Supporting Information

Energy Gap between the Poly-*p*-phenylene Bridge and Donor Groups Controls the Hole Delocalization in Donor–Bridge–Donor Wires

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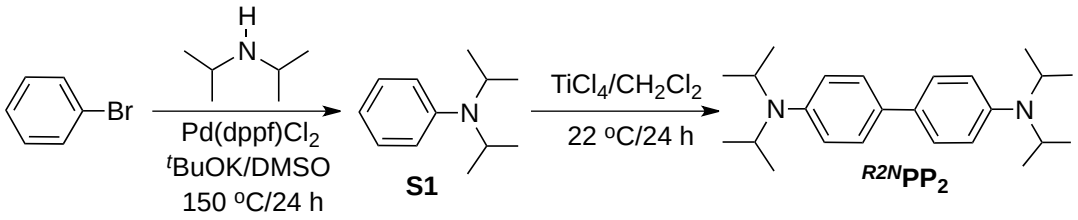
S1. General experimental methods and materials

All reactions were performed under an argon atmosphere unless otherwise noted. All commercial reagents were used without further purification unless otherwise noted. Dichloromethane (Aldrich) was repeatedly stirred with fresh aliquots of concentrated sulfuric acid (~10 % by volume) until the acid layer remained colorless. After separation, CH_2Cl_2 layer was washed successively with water, 5% aqueous sodium bicarbonate, water, and saturated aqueous sodium chloride and dried over anhydrous calcium chloride. The CH_2Cl_2 was distilled twice from P_2O_5 under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton *O*-rings. Acetonitrile was stirred with molecular sieves overnight, filtered, and again stirred with $CaCl_2$ overnight. After that it was filtered and distilled twice from P_2O_5 under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton *O*-rings. The hexanes and toluene were distilled over P_2O_5 under an argon atmosphere and then refluxed over calcium hydride (~12 h). After distillation from CaH_2, the solvents were stored in Schlenk flasks under an argon atmosphere. Tetrahydrofuran (THF) was dried initially by distilling over lithium aluminum hydride under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton *O*-rings. NMR spectra were recorded on Varian 400 MHz NMR spectrometers.

S2. Synthesis of compounds

Synthesis of $^{R2N}PP_2$

Scheme S1.

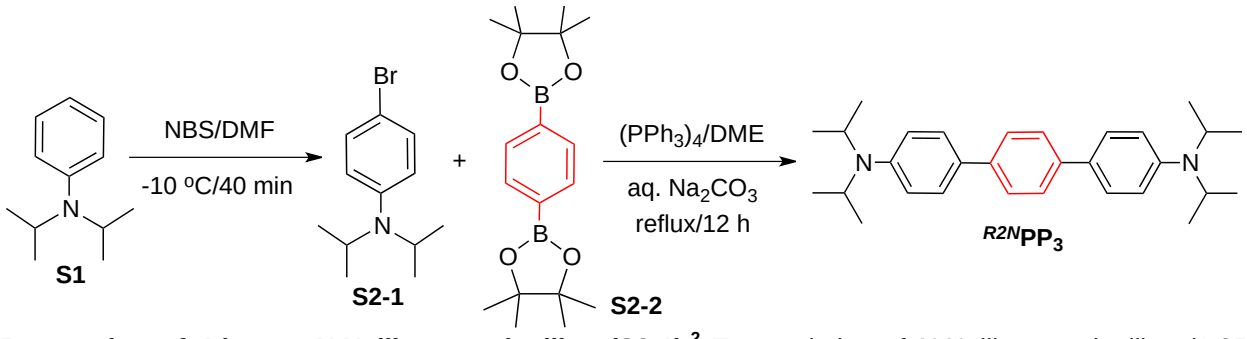


Preparation of *N*,*N*-diisopropylaniline (S1). A mixture of bromobenzene (4.71 g, 30 mmol), potassium *tert*-butoxide (5.05 g, 45 mmol), diisopropylamine (4.55 g, 45 mmol), $Pd(dppf)Cl_2$ (50 mg) and DMSO (40 mL) was placed in 200-mL Schlenk flask. The mixture was degassed (x3) and heated to 150 °C for 24 hour. After cooling to room temperature, the mixture was poured into brine solution (100 mL), then extracted with diethyl ether (2 x100 mL). The organic layer was dried over $MgSO_4$ and evaporated. The brown color residue was suspended into hexanes (100 mL) and extracted with 5% aqueous HCl solution (2 x 100 mL). The aqueous layer was made basic by adding NaOH pellets at 0 °C, then extracted with diethyl ether (2 x 100 mL). The organic layer was dried over $MgSO_4$ and evaporated to yield a light yellow oil. Yield: 2.92 g (55 %). ^{1}H NMR ($CDCl_3$) δ: 1.21 (d, 12H), 3.79 (m, 2H), 6.79 (t, 1H), 6.91 (d, 2H), 7.21 (t, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.37, 47.54, 118.21, 119.36, 128.42, 148.05.

Preparation of N^4,N^4,$N^{4'}$,$N^{4'}$-tetraisopropyl-[1,1'-biphenyl]-4,4'-diamine ($^{R2N}PP_2$). To a solution of *N*,*N*-diisopropylaniline (0.48 mL, 2.5 mmol) in CH_2Cl_2 (5 mL) at 0 °C was added dropwise a solution of $TiCl_4$ (274 uL, 2.5 mmol) in 5 mL of dichloromethane.[1] The reaction mixture was stirred for 24 h at room temperature. To the resulting red mixture, an aqueous solution of KOH (1 M, 10 mL) was added. The mixture was stirred for 1 h, then the aqueous layer was extracted with dichloromethane (3 × 50 mL). The organic layer was dried over $MgSO_4$ and evaporated to yield brown color solid. The crude product was purified by flash chromatography on silica gel using a mixture of ethyl acetate/hexanes as eluent to afford a pale white powder. Yield: 257 mg (73%), m.p. 101-103 °C. ^{1}H NMR ($CDCl_3$) δ: 1.25 (d, 24H), 3.81 (m, 4H), 6.95 (d, 4H), 7.43 (d, 4H). ^{13}C NMR ($CDCl_3$) δ: 21.38, 47.64, 119.48, 126.31, 131.19, 146.43.

Synthesis of $^{R2N}PP_3$

Scheme S2.



Preparation of 4-bromo-*N*,*N*-diisopropylaniline (S2-1).[2] To a solution of *N*,*N*-diisopropylaniline (1.95 mL, 10 mmol) in 30 mL of DMF at -10 °C was added dropwise to a solution of NBS (1.87 g, 10.5 mmol) in 20 mL of DMF. The mixture was stirred at -10 °C for 40 min. The mixture was diluted with brine (100 mL), extracted with ethyl acetate (3 × 100 mL), and the combined organic layers were dried over $MgSO_4$, and evaporated. The residue was redissolved into diethyl ether (75 mL) and filtered. The filtrate was washed with NaOH (3M, 100 mL), dried over $MgSO_4$, and evaporated to give 4-bromo-*N*,*N*-diisopropylaniline as light yellow oil which was used without further purification. Yield: 2.48 g (95%). ^{1}H NMR ($CDCl_3$) δ: 1.20

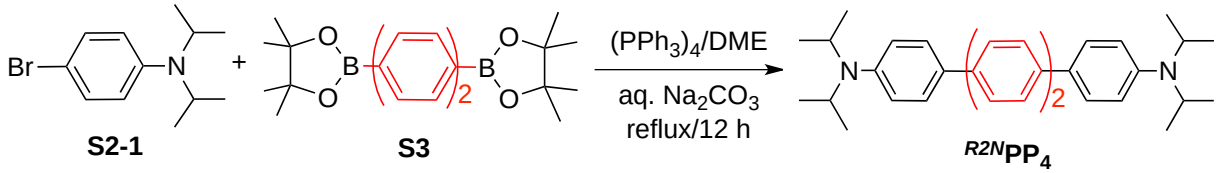
(d, 12H), 3.74 (m, 2H), 6.75 (d, 2H), 7.26 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.21, 47.60, 109.87, 120.24, 131.18, 147.07.

Preparation of 1,4-benzenediboronic acid bis(pinacol) ester (S2-2). 1,4-Dibromobenzene (1.28 g, 5 mmol), bis(pinacolato)diboron (2.66 g, 10.5 mmol), potassium acetate (1.03 g, 10.5 mmol) and 40 mL of 1,4-dioxane were placed in a 100-mL Schlenk flask under an argon atmosphere. Then catalyst Pd(dppf)Cl_2 (50 mg) was added to the flask. The mixture was degassed three times and refluxed for overnight (~12 h). The course of the reaction was monitored by NMR spectroscopy. After the reaction was completed, the mixture was poured into 100 mL of water, and then extracted with dichloromethane (2 x 75 mL). The organic layers were dried over $MgSO_4$ and evaporated. The crude product was redissolved in 150 mL of dichloromethane and passed through a short pad of silica gel. After removal of the solvent, the residue was recrystallized from acetone to produce pure product. Yield: 1.13 g (76%), m.p. 232-233 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.34 (s, 21H), 7.43 (d, 2H), 7.78 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 25.08, 31.44, 35.13, 83.84, 124.94, 134.92, 154.67.

Preparation of *N*^{4},*N*^{4},*N*$^{4'''}$,*N*$^{4'''}$-tetraisopropyl-[1,1':4',1''-terphenyl]-4,4''-diamine (*^{R2N}*PP$_3$). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (765 mg, 3 mmol), **S2-2** (330 mg, 1 mmol) and DME (60 mL) were placed in a 100-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst Pd(PPh_3)$_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). After the reaction was completed, the mixture was poured into 100 mL of water, and then extracted with dichloromethane (2 x 50 mL). The organic layers were dried over $MgSO_4$ and evaporated. The crude product was redissolved into 100 mL of dichloromethane and passed through a short pad of silica gel. After removal of the solvent, the residue was crystallized from a mixture of acetone/dichloromethane. Yield: 261 mg (61%), m.p. 150-151 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.30 (d, 24H), 3.87 (m, 4H), 6.98 (d, 4H), 7.52 (d, 4H), 7.62 (s, 4H). ^{13}C NMR ($CDCl_3$) δ: 21.37, 47.54, 118.22, 126.46, 126.91, 129.84, 138.84, 147.35.

Synthesis of *^{R2N}*PP$_4$

Scheme S3.



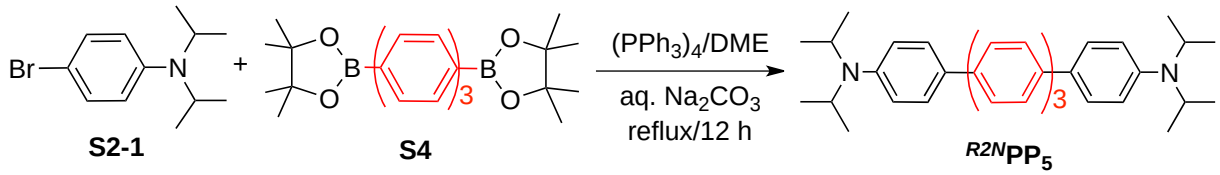
S2-1 **S3** ***^{R2N}*PP$_4$**

Preparation of 4,4'-biphenyldiboronic acid dipinacol ester (S3). 4,4'-Dibromobiphenyl (1.56 g, 5 mmol), bis(pinacolato)diboron (2.66 g, 10.5 mmol) and 40 mL of 1,4-dioxane were placed in a 100-mL Schlenk flask under an argon atmosphere and then Pd(dppf)Cl_2 (50 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). After the reaction was completed, the mixture was poured into 100 mL of water, extracted with dichloromethane (2 x 75 mL). The organic layers were dried over $MgSO_4$ and evaporated. The crude product was redissolved into 100 mL dichloromethane and passed through a short pad of silica gel. After evaporation of the solvent, the residue was crystallized from acetone to produce pure **S3**. Yield: 1.65 g. (81%), m.p. 262-264 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.37 (s, 24H), 7.64 (d, 4H), 7.89 (d, 4H). ^{13}C NMR ($CDCl_3$) δ: 25.02, 83.97, 126.65, 135.38, 143.76.

Preparation of *N*^{4},*N*^{4},*N*$^{4'''}$,*N*$^{4'''}$-tetraisopropyl-[1,1':4',1'':4'',1'''-quaterphenyl]-4,4'''-diamine (*^{R2N}*PP$_4$). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (319 mg, ~1.3 mmol), 4,4'-biphenyldiboronic acid dipinacol ester (**S3**) (203 mg, 0.5 mmol) and 40 mL of DME were placed in a 100-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst Pd(PPh_3)$_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (12 h). An aqueous workup as above and crystallization from acetone yielded ***^{R2N}*PP$_4$** as an off-white solid. Yield: 418 mg (83%), m.p. 193-195 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.28 (d, 24H), 3.87 (m, 4H), 6.95 (d, 4H), 7.51 (d, 4H), 7.65 – 7.69 (m, 8H). ^{13}C NMR ($CDCl_3$) δ: 21.46, 47.63, 118.07, 126.65, 127.12, 127.22, 128.94, 138.55, 140.04, 147.64.

Synthesis of $^{R2N}PP_5$

Scheme S4.



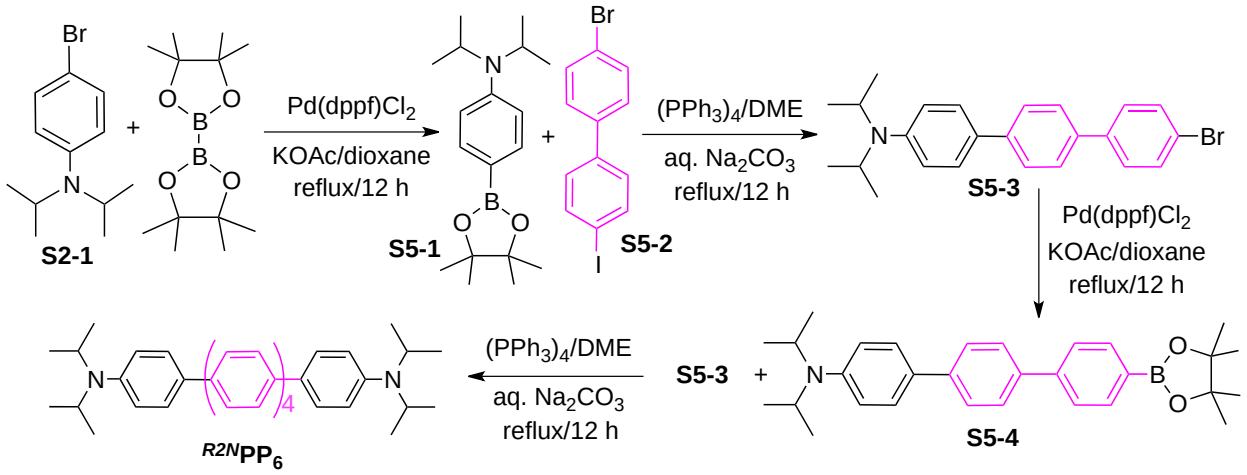
S2-1 **S4** $^{R2N}PP_5$

Preparation of 4,4''-terphenyldiboronic acid dipinacol ester (S4). 4,4''-Dibromoterphenyl (1.94 g, 5 mmol), bis(pinacolato)diboron (2.66 g, 10.5 mmol) and 40 mL of 1,4-dioxane were placed in a 100-mL Schlenk flask under an argon atmosphere and then $Pd(dppf)Cl_2$ (50 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from acetone afforded **S4** as a white solid. Yield: 976 mg. (40.5%), m.p. 1281-283 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.37 (s, 24H), 7.66 (d, 4H), 7.71 (s, 4H), 7.91 (d, 4H). ^{13}C NMR ($CDCl_3$) δ: 25.02, 83.97, 126.47, 127.73, 135.45, 140.31, 143.41.

Preparation of $N^4,N^4,N^{4''''},N^{4''''}$-tetraisopropyl-[1,1':4',1'':4'',1''':4''',1''''-quinquephenyl]-4,4''''-diamine ($^{R2N}PP_5$). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (319 mg, ~1.3 mmol), 4,4'-terphenyldiboronic acid dipinacol ester (**S4**) (241 mg, 0.5 mmol) and 40 mL of DME were placed in a 100-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from acetone yielded $^{R2N}PP_5$ as an off-white solid. Yield: 172 mg. (63%), m.p. 291-293 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.28 (d, 24H), 3.87 (m, 4H), 6.95 (d, 4H), 7.52 (d, 4H), 7.69 (m, 12H). ^{13}C NMR ($CDCl_3$) δ: 21.31, 47.50, 117.77, 126.55, 127.01, 127.18, 127.33, 129.84, 138.18, 139.57, 140.16, 147.56.

Synthesis of $^{R2N}PP_6$

Scheme S5.



S2-1 **S5-1** **S5-2** **S5-3** **S5-3** **S5-4** $^{R2N}PP_6$

Preparation of N,N-diisopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (S5-1). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (2.56 g, 10 mmol), bis(pinacolato)diboron (2.67 g, 10.5 mmol), potassium acetate (1.03 g, 10.5 mmol) and 40 mL of 1,4-dioxane were placed in a 100 mL Schlenk flask under an argon atmosphere and then catalyst $Pd(dppf)Cl_2$ (50 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from methanol yielded ***S5-1*** as a colorless solid. Yield: 1.6 g (53 %), m.p. 150-152 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.27 (d, 12H), 1.32 (s, 12H), 3.89 (m, 2H), 6.81 (d, 2H), 7.63 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.25, 24.96, 47.30, 83.23, 105.14, 115.20, 135.75, 150.69.

Preparation of 4-bromo-4'-iodobiphenyl (S5-2).[3] To a 250-mL round bottom flask, 4-bromobiphenyl (3 g, 12.9 mmol), iodide (1.8 g, 7 mmol), iodic acid (0.6 g, 3.4 mmol), acetic acid (22 mL), water (0.3 mL),

surfuric acid (1.8 mL) and carbon tetrachloride (5 mL) were added. The mixture was refluxed at 110 °C for overnight (~12 h). The resulting mixture was cooled to room temperature and additional amounts of iodine (0.18 g) and iodic acid (60 mg) were added and the refluxing was continued for an additional 4 h. After cooling, the reaction mixture was diluted with dichloromethane (50 mL) and $NaHSO_3$ (10%, 50 mL). The organic phase was washed with aqueous $NaHSO_3$ (10%, 3 × 50 mL), water and brine, then dried over $MgSO_4$. The solvent was evaporated and the crude product was crystallized from methanol. Yield: 3.6 g (68 %), m.p. 175-179 ºC. ^{1}H NMR ($CDCl_3$) δ: 7.29 (d, 2H), 7.41 (d, 2H), 7.56 (d, 2H), 7.77 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 93.45, 121.99, 128.45, 128.74, 132.02, 137.98, 138.95, 139.48.

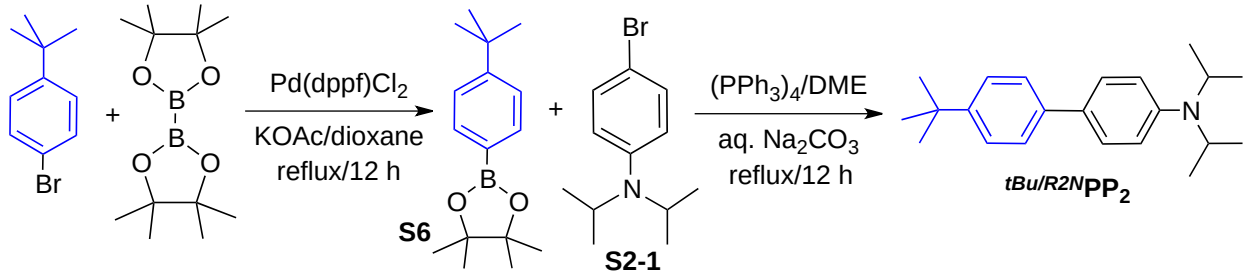
Preparation of 4''-bromo-N,N-diisopropyl-[1,1':4',1''-terphenyl]-4-amine (S5-3). *N*,*N*-Diisopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**S5-1**) (910 mg, 3 mmol), 4-bromo-4'-iodobiphenyl (**S5-2**) (1.6 g, 4.5 mmol, 1.5 equiv) and 40 mL of DME were placed in a 100 mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from acetone yielded **S5-1** as an off-white solid. Yield: 0.62 g (51 %), m.p. 192-194 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.28 (d, 12H), 3.86 (m, 2H), 6.95 (d, 2H), 7.48–7.65 (m, 10H). ^{13}C NMR ($CDCl_3$) δ: 21.44, 47.61, 117.76, 121.36, 126.74, 127.16, 127.26, 128.61, 128.88, 131.97, 132.16, 138.13, 140.69, 147.81.

Preparation of *N*,*N*-diisopropyl-4''-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1':4',1''-terphenyl]-4-amine (S5-4). 4''-Bromo-*N*,*N*-diisopropyl-[1,1':4',1''-terphenyl]-4-amine (**S5-3**) (0.82 g, 2 mmol), bis(pinacolato)diboron (0.66 g, 2.6 mmol), potassium acetate (0.26 g, 2.6 mmol) and 40 mL of 1,4-dioxane were placed in a 100 mL Schlenk flask under an argon atmosphere and then catalyst $Pd(dppf)Cl_2$ (30 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from methanol yielded ***S5-4*** as a colorless solid. Yield: 422 mg (46.3 %), m.p. 141-143 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.29 (d, 12H), 1.38 (s, 12H), 3.87 (m, 2H), 6.96 (d, 2H), 7.50 (d, 2H), 7.66 (m, 6H), 7.91 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.45, 25.03, 47.61, 83.92, 117.87, 126.32, 126.65, 127.18, 127.54, 128.88, 129.23, 135.39, 138.54, 140.62, 143.72, 147.73.

Preparation of ^{R2N}PP$_6$. A mixture of **S5-3** (204 mg, 0.5 mmol), **S5-4** (223 mg, 0.5 mmol) and 30 mL of DME were placed in a 100-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (2.5 g Na_2CO_3 in 10 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (30 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above yielded ^{R2N}**PP$_6$** as an off-white solid.. Yield: 230 mg (69 %), m.p. 448-452 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.28 (d, 24H), 3.87 (hept, 4H), 6.96 (d, 4H), 7.44 – 7.75 (m, 20 H). Note that owing to its very poor solubility, its ^{13}C NMR could not be recorded, and therefore ^{R2N}**PP$_6$** was not included in this study.

Synthesis of $^{tBu/R2N}$PP$_2$

Scheme S6.

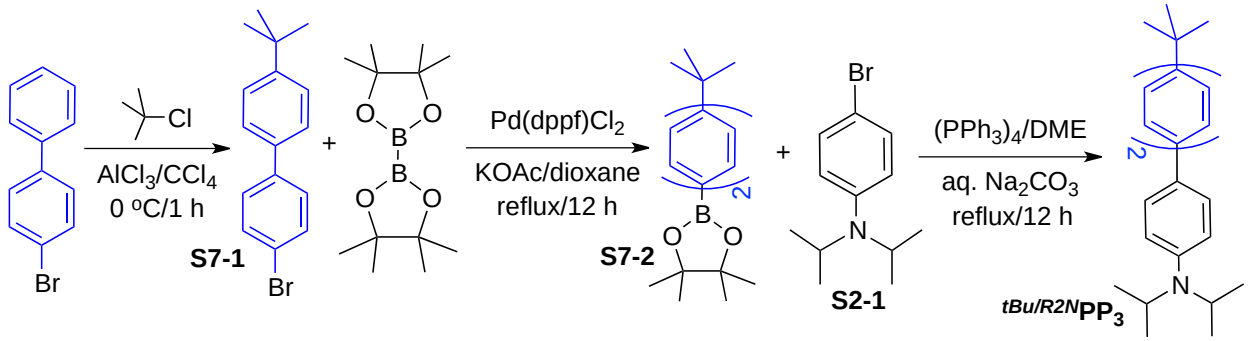


Preparation of 2-(4-(*tert*-butyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (S6). 1-Bromo-4-*tert*-butylbenzene (1.1 g, 5 mmol), bis(pinacolato)diboron (1.5 g, 6 mmol), potassium acetate (0.6 g, 6 mmol) and 40 mL of 1,4-dioxane were placed in a 100-mL Schlenk flask under an argon atmosphere and then catalyst $Pd(dppf)Cl_2$ (50 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from methanol yielded ***S6*** as a colorless solid. Yield: 804 mg (61%), m.p. 140-141 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.34 (s, 9H), 1.35 (s, 12H), 7.42 (d, 2H), 7.78 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 24.98, 31.34, 35.03, 83.73, 124.83, 134.82, 154.61.

Preparation of 4'-(*tert*-butyl)-*N*,*N*-diisopropyl-[1,1'-biphenyl]-4-amine (*tBu/R2N*PP$_2$). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (512 mg, 2.0 mmol), 4-*tert*-butylbenzeneboronic acid dipinacol ester (**S6**) (546 mg, 2.1 mmol) and 40 mL of DME were placed in a 200-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (2.5 g Na_2CO_3 in 10 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (30 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above yielded the crude product, which was redissolved in dichloromethane (~100 mL) and passed through a short pad of basic Al_2O_3. Evaporation of the solvent and crystallization from a mixture of acetone/methanol at -10 ^oC afforded pure **S6**. Yield: 424 mg (69%), m.p. 76-78 ^oC. ^1H NMR ($CDCl_3$) δ: 1.26 (d, 12H), 1.36 (s, 9H), 3.84 (m, 2H), 6.93 (d, 2H), 7.43 (t, 4H), 7.50 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.34, 31.41, 34.42, 47.49, 118.16, 125.53, 125.94, 126.98, 130.05, 138.37, 147.21, 148.83.

Synthesis of *tBu/R2N*PP$_3$

Scheme S7.



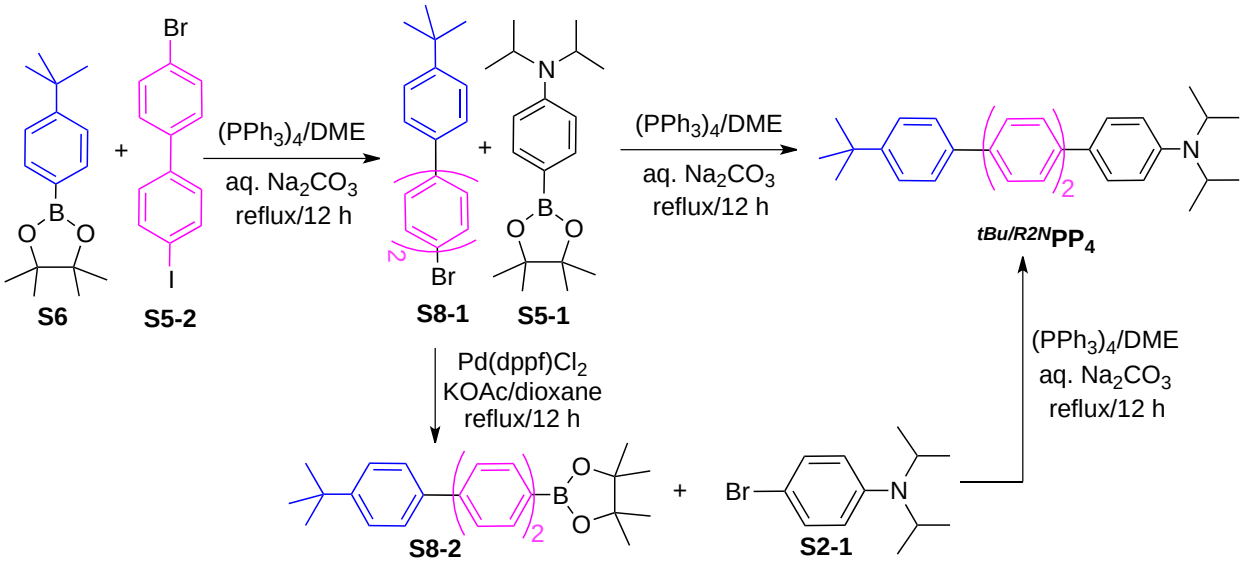
Preparation of 4-bromo-4'-(*tert*-butyl)-1,1'-biphenyl (S7-1).[4] To a solution of 4-bromobiphenyl (5.0 g, 21.5 mmol) and *tert*-butyl chloride (2.4 mL, 22 mmol) in dry CCl_4 (30 mL) was added $AlCl_3$ (267 mg, 2 mmol) at 0 ^oC. The reaction mixture was stirred for an additional 60 min at 0 ^oC during which time the color of the reaction mixture changed to dark green. The resulting mixture was diluted with $CHCl_3$ (100 mL) and washed with $NaHCO_3$ (3 × 20 mL) and water (3 × 20 mL), and finally dried over $MgSO_4$. Evaporation of the solvent afforded an yellow solid which was crystallization from methanol. Yield: 3.6 g (58%), m.p. 137-139 ^oC. ^1H NMR ($CDCl_3$) δ: 1.38 (s, 9H), 7.45-7.50 (m, 6H), 7.54 – 7.58 (m, 2H). ^{13}C NMR ($CDCl_3$) δ: 31.50, 34.99, 121.15, 125.82, 126.46, 128.56, 131.70, 137.02, 139.46, 151.34.

Preparation of 2-(4'-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (S7-2). 1-Bromo-4'-*tert*-butylbiphenyl (1.5 g, 5 mmol), bis(pinacolato)diboron (1.5 g, 6 mmol), potassium acetate (0.6 g, 6 mmol) and 40 mL of 1,4-dioxane were placed in a 100 mL Schlenk flask under an argon atmosphere and then catalyst $Pd(dppf)Cl_2$ (50 mg) was added to the flask. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from methanol yielded ***S7-2*** as a colorless solid. Yield: 1.24 g (73%), m.p. 155-158 ^oC. ^1H NMR ($CDCl_3$) δ: 1.37 (s, 21H), 7.48 (d, 2H), 7.58 (d, 2H), 7.62 (d, 2H), 7.88 (d, 2H). ^{13}C NMR ($CDCl_3$) δ: 25.02, 31.49, 34.70, 83.91, 125.87, 126.43, 126.98, 135.34, 138.19, 143.82, 150.75.

Preparation of 4''-(*tert*-butyl)-*N*,*N*-diisopropyl-[1,1':4',1''-terphenyl]-4-amine (*tBu/R2N*PP$_3$). 4-Bromo-*N*,*N*-diisopropylaniline (**S2-1**) (0.51 g, 2.0 mmol), 4'-tert-butylbiphenylboronic acid dipinacol ester (**S7-2**) (0.71 g, 2.1 mmol) and 60 mL of DME were placed in a 200 mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from a mixture of acetone and methanol yielded ***tBu/R2N*PP$_3$** as an off-white solid. Yield: 445 mg (67%), m.p. 119-121 ^oC. ^1H NMR ($CDCl_3$) δ: 1.28 (d, 12H), 1.37 (s, 9H), 3.86 (m, 2H), 6.95 (d, 2H), 7.49 (t, 4H), 7.58 (d, 2H), 7.62 (s, 4H). ^{13}C NMR ($CDCl_3$) δ: 21.32, 31.38, 34.53, 47.49, 117.91, 125.70, 126.48, 126.55, 126.99, 127.01, 127.19, 129.38, 138.56, 139.85, 147.50, 150.02.

Synthesis of $^{tBu/R2N}PP_4$

Scheme S8.



Preparation of 4-bromo-4''-(*tert*-butyl)-p-terphenyl (S8-1). 4-Bromo-4'-iodo-1,1'-biphenyl (**S5-2**) (1.4 g, 4 mmol), 4-*tert*-butylphenylboronic acid pinacol ester (**S6**) (1 g, 4 mmol) and 40 mL of DME were placed in a 200-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above afforded a solid which was washed with cold diethyl ether to produce pure **S8-1** as a white solid. Yield: 0.78 g (54%), m.p. 263-265 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.38 (s, 9H), 7.48-7.52 (m, 4H), 7.57-7.63 (m, 6H), 7.66-7.68 (m, 2H). ^{13}C NMR ($CDCl_3$) δ: 31.36, 34.58, 121.51, 125.82, 126.67, 127.23, 127.47, 128.58, 131.90, 137.58, 138.54, 139.67, 140.37, 150.54.

Preparation of 4'''-(*tert*-butyl)-*N*,*N*-diisopropyl-[1,1':4',1'':4'',1'''-quaterphenyl]-4-amine ($^{tBu/R2N}PP_4$). 4-Bromo-4''-(*tert*-butyl)-p-terphenyl (**S8-1**) (0.73 g, 2 mmol), *N*,*N*-diisopropyl-aniline-boronic acid pinacol ester (**S5-1**) (0.61 g, 2 mmol) and 40 mL of DME were placed in a 200-mL Schlenk flask under an argon atmosphere. The degassed aqueous Na_2CO_3 solution (5 g Na_2CO_3 in 20 mL of H_2O) and the catalyst $Pd(PPh_3)_4$ (50 mg) were added to the flask, successively. The mixture was degassed three times and refluxed overnight (~12 h). An aqueous workup as above and crystallization from a mixture of acetone and dichloromethane yielded $^{tBu/R2N}PP_4$ as a white solid. Yield: 0.76 g (81%), m.p. 184-186 ºC. ^{1}H NMR ($CDCl_3$) δ: 1.32 (d, 12H), 1.42 (s, 9H), 3.90 (m, 2H), 6.99 (d, 2H), 7.53 (t, 4H), 7.63 (d, 2H), 7.70-7.73 (m, 8H). ^{13}C NMR ($CDCl_3$) δ: 21.35, 31.42, 34.59, 47.52, 117.88, 125.80, 126.58, 126.68, 127.04, 127.22, 127.23, 127.37, 129.24, 137.86, 138.22, 139.55, 139.73, 140.17, 147.61, 150.31. Note that alternate preparation via boronic ester **S8-2** afforded similar yield of $^{tBu/R2N}PP_4$.

S3. UV/vis Absorption and Emission Spectra

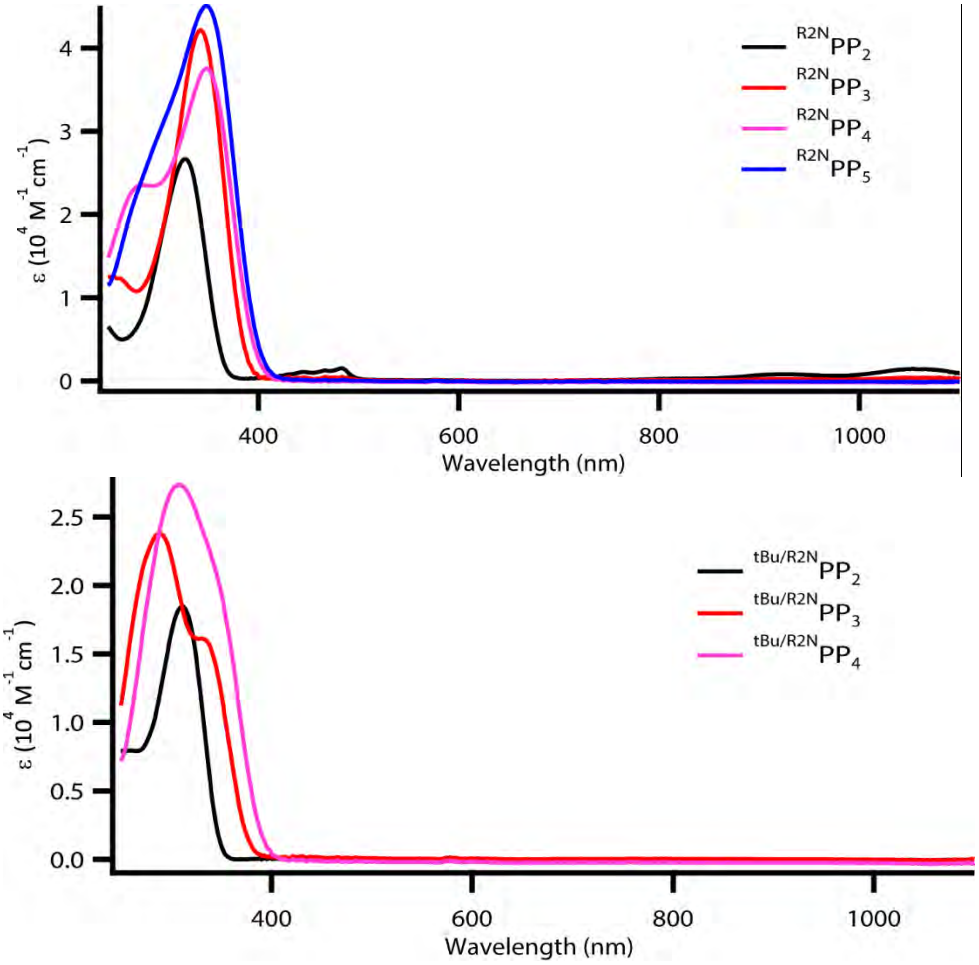


Figure S1. Absorption spectra of ^{R2N}**PP**$_n$ (*n* = 2-5) and $^{tBu/R2N}$**PP**$_n$ (*n* = 2-4) recorded in CH_2Cl_2 at 22 ºC. Note that additional bands in the absorption spectrum of ^{R2N}**PP**$_2$ arose due to the air oxidation. Note that position of the low-energy shold in the spectra of $^{tBu/R2N}$**PP**$_n$ (*n* = 3, 4) was used for determining the value of λ_{max}.

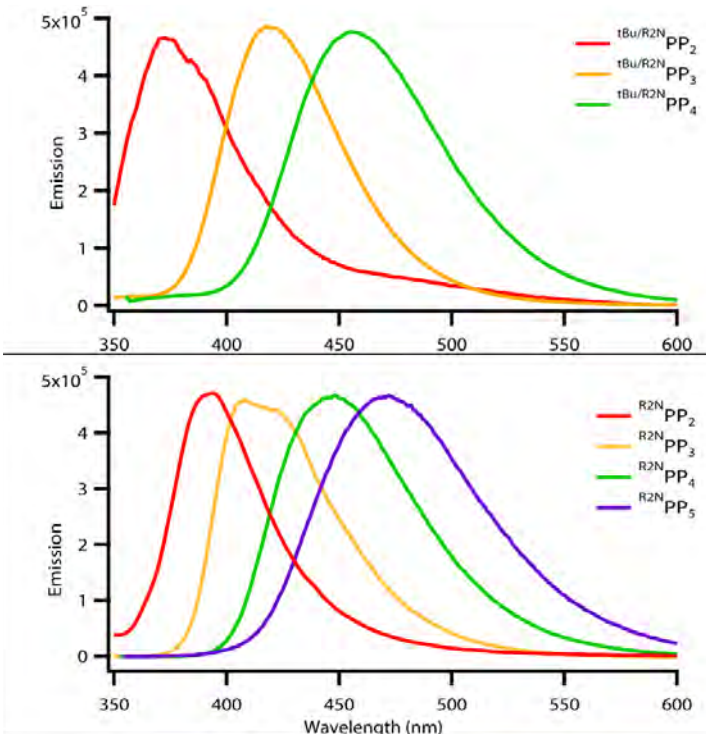


Figure S2. Emission spectra of ^{R2N}**PP**$_n$ (n = 2-5) and $^{tBu/R2N}$**PP**$_n$ (n = 2-4) recorded in CH_2Cl_2 at 22 ºC.

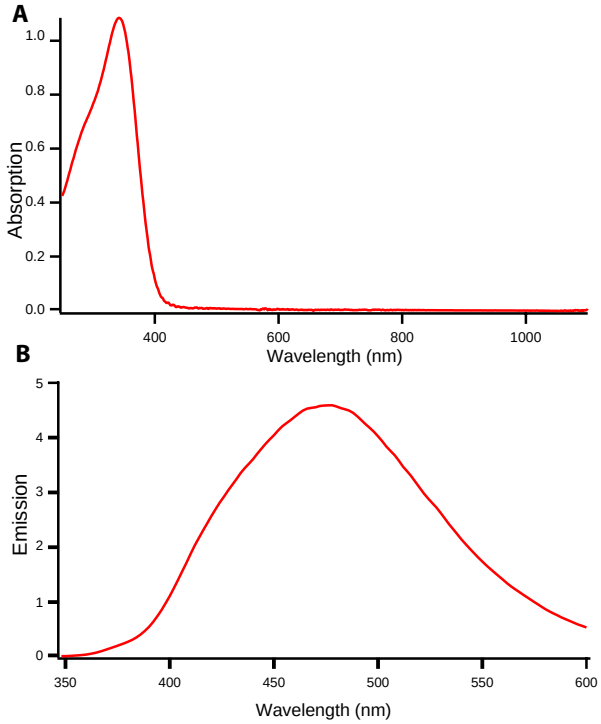


Figure S3. A: Absorption spectrum of 2.2×10^{-5} M ^{R2N}**PP**$_6$ recorded in CH_2Cl_2 at 22 ºC. **B**: Emission spectrum of ^{R2N}**PP**$_6$ recorded in CH_2Cl_2 at 22 ºC.

S4. Cyclic voltammetry of compounds

The CV cell was of an air-tight design with high vacuum Teflon valves and Viton O-ring seals to allow an inert atmosphere to be maintained without contamination by grease. The working electrode consisted of an adjustable platinum disk embedded in a glass seal to allow periodic polishing (with a fine emery cloth) without changing the surface area (~1 mm^2) significantly. The reference SCE electrode (saturated calomel electrode) and its salt bridge were separated from the catholyte by a sintered glass frit. The counter electrode consisted of a platinum gauze that was separated from the working electrode by ~3 mm. The CV measurements were carried out in a solution of 0.1 M supporting electrolyte (tetra-*n*-butylammonium hexafluorophosphate) and the substrate in dry CH_2Cl_2 under an argon atmosphere at 22 ºC. All the cyclic voltammograms were recorded at a sweep rate of 100 mV sec^{-1} and were IR compensated. The oxidation potentials (E_{ox}, calculated by taking the average of anodic and cathodic peaks) were referenced to ferrocene.

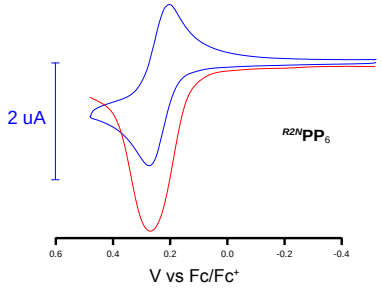
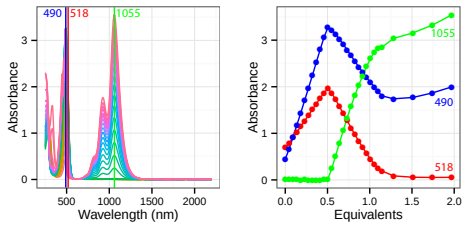


Figure S4. Cyclic (blue line) and square-wave (red line) voltammogram of 1 mM ^{R2N}**PP*6*** in CH_2Cl_2 (0.1 M *n*-Bu_4NPF_6) at a scan rate of 200 mV s^{-1} and 22 ºC. The scale for measure of current (in µA) for the cyclic voltammogram is shown in blue color.

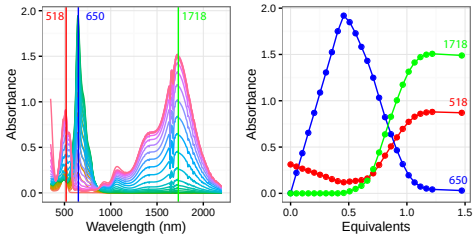
S5. Redox titration

The clean one-electron electron transfer from ^{R2N}**PP**$_n$ or $^{tBu/R2N}$**PP**$_n$ to **THE**$^{+\bullet}$ at the equivalence titration point (i.e. 1:1 ratio of electron donor:oxidant) was confirmed by the deconvolution of spectra at each titration point using the clean absorption spectra of **THE**$^{+\bullet}$, ^{R2N}**PP**$_n^{+\bullet}$, ^{R2N}**PP**$_n^{2+}$, or $^{tBu/R2N}$**PP**$_n^{+\bullet}$ and fitting of the obtained molar fractions to the equilibrium equations of the one- and two-electron oxidation.[5]

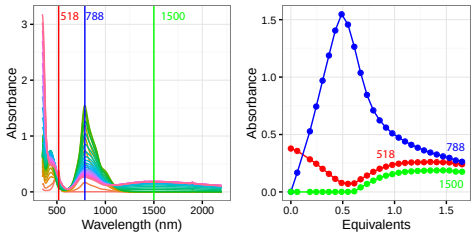
A: ^{R2N}**PP**$_2$ (1.30 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (94 uM) → ^{R2N}**PP**$_2^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}



B: ^{R2N}**PP**$_3$ (0.65 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (43 uM)→ ^{R2N}**PP**$_3^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}



C: ^{R2N}**PP**$_4$ (0.95 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (52 uM) → ^{R2N}**PP**$_4^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}



D: ^{R2N}**PP**$_5$ (1.46 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (65 uM) → ^{R2N}**PP**$_5^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}

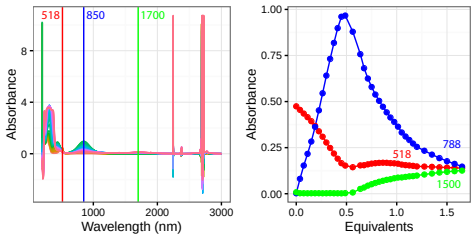
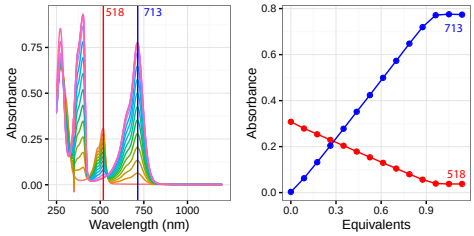
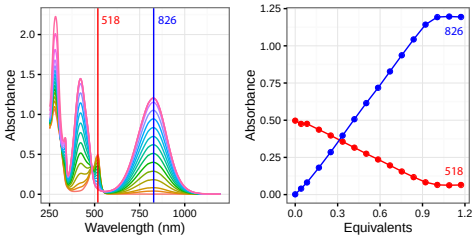


Figure S5. Spectral changes attendant upon the reduction of ^{R2N}**PP**$_n$ (*n* = 2-5 in panels **A**-**D**, respectively; see panel titles for the stock solution concentrations) by **THE**$^{+\bullet}$ $SbCl_6^-$ in CH_2Cl_2 at 22 ºC. Red, green and blue curves correspond to the absorbance at indicated wavelength (nm) against number of equivalents of added ^{R2N}**PP**$_n$.

A: $^{tBu/R2N}$**PP**$_2$ (1.11 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (42 uM) → ^{R2N}**PP**$_2^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}



B: $^{tBu/R2N}$**PP**$_3$ (0.86 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (68 uM)→ ^{R2N}**PP**$_3^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}



C: $^{tBu/R2N}$**PP**$_4$ (0.89 mM) + **THE**$^{+\bullet}$ $SbCl_6^-$ (49 uM) → ^{R2N}**PP**$_4^{+\bullet}$ $SbCl_6^-$ + **THE**^{0}

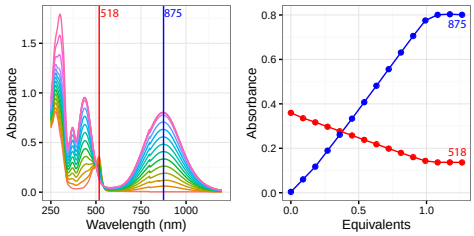


Figure S6. Spectral changes attendant upon the reduction of $^{tBu/R2N}$**PP**$_n$ (*n* = 2-4 in panels **A**-**C**, respectively; see panel titles for the stock solution concentrations) by **THE**$^{+\bullet}$ $SbCl_6^-$ in CH_2Cl_2 at 22 ºC. Red, and blue curves correspond to the absorbance at indicated wavelength (nm) against number of equivalents of added $^{tBu/R2N}$**PP**$_n$.

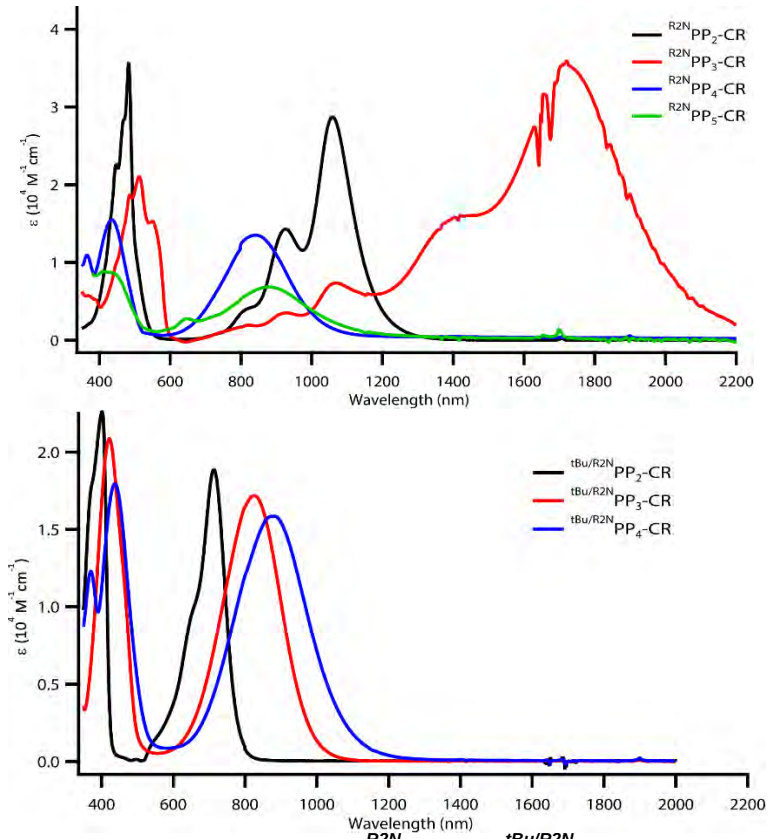


Figure S7. Absorption spectra of cation radicals of ^{R2N}**PP**$_n$ and $^{tBu/R2N}$**PP**$_n$ in CH_2Cl_2 at 22 ºC.

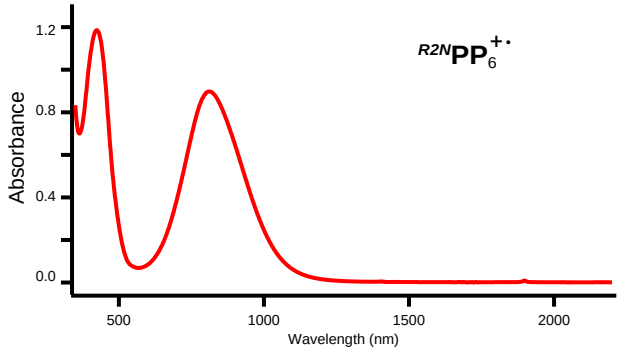


Figure S8. Absorption spectra of 1.6×10^{-4} M ^{R2N}**PP**$_6$ cation radical in CH_2Cl_2 at 22 ºC.

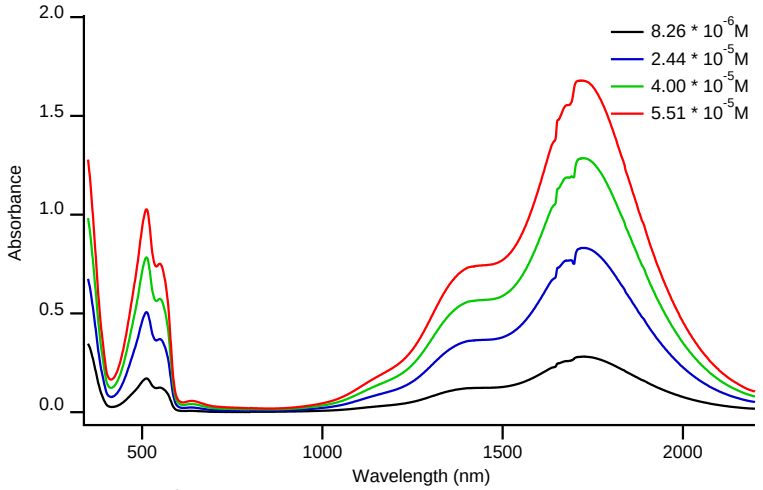


Figure S9. Absorption spectra of ^{R2N}**PP**$_{3}$ cation radical at different concentrations (indicated in the Figure) in CH_2Cl_2 at 22 ºC as a representative example of concentration-dependence on the cation radical spectra. The molar absorptivity determined from each spectrum was found to be (3.48 ± 0.05) × 10^4 M^{-1} cm^{-1} confirming that no aggregation occurs at higher concentrations used herein.

[Note that the spectra of other ^{R2N}PP$_n$ and $^{tBu/R2N}$PP$_n$ cation radicals and dications, similarly, did not show any concentration-dependent changes.]

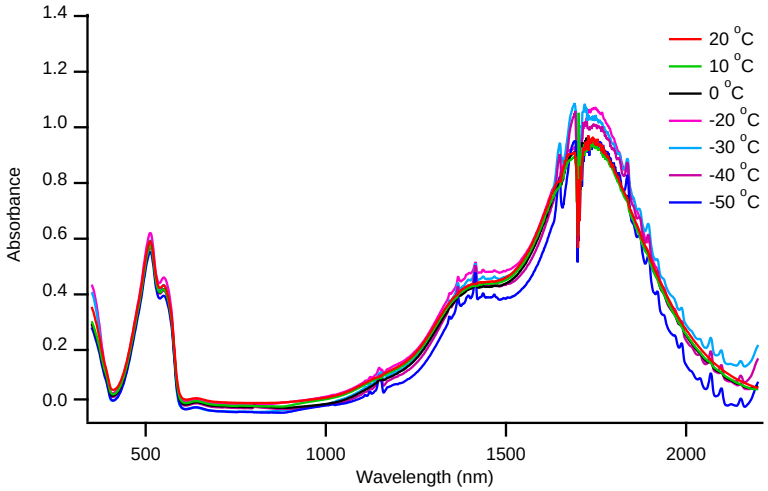


Figure S10. Absorption spectra of 3.0×10^{-5} M ^{R2N}**PP**$_{3}$ cation radical at different temperatures (indicated in the Figure) in CH_2Cl_2 as a representative example of temperature-dependent spectra of the cation radicals.

[Note that the spectra of other ^{R2N}PP$_n$ and $^{tBu/R2N}$PP$_n$ cation radicals and dications, similarly, did not show any temperature-dependent changes.]

S6. Crystal data and structure refinement

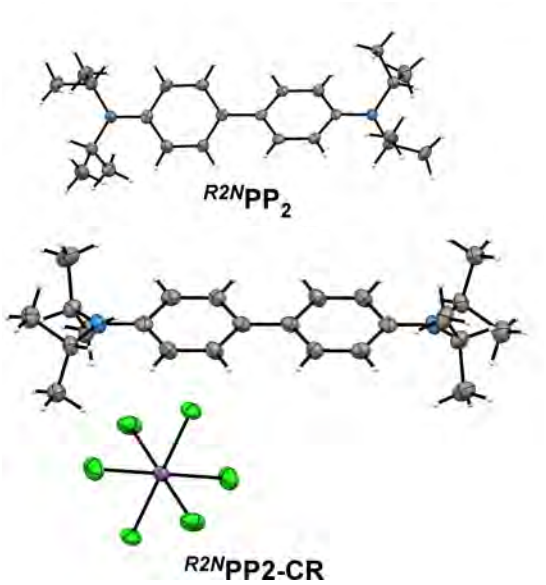


Figure S11. Thermal ellipsoid plots (50% probability) derived from the X-ray crystal structures of neutral ^{R2N}**PP**$_2$ and cation radical complexes ^{R2N}**PP**$_2^{+\bullet}$$(SbCl_6)^-$.

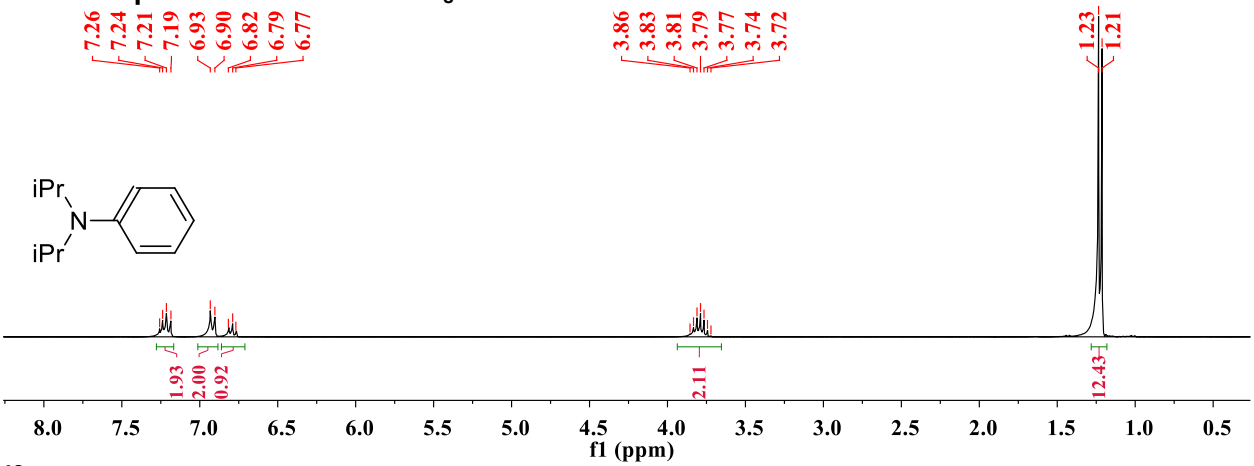
Table S1. Summary of X-ray crystallographic data collection and structure refine.

	^{R2N}**PP**$_2$	^{R2N}**PP**$_2^{+\bullet}$
CCDC Deposition Number	1492581	1492582
Empirical formula	$C_{24}H_{36}N_2$	$C_{24}H_{36}N_2Cl_6Sb$
Formula weight	352.55	687
Temperature/K	100.00(10)	100.00(10)
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	17.7621(3)	9.1227(6)
b/Å	22.2461(4)	12.7639(8)
c/Å	27.0076(4)	12.5204(9)
α/°	66.1403(16)	90
β/°	79.7820(13)	93.258(6)
γ/°	83.1039(13)	90
Volume/Å^3	9591.1(3)	1455.53(17)
Z	18	2
ρ_{calc}g/cm^3	1.099	1.568
μ/mm^{-1}	0.474	12.706
F(000)	3492	694
Crystal size/mm^3	0.38 × 0.32 × 0.25	0.1285 × 0.079 × 0.0208
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data	6.14 to 148.52	9.9 to 148.52

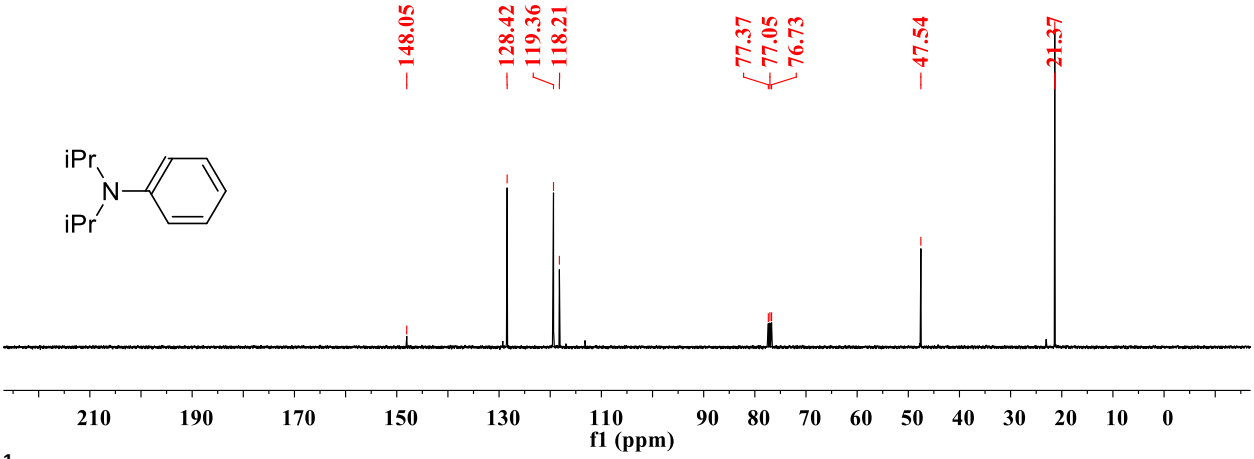
collection/°		
Index ranges	-20 ≤ h ≤ 22, -27 ≤ k ≤ 27, -33 ≤ l ≤ 33	-11 ≤ h ≤ 11, -15 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	182137	14114
Independent reflections	38524 [R_{int} = 0.0312, R_{sigma} = 0.0191]	2930 [R_{int} = 0.1097, R_{sigma} = 0.0634]
Data/restraints/parameters	38524/242/2495	2930/0/155
Goodness-of-fit on F^2	1.472	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.1082, wR_2 = 0.3071	R_1 = 0.0555, wR_2 = 0.1410
Final R indexes [all data]	R_1 = 0.1182, wR_2 = 0.3323	R_1 = 0.0675, wR_2 = 0.1507
Largest diff. peak/hole / e $Å^{-3}$	1.36/-0.46	1.77/-1.46

S7. NMR Spectroscopy

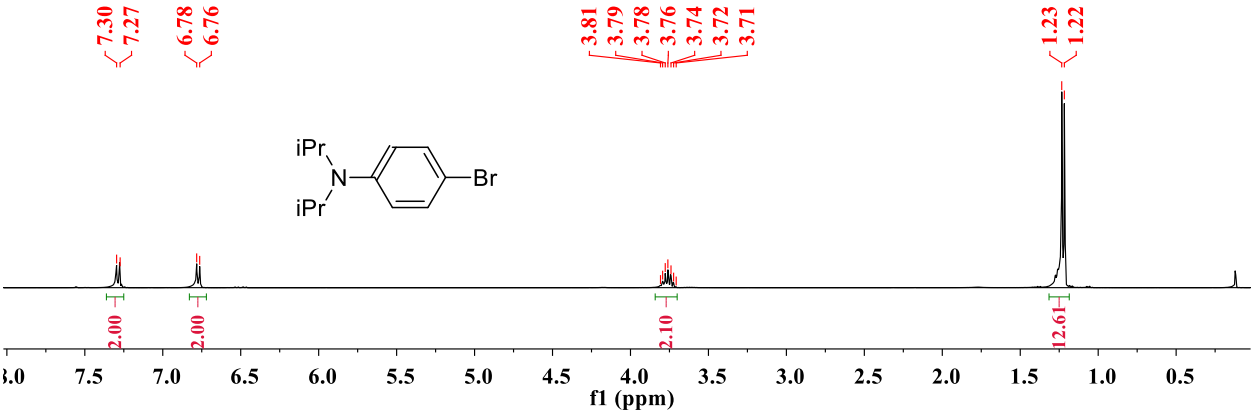
^{1}H NMR spectrum of S1 in $CDCl_3$



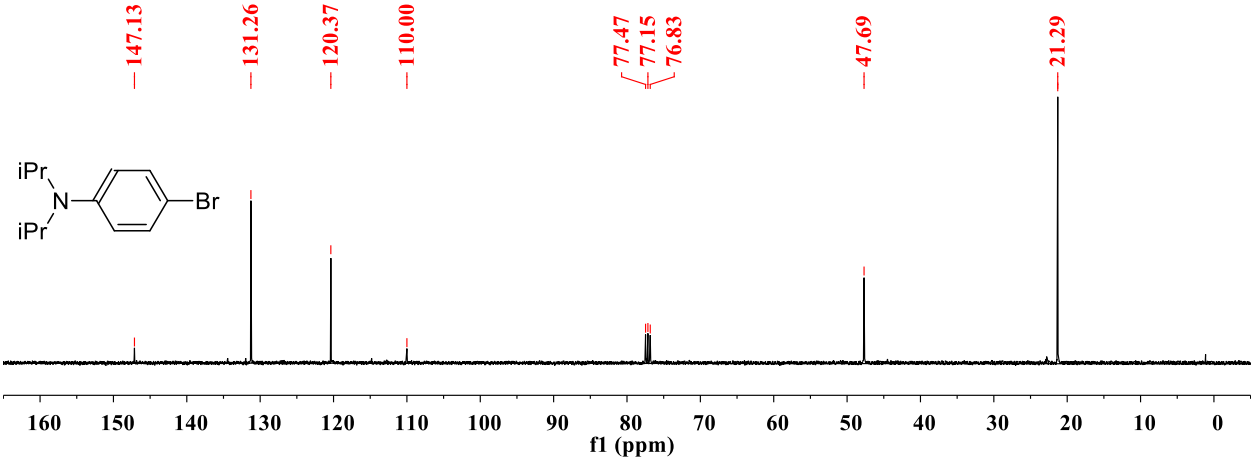
^{13}C NMR spectrum of S1 in $CDCl_3$



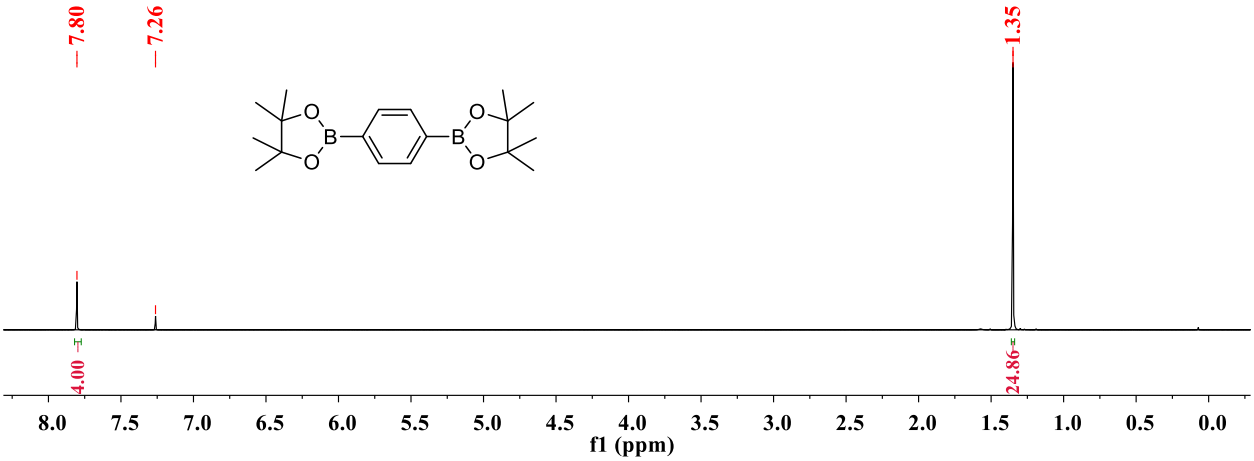
^{1}H NMR spectrum of S2-1 in $CDCl_3$



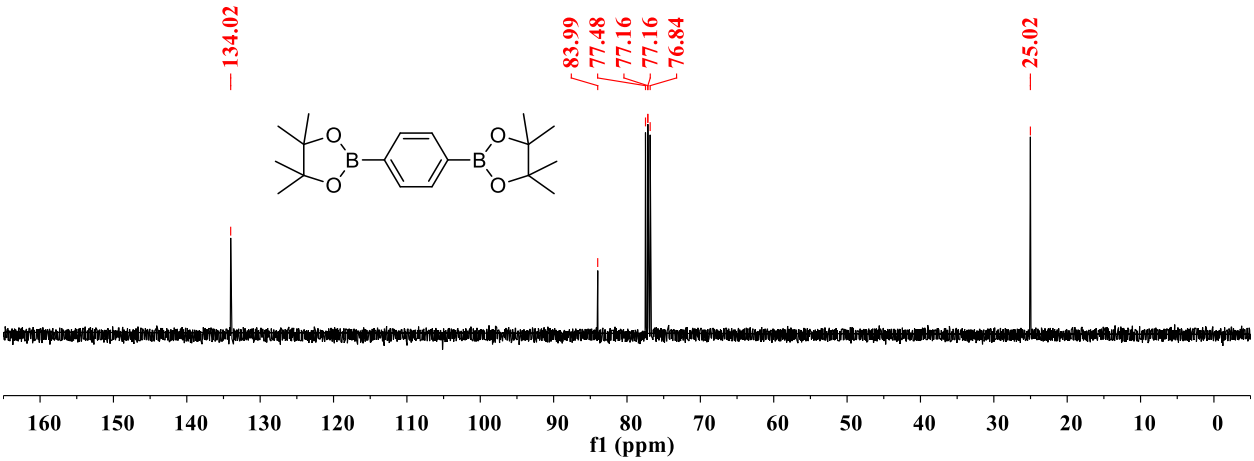
^{13}C NMR spectrum of S2-1 in $CDCl_3$



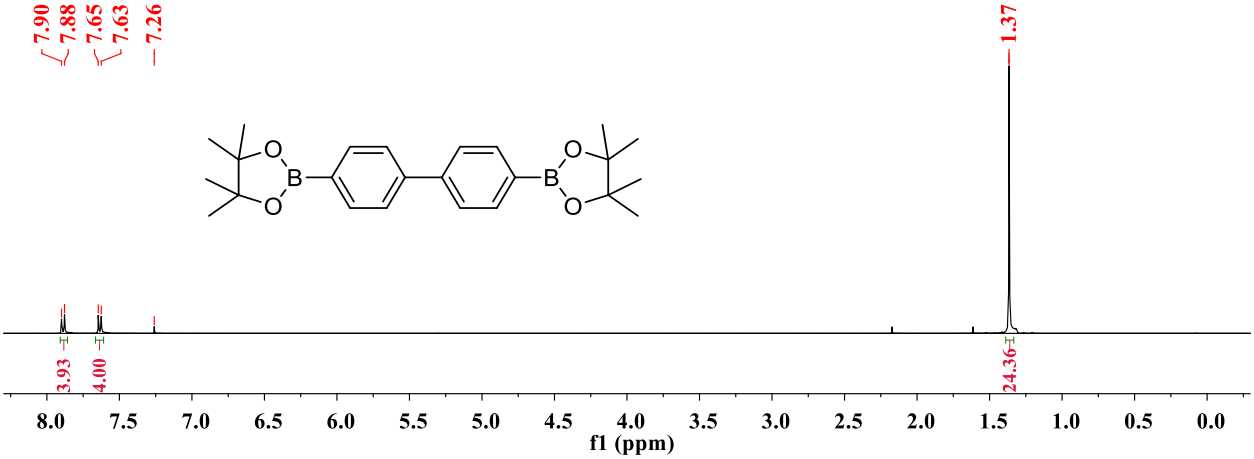
^{1}H NMR spectrum of S2-2 in $CDCl_3$



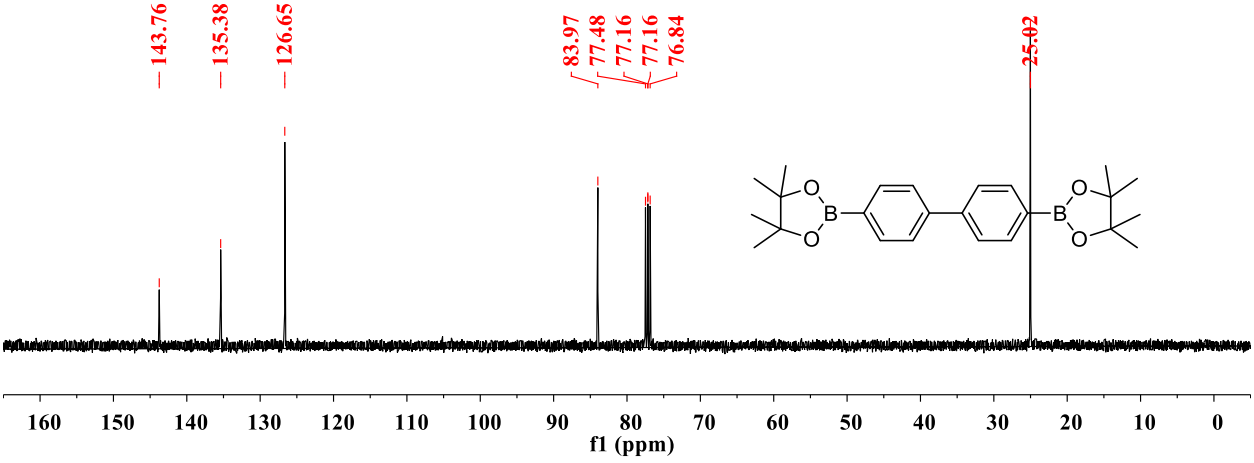
^{13}C NMR spectrum of S2-2 in $CDCl_3$



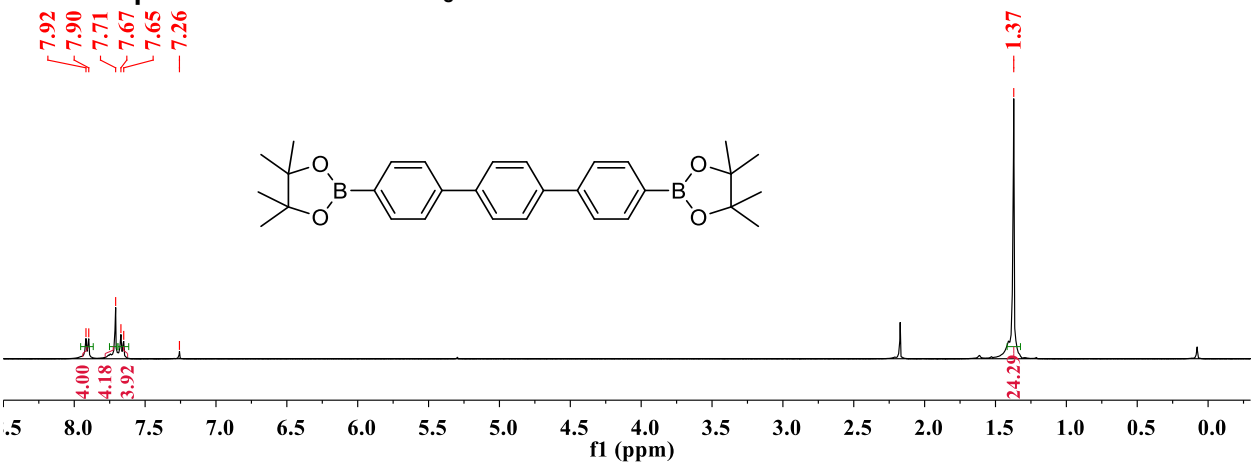
^{1}H NMR spectrum of S3 in $CDCl_3$



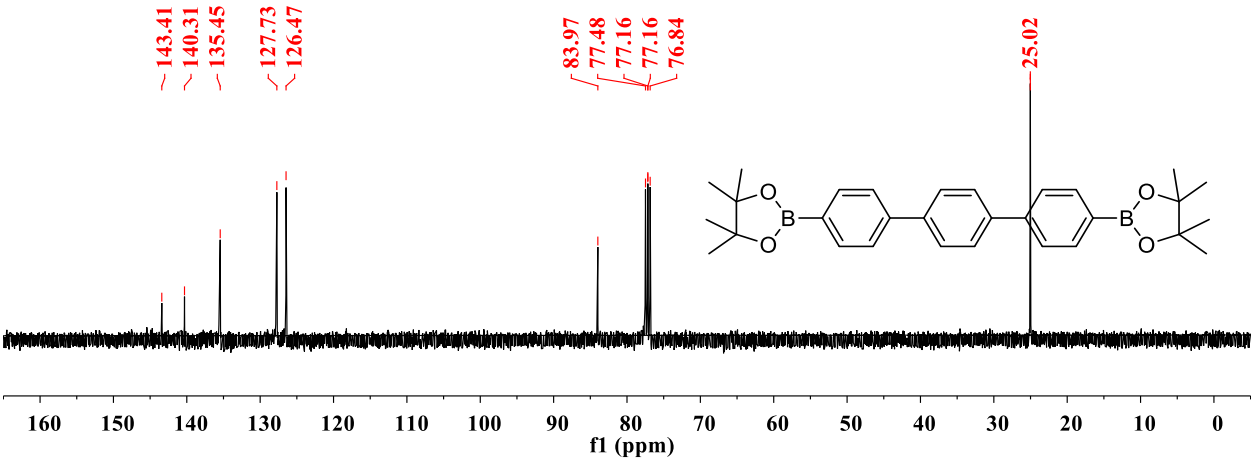
^{13}C NMR spectrum of S3 in $CDCl_3$



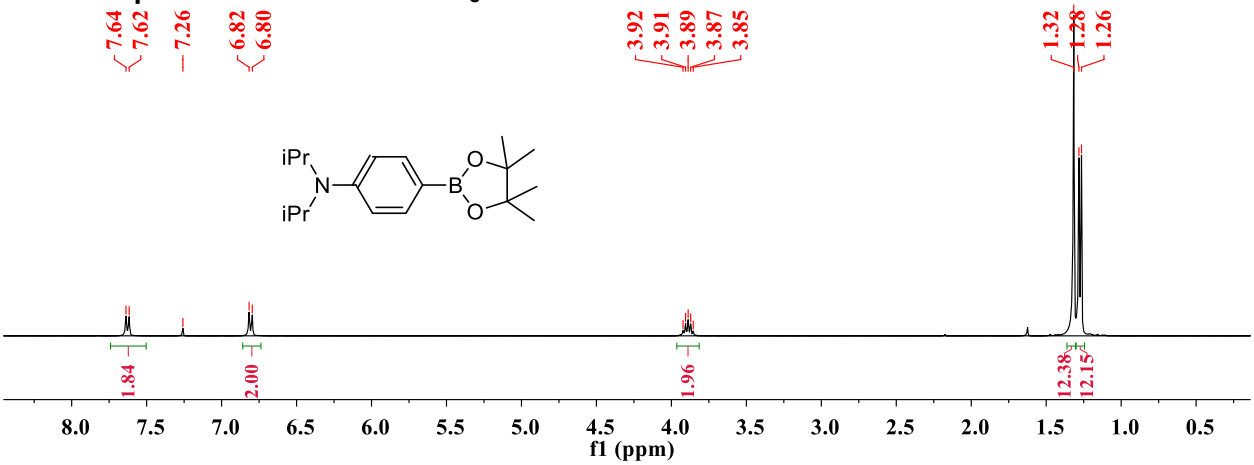
^{1}H NMR spectrum of S4 in $CDCl_3$



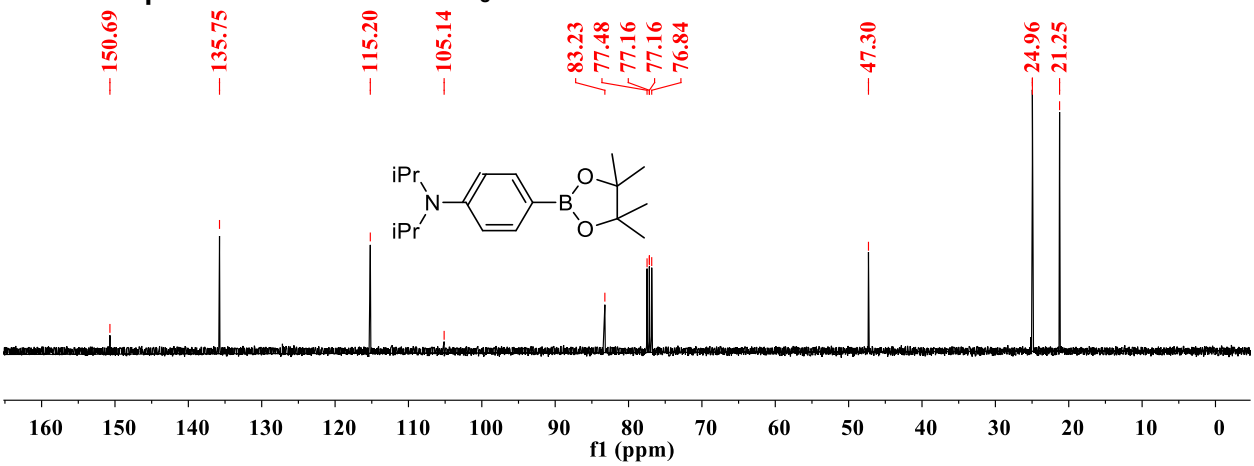
^{13}C NMR spectrum of S4 in $CDCl_3$



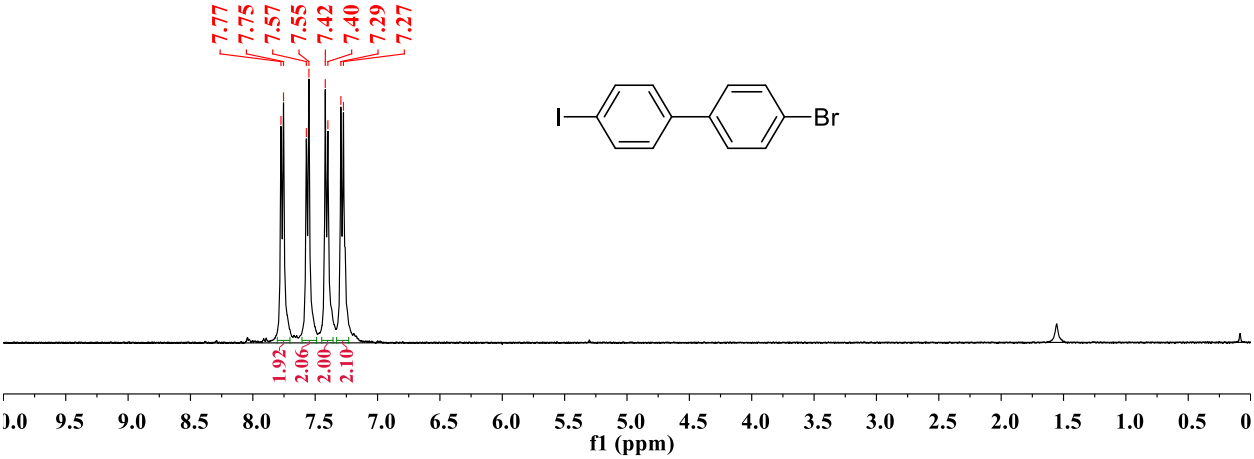
^{1}H NMR spectrum of S5-1 in $CDCl_3$



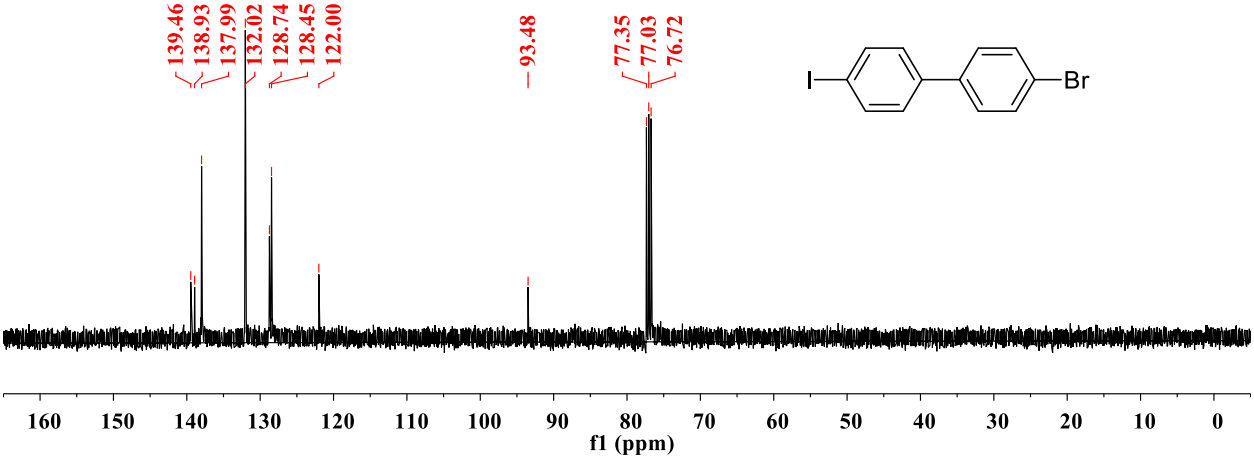
^{13}C NMR spectrum of S5-1 in $CDCl_3$



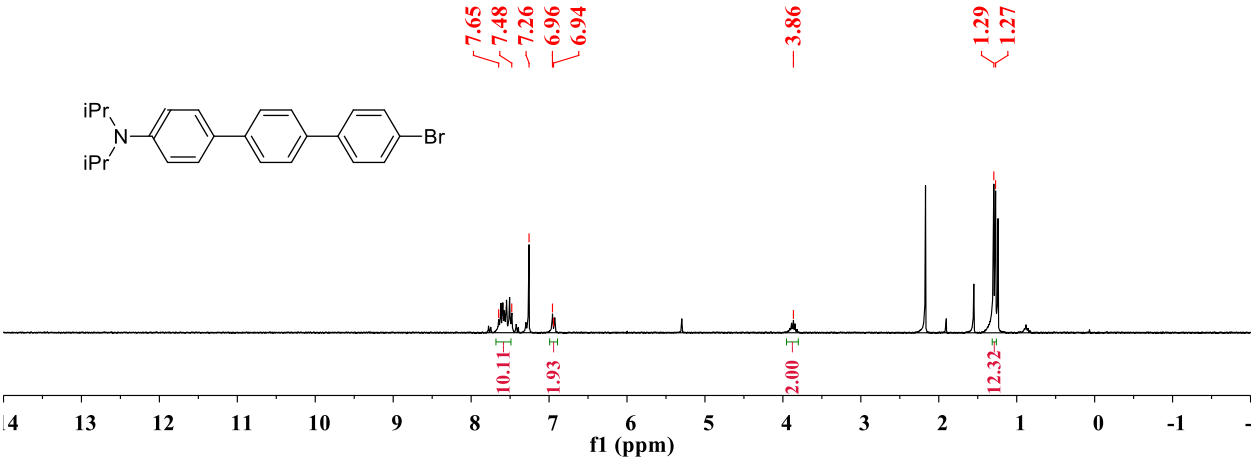
^{1}H NMR spectrum of S5-2 in $CDCl_3$



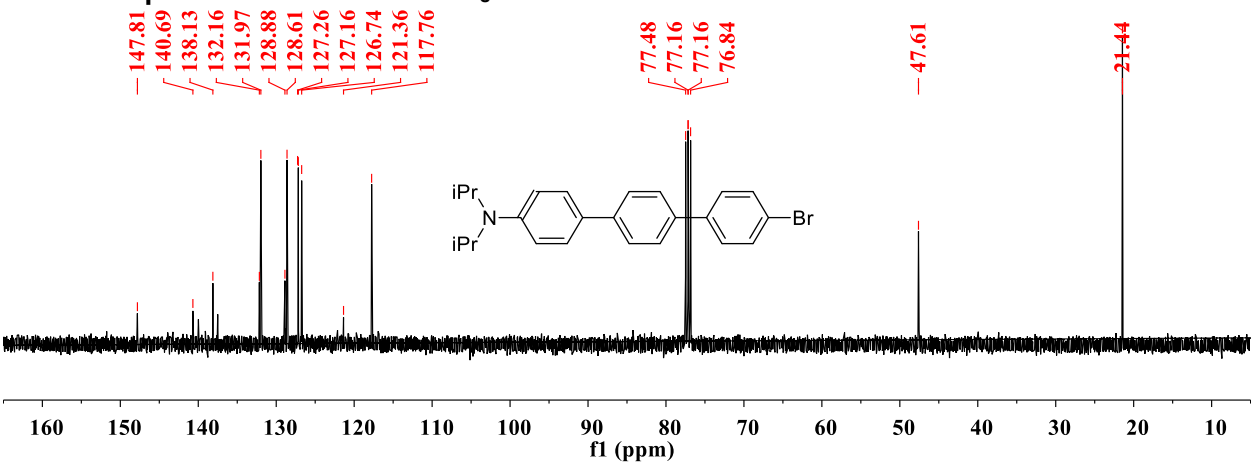
^{13}C NMR spectrum of S5-2 in $CDCl_3$



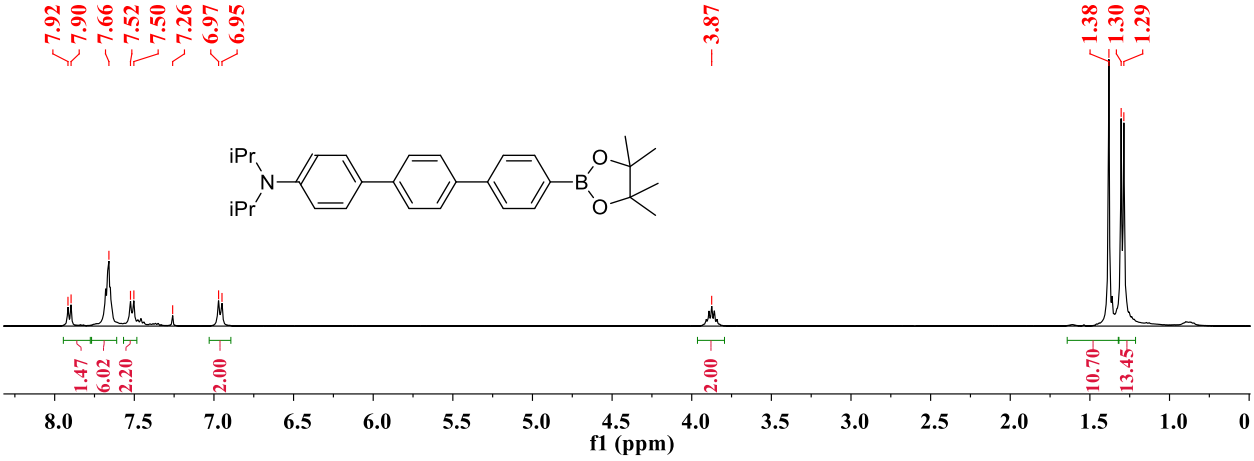
^{1}H NMR spectrum of S5-3 in $CDCl_3$



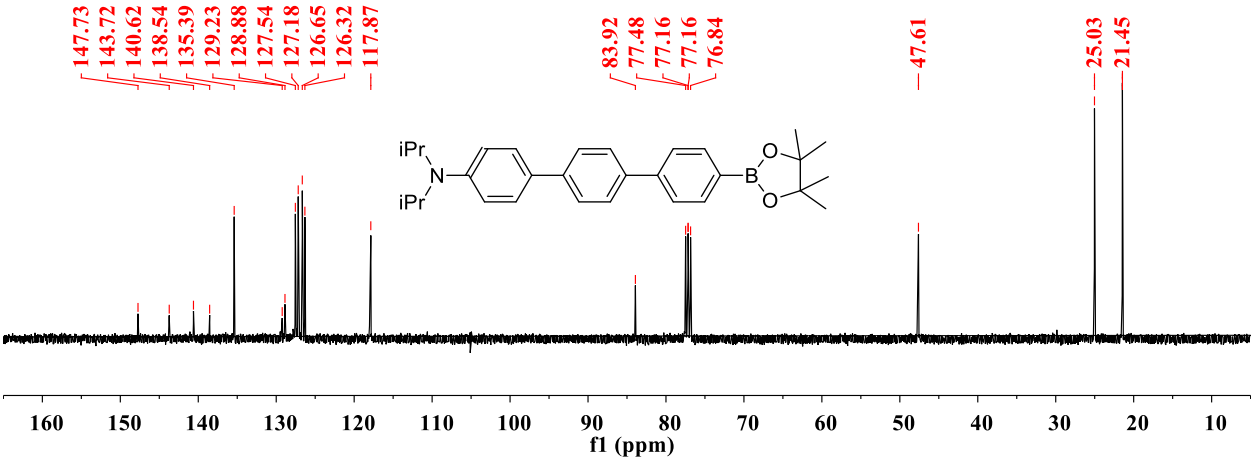
^{13}C NMR spectrum of S5-3 in $CDCl_3$



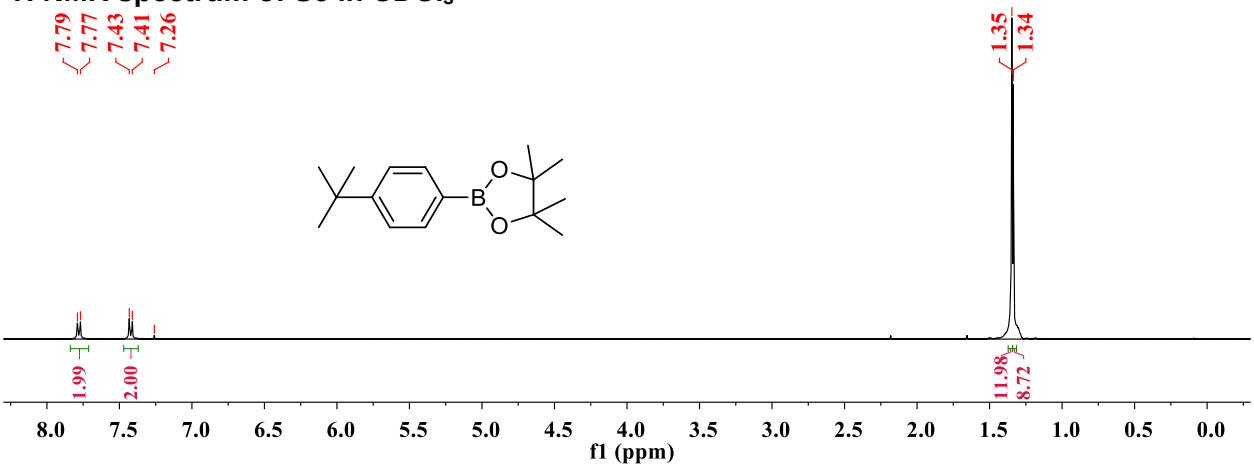
^{1}H NMR spectrum of S5-4 in $CDCl_3$



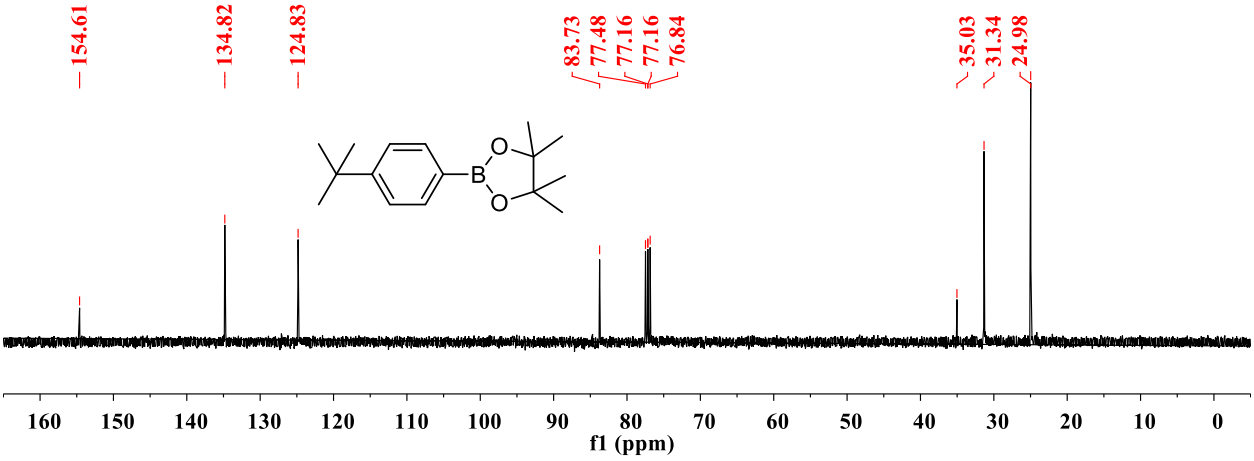
^{13}C NMR spectrum of S5-4 in $CDCl_3$



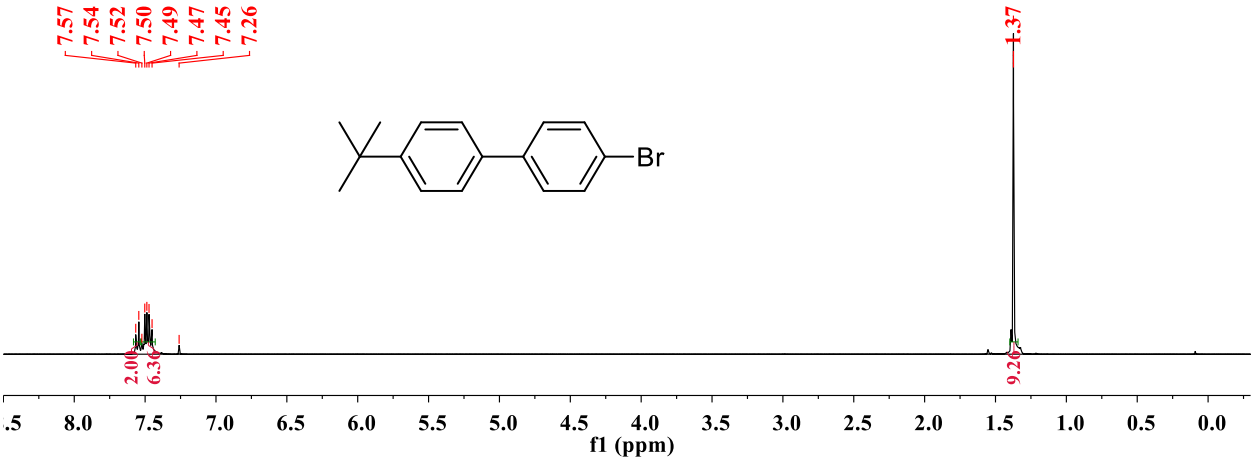
^{1}H NMR spectrum of S6 in $CDCl_3$



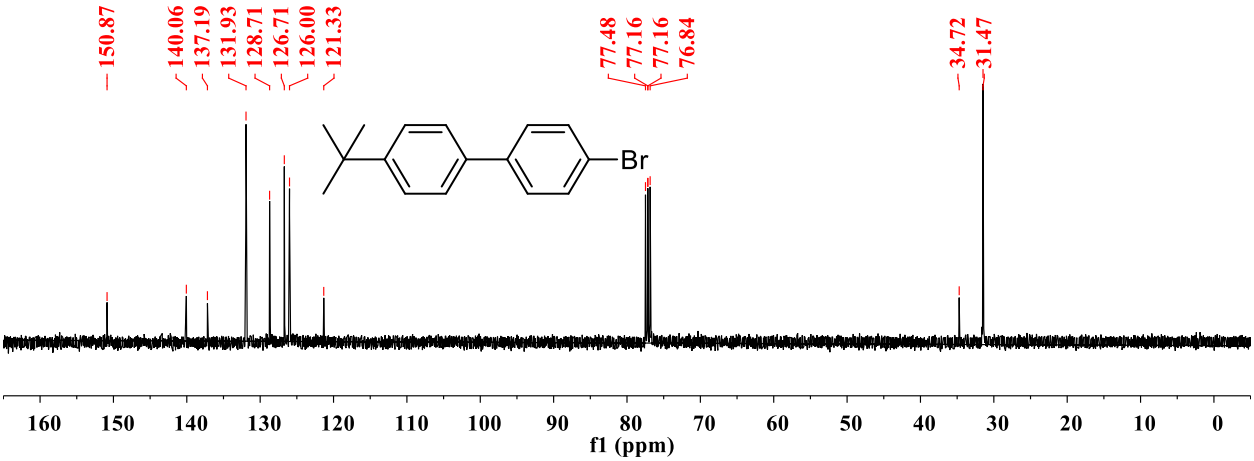
^{13}C NMR spectrum of S6 in $CDCl_3$



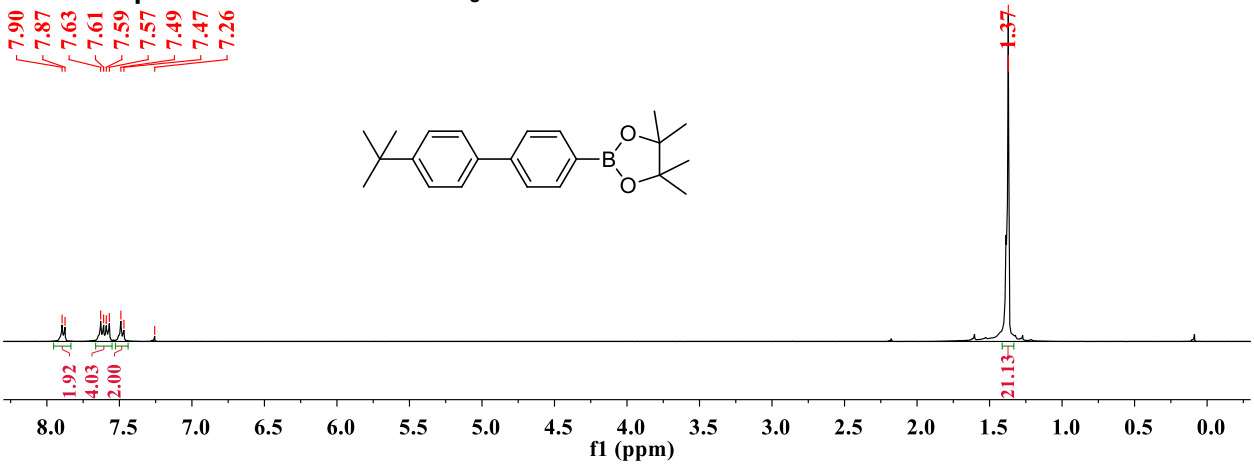
^{1}H NMR spectrum of S7-1 in $CDCl_3$



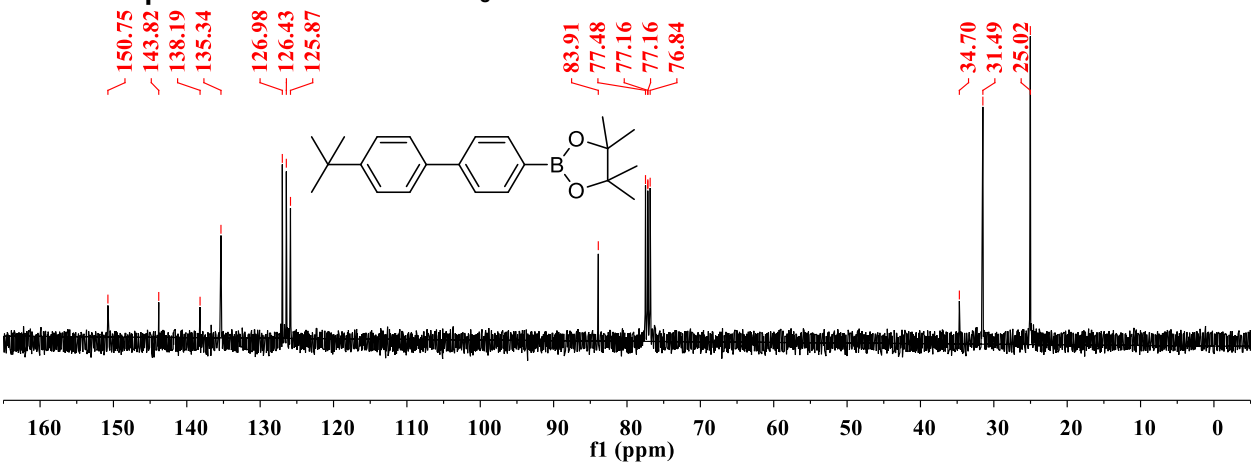
^{13}C NMR spectrum of S7-1 in $CDCl_3$



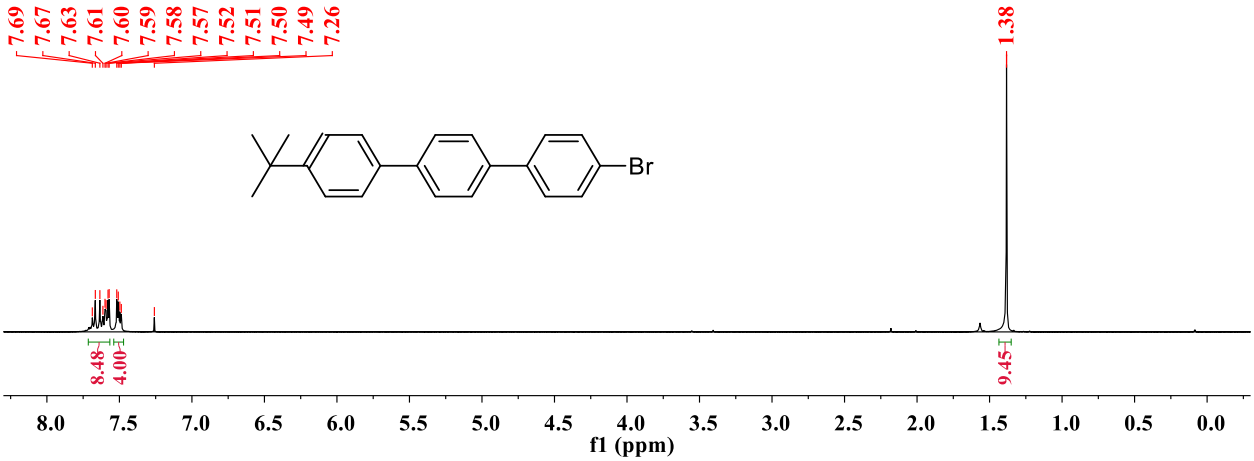
^{1}H NMR spectrum of S7-2 in $CDCl_3$



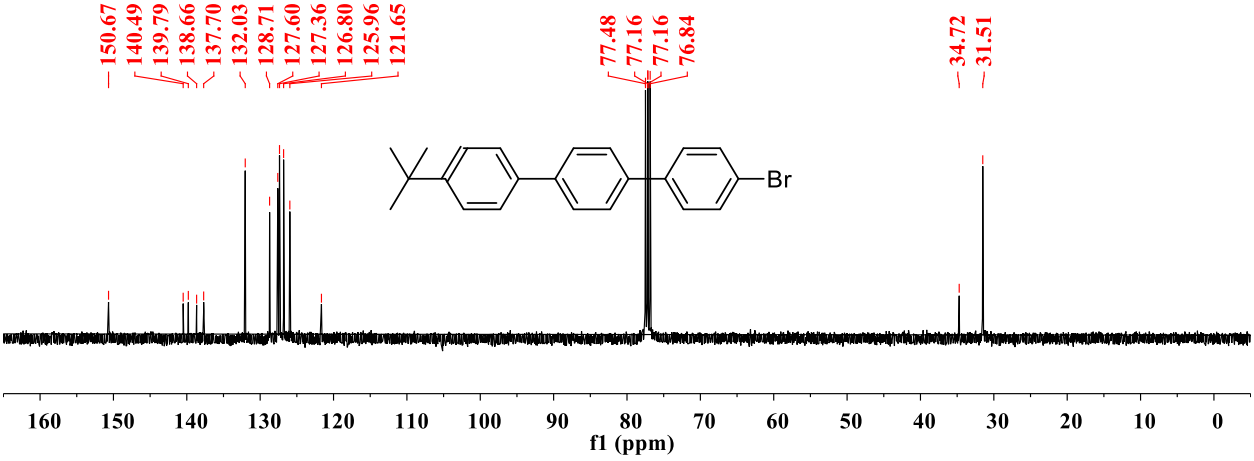
^{13}C NMR spectrum of S7-2 in $CDCl_3$



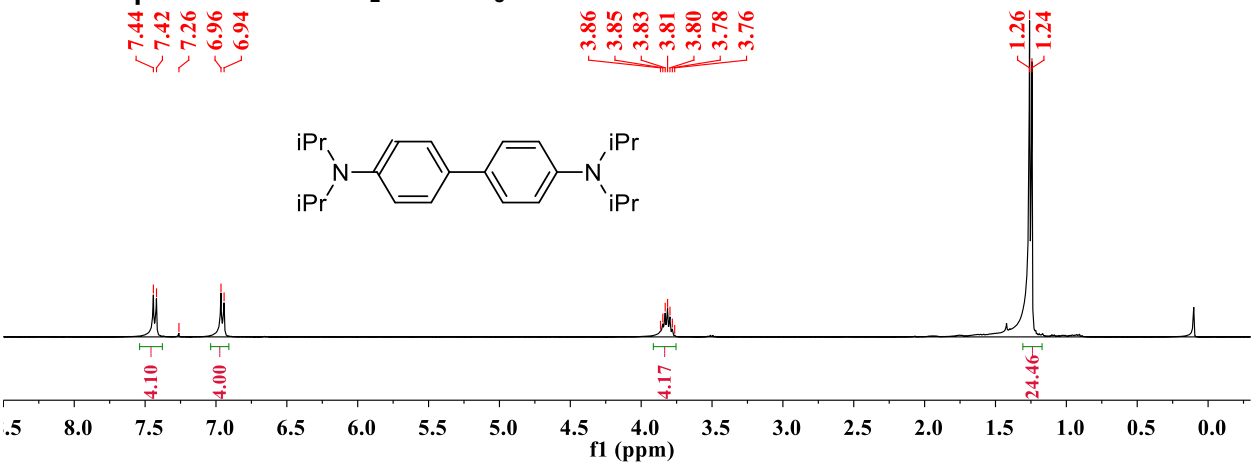
^{1}H NMR spectrum of S8 in $CDCl_3$



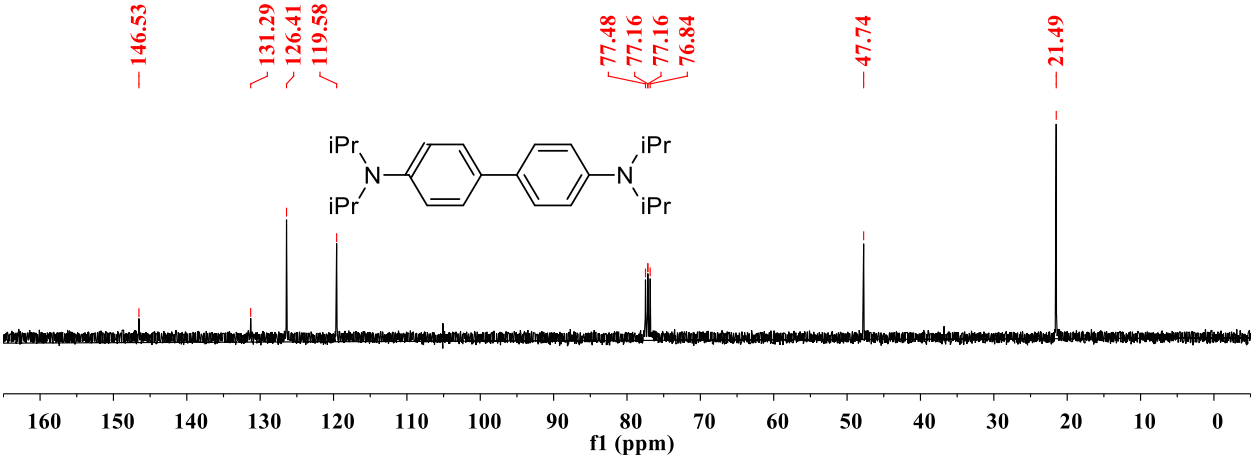
^{13}C NMR spectrum of S8 in $CDCl_3$



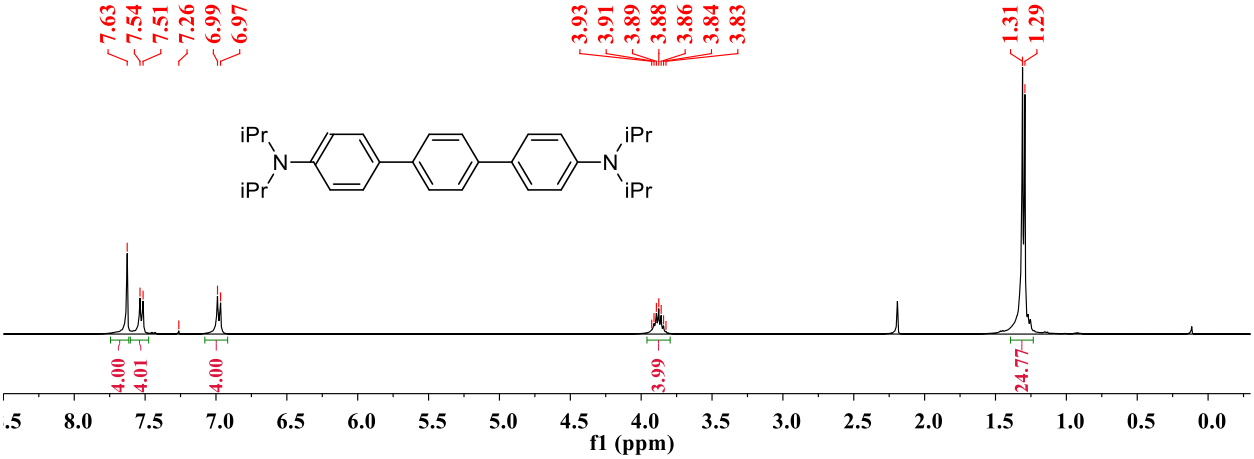
^{1}H NMR spectrum of $^{R2N}PP_2$ in $CDCl_3$



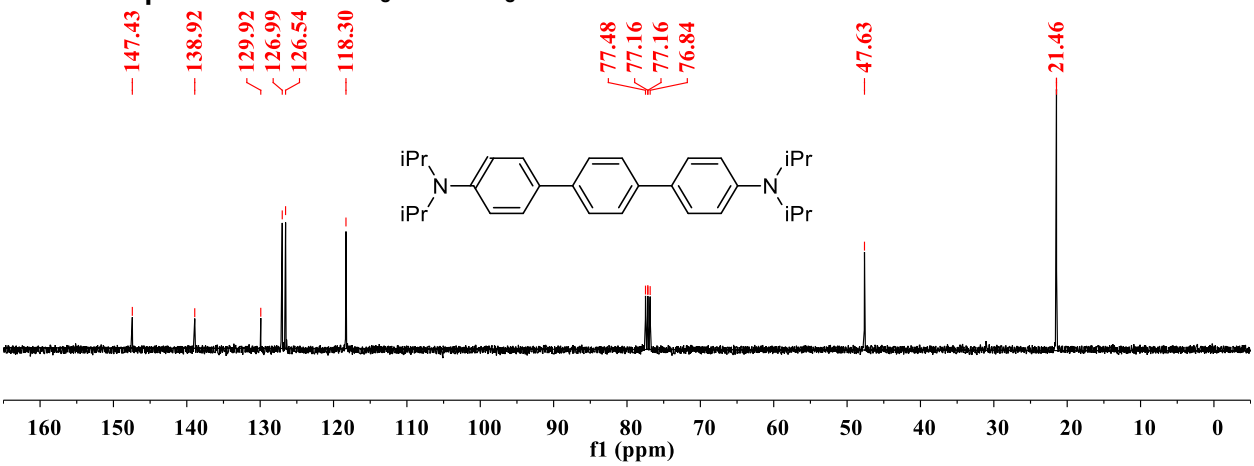
^{13}C NMR spectrum of $^{R2N}PP_2$ in $CDCl_3$



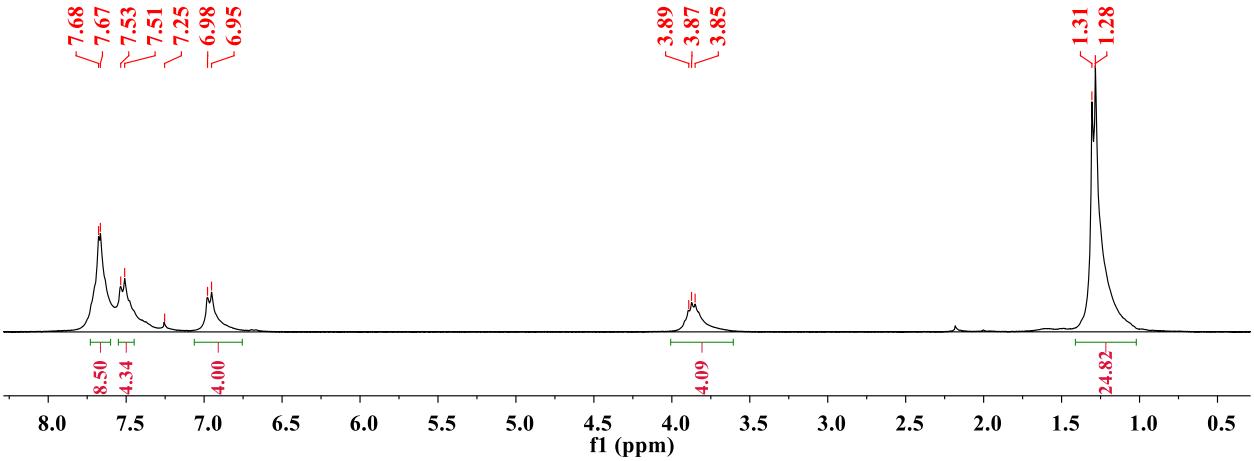
^{1}H NMR spectrum of $^{R2N}PP_3$ in $CDCl_3$



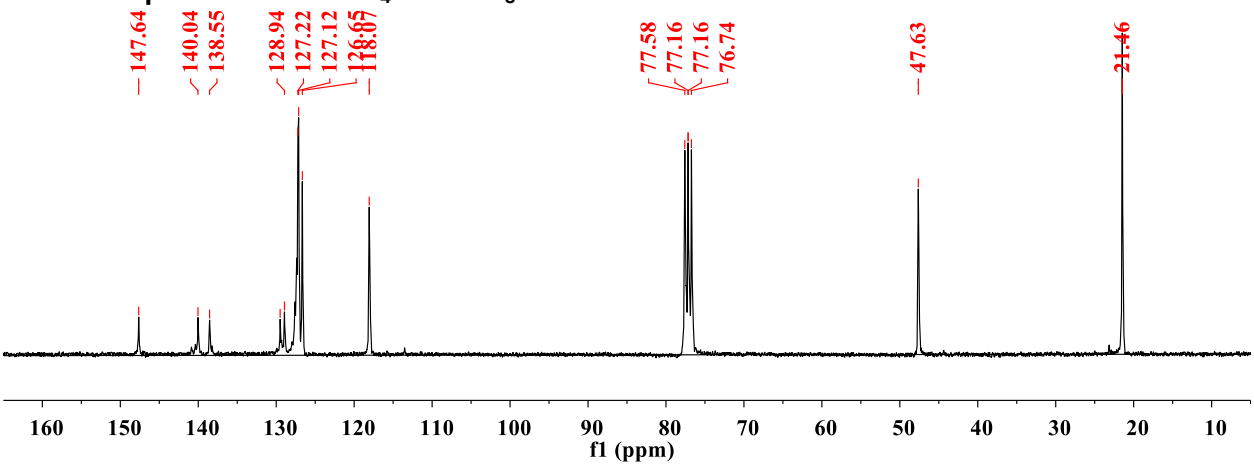
^{13}C NMR spectrum of $^{R2N}PP_3$ in $CDCl_3$



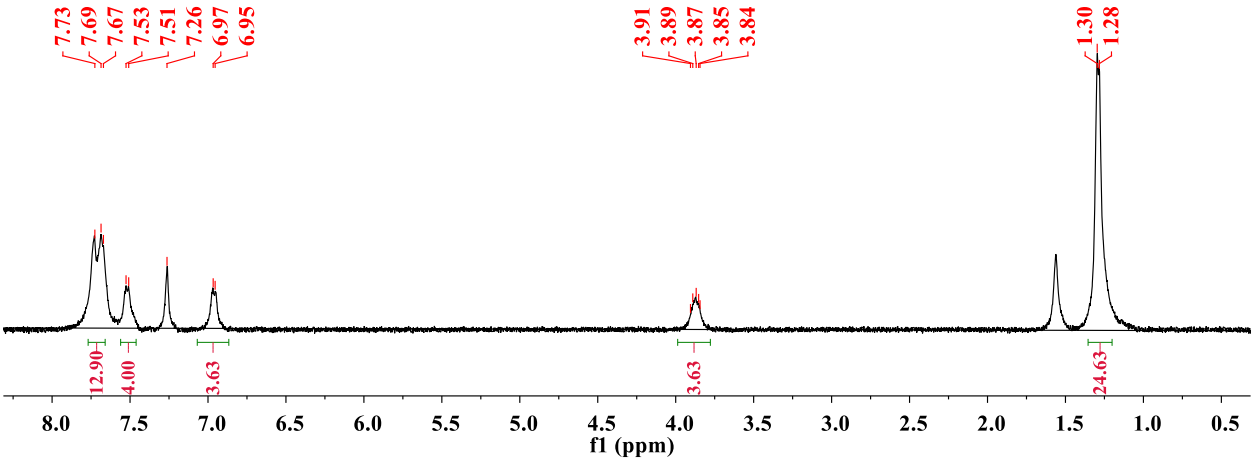
^{1}H NMR spectrum of $^{R2N}PP_4$ in $CDCl_3$



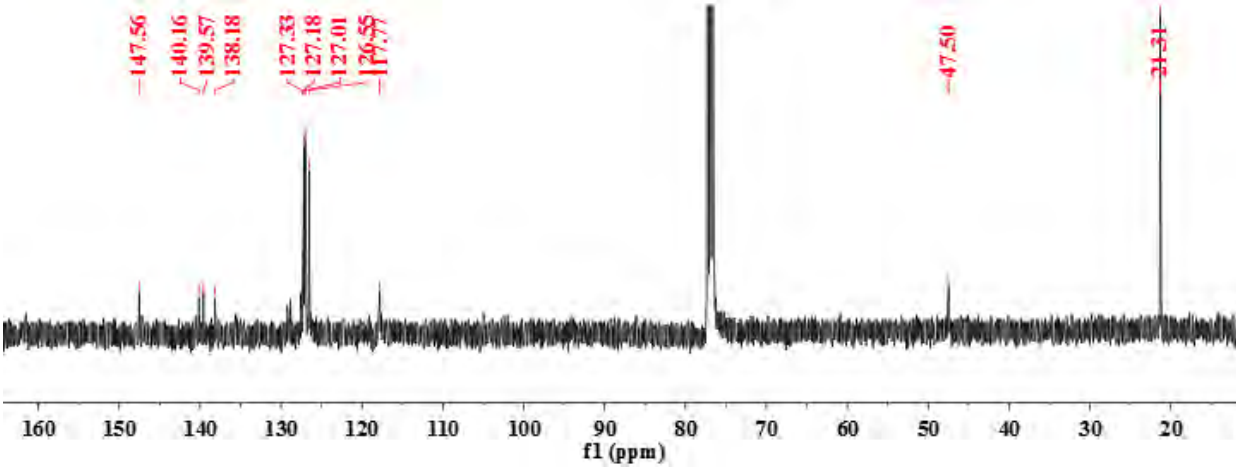
^{13}C NMR spectrum of $^{R2N}PP_4$ in $CDCl_3$



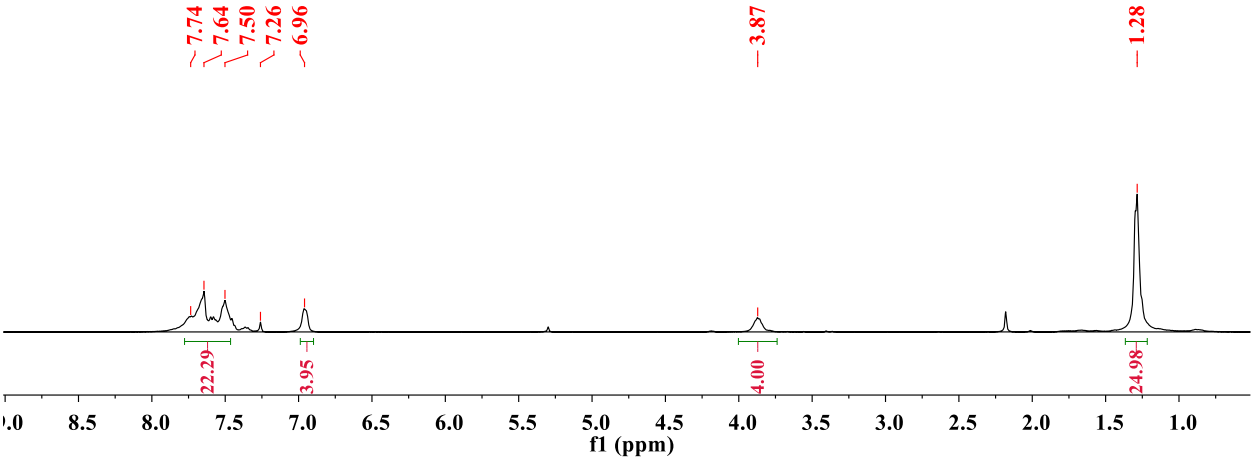
^{1}H NMR spectrum of $^{R2N}PP_5$ in $CDCl_3$



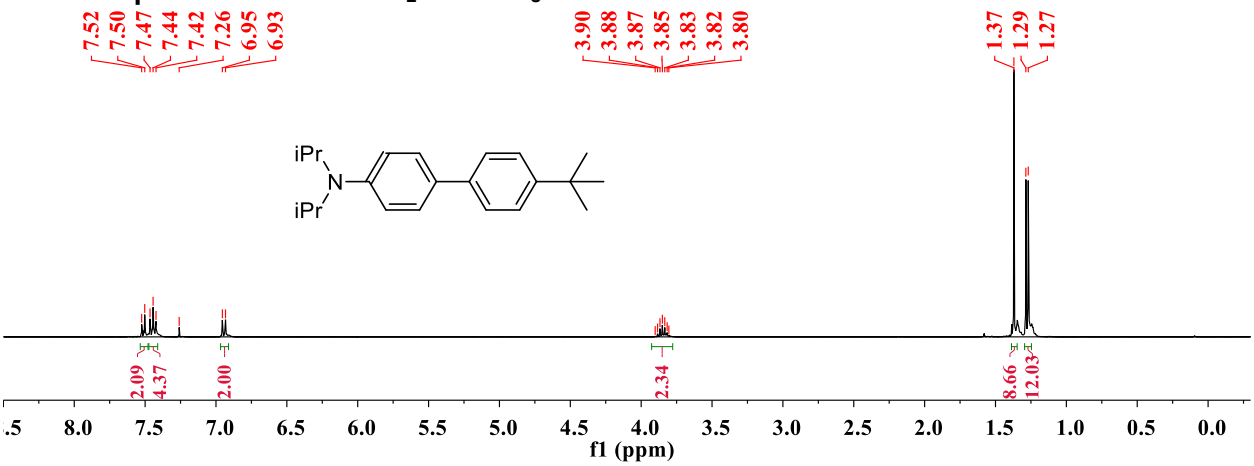
^{13}C NMR spectrum of $^{R2N}PP_5$ in $CDCl_3$



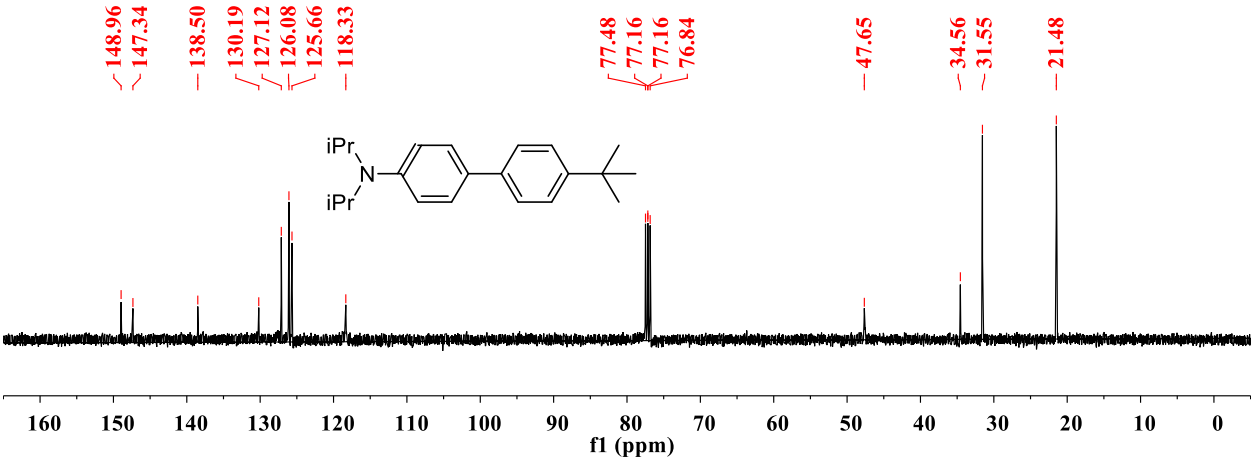
^{1}H NMR spectrum of $^{R2N}PP_6$ in $CDCl_3$



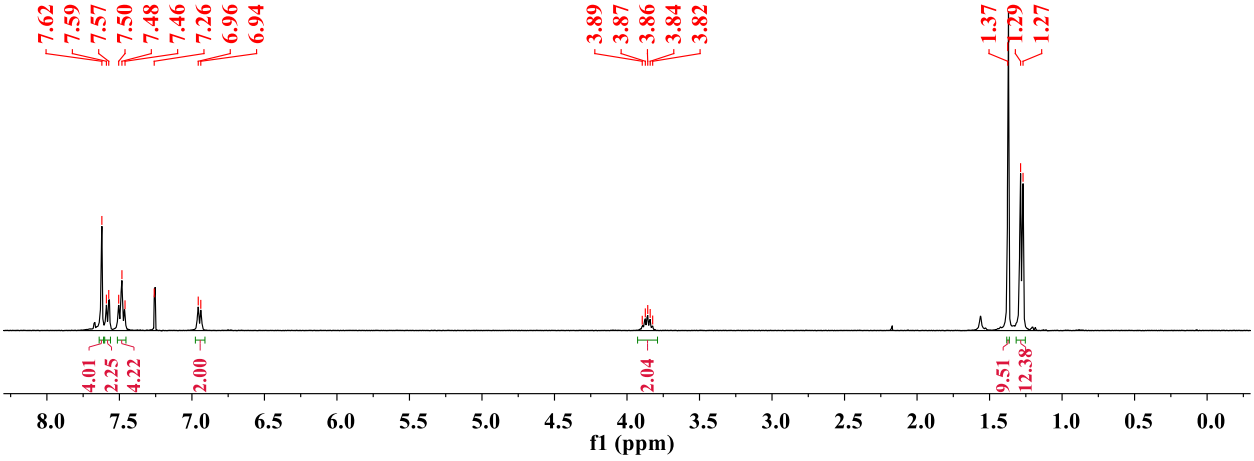
^{1}H NMR spectrum of $^{tBu/R2N}PP_2$ in $CDCl_3$



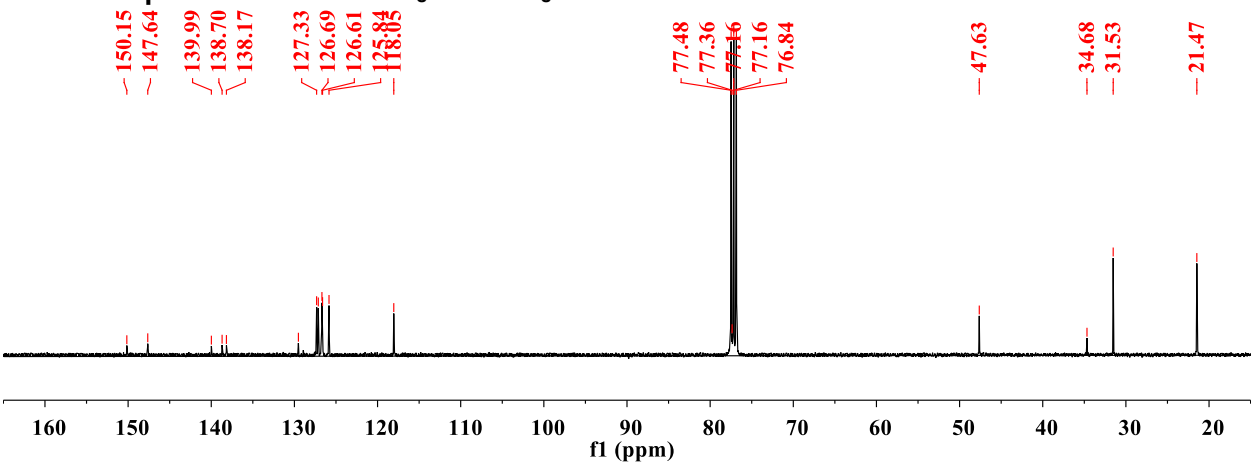
^{13}C NMR spectrum of $^{tBu/R2N}PP_2$ in $CDCl_3$



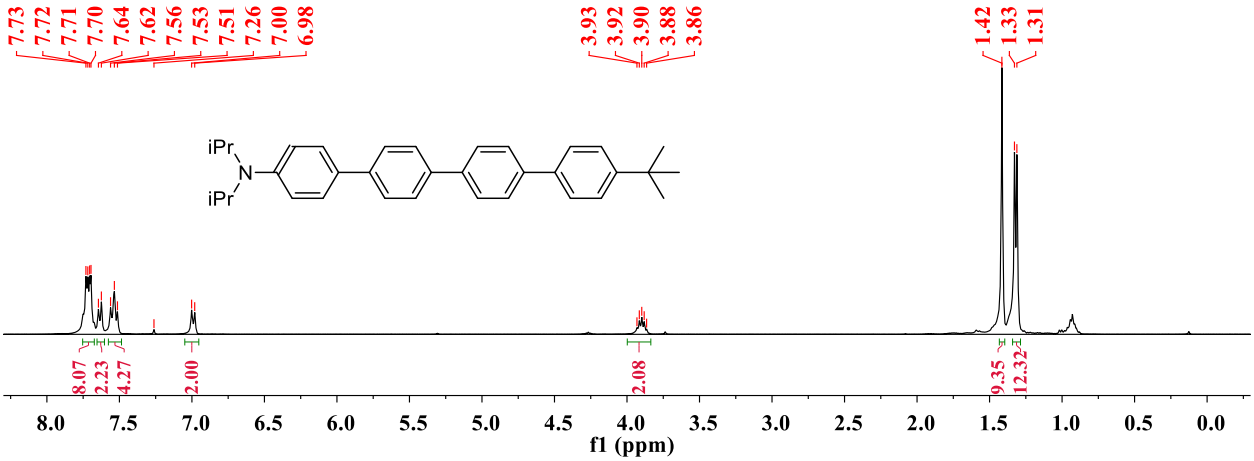
^{1}H NMR spectrum of $^{tBu/R2N}PP_3$ in $CDCl_3$



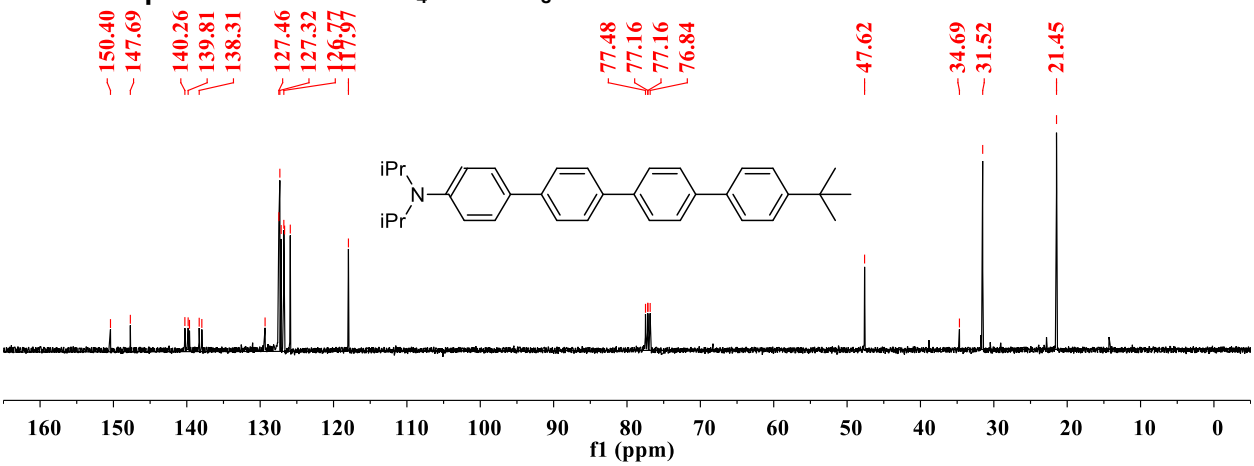
^{13}C NMR spectrum of $^{tBu/R2N}PP_3$ in $CDCl_3$



^{1}H NMR spectrum of $^{tBu/R2N}PP_4$ in $CDCl_3$



^{13}C NMR spectrum of $^{tBu/R2N}PP_4$ in $CDCl_3$



S8. Computational Details

Electronic structure calculations were performed with the Gaussian 09 package, revision D01.[NO STYLE for:] For the density functional theory (DFT) calculations we used calibrated (see Ref. [7] for details, also see refs [5,8-11]) B1LYP functional[12] that contains 40% contribution of the exact exchange with 6-31G(d) basis set by Pople and co-workers.[13] Solvent effects were included using the implicit integral equation formalism polarizable continuum model (IEF-PCM, also referred as PCM)[14-18] with the dichloromethane solvent parameters (ε = 8.93). In all DFT calculations, ultrafine Lebedev's grid was used with 99 radial shells per atom and 590 angular points in each shell. For the cation radical calculations, wave function stability tests[19,20] was performed to ensure absence of solutions with lower energy. The values of $\langle S^2 \rangle$ operator after spin annihilation were confirmed to be close to the expectation value of 0.75, thus indicating that spin contamination was not an issue for the performed calculations. Atomic charges were calculated using Natural Population Analysis approach,[21] which is a part of the Natural Bond Orbital analysis.[22] Energies of vertical electronic excitations and hole distribution in the first excited state of $^{R}\mathbf{PP}_{n}^{+\bullet}$ were computed using the time-dependent density functional theory (TD-DFT) method.[20,23-26]

Tight cutoffs on forces and atomic displacement were used to determine convergence in geometry optimization procedure. Hessians were calculated for the optimized structures to confirm absence of imaginary frequencies. Free energies were computed within harmonic oscillator approximation for T = 298.15 K and P = 1 atm. In the DFT calculations, only the electronic part of the oxidation energies (ΔE^{el}) of $^{R}\mathbf{PP}_{n}$ have been used due to the presence of highly anharmonic polymer-like vibrational modes in higher homologues that cannot be properly treated within the harmonic approximation.[7]

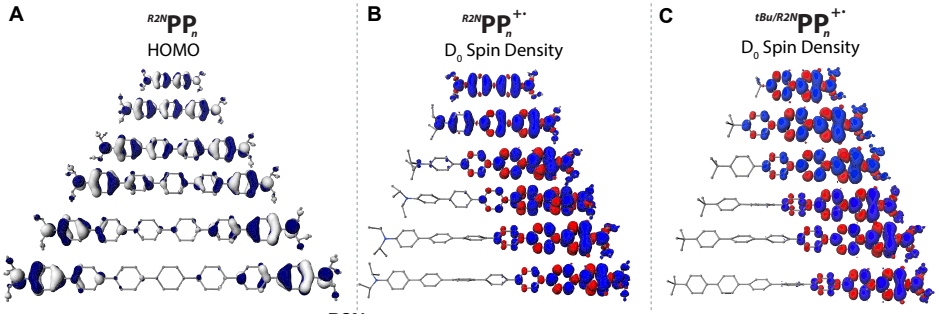


Figure S12. **A**: HOMOs (±0.03 au) of $^{R2N}\mathbf{PP}_{n}$ (n = 2-7). **B**: Spin density distribution plots (±0.001 au) of $^{R2N}\mathbf{PP}_{n}^{+\bullet}$ (n = 2-7) in the ground (D_0) electronic state. **C**: Spin density distribution plots (±0.001 au) of $^{tBu/R2N}\mathbf{PP}_{n}^{+\bullet}$ (n = 2-7) in the ground (D_0) electronic state.

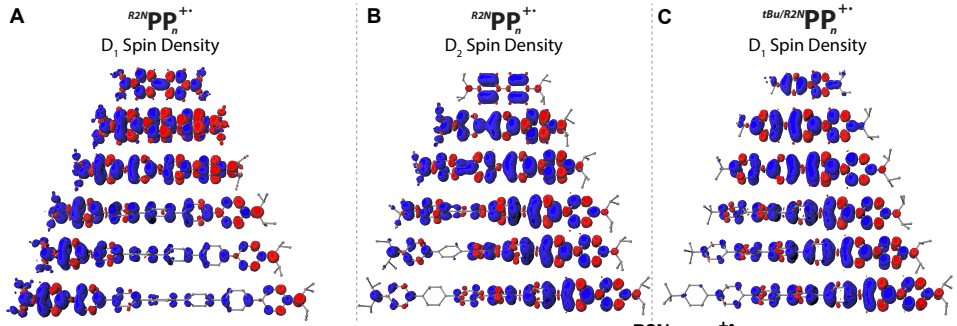


Figure S13. **A**: Spin density distribution plots (±0.001 au) of $^{R2N}\mathbf{PP}_{n}^{+\bullet}$ (n = 2-7) in the first vertically excited (D_1) electronic state. **B**: Spin density distribution plots (±0.001 au) of $^{R2N}\mathbf{PP}_{n}^{+\bullet}$ (n = 2-7) in the second vertically excited (D_2) electronic state. **C**: Spin density distribution plots (±0.001 au) of $^{tBu/R2N}\mathbf{PP}_{n}^{+\bullet}$ (n = 2-7) in the first vertically excited (D_1) electronic state.

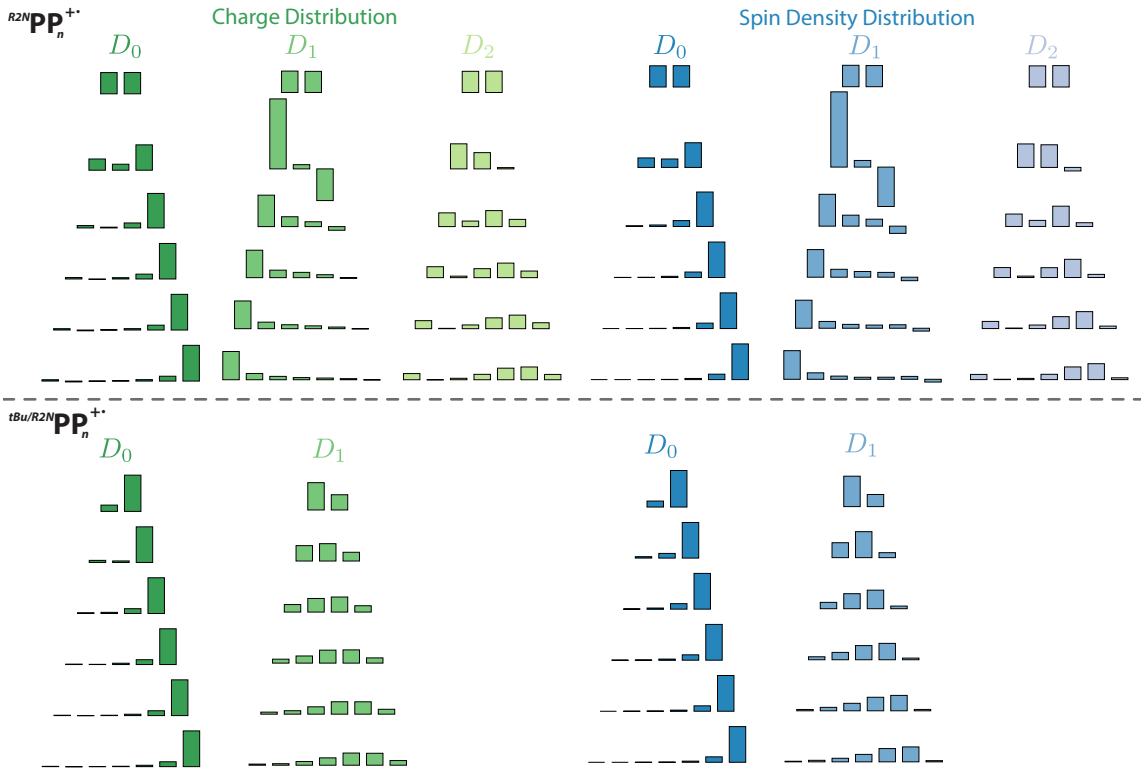


Figure S14. Per-unit barplot representation of NPA charge and spin-density distributions in ground (D_0), first (D_1) and second (D_2) vertically excited electronic states of $^{R2N}\mathbf{PP}_n^{+\bullet}$ and $^{tBu/R2N}\mathbf{PP}_n$ calculate using B1LYP-40/6-31G(d)+PCM(CH_2Cl_2).

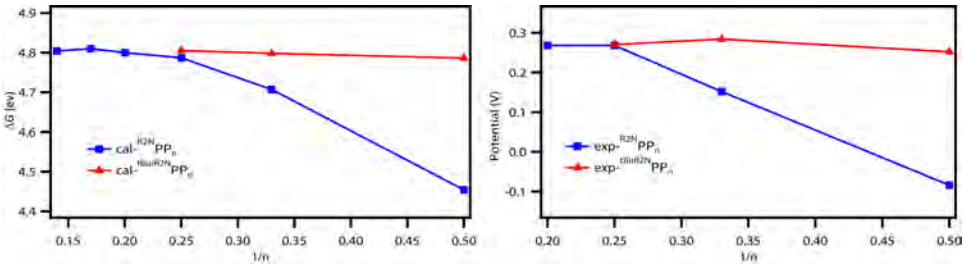


Figure S15. Calculated ([B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)]; left panel) and measured (electrochemistry; right panel) $^{R}\mathbf{PP}_n$ energies of oxidation of $^{R2N}\mathbf{PP}_n$ (n = 2-7) and $^{tBu/R2N}\mathbf{PP}_n$ (n = 2-4).

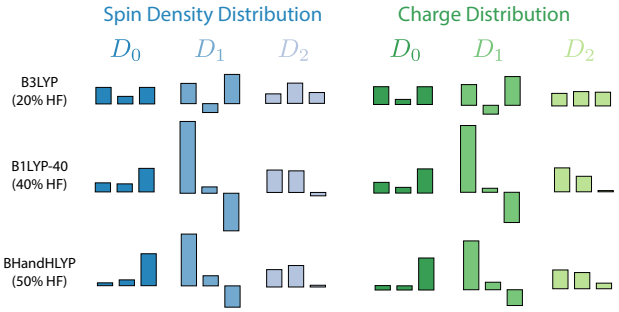


Figure S16. Effect of the amount of exact Hartree-Fock exchange on the hole distribution in the ground (D_0), first (D_1) and second (D_2) vertically excited electronic states of $^{R2N}\mathbf{PP}_3^{+\bullet}$ on the example of B3LYP, B1LYP-40 and BHandHLYP functionals with 6-31G(d) basis set.

Table S2. Comparison of the calculated [TD-B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] and experimental wavelength of vertical excitation in $^{R2N}PP_n^{+\bullet}$ and $^{tBu/R2N}PP_n^{+\bullet}$.

$^{R2N}PP_n^{+\bullet}$, *n*	λ_{max} (D_0->D_1), nm	f_{osc}	λ_{max} (D_0->D_2), nm	f_{osc}	λ_{max} (exp.), nm	λ_{max} (calc., scaled)[a], nm
2	984	0.74	472	0.00	1058	1105
3	1530	0.96	557	0.02	1718	1702
4	1165	0.48	653	0.27	840	742
5	1050	0.25	711	0.45	870	805
6	996	0.12	748	0.54	820	869
7	959	0.06	770	0.59		

$^{tBu/R2N}PP_n^{+\bullet}$, *n*	λ_{max} (D_0->D_1), nm	f_{osc}	λ_{max} (exp.), nm	λ_{max} (calc., scaled)[a], nm
2	615	0.47	713	700
3	725	0.58	826	821
4	769	0.60	880	869
5	788	0.62		
6	792	0.60		
7	794	0.60		

[a] Scaled values were obtained based on the linear correlation between λ_{max}(calc) and λ_{max}(exp), see Figure S10 below.

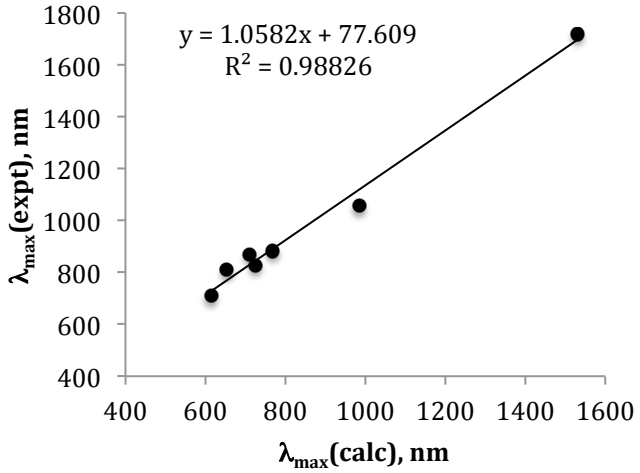


Figure S17. Comparison of the calculated [TD-B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] and experimental wavelength corresponding to the vertical excitation in $^{R2N}PP_n^{+\bullet}$ and $^{tBu/R2N}PP_n^{+\bullet}$.

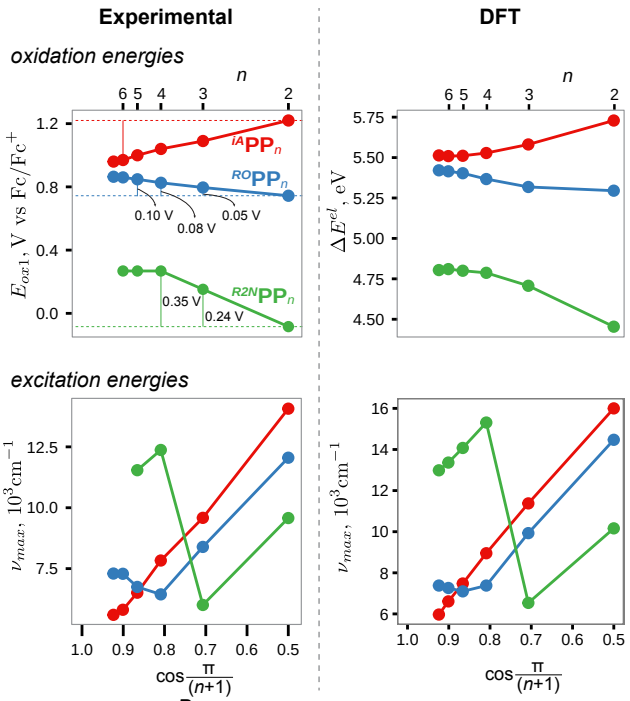


Figure S18. Left: Experimental E_{ox1} of ^{R}**PP**$_n$, where ***R*** = ***iA***, ***RO***, and ***R2N***, and vertical excitation energies of their cation radicals vs cos π/(*n*+1), where *n* is the number of *p*-phenylene units. Right: Calculated (TD-)DFT energies of oxidation of ^{R}**PP**$_n$, and vertical excitation energies of the corresponding ^{R}**PP**$_n^{+\bullet}$ [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)].

S9. Two- and three-state parabolic models

Lowest eigenvalues of the Hamiltonians **H2** and **H3** defined in eqs 1 and 2 of the Manuscript, respectively:

$$\varepsilon_0(\mathbf{H2}) = \frac{\lambda}{4} - \Delta\varepsilon - H_{ab} \qquad \text{(eq S1)}$$

$$\varepsilon_0(\mathbf{H3}) = \frac{\lambda - \Delta\varepsilon - \sqrt{(\Delta\varepsilon-\lambda)^2+8H_{ab}^2}}{2} \qquad \text{(eq S2)}$$

are equal to each other when:

$$\Delta\varepsilon = \frac{3\lambda^2 - 8\lambda H_{ab} + 16H_{ab}^2}{12\lambda + 16H_{ab}} \qquad \text{(eq S3)}$$

In the case of poly-*p*-phenylene wires, $H_{ab}/\lambda >> 1$, and eq S3 can be approximated as $\Delta\varepsilon \approx H_{ab}$.

Delocalization of the hole in the ground state of ^{R}**PP**$_3^{+\bullet}$ at $x_{min} = 1$ can be evaluated from the corresponding eigenvector of **H3**:

$$\psi_0 = \left(1; \left(\frac{\Delta\varepsilon - \lambda - \sqrt{(\Delta\varepsilon-\lambda)^2+8H_{ab}^2}}{2H_{ab}}\right)^2; 1\right) \qquad \text{(eq S4)}$$

The hole is evenly delocalized on all three units in a given ^{R}**PP**$_3^{+\bullet}$ when

$$\frac{\Delta\varepsilon - \lambda - \sqrt{(\Delta\varepsilon-\lambda)^2+8H_{ab}^2}}{2H_{ab}} = -1 \qquad \text{(eq S5)}$$

(note that the second element of ψ_0 is always negative), i.e., when $\Delta\varepsilon = \lambda + H_{ab}$. If $\Delta\varepsilon < \lambda + H_{ab}$ (or $\Delta\varepsilon > \lambda + H_{ab}$) then charge will be more concentrated (or depleted) on the central unit. Therefore, charge depletion on the central unit is only possible when $\Delta\varepsilon$ is positive and larger than $\lambda + H_{ab}$.

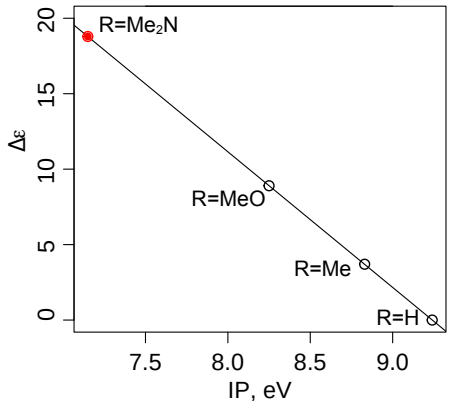


Figure S19. Correlation between the values of $\Delta\varepsilon$, obtained by fitting hole distribution produced by MPM vs pre-unit spin/charge distribution from the DFT calculations, vs the ionization potentials of model compounds, i.e. benzene (9.24 eV),[27] toluene (8.83 eV),[27] anisole (8.25 eV),[28] and dimethylaminobenzene (7.15 eV).[29] Note that $\Delta\varepsilon$(***R2N***) = 65.3 was obtained by multiplication of the value of $\Delta\varepsilon$(***R2N***) = 19.0 in MPM (shown in the Figure) by the value of reorganization energy (λ = 3.438) in MSM.

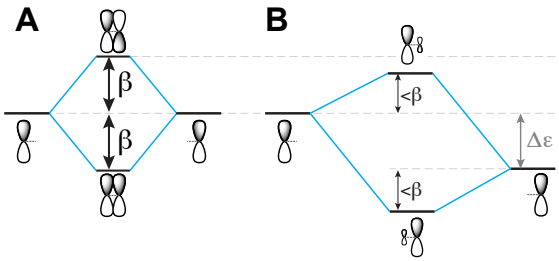


Figure S20. Schematic representation of molecular orbital diagrams for the interaction between orbitals of identical (A) and different (B) energies on the example of two p-type orbitals.

S10. Multistate Model

The effect of the electronic coupling H_{ab} on the free energies and hole distribution in polychromophoric wires can then be evaluated by a simple extension of the Hamiltonian matrix in Figure 9 of the Manuscript to an arbitrary number of states *n*, i.e. eqs S6-S8:

$$\mathbf{H}(X_\Lambda) = \begin{bmatrix} H_1(X_\Lambda) - \Delta\varepsilon & H_{ab} & 0 & . & 0 & 0 \\ H_{ab} & H_2(X_\Lambda) & H_{ab} & . & 0 & 0 \\ 0 & H_{ab} & H_3(X_\Lambda) & . & 0 & 0 \\ . & . & . & ... & . & . \\ 0 & 0 & 0 & . & H_i(X_\Lambda) & H_{ab} \\ 0 & 0 & 0 & . & H_{ab} & H_n(X_\Lambda) - \Delta\varepsilon \end{bmatrix} \quad \text{(eq S6)}$$

Quadratic function (used in MPM):

$$H_i(X_\Lambda) = \lambda\left(X_{Qi} - X_\Lambda\right)^2 \quad \text{(eq S7)}$$

We have recently shown, using examples of $^{iA}\mathbf{PP}_n^{+\bullet}$, $^{RO}\mathbf{PP}_n^{+\bullet}$, and cyclic poly-*p*-phenylene cation radicals, that a composite quadratic/reciprocal function rather than parabolic function allows for the improved description of the structural/solvent reorganization (see eq S8 in the Supporting Information) and the hole distribution in the excited states.[11] For the sake of consistency with our earlier results,[11] we reexamine $^{R2N}\mathbf{PP}_n^{+\bullet}$ using multistate model with composite quadratic/reciprocal function, simply referred to as MSM.

For ^{R2N}**PP**$_n^{+\bullet}$, we utilized the same parameters as used for ^{iA}**PP**$_n^{+\bullet}$ and ^{RO}**PP**$_n^{+\bullet}$ series, i.e. λ^{∞} = 45, H_{ab} = 26.16, λ = 3.438.[11] A value of the $\Delta\varepsilon$(***R2N***) = 64.8 was obtained by fitting the per-unit hole distributions in ^{R2N}**PP**$_n^{+\bullet}$ (n = 2-6) using MSM to those obtained by the DFT calculations. It is noteworthy that a very similar estimate of $\Delta\varepsilon$(***R2N***) = 65.3 was obtained based on the linear correlation between the values of $\Delta\varepsilon$ vs the ionization potentials of model monochromophoric units, Figure S12 in the Supporting Information. The hole distribution as well as the evolution of oxidation energies obtained by MSM was remarkably similar to those obtained by MPM (Figures S16 and S17 in the Supporting Information). The only difference between the MSM and MPM results was observed for the excitation energy trends for larger oligomers ^{R2N}**PP**$_n^{+\bullet}$ with hole localized on the terminal unit, which is consistent with our previous finding that shape of the reorganization energy function is much more critical for the excited states than for the ground electronic state.[11]

Composite quadratic/reciprocal function (used in MSM):

$$H_i(X_\Lambda) = \begin{cases} \lambda\left(X_{Qi} - X_\Lambda\right)^2, \ if \ \left|X_{Qi} - X_\Lambda\right| \leq \ t \\ \lambda^{\infty} - \frac{a}{\left|X_{Qi} - X_\Lambda\right|}, \ if \ \left|X_{Qi} - X_\Lambda\right| \geq \ t \end{cases} \qquad \text{(eq S8)}$$

where $X_{Qi} = i - 1$, H_i—diabatic free energy of i-th monomer, H_{ab}—the coupling strength between the interacting units, λ is the structural reorganization, λ^{∞} is the free energy of completely separated charge and reorganization ($|X_Q - X_\Lambda| \rightarrow \infty$), $\Delta\varepsilon$—the value of shift of terminal diabatic state, which serves to account for the better hole stabilization abilities of the terminal units with electron-donating capping group. The requirement of continuity of $H_i(X_\Lambda)$ and its first derivative at $|X_Q - X_\Lambda| = t$ is used to define the parameters $a = 2\lambda t^3$ and $t = \sqrt{\lambda^{\infty}/_{3\lambda}}$. The diabatic states were uniquely defined by two independent parameters, one indicating the position of the charge X_Q (i.e. X_Q = 0/1 denotes charge localized on the left/right chromophore in the two-state-model, respectively), and another indicating the extent of reorganization X_Λ (i.e. X_Λ = 0/1 corresponds to the case where structural/solvent reorganization, needed to accommodate charge, is fully localized on the left/right unit, respectively (see ref. [11] for the detailed description).

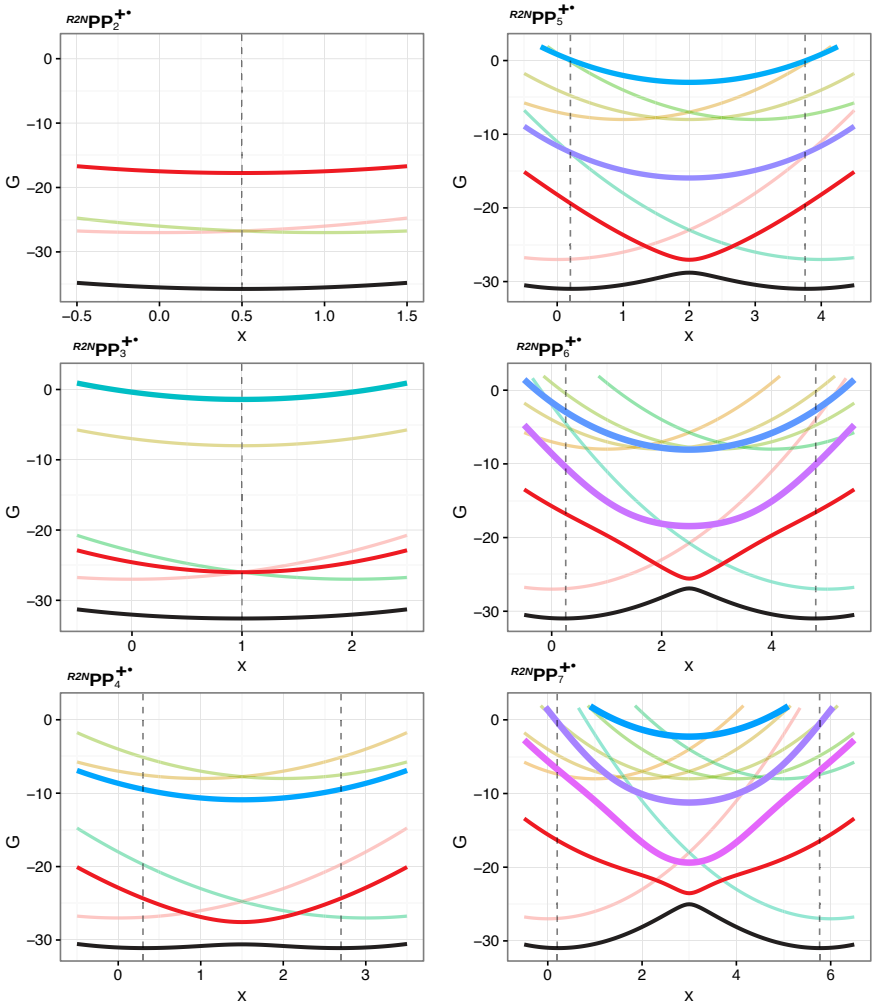


Figure S22. Ground and lowest excited states of $^{R2N}PP_n^{+\bullet}$, n = 2–7, along the hole transfer coordinate x, obtained by MPM. Thin lines represent diabatic 'pure' states, and thick lines represent adiabatic 'mixed' states. The dashed lines denote the positions of the minima of the ground adiabatic state.

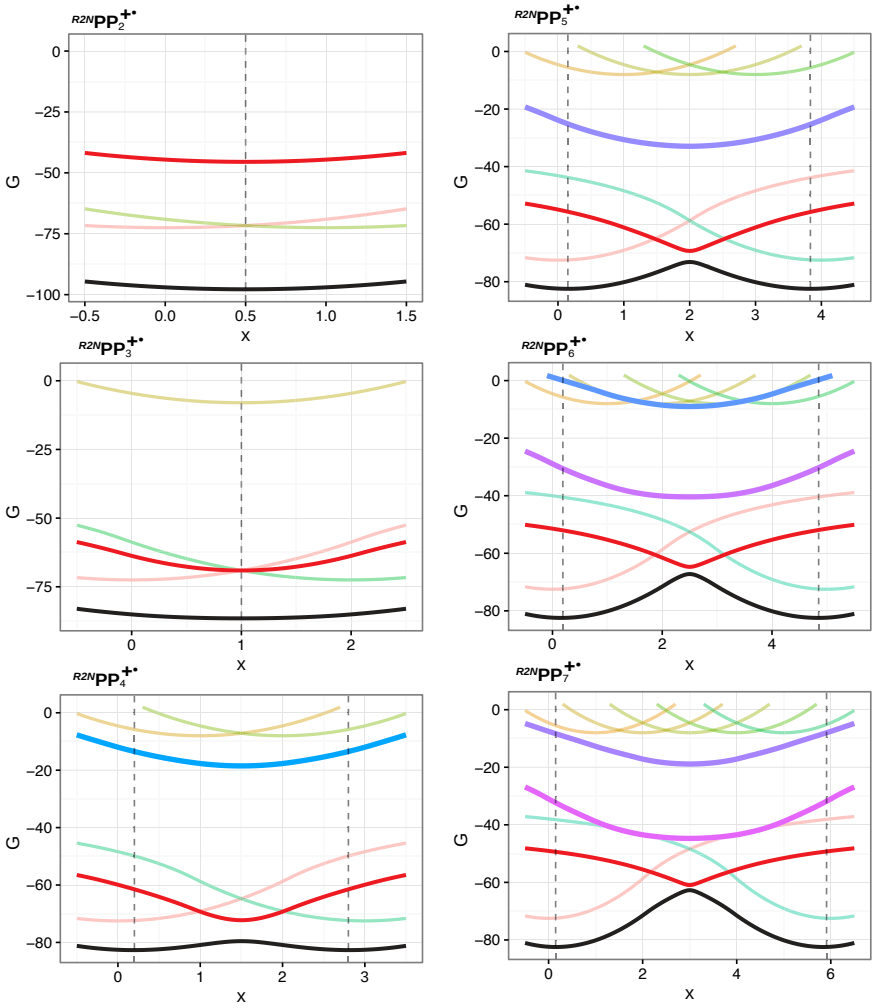


Figure S23. Ground and lowest excited states of $^{R2N}PP_n^{+\bullet}$, n = 2–7, along the hole transfer coordinate x, obtained by MSM. Thin lines represent diabatic 'pure' states, and thick lines represent adiabatic 'mixed' states. The dashed lines denote the positions of the minima of the ground adiabatic state.

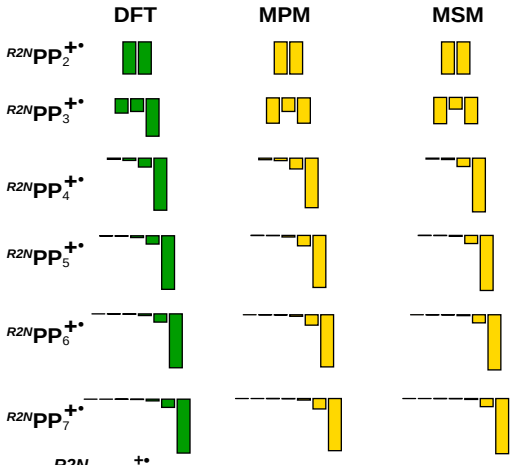


Figure S24. Hole delocalization in $^{R2N}PP_n^{+\bullet}$, n = 2–7, obtained from the DFT spin/charged distribution as well as from the MPM and MSM modeling.

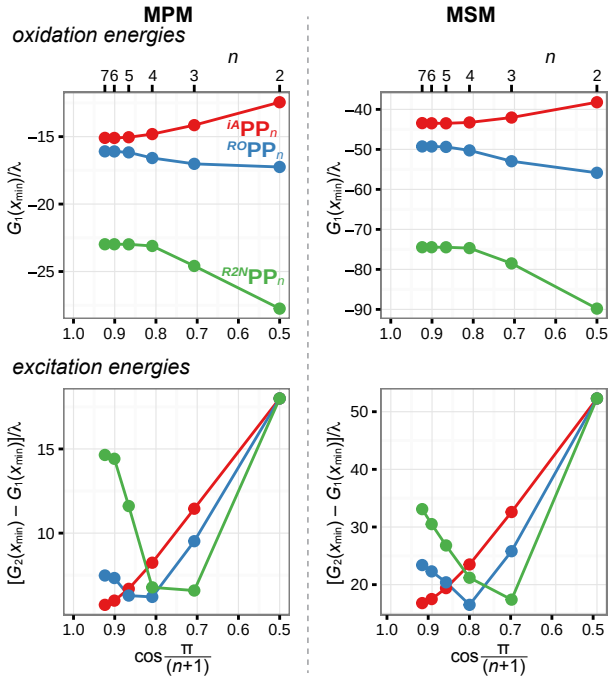


Figure S25. Oxidation energies $G_1(x_{min})$ and vertical excitation energies $G_2(x_{min}) - G_1(x_{min})$ of $^{R}\mathbf{PP}_n^{+\bullet}$ (n = 2-7, ***R*** = ***iA***, ***RO***, or ***R2N***) obtained from MPM (left) and MSM (right), vs cos π/(n+1).[NO STYLE for:]

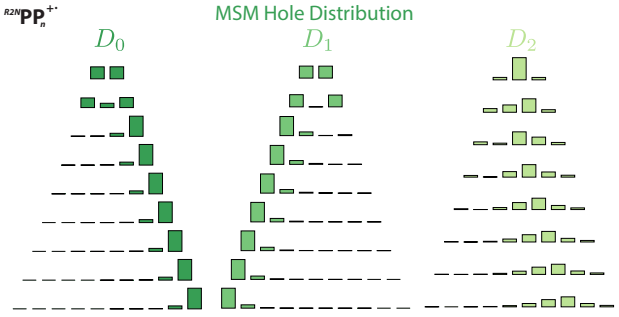


Figure S26. Hole distributions in the ground electronic state (D_0) of $^{R2N}\mathbf{PP}_n^{+\bullet}$, and in the vertically excited D_1 and D_2 states obtained by MSM. Compare with the results from DFT calculations in Figure S14.

S11. References

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S12. Archive entries from the calculation files

The archive entries, formerly intended for the Browse Quantum Chemistry Database System, are organized as a simple list of data fields separated by backslash symbols, which is wrapped in 70-char text lines. The script 'Parse.Archive.pl', written in Perl, converts archive entry into human readable format. To use this script,

1. Check if Perl interpreter is installed on the system. To do this, run the command 'perl –v' in console. If console returns a message like 'command not found', please obtain and install a Perl interpreter (www.perl.org/get.html; Perl is Open Source software licensed under GNU GPL).
2. Save the script code, listed below, as a file named 'Parse.Archive.pl'.
3. Select an archive entry of interest and save it as another file (e.g. 'A.txt').
4. Run the command 'perl Parse.Archive.pl A.txt > A-parsed.txt' in console. The parsed archive entry will be stored in the file 'A-parsed.txt' in this example. In some cases, absolute path to the Perl interpreter might need to be provided.

```
# --- Parse.Archive.pl ---

# Merge all strings in one line
my $s='';
while (<>) {chomp;$s .= $_}
$_ = $s;

#     Some     PDF     viewers     (like     Mac     OS's     Preview)     might     substitute
# 'end of line' symbols by the white space symbols,
# To remove these extra white spaces, please uncomment the following lines:
# my $str_length = 70;
# my $index = $str_length;
# while (length($_) > $index) {
#     substr $_,$index,1,'';
#     $index += $str_length;
# }

# Replace all backslashes by new-line symbols
s:\\:\n:g;

# Print the resulting output
print;

# --- END ---
```

R2NPP2

```
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hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
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```

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^{R2N}PP3

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hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
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30691,-5.8096747774,-3.8027237535\H,-0.1600634117,-5.2877050016,-6.931

6348805\H,-1.2738355291,-3.9572090483,-6.6318207747\H,-1.8682926684,-5
.446982757,-7.3475523087\H,0.4268383459,-7.6523291087,-5.7160385284\H,
1.801159105,-7.941682413,-4.6620063148\H,1.6920159623,-6.4280307527,-5
.5652023409\H,-0.8553059019,-7.1364567246,-2.1473210671\H,0.2920936546
,-8.3719452687,-2.673183156\H,-1.1557021964,-8.0547803021,-3.621536905
6\N,-0.1713937375,6.4400395122,3.8488248563\C,-0.4278185545,6.42112181
57,5.3010157638\C,0.8163475012,6.141971001,6.1547173498\C,-1.615454779
7,5.5440026193,5.7073911941\C,-0.223879011,7.7532615441,3.1923909764\C
,0.7720565408,8.7417501737,3.8053549271\C,-1.6358284743,8.348211683,3.
1351778528\H,1.6462318828,6.7749760258,5.8451953396\H,1.1447621004,5.1
058295984,6.0964247323\H,0.5975065864,6.3560332348,7.2020137518\H,-1.4
245495881,4.483231934,5.5614211471\H,-2.5026177483,5.8095832043,5.1330
481917\H,-1.8342953219,5.7000345044,6.7640026123\H,1.7779606506,8.3239
862203,3.8072384676\H,0.5132923626,9.0185501472,4.8272022096\H,0.78380
80685,9.6576835485,3.2140931161\H,-2.0127667323,8.5752572324,4.1333282
209\H,-2.335505984,7.6602235168,2.6618384146\H,-1.6340496945,9.2782443
273,2.5654497098\H,1.184313627,-6.1361865041,-3.1913155916\H,-1.452307
8864,-6.7210189804,-5.3725614754\H,-0.7257874855,7.4398562462,5.538617
4766\H,0.1144867397,7.5891573601,2.1725255462\\Version=EM64L-G09RevD.0
1\HF=-1276.005371\RMSD=6.969e-09\RMSF=6.246e-07\Dipole=-0.1956885,-0.0
346777,0.076166\Quadrupole=-24.0914303,22.9309782,1.1604522,-2.0106562
,2.669829,20.1642809\PG=C01 [X(C30H40N2)]\\@

^{R2N}PP4

1\1\GINC-HPC-CN42\FOpt\RBLYP\6-31G(d)\C36H44N2\TALIPOVM\20-Jun-2014\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
le\\0,1\H,1.7667068178,-2.4090527762,-1.1494692603\C,0.8926911337,-1.7
73522405,-1.1579650216\C,-1.3482182858,-0.1592181957,-1.0768725858\C,-
0.2449590155,-2.17307447,-1.8690195887\C,0.91070321,-0.5956489204,-0.4
281066039\C,-0.2098406904,0.2396788619,-0.3683792344\C,-1.3644667831,-
1.3347630907,-1.8104683822\H,1.7986740173,-0.338468318,0.1317780572\H,
-2.2515726999,-1.5897868053,-2.3725047715\H,-2.2233449886,0.4749904107
,-1.082120598\C,-0.1919469886,1.4954688718,0.4142197555\C,-0.157645364
9,3.9060742129,1.9181742112\C,-1.3312703868,1.9482526898,1.0879374788\
C,0.9649011496,2.2760935091,0.5100279425\C,0.9809683712,3.452732814,1.
242008625\C,-1.3138712728,3.1229565669,1.8228575936\H,-2.2355101477,1.
3567163958,1.0650012817\H,1.8565735835,1.9767856855,-0.0223988803\H,1.
8849753782,4.0445512574,1.2631410514\H,-2.2050696627,3.4204651392,2.35
6919053\C,-0.1399055242,5.1599814494,2.7011817505\C,-0.1038400401,7.59
29063372,4.218029325\C,-1.2592626861,5.9905029415,2.7866953463\C,0.998
9139011,5.5781838368,3.3967015524\C,1.023696342,6.7546291279,4.1242010
646\C,-1.2516671386,7.1632290765,3.5247704974\H,-2.1643131629,5.724201
7423,2.2585399653\H,1.8912452103,4.967992143,3.3779786183\H,1.94093217
79,7.0303992807,4.6147075684\H,-2.1621613521,7.7381749363,3.5647099082
\C,-0.2636641351,-3.4279934508,-2.6490061976\C,-0.3002503167,-5.865779
9402,-4.1573052335\C,0.8755734946,-3.9086180778,-3.2986145078\C,-1.423
7621019,-4.1986852232,-2.7764409694\C,-1.4446239297,-5.3798375027,-3.4
961097877\C,0.8626506351,-5.0806670533,-4.0372182404\H,1.7919765838,-3
.3357864254,-3.2641230319\H,-2.3271871574,-3.8926875235,-2.2672367361\
H,-2.357837656,-5.9487454436,-3.5152424865\H,1.7678083379,-5.363402211
6,-4.5491761134\N,-0.3184495855,-7.0654711616,-4.8619662954\C,-1.49838
65581,-7.5106567693,-5.6266443963\C,-2.5075528676,-8.3257868522,-4.807
0354737\H,-1.0983768298,-8.19723169,-6.3693131514\C,-2.1736107586,-6.3
930663104,-6.4265780017\C,0.9523043893,-7.7351445863,-5.1708572784\H,1
.6637550305,-7.3779323838,-4.4307973532\C,1.4983013798,-7.3900550474,-
6.5613610158\C,0.8677894761,-9.2503784184,-4.9667051506\N,-0.068052447

2,8.7872698091,4.9323752321\C,-1.0950472845,9.8064055467,4.6764258691\
H,-1.4571302289,9.6171649261,3.6692320358\C,-0.5061839038,11.219517889
7,4.6449477102\C,-2.2882754035,9.7208628375,5.6353594362\C,0.701539533
9,8.9317367672,6.1824919267\C,0.5840788205,7.7298133907,7.1241931193\H
,0.2205883699,9.7556406853,6.7047193486\C,2.158794932,9.3650732773,5.9
756610013\H,1.0479025447,7.9743696561,8.0800777381\H,1.074886858,6.840
3749442,6.7357707958\H,-0.4622709359,7.4858810722,7.306059558\H,2.5934
866058,9.6568621076,6.9329502847\H,2.2149648333,10.2191825194,5.302937
578\H,2.7809799352,8.5723611459,5.5641657965\H,0.3181726563,11.2778045
017,3.9354327566\H,-0.1440268607,11.5452805017,5.6198273296\H,-1.27608
61596,11.9254123247,4.33250383\H,-1.9916348907,9.9471383987,6.66038747
91\H,-2.7310481998,8.7254563128,5.6270308891\H,-3.0580883695,10.438866
0516,5.3500870939\H,-2.0034068611,-9.1077879581,-4.2418298226\H,-3.225
8332672,-8.799965706,-5.4776619254\H,-3.0726182794,-7.7151950817,-4.10
5084895\H,-1.4461237643,-5.8741314368,-7.0501944012\H,-2.66008637,-5.6
560552272,-5.7916281948\H,-2.9342541054,-6.8246282651,-7.0775858631\H,
2.480168595,-7.8418483562,-6.7073955144\H,1.596330397,-6.3127875548,-6
.6910920428\H,0.8439608656,-7.7643275804,-7.3498402503\H,0.5139615585,
-9.4853533103,-3.9637224605\H,1.8586863315,-9.6879799552,-5.0903176034
\H,0.2074619618,-9.734330468,-5.6860581341\\Version=EM64L-G09RevD.01\H
F=-1506.9291422\RMSD=5.565e-09\RMSF=4.562e-07\Dipole=-0.0620831,0.0152
817,-0.0478206\Quadrupole=-15.6752337,23.0060474,-7.3308137,-3.7391196
,0.3835425,39.8717001\PG=C01 [X(C36H44N2)]\\@

^{R2N}PP5

1\1\GINC-HPC-CN32\FOpt\RBLYP\6-31G(d)\C42H48N2\TALIPOVM\20-Jun-2014\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
le\\0,1\H,0.4590837489,0.337002913,-2.7560240226\C,0.1354378934,0.3115
911423,-1.7253112723\C,-0.6459323291,0.2857623839,0.9259856681\C,-0.26
98277108,-0.9006812526,-1.157137321\C,0.1471139071,1.4837418632,-0.986
0868937\C,-0.2426864994,1.4984174288,0.3572407415\C,-0.6607790875,-0.8
85761518,0.1858482105\H,0.4506558208,2.403890003,-1.4646048671\H,-0.99
47075631,-1.7999614418,0.655397808\H,-0.9394485739,0.2545447727,1.9655
129618\C,-0.2850535522,-2.152044074,-1.9473174932\C,-0.3159644644,-4.5
541056276,-3.4639152431\C,-0.6270180706,-2.1504228494,-3.3036536103\C,
0.0412313395,-3.3820053017,-1.366533086\C,0.029023935,-4.5531177445,-2
.1072182201\C,-0.6452347294,-3.3226468613,-4.0424394008\H,-0.916424662
6,-1.2247766199,-3.7805759101\H,0.3417746091,-3.4200952877,-0.32909528
94\H,0.3224371813,-5.4775713051,-1.6307220237\H,-0.9502640124,-3.28458
77884,-5.0784218929\C,-0.2297638008,2.7501429491,1.1468797732\C,-0.206
6613254,5.153750783,2.6609410055\C,-1.2033311747,3.0062814726,2.117997
2631\C,0.7559281068,3.7229478048,0.9503723099\C,0.7684931306,4.8941663
489,1.6908551581\C,-1.1933280586,4.1799847186,2.854664502\H,-1.9998750
769,2.2933480301,2.2770953054\H,1.5439464967,3.5475205676,0.2318443153
\H,1.5668715748,5.6052336477,1.5333573217\H,-1.9831282962,4.3558762872
,3.570962539\C,-0.1949635836,6.4048414227,3.4483857689\C,-0.178045335,
8.8322019009,4.9747108922\C,-0.6165903618,6.4405171424,4.7812443112\C,
0.237380846,7.6148899796,2.9016470064\C,0.2564127622,8.7897976372,3.63
58428526\C,-0.6167243912,7.6101664359,5.5199699163\H,-0.9486196532,5.5
307322211,5.2618523529\H,0.5630223188,7.6503385201,1.8712882112\H,0.62
83350368,9.6783975466,3.1529517156\H,-0.9781132978,7.5720372492,6.5327
941199\C,-0.3314760553,-5.8033982959,-4.2528232359\C,-0.3654603939,-8.
2272980826,-5.7836800444\C,0.0095696364,-5.8233845435,-5.6071602283\C,
-0.6879440817,-7.0300806813,-3.6833463259\C,-0.7137584345,-8.200919070
2,-4.4194257372\C,0.0048274091,-6.992395788,-6.3505360006\H,0.32786406
21,-4.9106557002,-6.09160586\H,-0.9937165919,-7.0696064843,-2.64702476

05\H,-1.0422744211,-9.1020629053,-3.9315779893\H,0.3254408629,-6.93708
59475,-7.3778829092\N,-0.4137279682,-9.402338042,-6.5271289632\C,-0.06
14325448,-10.7132426612,-5.9501122234\C,1.1790976009,-10.6801032278,-5
.052937673\H,0.2176175326,-11.3221031178,-6.8070950104\C,-1.2364037473
,-11.4430341479,-5.2858093636\C,-0.451594926,-9.3216891093,-7.99370424
07\C,-1.4361788428,-10.325913843,-8.5992368837\C,0.9320612615,-9.43633
1241,-8.6440265676\H,-0.853515883,-8.3390432886,-8.2266984667\N,-0.202
1719083,10.0119799158,5.7127378667\C,-0.1299397081,11.29981536,5.00901
77687\H,-0.4933417249,11.1096223221,4.002520811\C,1.2953847731,11.8546
089399,4.9038505833\C,-1.0882665929,12.3348306362,5.6049024918\C,0.077
0934368,10.0394314563,7.1608157443\C,-1.1584532284,9.8148333684,8.0425
056244\H,0.3971114565,11.0602077566,7.3568838179\C,1.256058957,9.15663
72764,7.5803988532\H,2.0164551391,-10.2156042731,-5.5730369694\H,1.463
1176373,-11.7000502395,-4.7928321215\H,1.0138123319,-10.1354515224,-4.
1261527358\H,-2.10554543,-11.451503248,-5.9412763883\H,-1.5332919087,-
10.9922361303,-4.34058318\H,-0.9558613242,-12.4771229558,-5.0797588259
\H,0.8597825994,-9.2835682353,-9.7215054933\H,1.3680594964,-10.4227889
989,-8.4806524672\H,1.6208396957,-8.6949953379,-8.2403751549\H,-0.9185
893591,10.0596025151,9.0783688737\H,-1.508999887,8.7845208605,8.024602
5928\H,-1.9800600129,10.4542770627,7.7242108001\H,1.4944992292,9.34736
94147,8.6270178495\H,2.1381263253,9.3859930923,6.9830918949\H,1.045804
2011,8.0946361523,7.4766880408\H,1.9669166353,11.1322343715,4.44108252
73\H,1.6980881903,12.1049617974,5.8862232368\H,1.3064720132,12.7644501
7,4.3025246304\H,-0.8011589477,12.6437403225,6.6098005844\H,-2.1037828
778,11.942829624,5.6431384252\H,-1.0904073402,13.22773487,4.9793430233
\H,-2.4248740795,-10.2111174895,-8.1569375939\H,-1.1174057494,-11.3593
14292,-8.4645836194\H,-1.5194596108,-10.1491438849,-9.6718244916\\Vers
ion=EM64L-G09RevD.01\HF=-1737.8526668\RMSD=5.062e-09\RMSF=2.307e-07\Di
pole=0.2650813,0.0538852,-0.1052733\Quadrupole=-42.8864643,40.4211182,
2.465346,3.8145154,-3.9489403,40.3377792\PG=C01 [X(C42H48N2)]\\@

^{R2N}PP6

1\1\GINC-HPC-CN43\FOpt\RBLYP\6-31G(d)\C48H52N2\TALIPOVM\20-Jun-2014\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
le\\0,1\H,-2.1466528076,0.708918524,-0.991928821\C,-1.2801669136,0.947
2711276,-0.3918463145\C,0.9472502867,1.6369827585,1.0931297384\C,-0.17
61707225,0.0884329646,-0.3989711437\C,-1.2703220601,2.123933389,0.3400
774577\C,-0.1563264748,2.4966172183,1.0997141809\C,0.9377456308,0.4605
927024,0.3607736069\H,-2.129338517,2.7779498018,0.2950928419\H,1.79699
12185,-0.1931758895,0.4054911758\H,1.8136285369,1.8753812755,1.6933148
233\C,-0.1860139506,-1.1673469065,-1.1823268637\C,-0.2048880167,-3.572
8143673,-2.6853011508\C,-1.354009547,-1.923342398,-1.3262350208\C,0.97
23726592,-1.6414047876,-1.8067255617\C,0.9630448507,-2.8164959971,-2.5
411598811\C,-1.3630825666,-3.0987433869,-2.0602238088\H,-2.2607908354,
-1.6055462601,-0.8317832594\H,1.8860681346,-1.06784721,-1.7445358331\H
,1.8696498751,-3.1341491031,-3.0359755269\H,-2.2766801223,-3.672426118
9,-2.1224291911\C,-0.1454117308,3.7539145875,1.8802202201\C,-0.1247871
09,6.169047596,3.3752932326\C,1.0225221905,4.5104646772,2.0216047572\C
,-1.3025967881,4.231693355,2.5039999809\C,-1.2916312289,5.4083491661,3
.2358282345\C,1.0316942509,5.6901806457,2.7484839499\H,1.9292764457,4.
1907364263,1.5279920528\H,-2.2169570187,3.6585419687,2.444850147\H,-2.
197488378,5.7253186985,3.7325475028\H,1.9452642214,6.2647080339,2.8036
681099\C,-0.114449198,7.4266796397,4.1508610287\C,-0.094078483,9.86649
16295,5.6562249682\C,1.0082842897,7.8346701475,4.8783056842\C,-1.22464
18731,8.2730567196,4.1956867018\C,-1.2184669195,9.4582445627,4.9129510
774\C,1.0204435816,9.0067372333,5.6127408721\H,1.884947314,7.202502917

,4.9075658486\H,-2.1083104824,8.0260254856,3.6236888229\H,-2.095397713
4,10.0824356626,4.8616073194\H,1.9000616578,9.2384979787,6.1877027944\
C,-0.2146662564,-4.8273943575,-3.4701691538\C,-0.2324724692,-7.2346793
94,-4.9781253567\C,-1.3274382304,-5.1990044517,-4.231751264\C,0.888807
8477,-5.6868738094,-3.4792086564\C,0.8788736088,-6.8624727946,-4.21268
25889\C,-1.3349285577,-6.3721646485,-4.9692860506\H,-2.1872571894,-4.5
456499764,-4.2756868191\H,1.7551254585,-5.4504080717,-2.8778245153\H,1
.7377128132,-7.5166579392,-4.1657353355\H,-2.2004152248,-6.6062577109,
-5.5725361067\C,-0.241204023,-8.4868886809,-5.7637856919\C,-0.26017574
01,-10.9127135962,-7.2927911862\C,0.9160782917,-8.9877006236,-6.363826
7097\C,-1.4091674847,-9.2337879277,-5.9469482316\C,-1.4251088317,-10.4
011488182,-6.6890347309\C,0.9161515471,-10.1637334227,-7.0964308155\H,
1.84653204,-8.4456755956,-6.266970894\H,-2.3329591641,-8.9022409681,-5
.4935138794\H,-2.3635563883,-10.9131074092,-6.8115069994\H,1.853983684
,-10.5000903388,-7.5068307445\N,-0.2843128707,-12.0741152329,-8.059196
847\C,-1.1613226613,-13.2140642419,-7.7319602558\C,-2.5594896539,-13.1
291487471,-8.3581846715\C,-1.2149816311,-13.5450127784,-6.2376384105\H
,-0.6806502244,-14.0702469614,-8.1996088065\C,0.8267131166,-12.3482650
926,-8.9809049648\C,1.9155631994,-13.2381051224,-8.370188331\H,1.26891
67564,-11.3821536459,-9.209576629\C,0.3383363357,-12.9055817813,-10.32
08941277\N,-0.0865003149,11.033702635,6.4134501261\C,1.1233907369,11.8
63439846,6.5667716999\C,2.0195568125,11.4553586722,7.7434639269\H,0.74
54846418,12.8530661787,6.8132113008\C,1.9184019159,12.0420803769,5.270
2867114\C,-1.364129291,11.6695136345,6.7632319841\C,-1.7783119375,12.7
774459764,5.7877557219\C,-1.3802649488,12.1679904163,8.2109042785\H,-2
.110975275,10.8812682294,6.7154175389\H,2.7544003596,-13.3410106161,-9
.0595954827\H,1.538377449,-14.2397449416,-8.1595410093\H,2.2907886624,
-12.818673476,-7.4373171159\H,1.1798103169,-12.9776242587,-11.01035227
71\H,-0.4090492355,-12.2479225349,-10.7628132003\H,-0.0921249078,-13.9
025506039,-10.229531084\H,-0.209351256,-13.6639094998,-5.8351670223\H,
-1.7517414583,-14.4832750629,-6.0955540309\H,-1.7233531843,-12.7809604
111,-5.6540744952\H,-3.1880375678,-12.3748946136,-7.8883073994\H,-3.06
73845112,-14.0889951931,-8.2523245639\H,-2.4923838046,-12.8960167677,-
9.419481283\H,1.4311023133,11.3295661259,8.6506882861\H,2.7624869037,1
2.2335418809,7.9250754337\H,2.5587255107,10.5273819863,7.5617198112\H,
2.3940491851,11.1220935567,4.938145697\H,2.7022355526,12.7834106559,5.
4272849347\H,1.2706959597,12.395952122,4.468617339\H,-1.8037881121,12.
4113965275,4.7619475955\H,-1.086693092,13.6201484371,5.8257498138\H,-2
.7699897981,13.1549598771,6.0398492732\H,-2.3811318814,12.5206635166,8
.4609685638\H,-0.6932492448,12.9975882468,8.3765812632\H,-1.1202002839
,11.3642487525,8.8984216848\\Version=EM64L-G09RevD.01\HF=-1968.7763166
\RMSD=3.374e-09\RMSF=6.867e-07\Dipole=0.0644253,0.0340231,-0.0547158\Q
uadrupole=-26.7398037,49.1392375,-22.3994338,-3.6240197,-1.8154076,58.
7746946\PG=C01 [X(C48H52N2)]\\@

^{R2N}PP7

1\1\GINC-HPC-CN56\FOpt\RBLYP\6-31G(d)\C54H56N2\TALIPOVM\20-Jun-2014\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
le\\0,1\C,10.0612951039,-0.050069037,-0.0807098572\C,7.2209768883,-0.0
831990627,-0.0690898261\C,9.3218507823,0.5071163116,-1.1305277736\C,9.
3436738224,-0.624198153,0.9750823527\C,7.9579871626,-0.6384459171,0.98
20442081\C,7.9362826036,0.4889306312,-1.1262079083\H,9.837225889,0.989
4846368,-1.9487250221\H,9.8767751267,-1.0940348512,1.7892127821\H,7.44
19623319,-1.1182696285,1.8014929026\H,7.4025150626,0.9568000263,-1.941
1903138\C,11.539457018,-0.0322362168,-0.0867062484\C,14.4065448866,-0.
0002293733,-0.0968925025\C,12.2793067269,0.1004177169,1.0925258153\C,1

2.2723833691,-0.1464403971,-1.2698640083\C,13.657729127,-0.1233131939,
-1.28317277\C,13.6626453834,0.1099166268,1.0937487315\H,11.7650904133,
0.2065594782,2.0376498324\H,11.7537900254,-0.2643994636,-2.2112039357\
H,14.152425945,-0.1903600074,-2.2381168311\H,14.1700391522,0.189591481
1,2.039316786\C,5.7411642034,-0.0996208228,-0.063083109\C,2.9049502573
,-0.128238512,-0.0522775512\C,5.0125696797,-0.2556730237,-1.2470598655
\C,5.0186427917,0.0411088383,1.1265122168\C,3.6329498498,0.026507283,1
.1319552703\C,3.6269023019,-0.2690505532,-1.2419471592\H,5.5358627855,
-0.3994873658,-2.1814611797\H,5.5460189701,0.1955529756,2.0569146472\H
,3.1095770731,0.1696322668,2.0664749082\H,3.0994111815,-0.4226824237,-
2.1724697669\C,1.4249048716,-0.1416048811,-0.0469612323\C,-1.410518424
,-0.1653743772,-0.036666711\C,0.6914325593,0.4229884541,-1.0956099272\
C,0.7086483454,-0.7185586229,1.0068500879\C,-0.6770841471,-0.730148360
4,1.011904008\C,-0.6942445995,0.4113540849,-1.0905833513\H,1.210064349
8,0.9059649626,-1.9112832585\H,1.2412487016,-1.1925615961,1.8187923996
\H,-1.1957656557,-1.2128928854,1.8276972181\H,-1.2268409421,0.88550214
42,-1.9024355061\C,-2.8905755076,-0.176786943,-0.0313131084\C,-5.72687
81276,-0.1952617717,-0.0218375078\C,-3.6125472258,-0.0332616069,1.1580
042675\C,-3.6185648503,-0.3305476115,-1.2156842113\C,-5.0042600488,-0.
3402417344,-1.210880397\C,-4.9982986654,-0.0416305705,1.1624609746\H,-
3.0849332956,0.1192174972,2.0886527343\H,-3.0952367265,-0.476132765,-2
.1498473728\H,-5.5317292188,-0.4934940702,-2.1414218085\H,-5.521483545
3,0.1048692761,2.0965067431\C,-7.2067724562,-0.2031602825,-0.017297562
4\C,-10.0472570605,-0.216321494,-0.0085958161\C,-7.9271216712,-0.76874
61091,1.0398676706\C,-7.9388475324,0.3555806605,-1.0700904323\C,-9.324
5149726,0.3511389452,-1.0645135204\C,-9.3128801949,-0.7770345305,1.042
864831\H,-7.3975108124,-1.2388640965,1.8562699939\H,-7.4186523901,0.83
08576182,-1.8895405721\H,-9.8535466985,0.8237557647,-1.8796800048\H,-9
.8324453074,-1.2541353341,1.8615137527\C,-11.5255219042,-0.2223059941,
-0.0040872049\C,-14.3926970744,-0.2352918633,0.0058170892\C,-12.259052
0357,-0.0985521138,1.1800438939\C,-12.2647995451,-0.3510594807,-1.1817
83287\C,-13.6503981237,-0.3498088127,-1.1853866177\C,-13.642335876,-0.
1108313505,1.1909701197\H,-11.7399286777,0.0178745143,2.1212670957\H,-
11.7509695686,-0.4632017085,-2.1264438274\H,-14.1506744143,-0.42712525
63,-2.1366419867\H,-14.1443190994,-0.0369254812,2.1399071493\N,15.7982
792223,-0.0141014263,-0.0895601969\C,16.5162734016,-0.5269006797,-1.26
45327822\C,17.7175246504,-1.3914237642,-0.8718196897\C,16.9192432109,0
.5706151147,-2.2562596066\H,15.8241742356,-1.1980532082,-1.7663292443\
C,16.5870765188,0.7935867492,0.8598574961\C,16.8736712162,0.0913320375
,2.1935656207\C,16.0514968925,2.2146071492,1.0574699432\H,17.553959665
5,0.91413342,0.3767689253\N,-15.7840117795,-0.2705462049,0.0229927665\
C,-16.578344535,0.5287385789,0.9749453352\C,-16.0621751428,1.957976346
9,1.1647455139\C,-16.8459781852,-0.1732857922,2.3126898443\H,-17.54998
84224,0.6337238397,0.4977808576\C,-16.5020931928,-0.7975806088,-1.1456
07655\C,-17.6878382562,-1.6784483776,-0.7422159141\H,-15.8034420198,-1
.4600293583,-1.6499105065\C,-16.9278298843,0.2906889806,-2.1379991858\
H,-17.2122893885,-1.1854613362,2.1499138505\H,-17.6051074483,0.3776140
797,2.8701229415\H,-15.9602735333,-0.2343050797,2.9424378541\H,-15.106
5386327,1.9957896894,1.6825798076\H,-16.7821789712,2.5257503569,1.7545
309647\H,-15.9443445677,2.4541653127,0.2017554546\H,-18.485748483,-1.1
140403695,-0.2600878051\H,-17.3679744683,-2.4685977301,-0.064197063\H,
-18.1118124341,-2.1436320525,-1.6324308893\H,-16.0755048942,0.88998371
69,-2.4563100242\H,-17.6649694107,0.9636254268,-1.6979201722\H,-17.379
4556848,-0.1574374443,-3.0238362974\H,17.4137788326,-2.1883882734,-0.1
943731283\H,18.5101753615,-0.8168638532,-0.3930254055\H,18.142426422,-
1.8474262706,-1.7663302577\H,17.6495131315,1.2528790738,-1.8190798164\
H,16.0560743783,1.1583660597,-2.5667997484\H,17.3712629084,0.131946902

8,-3.1466198743\H,15.9209344768,2.7121390025,0.0968183934\H,16.7666818
684,2.7907953487,1.6449581542\H,15.098426318,2.2369859569,1.580897271\
H,15.9932270811,0.0156190569,2.8290635027\H,17.6285515157,0.651362461,
2.747652905\H,17.2533896806,-0.9149553195,2.0250982314\\Version=EM64L-
G09RevD.01\HF=-2199.6996193\RMSD=5.359e-09\RMSF=2.042e-07\Dipole=-0.00
06153,0.2149256,-0.2231646\Quadrupole=97.2011111,-64.2933965,-32.90771
46,1.2779607,-0.4249461,-2.151984\PG=C01 [X(C54H56N2)]\\@

^{R2N}PP2+*

1\1\GINC-HPC-CN26\Stability\UBLYP\6-31G(d)\C24H36N2(1+,2)\TALIPOVM\20-
Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)
scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200
) int(grid=ultrafine)\\Title\\1,2\C,0,-0.206116825,1.1219189376,0.1958
798619\C,0,-0.1343517178,3.4701948695,1.8630199094\C,0,-0.7893182311,2
.3509534426,-0.2039214834\C,0,0.4248438978,1.1281269748,1.4654310813\C
,0,0.4657150153,2.2378920601,2.2617916851\C,0,-0.7568936572,3.46880974
19,0.5805263653\H,0,-1.3196306173,2.4153485111,-1.1404875531\H,0,0.937
3714997,0.2462484887,1.8147698076\H,0,1.0149816203,2.1703361912,3.1842
235458\H,0,-1.2585477916,4.3483690826,0.2255395294\C,0,-0.2484410639,-
0.0510134266,-0.6317204942\C,0,-0.346384914,-2.4064333983,-2.287550548
3\C,0,-0.6048112075,0.0037022028,-2.0028513288\C,0,0.0670223293,-1.340
0071052,-0.1322069834\C,0,0.0253129236,-2.4606174792,-0.9122831654\C,0
,-0.651489805,-1.1079954019,-2.7960795082\H,0,-0.8055714397,0.95525598
27,-2.4683667953\H,0,0.3110061595,-1.4678173359,0.9102137472\H,0,0.236
6594622,-3.4052420456,-0.4493380963\H,0,-0.8749591441,-0.9679843618,-3
.8389077009\N,0,-0.4072963474,-3.5161004943,-3.0625097228\C,0,0.287653
2614,-4.7876800158,-2.731716945\C,0,1.7753696073,-4.5992322359,-2.4235
412318\H,0,0.2559876572,-5.3444617,-3.6621934551\C,0,-0.4463102257,-5.
6504604545,-1.6994571149\C,0,-1.0713986392,-3.4728242002,-4.388064439\
C,0,-0.0542333396,-3.3589480674,-5.523721966\H,0,-1.6904458434,-2.5843
724919,-4.3881425702\C,0,-2.0389542207,-4.6414369331,-4.5868641816\N,0
,-0.1145531298,4.5701951244,2.6538144062\C,0,0.2793578444,4.4635540093
,4.0798127685\C,0,1.7324312436,4.888038135,4.2932651775\H,0,0.18109027
89,3.4178693399,4.3435066801\C,0,-0.6867146995,5.2069665481,5.00473027
87\C,0,-0.3265537912,5.950608266,2.1452396319\C,0,0.5705307525,6.29976
46501,0.9548436037\H,0,0.0208771392,6.5776885746,2.9593356403\C,0,-1.7
990661811,6.3170668175,1.9303363102\H,0,0.0132520486,-6.6382939246,-1.
6808620695\H,0,-1.4940341414,-5.7706197809,-1.9663369101\H,0,-0.399542
1859,-5.249248374,-0.6902604708\H,0,2.256177432,-4.0105495156,-3.20349
18901\H,0,2.2495381188,-5.579739709,-2.3987161605\H,0,1.9644806742,-4.
1178830604,-1.4680113536\H,0,-1.5373646327,-5.6032495391,-4.676696158\
H,0,-2.5896852931,-4.4748999902,-5.511786286\H,0,-2.7584145298,-4.6962
089837,-3.7716807829\H,0,0.5787099343,-4.2439497892,-5.5872538836\H,0,
0.5879860153,-2.4893649659,-5.3898405287\H,0,-0.5761108621,-3.25630330
61,-6.4745318445\H,0,0.5069959019,7.3728016259,0.777917949\H,0,0.28776
09644,5.7971905161,0.0341032525\H,0,1.6087623116,6.0537358492,1.172780
053\H,0,-1.8710699592,7.3923653768,1.7693037941\H,0,-2.3944689845,6.06
64255957,2.8055947304\H,0,-2.2447744614,5.8270144924,1.0683599413\H,0,
2.4073197391,4.3066382371,3.6662948083\H,0,2.0122067089,4.7319879582,5
.3345707749\H,0,1.8794421943,5.9435991055,4.0649632812\H,0,-1.71326217
67,4.8851259244,4.8383325608\H,0,-0.6367473323,6.2891141386,4.89796404
33\H,0,-0.4224653445,4.9702513162,6.0346184034\\Version=EM64L-G09RevD.
01\HF=-1044.9175857\S2=0.778196\S2-1=0.\S2A=0.750343\RMSD=5.763e-09\Di
pole=0.0014887,-0.0102049,-0.0084983\Quadrupole=-38.6790102,34.1148362
,4.564174,-1.7190507,7.8507035,41.509666\PG=C01 [X(C24H36N2)]\\@

^{R2N}PP3+*

1\1\GINC-HPC-CN59\Stability\UBLYP\6-31G(d)\C30H40N2(1+,2)\TALIPOVM\20-
Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)
scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200
) int(grid=ultrafine)\\Title\\1,2\H,0,-0.1181693072,0.6978347852,-2.61
75598535\C,0,-0.2583905914,0.6103428511,-1.5516868134\C,0,-0.572194550
1,0.4433367384,1.1936052657\C,0,-0.4299107356,-0.664063113,-0.96794076
93\C,0,-0.2313186609,1.7544465586,-0.7936353904\C,0,-0.390577975,1.719
1506578,0.6111082902\C,0,-0.5832297585,-0.700913326,0.4353962693\H,0,-
0.1059153882,2.697913929,-1.300307425\H,0,-0.7384282661,-1.6449702687,
0.9334145872\H,0,-0.683181641,0.3474993791,2.2618730514\C,0,-0.3660001
765,2.9223032209,1.4103952142\C,0,-0.291282871,5.3112906852,3.01229815
45\C,0,0.1449785121,4.1460888083,0.9128776647\C,0,-0.8528575357,2.9525
006862,2.7403314622\C,0,-0.8337457391,4.0858439745,3.5025730165\C,0,0.
1930665491,5.2835264415,1.6684521407\H,0,0.5323760041,4.1987615663,-0.
091632092\H,0,-1.2777120538,2.0637570949,3.1781110796\H,0,-1.213794496
2,4.0262040609,4.503755598\H,0,0.5754826852,6.1748432545,1.2042872583\
C,0,-0.4461933928,-1.8760644044,-1.7707544369\C,0,-0.4657603582,-4.271
4846828,-3.3619846886\C,0,-0.7289010037,-1.8548970347,-3.1500628483\C,
0,-0.181927184,-3.1424875789,-1.2166670306\C,0,-0.185750385,-4.2920995
938,-1.9710563085\C,0,-0.7479925921,-2.9965438772,-3.9142149727\H,0,-0
.9619491416,-0.921100692,-3.63861667\H,0,0.0522447064,-3.2337423652,-0
.1669292437\H,0,0.0043809445,-5.2223697981,-1.4642165212\H,0,-0.961241
8186,-2.8978833685,-4.9620951297\N,0,-0.4538456357,-5.4084196259,-4.12
50238256\C,0,-1.2080972047,-5.5415091755,-5.3915111376\C,0,-2.67127614
54,-5.1031941957,-5.279500483\C,0,-0.4963324111,-4.9490142751,-6.61381
52976\C,0,0.1517963937,-6.6470005811,-3.5963453027\C,0,1.0438082379,-7
.3439216929,-4.6268382529\C,0,-0.8945309945,-7.5974038698,-3.010205691
5\H,0,-3.198020136,-5.3998077171,-6.1862168556\H,0,-2.7926766137,-4.02
93259681,-5.1643309093\H,0,-3.1519152206,-5.5918175044,-4.432816114\H,
0,0.5340151224,-5.2951170814,-6.6669053552\H,0,-0.4855394682,-3.861444
5157,-6.6186672513\H,0,-1.0101549649,-5.2749577987,-7.5185189272\H,0,0
.4839075735,-7.7642108209,-5.4609872419\H,0,1.5639208906,-8.1674099493
,-4.1382573418\H,0,1.7918778321,-6.6579383411,-5.0211734241\H,0,-1.483
9625329,-7.1041480356,-2.238024447\H,0,-0.406602021,-8.465208374,-2.56
63811247\H,0,-1.5784370114,-7.9593286497,-3.7785004584\N,0,-0.24016293
83,6.4293446065,3.7721105636\C,0,-1.0606310795,6.6311978162,4.99750394
01\C,0,-0.517129873,5.9114309044,6.2364013339\C,0,-2.5568472525,6.4091
584183,4.7617913057\C,0,0.5689675923,7.6003844184,3.3471669029\C,0,1.4
63855118,8.1199139838,4.4743726865\C,0,-0.3098501997,8.6966944498,2.74
44957864\H,0,0.5444563604,6.1087416454,6.3676304141\H,0,-0.6596268638,
4.8344088299,6.2090259192\H,0,-1.0419374901,6.2896332601,7.1130658042\
H,0,-2.8271953008,5.36628853,4.6232031468\H,0,-2.8946125177,6.96851129
36,3.8907749613\H,0,-3.0987585705,6.7782359025,5.6315926041\H,0,2.0822
430698,7.322488668,4.8825342373\H,0,0.907116857,8.5837434847,5.2863259
506\H,0,2.124850776,8.8790504948,4.0584381803\H,0,-0.9926133918,9.1186
250112,3.481753974\H,0,-0.8982869346,8.3149901764,1.9112789679\H,0,0.3
206223178,9.5052261761,2.3766925203\H,0,0.8204406331,-6.3397475864,-2.
7996369622\H,0,-1.2446904668,-6.6132946036,-5.5618981476\H,0,-0.955268
5325,7.6913047308,5.1985715089\H,0,1.2467792182,7.2418129723,2.5837949
845\\Version=EM64L-G09RevD.01\HF=-1275.8324067\S2=0.784018\S2-1=0.\S2A
=0.750755\RMSD=6.525e-09\Dipole=0.1480171,2.9385062,1.9824362\Quadrupo
le=-67.0092717,70.0831545,-3.0738828,1.4174101,-1.5250548,74.2134649\P
G=C01 [X(C30H40N2)]\\@

^{R2N}PP4+*

1\1\GINC-HPC-CN41\Stability\UBLYP\6-31G(d)\C36H44N2(1+,2)\TALIPOVM\20-
Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)

scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200
) int(grid=ultrafine)\\Title\\1,2\H,0,1.5409931043,-1.3050282083,-2.87
1115614\C,0,0.774280302,-1.1600398736,-2.1259835834\C,0,-1.1394091271,
-0.7486794144,-0.1661673361\C,0,-0.198566592,-2.1544555869,-1.90884189
33\C,0,0.7915178632,-0.0006706606,-1.3796647454\C,0,-0.1668710794,0.24
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228,-0.7087189174\H,0,-1.8825735487,-0.6090515842,0.604028028\C,0,-0.1
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200526871\C,0,-1.3411179888,2.0503172994,0.8890705205\C,0,1.0439776901
,2.1486336614,0.6980059039\C,0,1.0538573123,3.318638368,1.4364897676\C
,0,-1.32926641,3.2211119072,1.6260617296\H,0,-2.2892831963,1.580804948
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2538\C,0,-0.1208150841,5.1364235236,2.7054136052\C,0,-0.0954729933,7.5
671207843,4.2284952693\C,0,-1.1751674196,6.0520453579,2.6494714892\C,0
,0.9463137288,5.4687939464,3.5473650123\C,0,0.9654650243,6.6404763535,
4.2802812403\C,0,-1.1726304028,7.223883619,3.3861981127\H,0,-2.0218898
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12\H,0,1.8280603366,6.8431733126,4.8900505972\H,0,-2.0335910328,7.8668
040902,3.3086909032\C,0,-0.2185739401,-3.3772319279,-2.6945576763\C,0,
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88,-3.9696624654\C,0,-0.856766288,-4.5529228039,-2.2298036176\C,0,-0.8
846747943,-5.7038607662,-2.963624037\C,0,0.3841914995,-4.5969321738,-4
.7154883559\H,0,0.8442047211,-2.5734154262,-4.3992498279\H,0,-1.303685
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,-6.9238716393,-4.971129532\C,0,-1.2253552183,-8.0460551508,-4.7404453
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\C,0,0.6256713347,-7.0818801007,-6.1537088154\H,0,1.37688194,-6.308443
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0.1177854513,9.7284903003,6.7278087195\C,0,2.0860949246,9.195105665,6.
1981285686\H,0,0.6717607199,7.9219923879,8.1973438928\H,0,0.7556683758
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659,5.5311693557\H,0,2.6896959666,8.3581760426,5.8521599457\H,0,0.6058
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\H,0,-2.957186663,10.6121902006,5.0352798793\H,0,0.199225137,-9.228695
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045686774,-8.4948255943,-2.5897347337\H,0,-2.8974515555,-6.971615947,-
5.6088799195\H,0,-2.959832018,-7.0224290577,-3.8466402667\H,0,-3.31768
37809,-8.4681440096,-4.777737689\H,0,0.5402238921,-6.9331156816,-8.293
1397371\H,0,-0.6424248977,-5.9092530035,-7.4739800424\H,0,-0.907896373
1,-7.6517575515,-7.5992041597\H,0,1.9355082562,-8.5184508483,-5.179456
5863\H,0,2.1187819263,-8.3902234785,-6.9258779455\H,0,0.7572936173,-9.
2767945928,-6.2638303479\\Version=EM64L-G09RevD.01\HF=-1506.7532259\S2
=0.801872\S2-1=0.\S2A=0.752132\RMSD=3.039e-09\Dipole=-0.2191449,-9.755
9237,-6.3592018\Quadrupole=-80.2040059,83.422723,-3.2187171,6.2178502,
-2.0286187,119.1577349\PG=C01 [X(C36H44N2)]\\@

^{R2N}PP5+*

1\1\GINC-HPC-CN15\Stability\UBLYP\6-31G(d)\C42H48N2(1+,2)\TALIPOVM\20-Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title\\1,2\H,0,0.1040196128,0.4072954569,-2.8784957428\C,0,-0.0638697847,0.3559019138,-1.8126996353\C,0,-0.4436457682,0.2721126394,0.9261154581\C,0,-0.2656077628,-0.8851402672,-1.1973241231\C,0,-0.0494360931,1.5267984789,-1.0742373828\C,0,-0.2386565842,1.5134591624,0.3125890093\C,0,-0.4553910636,-0.8999975218,0.1895639072\H,0,0.0960616887,2.4672040075,-1.5852654912\H,0,-0.632306044,-1.8362478897,0.6984647495\H,0,-0.5787060375,0.2200066542,1.9965248976\C,0,-0.2747502239,-2.1337402727,-1.9820310526\C,0,-0.2858450741,-4.5362890337,-3.4918724115\C,0,-0.7556475931,-2.1619202382,-3.2996676609\C,0,0.1996059151,-3.3365550538,-1.4376720974\C,0,0.2011816322,-4.5044974053,-2.1722322284\C,0,-0.7681074473,-3.3304827171,-4.033379757\H,0,-1.1429877366,-1.2594442334,-3.7478849833\H,0,0.5916225646,-3.3511720641,-0.4319997737\H,0,0.5615658522,-5.4076314245,-1.7046462152\H,0,-1.1322476551,-3.2984036852,-5.0485423484\C,0,-0.220352156,2.7646208797,1.1008260427\C,0,-0.1808959144,5.1662114843,2.6166973933\C,0,-1.04329329,2.9302844562,2.2198616594\C,0,0.6220485229,3.826925314,0.7560690166\C,0,0.6387524741,4.9992285293,1.4938705625\C,0,-1.0217300509,4.1007440886,2.9605241132\H,0,-1.7203904363,2.1393584359,2.5092139108\H,0,1.2845794555,3.7321546804,-0.0923770715\H,0,1.2895771195,5.8038468016,1.1834243504\H,0,-1.6586280905,4.1820535121,3.8294872148\C,0,-0.1586664586,6.4143960635,3.406300193\C,0,-0.1168229758,8.8392308232,4.9356451693\C,0,-1.3044585843,6.9061281265,4.0404485227\C,0,1.0079646951,7.1672655394,3.5608750471\C,0,1.037645572,8.3343699408,4.3059744048\C,0,-1.2915023146,8.0793856439,4.7724592452\H,0,-2.2443710726,6.3838758156,3.9278748235\H,0,1.932809103,6.8169665842,3.1240276071\H,0,1.9848884445,8.8354246745,4.4193597128\H,0,-2.2182722101,8.4260282893,5.1952637665\C,0,-0.2892185293,-5.7693868285,-4.2659810097\C,0,-0.3031900595,-8.2016931829,-5.7797297058\C,0,-1.1724749727,-5.9630089264,-5.3548086659\C,0,0.5944820383,-6.8346828409,-3.9706918999\C,0,0.6053600328,-7.9915484157,-4.6961055952\C,0,-1.1960275073,-7.1223982095,-6.0766689244\H,0,-1.8712643465,-5.1867487765,-5.6216742572\H,0,1.3054111323,-6.7339347199,-3.1665963153\H,0,1.297237792,-8.7604961692,-4.4145765922\H,0,-1.880264839,-7.1840464695,-6.9034737308\N,0,-0.3128646711,-9.3509378066,-6.4859051228\C,0,0.8076348962,-10.3402039786,-6.4765366517\C,0,2.1593727641,-9.7098842617,-6.8199697973\H,0,0.5691187472,-10.9907201421,-7.309504873\C,0,0.8280519132,-11.2312926812,-5.2304865574\C,0,-1.4276547792,-9.6669485471,-7.4236743871\C,0,-1.9911680709,-11.0685375161,-7.182656984\C,0,-1.0013781746,-9.4383777272,-8.8735411239\H,0,-2.2307002726,-8.9843829564,-7.1838870026\N,0,-0.1111587426,10.0295246356,5.6540391666\C,0,0.9897417847,10.9825547836,5.4554731786\H,0,1.3956209771,10.7664866267,4.4706029603\C,0,2.1188957371,10.8270620661,6.4806757427\C,0,0.492506605,12.4293098998,5.3903009238\C,0,-0.9426968487,10.2275087548,6.8562829027\C,0,-2.352155959,10.7595119098,6.5655085708\H,0,-0.4377198241,11.0163058606,7.4090868209\C,0,-0.9637757451,9.0197614036,7.7973194967\H,0,2.0811401724,-9.0935094158,-7.7138043267\H,0,2.8613824896,-10.516159863,-7.0269174282\H,0,2.5783583777,-9.1051088835,-6.0212811235\H,0,-0.1509734574,-11.6651399574,-5.0418592077\H,0,1.1484905689,-10.7130645083,-4.3310726357\H,0,1.5290413848,-12.0452185215,-5.4094901366\H,0,-1.8603388016,-9.5987211298,-9.5231546173\H,0,-0.2187797484,-10.1300659299,-9.1821313519\H,0,-0.6426972547,-8.4213363821,-9.0237406218\H,0,-2.8192358777,11.0853297717,7.4961504186\H,0,-3.0034195144,10.0094040272,6.1204981275\H,0,-2.3108784321,11.6121147087,5.889924923\H,0,-1.4654364992,9.294806023

2,8.7253507963\H,0,0.0508056351,8.7042907871,8.0392457254\H,0,-1.49085
70731,8.1668090566,7.3758041784\H,0,2.5005181773,9.8067306624,6.496549
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966554215,6.2401573991\H,0,0.0963596304,12.7802223118,6.3429690515\H,0
,-0.2846076187,12.5366749712,4.6347120425\H,0,1.3216580278,13.08462969
25,5.1226989412\H,0,-2.2865285538,-11.2003789691,-6.1435907581\H,0,-1.
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25,-7.8006966528\\Version=EM64L-G09RevD.01\HF=-1737.67627\S2=0.804125\
S2-1=0.\S2A=0.752326\RMSD=1.806e-09\Dipole=-0.0341896,-13.704053,-8.68
70298\Quadrupole=-141.8522723,144.4161262,-2.5638538,9.4565074,8.67348
52,197.311166\PG=C01 [X(C42H48N2)]\\@

^{R2N}PP6+*

1\1\GINC-HPC-CN20\Stability\UBLYP\6-31G(d)\C48H52N2(1+,2)\TALIPOVM\23-
Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)
scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200
) int(grid=ultrafine)\\Title\\1,2\H,0,-0.8690317823,1.4043070346,-2.14
31858336\C,0,-0.5796245181,1.382277928,-1.1026909999\C,0,0.187458354,1
.373220399,1.5557558887\C,0,-0.2020819625,0.1702758215,-0.5139757523\C
,0,-0.5705059084,2.5639273599,-0.3809347416\C,0,-0.1887165202,2.585319
4907,0.9654889257\C,0,0.1834995067,0.1935502149,0.831006293\H,0,-0.883
1822172,3.4770001872,-0.8661434995\H,0,0.4679960748,-0.7255594981,1.32
20774404\H,0,0.5050766154,1.3530886008,2.5880359867\C,0,-0.2113482705,
-1.0921540476,-1.2852213829\C,0,-0.2330080387,-3.5147071306,-2.7570220
156\C,0,-1.1916446356,-1.3440603588,-2.2504915807\C,0,0.7587280464,-2.
0770064619,-1.0728027606\C,0,0.7479917654,-3.2608473732,-1.792466938\C
,0,-1.2021489213,-2.5284660532,-2.9695342463\H,0,-1.9660056937,-0.6124
851153,-2.4315504346\H,0,1.5411131039,-1.910644144,-0.3463726535\H,0,1
.5044489537,-4.0054013943,-1.5905456602\H,0,-1.966670363,-2.6825682131
,-3.7172914607\C,0,-0.184488629,3.8423618106,1.7375245955\C,0,-0.17888
63012,6.2579706135,3.2232347059\C,0,-0.5031214078,3.8553485274,3.10345
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15766018,1.8551970201\C,0,-0.5079422743,5.0305860627,3.8265989127\H,0,
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0.0862677318\H,0,0.3889660646,7.161111056,1.3445672243\H,0,-0.74560684
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04777229,9.785900744,4.2904408426\C,0,-0.9379119132,8.8015109518,5.894
6629482\H,0,-1.5737590461,6.8387551608,5.5004972793\H,0,1.2312943995,8
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204,-3.5227263222\C,0,-0.2664990806,-7.2160978494,-4.9841774934\C,0,-1
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,-3.9133765464\C,0,0.9341317172,-6.5928917719,-4.6244728654\C,0,-1.456
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887311\C,0,-0.2765363268,-8.4853021265,-5.7421289902\C,0,-0.2946022084
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0888,12.3392381594,5.6227241467\C,0,1.7734220745,12.6324002496,6.22179
6823\C,0,-0.5698094018,13.5166767946,5.7535381542\H,0,0.5080204281,12.
1674363232,4.5611669918\H,0,2.3912587433,-12.81034317,-9.934824787\H,0
,1.7712272735,-13.8837811955,-8.6860804055\H,0,2.4026321359,-12.298421
8229,-8.2444776166\H,0,0.2105852793,-12.8938417803,-11.223444088\H,0,-
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90748,-10.0670249117\H,0,0.8345828578,-13.5352039579,-5.8956612491\H,0
,-0.492157182,-14.6673619656,-5.619656447\H,0,-0.6802525643,-12.970978
8987,-5.194355918\H,0,-2.8657451025,-13.0215604373,-6.7776566962\H,0,-
2.5086898961,-14.6901585118,-7.1932760275\H,0,-2.6362899578,-13.471992
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.3996867985,11.5392254383,8.7702088023\H,0,-2.6406441749,10.257761797,
7.596029419\H,0,-0.2778006832,9.16168247,8.3979240063\H,0,-0.164353465
5,10.4719472586,9.561850816\H,0,1.1334101414,10.2203966724,8.396457954
2\H,0,2.4522814719,11.7924361562,6.0834014647\H,0,1.7148801119,12.8582
752509,7.2855915714\H,0,2.1975052017,13.5015887064,5.7215705147\H,0,-0
.1495304101,14.352597486,5.1967380869\H,0,-0.7100442013,13.8471097668,
6.7805337522\H,0,-1.5397673727,13.2795983095,5.3208568442\\Version=EM6
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.121e-09\Dipole=0.2809418,17.4566745,10.576942\Quadrupole=-181.3992977
,228.1469058,-46.747608,-4.0044586,-9.3346615,226.999896\PG=C01 [X(C48
H52N2)]\\@

^{R2N}PP7+*

1\1\GINC-HPC-CN89\Stability\UBLYP\6-31G(d)\C54H56N2(1+,2)\TALIPOVM\21-
Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)
scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200
) int(grid=ultrafine)\\Title\\1,2\C,0,10.0573609428,0.051890844,-0.118
953085\C,0,7.2199800684,0.0649805381,-0.1156956835\C,0,9.3253062198,0.
0767306846,-1.320107074\C,0,9.3278042339,0.0363503683,1.0838879287\C,0
,7.9478872146,0.036724297,1.082996341\C,0,7.9454253506,0.0892541712,-1
.3160018172\H,0,9.8385488313,0.1119012327,-2.2684885901\H,0,9.84300978
14,-0.0039704382,2.0310189751\H,0,7.424776609,0.0339768563,2.027165362
7\H,0,7.4201886584,0.096774041,-2.2589653653\C,0,11.513571668,0.038137
6123,-0.1190551706\C,0,14.3783463139,-0.01794456,-0.107001753\C,0,12.2
619431735,0.4884410532,0.9944551705\C,0,12.2533719346,-0.4250273782,-1
.2331085104\C,0,13.618626187,-0.4660638425,-1.2350891544\C,0,13.627446
0453,0.4792191473,1.0036961893\H,0,11.7516783158,0.8770312081,1.860907
1039\H,0,11.7353658758,-0.7820868264,-2.1084371617\H,0,14.1079255961,-
0.809781733,-2.1282885374\H,0,14.1304390182,0.8286534899,1.8834907612\
C,0,5.7446768185,0.066097922,-0.1140768725\C,0,2.9117001216,0.06094678
47,-0.1133529147\C,0,5.0192121603,0.735482272,-1.1065917622\C,0,5.0220
824661,-0.6048392327,0.8794915534\C,0,3.6376203919,-0.6085738544,0.878
0037242\C,0,3.6346282461,0.7342881873,-1.1043280077\H,0,5.5406181928,1
.2794619015,-1.8805321726\H,0,5.5457713717,-1.1473428955,1.6528920578\
H,0,3.1132875961,-1.1263962027,1.6677252471\H,0,3.1079984231,1.2501100
878,-1.8938564955\C,0,1.4322768429,0.0553837183,-0.1140748945\C,0,-1.4
018920278,0.0425165711,-0.1157205019\C,0,0.7035144745,1.1742025829,-0.
5304588157\C,0,0.7131316034,-1.0699712772,0.3014775107\C,0,-0.67230839
86,-1.0759880482,0.3006330992\C,0,-0.6820589129,1.1676614865,-0.531135

8227\H,0,1.2245982178,2.0674205808,-0.8436951977\H,0,1.2418754264,-1.9
584945858,0.615161385\H,0,-1.1939894059,-1.9580077294,0.6429690516\H,0
,-1.2113833786,2.0449450209,-0.8739453492\C,0,-2.8820761594,0.03500516
35,-0.1162083955\C,0,-5.7180321792,0.0183788491,-0.1136319809\C,0,-3.6
003564582,-1.1213280041,-0.4371762545\C,0,-3.6132178802,1.183117396,0.
2052027113\C,0,-4.9989725345,1.1750889522,0.205485253\C,0,-4.986004030
7,-1.1295773032,-0.4348752423\H,0,-3.0701472483,-2.0235643491,-0.70633
1918\H,0,-3.0931097831,2.0915041949,0.4734605117\H,0,-5.5295023597,2.0
856866669,0.4439239167\H,0,-5.5062199589,-2.0464225474,-0.6720568019\C
,0,-7.1981274006,0.0083435527,-0.110323249\C,0,-10.0386116822,-0.01595
19719,-0.1002586027\C,0,-7.9211352866,-0.7451254068,-1.0408044317\C,0,
-7.9272801113,0.7504946198,0.8244324445\C,0,-9.3129763342,0.7411026301
,0.82701455\C,0,-9.3067400533,-0.7593252511,-1.033694785\H,0,-7.394159
0368,-1.319607219,-1.7893270894\H,0,-7.404922617,1.333898582,1.5692900
888\H,0,-9.8398138485,1.3429149736,1.5536146156\H,0,-9.8281735222,-1.3
700932144,-1.756717646\C,0,-11.5162146695,-0.0315742243,-0.0929992671\
C,0,-14.383318097,-0.0628837132,-0.079319068\C,0,-12.2579222623,-0.151
2739666,-1.2727419704\C,0,-12.2478347779,0.0701505099,1.0924942542\C,0
,-13.6328454394,0.0457183608,1.1075461669\C,0,-13.6410802253,-0.158551
7938,-1.2723963394\H,0,-11.7458602259,-0.1993820423,-2.22375673\H,0,-1
1.7275679298,0.1291874634,2.0384476423\H,0,-14.1264129478,0.0807349749
,2.0648310097\H,0,-14.1502925615,-0.2064139935,-2.2191669979\N,0,15.72
64219016,-0.0573980281,-0.0927793493\C,0,16.4852627288,-0.810822423,-1
.131388215\C,0,17.5115685198,-1.7579795378,-0.5071066971\C,0,17.100651
8717,0.1429875033,-2.1545794421\H,0,15.7691481398,-1.4455281426,-1.633
2578746\C,0,16.570447393,0.7058805907,0.8764812701\C,0,16.6259671403,0
.075659778,2.2717633026\C,0,16.264333924,2.2052048484,0.8754079091\H,0
,17.567364298,0.6102145964,0.4639104115\N,0,-15.7742532834,-0.04931656
49,-0.0838881808\C,0,-16.5653806749,-0.8443261288,-1.0420084579\C,0,-1
6.0288238575,-2.2618546224,-1.2601041666\C,0,-16.8553069366,-0.1249134
277,-2.3658249371\H,0,-17.5309652733,-0.9718452857,-0.5580512688\C,0,-
16.4903398914,0.4543851949,1.0962477859\C,0,-17.6883003122,1.327406417
2,0.7124958639\H,0,-15.7951129637,1.117117472,1.6049897795\C,0,-16.897
8027955,-0.6518930623,2.0763152778\H,0,-17.233066719,0.8797261308,-2.1
838986316\H,0,-17.612746192,-0.6770531308,-2.9242997709\H,0,-15.976741
589,-0.0428606663,-3.0031687096\H,0,-15.0769415317,-2.2754606572,-1.78
60837275\H,0,-16.7446622732,-2.8307666386,-1.8538208476\H,0,-15.895316
9084,-2.7723086911,-0.306667892\H,0,-18.4825008302,0.7606122467,0.2270
671914\H,0,-17.3816296988,2.1307179772,0.0439145138\H,0,-18.1121631082
,1.7749635102,1.6117404243\H,0,-16.0371570455,-1.2464347527,2.38086537
25\H,0,-17.6308025768,-1.326591392,1.6320794309\H,0,-17.348178183,-0.2
206100594,2.9710828743\H,0,17.0453884444,-2.4188599225,0.2210404903\H,
0,18.344309846,-1.2408268998,-0.035299314\H,0,17.9207616709,-2.3740910
124,-1.306122153\H,0,17.8585971709,0.785335336,-1.7083993728\H,0,16.34
01497779,0.7723094786,-2.6139941482\H,0,17.5808823388,-0.4418913975,-2
.937393717\H,0,16.2543784987,2.5960612894,-0.1406205321\H,0,17.0587831
721,2.7099370011,1.4229627453\H,0,15.3221457466,2.4603547031,1.3512028
176\H,0,15.7138620953,0.2095020332,2.8462884044\H,0,17.4351287022,0.55
13885681,2.8238938691\H,0,16.8386446171,-0.9892081763,2.2134705243\\Ve
rsion=EM64L-G09RevD.01\HF=-2199.5230907\S2=0.804923\S2-1=0.\S2A=0.7524
01\RMSD=4.584e-09\Dipole=24.4770922,-0.0828614,0.0605815\Quadrupole=53
7.8059269,-275.5777054,-262.2282215,3.1612919,-9.3135515,5.4829127\PG=
C01 [X(C54H56N2)]\\@

$^{tBu/R2N}$PP2

1\1\GINC-HPC-CN127\FOpt\RBLYP\6-31G(d)\C22H31N1\4688WANGD\23-Feb-2016\
0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=D

ichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\t
BuPP2-N\\0,1\C,-1.9521338326,-1.5898705853,4.4913374429\C,-2.698590156
2,-1.5014455519,3.2177908567\C,-4.0942285832,-1.5296760071,3.179257712
3\C,-4.8005218597,-1.4404523379,1.9903447989\H,-5.8767340728,-1.422626
7885,2.0438420214\C,-4.14604534,-1.3354676797,0.7482747071\N,-4.840678
8121,-1.2859873564,-0.4576148976\C,-6.2413497517,-1.7272389477,-0.4955
913223\C,-4.3767267789,-0.4745084723,-1.5982789483\C,-2.7390530334,-1.
3123603053,0.7916873652\H,-2.1742758799,-1.2704586446,-0.1234761403\C,
-2.0455005422,-1.3848768163,1.9868369934\H,-0.9647589633,-1.3905330951
,1.9529060081\C,-0.7448649296,-0.9063612787,4.6799814948\C,-0.04777285
05,-0.9925681425,5.8740141514\H,-0.3563913442,-0.2801640787,3.88906388
1\C,-0.5148713946,-1.7576641631,6.9490873091\H,0.8764803848,-0.4399063
493,5.9686875721\C,-2.4189734842,-2.3571389719,5.5601263674\C,-1.71919
43603,-2.4353148077,6.7588472845\H,-2.1283850222,-3.0487046399,7.54643
97921\C,0.2860247585,-1.8208703105,8.2545486607\H,-3.3337242894,-2.922
9388977,5.4517293188\H,-4.6525987826,-1.5834777898,4.1036522455\C,0.42
13209021,-0.4040003267,8.8432346228\C,1.6893616077,-2.3882486089,7.970
3539381\C,-0.3853897366,-2.7126176284,9.3064397733\C,-3.4105474379,-1.
2075726469,-2.5382729409\C,-3.8553678443,0.9093300669,-1.2007653805\H,
-5.2741643405,-0.288676437,-2.1840932386\C,-7.245438677,-0.5808735642,
-0.32595551\H,-6.3610454852,-2.4073137352,0.3439125315\C,-6.5489020103
,-2.5548084867,-1.7466660159\H,-8.2627587722,-0.9706807562,-0.27413523
6\H,-7.2023180228,0.1134943623,-1.1661571033\H,-7.0503647516,-0.016103
8671,0.585018698\H,-6.5006334369,-1.9649329182,-2.6618160295\H,-7.5587
626889,-2.9593223941,-1.6742368106\H,-5.8534022535,-3.3880369163,-1.83
81998764\H,-2.9220818649,0.8628497442,-0.6441275977\H,-4.5881405586,1.
4341277857,-0.5883166894\H,-3.6771960534,1.4997856221,-2.0998077683\H,
-2.4220290632,-1.3448499203,-2.1037027479\H,-3.285562017,-0.6321932845
,-3.4569167297\H,-3.8002989877,-2.1890011108,-2.8029143648\H,2.2729784
149,-2.4331265686,8.8914214962\H,1.6255085056,-3.3970158849,7.56068453
91\H,2.2385461348,-1.772330693,7.2589152438\H,0.9320899529,0.271986492
,8.1582061232\H,-0.558653729,0.0206341119,9.0642424748\H,0.9948859476,
-0.4330901876,9.771228563\H,-0.4849888706,-3.7420955337,8.9611752076\H
,-1.3763119533,-2.3459817767,9.5758753935\H,0.2192360098,-2.7259529212
,10.2135907594\\Version=EM64L-G09RevD.01\HF=-911.2031083\RMSD=4.765e-0
9\RMSF=2.861e-07\Dipole=-0.5284195,0.1641686,-0.7065807\Quadrupole=9.1
224122,-9.076113,-0.0462992,2.7220847,7.2951254,-0.8397574\PG=C01 [X(C
22H31N1)]\\@

$^{tBu/R2N}$PP3

1\1\GINC-HPC-CN122\FOpt\RBLYP\6-31G(d)\C28H35N1\4688WANGD\23-Feb-2016\
0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=D
ichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\T
itle\\0,1\C,-2.0275207891,-1.3874259402,5.0274998681\C,-2.6769011883,-
1.3665553666,3.7002074315\C,-4.019524608,-1.7126799106,3.5320043266\C,
-4.6367440214,-1.6873071056,2.2919101537\H,-5.687655471,-1.9216915789,
2.2477700271\C,-3.9355500883,-1.3289380628,1.124394635\N,-4.5310769826
,-1.3376184089,-0.1332787094\C,-5.7844817495,-2.0792897588,-0.32762794
16\C,-4.1824269145,-0.3535253822,-1.175091567\C,-2.5807181981,-0.98642
21079,1.2983892482\H,-1.9753361856,-0.7381855403,0.4439914335\C,-1.980
4656904,-0.9982314531,2.5446660718\H,-0.9295630953,-0.7523519515,2.609
726464\C,-1.0309035571,-0.4646172069,5.3658090923\C,-0.4210449454,-0.4
849403499,6.6101765802\H,-0.7497263422,0.3006560692,4.6564295297\C,-0.
7809226896,-1.42597123,7.5803171352\H,0.3233272254,0.2634657782,6.8425
130971\C,-2.3841667404,-2.3304891297,5.9984655101\C,-1.7778561666,-2.3
477452146,7.2445407519\H,-2.0607165673,-3.1105662155,7.956053727\C,-0.
1320730935,-1.4455671705,8.9109790191\H,-3.1251307154,-3.0818165944,5.

765280465\H,-4.6166732585,-1.9717943555,4.3953686605\C,-0.8463786709,-
1.7714654704,10.0643746156\C,-3.0049040318,-0.772521452,-2.0650843754\
C,-4.0282119008,1.0760225927,-0.648302721\H,-5.0515432316,-0.328868483
2,-1.8284957133\C,-7.0360611083,-1.2066391931,-0.1768399162\H,-5.80522
42213,-2.8366777556,0.4517185105\C,-5.7984513212,-2.8475277868,-1.6521
389319\H,-7.9365677972,-1.8183993225,-0.2428121215\H,-7.0927290743,-0.
4529241496,-0.9633604721\H,-7.0444613419,-0.6904090162,0.7824962199\H,
-5.8214204848,-2.187932509,-2.5193989653\H,-6.6895510411,-3.4740550531
,-1.6974034543\H,-4.924076639,-3.4918863862,-1.7338252943\H,-3.1548846
38,1.1982265309,-0.0116509592\H,-4.9073516852,1.3708895148,-0.07592354
94\H,-3.9242566124,1.761057259,-1.4900480401\H,-2.0471331972,-0.719674
6434,-1.5506629344\H,-2.9466853394,-0.111180296,-2.9309557711\H,-3.137
0122352,-1.7915740951,-2.4245653589\C,1.224286907,-1.1374953403,9.0641
062343\C,1.8277204999,-1.1561022414,10.3108144231\C,-0.2356989528,-1.7
903117042,11.3130776575\C,1.1158569193,-1.483241532,11.4708856525\H,1.
8208157888,-0.9020394039,8.1939886676\H,-1.9021077677,-1.9930103815,9.
9949121615\H,-0.839956683,-2.0426051275,12.1702916273\C,1.8241199249,-
1.4938398758,12.8302448393\H,2.8800646762,-0.9179409954,10.3744620221\
C,0.8765392034,-1.8659559005,13.9774472181\C,2.401958038,-0.0958364686
,13.119751868\C,2.9709276056,-2.5216934474,12.8026373573\H,0.053019064
9,-1.157201533,14.0692202993\H,1.4244335824,-1.8588424969,14.919945779
\H,0.45552198,-2.8634514968,13.8484427075\H,1.6100954011,0.6533660496,
13.1532468568\H,3.121058706,0.2106820549,12.3608141524\H,2.9135739656,
-0.091101642,14.0836016815\H,2.5897633837,-3.5249539642,12.6086262639\
H,3.488364168,-2.5359205304,13.7632971846\H,3.7057599929,-2.2880961207
,12.032899569\\Version=EM64L-G09RevD.01\HF=-1142.1269228\RMSD=4.221e-0
9\RMSF=2.720e-07\Dipole=-0.5214806,0.0909595,-0.8010432\Quadrupole=8.0
874612,-10.3390271,2.251566,6.2267321,9.675474,-1.172347\PG=C01 [X(C28
H35N1)]\\@

$^{tBu/R2N}$PP4

1\1\GINC-HPC-CN120\FOpt\RBLYP\6-31G(d)\C34H39N1\4688WANGD\23-Feb-2016\
0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=D
ichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\T
itle\\0,1\C,-2.1910503479,-1.3432272064,5.0393745064\C,-2.7890556168,-
1.3699267389,3.68612989\C,-3.6576368277,-2.3938134087,3.2903702345\C,-
4.2066239801,-2.4258128886,2.0209279397\H,-4.8453167111,-3.2529978169,
1.7477980192\C,-3.939180338,-1.4217988781,1.0760605252\N,-4.5217219481
,-1.4981625723,-0.2036621648\C,-5.9942495946,-1.57510781,-0.2367899571
\C,-3.7789723519,-1.1142543833,-1.4108912606\C,-3.078936962,-0.3922523
259,1.4787574044\H,-2.8465328598,0.4116680523,0.8006377333\C,-2.510003
1172,-0.3776601983,2.7448048866\H,-1.8309090529,0.4243818788,2.9980292
624\C,-1.9594671122,-0.1361715514,5.708146302\C,-1.3962730094,-0.11070
31027,6.974074505\H,-2.2514204034,0.7953625934,5.244715179\C,-1.040133
3403,-1.2916124998,7.6336076409\H,-1.2610858356,0.839951808,7.46997025
06\C,-1.8340620068,-2.5239111953,5.6999438046\C,-1.2733229009,-2.49892
68135,6.9670322272\H,-0.9825393734,-3.4305086785,7.4312719586\C,-0.438
3918211,-1.2644470626,8.9856069669\H,-1.9680101996,-3.4747198739,5.204
1692914\H,-3.9106105046,-3.1802949053,3.9874414661\C,-0.7276228835,-2.
2560724156,9.9287506615\C,-2.3508956612,-1.6644732762,-1.3905541855\C,
-3.7918608413,0.3738621753,-1.799591674\H,-4.2802008316,-1.6385006717,
-2.2224066552\C,-6.6877264567,-0.2443317339,0.0870413904\H,-6.27051519
38,-2.2665294698,0.5572946608\C,-6.5363609511,-2.1772928404,-1.5309147
694\H,-7.757278126,-0.4042095814,0.2335189728\H,-6.5678949181,0.483415
2762,-0.7145242505\H,-6.2839627097,0.1877179011,1.0025008821\H,-6.4291
888673,-1.504809528,-2.3821169264\H,-7.6008571772,-2.3770267741,-1.409
5721665\H,-6.0401856791,-3.1182854555,-1.7678198568\H,-3.2557882477,0.

9999950313,-1.0881678917\H,-4.8063044352,0.757201708,-1.8855135247\H,-
3.3101436019,0.4967170917,-2.7711593745\H,-1.7165854241,-1.1578318687,
-0.6657894704\H,-1.8999070442,-1.5335760196,-2.3741749215\H,-2.3540083
91,-2.7279140211,-1.1538569239\C,0.4411497727,-0.2460485408,9.36730578
59\C,1.0054927477,-0.2207616107,10.6328488822\C,-0.1633890586,-2.23046
0407,11.1943208143\C,0.7167257177,-1.212567001,11.5757622834\H,0.71280
82109,0.5199733953,8.6551628062\H,-1.4274085686,-3.0413651998,9.681049
8391\H,-0.4346371862,-2.996380082,11.906725786\H,1.7049774361,0.564713
3564,10.8808283111\C,1.3211395818,-1.1864744776,12.9272129498\C,1.6855
974179,-2.3624243687,13.5834434829\C,1.5509570388,0.0196695095,13.5980
932632\C,2.2534269224,-2.336494106,14.852008133\H,1.5471430783,-3.3148
896643,13.091428839\C,2.4854918411,-1.1367393705,15.5248480983\H,2.522
35441,-3.2765303934,15.3075222843\C,2.1178551687,0.0400002668,14.86174
23408\H,2.2675308396,0.9971203921,15.3409516086\C,3.1100938394,-1.0681
715847,16.9229734086\H,1.262045379,0.952918368,13.1355676717\C,3.44723
79343,-2.4574206568,17.4786528022\C,4.4112735586,-0.2462131417,16.8640
888898\C,2.1240931024,-0.3899659655,17.8926273312\H,5.1336682429,-0.70
86533771,16.1904818092\H,4.8637734144,-0.1844701998,17.8551278534\H,4.
2328314439,0.7708717946,16.5166469619\H,1.1944621851,-0.9560650688,17.
9616492598\H,1.8767211412,0.6229079143,17.5765546762\H,2.5587907925,-0
.3297201447,18.891708989\H,4.167865676,-2.9816348777,16.8503047324\H,2
.5590353095,-3.0826432399,17.5740091036\H,3.8872162668,-2.3562814684,1
8.4709704147\\Version=EM64L-G09RevD.01\HF=-1373.0456916\RMSD=4.546e-09
\RMSF=8.591e-07\Dipole=-0.2655622,0.0615177,-0.4245817\Quadrupole=-6.1
51785,-2.3725361,8.5243211,4.9165253,14.0552233,-0.2081828\PG=C01 [X(C
34H39N1)]\\@

$^{tBu/R2N}$PP2+*

1\1\GINC-HPC-CN61\Stability\UBLYP\6-31G(d)\C22H31N1(1+,2)\4688WANGD\23
-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo
) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=20
0) int(grid=ultrafine)\\Title\\1,2\C,0,-1.9764870512,-1.5457312933,4.4
975525417\C,0,-2.7223588637,-1.4354517164,3.2506968799\C,0,-4.12200334
95,-1.6409700981,3.2013398748\C,0,-4.829910666,-1.5548714303,2.0366800
516\H,0,-5.8978911382,-1.6665976082,2.0885667502\C,0,-4.1861530921,-1.
2429421666,0.7960071856\N,0,-4.8730456117,-1.1654425437,-0.3617745038\
C,0,-6.2723647661,-1.671312253,-0.4583693612\C,0,-4.3529979188,-0.4962
835554,-1.5930828786\C,0,-2.7761356203,-1.01247765,0.8543830335\H,0,-2
.2248202932,-0.8057569339,-0.0416265215\C,0,-2.0857078761,-1.113895172
9,2.0283335776\H,0,-1.0161447035,-0.981810326,2.0007624361\C,0,-0.7401
195834,-0.8977027993,4.6716629893\C,0,-0.0409352221,-1.0052541216,5.85
63139934\H,0,-0.3371749267,-0.2763673972,3.8865903419\C,0,-0.519797935
1,-1.7695557466,6.931141268\H,0,0.8970345575,-0.4781786554,5.947242017
2\C,0,-2.4606514891,-2.3061142527,5.5728297734\C,0,-1.7457931377,-2.41
72236967,6.7535934655\H,0,-2.1576669204,-3.0261263837,7.5417610174\C,0
,0.2936260536,-1.8656525209,8.2233626115\H,0,-3.3895345563,-2.84797718
97,5.4800327777\H,0,-4.6658167238,-1.8299501437,4.1127602037\C,0,0.478
7670716,-0.4541857543,8.8134134197\C,0,1.6741955048,-2.4735515973,7.90
90247471\C,0,-0.3903708464,-2.7427110756,9.2791830665\C,0,-3.336104686
7,-1.3402912775,-2.3685440784\C,0,-3.9082477864,0.9451130794,-1.337325
4422\H,0,-5.2299727865,-0.4259419469,-2.2252591021\C,0,-7.2717139782,-
0.5151104203,-0.4411570167\H,0,-6.4338490479,-2.2865765308,0.415476882
6\C,0,-6.4561241342,-2.6015667997,-1.6587986823\H,0,-8.2815169432,-0.9
223179326,-0.4375313889\H,0,-7.1735762879,0.1218324448,-1.3191306565\H
,0,-7.1477759188,0.100967965,0.4480198827\H,0,-6.3966965213,-2.0883157
054,-2.6161063841\H,0,-7.4492686803,-3.0416657309,-1.5859949634\H,0,-5
.7287168944,-3.4108337498,-1.6442410905\H,0,-2.9796081284,1.0235762718

,-0.779919525\H,0,-4.6791141466,1.4968738617,-0.802029569\H,0,-3.75715
70828,1.4258865999,-2.3025666447\H,0,-2.3592471041,-1.3891496638,-1.89
58792727\H,0,-3.2034961186,-0.8875608191,-3.3499591783\H,0,-3.69581319
94,-2.3563314937,-2.5122857503\H,0,2.266748504,-2.5422070694,8.8220536
891\H,0,1.5736797194,-3.4770318878,7.4944452822\H,0,2.232260985,-1.868
6603627,7.1953842581\H,0,1.0043838108,0.2088782605,8.127398496\H,0,-0.
4841076684,-0.0003939265,9.0497410909\H,0,1.0617160795,-0.5099041327,9
.7334638491\H,0,-0.5232358179,-3.7677206233,8.9322471775\H,0,-1.365510
8737,-2.3479203725,9.5654187734\H,0,0.2270438108,-2.7767839553,10.1764
186052\\Version=EM64L-G09RevD.01\HF=-911.0272403\S2=0.80395\S2-1=0.\S2
A=0.752262\RMSD=1.660e-09\Dipole=-2.2140164,0.2534983,-3.4628741\Quadr
upole=34.3645739,-37.7672856,3.4027117,21.017431,1.4057441,-11.9315825
\PG=C01 [X(C22H31N1)]\\@

$^{tBu/R2N}$PP3+*

1\1\GINC-HPC-CN121\Stability\UBLYP\6-31G(d)\C28H35N1(1+,2)\4688WANGD\2
3-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nb
o) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=2
00) int(grid=ultrafine)\\Title\\1,2\C,0,-2.0887772774,-1.3196717232,5.
0533016336\C,0,-2.7377586056,-1.2867338306,3.7513184125\C,0,-4.0443583
516,-1.7968434433,3.5569968433\C,0,-4.6572563474,-1.7854312991,2.33675
4488\H,0,-5.6720971879,-2.1361506097,2.2816999068\C,0,-4.0040671468,-1
.2481738938,1.1809678037\N,0,-4.5909588016,-1.2439648842,-0.032761906\
C,0,-5.8198302034,-2.0459033753,-0.2943081769\C,0,-4.1389698259,-0.388
0169604,-1.1716533239\C,0,-2.6948565678,-0.711631657,1.3863962025\H,0,
-2.1357952229,-0.3228384639,0.5584595699\C,0,-2.096835702,-0.740313555
9,2.6133498587\H,0,-1.0877717886,-0.3697390271,2.6931566681\C,0,-1.034
5806274,-0.442120027,5.3678912556\C,0,-0.4216731101,-0.4749207097,6.60
35379514\H,0,-0.7177978009,0.302888616,4.6547060198\C,0,-0.8164343761,
-1.3918876697,7.5892084022\H,0,0.3566282131,0.2409440463,6.8204727595\
C,0,-2.4882985808,-2.2334749377,6.046231158\C,0,-1.8640260244,-2.27098
73542,7.2761490575\H,0,-2.1712706356,-3.0138550661,7.996595316\C,0,-0.
1527409719,-1.4309696429,8.9061631375\H,0,-3.2654522768,-2.9530192288,
5.8398158067\H,0,-4.6028692213,-2.1699847449,4.400125379\C,0,-0.855195
6945,-1.7723339092,10.0635666582\C,0,-2.8907975683,-0.9168683615,-1.88
6276073\C,0,-4.0674705786,1.0948545168,-0.8022375337\H,0,-4.9515307261
,-0.4756256632,-1.8826137955\C,0,-7.0580441212,-1.1509085087,-0.339185
5737\H,0,-5.9167445526,-2.7336503204,0.5338186939\C,0,-5.6689931475,-2
.9184718478,-1.5418403697\H,0,-7.9417474588,-1.7774257865,-0.449709707
2\H,0,-7.0339579276,-0.4608858119,-1.1816118228\H,0,-7.1605945837,-0.5
729553743,0.5778242968\H,0,-5.6374234001,-2.3465734218,-2.4667165283\H
,0,-6.5361544527,-3.5747677858,-1.5932379848\H,0,-4.779172647,-3.54187
24472,-1.4800029741\H,0,-3.2342052789,1.3432737874,-0.1514158595\H,0,-
4.9888919567,1.4167561942,-0.320300085\H,0,-3.9507605131,1.6652243706,
-1.7224361399\H,0,-1.9698830208,-0.7533105615,-1.3336183408\H,0,-2.799
9076713,-0.391435206,-2.8358436378\H,0,-2.9779360479,-1.980084189,-2.0
96742896\C,0,1.2072786889,-1.1268468095,9.0425231348\C,0,1.8268434109,
-1.1683449961,10.2791736824\C,0,-0.2283310549,-1.8063094997,11.3024256
181\C,0,1.1275343791,-1.5077729725,11.4441200618\H,0,1.7945301093,-0.8
822160801,8.1691811203\H,0,-1.9123281658,-1.9888341183,10.0077126016\H
,0,-0.8212424983,-2.0656919327,12.164937756\C,0,1.8539929467,-1.539929
4334,12.7926727218\H,0,2.8807853757,-0.9369397003,10.3322952972\C,0,0.
9216430927,-1.9267919764,13.9472966611\C,0,2.4388435212,-0.1467621529,
13.0920768551\C,0,2.9977135113,-2.5701057655,12.7320194687\H,0,0.10170
72498,-1.2173147802,14.0620611925\H,0,1.4835208474,-1.9348271549,14.88
12505316\H,0,0.4967341766,-2.9214865217,13.809949897\H,0,1.649407839,0
.6035538701,13.1477701955\H,0,3.1483811563,0.1685535221,12.3278221409\

H,0,2.9635813556,-0.1576856834,14.0484797841\H,0,2.6117572309,-3.56931
39028,12.5272593426\H,0,3.526465952,-2.6002766067,13.6858052589\H,0,3.
723799664,-2.3255315373,11.957503127\\Version=EM64L-G09RevD.01\HF=-114
1.9506017\S2=0.80479\S2-1=0.\S2A=0.752381\RMSD=2.302e-09\Dipole=-3.430
7717,0.1058898,-6.6680843\Quadrupole=20.7059732,-43.616263,22.9102898,
24.3274944,0.5321948,-14.0555365\PG=C01 [X(C28H35N1)]\\@

$^{tBu/R2N}$PP4+*

1\1\GINC-HPC-CN120\Stability\UBLYP\6-31G(d)\C34H39N1(1+,2)\4688WANGD\2
3-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nb
o) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=2
00) int(grid=ultrafine)\\Title\\1,2\C,0,-2.1699481256,-1.2796521877,5.
0505985622\C,0,-2.7726411448,-1.2878453967,3.7256885231\C,0,-3.9382101
239,-2.0403288984,3.4437748859\C,0,-4.5118592126,-2.0578855734,2.20453
84198\H,0,-5.4298290662,-2.6043767175,2.0844948349\C,0,-3.9593268077,-
1.3058541569,1.1181937146\N,0,-4.5153139349,-1.3153890966,-0.110147035
3\C,0,-5.5569083252,-2.3189431134,-0.4718521724\C,0,-4.2293221013,-0.2
892347488,-1.1587537857\C,0,-2.789736586,-0.5370278838,1.4105460719\H,
0,-2.3012225055,0.0178287686,0.6339780825\C,0,-2.2282876352,-0.5385535
857,2.6552106386\H,0,-1.318484914,0.0208638346,2.8017247929\C,0,-1.353
4932404,-0.2155227573,5.475585083\C,0,-0.7941964365,-0.2037502989,6.73
69545655\H,0,-1.1902589529,0.6339188065,4.8305215064\C,0,-1.0064705626
,-1.257666891,7.6382324085\H,0,-0.2090936333,0.6507744517,7.0414244701
\C,0,-2.3839356176,-2.3342871314,5.9569884923\C,0,-1.8115819523,-2.324
7580267,7.2124717784\H,0,-1.9661382385,-3.1714291575,7.8640452209\C,0,
-0.4066215337,-1.2429336088,8.9857124238\H,0,-2.968122415,-3.192274891
4,5.6620889301\H,0,-4.4271553943,-2.5850625287,4.2352790849\C,0,-1.061
7127098,-1.8277117496,10.0758016094\C,0,-2.8916071756,-0.4976108402,-1
.8765197039\C,0,-4.4572071462,1.1411057543,-0.6651280994\H,0,-4.999006
9003,-0.4715176446,-1.8990410259\C,0,-6.949404131,-1.6889337433,-0.457
7623722\H,0,-5.5137857992,-3.0882738536,0.2862181343\C,0,-5.2345310895
,-3.0212542068,-1.7919971314\H,0,-7.6893515927,-2.4654852737,-0.644649
3167\H,0,-7.0623045307,-0.9305716629,-1.231283607\H,0,-7.1667175113,-1
.2336510871,0.5070948423\H,0,-5.316339769,-2.3691694406,-2.6587880621\
H,0,-5.9552405957,-3.8270553502,-1.9211873498\H,0,-4.2394785682,-3.461
2977294,-1.7715515182\H,0,-3.704339926,1.486554897,0.037184017\H,0,-5.
4349036613,1.2375506096,-0.1962540043\H,0,-4.4310647157,1.8019841162,-
1.530160062\H,0,-2.0288575483,-0.2128039081,-1.2808352148\H,0,-2.89130
5806,0.122956103,-2.7713753037\H,0,-2.7662940674,-1.5329037189,-2.1845
905369\C,0,0.835483658,-0.6413286788,9.2191032617\C,0,1.397466231,-0.6
281819163,10.484496832\C,0,-0.5014644383,-1.8073790648,11.3417973424\C
,0,0.7416097226,-1.2088658964,11.5757586677\H,0,1.3868194123,-0.209265
4679,8.3967864487\H,0,-2.0376305261,-2.271179489,9.9422627361\H,0,-1.0
512124523,-2.2366363854,12.1665911572\H,0,2.3731739914,-0.1853778426,1
0.6212676523\C,0,1.3399097312,-1.1897106503,12.9289758305\C,0,1.177931
9734,-2.2595439885,13.8096908333\C,0,2.0899310716,-0.0964168582,13.376
0511284\C,0,1.7391709433,-2.2392466255,15.0809587661\H,0,0.6261595162,
-3.1342067758,13.4953677468\C,0,2.4862164048,-1.1511598451,15.53302557
26\H,0,1.5888294725,-3.0976330867,15.7164322097\C,0,2.645449788,-0.081
0623612,14.6445024215\H,0,3.2082231436,0.7904838883,14.9468921332\C,0,
3.115464251,-1.0906169001,16.9292791494\H,0,2.2205296794,0.7630946965,
12.733863452\C,0,2.843195737,-2.3599881625,17.7459397967\C,0,4.6407994
405,-0.9218004775,16.7989507351\C,0,2.5348912217,0.1101295556,17.69990
48171\H,0,5.0812764814,-1.762854651,16.2623123304\H,0,5.0998744025,-0.
8732429227,17.7875610077\H,0,4.9041971101,-0.0089213197,16.2658347971\
H,0,1.4549028086,0.0127092189,17.8161919577\H,0,2.7335071742,1.0528646
284,17.1911065116\H,0,2.978553702,0.169228143,18.6949955255\H,0,3.2548

593217,-3.247734685,17.2649377396\H,0,1.7762464914,-2.5202971872,17.90
32842295\H,0,3.3107752393,-2.2694683745,18.7264924183\\Version=EM64L-G
09RevD.01\HF=-1372.8739398\S2=0.805041\S2-1=0.\S2A=0.752409\RMSD=4.599
e-09\Dipole=-4.7414201,-0.1439339,-10.3592333\Quadrupole=10.8574088,-4
1.1969414,30.3395326,28.6562242,5.8276322,-12.9951536\PG=C01 [X(C34H39
N1)]\\@