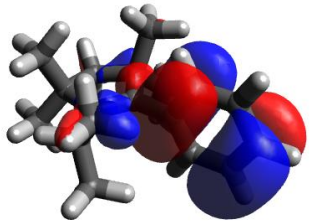
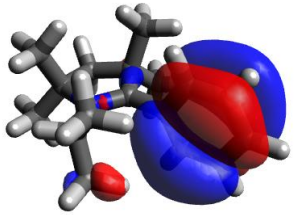
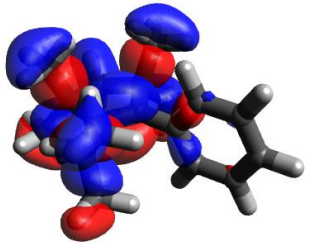
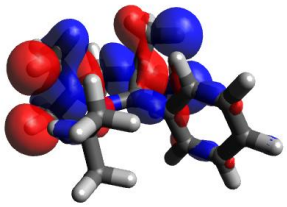
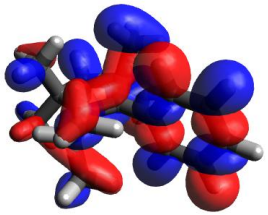
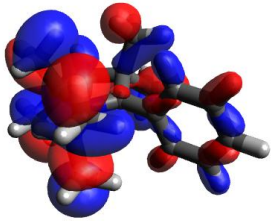
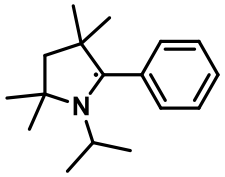
| LUMO | LUMO+1 | LUMO+2 | LUMO+3 |
|---|---|---|---|
|  |  |  |  |
| HOMO | HOMO-1 | HOMO-2 | HOMO-3 |
|  |  |  |  |
| HOMO-6 | HOMO-7 | | |
|  |  | | |

**Table S25.** Orbital energies for $\mathbf{3}^{H}$.

| Orbital No. | HOMO/LUMO | Energy (Eh) | Energy (eV) |
|---|---|---|---|
| 59 | HOMO-7 | -0.373473 | 10.1627 |
| 60 | HOMO-6 | -0.368433 | 10.0256 |
| 61 | HOMO-5 | -0.367359 | -9.9963 |
| 62 | HOMO-4 | -0.362142 | -9.8544 |
| 63 | HOMO-3 | -0.348688 | -9.4883 |
| 64 | HOMO-2 | -0.337256 | -9.1772 |
| 65 | HOMO-1 | -0.286633 | -7.7997 |
| 66 | HOMO | -0.286293 | -7.7904 |
| 67 | LUMO | -0.088517 | -2.4087 |
| 68 | LUMO+1 | -0.048959 | -1.3323 |
| 69 | LUMO+2 | -0.040165 | -1.0930 |
| 70 | LUMO+3 | 0.006274 | 0.1707 |

## Full TD-DFT Calculation $3^{H\bullet}$ (doublet state)



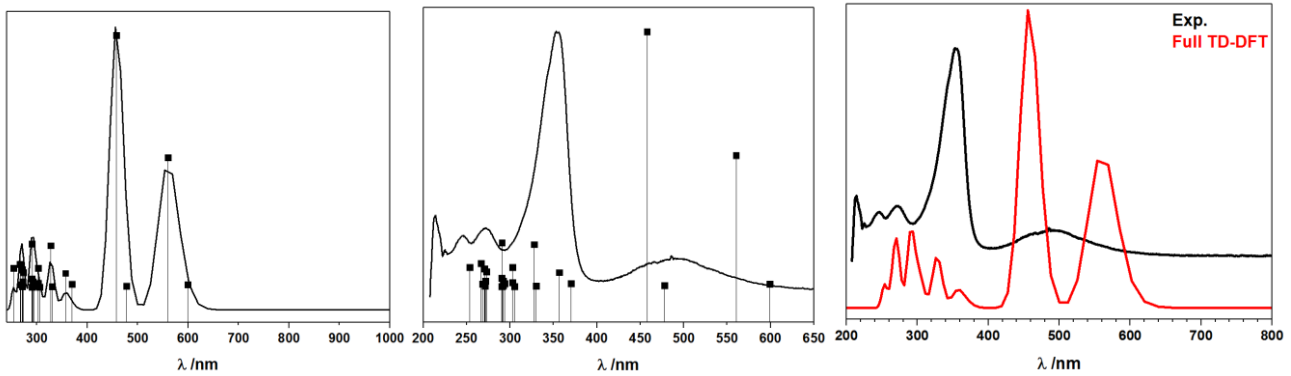



**Figure S68.** Calculated TD-DFT spectrum with discrete transitions (left), experimental spectrum with discrete calculated transitions (middle) and experimental (black) and calculated TD-DFT spectrum (red) (left).

**Table S26.** Full TD-DFT transitions for $\mathbf{3^{H\bullet}}$.

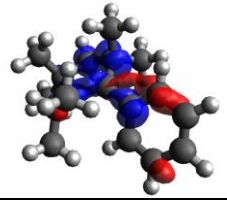
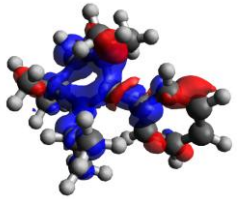
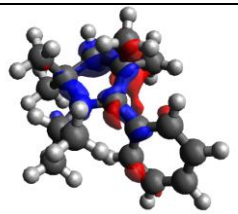
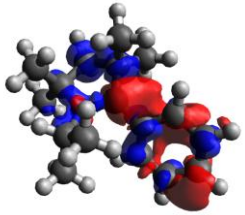
| State | Difference density (iso value 0.005) | Transition | Transition homo lumo | Calculated Transition energy | Oscillator strength | Experimental transition energy |
|---|---|---|---|---|---|---|
| 12 |  | 64b -> 67b (0.48) | HOMO-2β -> LUMOβ (0.48) | 290.7 | 0.0220 | 246 |
| 7 (0.3 iso) |  | 67a -> 72a (0.54) | HOMOα -> LUMO+4α (0.54) | 327.8 | 0.0211 | 271 |
| 4 |  | 66b -> 67b (0.73) | HOMOβ -> LUMOβ (0.73) | 457.8 | 0.1263 | 353 |
| 2 |  | 67a -> 69a (0.90) | HOMOα -> LUMO+1α (0.90) | 560.3 | 0.0653 | 487 |

**Table S27.** Selected molecular orbitals for $\mathbf{3}^{\mathbf{H\bullet}}$.

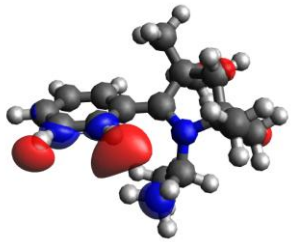
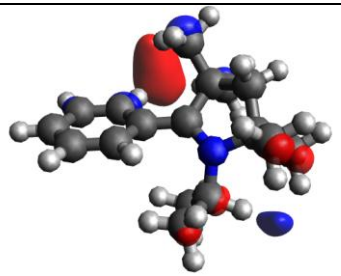
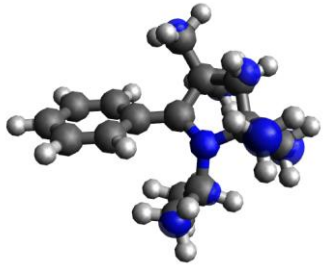
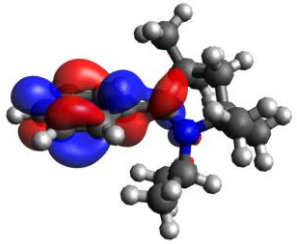
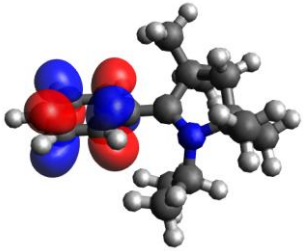
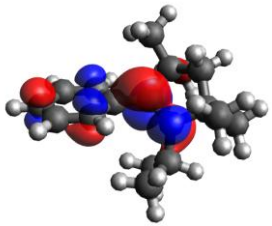
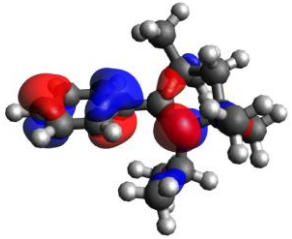
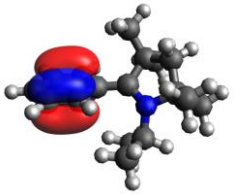
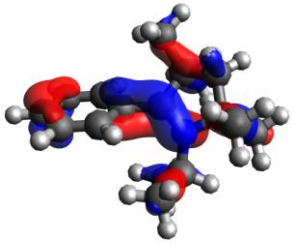
| LUMOα+4 | LUMOα+3 | LUMOα+2 | LUMOα+1 | LUMOα |
|---|---|---|---|---|
|  |  |  |  |  |
| HOMOα | HOMOα-1 | HOMOα-2 | HOMOα-3 | |
|  |  |  |  | |

**Table S28.** Selected molecular orbitals for $\mathbf{3}^{\mathbf{H\bullet}}$.

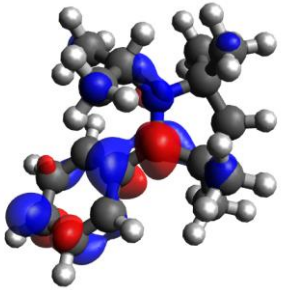
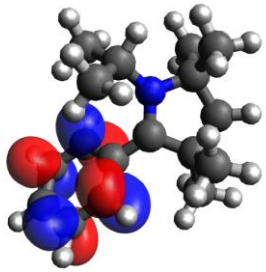
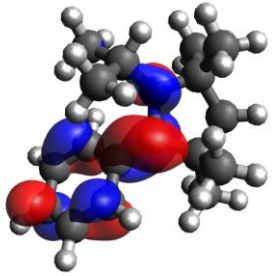
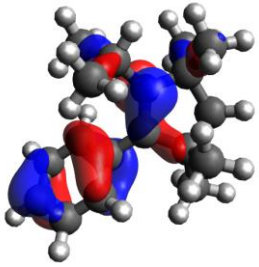
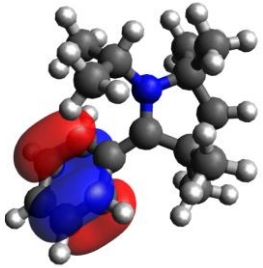
| LUMOβ+1 | LUMOβ | HOMOβ | HOMOβ-1 | HOMOβ-2 |
|---|---|---|---|---|
|  |  |  |  |  |

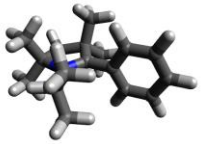
**Table S29.** Orbital energies for $\mathbf{3}^{H\bullet}$.

| Spin up Orbitals alpha | | | | Spin down orbitals beta | | | |
|---|---|---|---|---|---|---|---|
| Orbital No. | Orbital | Energy (Eh) | Energy (eV) | Orbital No. | Orbital | Energy (Eh) | Energy (eV) |
| 64 | HOMOα-3 | -0.279692 | -7.6108 | 63 | HOMOβ-3 | -0.301520 | -8.2048 |
| 65 | HOMOα-2 | -0.251411 | -6.8412 | 64 | HOMOβ-2 | -0.261491 | -7.1155 |
| 66 | HOMOα-1 | -0.240691 | -6.5495 | 65 | HOMOβ-1 | -0.245361 | -6.6766 |
| 67 | HOMOα | -0.124949 | -3.4000 | 66 | HOMOβ | -0.226126 | -6.1532 |
| 68 | LUMOα | -0.003691 | -0.1004 | 67 | LUMOβ | -0.042896 | -1.1673 |
| 69 | LUMOα+1 | 0.011238 | 0.3058 | 68 | LUMOβ+1 | 0.000016 | 0.0004 |
| 70 | LUMOα+2 | 0.031762 | 0.8643 | 69 | LUMOβ+2 | 0.029048 | 0.7904 |
| 71 | LUMOα+3 | 0.054668 | 1.4876 | 70 | LUMOβ+3 | 0.033730 | 0.9178 |
| 72 | LUMOα+4 | 0.059111 | 1.6085 | 71 | LUMOβ+4 | 0.055033 | 1.4975 |

# Coordinates of optimized structures

## $3^{H}$, $3^{H\bullet}$, and $3^{H-}$ coordinates

Cation



| | | | |
|---|---|---|---|
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| C | 5.41936861656645 | 5.51564634449475 | 16.72781335702993 |
| C | 4.61007829613500 | 5.02855621262387 | 19.12035192935314 |
| C | 6.91662378529766 | 6.87492237184885 | 19.89824242893203 |
| C | 7.25672200770801 | 7.04672116359897 | 17.32963369816216 |
| C | 6.43322972768453 | 8.05132228494046 | 20.46478672260445 |
| C | 7.84628931723432 | 6.10026346339789 | 20.58663729211465 |
| C | 4.14169949043673 | 6.21842295774085 | 16.27916811819180 |
| C | 5.38260552042153 | 4.03555375785450 | 16.36938942194270 |
| C | 6.69072394664420 | 6.18571029549299 | 16.19067786539662 |
| H | 3.90579980743249 | 4.55041653376307 | 18.44170233269622 |
| C | 3.81640034614861 | 6.00919794389951 | 19.97099903805910 |
| C | 5.27330724046344 | 3.93028520250575 | 19.93882057689478 |
| C | 6.90665793508990 | 8.53510982592672 | 17.18049717439667 |
| C | 8.77102978199262 | 6.89477596894815 | 17.47337623147840 |
| H | 5.71486974502143 | 8.66268909926872 | 19.93379454194204 |
| C | 6.85900112512780 | 8.43195089403672 | 21.72724264649415 |
| H | 6.47431938857879 | 9.34102195430712 | 22.16881805278661 |
| C | 7.77399764292482 | 7.65267822256580 | 22.41962339633756 |
| H | 3.24757298049777 | 5.78471468505993 | 16.72819784496087 |
| H | 4.03804611748574 | 6.11462978736180 | 15.19953884887480 |
| H | 4.15576445860732 | 7.28370373350342 | 16.50869945561416 |
| H | 8.24400739976144 | 5.19622700188914 | 20.14280161474211 |
| C | 8.26803843606756 | 6.48982355180643 | 21.84792544792069 |
| H | 6.24478694537314 | 3.50083979305061 | 16.76852078909081 |
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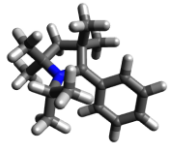
| H | 4.47480336702254 | 3.53183802877022 | 16.70081708809858 |
| H | 5.83347840670514 | 8.71095920512141 | 17.09824066876517 |
| H | 7.37236079347072 | 8.91596018709561 | 16.27151354291466 |
| H | 7.28874373946316 | 9.12410842079625 | 18.01355028643212 |
| H | 4.39975657705623 | 6.42130549952347 | 20.79034972922996 |
| H | 2.97208537796484 | 5.47614668938853 | 20.40683011301007 |
| H | 3.41179781144884 | 6.82819952652567 | 19.37612744208049 |
| H | 9.16344319713265 | 7.49327614887141 | 18.29458335753748 |
| H | 9.25242649325402 | 7.23364707318592 | 16.55580071911183 |
| H | 9.06599053293845 | 5.85685998511239 | 17.63347273683892 |
| H | 8.10560618248428 | 7.95434593812131 | 23.40374942872509 |
| H | 8.98714164599807 | 5.88364796731344 | 22.38158294802620 |
| H | 6.48435844731985 | 6.77196148279103 | 15.29532017356189 |
| H | 7.41914021681131 | 5.42264605288012 | 15.90889032146764 |
| H | 5.85366887211927 | 3.25071923688820 | 19.31543012536800 |
| H | 4.49595709607651 | 3.34283913010356 | 20.42597102940053 |
| H | 5.91666948710474 | 4.33190524397572 | 20.71861571435286 |

Radical



| | | | |
|---|---|---|---|
| N | 5.64879595220286 | 5.61187395732964 | 18.27569468545906 |
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| C | 5.65312804174928 | 5.32844039491407 | 16.83102814368184 |
| C | 4.48045047534268 | 5.22829325607194 | 19.06968343320795 |
| C | 7.08055848499904 | 6.80341105788719 | 19.91416771350407 |
| C | 6.98265430639391 | 7.34679485899257 | 17.36110106555624 |
| C | 7.37978658322865 | 8.08423337839775 | 20.42239609077161 |
| C | 7.38984476949352 | 5.70413803870474 | 20.73940917875373 |
| C | 4.33922737236741 | 5.68375581128289 | 16.12009077860369 |
| C | 5.95555464300838 | 3.85074316687231 | 16.58438757339258 |
| C | 6.80139617353398 | 6.21829170188266 | 16.33104486151158 |
| H | 3.72567396506797 | 4.92375098187951 | 18.34223201412798 |
| C | 3.88288427634721 | 6.39760007679257 | 19.84465827600534 |
| C | 4.68166932892221 | 4.01463943044761 | 19.97952523376934 |
| C | 6.10913719936811 | 8.56719436275221 | 17.03350924560898 |
| C | 8.44722596029724 | 7.77834104230624 | 17.39636110540777 |
| H | 7.13684225660539 | 8.96047339194491 | 19.83531445589960 |
| C | 7.93308977225391 | 8.24991263928981 | 21.67757606432991 |
| H | 8.13715983972205 | 9.24954450862744 | 22.03996182699553 |
| C | 8.21193795893834 | 7.15064373058656 | 22.48194754972931 |
| H | 3.52500091319745 | 5.00311213933943 | 16.37116717046755 |
| H | 4.48103962199185 | 5.61076171642563 | 15.04129080641539 |
| H | 4.00658623954309 | 6.69682772924844 | 16.34134889772120 |
| H | 7.24405348496485 | 4.70463335336623 | 20.35450436657358 |
| C | 7.93950936305492 | 5.87685763632024 | 21.99521995507331 |
| H | 6.87958594828669 | 3.55806765107014 | 17.08365131424094 |
| H | 6.06700313922580 | 3.64954045947605 | 15.51697114185792 |
| H | 5.15284238466028 | 3.20946214532210 | 16.95424010023633 |
| H | 5.04571995005957 | 8.33231304031259 | 17.04772112025966 |
| H | 6.35095968034370 | 8.96701346333786 | 16.04550719841758 |
| H | 6.26984948033600 | 9.36676546325510 | 17.75800551360572 |
| H | 4.53472524890383 | 6.73410932386073 | 20.64967225822461 |
| H | 2.93571242495871 | 6.09291972537457 | 20.29203734646747 |
| H | 3.68707643305971 | 7.24805825029258 | 19.19073598173968 |
| H | 8.62517907782093 | 8.59585363593299 | 18.09399308135868 |
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| H | 8.64001927921339 | 7.28392452534341 | 23.46622293746564 |
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| H | 6.62036509249136 | 6.59506844802481 | 15.32209496433670 |
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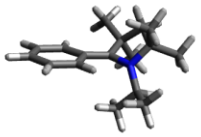
| H | 5.23202107586918 | 3.22235563043347 | 19.47194040537984 |
| H | 3.70969224767508 | 3.61079263841616 | 20.26813419975462 |
| H | 5.21126339183360 | 4.26888993547677 | 20.89546529200799 |

Anion



| | | | |
|---|---|---|---|
| N | 5.58604137806047 | 5.69370277648226 | 18.40625325122592 |
| C | 6.47721152881239 | 6.77562286972249 | 18.71428164455670 |
| C | 5.90084036021372 | 5.20434751244577 | 17.05895014652156 |
| C | 4.20624917957629 | 5.69277117219482 | 18.86924724388921 |
| C | 7.22794253109245 | 6.75668111328844 | 19.88346729230028 |
| C | 6.69263305364644 | 7.52930299960562 | 17.41943645812180 |
| C | 8.06001062015637 | 7.83543205436313 | 20.35244730230811 |
| C | 7.18008365099792 | 5.64406594799997 | 20.80002350638494 |
| C | 4.69428588799049 | 4.92235608806447 | 16.15719221187219 |
| C | 6.73794019850584 | 3.92606409703046 | 17.18034790697205 |
| C | 6.75629010275702 | 6.34018971486487 | 16.43608963136451 |
| H | 3.49834408557352 | 5.94196445293514 | 18.05906428222445 |
| C | 3.96962208848121 | 6.72272006120959 | 19.96595470165321 |
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| C | 5.49972657564609 | 8.43712611249553 | 17.06544671551354 |
| C | 7.97107093812234 | 8.34997363247400 | 17.27499239699264 |
| H | 8.10798752525307 | 8.75457242453876 | 19.78537025722068 |
| C | 8.76833246145604 | 7.77216244880035 | 21.53149268947976 |
| H | 9.36899367151563 | 8.63345878614775 | 21.81285722594061 |
| C | 8.72438577213841 | 6.66220543512455 | 22.37763041957490 |
| H | 4.02668568761311 | 4.15982052253587 | 16.56195536512906 |
| H | 5.05002399272351 | 4.55851148586734 | 15.19079572428040 |
| H | 4.10442566709832 | 5.82036666173055 | 15.96611524156633 |
| H | 6.57542995615687 | 4.78828249991333 | 20.52728196888372 |
| C | 7.90117935266728 | 5.60814199425223 | 21.97034921937874 |
| H | 7.57638384684917 | 4.10744251958785 | 17.85375536065477 |
| H | 7.13467635566218 | 3.60106018627626 | 16.21246806373661 |
| H | 6.14629771804166 | 3.10678081585241 | 17.59545511887441 |
| H | 4.55518013601753 | 7.89044751689831 | 17.09365266467881 |
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| H | 4.61980468757154 | 6.55011301071615 | 20.82345360494668 |
| H | 2.92917171735192 | 6.65980679990045 | 20.29860175380426 |
| H | 4.15980664634303 | 7.73463338302094 | 19.61430864778866 |
| H | 7.92361733968496 | 9.29304242138708 | 17.82074840491826 |
| H | 8.14022353885399 | 8.59911603695067 | 16.22214957085642 |
| H | 8.83913763405690 | 7.79857648571238 | 17.63880592137243 |
| H | 9.27693388748771 | 6.63041172086255 | 23.30772013469734 |
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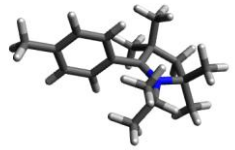
| H | 6.42150577454299 | 6.60272097132031 | 15.42346961534731 |
| H | 7.79762577938716 | 6.01546543279270 | 16.34850754708339 |
| H | 3.97984401390925 | 3.52682589970334 | 18.64324384927500 |
| H | 2.75677382665569 | 4.27133859820041 | 19.67146837087272 |
| H | 4.41065769081406 | 4.05174120946372 | 20.26604479125858 |

# $3^{Me}$, $3^{Me\bullet}$, and $3^{Me-}$ coordinates

**$3^{Me}$**



| | | | |
|---|---|---|---|
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| C | 4.09345715954557 | 0.37391026464399 | 5.67096247866540 |
| C | 3.73639731886475 | -1.56361982850817 | 4.15068252274382 |
| C | 6.02405424654232 | -0.74745113834573 | 4.99462439288888 |
| C | 5.19331673087435 | 1.10562175053515 | 6.39302085509084 |
| C | 2.68250733798944 | 0.76042800295649 | 5.82582300569551 |
| H | 4.47943549311207 | -2.27608382927037 | 3.79640643957882 |
| C | 3.10428396769769 | -0.91564213316068 | 2.92740801632276 |
| C | 2.73774381704141 | -2.34148059752136 | 4.99486908876602 |
| C | 5.07360803265392 | 2.61738768185152 | 6.20043744276831 |
| C | 5.11046559124086 | 0.77547715262974 | 7.89072239000026 |
| C | 6.45201783828485 | 0.53158161826235 | 5.72604598416590 |
| C | 2.11504895822269 | 1.67179638727278 | 4.94007651425985 |
| C | 1.93685579637176 | 0.30545618808097 | 6.90922146608100 |
| C | 6.60963046385249 | -0.80127874266446 | 3.58948556322839 |
| C | 6.35578766952854 | -2.01631750093018 | 5.77404342004622 |
| H | 2.68820610396564 | 2.05799875800992 | 4.10642101118969 |
| C | 0.81119471341090 | 2.09729921653844 | 5.12613214063644 |
| H | 6.35824175237306 | -1.71399832016214 | 3.04971071536821 |
| H | 7.69639707930280 | -0.77153847954372 | 3.66746189309164 |
| H | 6.30198341655258 | 0.05553345362102 | 2.98973597329761 |
| H | 2.26943987977330 | -0.27060124660454 | 3.19217199692876 |
| H | 2.71906989093993 | -1.70080304914705 | 2.27793936242550 |
| H | 3.82726007463702 | -0.34036541129434 | 2.34990244295147 |
| H | 3.19347485596904 | -2.73646243271746 | 5.90292094363778 |
| H | 2.38813257247579 | -3.19215466642413 | 4.41079816912506 |
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| H | 7.43817999796986 | -2.12089514382022 | 5.84169423866462 |
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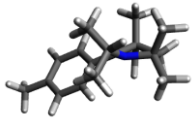

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| H | 6.27903252779416 | -2.13783973996931 | 6.17300216261891 |
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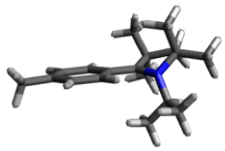

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## $3^{Et}$, $3^{Et\bullet}$, and $3^{Et-}$ coordinates

**$3^{Et}$**

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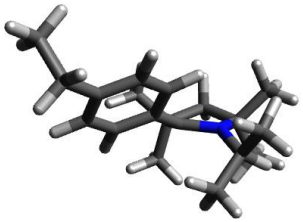

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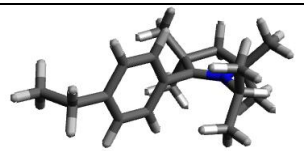

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| H | 18.37669481206169 | 6.36387576287042 | 5.70733192051535 |
| C | 17.43031150375683 | 5.93697287370601 | 7.58669555308924 |
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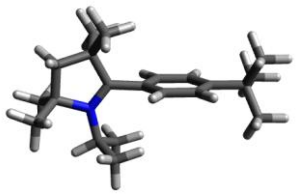
# $3^{tBu}$, $3^{tBu\bullet}$, and $3^{tBu-}$ coordinates



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| H | 2.36851300020123 | 3.06326184383959 | 17.21256908945339 |
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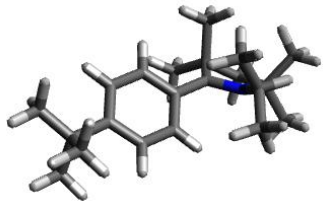

$3^{tBu\bullet}$

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| C | 0.03764218454986 | 4.71313647408823 | 18.44369160069594 |
| C | -0.30237011169297 | 3.22956753360262 | 18.65089556399717 |
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| C | 2.38191354680865 | 4.20909483874605 | 16.35245903532147 |
| C | 3.36925885578397 | 6.13519916116708 | 17.35883845030355 |
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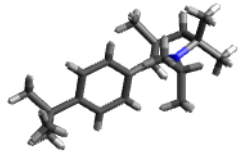

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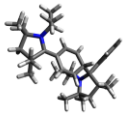
# $3^{H}_{2}$ and $3^{H}_{2}$' coordinates

$3^{H}_{2}$



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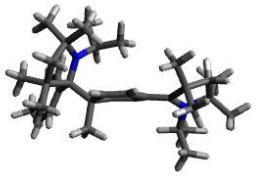
# $3^{Me}{}_2$ and $3^{Me}{}_2$' coordinates

$3^{Me}{}_2$



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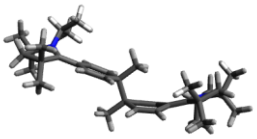

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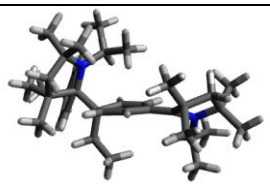

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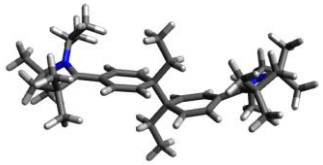

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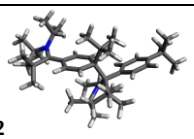
$3^{tBu}{}_2$



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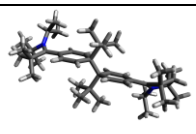

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| H | -4.312703114691 0 | 3.445539900957 85 | 0.20205042920976 |
| H | -6.662123834912 23 | 2.847784881844 46 | -2.70470290559891 |
| H | -5.123333520342 95 | 2.114594634105 13 | -3.15874598261158 |
| H | -6.480489793255 82 | 1.094759344332 81 | -2.79500825946064 |
| H | -5.526566839783 23 | -2.823299435993 99 | -2.33899708262013 |
| H | -5.610834530777 72 | -1.120323574340 64 | -2.75971215745747 |
| H | -7.008294456257 59 | -1.930619695105 197 | -2.04090247692781 |
| H | -3.258302302491 72 | -0.804461353916 9 | 0.90915148314077 |
| H | -0.939597759118 25 | -1.160349495947 54 | 0.86014636390604 |
| C | 0.084750809239 29 | -0.807860045042 62 | -1.83577439288571 |
| H | -0.555320334782 026 | 1.972494014929 11 | -2.15884718895081 |
| C | -2.871911110183 780 | 2.314022995068 621 | -2.07921798381068 |
| H | 1.686501260402 68 | 2.100424456148 94 | -1.54600825821296 |
| H | 3.910161979196 65 | 1.412027304110 89 | -1.37639249966977 |
| H | 2.899066778303 07 | -1.140425593349 05 | 1.97499461002288 |
| H | 7.977888105089 96 | -0.774930417819 50 | 0.08210737502173 |
| H | 7.365528814595 66 | -2.065580248064 35 | -0.93552742701069 |
| H | 7.261079582814 20 | -2.745533349453 81 | 2.99336979160866 |
| H | 8.312612162803 41 | -2.995681442458 32 | 1.61153328725359 |
| H | 8.196080542495 23 | -1.398676970691 92 | 2.32731421875785 |
| H | 6.454889117736 407 | -4.030404275228 82 | 0.30403552356268 |
| H | 5.336645232654 72 | -3.740602419131 83 | 1.63895716867555 |
| H | 4.961014356841 66 | -3.128018088881 08 | 0.03513313193305 |
| H | 4.639441734111 59 | -0.243819449937 36 | -2.43891337882785 |
| H | 6.214457409828 28 | -0.944324035537 08 | -2.78288241459260 |
| H | 4.996054162802 29 | -1.876835550082 31 | -1.91509172749597 |
| H | 5.905615852723 30 | 1.754429016467 13 | -1.29789815342648 |
| H | 6.986305080809 34 | 1.941409950982 93 | 0.04927294328638 |
| H | 7.456075896231 36 | 0.977160150980 96 | -1.59146411257437 |
| H | 6.520414283625 47 | -0.513328036846 42 | 3.24721755918990 |
| H | 5.168120484622 60 | 1.218777204853 36 | 4.08742757368415 |
| H | 5.524763081457 69 | 1.578548664587 54 | 2.39945543999136 |
| H | 3.923449299962 85 | 1.012138598319 25 | 2.86263856846640 |
| H | 4.952128763233 37 | -1.186703546436 3 | 4.89925225252667 |
| H | 5.080837176024 93 | -2.508912026052 27 | 3.74698126833365 |
| H | 3.669922765612 47 | -1.456672612446 56 | 3.72987503980999 |
| H | -4.279776745619 21 | -1.613657011940 56 | -0.74613345007208 |
| H | -6.853665734959 33 | -2.580474988667 09 | 0.55290022675362 |
| H | -5.319838500727 34 | -2.301331532529 13 | 1.38047542315332 |
| H | -5.440687327959 76 | -3.518407268752 86 | 0.11208274063692 |
| C | 0.386898577726 76 | 2.264347856273 09 | 0.99083463416281 |
| H | 0.658013667143 89 | -0.474557881741 37 | 1.82815104754563 |
| C | 0.230888880866 78 | 3.546384559263 80 | 0.15701408605431 |
| H | 1.509126442195 86 | 2.572103040606 65 | 1.99802144098747 |
| C | -0.897263977745 03 | 2.081370110355 74 | 1.80382388320535 |
| C | 0.704857652220 93 | -0.197986949142 50 | -3.10317500859048 |
| C | -1.157543772352 87 | -1.575814860949 24 | -2.32432486287076 |
| C | 1.062017558203 00 | -1.855056305788 57 | -1.29524279576278 |
| H | -1.959273231428 92 | -0.909155947638 84 | -2.64403190942829 |
| H | -1.560840846838 77 | -2.244212868566 83 | -1.56490689007914 |
| H | -0.879917850152 12 | -2.191124839611 01 | -3.18297711522426 |
| H | 2.488364776681 23 | 2.630273451259 90 | 1.52112376010701 |
| H | 1.568742630807 1 | 1.832926339157 56 | 2.79583643047667 |
| H | 1.313779214206 12 | 3.538938264524 16 | 2.46701302688440 |
| H | -1.792051056695 45 | 2.071110376563 17 | 1.18669989669179 |
| H | -0.992087689929 82 | 2.917982233490 85 | 2.50150346983414 |
| H | -0.890217518380 87 | 1.168956411928 65 | 2.40036778617648 |
| H | 2.060429541598 34 | -1.459305443311 27 | -1.12791452481146 |
| H | 1.151501731876 32 | -2.661108642062 74 | -2.02873934978832 |
| H | 0.718991485198 56 | -2.307413537145 78 | -0.36466388477936 |
| H | 0.004452629894 07 | 0.442975957760 13 | -3.63944907201860 |
| H | 0.972204633828 31 | -1.008900006081 03 | -3.78447395833907 |
| H | 1.613685866858 99 | 0.364175487569 09 | -2.91228424382314 |
| H | 1.157888513273 18 | 3.834389861123 50 | -0.33977312058052 |
| H | -0.030768858233 74 | 4.367128792125 23 | 0.82867521731469 |
| H | -0.558154454937 01 | 3.485400552108 63 | -0.58594090094120 |

**Crystallographic Tables**

**Table S30.** Crystal data and structure refinement for compound $\mathbf{3^H}$ (CCDC:1868053).

| | |
|---|---|
| Identification code | AJ0168RT1 |
| Empirical formula | $C_{18}H_{26}F_3NO_3S$ |
| Formula weight | 393.46 |
| Temperature/K | 293(2) |
| Wavelength | 0.71073 Å |
| Crystal system | Orthorhombic |
| space group | *Pbca* |
| Unit cell dimensions | a = 8.2322(9) Å α = 90°. |
| | b = 16.0090(15) Å β = 90°. |
| | c = 30.617(3) Å γ = 90°. |
| Volume | 4035.0(7) $Å^3$ |
| *Z*, Calculated density | 8, 1.295 $g/cm^3$ |
| Absorption coefficient | 0.204 $mm^{-1}$ |
| *F*(000) | 1664.0 |
| Crystal size | 0.55 × 0.413 × 0.261 $mm^3$ |
| Theta range for data collection | 2.861 to 25.498°. |
| Limiting indices | −9 ≤ h ≤ 9, −17 ≤ k ≤ 17, −37 ≤ l ≤ 36 |
| Reflections collected / unique | 17681 / 3642 [*R*(int) = 0.0553] |
| Completeness to theta= 25.498 | 97.3% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3642 / 0 / 241 |
| Goodness-of-fit on $F^2$ | 1.095 |
| Final *R* indices [*I*>2sigma(*I*)] | $R_1$ = 0.0570, $wR_2$ = 0.1583 |
| *R* indices (all data) | $R_1$ = 0.0742, $wR_2$ = 0.1716 |
| Largest diff. peak and hole | 0.45 and −0.32 e. $Å^{-3}$ |

**Table S31.** Crystal data and structure refinement for compound $\mathbf{3^{Me}}$ (CCDC: 1868056)

| | |
|---|---|
| Identification code | aj0284 |
| Empirical formula | $C_{19}H_{28}F_3NO_3S$ |
| Formula weight | 407.48 |
| Temperature/K | 293(2) |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| space group | *C*2/*c* |
| Unit cell dimensions | a = 34.1987(12) Å α = 90°. |
| | b = 8.2153(3) Å β = 101.860(4)°. |
| | c = 15.7716(6) Å γ = 90°. |
| Volume | 4336.5(3) $Å^3$ |
| *Z*, Calculated density | 8, 1.248 $g/cm^3$ |
| Absorption coefficient | 0.192 $mm^{-1}$ |
| *F*(000) | 1728.0 |
| Crystal size | 0.89 × 0.773 × 0.235 $mm^3$ |
| Theta range for data collection | 2.553 to 26.498°. |
| Limiting indices | −34 ≤ h ≤ 42, −10 ≤ k ≤ 9, −19 ≤ l ≤ 18 |
| Reflections collected / unique | 23027 / 4493 [*R*(int) = 0.0344] |
| Completeness to theta= 26.498 | 99.7% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4493 / 0 / 251 |
| Goodness-of-fit on $F^2$ | 1.057 |
| Final *R* indices [*I*>2sigma(*I*)] | $R_1$ = 0.0407, $wR_2$ = 0.1050 |
| *R* indices (all data) | $R_1$ = 0.0467, $wR_2$ = 0.1087 |
| Largest diff. peak and hole | 0.51 and −0.38 e. $Å^{-3}$ |

**Table S32.** Crystal data and structure refinement for compound $\mathbf{3}^{\mathbf{Et}}$ (CCDC: 1868057).

| | |
|---|---|
| Identification code | AJ0300 |
| Empirical formula | $C_{20}H_{30}F_3NO_3S$ |
| Formula weight | 421.51 |
| Temperature/K | 293(2) |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| space group | *C*2/*c* |
| Unit cell dimensions | a = 33.4373(11) Å α = 90°. |
| | b = 8.2621(2) Å β = 93.540(3)°. |
| | c = 15.8008(6) Å γ = 90°. |
| Volume | 4356.8(2) $Å^3$ |
| *Z*, Calculated density | 8, 1.285 $g/cm^3$ |
| Absorption coefficient | 0.193 $mm^{-1}$ |
| *F*(000) | 792.0 |
| Crystal size | 0.45 × 0.327 × 0.097 $mm^3$ |
| Theta range for data collection | 2.832 to 26.5°. |
| Limiting indices | −41 ≤ h ≤ 40, −10 ≤ k ≤ 10, −16 ≤ l ≤ 19 |
| Reflections collected / unique | 26737 / 4422 [*R*(int) = 0.0851] |
| Completeness to theta= 26.5 | 97.9% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4422 / 0 / 260 |
| Goodness-of-fit on $F^2$ | 1.103 |
| Final *R* indices [*I*>2sigma(*I*)] | $R_1$ = 0.0588, $wR_2$ = 0.1463 |
| *R* indices (all data) | $R_1$ = 0.0680, $wR_2$ = 0.1517 |
| Largest diff. peak and hole | 0.86 and −0.33 e. $Å^{-3}$ |

**Table S33.** Crystal data and structure refinement for compound $\mathbf{3}^{t\mathbf{Bu}}$ (CCDC: 1868055).

| | |
|---|---|
| Identification code | AJ0254 |
| Empirical formula | $C_{34.5}H_{50.5}F_{4.75}N_{1.5}O_{4.5}S_{1.5}$ |
| Formula weight | 696.60 |
| Temperature/K | 293(2) |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| space group | *I*2/*m* |
| Unit cell dimensions | a = 18.9188(12) Å α = 90°. |
| | b = 10.3807(6) Å β = 97.509(4)° |
| | c = 35.7997(16) Å γ = 90° |
| Volume | 6970.4(7) $Å^3$ |
| *Z*, Calculated density | 8, 1.328 $g/cm^3$ |
| Absorption coefficient | 0.189 $mm^{-1}$ |
| *F*(000) | 2966.0 |
| Crystal size | 0.498 × 0.4 × 0.097 $mm^3$ |
| Theta range for data collection | 2.583 to 26.499°. |
| Limiting indices | −23 ≤ h ≤ 23, −13 ≤ k ≤ 12, −44 ≤ l ≤ 44 |
| Reflections collected / unique | 47739 / 7598 [*R*(int) = 0.1046] |
| Completeness to theta= 26.499 | 99.5% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7598 / 54 / 545 |
| Goodness-of-fit on $F^2$ | 1.173 |
| Final *R* indices [*I*>2sigma(*I*)] | $R_1$ = 0.1590, $wR_2$ = 0.3768 |
| *R* indices (all data) | $R_1$ = 0.1916, $wR_2$ = 0.3962 |
| Largest diff. peak and hole | 1.11 and −0.75 e. $Å^{-3}$ |

**Table S34.** Crystal data and structure refinement for compound $\mathbf{3^H_2}$ (CCDC: 1868054).

| | |
|---|---|
| Identification code | AJ0212 |
| Empirical formula | $C_{34}H_{52}N_2$ |
| Formula weight | 488.77 |
| Temperature/K | 120.01(2) |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| space group | $P2_1/c$ |
| Unit cell dimensions | a = 15.1760(14) Å α = 90°. |
| | b = 15.7667(14) Å β = 96.938(8)°. |
| | c = 12.4170(9) Å γ = 90°. |
| Volume | 2949.3(4) $Å^3$ |
| *Z*, Calculated density | 4, 1.101 $g/cm^3$ |
| Absorption coefficient | 0.063 $mm^{-1}$ |
| *F*(000) | 1080.0 |
| Crystal size | 0.204 × 0.152 × 0.112 $mm^3$ |
| Theta range for data collection | 2.704 to 26.5°. |
| Limiting indices | −19 ≤ h ≤ 17, −19 ≤ k ≤ 18, −15 ≤ l ≤ 15 |
| Reflections collected / unique | 32924 / 6102 [*R*(int) = 0.1013] |
| Completeness to theta= 26.5 | 99.8% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 6102 / 0 / 337 |
| Goodness-of-fit on $F^2$ | 1.039 |
| Final *R* indices [*I*>2sigma(*I*)] | $R_1$ = 0.0907, $wR_2$ = 0.2111 |
| *R* indices (all data) | $R_1$ = 0.1182, $wR_2$ = 0.2237 |
| Largest diff. peak and hole | 0.34 and −0.38 e. $Å^{-3}$ |

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