Supporting Information

S1: Synthetic Details

General: All manipulations were performed under an inert atmosphere of dry nitrogen, using standard Schlenk techniques. Dry, oxygen-free solvents were employed unless otherwise mentioned. The compound **IDP and 1b** were prepared following reported procedure,[1] while all other starting materials were purchased from commercial sources. NMR spectra were recorded on Bruker Avance 400 MHz spectrometers (^{1}H, 400.1 MHz; ^{13}C, 100.5 MHz; ^{19}F, 376.3 MHz; ^{31}P, 161.9 MHz). All spectra were obtained in the solvent indicated at 25 °C. The chemical shifts (δ) were measured according to IUPAC and expressed in ppm relative to $SiMe_4$ (^{1}H, ^{13}C), and 85% H_3PO_4 (^{31}P). Coupling constants *J* are reported in Hertz [Hz] as absolute values. Because of high sensitivity of these compounds or the contamination of solvents, the elemental analyses gave unsatisfying results. The high purity of these isolated compounds has been proved mainly by NMR or EPR spectra. UV/vis spectra were measured on Shimadzu UV/vis/NIR UV-3600-spectrometer. ESI-MS spectra were measured on Bruker ESI-Q-TOF maxis 4G. Melting point (M. P.) were measured on Buchi M-560 apparatus.

Preparation of 1a: Tert-butyl-3-phenylpropiolate (1.0 equivalent) was added to a stirred solution of **IDP** (86.7 mg, 0.1 mmol) in Tol (4 mL) at room temperature and then heated to 110°C. After stirring for overnight, the solvent was removed under reduced pressure. The remaining solid was washed with acetonitrile and dried *in vacuo* to afford **1a** as yellowish powder, 101.8 mg, 0.095 mmol, 95.0% yield. Yellowish crystals of **1a** were obtained from a saturated hexane solution via slow evaporation at room temperature. M. P. > 250 °C. ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.21 (m, 2 H, $C_{ar}H$), 7.15 (m, 5 H, $C_{ar}H$), 7.13 (m, 3 H, $C_{ar}H$), 7,02 (m, 3 H, $C_{ar}H$), 6.84 (d, J = 8.0 Hz, 2 H, $C_{ar}H$), 6.61 (d, J = 8.0 Hz, 2 H, $C_{ar}H$), 3.57 (m, 4 H, CHMe$_2$), 3.41 (m, 2 H, NCH_2), 3.31 (m, 2 H, NCH_2), 3.22 (m, 2 H, NCH_2), 3.12 (m, 2 H, NCH_2), 3.06 (m, 2 H, CHMe$_2$), 2.98 (m, 2 H, CHMe$_2$), 1.43 (d, J = 8.0 Hz, 11 H, CH_3), 1.37 (s, 11 H, CH_3), 1.29 (m, 17 H, CH_3), 1.09 (d, J = 8.0 Hz, 6 H, CH_3), 0.97 (d, J = 8.0 Hz, 6 H, CH_3), 0.69 (d, J = 8.0 Hz, 6 H, CH_3); ^{13}C{^{1}H} NMR (C_6D_6, 100.5 MHz): δ =191.7 (d, $^{2}J_{PC}$ = 40.2 Hz, PCCO), 169.3 (d, $^{1}J_{PC}$ = 40.2 Hz, PCC$_{ar}$), 148.3 (s, C_{ar}), 148.0 (s, C_{ar}), 147.6 (s, C_{ar}), 144.3 (t, $^{1}J_{PC}$ = 40.2 Hz, PCC), 139.4 (s, C_{ar}), , 127.9 (s, C_{ar}), 127.7 (s, C_{ar}), 127.4 (s, C_{ar}), 124.7 (s, C_{ar}), 124.4 (s, C_{ar}), 102.5 (t, $^{1}J_{PC}$ = 10.1 Hz, PCC), 78.4 (s, OCtBu), 52.1 (s, NCH$_2$), 28.2 (CH$_3$), 27.9 (CH$_3$), 27.7 (CH$_3$), 25.6 (CH$_3$), 25.3 (CH$_3$), 25.1 (CH$_3$), 25.0 (CH$_3$), 24.0 (CH$_3$), 22.5 (CH$_3$). ^{31}P{^{1}H} NMR (C_6D_6, 161.9 MHz) δ = 158.9 (d, J = 6.5 Hz), 153.8 (d, J = 6.5 Hz). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 282 (4190.5), 332 (2501.3); ESI-MS $[M+H]^+$ $C_{69}H_{90}N_4O_2P_2^+$ calc. 1069.661 m/z, found 1069.660 $[M+H]^+$.

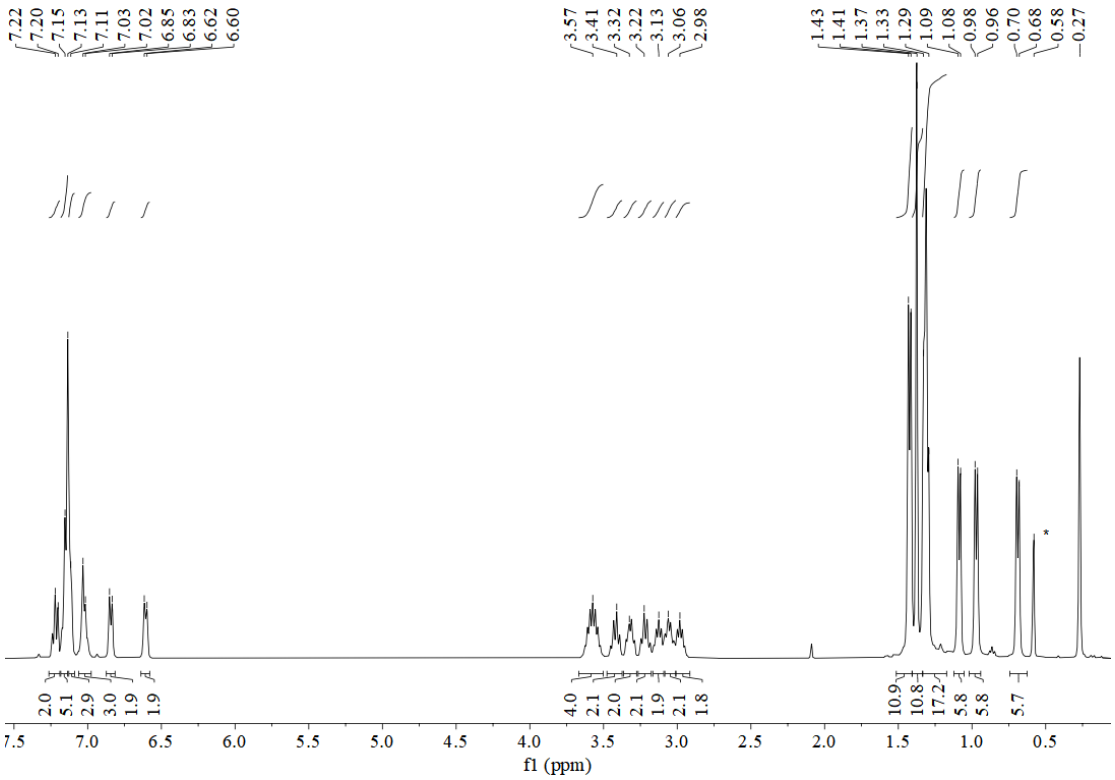

Figure S1. ^{1}H NMR spectrum of **1a** in C_6D_6. *Acetonitrile $^{\#}$Silicon grease.

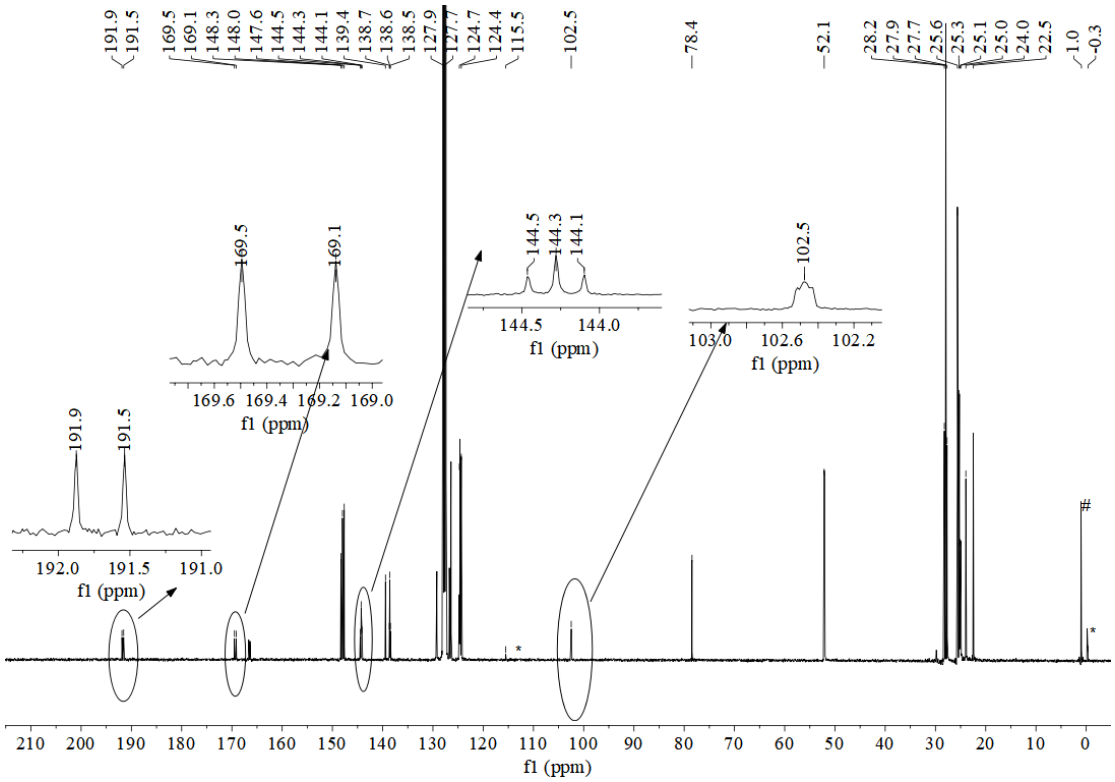

Figure S2. ^{13}C{^{1}H} NMR spectrum of **1a** in C_6D_6. *Acetonitrile $^{\#}$Silicon grease.

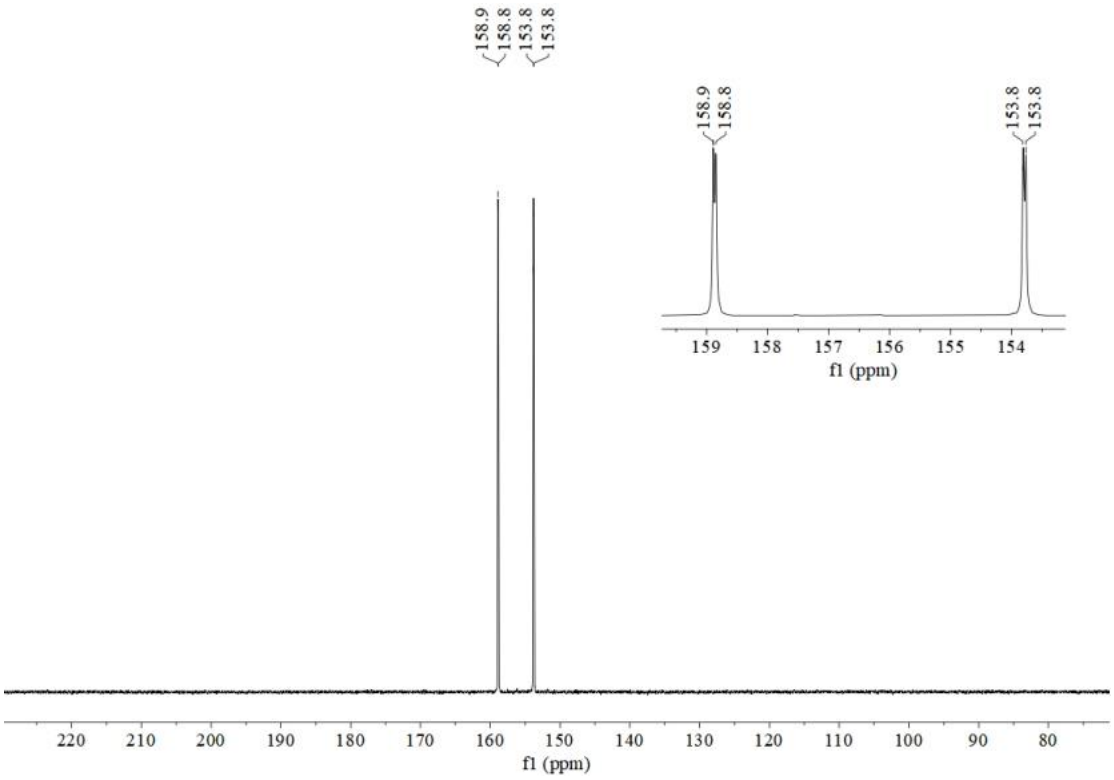

Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of **1a** in C_6D_6.

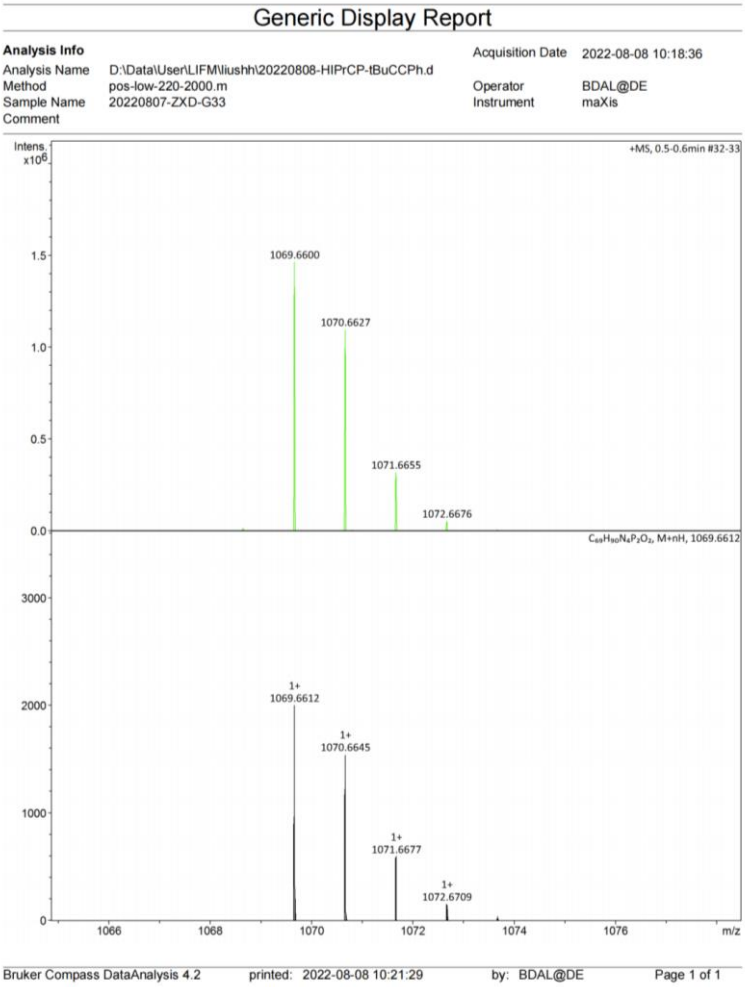

Figure S4. ESI-MS of **1a**.

Preparation of $2a^{\bullet+}(BAr^F)$: $Fc^+(BAr^F)$ (0.8 equivalent in diethyl ether 2 mL) was added dropwise to a stirred solution of **1a** (53.6 mg, 0.05 mmol) in diethyl ether (10 mL) at -30 ℃. After stirring for 0.5 hour, the solvent was removed under reduced pressure. Then, the remaining solid was washed with hexane and dried in vacuo to afford green powder as $\mathbf{2a}^{\bullet+}(BAr^F)$, 67.6 mg, 0.035 mmol, 87.5% yield (based on oxidant). Green crystals of $\mathbf{2a}^{\bullet+}(BAr^F)$ were obtained from a saturated solution of mixed hexane and diethyl ether (1:1) via slow evaporation at room temperature. M. P. = 160.6 °C (Decomposition, green to dark-brown). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 269 (4681.5), 473 (880.4), 665 (182.3).

Preparation of $2b^{\bullet+}(BAr^F)$: $Fc^+(BAr^F)$ (0.8 equivalent in diethyl ether 2 mL) was added dropwise to a stirred solution of **1b** (51.9 mg, 0.05 mmol) in diethyl ether (10 mL) at -30 ℃. After stirring for 0.5 hour, the solvent was removed under reduced

pressure. Then, the remaining solid was washed with hexane and dried in vacuo to afford green powder as **2b**$^{\bullet+}$(BAr^F), 60.3 mg, 0.032 mmol, 80.0% yield (based on oxidant). Green crystals of **2b**$^{\bullet+}$(BAr^F) were obtained from a saturated solution of mixed hexane and diethyl ether (1:1) via slow evaporation at room temperature. M. P. = 167.1 °C (Decomposition, green to red-brown). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 268 (6178.5), 472 (1356.8), 657 (642.5).

Preparation of 3: Magnesium powder (28.8 mg, 1.2 mmol) was added to a stirred solution of **2a**$^{\bullet+}$(BAr^F) (192.8 mg, 0.1 mmol) in tetrahydrofuran (3 mL) at room temperature. After stirring for overnight, the solvent was removed under reduced pressure. The remaining solid was washed with acetonitrile and dried *in vacuo* to afford **3** as reddish powder, 97.5 mg, 0.091 mmol, 91.0% yield. Reddish crystals of **3** were obtained from a saturated hexane solution via slow evaporation at room temperature. M. P. = 247.7 °C. ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.29 (m, 2 H, $C_{ar}H$), 7.15 (m, 6 H, $C_{ar}H$), 6.96 (m, 5 H, $C_{ar}H$), 6.85 (d, *J* = 4.0 Hz, 1 H, $C_{ar}H$), 6.77 (d, *J* = 8.0 Hz, 1 H, $C_{ar}H$), 5.68 (d, *J* = 4.0 Hz, 2 H, $C_{ar}H$), 4.22 (m, 1 H, C*H*Me$_2$), 3.97 (m, 1 H, C*H*Me$_2$), 3.82 (m, 2 H, NCH_2), 3.69(m, 2 H, NCH_2), 3.56 (m, 2 H, NCH_2), 3.18 (m, 1 H, NCH_2), 3.08 (m, 1 H, NCH_2), 2.94 (m, 5 H, C*H*Me$_2$), 2.73 (m, 1 H, C*H*Me$_2$), 1.69 (d, *J* = 4.0 Hz, 3 H, CH_3), 1.59 (d, *J* = 8.0 Hz, 3 H, CH_3), 1.33 (m, 6 H, CH_3), 1.21 (m, 27 H, CH_3), 1.07 (m, 12 H, CH_3), 0.99 (d, *J* = 4.0 Hz, 3 H, CH_3), 0.81 (d, *J* = 8.0 Hz, 3 H, CH_3); ^{13}C{^{1}H} NMR (C_6D_6, 100.5 MHz): δ =164.3 (s, C*C*OO), 158.6 (d, $^1J_{PC}$ = 30.2 Hz, P*C*C$_{ar}$), 153.1 (t, $^1J_{PC}$ = 40.2 Hz, P*C*C), 149.6 (s, C_{ar}), 148.0 (s, C_{ar}), 147.4 (s, C_{ar}), 146.6 (s, C_{ar}), 141.8 (s, C_{ar}), 141.3 (d, $^1J_{PC}$ = 20.1 Hz, P*C*C), 139.7 (s, C_{ar}),148.0 (s, C_{ar}), 139.4 (s, C_{ar}), 138.3 (s, C_{ar}), 131.9 (d, $^1J_{PC}$ = 11 Hz, C*C*CO), 131.0 (s, C_{ar}), 127.9 (s, C_{ar}), 127.7 (s, C_{ar}), 127.4 (s, C_{ar}), 126.5 (s, C_{ar}), 125.7 (s, C_{ar}), 125.1 (s, C_{ar}), 125.0 (s, C_{ar}), 124.4 (s, C_{ar}), 123.7 (s, C_{ar}), 94.7 (s, OCMe$_3$), 77.5 (s, P*C*P), 52.3 (s, N*C*H$_2$), 29.9 (*C*H$_3$), 28.9 (*C*H$_3$), 28.7 (*C*H$_3$), 28.6 (*C*H$_3$), 28.4 (*C*H$_3$), 27.9 (*C*H$_3$), 27.3 (*C*H$_3$), 27.2 (*C*H$_3$), 26.4 (*C*H$_3$), 26.1 (*C*H$_3$), 25.5 (*C*H$_3$), 25.4 (*C*H$_3$), 24.8 (*C*H$_3$), 24.5 (*C*H$_3$), 24.1 (*C*H$_3$), 23.4 (*C*H$_3$), 23.0 (*C*H$_3$), 22.8 (*C*H$_3$), 22.7 (*C*H$_3$). ^{31}P{^{1}H} NMR (C_6D_6, 161.9 MHz) δ = -154.1 (d, $^1J_{PC}$ = 64.8 Hz), -197.1 (d, $^1J_{PC}$ = 64.8 Hz). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-}$

[1])): 270 (7760.0), 324 (3658.7), 443 (1541.4); ESI-MS $[M+H]^+$ $C_{69}H_{90}N_4O_2P_2^+$ calc. 1069.661 m/z, found 1069.654 $[M+H]^+$.

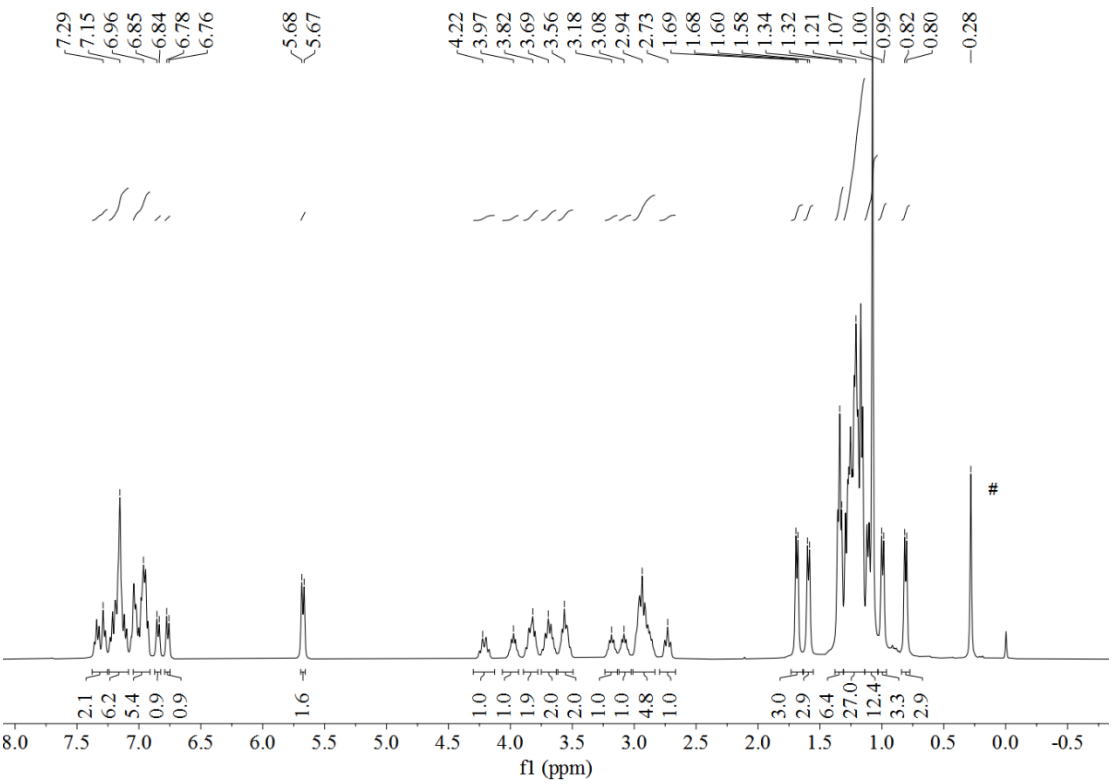

Figure S5. ^{1}H NMR spectrum of **3** in C_6D_6. $^{\#}$Silicon grease.

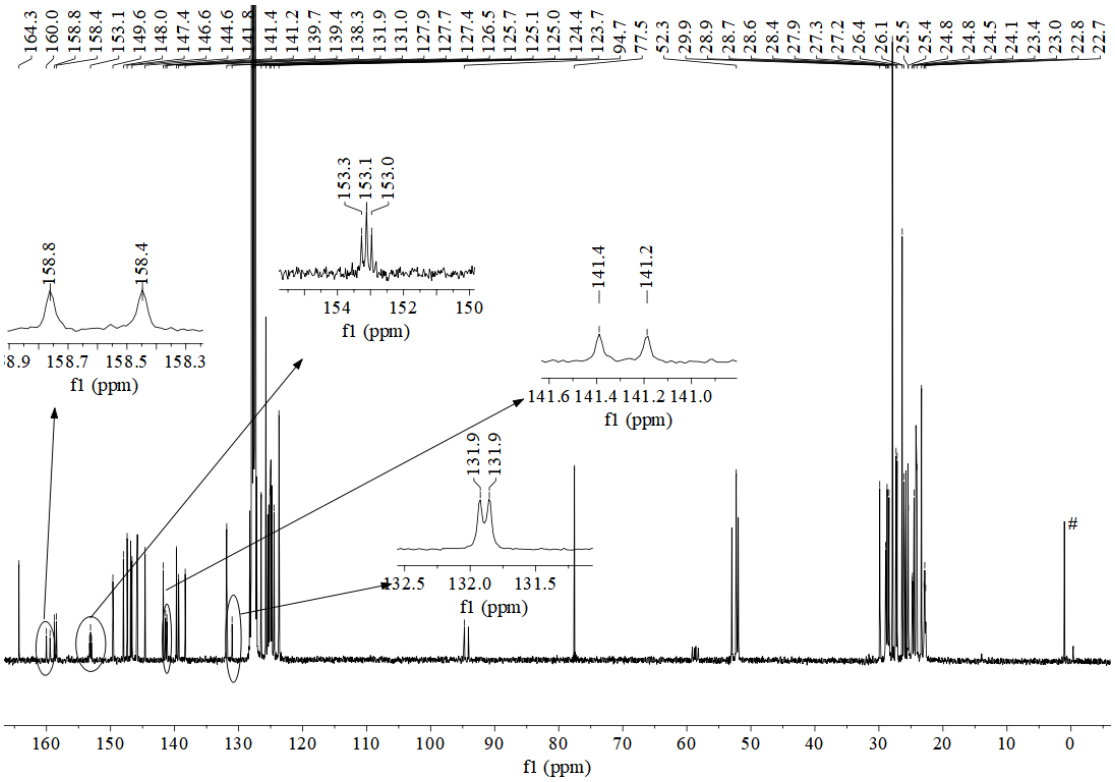

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6. #Silicon grease.

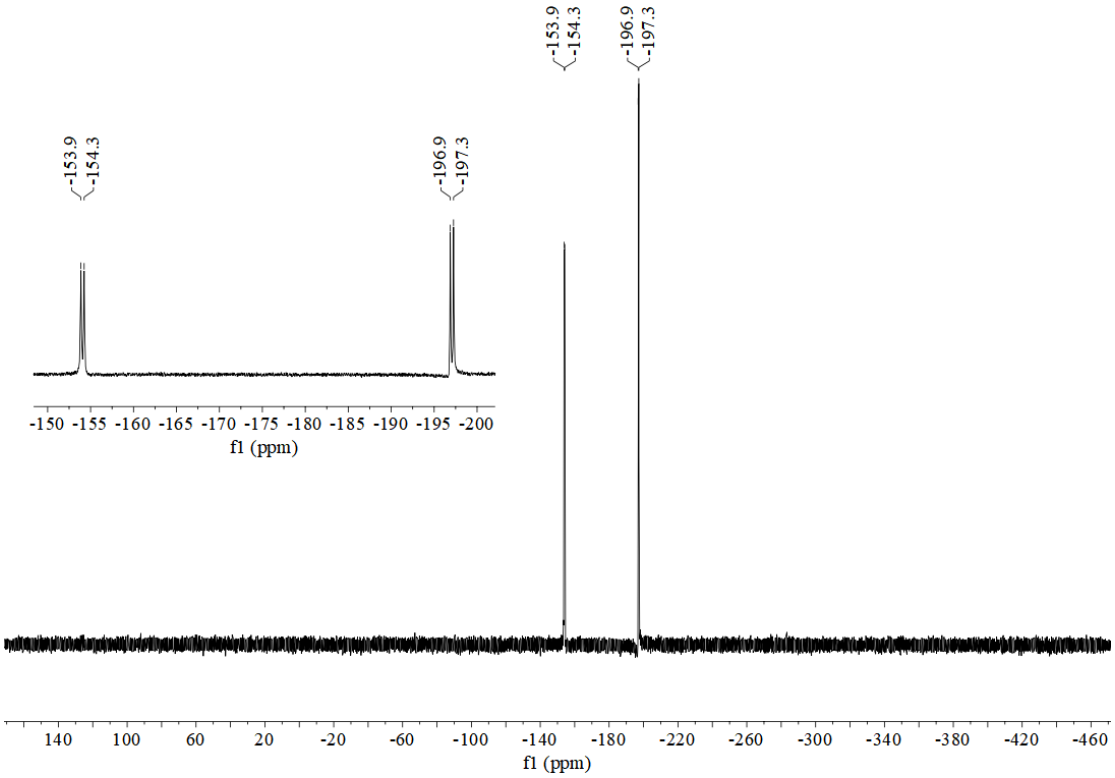

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in C_6D_6.

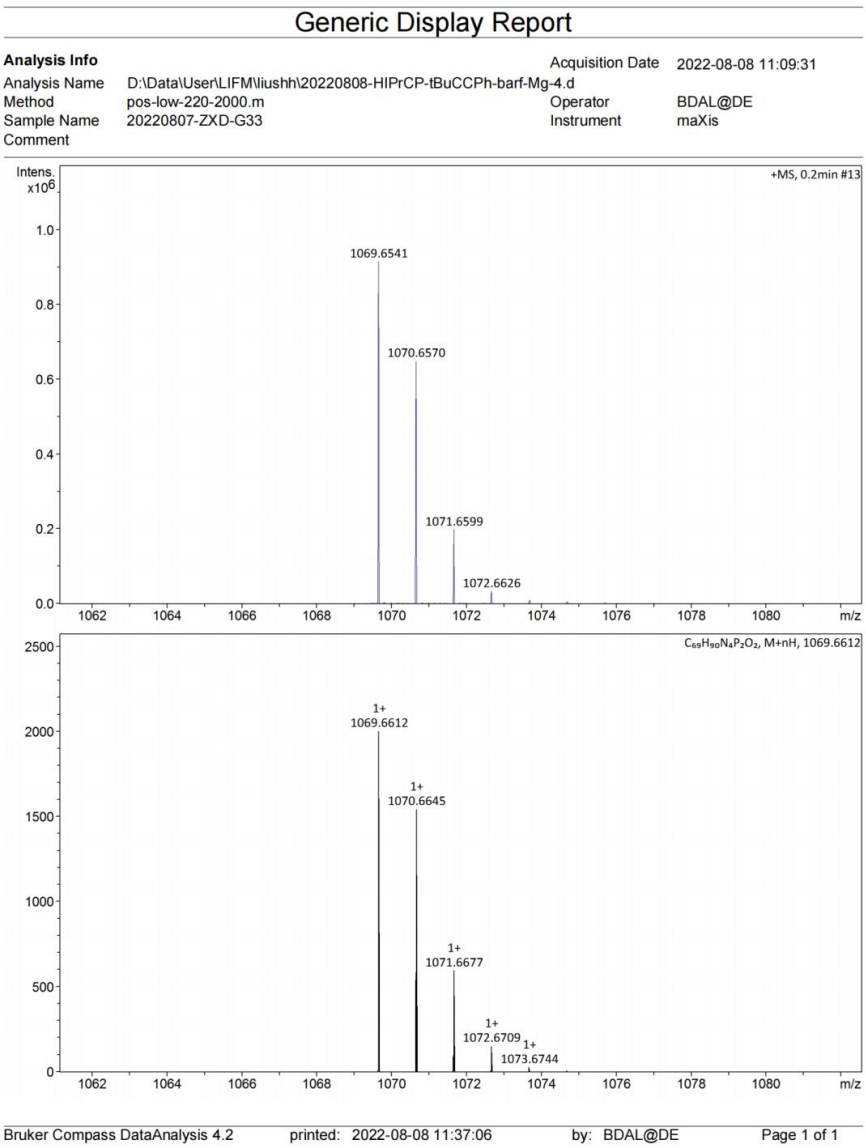

Figure S8. ESI-MS of **3**.

Preparation of $4^{+}(BAr^{F})$: Diphenyl disulfide (0.5 equivalent) was added to a stirred solution of $\mathbf{2a}^{\bullet+}(BAr^{F})$ (192.8 mg, 0.1 mmol) in diethyl ether (5 mL) at room temperature. After stirring for overnight, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford $\mathbf{4}^{+}(BAr^{F})$ as red powder. 183.3 mg, 0.09 mmol, 90.0% yield. Red crystals of $\mathbf{4}^{+}(BAr^{F})$ were obtained from a saturated acetonitrile and diethyl ether solution via slow evaporation at room temperature. M. P. = 204.3 °C. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.76 (s, 8 H, $C_{ar}H$), 7.60 (s, 4 H, $C_{ar}H$), 7.49 (m, 2 H, $C_{ar}H$), 7.38 (d, J = 8.0 Hz, 2 H, $C_{ar}H$), 7.26 (m, 6 H, $C_{ar}H$), 7.07 (m, 10 H, $C_{ar}H$), 6.78 (s, 2 H, $C_{ar}H$), 4.66 (m, 1 H, $CHMe_2$), 4.07 (m, 5 H, $CHMe_2$), 3.80 (m, 2 H, $CHMe_2$), 3.43(m, 2 H, NCH_2), 3.05 (m,

6 H, NCH_2), 1.45-071 (57 H, CH_3); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 100.5 MHz): δ = 162.3 (dd, $^2J_{PC}$ = 50.3 Hz, PC*C*O), 161.3 (dd, $^2J_{PC}$ = 50.3 Hz, PCC_{ar}), 147.8 (s, C_{ar}), 146.6 (s, C_{ar}), 143.5 (d, $^1J_{PC}$ = 60.3 Hz, P*C*CO), 134.8 (s, C_{ar}), 130.8 (s, C_{ar}), 130.2 (s, C_{ar}), 129.0 (s, C_{ar}), 128.0 (s, C_{ar}), 126.5 (s, C_{ar}), 125.8 (s, C_{ar}), 123.2 (s, C_{ar}), 120.5 (s, C_{ar}), 117.4 (s, C_{ar}), 116.5 (s, C_{ar}), 83.1 (s, O*C*Me$_3$), 30.2 (*C*H$_3$), 29.7 (*C*H$_3$), 29.2 (*C*H$_3$), 28.9 (*C*H$_3$), 28.3 (*C*H$_3$), 27.5 (*C*H$_3$), 27.2 (*C*H$_3$), 26.7 (*C*H$_3$), 26.0 (*C*H$_3$), 25.3 (*C*H$_3$), 25.0 (*C*H$_3$), 24.9 (*C*H$_3$), 24.1 (*C*H$_3$), 23.7 (*C*H$_3$), 23.2 (*C*H$_3$). $^{31}P\{^1H\}$ NMR (CD_2Cl_2, 161.9 MHz) δ = 310.0 (s), 6.1 (s). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 263 (7793.4), 393 (2261.5), 501 (1890.6); ESI-MS $[M]^+$ $C_{75}H_{95}N_4O_2P_2S^+$ calc. 1177.665 m/z, found 1177.658 $[M]^+$.

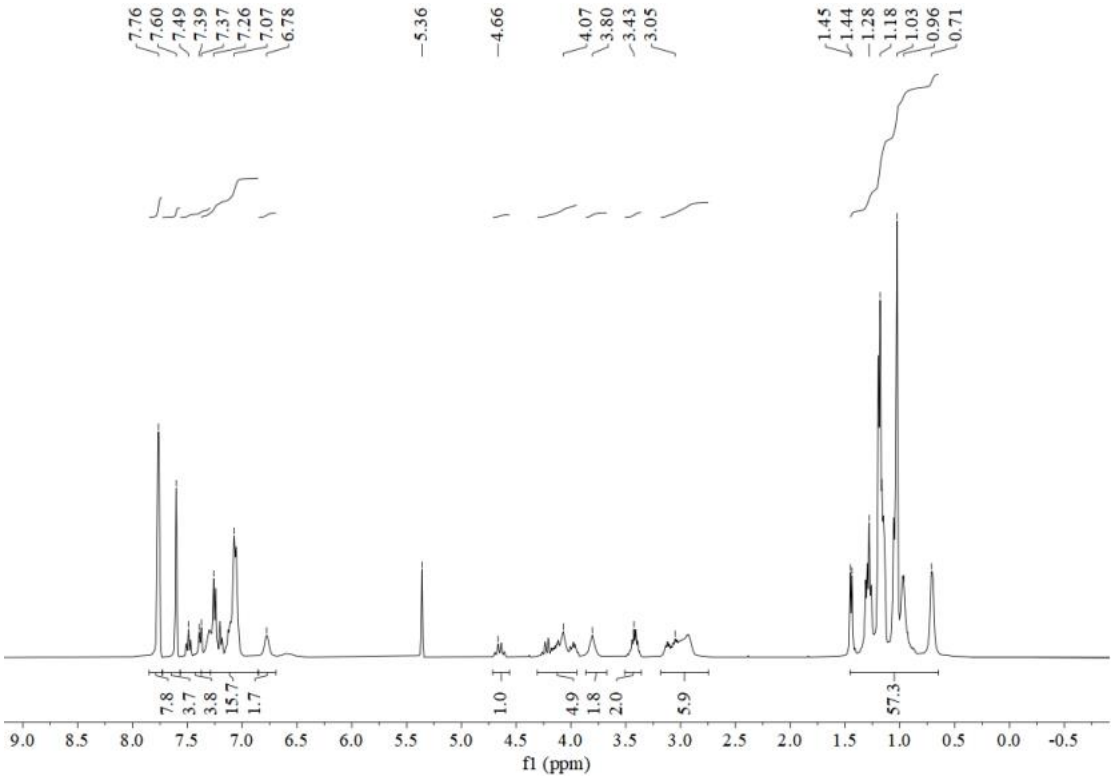

Figure S9. ^1H NMR spectrum of **4^+(BAr^F)** in CD_2Cl_2.

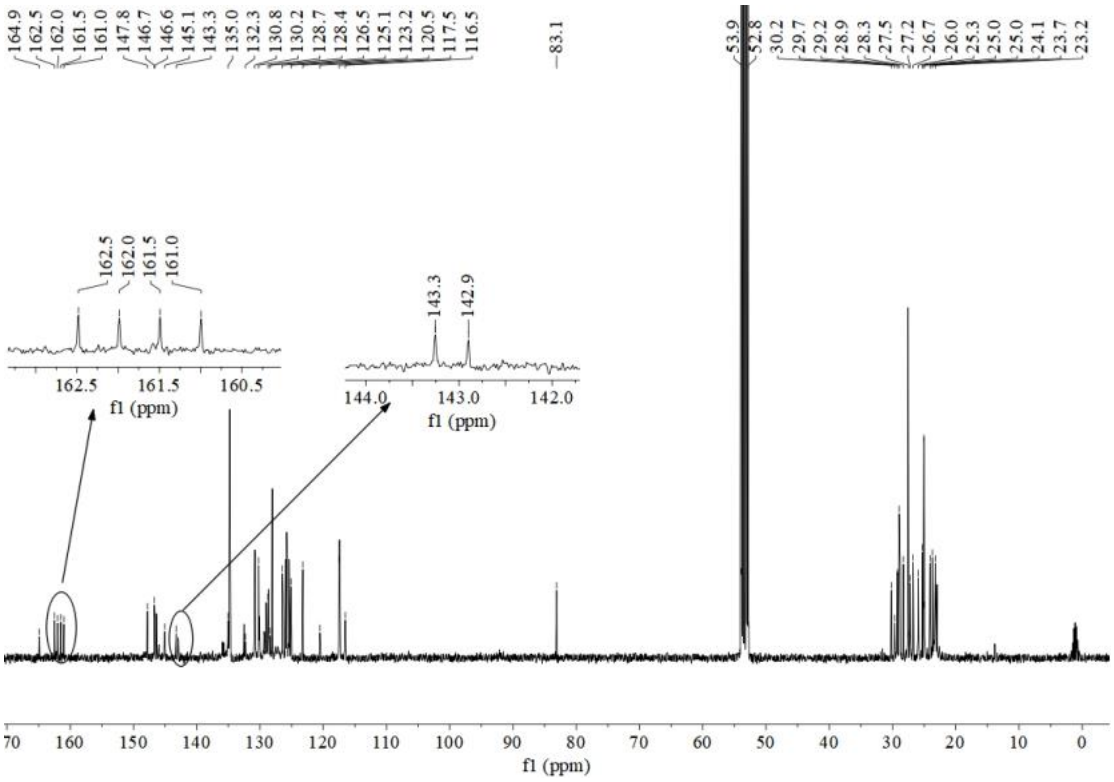

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4^{+}(BAr^{F})** in CD_2Cl_2.

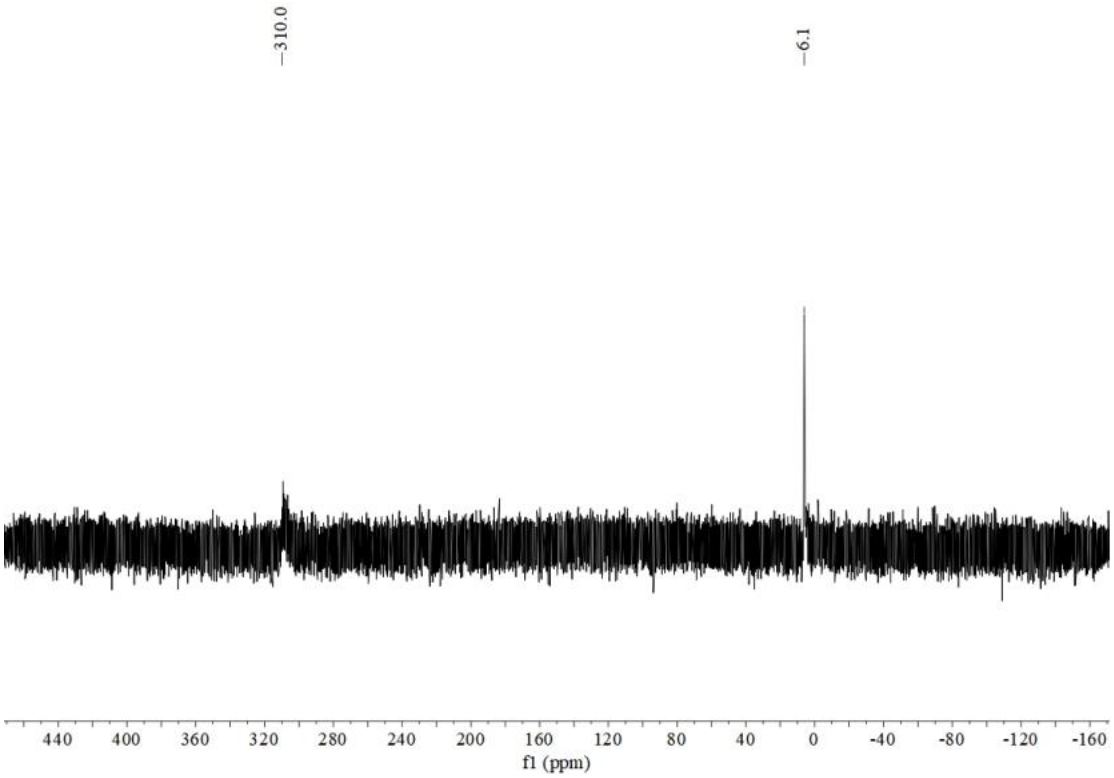

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **4^{+}(BAr^{F})** in CD_2Cl_2.

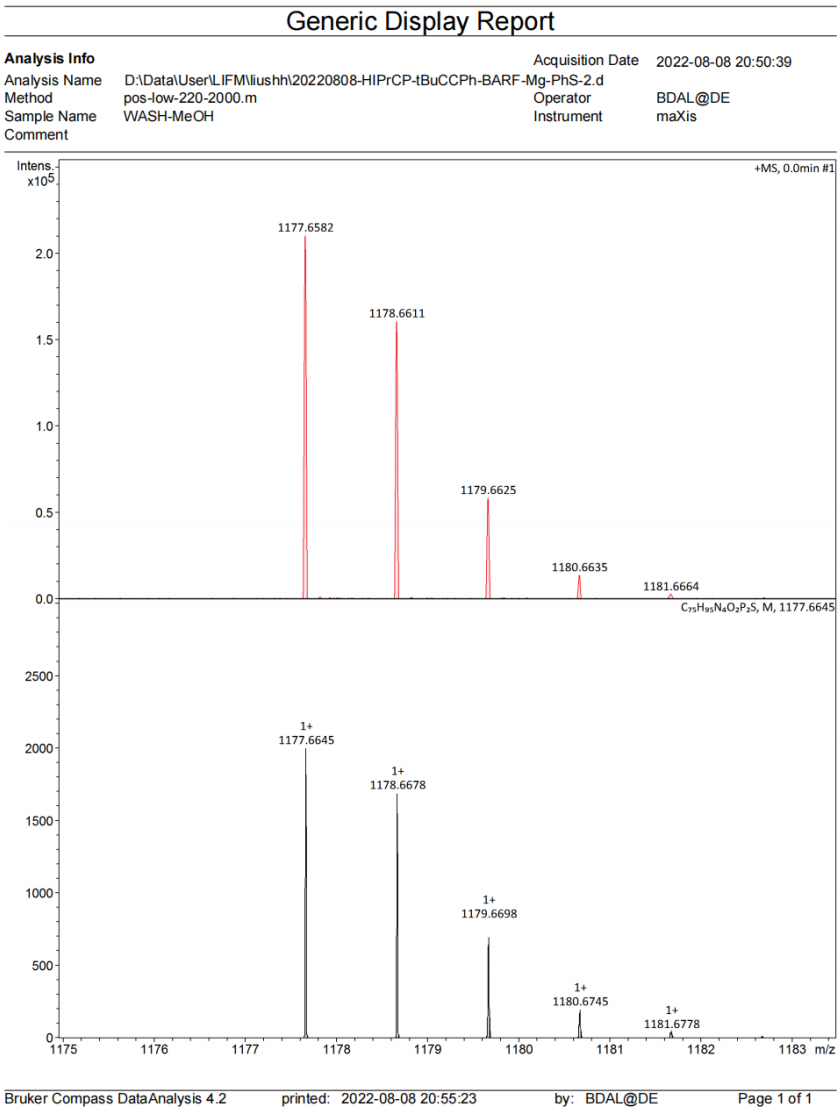

Figure S12. ESI-MS of $\mathbf{4}^{+}\mathbf{(BAr^{F})}$.

Preparation of 5: Potassium fluoride (3.0 equivalent) and 18-crown-6 (1.0 equivalent) was added to a stirred solution of $\mathbf{4}^{+}(BAr^{F})$ (117.8 mg, 0.1 mmol) in tetrahydrofuran (10 mL) at room temperature. After stirring for one week, the solvent was removed under reduced pressure. The remaining solid was extracted with hexane, then washed with acetonitrile and dried in vacuo to afford **5** as yellow powder, 87.3 mg, 0.073 mmol, 73.0% yield. Yellow crystals of **5** were obtained from a saturated hexane solution via slow evaporation at room temperature. M. P. = 232.1 °C (Decomposition). The detailed ^{1}H and ^{13}C NMR data were not available because the presence of two isomers. $^{31}P\{^{1}H\}$ NMR (C_6D_6, 161.9 MHz) δ = 149.7 (d, $^{2}J_{PF}$ = 921.2 Hz, PF), 13.5 (s, PSC_{ar}); ^{19}F NMR (C_6D_6, 376.6 MHz) δ = –124.2 (d, ^{2}J = 919.3 Hz, PF, 77%), -127.6 (d, ^{2}J = 926.4 Hz,

PF, 23%); UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 331 (1235.8), 416 (780.2); ESI-MS $[M]^+$ $C_{75}H_{95}FN_4O_2P_2S^+$ calc. 1196.663 m/z, found 1196.664 $[M]^+$.

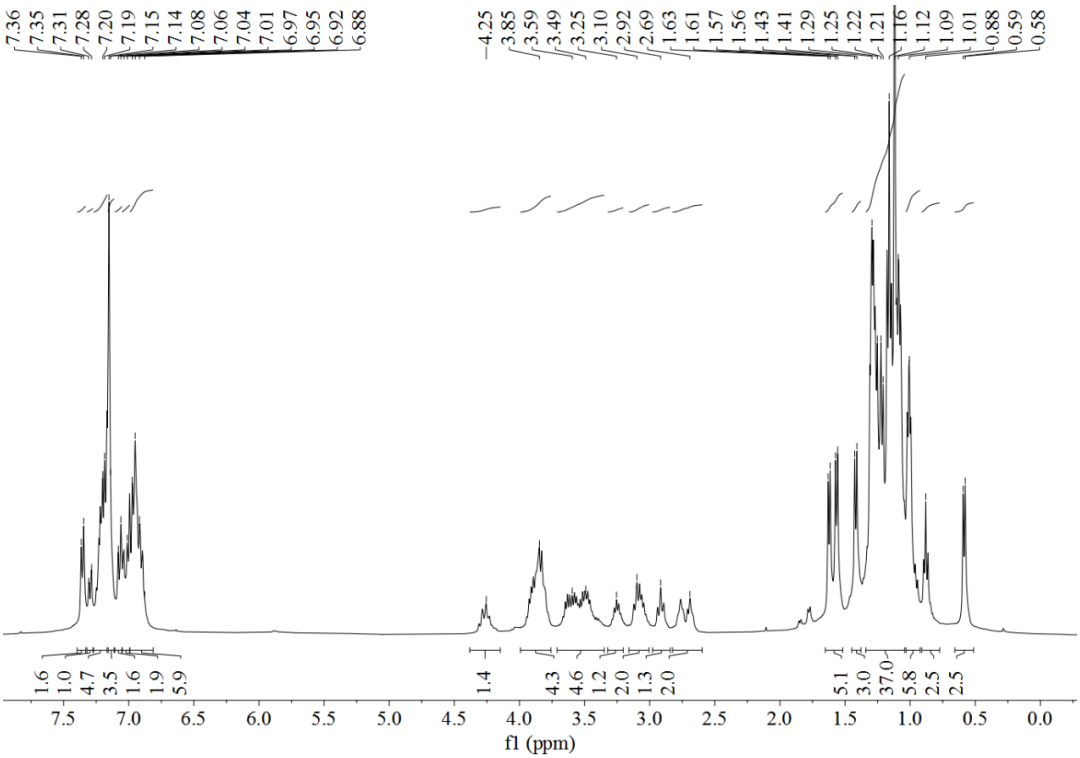

Figure S13. ^{1}H NMR spectrum of **5** in C_6D_6.

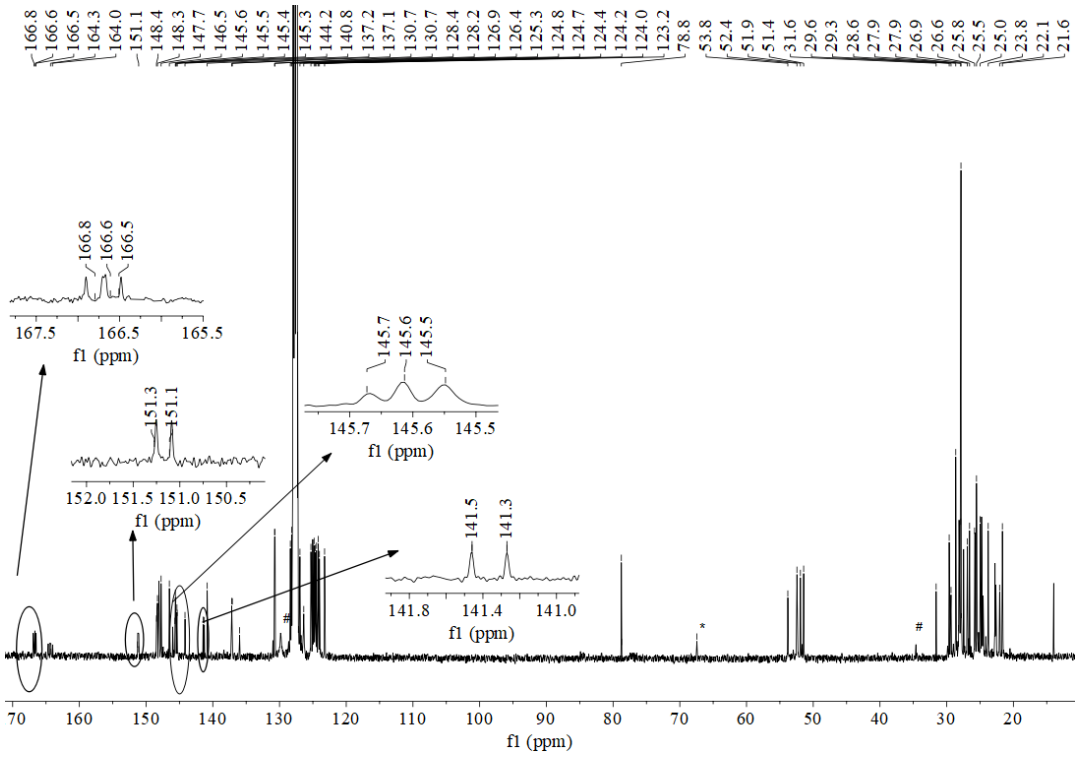

Figure S14. $^{13}C\{^1H\}$ NMR spectrum of **5** in C_6D_6.

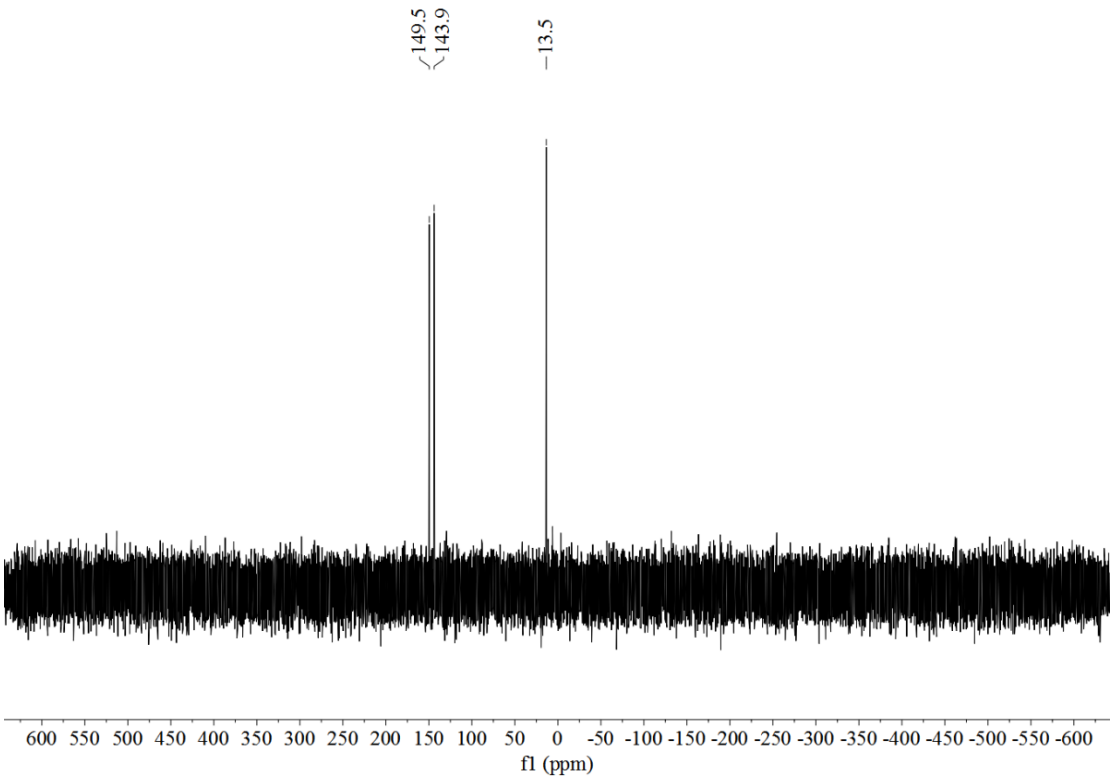

Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

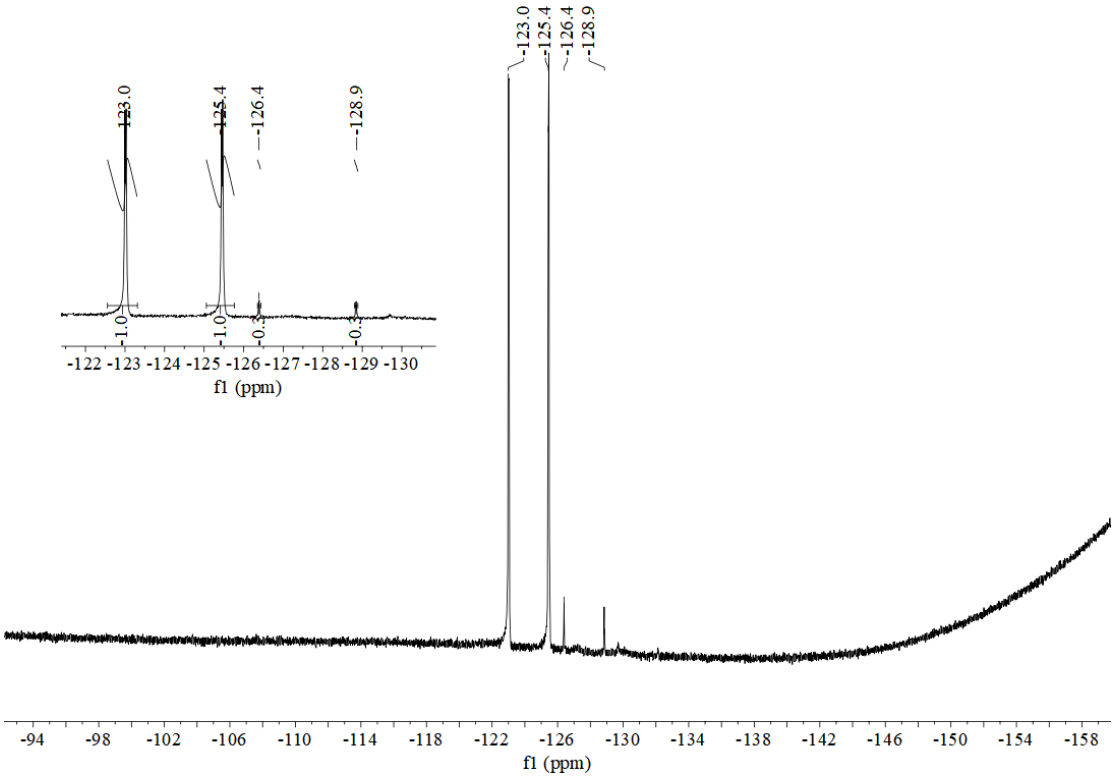

Figure S16. $^{19}F\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

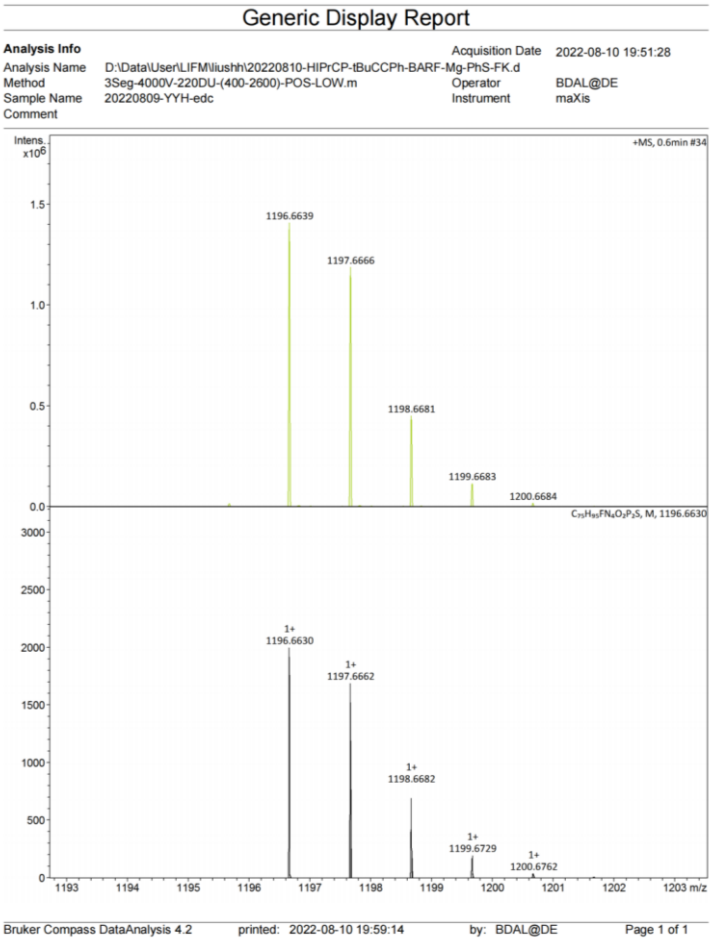

Figure S17. ESI-MS of **5**.

Preparation of $\mathbf{6}^{+}(BAr^{F})$: Sodium azide powder (130 mg, 2 mmol) was added to a stirred solution of $\mathbf{2a}^{\bullet+}(BAr^{F})$ (192.8 mg, 0.1 mmol) in tetrahydrofuran (5 mL) at room temperature. After stirring overnight, the resulting suspension was filtered and the filtrate was dried under reduced pressure. The remaining solid was extracted with the mixture of hexane and toluene (1:1), then filtered through celite and the resulting filtrate was dried under reduced pressure. Then, the remaining residue was washed with hexane and dried in vacuo to afford $\mathbf{6}^{+}(BAr^{F})$ as reddish powder, 143.6 mg. The powder was further purified via slow evaporation from a saturated hexane and tetrahydrofuran (1:1) solution at room temperature yielding crystalline reddish materials of $\mathbf{6}^{+}(BAr^{F})$, 30 mg, 14.6% yield. M. P. = 238.2 °C. ^{1}H NMR (CD_3CN, 400 MHz): δ = 7.71 (m, 7H, $C_{ar}H$), 7.69 (m, 4 H, $C_{ar}H$), 7.52 (m, 1 H, $C_{ar}H$), 7.44 (m, 4 H, $C_{ar}H$), 7.27 (m, 3 H, $C_{ar}H$), 7.17 (m, 6 H, $C_{ar}H$), 7.07 (m, 1 H, $C_{ar}H$), 6.99 (m, 1 H, $C_{ar}H$), 4.71 (m, 1 H, CHMe$_2$), 4.31 (m, 3 H, CHMe$_2$), 4.07 (m, 2 H, NCH_2), 3.78(m, 1 H, NCH_2), 3.67 (m, 4 H, CHMe$_2$),

3.48 (m, 1 H, NCH_2), 3.22 (m, 2 H, NCH_2), 3.06 (m, 1 H, NCH_2), 2.93 (m, 1 H, NCH_2), 1.85 (m, 4 H, CH_3), 1.51 (d, J = 8.0 Hz, 3 H, CH_3), 1.44 (d, J = 8.0 Hz, 3 H, CH_3), 1.38 (d, J = 8.0 Hz, 1H, CH_3), 1.30 (m, 5 H, CH_3), 1.20 (m, 11 H, CH_3), 1.13 (m, 4 H, CH_3), 1.09 (m, 10 H, CH_3), 1.01 (m, 9 H, CH_3), 0.95 (m, 3 H, CH_3), 0.86 (d, J = 4.0 Hz, 2 H, CH_3), 0.79 (d, J = 8.0 Hz, 2 H, CH_3); $^{13}C\{^1H\}$ NMR (CD_3CN, 100.5 MHz): δ = 162.2 (d, $^2J_{PC}$ = 50.3 Hz, PC*C*O), 161.2 (d, $^2J_{PC}$ = 50.3 Hz, PC*C*O), 144.3 (d, $^2J_{PC}$ = 40.0 Hz, P*C*C), 134.6 (s, C_{ar}), 130.6 (s, C_{ar}), 128.9 (s, C_{ar}), 128.2 (s, C_{ar}), 125.1 (s, C_{ar}), 123.1 (s, C_{ar}), 67.3 (s, OCH_2CH_3), 53.5 (s, NCH_2), 52.4 (s, NCH_2), 30.1 (CH_3), 29.8 (CH_3), 29.4 (CH_3), 27.9 (CH_3), 27.2 (CH_3), 25.7 (CH_3), 25.0 (CH_3), 24.2 (CH_3); $^{31}P\{^1H\}$ NMR (CD_3CN, 161.9 MHz) δ = 305.7 (s), 42.7 (s); UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)): 317.5 (4636.1), 389 (2226.6), 479 (3067.6); ESI-MS $[M]^+$ $C_{69}H_{90}N_7O_2P_2^+$ calc. 1110.663 m/z, found 1110.639 $[M]^+$.

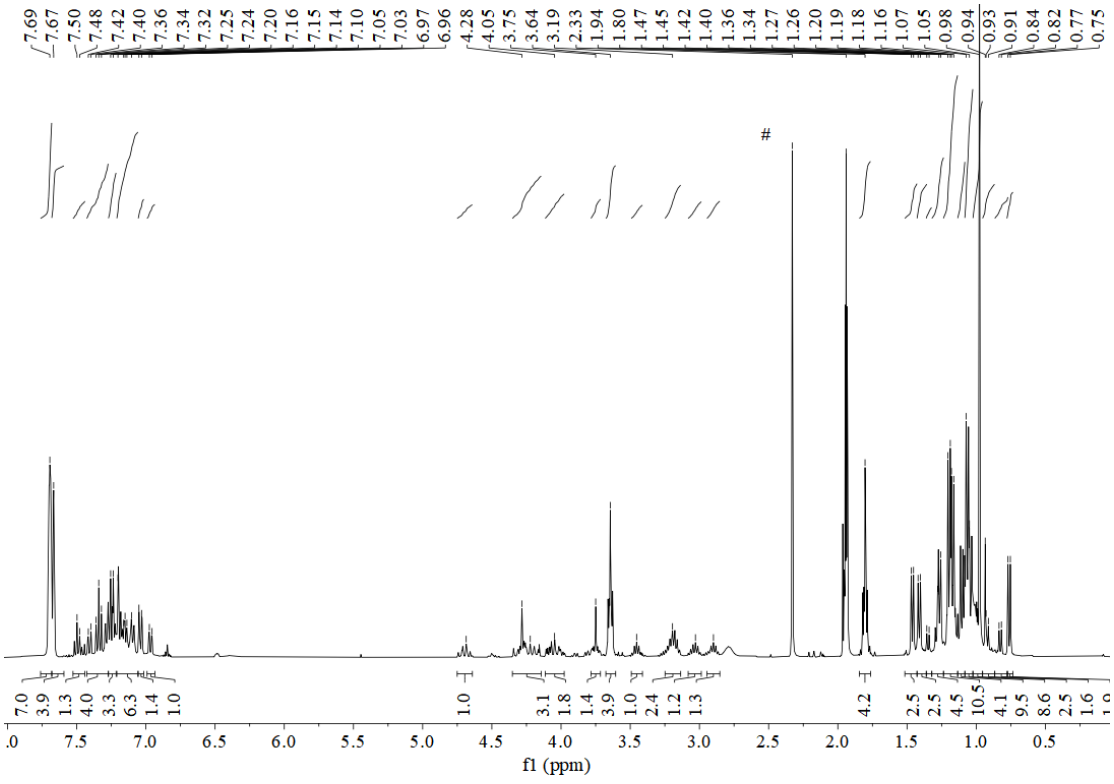

Figure S18. ^1H NMR spectrum of **6**$^+$(BAr^F) in CD_3CN. #Toluene

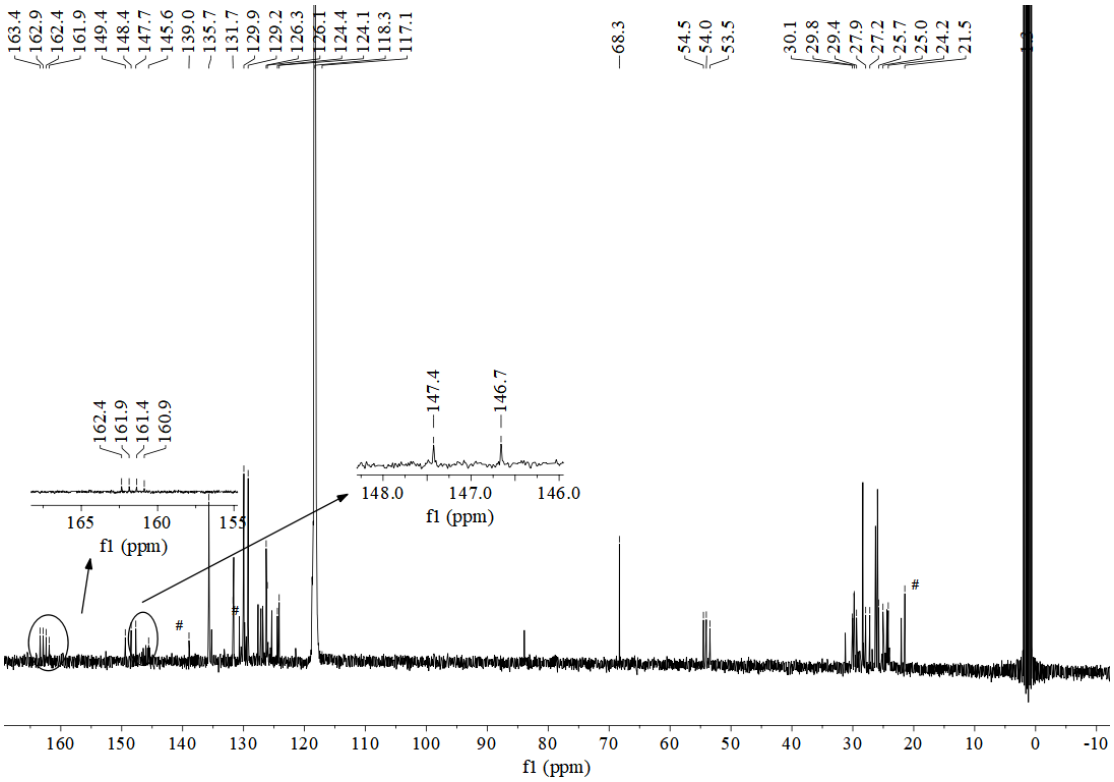

Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{6}^{+}(BAr^{F})$ in CD_3CN. #Toluene

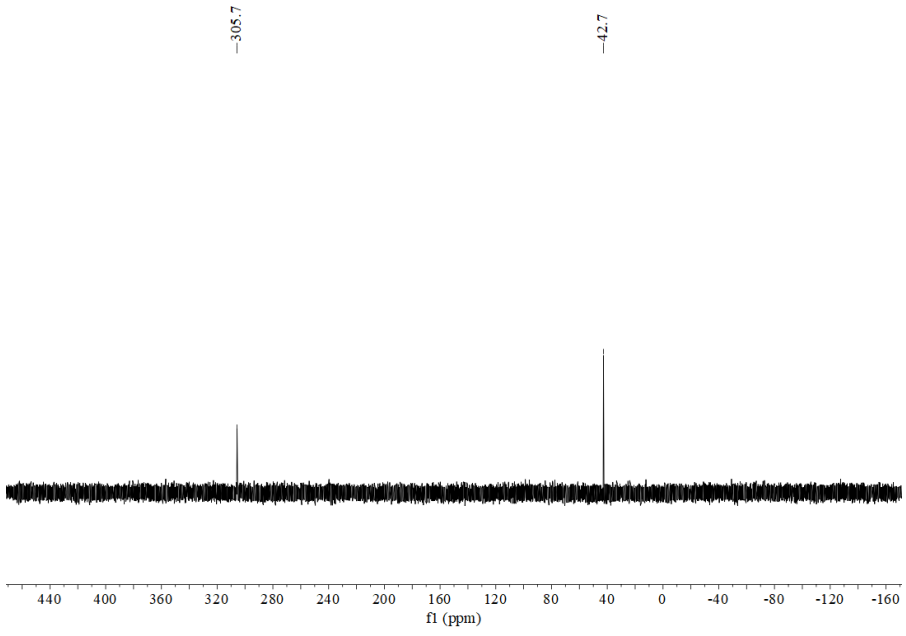

Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of $\mathbf{6}^{+}(BAr^{F})$ in CD_3CN.

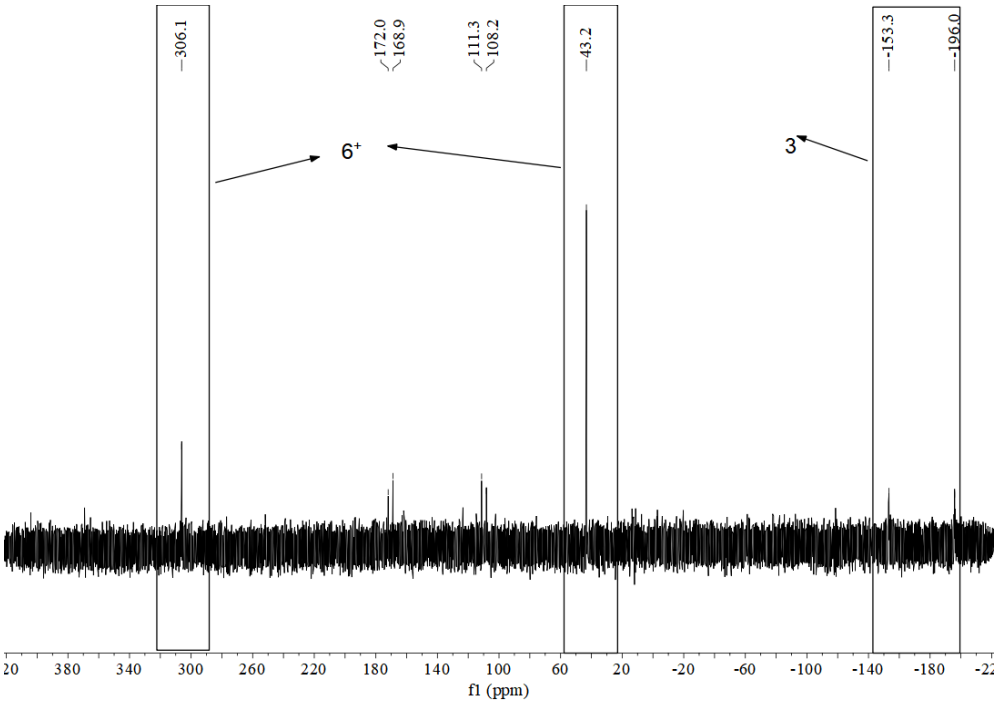

Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum of the mixture of Sodium azide powder and **2a**$^{\bullet+}$(BAr^{F}) in tetrahydrofuran.

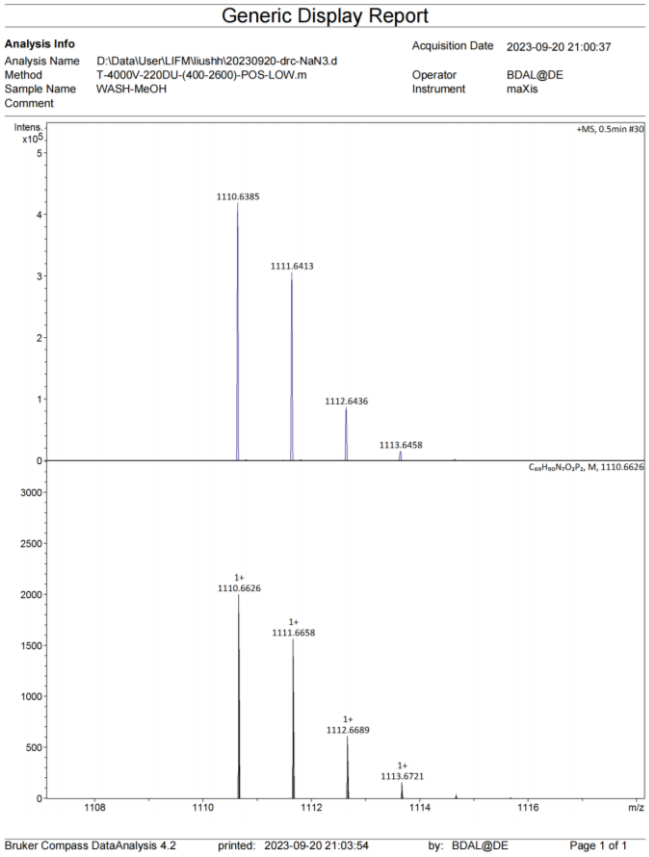

Figure S22. ESI-MS of **6**$^{+}$(BAr^{F}).

Preparation of $7^{\bullet+}(BAr^F)$: (Trimethylsilyl)diazomethane (1 equivalent in hexane, 1.0 M) was added dropwise to a stirred solution of $\mathbf{2b}^{\bullet+}(BAr^F)$ (188.9 mg, 0.1 mmol) in tetrahydrofuran (10 mL) at room temperature. After stirring for 0.5 hour, the solvent was removed under reduced pressure. Then, the remaining solid was washed with hexane and dried *in vacuo* to afford green powder as $\mathbf{7}^{\bullet+}(BAr^F)$, 148.0 mg, 0.075 mmol, 75.0% yield. Green crystals of $\mathbf{7}^{\bullet+}(BAr^F)$ were obtained from a solution of hexane and tetrahydrofuran at room temperature. M. P. = 210.2 °C (Decomposition). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$)):325 (37201), 382.5 (9900), 522 (13621).

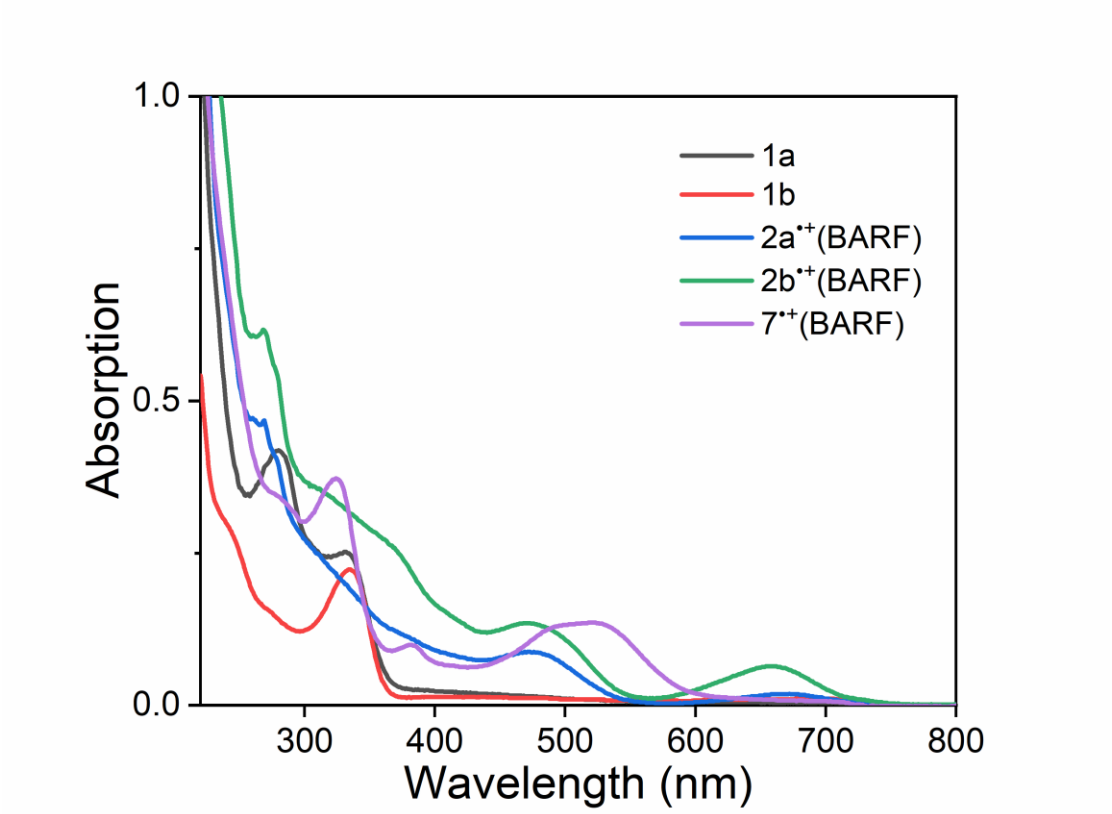

Figure S23. UV/Vis absorption spectra for 10^{-5} M tetrahydrofuran solution of **1a**, **1b**, $\mathbf{2a}^{\bullet+}(BAr^F)$, $\mathbf{2b}^{\bullet+}(BAr^F)$ and $\mathbf{7}^{\bullet+}(BAr^F)$.

S2. X-Ray Diffraction Studies

These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi, or by emailing data_request@ccdc.cam.ac.uk. The CCDC reference numbers are 2215136 - 2215138, 2215140 - 221543 and 2314776.

Table *S1*. The summary of crystal data and structure refinement.

Compounds	**1a**	**2a**$^{\bullet+}$(BAr^{F})	**2b**$^{\bullet+}$(BAr^{F})	**3**
CCDC	2215137	2215142	2215138	2215136
Empirical formula	$C_{71}H_{93}N_5O_2P_2$	$C_{101}H_{102}BF_{24}N_4O_2P_2$	$C_{195}H_{203}N_8O_8B_2F_{48}P_4$	$C_{72}H_{97}N_4O_2P_2$
Formula weight	1110.44	1932.61	3844.14	1112.47
Temperature/K	149.99(10)	150.0	103(5)	149.99(10)
Crystal system	orthorhombic	triclinic	triclinic	monoclinic
Space group	$Pna2_1$	P-1	P-1	$P2_1/n$
a/Å	30.4484(2)	12.9969(5)	14.7749(2)	12.33630(10)
b/Å	15.17880(10)	20.0236(7)	16.5982(2)	22.0219(2)
c/Å	14.02580(10)	20.1523(7)	20.9941(2)	24.3308(3)
α/°	90	106.472(2)	72.2590(10)	90
β/°	90	101.180(2)	77.1930(10)	96.0520(10)
γ/°	90	96.412(2)	89.9430(10)	90
Volume/Å^3	6482.31(8)	4855.8(3)	4769.40(10)	6573.08(11)
Z	4	2	1	4
ρ_{calc}g/cm^3	1.138	1.322	1.338	1.124
μ/mm^{-1}	0.967	0.141	1.279	0.949
F(000)	2400.0	2006.0	1995.0	2412.0
Crystal size/mm^3	0.2 × 0.1 × 0.1	0.03 × 0.03 × 0.01	0.21 × 0.16 × 0.14	0.3 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.806 to 148.304	2.154 to 54.286	5.604 to 148.584	5.426 to 148.152
Index ranges	-37 ≤ h ≤ 33, -18 ≤ k ≤ 18, -17 ≤ l ≤ 16	-16 ≤ h ≤ 16, -25 ≤ k ≤ 25, -24 ≤ l ≤ 24	-14 ≤ h ≤ 18, -20 ≤ k ≤ 20, -26 ≤ l ≤ 26	-15 ≤ h ≤ 13, -27 ≤ k ≤ 19, -30 ≤ l ≤ 28
Reflections collected	44409	92619	57770	37571
Independent reflections	12612 [R_{int} = 0.0382,	20436 [R_{int} = 0.0901,	18754 [R_{int} = 0.0397,	12964 [R_{int} = 0.0677,

	R_{sigma} = 0.0340]	R_{sigma} = 0.0924]	R_{sigma} = 0.0374]	R_{sigma} = 0.0608]
Data/restraints/parameters	12612/7/741	20436/258/1511	18754/0/1211	12964/0/726
Goodness-of-fit on F^2	1.034	1.024	1.041	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0331, wR_2 = 0.0800	R_1 = 0.0890, wR_2 = 0.1776	R_1 = 0.0607, wR_2 = 0.1652	R_1 = 0.0572, wR_2 = 0.1634
Final R indexes [all data]	R_1 = 0.0341, wR_2 = 0.0895	R_1 = 0.1929, wR_2 = 0.2327	R_1 = 0.0694, wR_2 = 0.1720	R_1 = 0.0640, wR_2 = 0.1699
Largest diff. peak/hole / e Å^{-3}	0.38/-0.27	0.38/-0.32	1.37/-0.60	0.55/-0.53
Flack parameter	0.007(6)			

to be continued:

Compounds	**4**$^{+}$(BAr^{F})	**5**	**6**$^{+}$(BAr^{F})	**7**$^{\bullet+}$(BAr^{F})
CCDC	2215140	2215143	2314776	2215141
Empirical formula	$C_{107}H_{107}BF_{24}N_4O_2P_2S$	$C_{300}H_{380}F_4N_{16}O_8P_8S_4$	$C_{102}H_{104}BF_{24}N_7O_2P_2$	$C_{100}H_{108}BF_{24}N_4O_4P_2Si$
Formula weight	2041.77	4790.18	1988.67	1986.74
Temperature/K	149.98(10)	149.99(10)	100.00(10)	150.0
Crystal system	triclinic	monoclinic	triclinic	triclinic
Space group	P-1	P2/n	P-1	P-1
a/Å	15.1726(2)	26.0037(8)	12.4929(2)	13.4882(6)
b/Å	16.6364(2)	13.0979(3)	18.7651(3)	17.4109(7)
c/Å	21.9306(2)	40.7620(9)	22.0705(2)	22.7720(9)
α/°	103.6170(10)	90	106.6200(10)	87.067(2)
β/°	108.0100(10)	95.402(2)	95.6430(10)	73.300(2)
γ/°	91.8250(10)	90	92.8630(10)	89.995(2)
Volume/Å^3	5083.56(11)	13821.6(6)	4917.25(12)	5115.0(4)
Z	2	2	2	2
ρ_{calc}g/cm^3	1.334	1.151	1.343	1.290

μ/mm^{-1}	1.405	1.235	1.253	0.149
F(000)	2120.0	5152.0	2064.0	2066.0
Crystal size/mm^3	0.1 × 0.1 × 0.05	0.06 × 0.06 × 0	0.2 × 0.2 × 0.15	0.2 × 0.2 × 0.15
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.502 to 148.654	7.082 to 148.88	4.208 to 151.558	2.342 to 54.274
Index ranges	-15 ≤ h ≤ 18, -20 ≤ k ≤ 15, -27 ≤ l ≤ 27	-32 ≤ h ≤ 32, -16 ≤ k ≤ 16, -30 ≤ l ≤ 49	-15 ≤ h ≤ 15, -23 ≤ k ≤ 23, -27 ≤ l ≤ 27	-17 ≤ h ≤ 17, -22 ≤ k ≤ 22, -29 ≤ l ≤ 29
Reflections collected	63197	85375	160084	157333
Independent reflections	20085 [R_{int} = 0.0309, R_{sigma} = 0.0302]	27437 [R_{int} = 0.0798, R_{sigma} = 0.0844]	19570 [R_{int} = 0.0974, R_{sigma} = 0.0441]	22499 [R_{int} = 0.0465, R_{sigma} = 0.0309]
Data/restraints/parameters	20085/172/1383	27437/0/1589	19570/290/1527	22499/79/1275
Goodness-of-fit on F^2	1.073	1.052	1.080	1.079
Final R indexes [I>=2σ(I)]	R_1 = 0.0781, wR_2 = 0.2170	R_1 = 0.0721, wR_2 = 0.1984	R_1 = 0.0953, wR_2 = 0.2679	R_1 = 0.0638, wR_2 = 0.1762
Final R indexes [all data]	R_1 = 0.0909, wR_2 = 0.2281	R_1 = 0.0996, wR_2 = 0.2163	R_1 = 0.1259, wR_2 = 0.2913	R_1 = 0.0787, wR_2 = 0.1867
Largest diff. peak/hole / e $Å^{-3}$	1.27/-0.75	1.42/-1.25	1.20/-0.83	1.31/-0.87
Flack parameter				

Table *S2*. The comparison of structure parameters.

	P2-C1	P2-C3	C1-C2	C3-C4	P1-C1	P1-C6	C6-C5	C5-C3
2a$^{\bullet+}$	1.735(4)	1.719(4)	1.444(6)	1.470(5)	1.785(5)	1.725(5)	1.412(6)	1.455(6)
2b$^{\bullet+}$	1.767(2)	1.724(2)	1.424(3)	1.479(3)	1.793(2)	1.747(3)	1.373(3)	1.458(3)
3	1.7911(19)	1.8387(17)	1.365(3)	1.383(2)	1.8075(19)	1.8408(17)	1.376(2)	1.468(2)
4^{+}	1.752(3)	1.723(3)	1.432(5)	1.473(4)	1.808(4)	1.818(3)	1.363(4)	1.487(4)
5	1.801(3)	1.798(3)	1.393(4)	1.395(3)	1.798(3)	1.825(3)	1.361(4)	1.489(3)
6^{+}	1.746(4)	1.723(4)	1.415(5)	1.470(5)	1.794(3)	1.814(4)	1.359(5)	1.483(4)
7$^{\bullet+}$	1.743(2)	1.789(2)	1.414(3)	1.498(3)	1.743(2)	1.867(2)	1.487(3)	1.381(3)

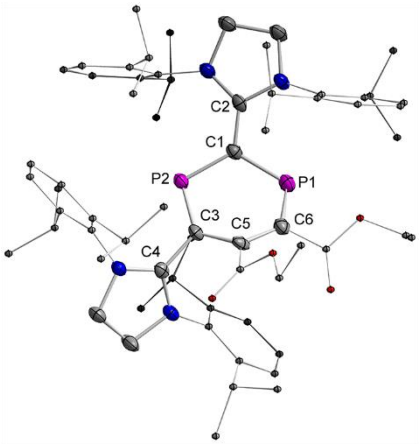

Figure S24. Molecular structure of **2b**$^{\bullet+}$(BAr^{F}) in the solid state (H atoms, solvents and anions were omitted for clarity; 50% probability thermal ellipsoids). Selected distances [Å] and angles [°]: P1-C1 1.793(2), P1-C6 1.747(3), C6-C5 1.373(3), C5-C3 1.458(3), C3-P2 1.724(2), P2-C1 1.767(2), C1-C2 1.424(3), C3-C4 1.479(3), P1-C1-P2 120.41(13), P1-C1-C2 113.38(16), C2-C1-P2 125.47(18), C1-P2-C3 103.82(11), P2-C3-C4 118.81(16), P2-C3-C5 125.59(17), C4-C3-C5 115.6(2), C3-C5-C6 122.7(2), C5-C6-P1 125.87(19), C6-P1-C1 102.01(11).

S3: EPR analysis

Table *S3*. Spin Hamiltonian parameters and spin populations from CW EPR experiments at RT and 100 K. All EPR data was processed and analyzed in Matlab R2019b and simulated using the EasySpin package (v. 5.2)

Interaction	Principal Values			Isotropic Values
	1	2	3	
2a$^{\bullet+}$(BAr^{F})				
g-matrix	2.0042	2.0091	2.0130	2.0105
^{31}P	-23.1	5.05	342.1	108
^{31}P	-25.3	10.58	49.23	11.5
2b$^{\bullet+}$(BAr^{F})				
g-matrix	N.A.	N.A.	N.A.	2.0077
^{31}P	N.A.	N.A.	N.A.	85.7
7$^{\bullet+}$(BAr^{F})				
g-matrix	2.0041	2.0165	2.0081	2.0096

^{31}P	-1.9	-2.8	317.7	104.4

N.A. equals “not available”.

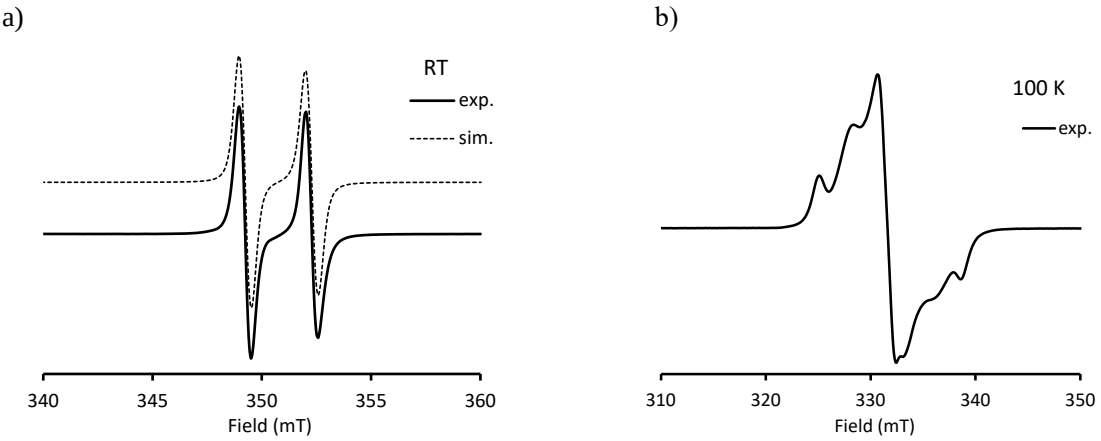

Figure S25. Continuous wave EPR spectra of **2b**$^{\bullet+}$(BAr^{F}) at RT and at 100 K.

S4: Theoretical Details

Geometry optimizations were performed using the Gaussian16 optimizer.[2] All geometry optimizations were computed using the functional M06-2X functional. The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima. The single-point energy calculations were performed at the M06-2X/Def2-TZVP level of theory for solution-phase (diethyl ether). The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with the corresponding solvent, while the Bondi radii were chosen as the atomic radii to define the molecular cavity.[3] The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution, respectively. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. NBO calculations were carried out using NBO 7.0 program[4] at the M06-2X/Def2-TZVP//M06-2X/Def2-SVP level of theory.

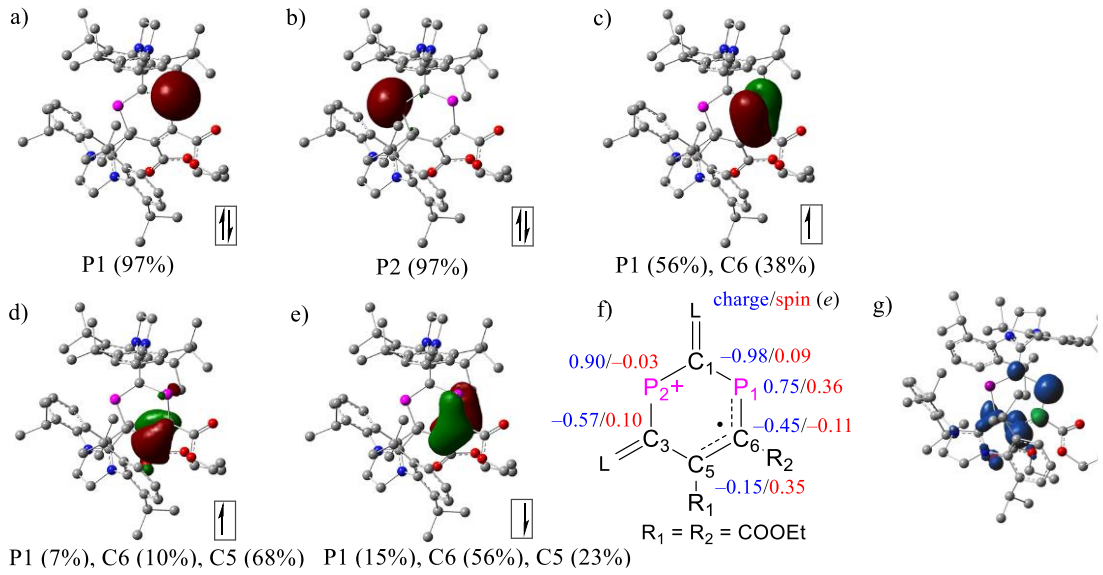

Figure S26. Selected NLMOs resulting from an NBO analysis of **2b**$^{\bullet+}$ (isovalue = 0.05; results for doubly occupied orbitals were obtained by averaging over the α and β spin orbitals: a) and b) unpaired s-type lone pairs; c) a π-bond α-electron; d) a π-type α-electron lone pair; e) a π-bond β-electron; f) selected NPA charges and spin populations; g) calculated spin density (density = 0.004) of **2b**$^{\bullet+}$.

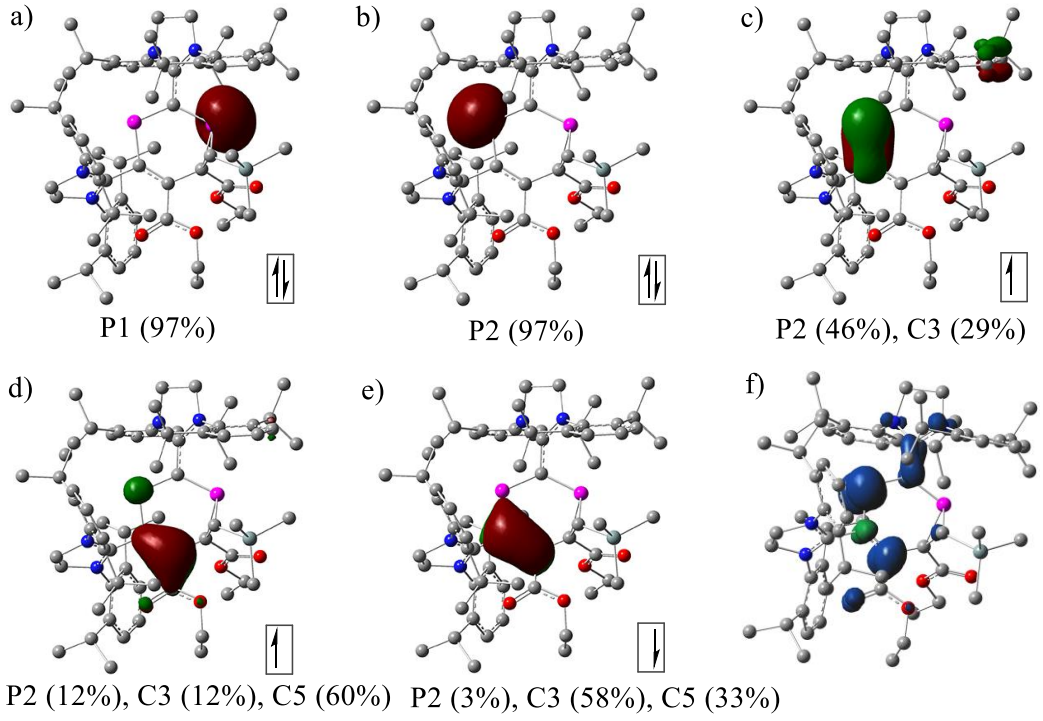

Figure S27. Selected NLMOs resulting from an NBO analysis of **7**$^{\bullet+}$ (isovalue = 0.05; results for doubly occupied orbitals were obtained by averaging over the α and β spin orbitals: a) and b) unpaired s-type lone pairs; c) a π-bond α-electron; d) a π-type α-electron lone pair; e) a π-bond β-electron; f) calculated spin density (density = 0.004) of **7**$^{\bullet+}$.

Cartesian Coordinates:

1a$^{\bullet+}$, E(solvation) = -3735.36793354

P	19.00888400	10.16822900	6.61340500
P	19.14040000	12.30749100	7.79670700
O	22.74970800	10.61496900	5.06769000
N	19.33735800	8.53701400	9.57513700
N	16.41234100	11.68261300	4.67763200
N	16.96946600	13.68342600	5.49489400
N	18.78763900	10.30374900	10.79298400
C	18.98513500	10.60992600	8.37116300
C	20.86867000	12.03472200	6.92852200
C	17.24612500	12.33335000	5.54197900
C	20.75004200	10.86566300	6.28281900
O	21.03991800	9.20839000	4.64709900
C	17.96977300	14.70225900	5.65556200
C	15.28313500	9.59123300	5.27387100
C	18.17486200	11.75491800	6.36316800
C	19.05523500	9.87348600	9.53023200
C	17.34989900	12.23590700	11.23779400
C	16.25464600	10.27037700	4.51656500
C	21.88864400	13.08179200	7.06369400
C	17.84558600	15.61754800	6.71785900
C	19.58662000	13.63135700	12.21423800
H	20.45086600	14.18612800	12.58511100
C	17.82207300	6.55149400	8.09889900
H	17.43039200	7.38636200	8.70144300
C	16.99342500	9.62473000	3.50223900
C	16.13149900	11.54031600	10.65686900
H	16.45355700	10.56084700	10.27230000
C	20.00079000	7.80734800	8.54249200
C	22.15743200	9.09770700	9.08252500
H	21.53983600	10.00728200	9.17512300
C	16.73568900	15.50636500	7.74536300
H	16.26335800	14.52185000	7.61189800
C	21.36570100	8.07899100	8.27281600
C	17.21544700	13.50595200	11.80487400
H	16.22591400	13.96501500	11.85816500
C	19.76769000	12.35030600	11.68514500
C	18.63332900	11.65801200	11.21469000
C	19.28858700	6.82896500	7.82851100
C	19.96358300	6.10107400	6.84118500
H	19.43006600	5.33253100	6.28031100
C	15.62682100	7.65031900	3.86016100
H	15.36158900	6.62893100	3.58284800
C	14.95762300	8.28319800	4.89997900
H	14.18517800	7.74335500	5.45209000
C	22.45652900	8.56837700	10.49133000
H	21.54151200	8.33211000	11.05012700
H	23.02249300	9.31471400	11.06942200
H	23.06221700	7.65189900	10.43200500
C	21.52960400	10.13253200	5.25210100
C	16.66546800	8.30125900	3.19777400
H	17.21603100	7.77392300	2.41933900
C	18.93954900	9.22421500	11.76749000
H	18.09482800	9.22580000	12.46916900
H	19.87170600	9.34539800	12.34680000
C	21.16089600	11.74818700	11.62610000
H	21.06984400	10.72115400	11.24721200
C	23.65979000	10.07899600	4.05590700
C	21.47272000	14.39317300	7.35151700
H	20.40811200	14.62979200	7.42677500
C	18.97224900	14.85154200	4.66924900
C	21.29560100	6.35799400	6.55535800
H	21.80646000	5.79302400	5.77437500
C	17.64996500	5.25158900	8.89315700
H	18.01611900	4.39453000	8.30778300
H	16.58993800	5.07462900	9.12663000
H	18.21485500	5.27181400	9.83646600
C	15.91334500	13.94958500	4.51252800
H	16.35417500	14.37736100	3.59624600
H	15.17799400	14.66262100	4.90799300
C	18.74339700	16.69066500	6.77967200
H	18.64780600	17.42233600	7.58404500
C	23.26773300	12.82033700	6.97341000
H	23.60709600	11.81167500	6.76074200
C	18.31865400	14.19798200	12.29363400
H	18.19039400	15.18941100	12.73079500
C	15.32195300	12.56571300	4.26336300
H	14.42572900	12.38580300	4.88114800
H	15.05443900	12.38949000	3.21341500
C	18.96129900	7.97854400	10.87314800
H	19.69241100	7.22524200	11.19437100
H	17.96828700	7.50121300	10.82466100
C	21.98461500	7.34109600	7.26264600
H	23.03037500	7.52609300	7.02227700
C	14.64580100	10.19507800	6.51487700
H	15.00783200	11.22920700	6.62540400

C	24.19287500	13.84016700	7.16933900	H	16.45735200	15.47163400	9.89708700
H	25.25918300	13.61757800	7.10734000	H	17.76043700	16.54880800	9.37416700
C	19.85833700	15.92547000	4.78770400	C	18.88028700	14.75060500	2.16086400
H	20.64316700	16.05570000	4.03992100	H	17.92711900	15.29953800	2.16770200
C	23.46620700	9.51214000	8.41138200	H	18.88811400	14.08455400	1.28635900
H	24.20428000	8.69559300	8.43473000	H	19.68497400	15.48803800	2.02498400
H	23.90550400	10.36781500	8.94371700	C	17.50659500	11.29107000	1.67975900
H	23.31065700	9.80231400	7.36275400	H	16.93652900	10.70696900	0.94176400
C	23.76527900	15.14013000	7.44533000	H	18.31488400	11.81332600	1.14598500
H	24.49532700	15.93621400	7.59836200	H	16.83664600	12.05094000	2.10479300
C	19.73984900	16.84700200	5.82326900	C	22.04141900	12.51025800	10.63254800
H	20.42634200	17.69327400	5.88021100	H	21.59232200	12.51489000	9.62872300
C	15.05296500	11.30606000	11.71868200	H	23.03617900	12.04430300	10.55821700
H	15.44851600	10.73996000	12.57397200	H	22.18151800	13.55825100	10.93897400
H	14.21002500	10.74197700	11.29291900	C	20.41469400	13.19082400	3.41486300
H	14.65629800	12.25834400	12.10155900	H	21.26640600	13.88326300	3.32752200
C	18.09203300	10.36237800	2.75067200	H	20.43920900	12.51272400	2.54713800
H	18.62739200	10.98412900	3.49105300	H	20.55795200	12.59397400	4.32601800
C	21.81171900	11.67752900	13.01038700	C	19.11695600	9.42548100	2.11376600
H	21.98576300	12.68326500	13.42088900	H	19.52570900	8.71586100	2.84489900
H	22.78665700	11.17170000	12.95108700	H	19.95224000	10.01729600	1.71115300
H	21.18072600	11.12973500	13.72542300	H	18.68080600	8.86875900	1.27072300
C	17.01734200	6.51999600	6.80063300	C	23.03967300	10.23002900	2.67154900
H	17.16216300	7.44530100	6.22374000	H	22.16720700	9.57716700	2.55270100
H	15.94409600	6.41218600	7.01547600	H	23.78736800	9.96349000	1.91169000
H	17.30675300	5.67362200	6.16003600	H	22.73902700	11.27487500	2.50597800
C	22.40118900	15.41409500	7.52955700	C	13.11720600	10.22346600	6.43654700
H	22.05194600	16.42557900	7.74158700	H	12.76590100	10.75302800	5.53913200
C	15.67183800	16.58482000	7.50690800	H	12.69570300	10.72451300	7.32032200
H	16.09673800	17.58971400	7.65271400	H	12.70220800	9.20511800	6.40458800
H	14.83561900	16.46563800	8.21117100	C	24.88891900	10.96633700	4.19862700
H	15.27056200	16.54023800	6.48435800	H	24.62197600	12.01945600	4.03216000
C	15.58073500	12.34759300	9.47451100	H	25.65079800	10.67247900	3.46422400
H	15.34571800	13.37990800	9.77631600	H	25.32090800	10.86731400	5.20533700
H	14.65385700	11.89841000	9.08899400	C	23.99705500	8.62873700	4.38365200
H	16.31008700	12.38774200	8.64850900	H	24.44291700	8.56135000	5.38729900
C	15.12312700	9.41991600	7.75082400	H	24.73578200	8.25872400	3.65897600
H	14.87115900	8.35259600	7.66356000	H	23.10470600	7.99259800	4.33437300
H	14.64252800	9.80113100	8.66344000				
H	16.21586500	9.50909000	7.87218900	**TS1**, E(solvation) = -3735.35414109			
C	19.08307300	13.94620100	3.45132500	P	0.84075500	0.83292300	0.5209350
H	18.28712200	13.19047500	3.49908700	P	-0.28940800	-1.22992400	-0.8184690
C	17.27719200	15.58076400	9.17278100	O	-1.36548200	0.70563800	3.4561690
H	18.01066100	14.78375100	9.37059200	N	3.73105700	-0.94222700	0.4091920

N	-1.16606000	2.96860900	-1.0949730	C	-1.46365400	1.11674000	2.2020230
N	-2.76861200	1.46258600	-1.4208760	C	1.94412500	5.00068300	-0.9496630
N	2.77120400	-2.76648100	-0.3795480	H	2.48846600	5.63131700	-0.2451650
C	1.33104500	-0.79266000	-0.1003350	C	4.19921000	-3.06432800	-0.3992230
C	-1.19378800	-1.12098800	0.8339790	H	4.60711200	-2.97072700	-1.4207800
C	-1.47272500	1.64563200	-1.0770390	H	4.38689300	-4.08511700	-0.0397970
C	-0.82773400	0.15464400	1.2488540	C	1.51737600	-4.61758500	1.4299070
O	-1.93005900	2.17014100	1.8362170	H	2.53695500	-4.21021700	1.5165370
C	-3.52146600	0.24057800	-1.3571470	C	-1.57944900	1.59831500	4.6033470
C	0.53897700	3.42137300	-2.7965070	C	-2.46642600	-3.20037900	0.4931880
C	-0.55681100	0.65090700	-0.6463340	H	-2.02224000	-3.27758400	-0.5008120
C	2.53512900	-1.46945300	-0.0147310	C	-4.50670900	0.10029700	-0.3574960
C	1.55421500	-3.65478100	-2.3049270	C	4.19353000	2.57130500	2.6610920
C	0.09464700	3.54976700	-1.4631890	H	4.32395400	3.48384300	3.2451460
C	-2.15037200	-2.09623800	1.3125760	C	5.71624200	2.49449600	-1.3306470
C	-3.31156400	-0.75633400	-2.3387600	H	5.21204500	3.47285000	-1.3079150
C	0.12057400	-5.33904000	-0.5685560	H	6.06902800	2.33382400	-2.3587010
H	-0.43081100	-6.01275700	0.0894060	H	6.59384400	2.54154800	-0.6704680
C	4.75728500	1.37405000	-0.9322570	C	-3.37978000	2.74946000	-1.7910640
H	5.26268400	0.41174300	-1.1170750	H	-4.38830900	2.83047200	-1.3752160
C	0.78050900	4.34819900	-0.5281410	H	-3.44573300	2.84040200	-2.8867970
C	2.38550200	-2.80564600	-3.2505600	C	-4.07413600	-1.92408300	-2.2537160
H	2.93214200	-2.06560400	-2.6456540	H	-3.92783600	-2.71658900	-2.9863200
C	3.86139000	0.25633500	1.1747220	C	-2.71961100	-2.04023400	2.6036500
C	3.00082500	-0.99985000	3.2450220	H	-2.44057300	-1.23195500	3.2779310
H	2.80559400	-1.77727700	2.4899200	C	-0.17504400	-5.31263700	-1.9296870
C	-2.38190800	-0.53288500	-3.5234000	H	-0.96108100	-5.95768700	-2.3262110
H	-1.47784800	-0.01897000	-3.1603520	C	-2.40255000	3.75370200	-1.1849670
C	3.51976100	0.24416700	2.5399650	H	-2.24756900	4.63868200	-1.8139000
C	0.55225600	-4.49750800	-2.7934630	H	-2.71029600	4.06897600	-0.1740200
H	0.33787100	-4.51805200	-3.8638790	C	4.74801800	-1.98550400	0.5280280
C	1.12917800	-4.52863700	-0.0382690	H	4.81949400	-2.34073300	1.5709800
C	1.79769700	-3.65498000	-0.9195210	H	5.73161100	-1.60665700	0.2207850
C	4.38394100	1.40340500	0.5421690	C	3.69475100	1.42610300	3.2691250
C	4.53180900	2.56104000	1.3094500	H	3.44989800	1.44484600	4.3330850
H	4.92956300	3.46739800	0.8534960	C	-0.18481900	2.58042100	-3.8350710
C	2.40169600	4.88272300	-2.2579340	H	-1.15225400	2.25980000	-3.4213250
H	3.30391600	5.41056100	-2.5710300	C	-3.59126200	-3.03205400	3.0357200
C	1.70402000	4.09803000	-3.1693260	H	-4.01707300	-2.97549700	4.0386560
H	2.06841800	4.01169100	-4.1946540	C	-5.25325900	-1.08282400	-0.3313810
C	4.04261300	-1.54291900	4.2312880	H	-6.02114900	-1.21451600	0.4325090
H	5.00877700	-1.73565100	3.7433550	C	1.67817200	-0.72436400	3.9624880
H	3.68978000	-2.48007400	4.6865730	H	1.81714600	0.02122100	4.7605770
H	4.22226800	-0.82078200	5.0421010	H	1.29137200	-1.64148300	4.4302030

H	0.90744000	-0.34682500	3.2750890
C	-3.90741700	-4.11043600	2.2042010
H	-4.58630600	-4.88993600	2.5527220
C	-5.03506800	-2.08906200	-1.2607150
H	-5.62151500	-3.00793300	-1.2171220
C	3.40843400	-3.68096600	-3.9861580
H	4.04446000	-4.24215900	-3.2865890
H	4.05486400	-3.06612100	-4.6293410
H	2.89359300	-4.41519800	-4.6242170
C	0.23590900	4.58573600	0.8686290
H	-0.51934700	3.81038800	1.0663440
C	1.55378300	-6.06410900	1.9287900
H	0.54374900	-6.49566900	1.9873350
H	1.98057500	-6.10124900	2.9411290
H	2.16150300	-6.70414300	1.2736560
C	3.50182200	1.41902000	-1.8134050
H	2.89993500	0.50600700	-1.7167800
H	3.77898100	1.53716500	-2.8725470
H	2.87171400	2.27766500	-1.5311890
C	-3.33467800	-4.19238300	0.9348220
H	-3.56581800	-5.03621700	0.2821660
C	-3.05505100	0.37490200	-4.5616450
H	-3.95213600	-0.11433100	-4.9696080
H	-2.36823300	0.57876200	-5.3970830
H	-3.36743200	1.33565500	-4.1339280
C	1.52608000	-2.02617100	-4.2429580
H	1.02946300	-2.69727300	-4.9603370
H	2.14741100	-1.32499100	-4.8197420
H	0.74993500	-1.45272000	-3.7182480
C	0.62440200	1.31612300	-4.1363120
H	1.59500400	1.57285000	-4.5891170
H	0.08578400	0.65992600	-4.8378140
H	0.82676200	0.75038700	-3.2127700
C	-4.85492800	1.20296900	0.6299320
H	-4.06712000	1.96871100	0.5917370
C	-1.93743500	-1.82777800	-4.1997100
H	-1.46760800	-2.51948400	-3.4839990
H	-1.20761700	-1.59902500	-4.9886890
H	-2.78366400	-2.33586800	-4.6850430
C	-6.20493900	1.83577700	0.2572750
H	-6.24651600	2.15881000	-0.7929740
H	-6.41542100	2.70419100	0.8982690
H	-7.01768300	1.10777700	0.3995880
C	-0.45272300	5.95602800	0.9349550
H	0.27793900	6.76421800	0.7773100
H	-0.91873000	6.10599000	1.9200210
H	-1.23227200	6.06117000	0.1665980
C	0.60922200	-3.76372900	2.3185520
H	0.61658400	-2.70686900	2.0089040
H	0.94378200	-3.81974800	3.3658740
H	-0.43101200	-4.12320200	2.2728400
C	-4.90887200	0.70541200	2.0740250
H	-5.68175400	-0.06509200	2.2113600
H	-5.15017800	1.54103400	2.7455740
H	-3.95041000	0.27368700	2.3895700
C	1.31819900	4.47262900	1.9422580
H	1.77569000	3.47350000	1.9368680
H	0.88776800	4.65643400	2.9368600
H	2.11643800	5.21649500	1.7973460
C	-3.02947100	2.05721000	4.6668310
H	-3.29301200	2.66607200	3.7943230
H	-3.16802100	2.66001600	5.5754240
H	-3.70468300	1.19184300	4.7254040
C	-0.48971900	3.37003400	-5.1111560
H	-1.05743100	4.28526200	-4.8893050
H	-1.08233700	2.75634300	-5.8050350
H	0.43075600	3.66392300	-5.6359080
C	-1.24451800	0.71382100	5.7950430
H	-1.90938400	-0.16101000	5.8222600
H	-1.37581200	1.28056300	6.7265150
H	-0.20632000	0.36267300	5.7370510
C	-0.60846600	2.76650300	4.4888420
H	0.41264700	2.39452300	4.3118230
H	-0.61393500	3.34096200	5.4256390
H	-0.89208400	3.43424100	3.6656930

IN1, E(solvation) = -3735.39203599

P	18.55031800	9.79855300	6.68965500
P	18.65066900	12.31859400	7.92402800
O	21.99655000	11.51845600	4.82466500
N	19.21262100	8.48581500	9.57422100
N	16.76512500	11.51550300	4.35776800
N	17.72664500	13.46681000	4.67743200
N	18.99597900	10.33073300	10.77724000
C	18.82681900	10.52727100	8.29971900
C	20.32069900	12.63827900	7.12981800
C	17.66029600	12.18233700	5.08232400
C	19.98799500	12.04007900	5.96022700

O	20.03728800	11.26843200	3.74159200	H	21.36862500	10.61073100	11.04490400
C	18.25502700	14.59590000	5.39856300	C	22.83001900	10.80367600	3.85232700
C	15.39771800	9.76780900	5.42264600	C	21.14628400	14.42799100	8.57598300
C	18.54553100	11.61899900	6.12420900	H	20.11009500	14.57993400	8.88777100
C	19.01051600	9.83964800	9.50047900	C	19.44561800	15.20195700	4.95691000
C	17.74820900	12.38235300	11.22458100	C	20.81780800	6.07561200	6.52914200
C	16.29299500	10.15653300	4.40495600	H	21.23987200	5.44520700	5.74517600
C	21.44543100	13.40835600	7.65571400	C	17.42761800	5.20534000	9.34488200
C	17.51670800	15.10758600	6.48939900	H	17.71905100	4.29437100	8.80023000
C	20.16952100	13.72143400	11.72620400	H	16.39593800	5.07135800	9.70183600
H	21.10102800	14.24431800	11.95160100	H	18.08890600	5.29227500	10.21909100
C	17.53181000	6.42901800	8.42739400	C	17.05686700	13.60977400	3.37727600
H	17.22663200	7.32203700	8.99598100	H	17.80648900	13.53594600	2.57284600
C	16.61001000	9.31919700	3.32262900	H	16.54898300	14.57762100	3.30206500
C	16.43600400	11.62118600	11.12800700	C	18.05949800	16.19569400	7.18167700
H	16.63455100	10.67138300	10.60854000	H	17.53229700	16.60583200	8.04110700
C	19.75339100	7.67582300	8.53162600	C	22.78165000	13.22354800	7.25772800
C	21.93815500	8.99850100	8.72690000	H	23.02352100	12.43086600	6.55341500
H	21.28444300	9.82650400	9.03548000	C	18.96323000	14.41339000	11.76578000
C	16.13304400	14.58590100	6.86118100	H	18.95337700	15.47660700	12.01162200
H	16.14862200	13.48256200	6.81955700	C	16.11942500	12.40947100	3.37872900
C	21.07241400	7.92241600	8.08820500	H	15.09870100	12.64483300	3.72070800
C	17.76322800	13.74533000	11.53340500	H	16.05726500	11.90932900	2.40564500
H	16.82208300	14.29107100	11.61926400	C	19.03093300	8.00257100	10.93926400
C	20.20765700	12.35941400	11.41186300	H	19.76790100	7.22312900	11.17378500
C	18.98489900	11.71395700	11.12680700	H	18.02166700	7.57746400	11.07416300
C	18.96393100	6.65358400	7.97922700	C	21.57971800	7.10733100	7.07530300
C	19.52431000	5.84962300	6.98094100	H	22.59574600	7.26700600	6.71279800
H	18.93136600	5.04578200	6.54155200	C	15.14102500	10.61850600	6.65734100
C	15.02217300	7.70539800	4.19146100	H	16.03626500	11.23714700	6.83256000
H	14.50733800	6.74772800	4.10232100	C	23.78405400	14.04113200	7.77255000
C	14.75966200	8.53510000	5.27906900	H	24.81903600	13.88262500	7.46566900
H	14.05331800	8.20515300	6.04074300	C	19.93392500	16.29736200	5.67488300
C	22.62727100	8.44522100	9.98005100	H	20.86083000	16.77691200	5.35949500
H	21.89239500	8.07848900	10.71310800	C	22.94909800	9.61640200	7.76364500
H	23.23717600	9.22241300	10.46523000	H	23.71991500	8.89688300	7.44629800
H	23.28655900	7.60360500	9.71969200	H	23.46647300	10.45379000	8.25644000
C	20.67957600	11.59336500	4.71731600	H	22.44103300	10.01160000	6.86971100
C	15.95959900	8.08298300	3.24027200	C	23.47297000	15.06105900	8.67428300
H	16.19098700	7.41220600	2.41084100	H	24.26320700	15.70264200	9.06704300
C	19.22022700	9.27631700	11.76660700	C	19.25790000	16.77997800	6.78678100
H	18.49555300	9.35817700	12.58770100	H	19.66045400	17.62661000	7.34482800
H	20.23402600	9.34193300	12.19274700	C	15.93577600	11.29713200	12.54276600
C	21.51402500	11.58827300	11.52480200	H	16.69450900	10.75661200	13.12627300

H	15.02557200	10.68133700	12.50238500
H	15.69896700	12.22369800	13.08756500
C	17.65931900	9.68218000	2.28777100
H	18.04132200	10.68687400	2.51489300
C	21.83595500	11.35679100	13.00939800
H	22.08057900	12.31240200	13.49767200
H	22.70410400	10.68940100	13.11695800
H	20.98782700	10.91885000	13.55494200
C	16.58177600	6.30681800	7.23442800
H	16.71737900	7.14743600	6.53875800
H	15.53613100	6.30347800	7.57829500
H	16.74742300	5.37155700	6.67865500
C	22.15039000	15.25405800	9.07229100
H	21.89912100	16.04874700	9.77716500
C	15.07801100	15.08824200	5.86503700
H	15.08031700	16.18793500	5.83253600
H	14.07509400	14.75873700	6.17314400
H	15.25156700	14.72172900	4.84557300
C	15.36330900	12.36246900	10.33536600
H	15.13168700	13.34413800	10.77369900
H	14.42780300	11.78398100	10.33118100
H	15.68482700	12.51707100	9.29439000
C	14.96531400	9.74830600	7.90417500
H	14.00069500	9.21975700	7.89881200
H	14.99014200	10.37429900	8.80369400
H	15.77303700	9.00448800	7.97610100
C	20.16268000	14.75503400	3.69705400
H	19.82415900	13.73733300	3.45317200
C	15.70925500	14.98827600	8.27177400
H	16.46631700	14.70351700	9.01712600
H	14.76231900	14.49499000	8.53011900
H	15.53575200	16.07247100	8.33727100
C	19.78637000	15.68229800	2.53165500
H	18.69847300	15.74016000	2.38390600
H	20.24589500	15.33353100	1.59536000
H	20.14511100	16.70395300	2.72772800
C	17.09857300	9.67290600	0.86269900
H	16.76647500	8.66553400	0.57122500
H	17.87203000	9.98577800	0.14684800
H	16.23570800	10.34696000	0.75159400
C	22.70213600	12.25122700	10.83021500
H	22.53049300	12.36363100	9.75235500
H	23.60480100	11.63817600	10.97450100
H	22.91773900	13.24691900	11.24561200
C	21.68244400	14.71487500	3.86693000
H	22.09628900	15.72054200	4.02840200
H	22.14438900	14.32216000	2.95121200
H	21.98457000	14.08132500	4.71344700
C	18.85253700	8.72990800	2.42007600
H	19.23004800	8.72814400	3.45278800
H	19.66640200	9.04555500	1.75073800
H	18.56747600	7.70065400	2.15319700
C	22.75832100	11.45554200	2.47674100
H	21.73792400	11.43655000	2.07715200
H	23.41566200	10.90080800	1.79247900
H	23.11787500	12.49164200	2.52278800
C	13.95407700	11.56761200	6.46769900
H	14.11016400	12.24661100	5.61630600
H	13.80741400	12.18347700	7.36901800
H	13.02886500	11.00156600	6.28298000
C	24.23015000	10.94168400	4.43496000
H	24.50412700	12.00308000	4.52253800
H	24.95796600	10.44790900	3.77711100
H	24.28427900	10.47668700	5.42929100
C	22.39025800	9.34429400	3.81509600
H	22.34930500	8.92957900	4.83292800
H	23.11561200	8.76251100	3.22930800
H	21.40255300	9.24113800	3.35191100

TS2, E(solvation) = -3735.37224976

P	0.13668400	1.45717800	-0.21997300
P	-0.83813200	-0.91810600	1.10926600
O	1.64768000	-2.43868300	-2.56913900
N	-2.98248000	2.21093800	-0.68171400
N	3.26505000	1.24732500	0.77644800
N	3.18469900	-0.93485800	1.17770100
N	-3.78081000	0.63212200	0.63231400
C	-1.33182200	0.59497700	0.19807500
C	-0.18027700	-1.90370500	-0.30744000
C	2.50790200	0.14280100	0.68752200
C	0.93442500	-1.21522600	-0.65230800
O	2.87815900	-0.69487300	-1.89994700
C	2.54672400	-2.01089200	1.90305900
C	2.39680300	3.46838100	1.34685300
C	1.16860700	0.02239600	0.16702600
C	-2.65220300	1.11572700	0.05356700
C	-3.72529800	-0.87020100	2.58659200
C	2.95528600	2.59711700	0.38506900

C	-0.82334700	-3.15095000	-0.75769300
C	2.05389000	-1.74132300	3.19564700
C	-4.77065400	-2.91899600	0.96711500
H	-5.17072500	-3.72373500	0.34800800
C	-2.30964800	4.94997500	-0.01815300
H	-2.81938100	4.19804100	0.60398600
C	3.29385800	3.04101900	-0.90524500
C	-3.20017400	0.24661900	3.47132300
H	-2.59928300	0.91858900	2.83545900
C	-2.13031400	2.92992800	-1.57837900
C	-2.24866900	0.96852200	-3.23136700
H	-2.80328800	0.51487400	-2.39696000
C	2.36985300	-0.45803400	3.94189200
H	2.86658800	0.23210500	3.24837200
C	-1.71858900	2.31866200	-2.78001800
C	-3.97129800	-2.14276400	3.10758200
H	-3.75793600	-2.34582000	4.15697100
C	-4.55317300	-1.65897600	0.40230000
C	-3.99958400	-0.65669700	1.22249400
C	-1.74771400	4.23924700	-1.23643200
C	-0.85448600	4.90111000	-2.08304300
H	-0.52780600	5.91233100	-1.83416100
C	2.47823300	5.24851100	-0.30124600
H	2.29551100	6.29062100	-0.56927700
C	2.18513700	4.79828200	0.98215500
H	1.77643100	5.49456600	1.71672400
C	-3.23059000	1.15335100	-4.39600500
H	-4.04890100	1.83861500	-4.13121100
H	-3.66690700	0.18735200	-4.69032900
H	-2.71771700	1.57473700	-5.27378600
C	1.91883800	-1.42099300	-1.76754800
C	3.02198800	4.37430600	-1.23228000
H	3.26626800	4.73485400	-2.23336700
C	-4.91432600	1.53574300	0.40606100
H	-5.08891600	2.15092900	1.30256000
H	-5.82536400	0.96157200	0.19414000
C	-4.87536800	-1.42577200	-1.06500800
H	-4.86417800	-0.34282500	-1.25734200
C	2.39654800	-2.66822200	-3.80662300
C	-1.39592900	-3.97315900	0.22831800
H	-1.35334700	-3.66603300	1.27631300
C	2.46075000	-3.30296700	1.34752200
C	-0.37679100	4.28908200	-3.23678500
H	0.32997200	4.81565700	-3.88011800
C	-3.33654400	6.00707700	-0.44518300
H	-2.85009800	6.79154800	-1.04437200
H	-3.78904400	6.48591200	0.43529200
H	-4.14110500	5.57907000	-1.06077500
C	4.58649100	-0.57456300	1.42311600
H	5.22164000	-0.98518200	0.62288900
H	4.92026500	-0.98220900	2.38591900
C	1.33238300	-2.73995700	3.85740000
H	0.93240600	-2.54219600	4.85388700
C	-0.91709000	-3.55512500	-2.09954900
H	-0.52377900	-2.90612000	-2.87676600
C	-4.47934300	-3.16038700	2.30486300
H	-4.65770200	-4.14936000	2.73013300
C	4.56281900	0.95905700	1.39649300
H	4.61116900	1.41762900	2.39811800
H	5.36630900	1.38451400	0.78125500
C	-4.43246000	2.37768400	-0.76834000
H	-4.79168500	2.00315800	-1.74348000
H	-4.70712000	3.43614200	-0.67959900
C	-0.82385400	3.01953400	-3.59165000
H	-0.47490000	2.56774200	-4.52212600
C	2.04489300	3.01957100	2.75412900
H	2.09481100	1.92454400	2.77097600
C	-1.52469400	-4.76025100	-2.43647600
H	-1.58850300	-5.05753400	-3.48476800
C	1.72386100	-4.26748400	2.04155500
H	1.61122200	-5.26456500	1.61722900
C	-1.13131900	-0.00327500	-3.61670300
H	-0.55810800	0.36971400	-4.47875900
H	-1.56078000	-0.97713700	-3.89799800
H	-0.43321500	-0.16442700	-2.78061600
C	-2.06174500	-5.58363400	-1.44467600
H	-2.53235700	-6.53063000	-1.71281800
C	1.13729100	-3.98322400	3.27102000
H	0.56018800	-4.75002400	3.79011800
C	-4.36461600	1.05364800	4.06112900
H	-5.02520000	1.45596900	3.28152000
H	-3.98906400	1.89359500	4.66341600
H	-4.97675800	0.41188900	4.71235900
C	3.95499000	2.15230400	-1.93943000
H	4.07217200	1.15075400	-1.51042600
C	-6.26499100	-1.94161100	-1.44599700
H	-6.31773700	-3.03831000	-1.38719800
H	-6.50143800	-1.65925900	-2.48179800

H	-7.04437000	-1.53034400	-0.78816200
C	-1.21140100	5.57955200	0.83688400
H	-0.44378400	4.83676600	1.08398800
H	-1.63315500	5.97976800	1.77076800
H	-0.72088300	6.41328200	0.31131100
C	-2.00256600	-5.18091600	-0.11137700
H	-2.42984600	-5.80927500	0.67179600
C	3.35637000	-0.74029100	5.08300400
H	2.89924500	-1.39425100	5.84048100
H	3.65066700	0.19709800	5.57814100
H	4.26507600	-1.24252000	4.72026200
C	-2.29707700	-0.26576700	4.59266800
H	-2.87643000	-0.79951900	5.36075600
H	-1.80003700	0.57928500	5.09053000
H	-1.52460600	-0.94405200	4.20160700
C	0.61651900	3.40465800	3.14993500
H	0.48256100	4.49610200	3.17031900
H	0.38748000	3.02993700	4.15737900
H	-0.11875800	2.97843600	2.44942500
C	3.24264600	-3.69645900	0.10871100
H	3.36973900	-2.79903400	-0.51392600
C	1.11840400	0.23965900	4.46844600
H	0.41577900	0.46891700	3.65180500
H	1.39045300	1.17807300	4.97400600
H	0.59587600	-0.38908900	5.20348800
C	4.64957900	-4.14886000	0.53192900
H	5.17147600	-3.37303600	1.11044300
H	5.26005300	-4.38942700	-0.35130700
H	4.58843600	-5.04871800	1.16219600
C	5.34242000	2.68537600	-2.31447600
H	5.27670500	3.67084600	-2.79980200
H	5.83636300	1.99925600	-3.01757400
H	5.98761700	2.79416600	-1.43013600
C	-3.78659500	-2.04501600	-1.94133600
H	-2.80542800	-1.60519500	-1.71101100
H	-4.00151800	-1.88255900	-3.00940700
H	-3.71038800	-3.12871700	-1.76185500
C	2.56205700	-4.79443300	-0.70852700
H	2.55098200	-5.74675500	-0.15882800
H	3.12309500	-4.97872100	-1.63508400
H	1.52927700	-4.52888900	-0.97647800
C	3.06686100	2.00555800	-3.17803000
H	2.07816700	1.60538500	-2.90675700
H	3.53630600	1.31816500	-3.89669800
H	2.92216300	2.97458600	-3.68134300
C	3.89683800	-2.80549400	-3.55216200
H	4.35957200	-1.84197700	-3.31677900
H	4.36707100	-3.21796100	-4.45586200
H	4.08770400	-3.50212800	-2.72434100
C	3.05197200	3.56716000	3.77294000
H	4.08769700	3.30998300	3.50804100
H	2.84286800	3.17215700	4.77873800
H	2.99032100	4.66492100	3.82425800
C	1.82286600	-3.97853300	-4.33134300
H	1.96909200	-4.78711700	-3.60246200
H	2.32362400	-4.25146700	-5.26996700
H	0.74669800	-3.88113200	-4.53002400
C	2.08981700	-1.52496000	-4.76698600
H	1.01049200	-1.48137700	-4.97244400
H	2.61622300	-1.69214100	-5.71716200
H	2.41730600	-0.56457000	-4.34931800

2a$^{\bullet+}$, E(solvation) = -3735.40759355

P	0.80387700	0.74056800	-0.21873900
P	0.31686200	-2.31128800	0.44927700
O	-3.40019300	1.27337000	0.98469400
N	-2.64934300	1.27776300	-1.86309900
O	-3.31835300	-0.61704600	2.19580200
N	3.35106400	-2.26529700	0.35661000
N	-1.45452600	2.94841000	-1.07710000
C	-0.91923400	0.64179500	-0.21295500
C	-2.04007700	-0.73652600	-3.13792400
C	-1.65728300	1.62343300	-1.01995300
C	1.33706700	-0.83172200	0.32808700
C	3.68018800	-2.34354400	-2.05968700
C	-1.72415700	-0.36386800	0.48731400
C	-2.98551200	-0.02260600	-2.37030100
C	-1.29637600	-1.68386800	0.66731000
C	3.45163000	-2.98164900	-3.28234000
H	3.80259900	-2.51687300	-4.20629600
C	4.52713100	-1.07797800	-2.01894700
H	4.71031900	-0.82066100	-0.96568500
C	3.18980200	-2.96219400	-0.89271000
C	2.71007500	-1.10181300	0.65689800
N	3.50275400	-0.33708200	1.42648900
C	-2.92075900	0.17863800	1.21271900
C	-2.42820600	-1.97302600	-3.66256600
H	-1.70957500	-2.55457800	-4.24162300

C	-0.38283900	3.76815000	-0.59221100
C	-3.39585100	-2.97755400	0.28327400
H	-3.57899300	-2.33100000	-0.57502700
C	-4.31320600	-0.47207400	-2.22790700
C	-0.68783700	-0.17174400	-3.54582400
H	-0.45797400	0.70517600	-2.92450000
C	2.80420700	-4.21170700	-3.33289100
H	2.62908800	-4.69527900	-4.29511100
C	-2.24290100	-2.77143800	1.05121200
C	-0.36402500	4.20664500	0.73962400
C	2.62209700	-4.25025000	-0.91034000
C	-4.66314400	-1.68925200	-2.82191400
H	-5.68850500	-2.05195300	-2.73101600
C	-3.72548400	-2.44962300	-3.50914800
H	-4.01059600	-3.40715900	-3.94676200
C	2.42178400	-4.85059700	-2.15638200
H	1.96603100	-5.84021600	-2.20607900
C	0.53963500	4.23324400	-1.55487300
C	-4.28343200	-4.00146700	0.59808500
H	-5.17576300	-4.15003600	-0.01301300
C	0.64579900	5.10159000	1.11324300
H	0.68874900	5.45315200	2.14621500
C	0.45206700	-1.17478100	-3.36098400
H	0.48903500	-1.57524300	-2.33645200
H	1.41543400	-0.69300500	-3.57687400
H	0.35783100	-2.02790300	-4.04945700
C	-3.14075800	2.44571800	-2.60245600
H	-4.23597700	2.46743400	-2.61732700
H	-2.77635300	2.39078200	-3.64203600
C	-5.38108900	0.31830500	-1.49065600
H	-4.89091900	1.15419800	-0.97090700
C	2.34186200	-5.01613300	0.37072700
H	2.23554300	-4.27806700	1.17972100
C	-1.40965400	3.78183300	1.75059900
H	-2.08960800	3.06645000	1.26950800
C	-4.17768700	-0.20747100	3.29860100
C	-1.98113300	-3.63181800	2.12516900
H	-1.08364700	-3.47913200	2.72748900
C	-0.74799200	0.30981800	-5.00258800
H	-0.95402000	-0.53101500	-5.68172300
H	0.21236000	0.75825300	-5.29745000
H	-1.54046300	1.05779400	-5.15343400
C	-2.87167800	-4.65729600	2.44130600
H	-2.66357200	-5.31238300	3.28858500
C	-6.42927300	0.86244700	-2.47082700
H	-5.98062400	1.45426800	-3.28209600
H	-7.15877200	1.49354400	-1.94302000
H	-6.98105700	0.03544300	-2.94251300
C	1.50520400	5.14976000	-1.13825900
H	2.23082300	5.53019400	-1.86072400
C	3.83089400	0.12636700	-2.65110000
H	3.61766500	-0.05240200	-3.71685300
H	4.46640200	1.02221300	-2.58192100
H	2.88032000	0.34047900	-2.14193200
C	-4.02714400	-4.84223400	1.68338300
H	-4.72235900	-5.64543700	1.93153200
C	0.50073900	3.79742600	-3.01374000
H	-0.34783000	3.10899400	-3.14944800
C	4.60712400	-2.38111400	1.10723400
H	4.50807500	-3.14053300	1.89807300
H	5.41768800	-2.68551500	0.43189600
C	-2.53583600	3.60271800	-1.82076800
H	-2.13837200	4.40344200	-2.45576900
H	-3.24421000	4.03800700	-1.09753000
C	-3.55570000	0.99238000	4.00212400
H	-2.50717200	0.77554400	4.25276300
H	-4.10193900	1.19097200	4.93478400
H	-3.60051700	1.88792500	3.36875900
C	1.56490700	5.57605700	0.18624500
H	2.32889100	6.29289500	0.49283400
C	3.16073600	0.85515300	2.14129800
C	5.89867200	-1.32019400	-2.65936400
H	6.40452300	-2.18738000	-2.21101600
H	6.54094800	-0.43676400	-2.52954100
H	5.80687100	-1.50836300	-3.73895400
C	-0.75212100	3.07501800	2.93485300
H	-0.17894400	2.19671100	2.60125100
H	-1.50955800	2.74567400	3.65866300
H	-0.05556300	3.74541300	3.46080200
C	3.73776900	2.06341600	1.71158800
C	-6.05923700	-0.53516200	-0.41794000
H	-6.60740800	-1.37930600	-0.86338700
H	-6.78460400	0.06893600	0.14482000
H	-5.32556300	-0.94107500	0.29187500
C	1.75310600	-0.53913000	3.78680800
H	2.01696800	-1.33896400	3.07844700
C	1.05582500	-5.84119500	0.31913500
H	0.19520700	-5.22734800	0.01829200

H	0.84361600	-6.26591100	1.31081900
H	1.14604400	-6.68496500	-0.38114300
C	2.18196700	1.93314800	4.04412100
H	1.57696500	1.89782000	4.95277800
C	-5.59261300	0.09870800	2.82776300
H	-5.59452000	0.91223900	2.09210500
H	-6.19305900	0.40502600	3.69612100
H	-6.05687800	-0.79513700	2.39072000
C	3.54547800	-5.91384200	0.69475700
H	3.68223200	-6.67256900	-0.09045000
H	3.39158200	-6.43643400	1.65013000
H	4.48009200	-5.33740100	0.76154800
C	2.37444700	0.76254000	3.30610500
C	-4.16472500	-1.43693900	4.19725200
H	-4.51154500	-2.31519300	3.63341500
H	-4.82277900	-1.28096400	5.06304600
H	-3.14483000	-1.63854800	4.55461400
C	4.80314000	-0.97002700	1.67550700
H	5.00449700	-0.96815200	2.75504700
H	5.60578400	-0.40647100	1.17335800
C	2.74317400	3.14134700	3.64149200
H	2.58349200	4.04002800	4.23996300
C	0.22354200	-0.44270000	3.81070500
H	-0.10720000	0.32339000	4.52994800
H	-0.21815400	-1.40376900	4.11489300
H	-0.18099700	-0.18392900	2.82006300
C	-2.24277500	4.98177900	2.21423800
H	-1.62188600	5.71696400	2.74862400
H	-3.03647600	4.65049900	2.89966600
H	-2.71575300	5.49646800	1.36539500
C	0.29211900	4.99277200	-3.95017600
H	-0.59988100	5.57702200	-3.68011300
H	0.18122000	4.65141300	-4.98949000
H	1.15416900	5.67510100	-3.91451600
C	1.76118700	3.01819800	-3.39918300
H	2.66358200	3.63667800	-3.27560700
H	1.71053800	2.70380000	-4.45233000
H	1.87516700	2.12260000	-2.77216000
C	4.62328900	2.13983600	0.47888700
H	4.58635100	1.16183500	-0.02463300
C	3.50689600	3.20676400	2.48117000
H	3.94242200	4.15920800	2.17208800
C	2.30265500	-0.93803400	5.16093400
H	3.39902200	-1.02199300	5.14843200
H	1.88563100	-1.90582100	5.47411700
H	2.03393600	-0.19444100	5.92586400
C	4.10197200	3.16955100	-0.52176800
H	3.06399700	2.94679700	-0.80754800
H	4.72700600	3.17577300	-1.42806500
H	4.12219900	4.18447400	-0.09720700
C	6.07778900	2.43314600	0.86501700
H	6.46348600	1.70886000	1.59730100
H	6.16386500	3.43304300	1.31644000
H	6.72636200	2.40921100	-0.02300700

TS3, E(solvation) = -3735.333758

P	-0.71467400	-0.59244200	-0.91361400
P	1.15185100	0.91045400	0.26903600
O	-2.66252600	-1.86492900	2.47221900
N	-2.29985300	2.40221200	-1.50982900
N	2.06921100	-2.62074500	-1.63114600
N	3.25920200	-1.67961300	-0.01907800
N	-0.65034200	3.64268000	-0.70675100
C	-0.36376400	1.21435200	-0.56164400
C	-0.58567600	-0.10551600	1.83564600
C	2.06724800	-1.63330200	-0.69697500
C	-1.26465100	-0.78024300	0.92519300
O	-2.84167300	-2.43240600	0.29971100
C	3.47208300	-1.32984000	1.35315900
C	1.35482300	-2.00771300	-3.89215200
C	1.07515200	-0.67557000	-0.50747100
C	-1.09442500	2.37048600	-0.87471300
C	1.67379800	4.40265200	-0.62585400
C	1.19530200	-2.81230000	-2.74592800
C	-0.33582100	0.21043300	3.21737700
C	4.21320200	-0.17323700	1.65543100
C	1.44554900	4.70549600	2.15572200
H	1.38511700	4.81430800	3.23777900
C	-2.48930500	0.63776900	-3.79488300
H	-1.54952500	1.10662500	-3.46160500
C	0.33067600	-3.92244600	-2.73050200
C	1.85185300	4.18686600	-2.11908600
H	1.00244900	3.58395100	-2.47881400
C	-3.26843000	1.33976400	-1.47357900
C	-4.09050600	2.21871200	0.79739200
H	-3.19081100	2.84104400	0.69225300
C	4.73816300	0.73606900	0.55935500
H	4.12460400	0.55245600	-0.33854200

C	-4.12001300	1.23063000	-0.35552500	H	3.68387800	-3.59412200	-2.56811800
C	2.71843700	4.95631800	0.12253300	H	3.05499100	-4.42920200	-1.12288600
H	3.64037700	5.25585600	-0.37952800	C	-2.72000700	3.78705500	-1.74566600
C	0.35595800	4.19076200	1.45004200	H	-3.48940700	4.08164400	-1.01424800
C	0.48694900	4.06368800	0.04709700	H	-3.13662700	3.90470300	-2.75283600
C	-3.36395200	0.45951500	-2.56814200	C	-5.05537900	0.19168400	-0.34101100
C	-4.30720600	-0.56835800	-2.50188200	H	-5.72743800	0.08742800	0.51304400
H	-4.38604000	-1.27987500	-3.32321200	C	2.24946300	-0.78012100	-3.91256300
C	-0.20456600	-3.46472500	-5.05254700	H	2.80748600	-0.74099900	-2.96476500
H	-0.74492200	-3.72683700	-5.96342100	C	-1.10710200	0.55456300	5.49710000
C	0.64515000	-2.36253600	-5.04128600	H	-1.92521100	0.59279900	6.21797000
H	0.75946500	-1.76333800	-5.94717100	C	3.40112100	-1.94365000	3.67993800
C	-5.32063200	3.13486500	0.76509400	H	3.10417400	-2.62606800	4.47680300
H	-5.42648500	3.65687800	-0.19666200	C	-3.98606100	1.51509200	2.15051500
H	-5.26591800	3.88747300	1.56583200	H	-4.93190300	1.02045100	2.42093100
H	-6.23763500	2.54611800	0.91769400	H	-3.75467400	2.24016600	2.94672100
C	-2.34081200	-1.78663500	1.18435200	H	-3.19680800	0.75367700	2.12770600
C	-0.37138700	-4.22622900	-3.90160500	C	0.20523100	0.78407300	5.91460300
H	-1.04353200	-5.08625400	-3.91505200	H	0.41411900	1.01142400	6.96095400
C	-1.41695700	4.55943100	-1.55049600	C	4.13290500	-0.80205600	3.99716400
H	-0.89579200	4.72048800	-2.50914400	H	4.40476500	-0.60466200	5.03557200
H	-1.54768800	5.53009300	-1.05623800	C	1.86465500	5.52259200	-2.87187500
C	-0.93972700	3.82933100	2.16750200	H	0.96237400	6.11641000	-2.66675700
H	-1.28366700	2.85899500	1.76370700	H	1.93334300	5.35783200	-3.95684900
C	-3.65793300	-2.81781200	2.95682000	H	2.73192000	6.12742500	-2.56669300
C	0.98556000	0.43839600	3.65402300	C	0.18869100	-4.81351400	-1.50882500
H	1.80656900	0.39880700	2.93613000	H	0.71465200	-4.31993500	-0.67590000
C	3.06753600	-2.24059500	2.35584300	C	-2.02813200	4.87993500	1.90700200
C	-5.14190900	-0.70622400	-1.39790200	H	-1.70307800	5.86108600	2.28395300
H	-5.86683700	-1.52068900	-1.36322500	H	-2.95566200	4.60504000	2.43169900
C	-3.16427500	1.58255300	-4.79768600	H	-2.26686800	4.98866000	0.84156700
H	-4.11074300	1.14762400	-5.15246600	C	-2.13450000	-0.68494700	-4.46611200
H	-2.51557100	1.74836400	-5.67019400	H	-1.69616800	-1.39433800	-3.74865700
H	-3.39599000	2.55960600	-4.35207400	H	-1.40401700	-0.51156300	-5.26846700
C	4.19639300	-2.59806200	-0.67311200	H	-3.01450900	-1.15489200	-4.93100400
H	4.73219000	-3.18996600	0.08088200	C	1.24838400	0.71848200	4.99039000
H	4.93576400	-2.03687100	-1.26716500	H	2.27720900	0.89300200	5.30670000
C	4.52976500	0.07724800	2.99618700	C	6.19254300	0.37655300	0.22713100
H	5.11373600	0.96168800	3.25479900	H	6.83930300	0.56455800	1.09764100
C	-1.38176500	0.26985000	4.16499600	H	6.56178000	0.98722300	-0.60966000
H	-2.40000000	0.05914700	3.85078500	H	6.30220900	-0.68324900	-0.04234000
C	2.60529400	5.11031600	1.49698700	C	3.12523400	3.38753300	-2.41297900
H	3.43226500	5.53558200	2.06767000	H	4.02431800	3.93394900	-2.09183500
C	3.27994100	-3.44116700	-1.55834700	H	3.22268500	3.20912900	-3.49367200

H	3.11082000	2.41459600	-1.89646100
C	1.39202500	0.48819600	-3.99163600
H	0.79255300	0.49746500	-4.91565000
H	2.02627200	1.38553000	-3.98962200
H	0.70299700	0.55114300	-3.13452000
C	2.32447600	-3.52771800	2.02278700
H	2.59434200	-3.80915800	0.99287000
C	4.61904100	2.21577700	0.92048500
H	3.59452400	2.47215500	1.22525300
H	4.88269900	2.83863900	0.05327700
H	5.30524000	2.48994600	1.73622200
C	2.72505000	-4.69492600	2.92767300
H	3.81672200	-4.80785800	2.98906800
H	2.30185800	-5.63098300	2.53670100
H	2.33613600	-4.56685900	3.94840700
C	0.83844800	-6.18183200	-1.75192300
H	0.29992700	-6.72726900	-2.54177600
H	0.80383700	-6.79423000	-0.83870600
H	1.88679600	-6.09330300	-2.07163100
C	-0.77180900	3.66034300	3.67644800
H	0.03448900	2.95832700	3.92869000
H	-1.70450000	3.27307900	4.11021700
H	-0.56117800	4.62436900	4.16383300
C	0.80467500	-3.32386600	2.04706000
H	0.47587300	-2.94251200	3.02779100
H	0.28717800	-4.27633500	1.85339500
H	0.49063400	-2.60070300	1.28312100
C	-1.27577000	-4.97971900	-1.09565900
H	-1.77018500	-4.01000700	-0.94971100
H	-1.33986900	-5.54929700	-0.15580500
H	-1.83907900	-5.54302900	-1.85509100
C	-3.18605600	-4.24029400	2.67372400
H	-3.14619600	-4.43906800	1.59613000
H	-3.88376100	-4.95162200	3.13717600
H	-2.19000900	-4.40085400	3.11117300
C	3.27283800	-0.82912100	-5.05068100
H	3.88126600	-1.74377400	-5.00468300
H	3.94791600	0.03720700	-4.99478300
H	2.78218500	-0.80250400	-6.03469300
C	-3.69266900	-2.55047200	4.45577200
H	-2.68849300	-2.66401600	4.88816200
H	-4.37295400	-3.25904300	4.94712900
H	-4.05098300	-1.53054600	4.65915200
C	-5.01494700	-2.52077900	2.32685000
H	-5.28056600	-1.46678100	2.49532200
H	-5.77976800	-3.14814700	2.80579500
H	-5.00972700	-2.72327900	1.24949600

IN2, E(solvation) = -3735.3492702

P	0.67902000	-0.39872200	-0.91618300
P	-1.51793600	0.92548800	-0.13329500
O	3.22497500	-2.31558100	1.61078100
N	-1.54301900	-2.96491400	-1.44122900
N	1.53055000	3.04226800	-1.44421400
N	0.20126700	3.67573300	0.20208500
N	-3.30423500	-1.76495900	-0.86637900
C	-1.10018600	-0.71651400	-0.54873200
C	0.95977600	-0.80423700	1.82359500
C	0.65424700	2.60971000	-0.51790500
C	1.49333400	-1.06620300	0.64994500
O	3.42507400	-1.75765800	-0.56631800
C	-0.19471100	3.65557100	1.58182400
C	1.33512800	2.05878500	-3.67953200
C	0.16142200	1.29097300	-0.36619400
C	-1.94450800	-1.77913500	-0.91920100
C	-4.88368400	0.10107200	-0.93297500
C	2.11117900	2.31722200	-2.53360300
C	0.85129900	-0.79504300	3.24721900
C	-1.55268500	3.80245400	1.91511400
C	-5.33141000	-0.20994100	1.82177600
H	-5.50301600	-0.31317800	2.89513500
C	0.27483200	-2.59866500	-3.69200400
H	-0.51819400	-1.88680400	-3.41084800
C	3.48368400	2.01739800	-2.47200500
C	-4.63051500	0.31581600	-2.41529400
H	-3.68899000	-0.19710700	-2.66891900
C	-0.23152600	-3.53673000	-1.37280900
C	-0.93698500	-4.64754600	0.83348100
H	-1.90643400	-4.22367400	0.53229200
C	-2.60514800	4.07820300	0.85588800
H	-2.20661300	3.72762000	-0.10942800
C	0.07131100	-4.35408400	-0.26599200
C	-5.87257900	0.83972000	-0.27820600
H	-6.47051800	1.55665300	-0.84384000
C	-4.34420300	-0.98796900	1.20859200
C	-4.15355200	-0.83891400	-0.17983200
C	0.67025100	-3.35851400	-2.44012600
C	1.91742900	-3.97996700	-2.35112100

H	2.64239700	-3.84997400	-3.15440300
C	3.32973500	1.16358800	-4.73759900
H	3.80848800	0.71069600	-5.60702800
C	1.97562900	1.48214800	-4.77795800
H	1.40215500	1.27882000	-5.68484500
C	-1.14062800	-6.15337900	1.02685200
H	-1.40676600	-6.65015300	0.08252100
H	-1.94453900	-6.33752100	1.75424300
H	-0.22990700	-6.63470600	1.41232700
C	2.81394000	-1.75458800	0.47225000
C	4.07317400	1.42290400	-3.59203900
H	5.13596600	1.17548100	-3.57026100
C	-3.85297000	-3.08519100	-1.18178000
H	-4.75277200	-2.99122800	-1.80214000
H	-4.12718600	-3.60915400	-0.24846100
C	-3.51292000	-1.93737600	2.05463000
H	-2.79383800	-2.44850700	1.39745900
C	4.59028700	-2.79720300	1.78838200
C	0.22142700	0.30159500	3.86822900
H	-0.16218800	1.11387700	3.24639800
C	0.82031500	3.62052700	2.56192900
C	2.24913100	-4.76374900	-1.25148500
H	3.22556200	-5.24681500	-1.20762900
C	-0.29621200	-3.57195500	-4.73322700
H	0.48215000	-4.27970800	-5.05612900
H	-0.65059100	-3.02686200	-5.62043700
H	-1.13132000	-4.16408900	-4.33340300
C	0.64372300	4.93858600	-0.40059800
H	1.00543100	5.62072400	0.38022500
H	-0.19572400	5.42217400	-0.92472400
C	-1.89411500	3.81019300	3.27223200
H	-2.94107700	3.90946000	3.56179100
C	1.31750100	-1.86203800	4.04135100
H	1.81554600	-2.69825100	3.55463400
C	-6.10811700	0.67580900	1.08314100
H	-6.88995100	1.25662400	1.57486500
C	1.74510300	4.49074800	-1.36423500
H	1.64326800	4.93067600	-2.36516800
H	2.75949700	4.70790700	-0.99253900
C	-2.68768400	-3.74882700	-1.90883400
H	-2.55700600	-4.80807900	-1.65072900
H	-2.78637800	-3.66112300	-3.00266000
C	1.33648600	-4.94734200	-0.21851000
H	1.59959200	-5.58238600	0.63026800
C	-0.14529700	2.39081300	-3.76767200
H	-0.46314300	2.83283700	-2.81078500
C	1.14999100	-1.82594900	5.42168100
H	1.50955000	-2.65597800	6.03160100
C	0.43116200	3.65673000	3.90379000
H	1.19061400	3.62142400	4.68618500
C	-0.53511000	-3.96726400	2.14179000
H	0.45388200	-4.32013600	2.47309800
H	-1.26033500	-4.18947600	2.93985600
H	-0.48193500	-2.87688400	2.01515600
C	0.53608200	-0.72814800	6.02876200
H	0.41174000	-0.70454400	7.11235100
C	-0.91376600	3.73357300	4.25627200
H	-1.19907400	3.76095400	5.30941800
C	-5.75456600	-0.29281800	-3.26113600
H	-5.88016300	-1.36592200	-3.05852800
H	-5.54575000	-0.16846200	-4.33347800
H	-6.71389400	0.20014500	-3.04217100
C	4.33661700	2.37710800	-1.26704800
H	3.66014400	2.70672700	-0.46293700
C	-4.37517800	-3.00710700	2.73171700
H	-5.07827400	-2.55455700	3.44680500
H	-3.74216800	-3.71216500	3.29043900
H	-4.96707500	-3.57790500	2.00105800
C	1.43075200	-1.80088300	-4.29179900
H	1.90889700	-1.15721900	-3.53945700
H	1.05976200	-1.16611400	-5.10914800
H	2.19590800	-2.46426500	-4.72275100
C	0.07901800	0.33744800	5.25012700
H	-0.40509900	1.19488500	5.71993900
C	-2.83709700	5.59261200	0.75037500
H	-3.25125600	5.98255900	1.69241400
H	-3.55004200	5.81956400	-0.05563400
H	-1.90278600	6.13712200	0.55117400
C	-4.45126000	1.80260500	-2.73873500
H	-5.36871800	2.37381600	-2.53370900
H	-4.21961500	1.93624200	-3.80570200
H	-3.63452300	2.24154900	-2.14407500
C	-0.97177000	1.11809200	-3.97879100
H	-0.73286400	0.64861500	-4.94593100
H	-2.04586000	1.35099100	-3.97379200
H	-0.77129100	0.38032500	-3.18714900
C	2.29616800	3.55207800	2.19395400
H	2.40547600	3.93434400	1.16706000

C	-3.92246200	3.34960000	1.11201900
H	-3.76795600	2.27120000	1.25753800
H	-4.59808900	3.48077900	0.25389000
H	-4.44103900	3.74836800	1.99730500
C	3.16755900	4.43341500	3.09175100
H	2.77839100	5.45953900	3.15592900
H	4.19126100	4.47523700	2.69324000
H	3.23479300	4.02910000	4.11208900
C	5.29126600	3.52977800	-1.60371200
H	6.02257000	3.21313200	-2.36266100
H	5.85001700	3.84301700	-0.70942100
H	4.76009000	4.40438100	-2.00680100
C	-2.69584400	-1.14705100	3.08112700
H	-2.07332300	-0.39126300	2.58006800
H	-2.02769900	-1.81013600	3.65205600
H	-3.35082200	-0.62803400	3.79785800
C	2.80425800	2.10633800	2.19246500
H	2.69415400	1.65695000	3.19191400
H	3.86932500	2.07333900	1.91628500
H	2.24374200	1.48266700	1.48034700
C	5.11044200	1.17087800	-0.73484400
H	4.43584800	0.33288600	-0.51886800
H	5.65565900	1.44102700	0.18219500
H	5.85442100	0.81871300	-1.46558700
C	5.57550700	-1.66203900	1.52563600
H	5.62016900	-1.41078200	0.45944500
H	6.57760700	-1.96898500	1.85595900
H	5.28186900	-0.76861300	2.09695900
C	-0.42493200	3.41907600	-4.86865100
H	0.15381900	4.34144700	-4.71579800
H	-1.49306500	3.68069900	-4.88727700
H	-0.16038600	3.02023500	-5.85914700
C	4.62699800	-3.20775200	3.25483700
H	4.39291700	-2.34955400	3.90067400
H	5.62565000	-3.58419200	3.51427600
H	3.89566700	-4.00622500	3.44817800
C	4.85607900	-3.99648400	0.88726500
H	4.11566400	-4.78594100	1.08067700
H	5.85497600	-4.39886000	1.10796200
H	4.81232100	-3.70787200	-0.16945500

TS4, E(solvation) = -3735.332688

P	-0.67853900	0.10211500	-0.92469800
P	1.76196900	-0.10164600	0.18276000
O	-4.55108400	0.07709700	1.06773600
N	-0.07997500	3.42801200	-0.88912600
N	-0.11546800	-3.27622900	-1.59430800
N	1.68546900	-3.32906100	-0.32285200
N	2.09931300	3.14084900	-0.68034000
C	0.65170400	1.16750000	-0.31358700
C	-1.73504100	0.08213000	1.95511700
C	0.65017200	-2.55042800	-0.74664800
C	-2.26319900	0.03179700	0.83185900
O	-3.75269500	-0.45277700	-0.97444800
C	2.45590000	-3.09093200	0.85622700
C	-1.37250900	-2.11822900	-3.35370200
C	0.49777200	-1.18285200	-0.42338900
C	0.89327700	2.52763900	-0.59454900
C	4.23767000	2.44950500	-1.61677600
C	-1.36823100	-2.90277000	-2.18237700
C	-1.18238600	0.17730000	3.26714200
C	3.74936900	-2.55029500	0.74379300
C	5.28887000	2.20565600	0.97671900
H	5.70863700	2.10670800	1.97898100
C	-2.25144600	2.81070800	-2.69573700
H	-1.19891000	2.51332300	-2.83901900
C	-2.55086200	-3.42510700	-1.62548100
C	3.64215200	2.48825200	-3.01490500
H	2.86426500	3.26832200	-3.03289300
C	-1.40437500	3.34936500	-0.35435600
C	-0.47844300	4.25982000	1.86430700
H	0.46815000	4.18432800	1.30892200
C	4.39667600	-2.37072100	-0.61710200
H	3.58253400	-2.30183800	-1.35832500
C	-1.59346800	3.68606500	1.00078300
C	5.59337400	2.18315100	-1.41613100
H	6.25344000	2.05703200	-2.27412400
C	3.92774700	2.49816800	0.82917500
C	3.42281100	2.63043200	-0.47781700
C	-2.46704700	2.99339100	-1.20262800
C	-3.74322200	2.91820100	-0.64020200
H	-4.58659300	2.64196900	-1.27204100
C	-3.78113100	-2.41065400	-3.45155100
H	-4.72938500	-2.21963500	-3.95578600
C	-2.60421100	-1.87021100	-3.96257500
H	-2.64741300	-1.25799800	-4.86327400
C	-0.73650800	5.74863900	2.13313200
H	-0.88258600	6.31386300	1.20100400

H	0.10795600	6.19256400	2.68088600	H	-1.20049300	3.49890500	3.78296600
H	-1.64234800	5.88158200	2.74355000	H	0.50641800	3.97723900	3.77584500
C	-3.58873500	-0.14261200	0.17400800	H	0.00388000	2.45525300	2.99437800
C	-3.75179000	-3.18284700	-2.29893300	C	-0.19699400	0.44298900	5.87065900
H	-4.68130400	-3.59819000	-1.90414100	H	0.18881600	0.54822000	6.88560600
C	1.94727100	4.58336300	-0.90730800	C	3.83629400	-2.45232900	3.16527900
H	2.66352500	4.92651000	-1.66506500	H	4.37208300	-2.17830400	4.07581600
H	2.14545500	5.13507200	0.02590400	C	4.66076700	2.82801300	-4.10185700
C	3.06907600	2.73130100	2.06108700	H	5.22682300	3.73899600	-3.86102800
H	2.01244900	2.67172000	1.75873200	H	4.14646900	2.98593100	-5.05977600
C	-5.96843800	-0.10556300	0.75945100	H	5.37833900	2.00761600	-4.25103600
C	0.12947800	-0.22827400	3.57086600	C	-2.56213300	-4.26637600	-0.35811400
H	0.76296400	-0.64744500	2.78674900	H	-1.56238800	-4.21228300	0.09868600
C	1.88205800	-3.41846900	2.10004800	C	3.33086300	4.13069800	2.63386900
C	-3.94785900	3.19014700	0.71011300	H	4.38682400	4.23143300	2.92730100
H	-4.95008300	3.11692700	1.13548200	H	2.71418600	4.30750800	3.52676200
C	-2.47115100	4.15475300	-3.40575500	H	3.11539200	4.92396500	1.90365200
H	-3.52122700	4.46859400	-3.30471500	C	-3.13298000	1.72806800	-3.31739400
H	-2.24250800	4.06946000	-4.47810600	H	-3.00544100	0.75989300	-2.81245300
H	-1.84758700	4.95387500	-2.97967800	H	-2.87728600	1.61123000	-4.38127300
C	1.76017200	-4.57124400	-1.08834200	H	-4.19827900	2.00335600	-3.27444000
H	2.00215900	-5.41501200	-0.42828400	C	0.61217600	-0.09672000	4.86854700
H	2.53920600	-4.49628800	-1.86557400	H	1.63159800	-0.41435700	5.09511800
C	4.42626600	-2.22952300	1.92290700	C	5.25269600	-3.60118200	-0.94871000
H	5.42260300	-1.78843100	1.87101100	H	6.08890000	-3.68245700	-0.23787900
C	-1.99747100	0.71002300	4.28423900	H	5.67284400	-3.52126200	-1.96192300
H	-3.01587300	1.01437100	4.03684100	H	4.67490000	-4.53434000	-0.88363700
C	6.11785300	2.07471800	-0.13024000	C	2.95151200	1.15189300	-3.32528600
H	7.18148000	1.87366300	0.00664000	H	3.66737200	0.32138400	-3.21988700
C	0.35883100	-4.66131100	-1.69011400	H	2.57639000	1.15310100	-4.35881100
H	0.35580900	-4.99442200	-2.73543500	H	2.10309700	0.95972500	-2.65041300
H	-0.29499100	-5.33256800	-1.11294500	C	-0.25211700	-0.29915600	-4.72803500
C	0.49256000	4.68926500	-1.36273800	H	-0.87322200	-0.42135900	-5.62769900
H	-0.03980400	5.53957400	-0.91758100	H	0.72594800	0.07315900	-5.06109700
H	0.41011300	4.75720200	-2.45965200	H	-0.71726300	0.46284800	-4.08470400
C	-2.88664200	3.58100300	1.51975500	C	0.57335100	-4.18753600	2.19864800
H	-3.06948500	3.83007400	2.56722300	H	0.34897400	-4.58192900	1.19517800
C	-0.07720700	-1.61755600	-3.97603100	C	5.22152900	-1.09180000	-0.72303800
H	0.64002400	-1.43448700	-3.16040800	H	4.62815000	-0.21425700	-0.43177500
C	-1.50203500	0.84278100	5.57681000	H	5.56919900	-0.94692600	-1.75691600
H	-2.13642700	1.25726100	6.36125800	H	6.11731700	-1.12827800	-0.08423400
C	2.58611600	-3.05982000	3.25406900	C	0.70357200	-5.39217700	3.13596000
H	2.15885300	-3.27843000	4.23497200	H	1.56105300	-6.02412700	2.86454500
C	-0.28279800	3.50029900	3.17626600	H	-0.20792500	-6.00538000	3.09009900

H	0.83254600	-5.07574300	4.18136100
C	-2.89037300	-5.73201300	-0.67511100
H	-3.92575900	-5.81914200	-1.03764700
H	-2.79740400	-6.35565700	0.22637400
H	-2.23852600	-6.14750700	-1.45655900
C	3.28750800	1.66788200	3.14061700
H	3.17564600	0.65040300	2.73452200
H	2.54991300	1.80530200	3.94509700
H	4.28751100	1.75062200	3.59265600
C	-0.60130200	-3.29993000	2.61273900
H	-0.43178200	-2.87098900	3.61199300
H	-1.52783600	-3.89050600	2.65362200
H	-0.75339300	-2.47076100	1.90306600
C	-3.54972900	-3.72916800	0.67785100
H	-3.32482100	-2.68924700	0.95925900
H	-3.51683600	-4.34505900	1.58886700
H	-4.57770700	-3.77044200	0.29429500
C	-6.23629800	-1.56855300	0.43193200
H	-5.71127700	-1.86610700	-0.48508700
H	-7.31559600	-1.71438600	0.28545000
H	-5.91122700	-2.20712600	1.26454400
C	0.52233000	-2.68750400	-4.89678300
H	0.72104000	-3.62298800	-4.35494200
H	1.47056500	-2.33791500	-5.33094300
H	-0.16926800	-2.91758200	-5.72101100
C	-6.65111400	0.28548200	2.06312700
H	-6.30783000	-0.36062900	2.88249800
H	-7.74008900	0.18285000	1.96344100
H	-6.41828400	1.32850100	2.31950300
C	-6.42272200	0.80519200	-0.37694700
H	-6.29896100	1.86200700	-0.10567600
H	-7.49325700	0.63141100	-0.55464300
H	-5.87515100	0.59351800	-1.30335600

1$^{\bullet+}$, E(solvation) = -3081.1635544

P	1.37704600	0.00111900	0.00011700
P	-1.32030500	-0.00105600	-0.00009600
N	-1.07354600	-3.35943000	0.01247900
N	1.12507800	-3.36628900	-0.16030800
N	-1.07892700	3.35775100	-0.01243800
N	1.11966900	3.36809200	0.16044600
C	0.02651600	1.16899900	0.02544200
C	-0.71945000	-4.77671600	0.07682200
C	0.02760500	-2.57967000	-0.05391800
C	0.02346300	2.57973300	0.05400100
C	0.74513000	-4.76396500	-0.37636800
C	0.02841400	-1.16893600	-0.02536500
C	0.73749200	4.76516000	0.37649700
C	-0.72705700	4.77558800	-0.07684200
C	2.41288800	-2.86189200	-0.52765500
C	2.63107400	-2.43967600	-1.85211200
C	3.40175700	-2.76759000	0.46951200
C	3.86973400	-1.86501200	-2.15381300
C	4.62108700	-2.18264400	0.12009800
C	4.84780400	-1.72352400	-1.17522400
H	4.07040900	-1.52449500	-3.17180600
H	5.40814100	-2.08527300	0.86808500
C	-2.36395200	-2.87167500	0.38700100
C	-2.61699800	-2.60116000	1.74619400
C	-3.31502900	-2.62611800	-0.61924100
C	-3.86229800	-2.06384000	2.08108100
C	-4.54871400	-2.09396200	-0.23311200
C	-4.81792600	-1.80844100	1.10123100
H	-4.08743800	-1.83940200	3.12594000
H	-5.30673000	-1.89111500	-0.99197200
C	-2.36856000	2.86794200	-0.38694600
C	-2.62116600	2.59688100	-1.74611600
C	-3.31927200	2.62101700	0.61930600
C	-3.86558900	2.05750100	-2.08095000
C	-4.55207500	2.08677700	0.23323000
C	-4.82079800	1.80063200	-1.10107500
H	-4.09037100	1.83260300	-3.12578700
H	-5.30977600	1.88280900	0.99210700
C	2.40832200	2.86574800	0.52763700
C	2.62732900	2.44384300	1.85205500
C	3.39721900	2.77303600	-0.46964900
C	3.86695000	1.87117700	2.15360900
C	4.61752500	2.19003600	-0.12038800
C	4.84513500	1.73127700	1.17490400
H	4.06828200	1.53095000	3.17156800
H	5.40463400	2.09390500	-0.86847800
C	1.58400700	-2.59259800	-2.94412400
H	0.65032500	-2.95145400	-2.48453400
C	3.13086900	-3.24570300	1.88805700
H	2.44519900	-4.10526900	1.81721000
C	-1.58986900	-2.86335200	2.83643300
H	-0.66165500	-3.22096400	2.36373200
C	-3.03223100	-2.91092800	-2.08361600

H	-1.96448500	-3.16376600	-2.17202800
C	1.58010300	2.59499100	2.94415600
H	0.64576400	2.95222600	2.48463200
C	3.12535900	3.25064800	-1.88817300
H	2.43819300	4.10901200	-1.81727800
C	-3.03703300	2.90655400	2.08365000
H	-1.96988100	3.16190300	2.17199000
C	-1.59449000	2.86069400	-2.83639100
H	-0.66679600	3.21968600	-2.36371500
H	5.80566800	-1.26578200	-1.42739900
H	5.80375600	1.27505200	1.42695400
H	-5.78443300	-1.38715000	1.38267300
H	-5.78660800	1.37771800	-1.38247800
C	2.02977400	-3.63741900	-3.97436200
H	2.94959900	-3.31338000	-4.48376300
H	2.23788500	-4.60874900	-3.50260300
H	1.25346100	-3.78112700	-4.73974100
C	1.26323200	-1.25719900	-3.62109200
H	2.12749300	-0.87718100	-4.18709900
H	0.42960800	-1.37719100	-4.32899000
H	0.98076000	-0.49511100	-2.88012600
C	-3.28858500	-1.68131400	-2.96011800
H	-2.97181300	-1.87795800	-3.99510000
H	-4.35869700	-1.42424200	-2.98517600
H	-2.74037000	-0.80438800	-2.58570200
C	-3.84898500	-4.11415200	-2.56856700
H	-3.64902200	-5.00989800	-1.96298500
H	-4.92706900	-3.90306600	-2.50265100
H	-3.61375000	-4.34512600	-3.61753700
C	-2.07657100	-3.95729800	3.79363800
H	-2.98803300	-3.63841500	4.32093900
H	-2.31215000	-4.88788600	3.25720800
H	-1.30976100	-4.17658600	4.55052900
C	-1.23886400	-1.58130300	3.59640200
H	-2.10951200	-1.19192500	4.14598900
H	-0.43922300	-1.77362300	4.32712400
H	-0.89229700	-0.79739200	2.90651200
C	4.39393200	-3.71826800	2.60815700
H	4.96430800	-4.43619700	2.00221600
H	5.05560800	-2.87476600	2.85488400
H	4.12426300	-4.20461800	3.55579800
C	2.42248000	-2.15820300	2.70578000
H	2.28249500	-2.48844900	3.74646400
H	3.02197600	-1.23359700	2.71129200
H	1.43497800	-1.91145900	2.28859500
C	-3.85656000	4.10787300	2.56863400
H	-3.62169200	4.33947900	3.61754800
H	-3.65879800	5.00403600	1.96294800
H	-4.93415800	3.89425600	2.50293600
C	-3.29044400	1.67634500	2.96017400
H	-4.35990700	1.41656400	2.98499600
H	-2.73994300	0.80079100	2.58590900
H	-2.97437800	1.87383100	3.99521200
C	1.26168500	1.25906700	3.62119300
H	0.42793600	1.37765900	4.32918000
H	0.98042500	0.49647600	2.88028100
H	2.12664900	0.88053200	4.18711900
C	2.02418300	3.64061100	3.97431800
H	2.23060200	4.61227600	3.50250500
H	1.24770000	3.78302700	4.73976500
H	2.94460600	3.31814900	4.48364100
C	4.38752500	3.72540600	-2.60841000
H	4.95671200	4.44432900	-2.00253000
H	5.05064400	2.88305800	-2.85520400
H	4.11691200	4.21128000	-3.55602600
C	2.41878700	2.16188200	-2.70578800
H	2.27806700	2.49187300	-3.74645400
H	3.01992900	1.23834600	-2.71137800
H	1.43178400	1.91338200	-2.28845700
C	-2.08292200	3.95395700	-3.79349900
H	-2.31987900	4.88415900	-3.25700700
H	-1.31650700	4.17444900	-4.55044100
H	-2.99394400	3.63371000	-4.32073700
C	-1.24157000	1.57924300	-3.59647700
H	-0.89385600	0.79577200	-2.90666500
H	-2.11161900	1.18862900	-4.14613400
H	-0.44220000	1.77282500	-4.32716400
H	0.84433200	5.01890900	1.44503100
H	1.37630200	5.44281400	-0.20468300
H	-0.84289300	5.14430500	-1.11050400
H	-1.37813500	5.36935500	0.57822300
H	1.38494700	-5.44060000	0.20489200
H	0.85248800	-5.01756800	-1.44488400
H	-1.36952800	-5.37146200	-0.57834500
H	-0.83481700	-5.14568100	1.11044800

PTP, E(solvation) = -654.2035489

O	2.14517700	0.39283900	-0.00043400

C	-1.19020400	-0.26380600	0.00010600
C	0.00786900	-0.44823300	0.00008100
O	1.88906200	-1.85069100	0.00067300
C	-2.60951400	-0.04947400	0.00007100
C	1.44088300	-0.73599600	0.00019400
C	3.60078900	0.37387300	-0.00013900
C	-3.48675300	-1.14601900	-0.00029400
H	-3.07556300	-2.15593700	-0.00049200
C	-3.12940600	1.25492500	0.00034300
H	-2.44229600	2.10162700	0.00063500
C	-4.50610300	1.45500000	0.00024700
H	-4.90575200	2.46990400	0.00044600
C	-5.37333900	0.36176600	-0.00013700
H	-6.45243200	0.52236100	-0.00022200
C	-4.86200700	-0.93660100	-0.00040600
H	-5.53967600	-1.79127900	-0.00070000
C	4.11424800	-0.30628000	-1.26623400
H	3.86980600	-1.37466600	-1.27095500
H	5.20604900	-0.19089500	-1.32055100
H	3.67234000	0.16898300	-2.15381000
C	3.96202700	1.85337200	-0.00046200
H	3.54894900	2.34485100	-0.89195000
H	5.05377800	1.97498600	-0.00088200
H	3.54959200	2.34519400	0.89113700
C	4.11390500	-0.30560400	1.26646000
H	3.67089200	0.16944700	2.15360400
H	5.20554500	-0.18907800	1.32155600
H	3.87048200	-1.37420900	1.27129500

3d$^{\bullet+}$, E = -3689.3149226

P	0.73614200	-0.73864500	-0.25861700
P	0.30312600	2.24565700	0.75637600
C	2.68334900	1.06390500	0.59671500
N	-2.96139900	-1.20070700	-1.46595200
O	-3.23667300	-1.43771000	1.45945400
N	3.48722700	0.34473700	1.38803300
O	-3.39791800	2.57966000	0.93980300
O	-1.90365100	3.42991300	2.37952500
N	3.30858600	2.19419600	0.20901200
C	1.28105200	0.79133500	0.35100900
C	-5.56505000	-0.38239700	-0.42743800
H	-4.97135700	-1.25955200	-0.13624700
O	-3.06211200	0.42846900	2.68229900
C	-0.45276100	-3.69724500	-0.78693400
C	-1.81501700	-1.58450000	-0.86987700
N	-1.56487200	-2.87283700	-1.15147400
C	-2.21534900	2.61487800	1.55278200
C	-5.14572200	1.79878000	-1.60932500
H	-6.13266900	2.11689500	-1.26680000
C	3.19715700	-0.90889500	2.01601000
C	-4.67807000	0.52936500	-1.25786200
C	-1.27228600	1.57582300	0.99820900
C	1.51517100	-4.88230600	-1.48154700
H	2.25130300	-5.14310300	-2.24541900
C	2.41775700	-0.93556800	3.18650000
C	-2.75912500	-0.33556400	1.62963100
C	0.36545600	-3.44478300	-3.21130400
H	-0.52270300	-2.79524200	-3.25284700
C	-0.39143100	-4.26890400	0.49488900
C	-3.41071800	0.13803300	-1.72996900
C	-3.51916100	-2.28484600	-2.28001200
H	-3.37349600	-2.04225400	-3.34580200
H	-4.59380400	-2.40031600	-2.09343200
C	0.68695100	-5.11585100	0.77275400
H	0.76909100	-5.56420500	1.76511100
C	-3.13771700	2.24330700	-2.85900200
H	-2.55481400	2.90969100	-3.49757100
C	-2.70276800	-3.49396000	-1.83323300
H	-3.24330600	-4.12931200	-1.11279400
H	-2.35772500	-4.12243400	-2.66456300
C	3.77623500	-2.06348200	1.45818200
C	-1.69593000	0.26024400	0.78134600
C	2.98915000	2.97074800	-0.95749700
C	-0.98568400	-0.67467900	-0.08881200
C	2.30604600	5.05153500	-1.94532700
H	1.98694200	6.08998400	-1.84761000
C	1.62838200	-5.42264400	-0.20300000
H	2.44917100	-6.10468800	0.02729500
C	-3.94480500	-0.09851400	3.67706100
H	-3.34817400	-0.73118000	4.35308600
H	-4.69418600	-0.73732900	3.19240000
C	4.77616900	1.01336500	1.60415700
H	5.58650100	0.44969500	1.11567900
H	4.98491300	1.05733800	2.68102600
C	3.54512800	-3.28095500	2.10210400
H	3.97822300	-4.19599000	1.69275000
C	4.53704500	2.39890700	0.98898100
H	4.36557200	3.16492800	1.76033600

H	5.35220100	2.73847100	0.33832800	H	-5.18044300	0.71066600	5.24181400
C	-2.64294500	0.96831300	-2.57255000	H	-5.20965400	1.64864700	3.72798700
C	2.58129800	4.30691800	-0.79337000	H	-3.78765700	1.73672700	4.80127300
C	3.15411100	2.37909500	-2.23342100	C	0.28063400	0.20623400	3.86883900
C	2.77434100	-3.33815600	3.25947700	H	-0.13744100	-0.07271000	2.89150500
H	2.60825800	-4.29643100	3.75499500	H	-0.16485400	1.17017500	4.15723900
C	1.21922600	5.80366400	0.74634900	H	-0.02998300	-0.55331700	4.60384400
H	1.22202600	6.68718400	0.09136500	C	3.52961800	0.40836100	-3.83023400
H	1.15091200	6.16470000	1.78214900	H	2.49067700	0.45571700	-4.18277000
H	0.31904500	5.21100400	0.53388000	H	3.84399400	-0.64464700	-3.84979500
C	-4.07527700	4.90458200	0.68378000	H	4.15975700	0.95232600	-4.54936200
H	-3.11531700	5.30883500	1.02997500	C	2.49072300	4.96991700	0.57129100
H	-4.86624200	5.62130400	0.94358000	H	2.45833700	4.17289200	1.32949000
H	-4.04651000	4.79361900	-0.40873600	C	5.19494700	0.89926100	-2.06076700
C	0.47924800	-4.00319600	-1.79964000	H	5.76501400	1.58635600	-2.70348400
C	2.21847400	-2.17905000	3.79281200	H	5.58244300	-0.11788400	-2.22190200
H	1.61547400	-2.23831200	4.70139600	H	5.39711700	1.17036100	-1.01807000
C	1.56896900	-2.57407100	-3.58396100	C	-1.59376800	0.30865700	-4.75659500
H	1.68269100	-1.73184200	-2.88489800	H	-2.39549900	-0.41945500	-4.94819100
H	1.44597700	-2.16754100	-4.59917200	H	-0.67422300	-0.05435200	-5.24029400
H	2.50192700	-3.15895600	-3.56800200	H	-1.88165500	1.25314400	-5.24178900
C	-4.37842300	2.65775900	-2.38622600	C	2.43247900	4.48745300	-3.20712700
H	-4.75842800	3.64672600	-2.64768700	H	2.21074100	5.08177200	-4.09464600
C	-0.91560400	-3.23938500	2.73000900	C	1.80732600	0.31349500	3.79884500
H	-0.16752300	-3.82834700	3.28389800	H	2.04252500	1.16890800	3.14688400
H	-1.73306100	-2.98060300	3.41928900	C	0.17328800	-4.57114400	-4.23344900
H	-0.43097500	-2.30730700	2.40171800	H	1.06326900	-5.21631900	-4.27794300
C	-1.36139800	0.51628400	-3.25442000	H	0.01104300	-4.15618400	-5.23862400
H	-1.05588100	-0.45391900	-2.83811600	H	-0.68426100	-5.21133300	-3.97955800
C	-6.01376000	0.30641800	0.86535800	C	-6.78619700	-0.84213500	-1.23420000
H	-5.15942800	0.75645100	1.39041800	H	-7.42031300	0.01671700	-1.50123500
H	-6.50602600	-0.41642700	1.53270500	H	-7.39741100	-1.54030200	-0.64397100
H	-6.74219000	1.10577100	0.65669100	H	-6.50251200	-1.33945800	-2.17331900
C	2.85461000	3.16725300	-3.34700600	C	3.73491200	5.83566900	0.81679100
H	2.95694200	2.75049200	-4.34810100	H	4.66757400	5.26369900	0.70517900
C	-1.46372300	-4.02755900	1.53924800	H	3.71122900	6.26935500	1.82706300
H	-2.25169400	-3.41139500	1.09046400	H	3.77177300	6.66419700	0.09358000
C	-2.10095200	-5.34420800	1.99509500	C	6.11048100	-2.33794000	0.56033900
H	-2.50147000	-5.91394900	1.14395900	H	6.50128300	-1.69905800	1.36596000
H	-2.92658600	-5.14134700	2.69206100	H	6.75311400	-2.21520100	-0.32402800
H	-1.37466900	-5.98616200	2.51606200	H	6.19895900	-3.38172400	0.89745200
C	4.65423400	-2.00198500	0.21924100	C	3.70207700	0.96401700	-2.41544900
H	4.62296800	-0.97320400	-0.16666800	H	3.15186100	0.28842900	-1.73569900
C	-4.56605600	1.06996500	4.40579800	C	4.12858700	-2.90075600	-0.89866800

H	4.17874700	-3.96297200	-0.61501600
H	4.73309200	-2.76965500	-1.81001000
H	3.07998800	-2.66682600	-1.13110700
C	2.40858800	0.60203500	5.17849100
H	2.18926400	-0.21553300	5.88134200
H	1.98290400	1.52622900	5.59440000
H	3.50137700	0.71512500	5.12897000
C	-4.35315100	3.56766700	1.34072100
H	-4.33365000	3.65372700	2.43651400
H	-5.32148000	3.15750900	1.02647000
C	-0.21028500	1.49537100	-3.01478400
H	-0.35224600	2.43353400	-3.57295600
H	0.74023800	1.05679900	-3.34942200
H	-0.10844100	1.75301700	-1.95114900

7$^{\bullet+}$, E= -4136.9952281

P	0.20181200	1.14242500	0.50838200
P	1.67144500	-1.40575300	-0.82016100
Si	1.04144300	-4.42241800	0.45514200
O	-1.09227700	-2.00174500	-3.00397400
O	-3.63532000	-1.44996400	0.06866300
O	-2.46370200	-3.12442100	-0.82339100
O	0.22565300	-3.70516100	-2.39816700
N	-2.44665900	1.27288600	2.07695200
N	4.02273000	0.42932000	0.22978700
N	-3.43652000	1.36910700	0.11006200
N	2.96119100	2.31174200	-0.29647400
C	-1.24082400	0.10262900	0.25642800
C	-1.31273100	-1.12230800	-0.37925700
C	-2.42136400	0.83751600	0.80474100
C	0.68570000	-2.55784400	0.23468000
H	0.43511100	-2.10860600	1.20272600
C	-2.59000600	-1.88167600	-0.36334100
C	-1.77489900	0.78278000	3.25818200
C	-0.14015600	-1.90422200	-0.86033300
C	-0.98982200	1.68971500	4.00221300
C	2.81304300	0.96759500	-0.06079800
C	-3.92681400	1.07132800	-1.21095000
C	4.31241600	-0.84933200	0.81061600
C	1.58370700	0.26037200	-0.09538200
C	-0.32384300	-2.66574000	-2.13833100
C	-0.62242500	3.07884900	3.50918400
H	-0.96765200	3.17437700	2.46853800
C	2.36524900	3.02524400	-1.39950900
C	-4.07436400	2.43326400	0.89669300
H	-5.15698300	2.43921400	0.74585000
H	-3.66253400	3.40378400	0.57096500
C	-2.10337800	-0.49282900	3.76238400
C	-5.19409900	0.44880900	-1.32462300
C	5.01990700	-1.79564700	0.04112100
C	-0.53838400	1.28777500	5.26157700
H	0.05390500	1.98148300	5.86117800
C	-3.20011800	1.48134700	-2.33698800
C	5.40626900	-2.98597300	0.66232300
H	5.96075000	-3.73212900	0.08998100
C	3.99156800	-1.07641300	2.16212200
C	1.62843200	4.19297300	-1.12637000
C	-1.93567200	2.30693700	-2.24269700
H	-1.68045900	2.43449900	-1.18096500
C	-3.65642400	2.07420300	2.31140900
H	-3.42325900	2.94423500	2.93517000
H	-4.39847800	1.44715600	2.83486800
C	2.66624000	2.64171100	-2.72511500
C	5.40925500	-1.54398700	-1.40666200
H	4.87633000	-0.64258300	-1.74232900
C	5.09420500	1.42133900	0.08626200
H	5.63249100	1.27240900	-0.86562900
H	5.80716900	1.31952500	0.91411900
C	1.32407000	4.63451400	0.29180300
H	1.54465600	3.78266600	0.94866100
C	4.38922200	-2.28982900	2.73152100
H	4.14931800	-2.49188900	3.77760900
C	-0.81271700	0.01809800	5.75792200
H	-0.43937500	-0.27960000	6.73864700
C	5.09385100	-3.23544000	1.99472000
H	5.40104300	-4.17249400	2.46127600
C	-0.51610000	-5.43356100	0.16005900
H	-1.34899500	-5.04432100	0.76589900
H	-0.33893300	-6.47978000	0.45378000
H	-0.80371500	-5.40498000	-0.89927700
C	0.89916600	3.26769900	3.51053100
H	1.30429000	3.20588400	4.53158500
H	1.16241300	4.25936500	3.11387900
H	1.39355200	2.50036900	2.89523400
C	3.25282400	-0.06469800	3.01874600
H	3.04807700	0.82735800	2.40848300
C	-3.06737300	-1.44130000	3.07649800
H	-3.43537100	-0.97201700	2.15812600

C	1.22083400	4.98765200	-2.20237200	H	7.19023700	-1.02177000	-2.55116700
H	0.66688600	5.90795800	-2.00705100	H	7.48466500	-2.18409100	-1.23868000
C	4.31021900	2.73098900	0.12369600	C	1.52018900	4.63430000	-3.51365300
H	4.27163400	3.15517800	1.14041200	H	1.19971500	5.27089700	-4.33956500
H	4.69998100	3.49091600	-0.56356200	C	-4.93363200	0.52870000	-3.74218800
C	2.22663600	3.46477200	-3.76672600	H	-5.32628800	0.30680500	-4.73581200
H	2.45104400	3.18271800	-4.79733100	C	-1.26733200	-2.61823800	-4.28282200
C	-3.65706400	-3.90055900	-0.96972200	H	-1.65487100	-3.63732300	-4.13175500
H	-4.28472600	-3.75693300	-0.07860900	H	-0.28243500	-2.71848900	-4.76266300
H	-3.31043500	-4.94037900	-0.99783800	C	3.43556900	1.38191600	-3.08297300
C	-6.09188000	0.13065800	-0.13609700	H	3.68890100	0.85394200	-2.15859100
H	-5.48725700	0.21490000	0.77983800	C	-7.26081400	1.12842800	-0.07831500
C	-2.17412300	3.70662300	-2.81976400	H	-6.93790200	2.17857400	-0.12464300
H	-2.40332100	3.65728300	-3.89494900	H	-7.84872500	0.98385800	0.83978600
H	-1.27456900	4.32429600	-2.69372100	H	-7.93352000	0.96834800	-0.93405500
H	-3.01709600	4.20696200	-2.32029900	C	1.90478200	-0.62467200	3.47560800
C	-1.28436200	4.17225800	4.35761600	H	1.29050500	-0.92324700	2.61419900
H	-2.37703300	4.06186200	4.40904300	H	1.34738500	0.13297300	4.04106600
H	-1.05907000	5.16801200	3.94773900	H	2.03681200	-1.50445800	4.12484700
H	-0.90655700	4.14449500	5.39050900	C	-6.65481500	-1.29408100	-0.16365900
C	-1.57185600	-0.86514400	5.00262300	H	-7.31622700	-1.44883400	-1.02890600
H	-1.80273500	-1.85526400	5.40017800	H	-7.25835900	-1.46971700	0.73889900
C	-3.71563400	1.17686500	-3.60298400	H	-5.84679000	-2.03276700	-0.19359100
H	-3.15728900	1.48094600	-4.49036200	C	4.98412200	-2.68415100	-2.33598100
C	-5.67036100	0.18755700	-2.60978800	H	5.49452600	-3.62518300	-2.08171300
H	-6.64464000	-0.28958400	-2.72873700	H	5.25043300	-2.43830900	-3.37481900
C	2.48932200	-5.00867000	-0.57775700	H	3.89994100	-2.85565800	-2.28682800
H	2.25272900	-4.94389400	-1.64808000	C	-2.38550300	-2.75198700	2.67221500
H	2.73200200	-6.05344200	-0.33004800	H	-1.51388400	-2.57361800	2.02521900
H	3.37730800	-4.39354800	-0.36834600	H	-3.09135100	-3.39170600	2.12161500
C	-0.15310600	4.99117500	0.47361400	H	-2.04094900	-3.31250700	3.55499800
H	-0.43934000	5.86582100	-0.12945500	C	-4.29284600	-1.71598100	3.95689600
H	-0.35804500	5.24175500	1.52580500	H	-4.02045000	-2.26794100	4.86873800
H	-0.79727400	4.14595100	0.18301300	H	-5.02390200	-2.32278200	3.40292800
C	-0.75403000	1.61075200	-2.91664000	H	-4.78506900	-0.78235300	4.26664600
H	-0.64761700	0.57191900	-2.56616400	C	2.22463500	5.80615100	0.70051200
H	0.17260100	2.15783500	-2.70099100	H	3.28950400	5.55226500	0.59671200
H	-0.87948200	1.58568100	-4.01149800	H	2.04129900	6.09492000	1.74658400
C	1.47013100	-4.54784000	2.28870400	H	2.02979500	6.68648700	0.06926500
H	2.32300300	-3.90028100	2.53875700	C	-4.39200200	-3.51132600	-2.23687900
H	1.73457000	-5.58112400	2.56083000	H	-3.76690200	-3.70439500	-3.11933500
H	0.61368400	-4.24357700	2.91112600	H	-4.65869600	-2.44402000	-2.21764400
C	6.91713300	-1.28363500	-1.51831500	H	-5.31576100	-4.09851100	-2.33206700
H	7.24427700	-0.46968400	-0.85489200	C	4.09925700	0.38693800	4.21314100

H	4.30698500	-0.45159200	4.89415100	H	1.63476500	0.18356600	-3.39513500
H	3.56495400	1.15874800	4.78684600	H	3.11905900	-0.52543100	-4.07614000
H	5.06463900	0.80242600	3.88938800	H	2.33398800	0.84841100	-4.89449800
C	4.75579500	1.70367100	-3.79093200	C	-2.21180100	-1.75729500	-5.08512000
H	4.57985300	2.17551000	-4.76910900	H	-1.79233900	-0.75092900	-5.22224000
H	5.33030800	0.78089400	-3.96488800	H	-3.17674500	-1.65795400	-4.56869800
H	5.37628300	2.39214900	-3.19738400	H	-2.38138200	-2.20395300	-6.07382500
C	2.57764800	0.41840700	-3.91073300				

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