Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

for

A crystalline C5-protonated 1,3-imidazol-4-ylidene

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Experimental

All syntheses and manipulations were carried out under an inert gas atmosphere (Ar or N_2) using standard Schlenk techniques or a glove box (MBraun LABMasterPro). Solvents were dried over appropriate drying agents, distilled, and stored over 3Å molecular sieve prior to use. Deuterated solvents were dried over appropriate drying agents, distilled, and stored inside a glove box. NMR spectra were recorded on a Bruker Avance III 500, Bruker Avance III 500 HD or Bruker NEO 600 spectrometer. Chemical shifts (in δ, ppm) are referenced to the solvent residual signals of C_6D_6: ^{1}H, 7.16 ppm and ^{13}C, 128.06 ppm; THF-d_8: ^{1}H, 3.58 ppm and ^{13}C, 67.21 ppm, $CDCl_3$: ^{1}H, 7.26 ppm and ^{13}C, 77.7 ppm; and DMSO-d_6: ^{1}H, 2.50 ppm and ^{13}C, 39.52 ppm. Nano-ESI mass spectra were recorded using an Esquire 3000 ion trap mass spectrometer (Bruker Daltonik GmbH, Bremen, Germany) equipped with a nano-ESI source. Samples were dissolved in acetonitrile (**1**, **3**, **5**) or THF (**4**) and introduced by static nano-ESI using *in-house* pulled glass emitters. Nitrogen served both as nebulizer gas and dry gas and was generated by a Bruker nitrogen generator NGM 11. Helium served as cooling gas for the ion trap. The mass axis was externally calibrated with ESI-L Tuning Mix (Agilent Technologies, Santa Clara, CA, USA) as calibration standard. Infrared spectra were recorded using a Bruker Alpha-T FTIR spectrometer. Elemental analyses were carried out with a EURO EA Element Analyzer. $KN(SiMe_3)_2$ (Aldrich) was used as received. 4-Bromobiphenyl (BpBr) was dried in vacuo prior to use. $(Me_2S)AuCl$ was prepared following a literature protocol.[1]

Synthesis of (IPr^{Bp})Br (1)

To a Schlenk flask containing a mixture of IPr (2.00 g, 5.15 mmol) and 4-bromobiphenyl (1.20 g, 5.15 mmol) in 30 mL of *o*-xylene was added 7 mol% of $Ni(cod)_2$ (100 mg, 0.36 mmol) at room temperature (rt). The resulting suspension was stirred under reflux for 4h, then brought to rt and filtered through a G4 frit. The residue was washed with toluene (15 mL) and dried under vacuum to obtain **1** as an off-white solid in 62% (1.99 g) yield. Crystals suitable for X-ray diffraction analysis were obtained by a slow diffusion of *n*-hexane into a saturated methanol solution of **1**. Elemental analysis (%) calcd for $C_{39}H_{45}BrN_2$ (621.71) **1**: C 75.35; H 7.30; N 4.51; found: C 74.77, H 7.01, N 4.23. ^{1}H NMR (500 MHz, DMSO-d_6, 298 K): δ = 8.75 (s, 2H, NC*H*), 7.83 (d, J = 8.5 Hz, 2H, *o*-$C_{12}H_9$), 7.64 (d, J = 7.6 Hz, 4H, *o'*-, *m'*-$C_{12}H_9$), 7.50 (d, J = 7.8 Hz, 4H, *m*-C_6H_3), 7.39 (m, 3H, *p*-C_6H_3, *p*'-$C_{12}H_9$), 7.01 (d, J = 8.5 Hz, 2H, *m*-$C_{12}H_9$), 2.43 (sept, J = 6.6 Hz, 4H, C*H*$(CH_3)_2$), 1.26 (d, J = 6.7 Hz, 12H, CH(C*H*$_3)_2$), 1.07 (d, J = 6.7 Hz, 12H, CH(C*H*$_3)_2$) ppm. ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6, 298 K): δ = 144.5, 143.7, 136.88, 132.1, 129.8, 129.37,

129.1, 127.1, 126.8, 126.5 (N*C*N, C_6H_3, $C_{12}H_9$), 125.2 (N*C*H), 125.0, 124.4, 118.6 ($C_{12}H_9$), 28.9 ($CH(CH_3)_2$, 24.9, 22.1 ($CH(CH_3)_2$ ppm. MS (ESI pos): *m*/*z* = 541.5 [**1**−Br]$^+$.

Synthesis of (iMIC^{Bp}) (2)

To a mixture of **1** (1.14 g , 1.83 mmol) and $KN(SiMe_3)_2$ (0.36 g, 1.83 mmol) was added 20 mL THF at −78 °C. The resulting bright green suspension allowed to reach room temperature (rt) and was further stirred for 1h, giving a dark green solution. The volatiles were removed in vacuo and then 20 mL toluene was added. The green suspension was filtered over a plug of Celite and washed twice with 10 mL toluene. The volatiles from the filtrate were removed under vacuum to obtain the carbene **2** as a pale green solid in 85% (0.91 g) yield. Crystals suitable for X-ray diffraction analysis were obtained by storing a toluene solution of **2** at −30 °C for two days. Elemental analysis (%) calcd for $C_{39}H_{44}N_2$ (540.80) **2**: C 86.62, H 8.20, N 5.18; found: C 85.43, H 8.01, N 4.93. ^{1}H NMR (500 MHz, C_6D_6, 298 K) δ = 7.22 (t, *J* = 7.6 Hz, 2H, *p*-C_6H_3), 7.12–7.07 (m, 7H, *m*-C_6H_3, $C_{12}H_9$), 7.04–6.98 (m, 5H, $C_{12}H_9$), 6.95 (d, *J* = 6.1 Hz, 2H, $C_{12}H_9$), 3.05 (s, br, 4H, C*H*$(CH_3)_2$), 1.29 (d, 12H, *J* = 6.6 Hz, CH(C*H*$_3)_2$), 1.02 (d, 12H, *J* = 6.7 Hz, CH(C*H*$_3)_2$) ppm. ^{1}H NMR (500 MHz, THF-d_8, 298 K) δ = 7.51 (d, *J* = 7.8 Hz, 2H, *m*-C_6H_3), 7.41 (d, *J* = 8.3 Hz, 2H, $C_{12}H_9$), 7.37 (t, *J* = 7.7 Hz, 2H, *p*-C_6H_3), 7.31 (t, *J* = 7.5 Hz, 2H, $C_{12}H_9$), 7.24 (d, *J* = 7.7 Hz, 5H, *m*-C_6H_3), 6.95 (d, *J* = 8.3 Hz, 2H, $C_{12}H_9$), 2.77 (sept, *J* = 6.1 Hz, 4H, C*H*$(CH_3)_2$), 1.24 (d, *J* = 6.7 Hz, 12H, CH(C*H*$_3)_2$), 1.01 (d, *J* = 6.9 Hz, 12H, CH(C*H*$_3)_2$) ppm. ^{1}H NMR (600 MHz, THF-d_8, 163 K): δ = 7.80–7.62 (m, 4H, C_6H_3), 7.52 (br, 1H, *p*'-$C_{12}H_9$), 7.41 (br, 5H, C_6H_3, $C_{12}H_9$), 7.34 (br, 2H, $C_{12}H_9$) 6.93 (br, 2H, $C_{12}H_9$), 6.76 (s, 1H, NC*H*), 2.74 (br, 2H, C*H*$(CH_3)_2$), 2.60 (br, 2H, C*H*$(CH_3)_2$), 1.23 (br, 12H, CH(C*H*$_3)_2$), 0.99 (br, 12H, CH(C*H*$_3)_2$) ppm. ^{13}C{^{1}H} NMR (126 MHz, THF-d_8, 298 K) δ = 203.7 (N$C_{carbene}$), 146.9, 146.0, 144.9, 142.1, 140.1, 138.6, 130.0, 129.8, 129.7, 129.1, 128.8, 127.6, 127.1, 126.2, 125.4 (C_6H_3, $C_{12}H_9$); 124.8 (br, N*C*H); 124.1 ($C_{12}H_9$); 29.6 ($CH(CH_3)_2$; 25.8 ($CH(CH_3)_2$, overlaps with THF), 23.0 ($CH(CH_3)_2$) ppm. UV/vis (THF, $1.05\cdot10^{-5}$ M): λ / nm (ε / M^{-1} cm^{-1})) 299 (80937), 417 (shoulder, 16937).

Synthesis of (iMIC^{Bp})Ni(CO)$_3$ (3)

To a 5 mL toluene solution of **2** (280 mg, 0.5 mmol) was added a freshly prepared toluene solution of $Ni(CO)_4$ (0.5 M, 1.04 mL, 0.5 mmol) at rt. The resulting solution was stirred overnight and then the volatiles were removed under vacuum to afford **3** as a pale yellow solid in 99% yield (355 mg) yield. Crystals suitable for X-ray diffraction analysis were obtained by a slow diffusion of *n*-hexane into a saturated benzene solution of **5** at rt. Elemental analysis (%) calcd for $C_{42}H_{44}N_2NiO_3$ (683.52) **3**: C 73.80, H 6.49, N 4.10; found: C 73.49, H 6.17, N 3.84. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 7.34 (t, *J* = 7.8 Hz, 1H, *p*-C_6H_3), 7.17 (d, *J* = 7.9 Hz, 2H, *m*-C_6H_3, overlaps with

benzene), 7.14–7.09 (m, 2H, $C_{12}H_9$), 7.05 (d, J = 8.6 Hz, 2H, $C_{12}H_9$), 7.02–6.99 (m, 3H, $C_{12}H_9$), 6.94 (d, J = 7.9 Hz, 2H, *m*-C_6H_3), 6.91–6.90 (m, 3H, *p*-C_6H_3, $C_{12}H_9$), 6.87 (s, 1H, NC*H*), 2.98 (sept, J = 7.0 Hz, 2H, C*H*$(CH_3)_2$), 2.75 (sept, J = 6.6 Hz, 2H, C*H*$(CH_3)_2$), 1.51 (d, J = 6.8 Hz, 6H, CH(C*H*$_3)_2$), 1.08 (d, J = 6.8 Hz, 6H, CH(C*H*$_3)_2$), 0.96 (d, J = 6.9 Hz, 6H, CH(C*H*$_3)_2$), 0.89 (d, J = 6.9 Hz, 6H, CH(C*H*$_3)_2$) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ = 170.2 (*C*O), 145.5, 145.3, 143.5, 142.3, 138.8, 137.7, 133.2, 131.3 (C_6H_3, $C_{12}H_9$); 130.7 (N*C*H); 130.5, 129.3; 129.1, 128.9, 127.1, 126.8, 124.9, 124.8 (C_6H_3, $C_{12}H_9$); 29.1, 29.0 (*C*H$(CH_3)_2$; 25.2, 24.4, 23.4, 22.7 (CH(*C*$H_3)_2$) ppm. MS (ESI, positive mode): m/z = 541.5 [**2**+H]$^+$, 627.5 [(**3**−2 CO)+H]$^+$. IR (KBr, neat): $\tilde{\nu}_{CO}$ = 2033.5, 1941.7 cm^{-1}. IR (KBr, DCM): $\tilde{\nu}_{CO}$ = 2039.6, 1954.0 cm^{-1}.

Synthesis of (iMIC^{Bp})AuCl (4)

To an 8 mL toluene solution of **2** (150 mg, 0.26 mmol) was added (Me_2S)AuCl (76 mg, 0.26 mmol) at rt. The resulting brown solution was stirred for 3h and then dried under vacuum, affording **4** as a colorless solid. Yield: 212 mg, 99%. Crystals suitable for X-ray diffraction analysis were obtained by a slow diffusion of *n*-hexane into a saturated toluene solution of **4** at rt. Elemental analysis (%) calcd for $C_{39}H_{44}AuClN_2$ (773.21) **4**: C 60.58, H 5.74, N 3.62; found: C 60.15, H 5.55, N 3.36. ^1H NMR (500 MHz, $CDCl_3$, 298 K) δ = 7.52–7.40 (m, 4H, C_6H_3, $C_{12}H_9$), 7.38–7.32 (m, 5H, C_6H_3, $C_{12}H_9$), 7.28 (d, J = 7.8 Hz, 2H, $C_{12}H_9$), 7.22 (d, J = 7.8 Hz, 2H, $C_{12}H_9$), 6.92–6.91 (m, 3H, NC*H*, $C_{12}H_9$), 2.68–2.50 (m, 4H, C*H*$(CH_3)_2$), 1.47 (d, J = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.26 (d, J = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.03 (d, J = 7.0 Hz, 6H, CH(C*H*$_3)_2$), 0.98 (d, J = 6.8 Hz, 6H, CH(C*H*$_3)_2$). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ = 154.1 (*C*Au); 145.2, 145.0, 143.7, 143.5, 138.6, 134.9, 131.6; 131.39, 130.93, 129.54, 129.18, 129.08 (N*C*N, C_6H_3, $C_{12}H_9$); 128.98 (N*C*H); 128.68, 128.37, 127.02, 126.90, 125.60, 125.44, 125.03, 124.87, 121.74 (C_6H_3, $C_{12}H_9$); 29.11 (*C*H$(CH_3)_2$); 25.81, 25.78, 22.91, 22.77 (CH(*C*$H_3)_2$) ppm. MS (ESI, negative mode) m/z = 807.0 [**4**+Cl]$^-$

Synthesis of (iMIC^{Bp})CO_2 (5)

A toluene (5 mL) solution of **2** (196 mg, 0.36 mmol) was stirred under one atmosphere of CO_2 for 1h at rt, resulting in an immediate color change from green to red-brown. The volatiles were removed in vacuo, affording **5** as an off-white solid in >99% (211 mg) yield. Elemental analysis (%) calcd for $C_{40}H_{44}N_2O_2$ (584.80) **5**: C 82.15, H 7.58, N 4.79; found: C 82.32, H 7.32, N 4.63. ^1H NMR (500 MHz, $CDCl_3$, 298 K): δ = 7.85 (s, 1H, NC*H*), 7.54 (t, J = 7.8 Hz, 1H, *p*-C_6H_3), 7.48–7.40 (m, 3H, *p*-C_6H_3, $C_{12}H_9$), 7.37–7.35 (m, 4H, $C_{12}H_9$), 7.30 (m, 3H, *m*-C_6H_3, *p*'-$C_{12}H_9$), 7.21 (d, J = 7.8 Hz, 2H, *m*-C_6H_3), 6.90 (d, J = 8.2 Hz, 2H, $C_{12}H_9$), 2.55 (sept, J = 6.4 Hz, 4H, C*H*$(CH_3)_2$), 1.34 (d, J = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.26 (d, J = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.00 (d, J = 6.7 Hz, 6H,

$CH(CH_3)_2$), 0.96 (d, J = 6.8 Hz, 6H, $CH(CH_3)_2$) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K): δ = 157.6 (CO_2); 145.0, 144.5, 138.3 (N*C*N, C_6H_3, $C_{12}H_9$); 137.8 (N*C*CO_2); 132.0, 131.3, 131.0, 130.7, 130.0, 129.1, 127.1, 127.0 (C_6H_3, $C_{12}H_9$); 125.8 (N*C*H); 125.4, 125.3, 124.6, 120.3 (C_6H_3, $C_{13}H_9$)); 29.6, 29.3 ($CH(CH_3)_2$)); 25.7, 24.9, 22.9, 22.7 ($CH(CH_3)_2$ ppm. MS (ESI, positive mode) m/z = 541.4 [**2**+H]$^+$, 585.4 [**3**+H]$^+$.

Synthesis of (ADC^{Bp})P$_3$ (6)

To a 5 mL THF solution of **2** (178 mg, 0.3 mmol) was added P_4 (51 mg, 0.4 mmol) and the resulting green solution was stirred overnight at room temperature and then under reflux for 2h. The volatiles were removed and the brown residue was suspended in 5 mL toluene, filtered, and dried under vacuum to afford **6** as a pale yellow solid in 48% (100 mg) yield. Elemental analysis (%) calcd for $C_{39}H_{43}N_2P_3$ (632.71) **6**: C 74.04, H 6.85, N 4.43; found: C 73.71, H 6.39, N 4.22. ^1H NMR (500 MHz, $CDCl_3$, 298 K): δ = 7.57 (t, J = 7.8 Hz, 2H, p-C_6H_3), 7.47 (d, J = 7.4 Hz, 2H, m-C_6H_3), 7.42 – 7.33 (m, 9H, C_6H_3, $C_{12}H_9$), 7.19 (d, J = 8.4 Hz, 2H, $C_{12}H_9$), 2.65 (sept, J = 6.7 Hz, 4H, $CH(CH_3)_2$), 1.26 (d, J = 6.7 Hz, 12H, $CH(CH_3)_2$), 1.00 (d, J = 6.8 Hz, 12H, $CH(CH_3)_2$) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K): δ = 167.2 (d, J_{PC} = 83.9 Hz), 147.9, 145.7, 144.9, 143.7, 138.5, 133.4, 132.4, 131.3, 129.6, 129.2, 129.1, 128.7, 127.0, 125.5, 122.2 (N*C*N; C_6H_3, $C_{12}H_9$); 29.2 ($CH(CH_3)_2$); 25.8, 23.3 ($CH(CH_3)_2$. $^{31}P\{^1H\}$ NMR (202 MHz, $CDCl_3$, 298 K): δ = 331.9 (t, J_{PP} = 505 Hz), 174.5 (d, J_{PP} = 505 Hz). MS (ESI, positive mode): m/z = 633.3 [**6**+H]$^+$.

NMR spectra of compounds 1–6

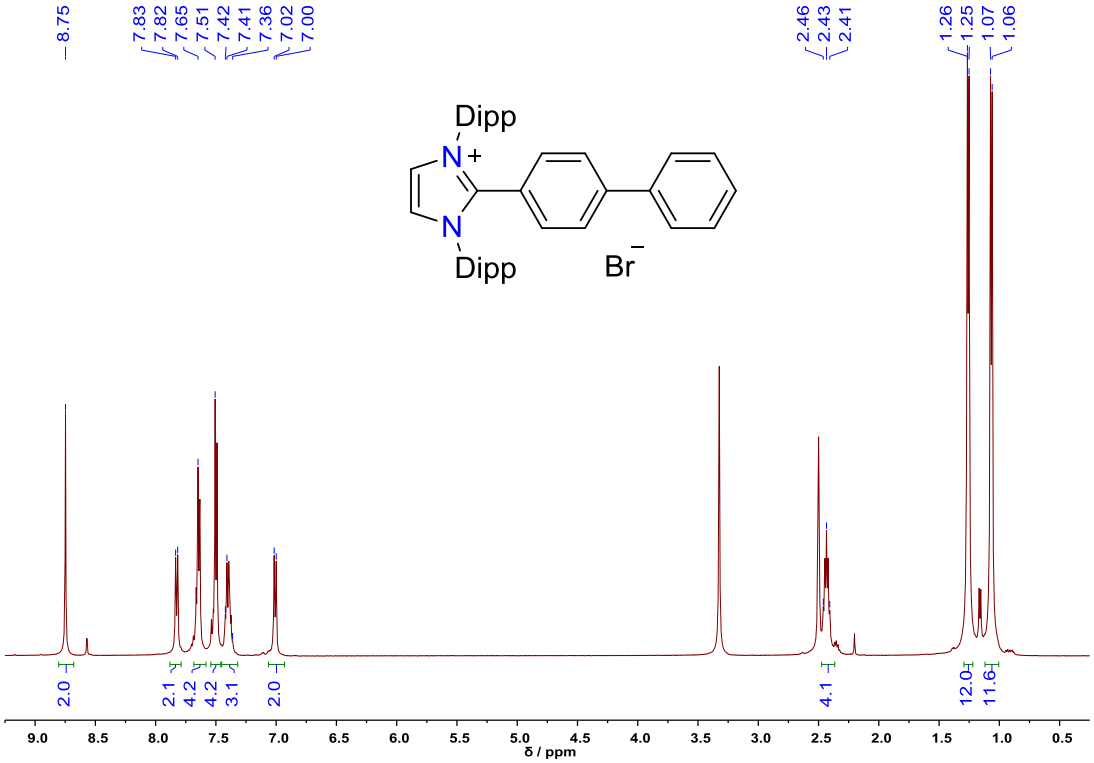


Fig. S1 ^{1}H NMR spectrum (500 MHz, DMSO-d_6, 298 K) of **1**.

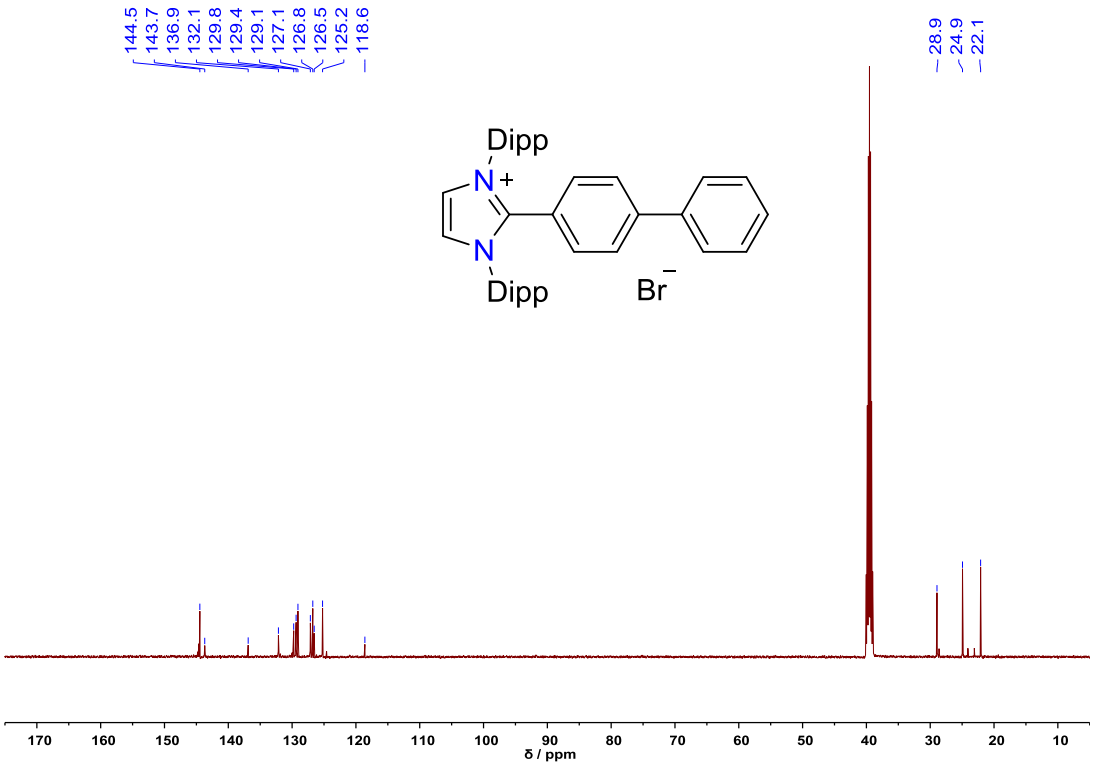


Fig. S2 ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6, 298 K) spectrum of **1**.

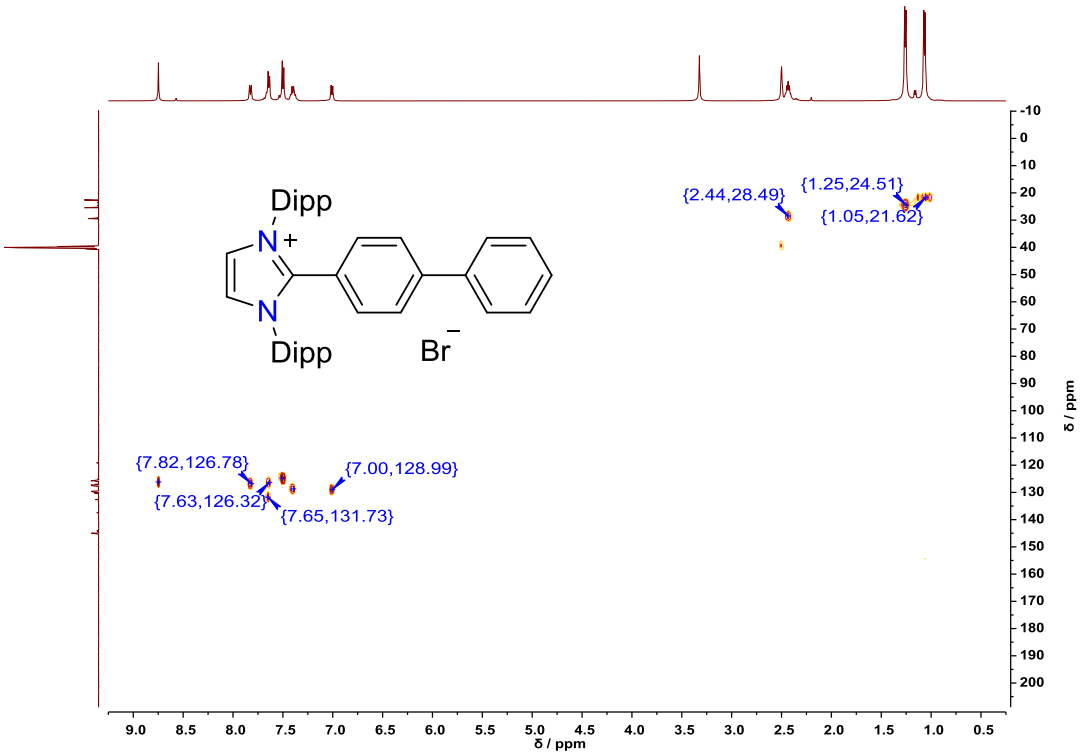


Fig. S3 ^{1}H-^{13}C HMQC NMR spectrum (DMSO-d_6, 298 K) of **1**.

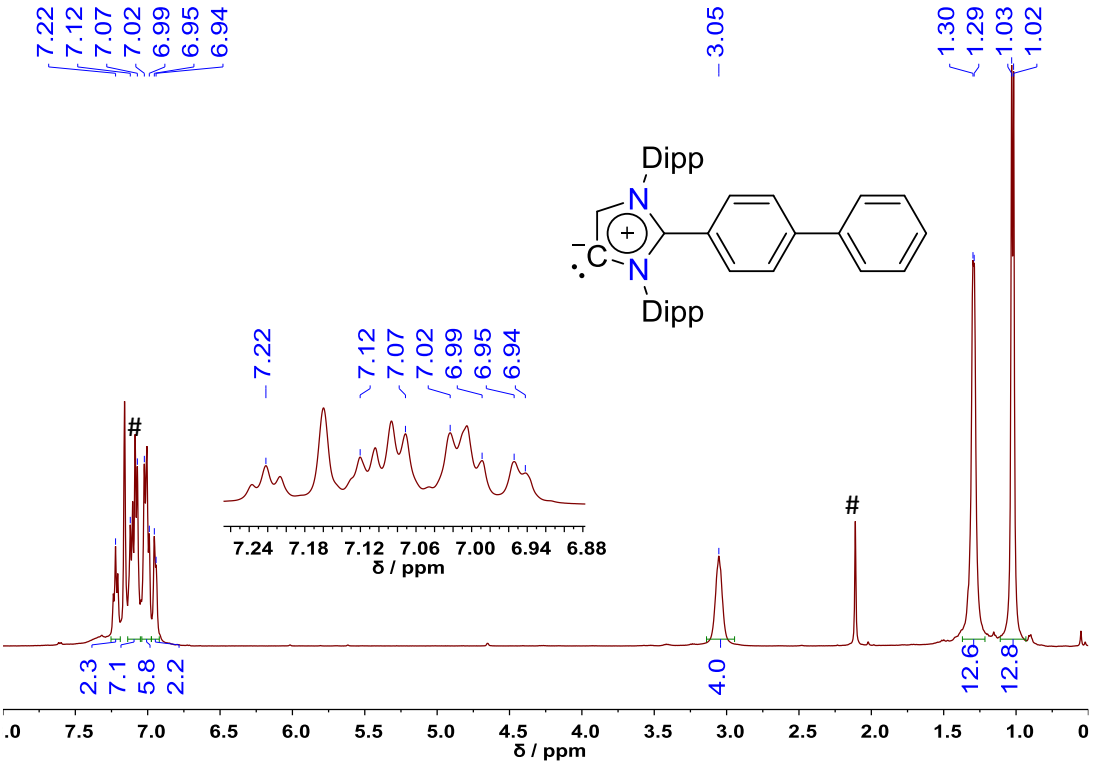


Fig. S4 ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of **2**. # = toluene.

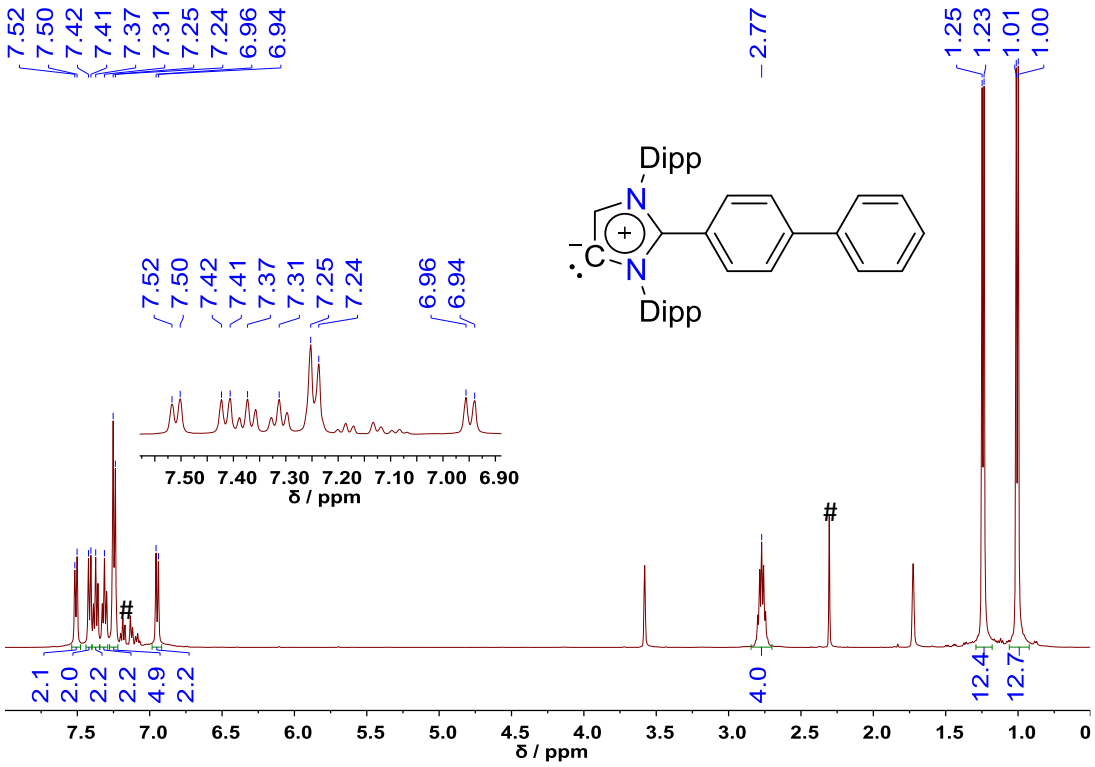


Fig. S5 ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of **2**. # = toluene.

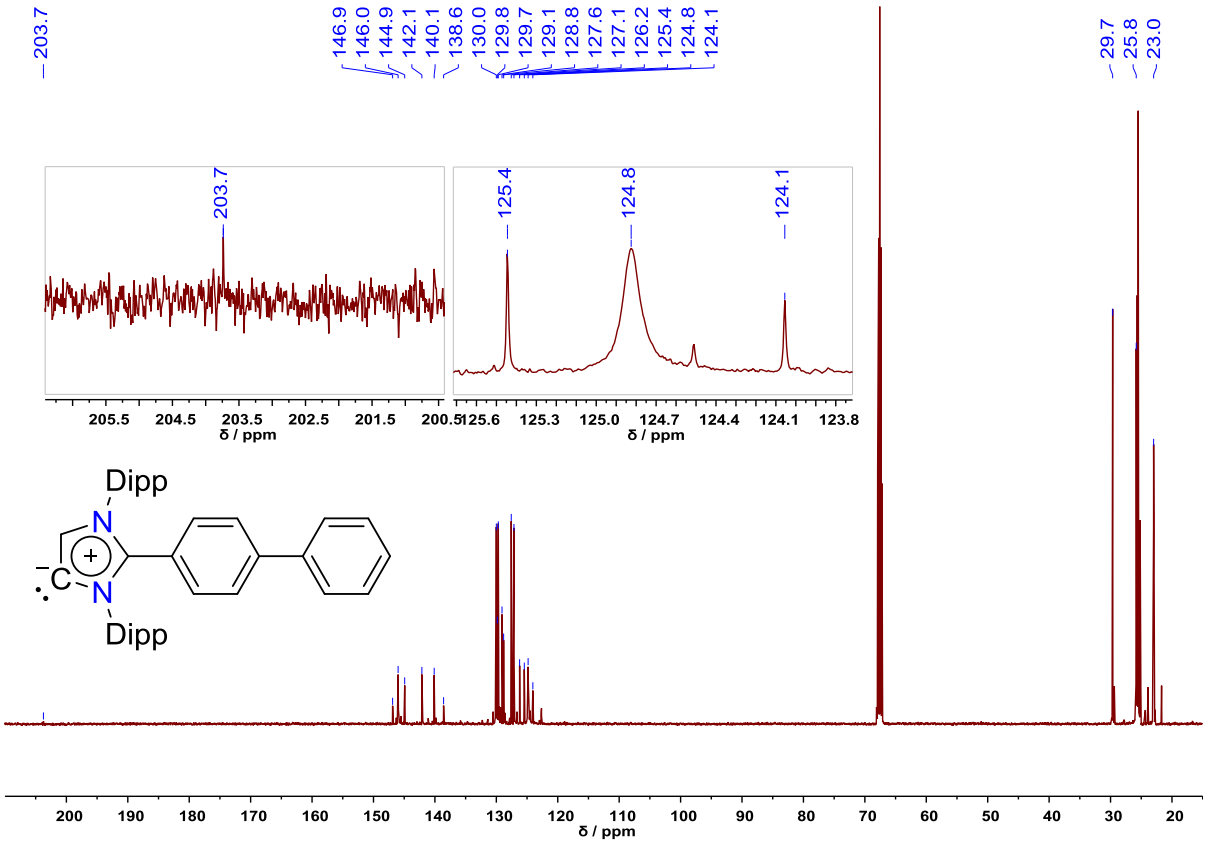


Fig. S6 ^{13}C{^{1}H} NMR (126 MHz, THF-d_8, 298 K) spectrum of **2**.

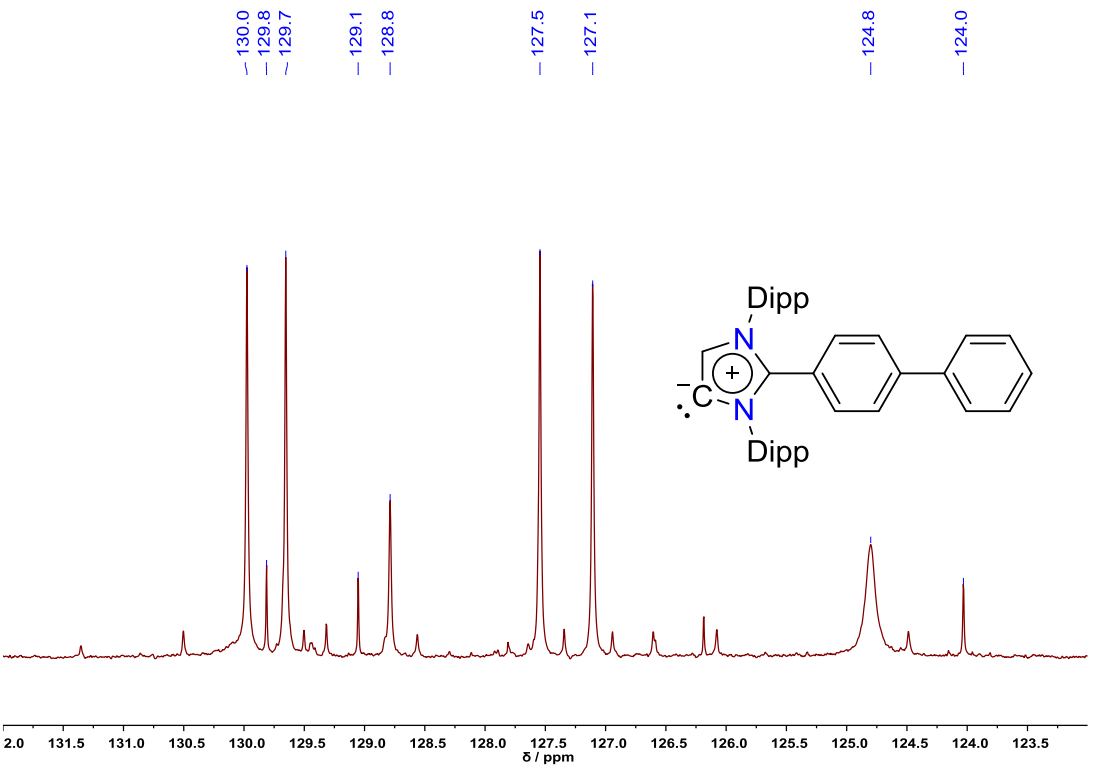


Fig. S7 ^{13}C-DEPT135 NMR (126 MHz, THF-d_8, 298 K) spectrum of the aromatic region of **2**.

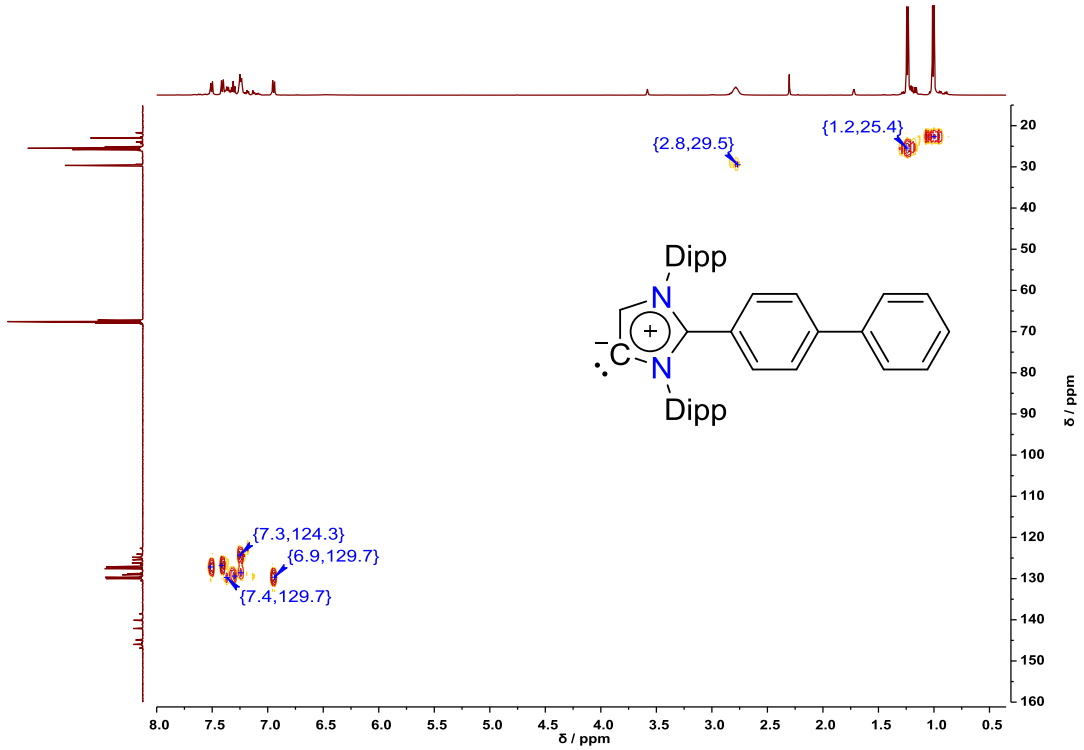


Fig. S8 ^{1}H-^{13}C HMQC NMR (THF-d_8, 298 K) spectrum of **2**.

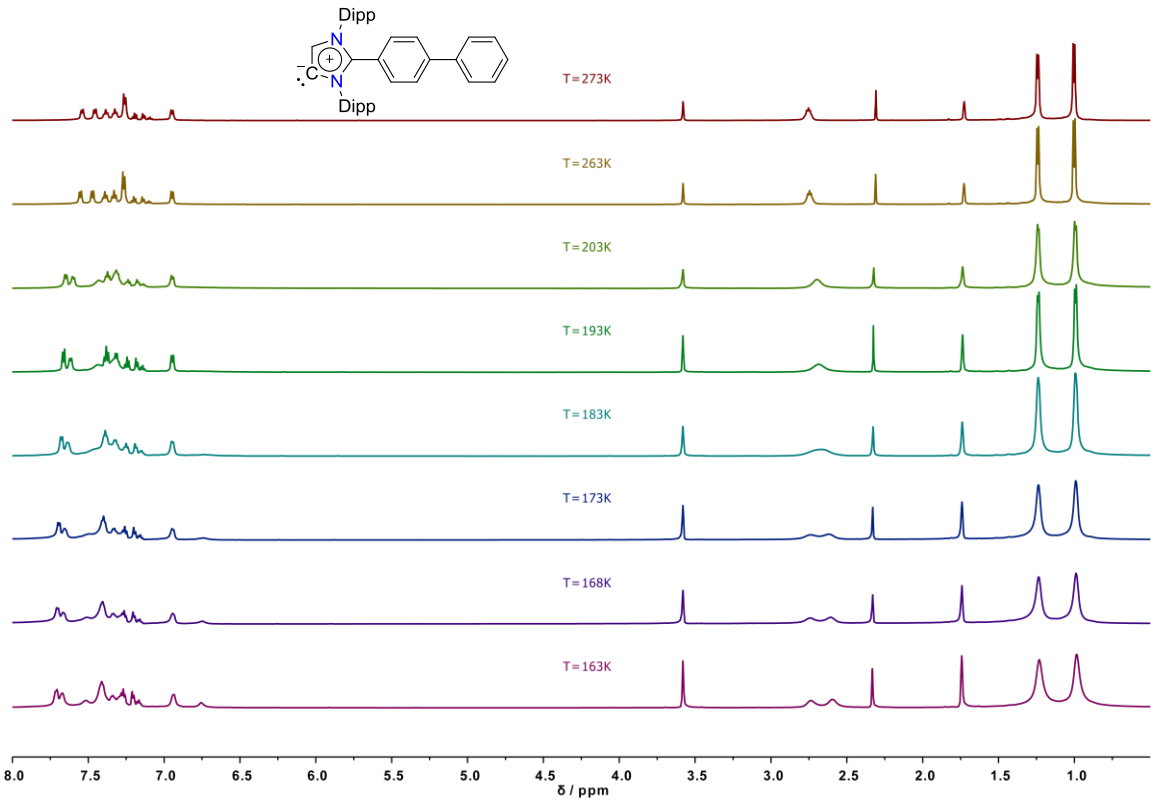


Fig. S9a Variable temperature ^{1}H NMR (600 MHz, THF-d_8) spectra of **2** (273-163 K).

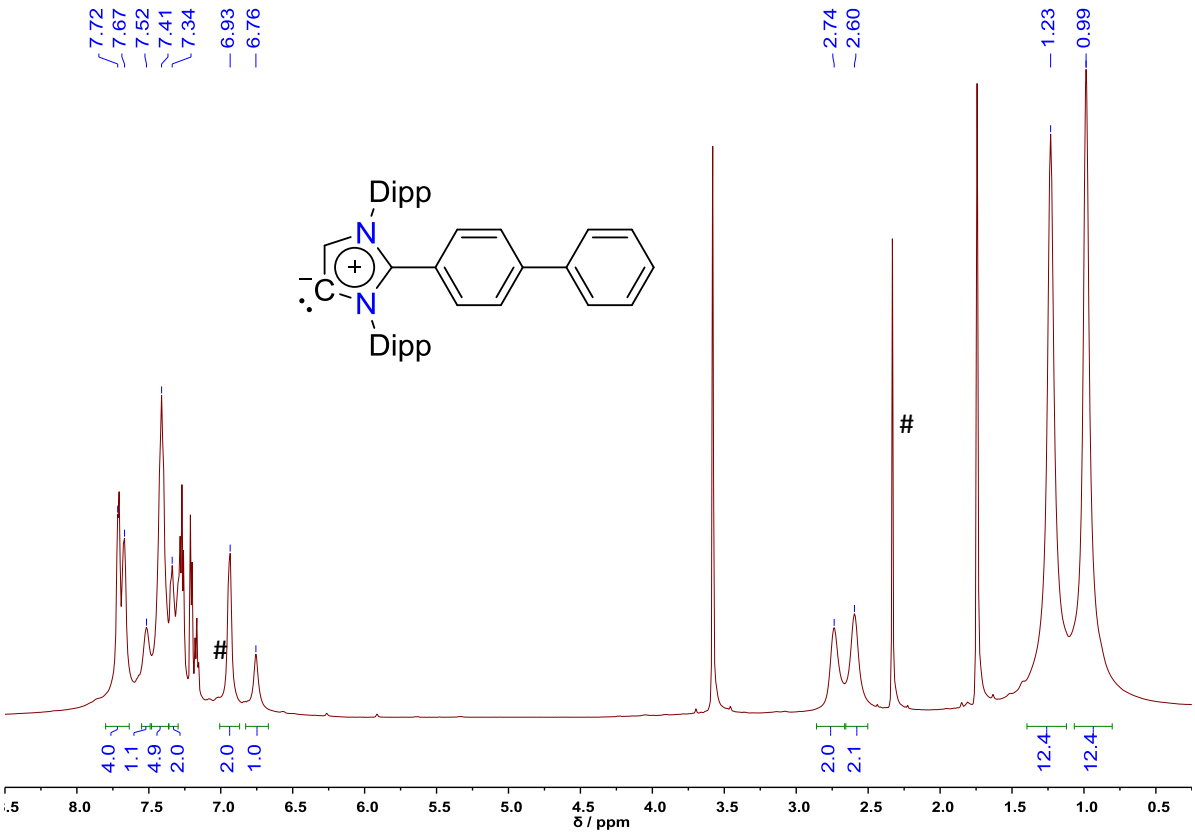


Fig. S9b ^{1}H NMR (600 MHz, THF-d_8, 163 K) spectrum of **2**. # = toluene.

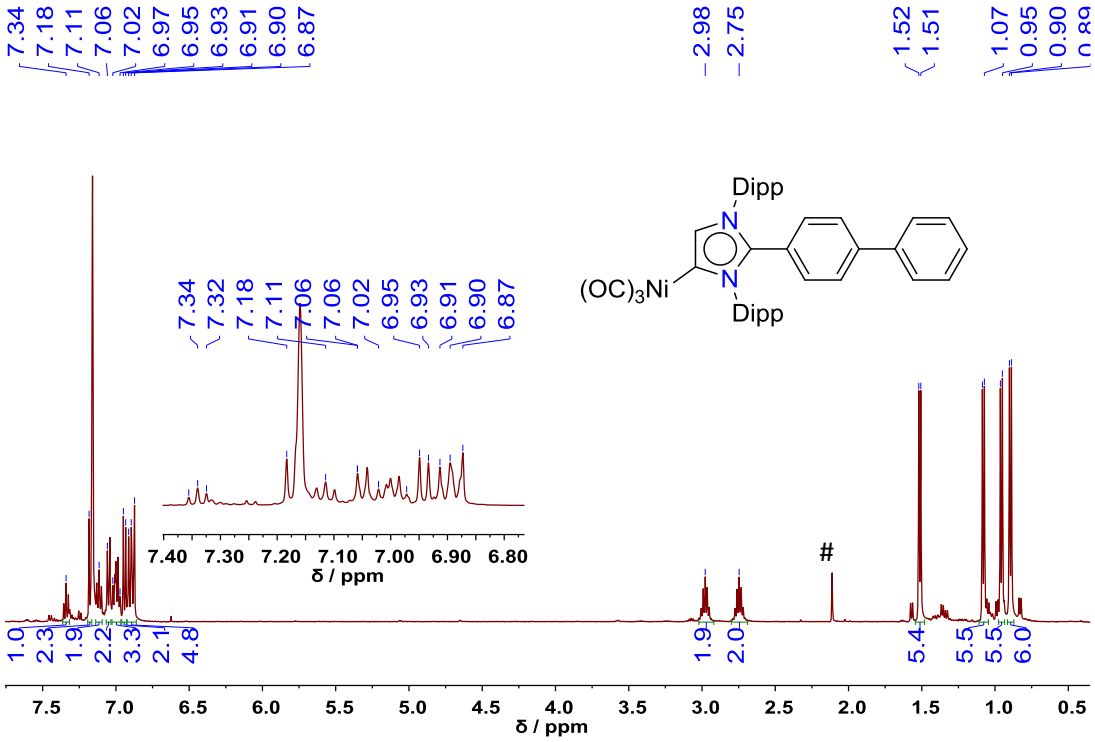


Fig. S10 ^{1}H NMR (500 MHz, C_6D_6, 298 K) spectrum of **3**. # = toluene.

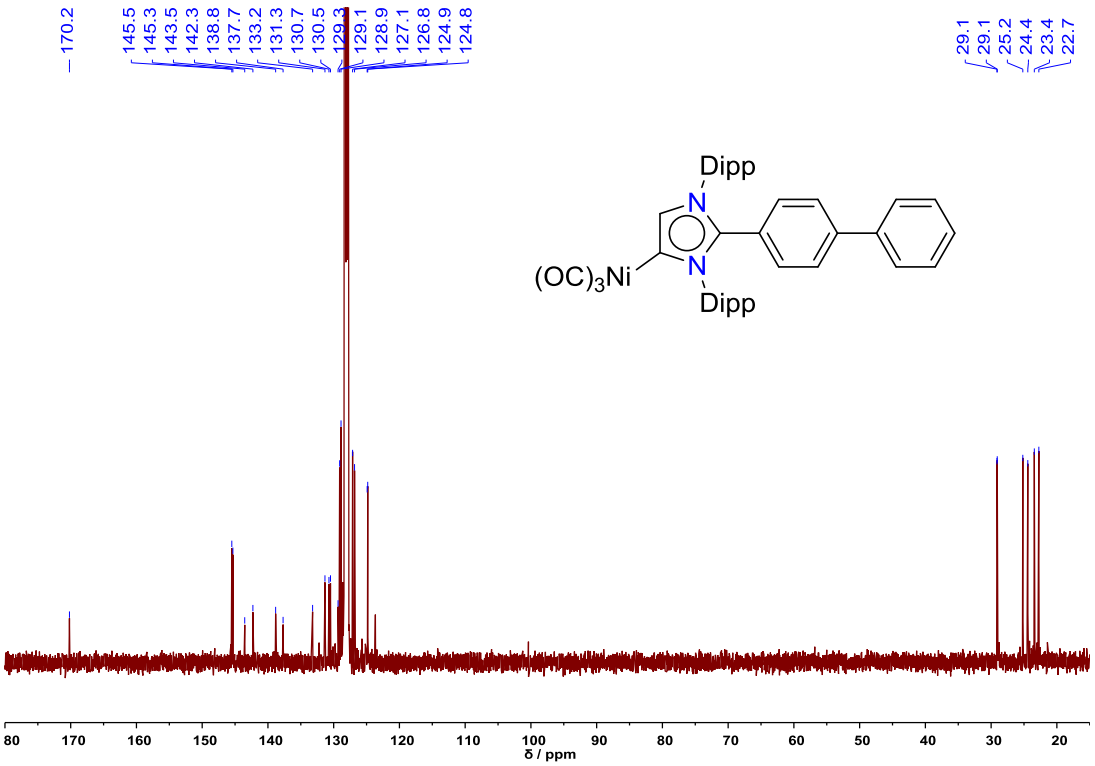


Fig. S11 ^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 298 K) spectrum of **3**.

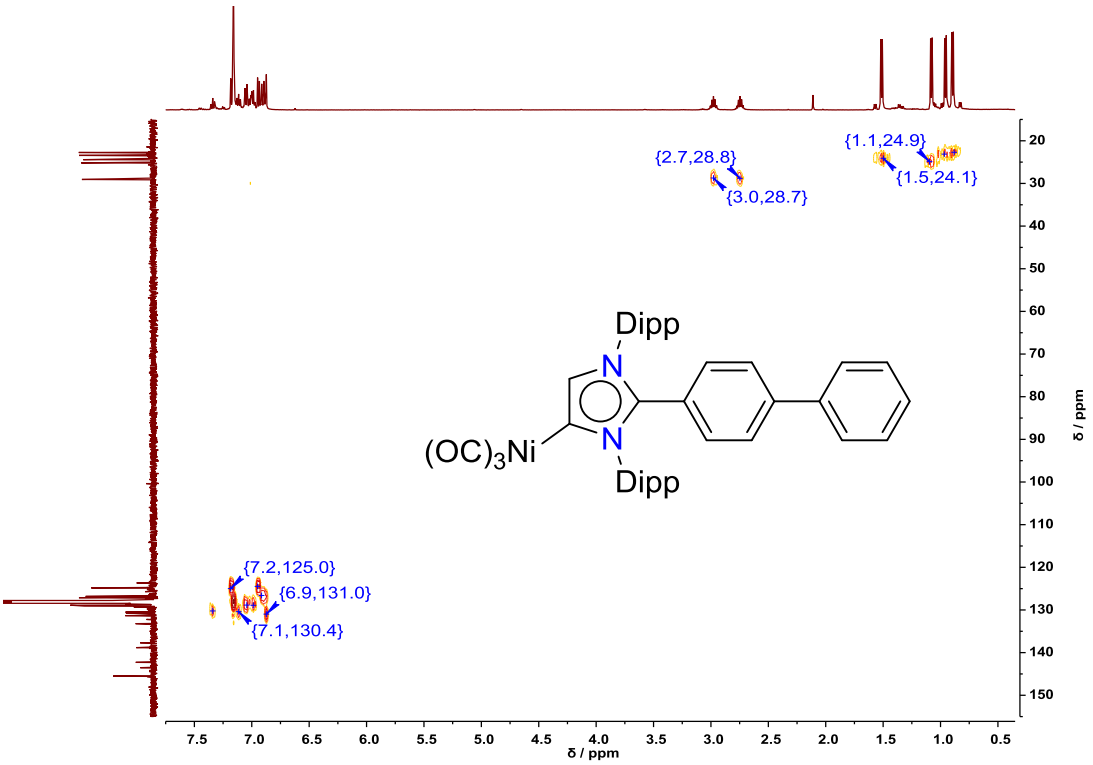


Fig. S12 ^{1}H-^{13}C HMQC NMR (C_6D_6, 298 K) spectrum of **3**.

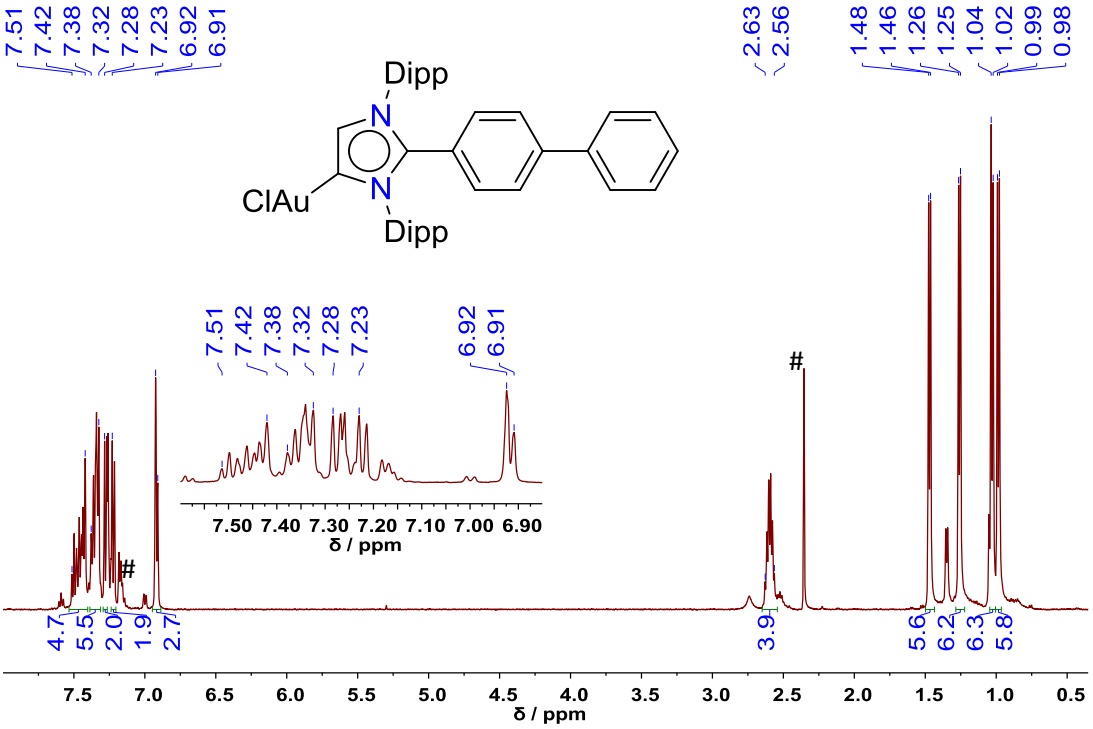


Fig. S13 ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of **4**. # = toluene.

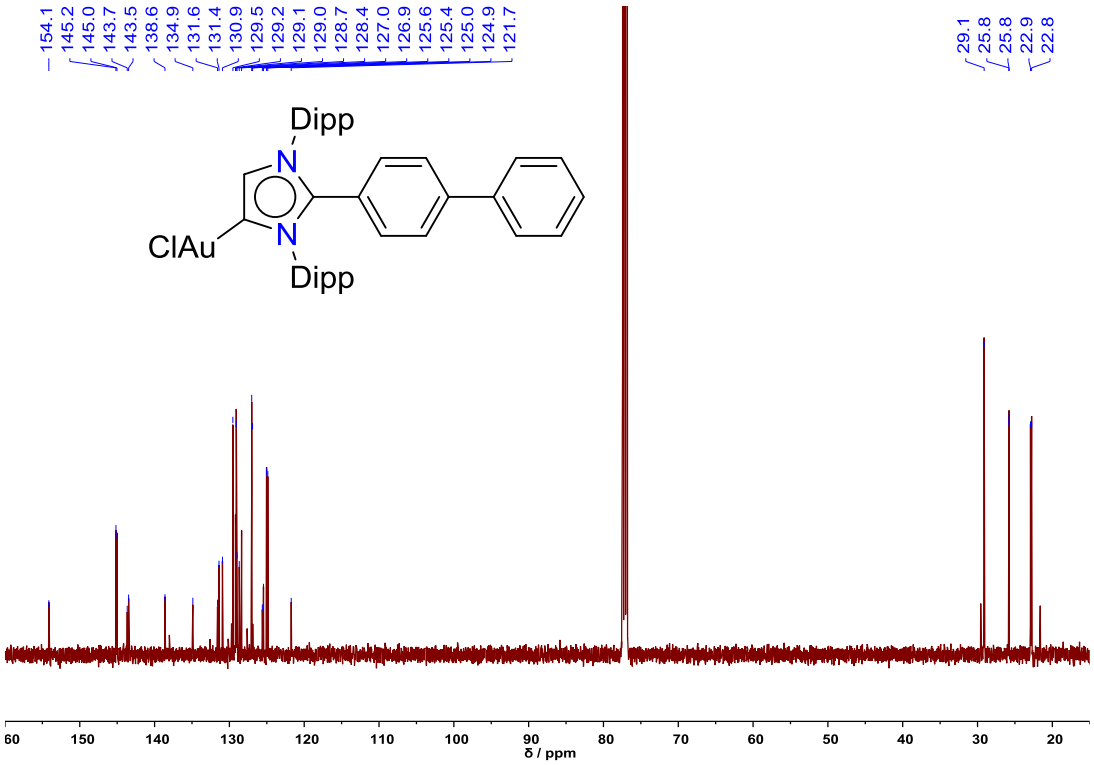


Fig. S14 $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 298 K) spectrum of **4**.

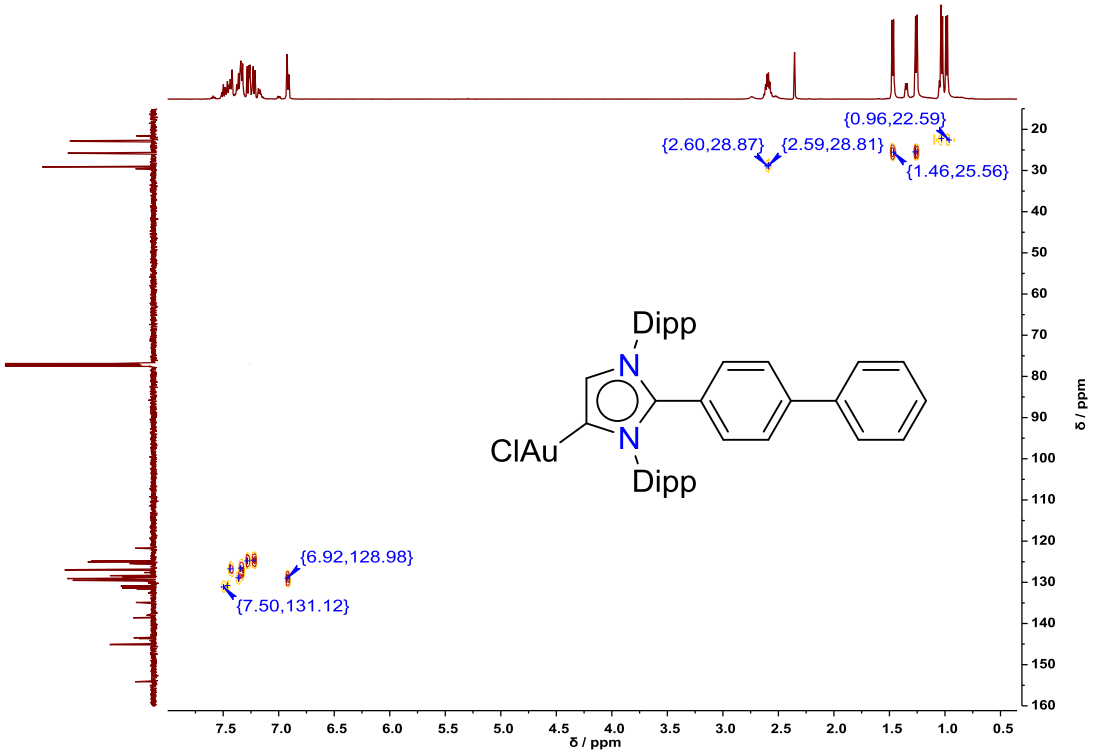


Fig. S15 ^{1}H-^{13}C HMQC NMR ($CDCl_3$, 298 K) spectrum of **4**.

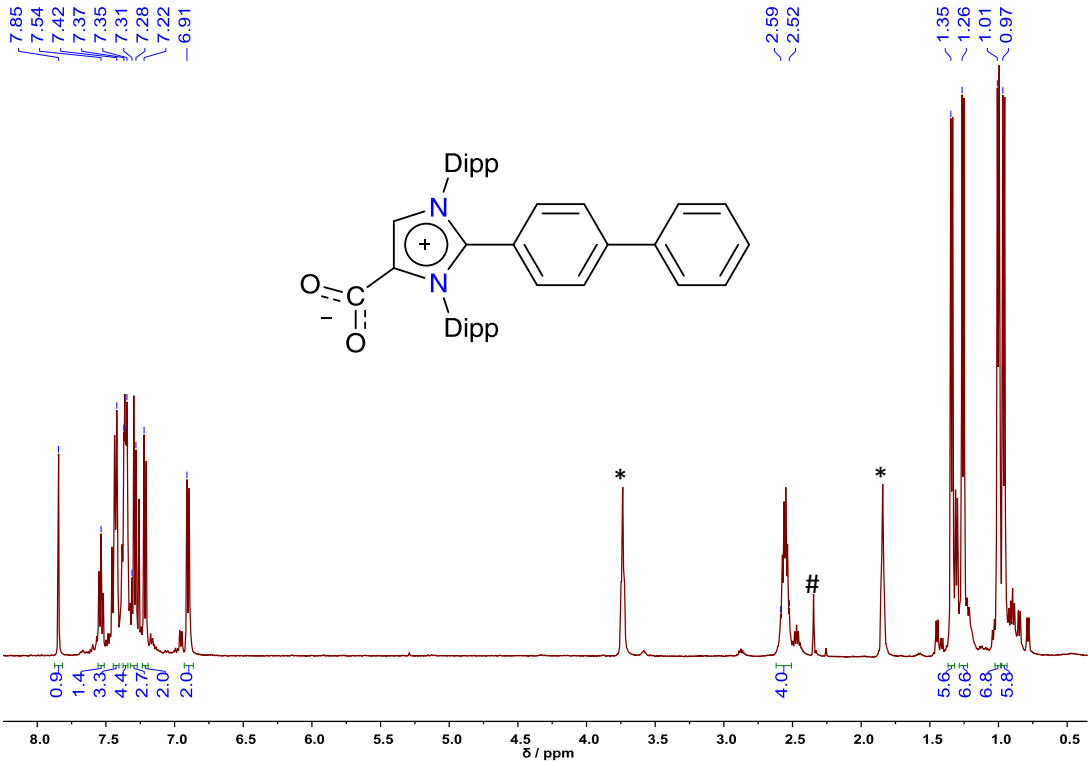


Fig. S16 ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of **5**. * THF, # = toluene.

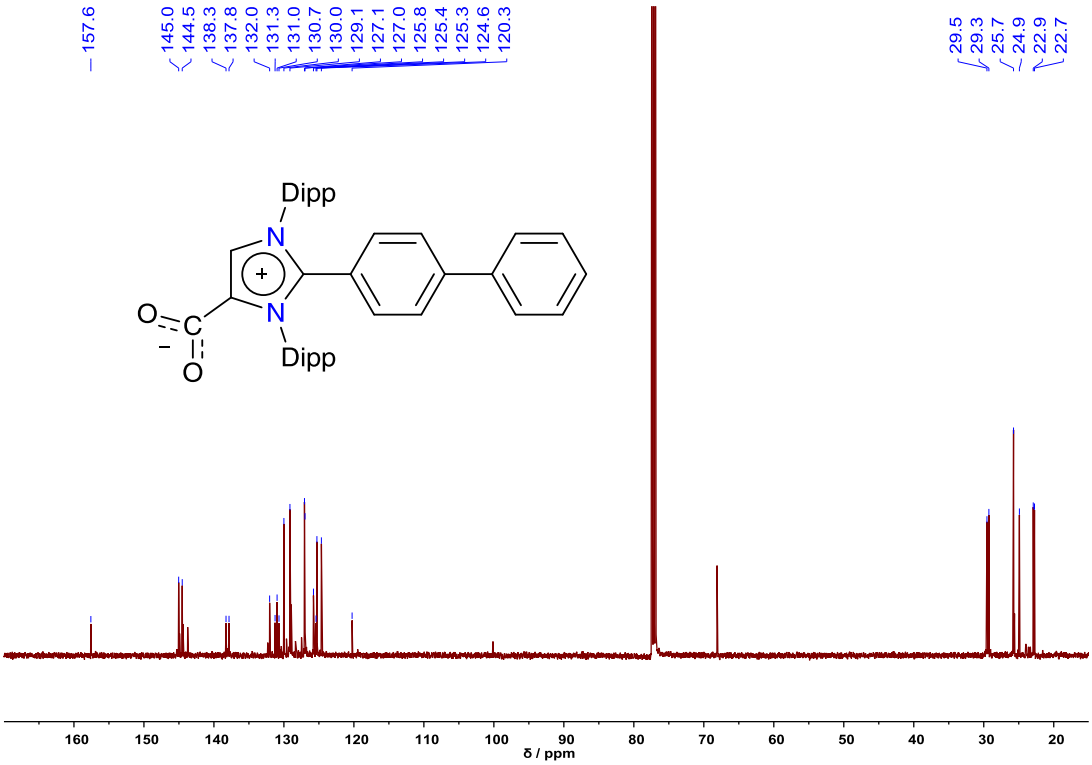


Fig. S17 $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 298 K) spectrum of **5**.

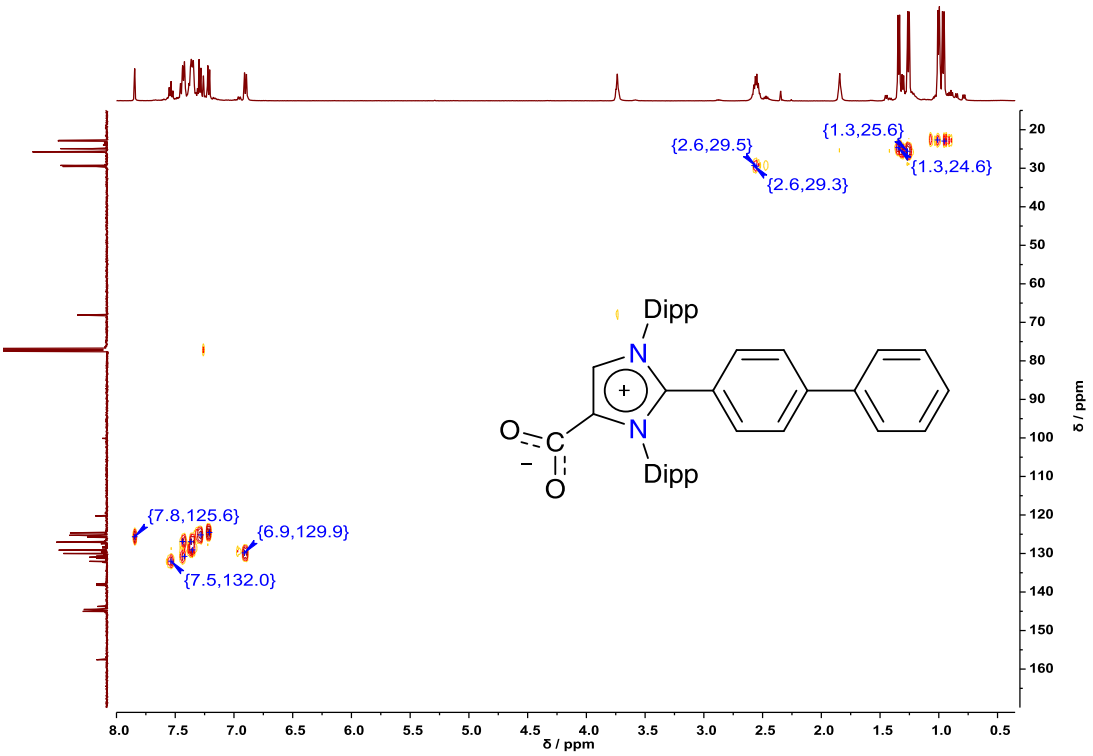


Fig. S18 ^{1}H- ^{13}C HMQC NMR ($CDCl_3$, 298 K) spectrum of **5**.

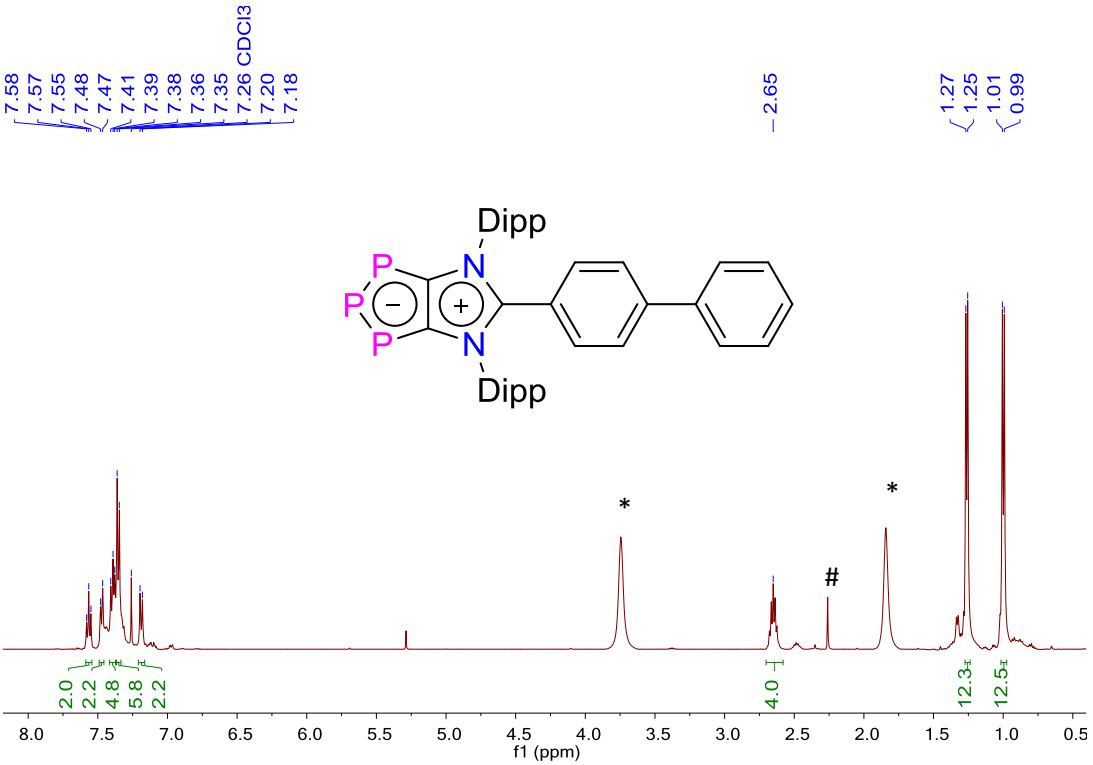


Fig. S19 ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of **6**. * = THF, # = toluene.

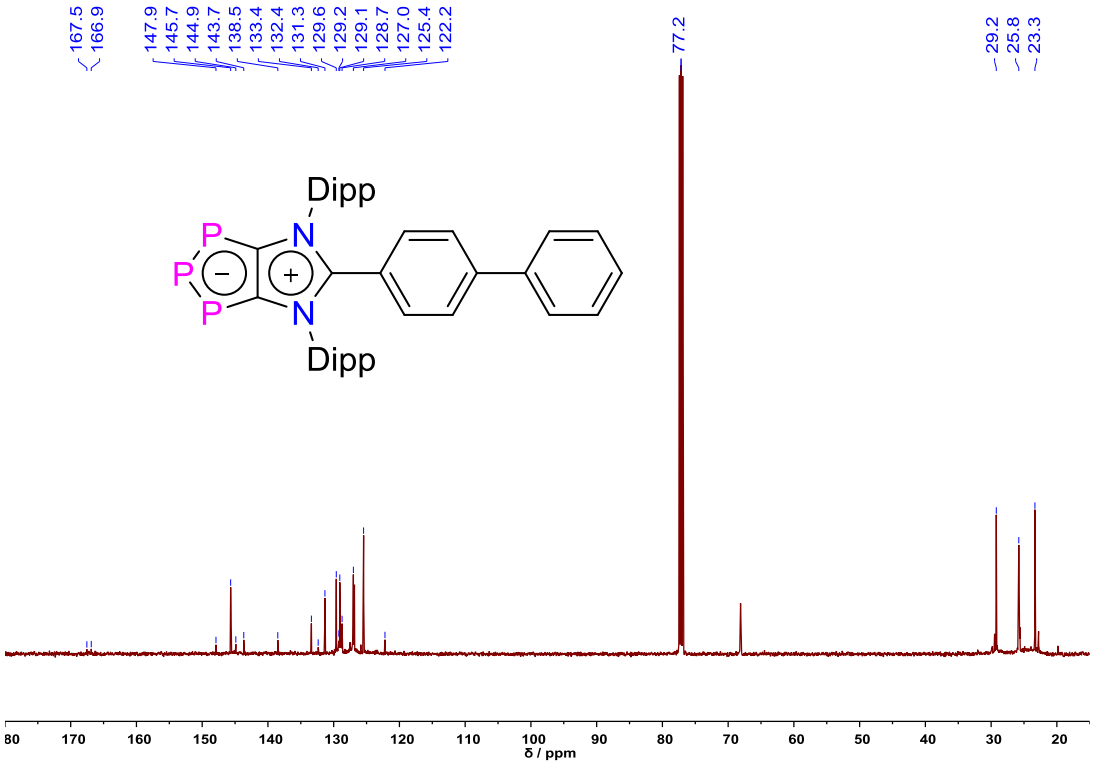


Fig. S20 $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 298 K) spectrum of **6**.

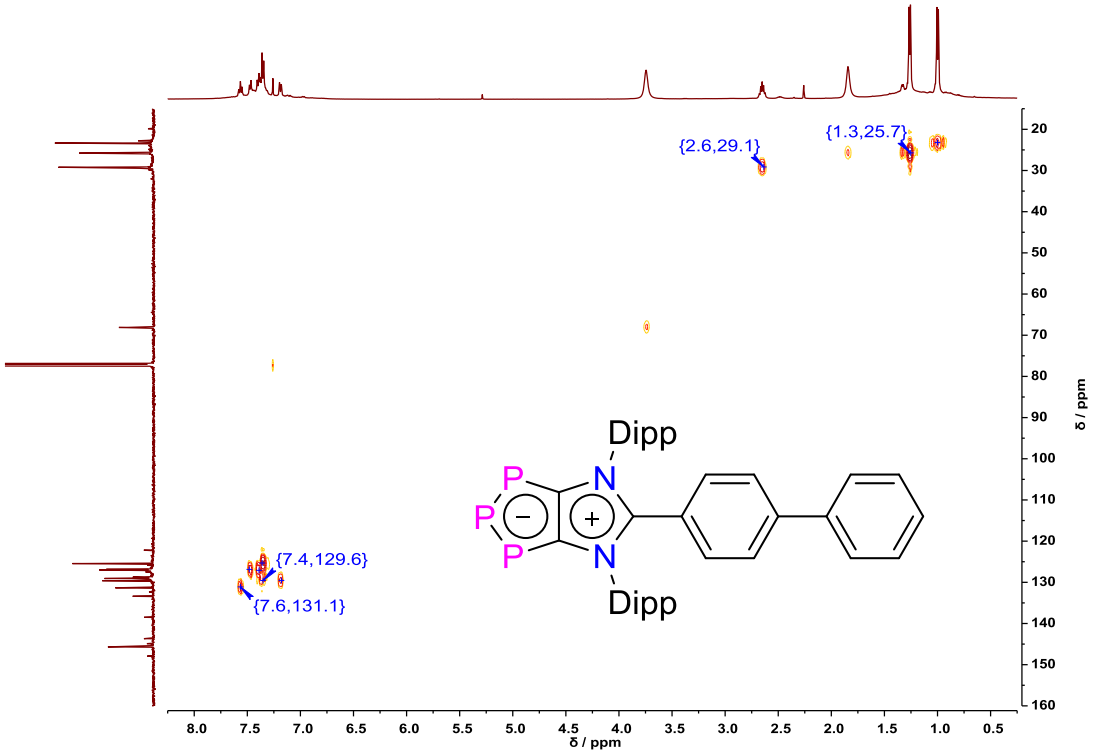


Fig. S21 ^{1}H-^{13}C HMQC ($CDCl_3$, 298 K) NMR spectrum of **6**.

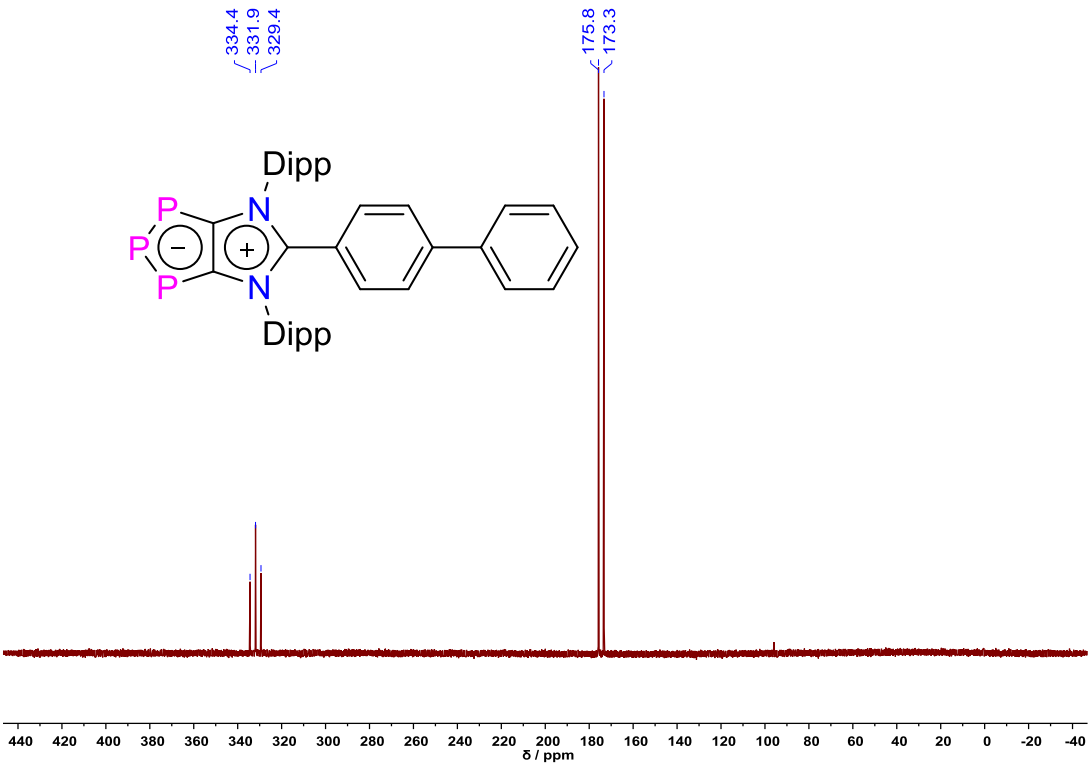


Fig. S22 $^{31}P\{^{1}H\}$ NMR (202 MHz, $CDCl_3$, 298 K) spectrum of **6**.

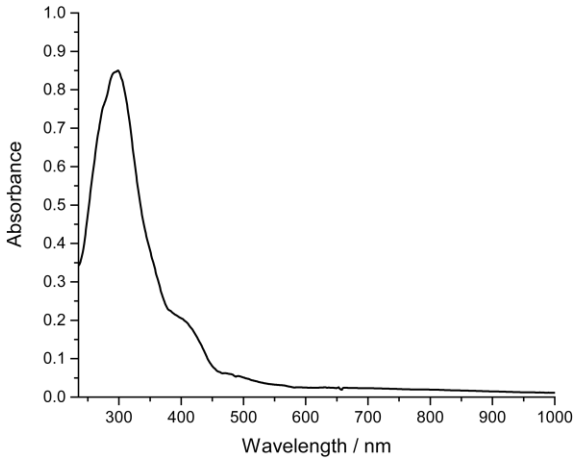


Fig. S23 UV-Visible spectrum of **2** in THF ($1.05x10^{-5}$ M)

Crystallographic Details

Single crystals were examined on a Rigaku Supernova diffractometer using Cu Kα (λ = 1.54184 Å) or MoKα (λ = 0.71073 Å) radiation. The crystals were kept at 100.0(1) K during data collection. Using Olex2,[2] the structure was solved with the ShelXT[3] (**1**, **3**, **4**) or ShelXD[4] (**2**) structure solution program using Intrinsic Phasing (**1**, **3**, **4**) or Dual Space (**2**) and refined with the ShelXL[5] refinement package using Least Squares minimisation. For the structure of **2**, a solvent mask was calculated and 448 electrons were found in a volume of 2272 Å^3 in two voids. This is consistent with the presence of 0.5 *toluene* per formula unit, which account for 400.0 electrons. All hydrogens were refined isotropically for **2**, apart from that hydrogen atoms were taken into account using a riding model. Further details of the X-ray investigation are given in Tables S1 and S2. CCDC 1947027-1947030 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html.

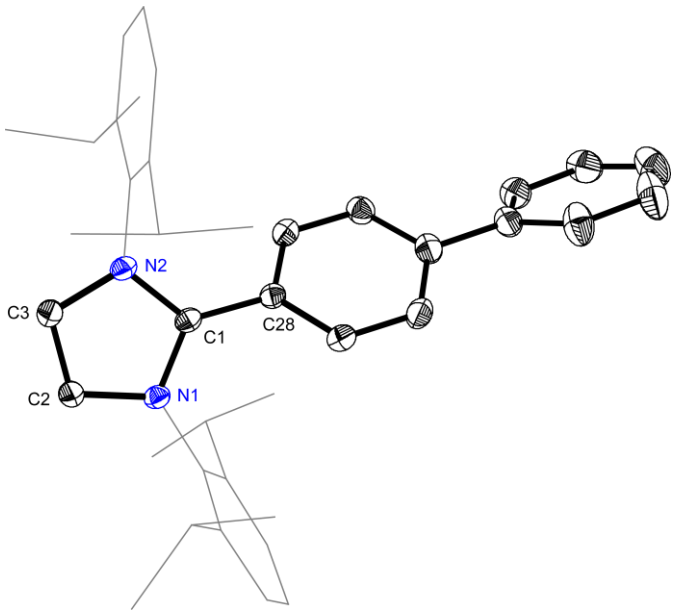


Fig. S24 Solid-state molecular structure of **1**. Hydrogen atoms, the bromide counter anion, and one co-crystallized solvent methanol molecule were omitted for clarity. Selected bond lengths (Å) and angles (°) for one out of two molecules in the asymmetric unit: C1–C28 1.465(2), C2–C3 1.355(2), N1–C1 1.352(2), N2–C1 1.349(2), N1–C2 1.385(2), N2–C3 1.388(2); N1–C1–N2 107.2(2), C2–C3–N2 107.3(1), C3–C2–N1 107.1(1).

Table S1. Crystallographic details of 1 and 2.

	1(methanol)	**2**(0.5 toluene)
Empirical formula	$C_{40}H_{49}BrN_2O$	$C_{42.5}H_{48}N_2$
Formula weight	653.72	540.76
Crystal system	monoclinic	tetragonal
Space group	$P2_1/n$	$I4_1/a$
a/Å	11.10880(10)	38.4682(4)
b/Å	21.1979(2)	38.4682(4)
c/Å	15.9518(2)	9.5772(2)
β/°	108.6410(10)	90
Volume/Å3	3559.32(7)	14172.4(4)
Z	4	16
ρcalcg/cm3	1.220	1.014
μ/mm-1	1.187	0.438
F(000)	1384.0	4672.0
Crystal size/mm3	0.41 × 0.25 × 0.21	0.48 × 0.07 × 0.05
Radiation	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection	3.31 to 60.10	6.50 to 153.03
Index ranges	$-15 \le h \le 15$ $-29 \le k \le 29$ $-22 \le l \le 22$	$-48 \le h \le 46$ $-47 \le k \le 44$ $-11 \le l \le 11$
Reflections collected	206381	72087
Independent reflections	10453 [R_{int} = 0.0385, R_{sigma} = 0.0137	7319 [R_{int} = 0.0564, R_{sigma} = 0.0272]
Reflections with I > 2σ(I)	9367	6284
Completeness up to Θ max	0.999	0.983
Data/restraints/parameters	10453/0/407	7319/0/547
Goodness-of-fit on F2	1.046	1.041
Final R indexes [I > 2σ(I)]	R_1 = 0.0302, wR_2 = 0.0775	R_1 = 0.0441, wR_2 = 0.1020
Final R indexes [all data]	R_1 = 0.0354, wR_2 = 0.0800	R_1 = 0.0519, wR_2 = 0.1068
Largest diff. peak/hole / e Å-3	0.46/-0.37	0.18/-0.26
CCDC number	1947027	1947028

Table S2. Crystallographic details of 3 and 4.

	3	**4**(toluene)
Empirical formula	$C_{42}H_{44}N_2NiO_3$	$C_{46}H_{52}N_2ClAu$
Formula weight	683.50	865.31
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/c$
a/Å	10.35522(15)	12.2795(3)
b/Å	11.18263(16)	16.8120(3)
c/Å	16.4194(2)	19.2885(4)
α/°	100.3074(12)	90
β/°	95.6535(12)	93.6946(19)
γ/°	99.0466(12)	90
Volume/Å3	1831.62(5)	3973.69(14)
Z	2	4
ρcalcg/cm3	1.239	1.446
μ/mm-1	1.073	7.817
F(000)	724.0	1752.0
Crystal size/mm3	0.33 × 0.30 × 0.15	0.24 × 0.07 × 0.06
Radiation	Cu Kα (λ = 1.54184 Å)	Cu Kα (λ = 1.54184)
2Θ range for data collection	5.52 to 152.95	6.98 to 153.69
Index ranges	$-13 \le h \le 13$ $-14 \le k \le 14$ $-20 \le l \le 19$	$-14 \le h \le 14$ $-20 \le k \le 20$ $-23 \le l \le 24$
Reflections collected	53689	52376
Independent reflections	7620 [R_{int} = 0.0307, R_{sigma} = 0.0161]	8070 [R_{int} = 0.0482, R_{sigma} = 0.0286]
Reflections with I > 2σ(I)	7232	7300
Completeness up to Θ max	0.991	0.990
Data/restraints/parameters	7620/0/441	8070/0/460
Goodness-of-fit on F2	1.036	1.166
Final R indexes [I > 2σ(I)]	R_1 = 0.0319, wR_2 = 0.0850	R_1 = 0.0351, wR_2 = 0.0971
Final R indexes [all data]	R_1 = 0.0335, wR_2 = 0.0863	R_1 = 0.0389, wR_2 = 0.0993
Largest diff. peak/hole / e Å-3	0.31/-0.42	1.35/-2.03
CCDC number	1947029	1947030

Computational Details

All structures were optimized on the BP86/def-SVP level of theory as implemented in the Turbomole software package.[6] The nature of the ground states was verified by frequency analyses (N_{imag} = 0). The HOMO/LUMO Gaps and other electronic properties were calculated at the BP86/def2-TZVPP, B3LYP/def2-TZVPP and M06-2x/def2-TZVPP level on optimized structures on BP86/def-SVP. Standard grid size utilized was m3 and the convergence criteria of the self-consistent field (SCF) was set to $\Delta E_{SCF} = 0.1 \cdot 10^{-6}\ E_H$.

The proton affinities (PA) were calculated according to the literature[7, 8] on and the B3LYP/def2-SVP level and have been referenced against 1-Ethyl-3-methylimidazol-2-ylidene at the CBS-QB3 level.[8-10] Standard grid size utilized was 5 and the convergence criteria of the self-consistent field (SCF) was set to $\Delta E_{SCF} = 1 \cdot 10^{-7} E_H$. The procedure is derived from the fluoride ion affinity (FIA) by Kögel *et al.*[7]

The Enthalpy of each compound is given by

$$\Delta H_{DFT} = E_{\mathrm{SCF}}(B+H)_{\mathrm{DFT}} - E_{\mathrm{SCF}}(B)_{\mathrm{DFT}} + H(B+H)_{\mathrm{DFT}} - H(B))_{\mathrm{DFT}} \quad (1)$$

Equation 1 obtains the Enthalpy for the protonation on the chosen DFT level for the compound of interest.

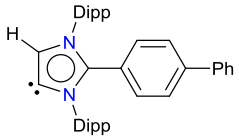
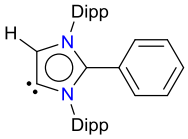
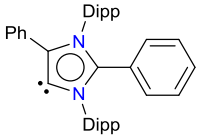
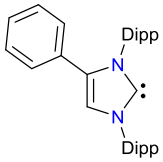
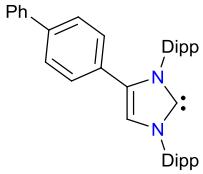
$$\Delta H_{ref,DFT} = E_{\mathrm{SCF}}(B+H)_{\mathrm{ref,DFT}} - E_{\mathrm{SCF}}(B)_{\mathrm{ref,DFT}} + H(B+H)_{\mathrm{ref,DFT}} - H(B)_{\mathrm{ref,DFT}} \quad (2)$$

Equation 2 obtains the Enthalpy for the protonation on the chosen DFT level for the reference.

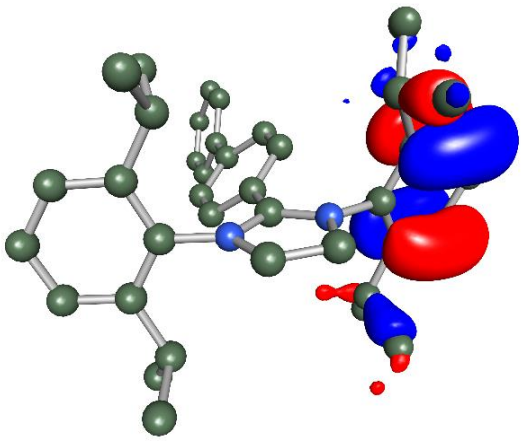
$$PA_{\mathrm{DFT}} = \Delta H_{DFT} + \Delta H_{ref,DFT} - PA_{ref,CBS-QB3} \quad (3)$$

Nucleus-independent chemical shifts (NICS) were calculated at the B3LYP/def2-SVP level of theory. The points for the NICS calculation were obtained along the centroid along the orthogonal coordinate of the imidazole-plane. The plane equations have been obtained using the Olex2 software.[1]

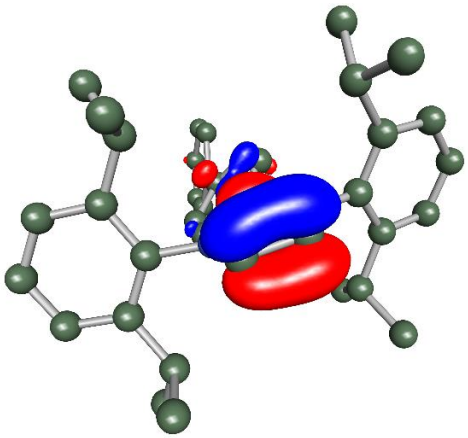
Table S3: Summary of calculated HOMO/LUMO energies and energy gaps for **2**, **VI**, **V**, **IPr^{Ph}** and **IPr^{Bp}**. All values were calculated using the def2-TZVPP basis set. The singlet-triplet energy gap $\Delta E_{S\text{-}T}$ for compound **2** was calculated at the BP89/def2-TZVPP as well was the M06-2x/def2-TZVPP level of theory.

			BP86	**M06-2X**	**B3LYP**
	**2**	E_{HOMO} / eV	−4.310	−6.646	−5.040
		E_{LUMO} / eV	−2.486	−0.999	−1.640
		$\Delta E_{HOMO\text{-}LUMO}$ / eV	1.824	5.647	3.400
		$\Delta E_{S\text{-}T}$ / kcal mol^{-1}	56.1	66.7	-[a]
	**VI**	E_{HOMO} / eV	−4.305	−6.671	−5.103
		E_{LUMO} / eV	−2.223	−0.642	−1.445
		$\Delta E_{HOMO\text{-}LUMO}$ / eV	2.082	6.029	3.658
	**V**[11]	E_{HOMO} / eV	−4.396	−6.401	−5.135
		E_{LUMO} / eV	−2.325	−0.779	−1.565
		$\Delta E_{HOMO\text{-}LUMO}$ / eV	2.071	5.622	3.570
	**IPr^{Ph}**	E_{HOMO} / eV	−5.028	−7.247	−5.886
		E_{LUMO} / eV	−1.923	−0.270	−1.093
		$\Delta E_{HOMO\text{-}LUMO}$ / eV	3.105	6.977	4.793
	**IPr^{Bp}**	E_{HOMO} / eV	−5.017	−7.058	−5.763
		E_{LUMO} / eV	−2.256	−0.694	−1.462
		$\Delta E_{HOMO\text{-}LUMO}$ / eV	2.761	6.364	4.301

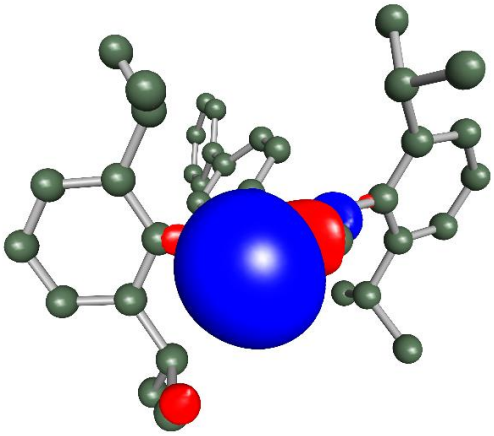
[a] B3LYP failed to converge during the energy calculation.



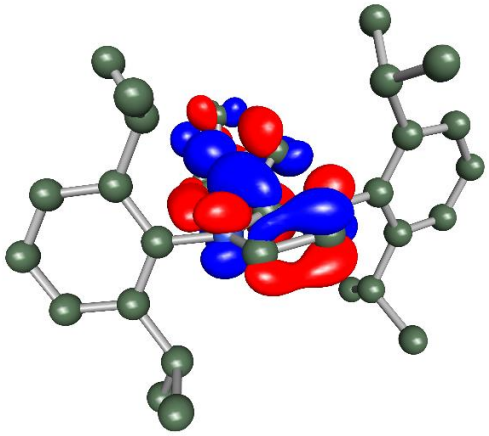
HOMO−2 (ε = −5.911 eV)



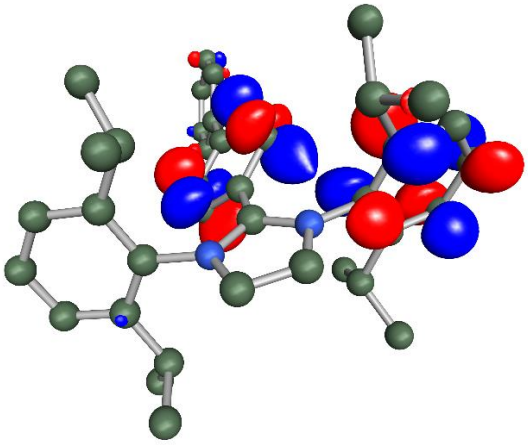
HOMO−1 (ε = −5.165 eV)



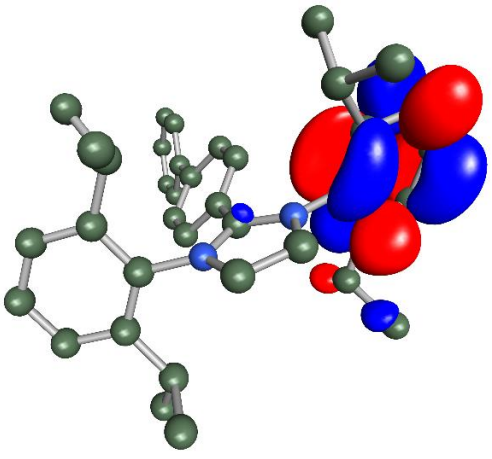
HOMO (ε = −4.310 eV)



LUMO (ε = −2.486 eV)

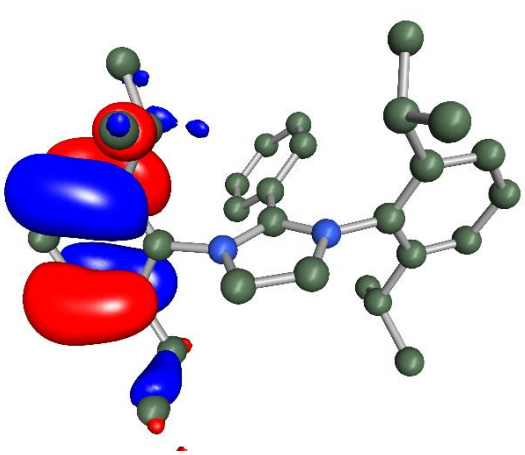


LUMO+1 (ε = −1.753 eV)

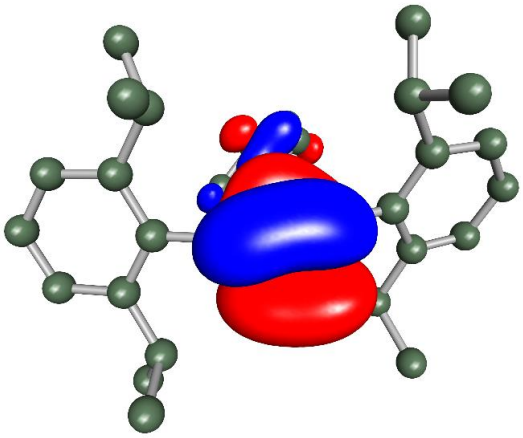


LUMO+2 (ε = −1.614 eV)

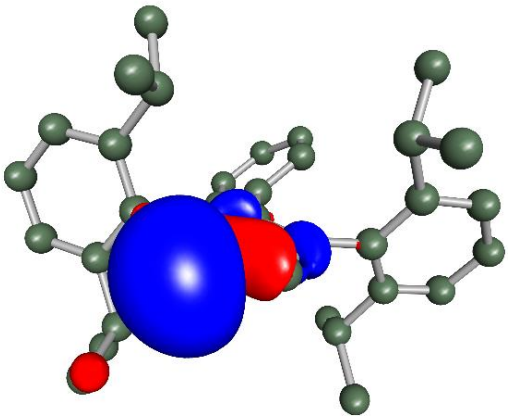
Fig. S25 Selected molecular orbitals of compound **2** at the BP86/def2-TZVPP level of theory. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms were omitted for clarity reasons.



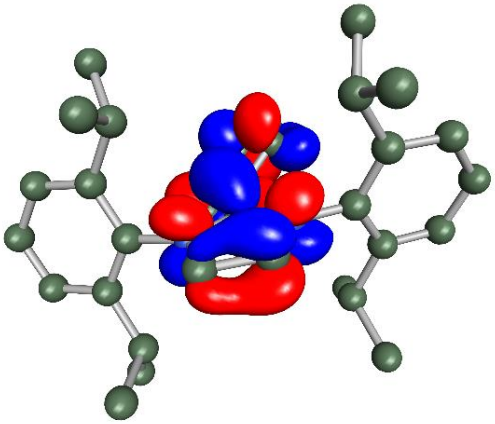
HOMO−2 (ε = −5.910 eV)



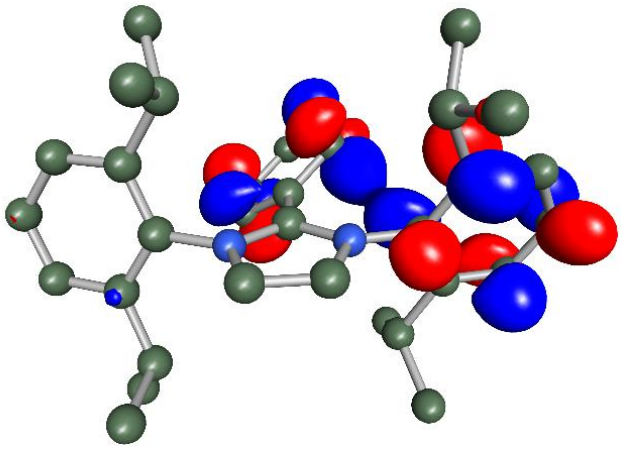
HOMO−1 (ε = −5.228 eV)



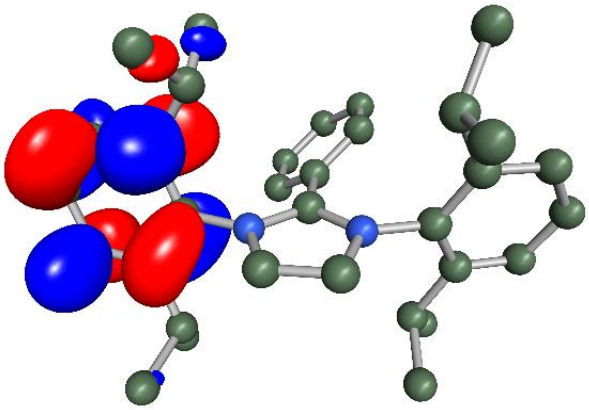
HOMO (ε = −4.305 eV)



LUMO (ε = −2.223 eV)



LUMO+1 (ε = −1.726 eV)



LUMO+2 (ε = −0.725 eV)

Fig. S26 Selected molecular orbitals of compound **VI** at the BP86/def-SVP level of theory. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms were omitted for clarity reasons.

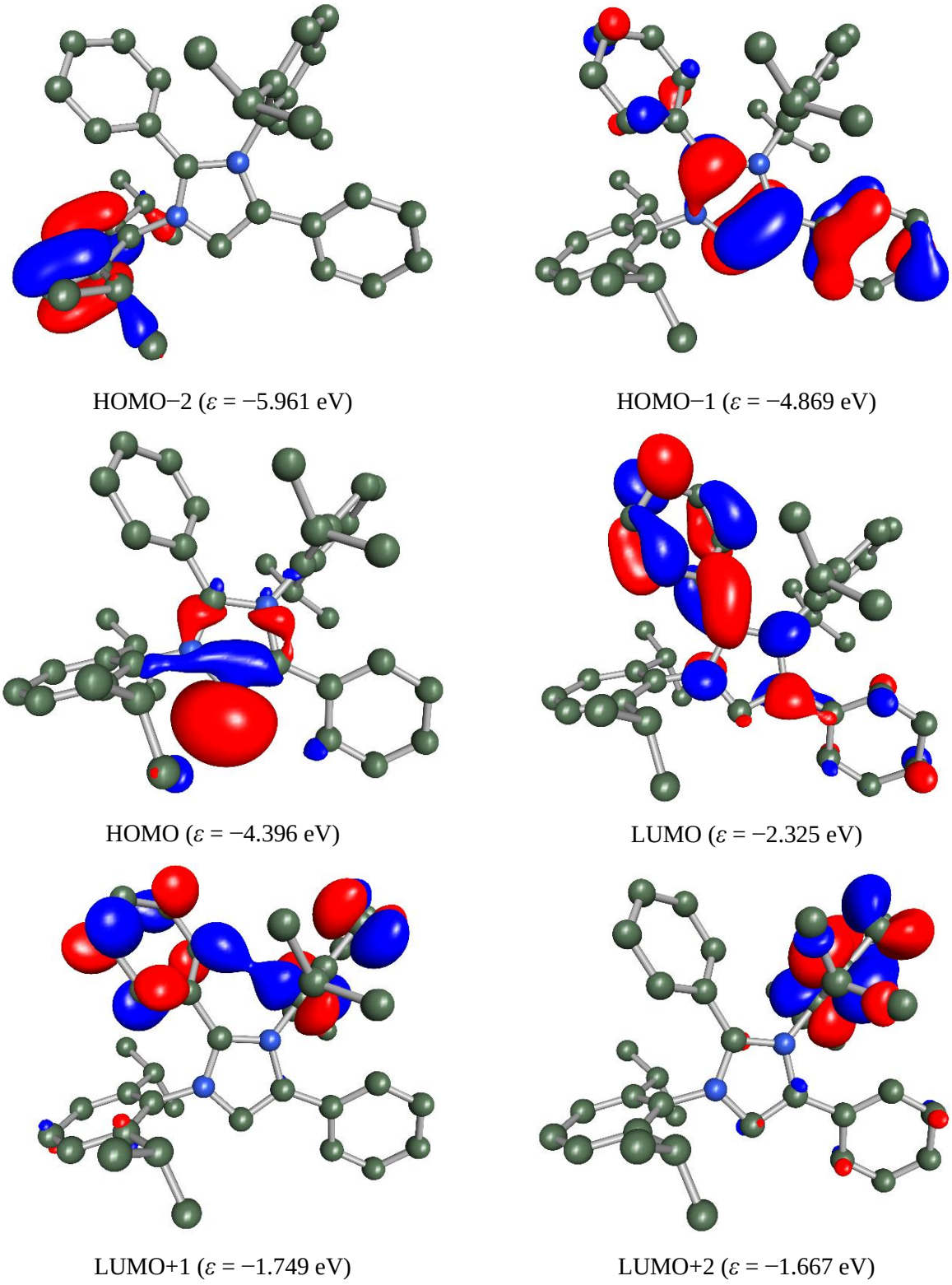
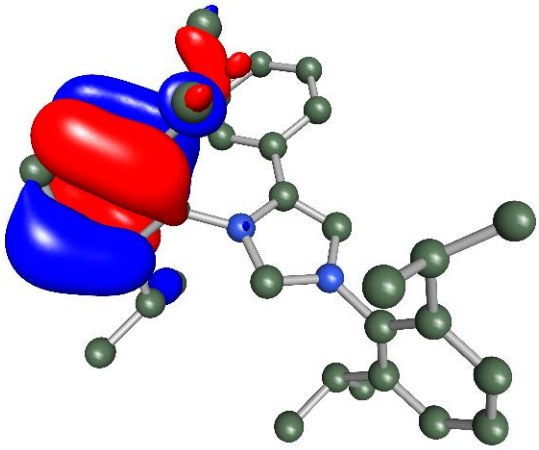
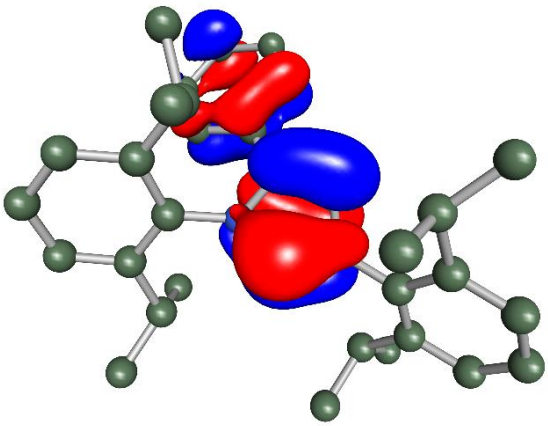


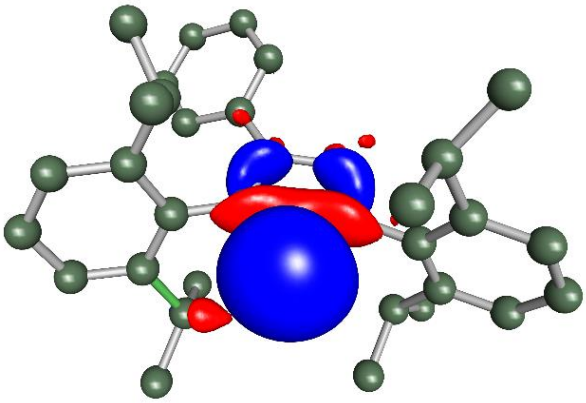
Fig. S27 Selected molecular orbitals of compound **V**[12] at the BP86/def-SVP level of theory. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms were omitted for clarity reasons.



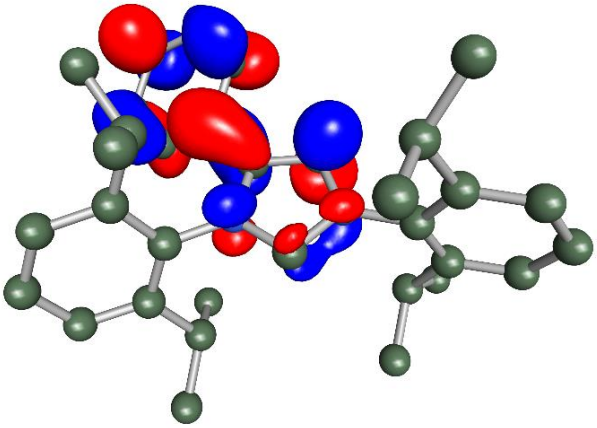
HOMO−2 (ε = −5.982 eV)



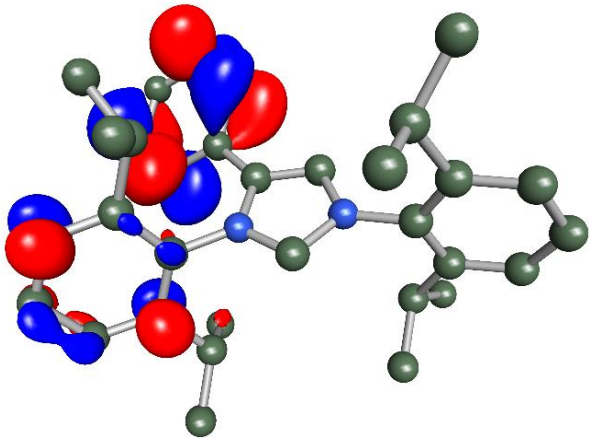
HOMO-1 (ε = −5.432 eV)



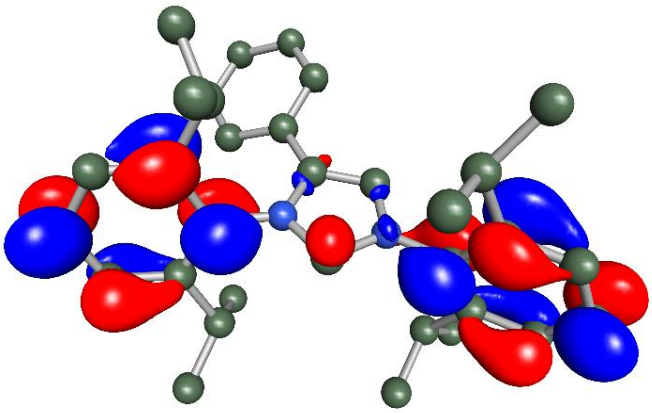
HOMO (ε = −5.028 eV)



LUMO (ε = −1.923 eV)

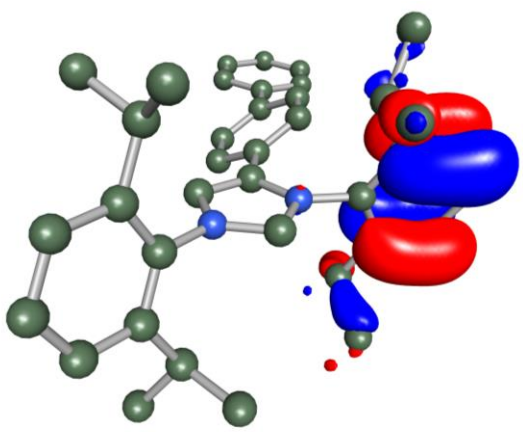


LUMO+1 (ε = −1.515 eV)

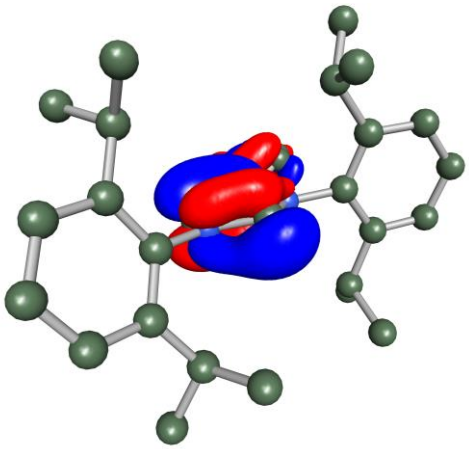


LUMO+2 (ε = −1.411 eV)

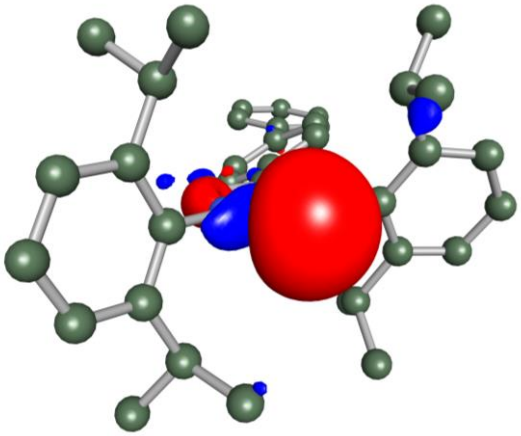
Fig. S28 Selected molecular orbitals of **IPr^{Ph}** at the BP86/def-SVP level of theory. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms were omitted for clarity reasons.



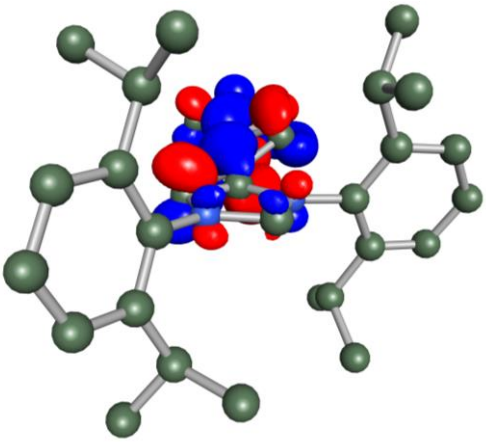
HOMO−2 (ε = −5.974 eV)



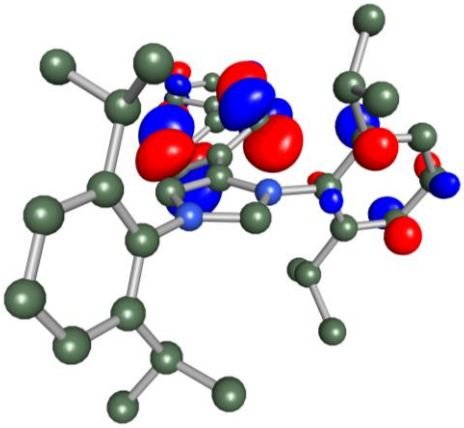
HOMO−1 (ε = −5.344 eV)



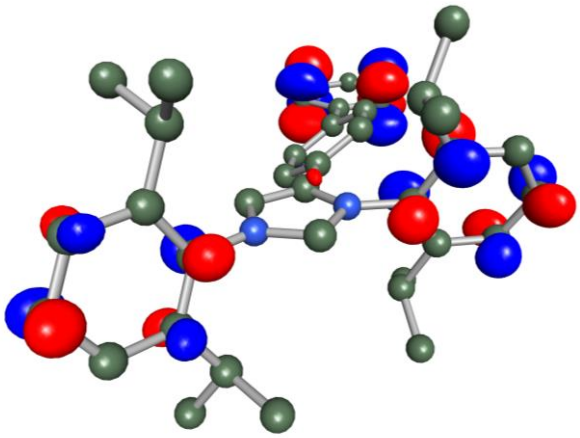
HOMO (ε = −5.017 eV)



LUMO (ε = −2.256 eV)



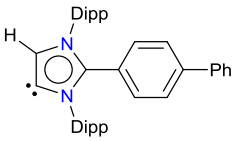
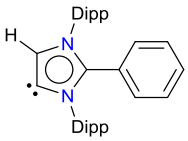
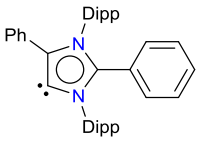
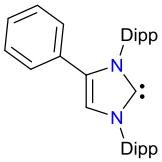
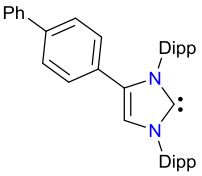
LUMO+1 (ε = −1.577 eV)



LUMO+2 (ε = −1.402 eV)

Fig. S29 Selected molecular orbitals of **IPr^{Bp}** at the BP86/def-SVP level of theory. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms were omitted for clarity reasons.

Table S4. 1st proton affinities (PA) of compounds **2**, **VI**, **V**, **IPr^{Ph}**, and **IPr^{Bp}** at the B3LYP/def2-SVP level of theory. All values are given in kcal mol^{-1}.

	 **2**	 **VI**	 **V**	 **IPr^{Ph}**	 **IPr^{Bp}**
PA$_{B3LYP}$	293.4	292.2	293.0	274.7	275.5
PA$_{BP86}$	289.1	287.8	288.9	274.4	274.1

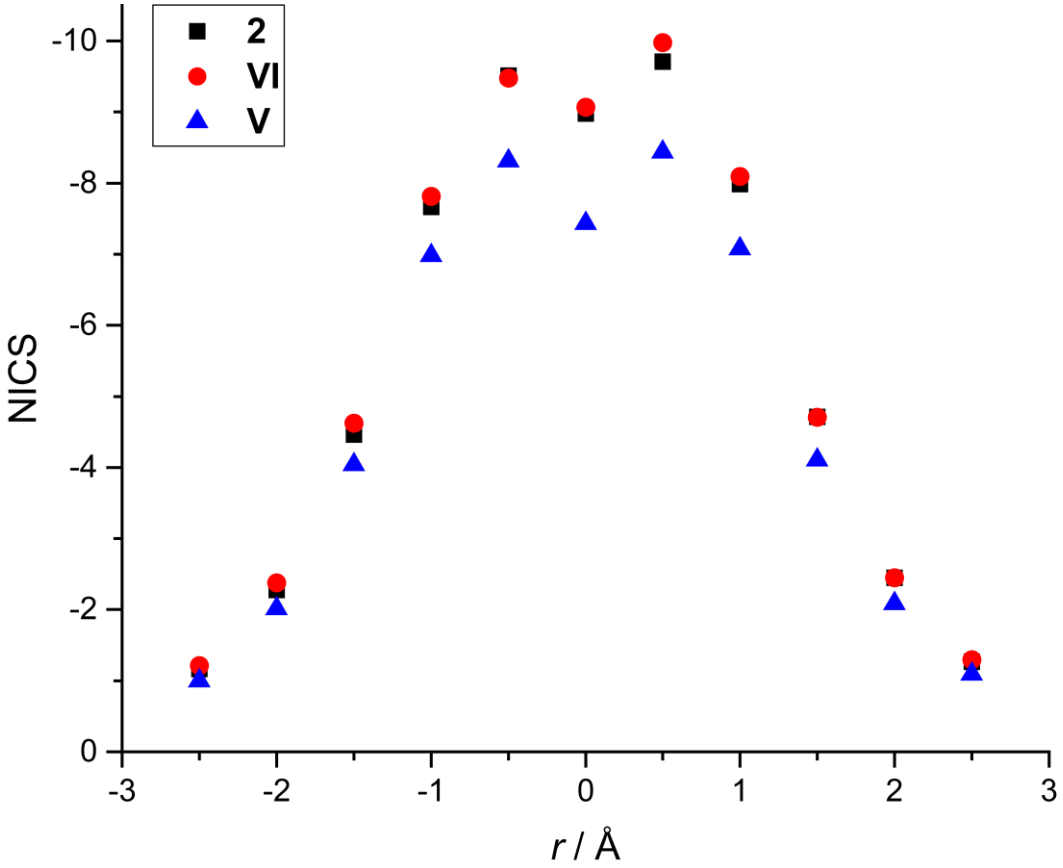
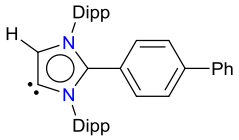
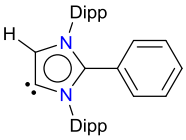
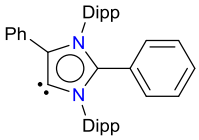


Fig. S30 Calculated NICS values at the B3LYP/def2-SVP level of theory.

Table S5. Selected NICS values for compounds **2**, **VI**, and **V**.

	 **2**	 **VI**	 **V**
NICS−2	−2.277	−2.377	−2.013
NICS−1	−7.665	−7.815	−6.981
NICS0	−8.979	−9.066	−7.434
NICS+1	−7.987	−8.092	−7.077
NICS+2	−2.450	−2.448	−2.088

Optimized Geometries

2

$E_{B3LYP/def\text{-}SVP}$ = -1619.885142

$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1619.156530

N	31.63504	11.51563	6.04728
C	32.5689	12.38279	5.5884
C	31.30703	10.63954	5.00343
C	31.11086	11.39937	7.38433
N	32.78282	12.03358	4.28307
C	33.2093	13.46438	6.35315
H	30.58629	9.8483	5.20118
C	32.00573	10.94121	3.84899
C	29.80545	11.87998	7.64641
C	31.88322	10.74257	8.36931
C	33.64539	12.74451	3.36852
C	34.59269	13.71317	6.24498
C	32.46469	14.29151	7.21824
C	29.2966	11.70816	8.9418
C	28.94344	12.5406	6.57081
C	31.32606	10.60765	9.6499
C	33.26193	10.15374	8.08026
C	34.90656	12.1906	3.05283
C	33.17664	13.93722	2.77373
H	35.20502	13.0983	5.58674
C	35.19774	14.73789	6.96895
C	33.07576	15.31331	7.94157
H	31.39211	14.1368	7.32763
H	28.29189	12.06791	9.1759
C	30.04887	11.0854	9.93721
H	29.58778	12.74156	5.70166
C	27.82779	11.59005	6.09467
C	28.35164	13.88702	7.02464
H	31.90138	10.10961	10.43418
H	33.52801	10.40831	7.04429
C	33.23692	8.61603	8.16839
C	34.34973	10.75048	8.99083
C	35.71395	12.88636	2.14077
C	35.36847	10.85322	3.62814
C	34.02795	14.5951	1.87345

C	31.75907	14.45129	3.01495
H	36.26853	14.9118	6.8407
C	34.45704	15.56389	7.8359
H	32.46696	15.9181	8.61761
H	29.63343	10.96543	10.9414
H	27.23984	12.05775	5.28802
H	27.13635	11.34362	6.91778
H	28.24009	10.6468	5.70622
H	27.81618	14.36679	6.18942
H	27.62857	13.7643	7.84734
H	29.13128	14.58551	7.36829
H	34.22222	8.19937	7.90204
H	32.49156	8.18805	7.47998
H	32.99309	8.27197	9.18731
H	35.34046	10.355	8.71265
H	34.18013	10.49603	10.05022
H	34.38645	11.84766	8.90841
H	36.69429	12.48507	1.87515
C	35.28548	14.08021	1.56233
H	34.78416	10.66717	4.54308
C	35.03689	9.70831	2.65047
C	36.85391	10.83725	4.02426
H	33.69711	15.52054	1.39801
H	31.43277	14.08433	3.9998
C	30.79943	13.84821	1.96859
C	31.6549	15.98314	3.0568
C	35.10649	16.65609	8.60723
H	35.9324	14.60835	0.85639
H	35.57291	9.84146	1.69534
H	35.33874	8.73659	3.07707
H	33.95484	9.68294	2.45151
H	37.09732	9.89281	4.53774
H	37.11176	11.66681	4.70346
H	37.51879	10.90549	3.14781
H	31.0706	14.1821	0.95279
H	30.8377	12.7481	1.99145
H	29.7612	14.16643	2.16416
H	32.36215	16.42054	3.77955
H	31.84907	16.44059	2.07279
H	30.63653	16.28379	3.35268
C	36.40876	16.50539	9.12272

2

$E_{BP86/def\text{-}SVP}$ = -1621.014034
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.305300
$E_{BP86/def2\text{-}TZVPP//BP86/def\text{-}SVP}$ = -1622.746128

N	31.61852	11.52852	6.03573
C	32.5731	12.39632	5.58685
C	31.2879	10.65719	4.98236
C	31.09145	11.40146	7.37237
N	32.78865	12.03997	4.26942
C	33.21121	13.47075	6.3574
H	30.55812	9.86311	5.17822
C	32.00038	10.95889	3.82563
C	29.77159	11.86518	7.63018
C	31.87206	10.74569	8.36182
C	33.66561	12.74225	3.35695
C	34.5793	13.7967	6.17073
C	32.48564	14.22729	7.31414
C	29.25472	11.67379	8.92684
C	28.91241	12.53151	6.55402
C	31.30536	10.59257	9.64298
C	33.2654	10.187	8.0774
C	34.92851	12.16994	3.05125
C	33.21192	13.947	2.75957
H	35.17789	13.24042	5.43834
C	35.1845	14.82189	6.90479
C	33.09874	15.24956	8.04556
H	31.42394	14.01161	7.49051
H	28.23613	12.02152	9.15791
C	30.01269	11.0506	9.92716
H	29.56359	12.72229	5.67643
C	27.78203	11.58968	6.08606
C	28.34033	13.88858	7.01103
H	31.8892	10.09444	10.43239
H	33.52071	10.43553	7.0277
C	33.28116	8.64842	8.19357
C	34.33792	10.83255	8.97784
C	35.7547	12.86106	2.14207
C	35.36326	10.82535	3.6346
C	34.08253	14.59897	1.86326
C	31.79535	14.46843	2.99557
H	36.24205	15.05731	6.71262
C	34.46372	15.5761	7.86195
H	32.50578	15.7949	8.79511

H	29.58967	10.91561	10.93454
H	27.19013	12.06322	5.27593
H	27.08719	11.35111	6.9184
H	28.18377	10.63395	5.69615
H	27.79108	14.37429	6.17876
H	27.62639	13.77474	7.85292
H	29.1379	14.58562	7.33896
H	34.28208	8.24942	7.92895
H	32.53937	8.18368	7.51387
H	33.04992	8.31447	9.22667
H	35.34619	10.45513	8.71043
H	34.16911	10.59614	10.04946
H	34.34688	11.93559	8.87127
H	36.74012	12.44552	1.88444
C	35.34255	14.06697	1.55991
H	34.79399	10.67684	4.57729
C	34.95449	9.67951	2.68195
C	36.86073	10.76192	3.98461
H	33.76285	15.53708	1.3866
H	31.48715	14.14415	4.0112
C	30.82695	13.80407	1.98996
C	31.68226	16.00181	2.95923
C	35.1113	16.66404	8.64034
H	36.00614	14.59318	0.85623
H	35.46376	9.78401	1.7008
H	35.23713	8.69563	3.11192
H	33.85673	9.69601	2.52177
H	37.09032	9.81027	4.50636
H	37.17219	11.59607	4.6468
H	37.50186	10.79303	3.07947
H	31.08508	14.09471	0.94981
H	30.87968	12.69823	2.06331
H	29.7807	14.12145	2.18367
H	32.40086	16.48576	3.65126
H	31.85973	16.41016	1.94222
H	30.66012	16.31521	3.25439
C	36.46782	16.57149	9.03603
C	34.39073	17.8257	9.00982
H	37.04456	15.66749	8.78726
C	37.07831	17.59792	9.77151
C	35.0015	18.8526	9.74434
H	33.34322	17.93785	8.6908
H	38.13174	17.49725	10.0756

C	36.34847	18.74403	10.12966
H	34.42213	19.7504	10.01009
H	36.82757	19.54969	10.70673

2 + H

$E_{B3LYP/def\text{-}SVP}$ =-1620.365051
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1619.622672

C	36.27453	18.76694	9.95345
C	36.97998	17.58608	9.70055
C	36.37785	16.54714	8.98911
C	35.0538	16.66454	8.52175
C	34.35498	17.85879	8.78779
C	34.96062	18.89993	9.49301
C	34.41187	15.55896	7.76882
C	35.15534	14.73652	6.89724
C	34.55716	13.70069	6.18674
C	33.17944	13.43653	6.32325
C	32.42796	14.25078	7.19435
C	33.03369	15.28827	7.89597
C	32.54457	12.34332	5.57855
N	31.61606	11.47073	6.05457
C	31.26395	10.58549	5.04913
C	31.97962	10.9233	3.94312
N	32.77183	12.00843	4.27996
C	31.09557	11.36825	7.409
C	29.79021	11.85048	7.66292
C	29.29781	11.69828	8.9667
C	30.06591	11.09868	9.96435
C	31.34453	10.62536	9.67727
C	31.8925	10.73888	8.39058
C	33.62626	12.686	3.31728
C	34.86556	12.08991	2.98595
C	35.64796	12.74167	2.02234
C	35.21868	13.92501	1.42212
C	33.98743	14.47991	1.76477
C	33.15275	13.87252	2.71509
C	28.9092	12.48683	6.58717
C	28.31014	13.83453	7.02875
C	33.27684	10.15857	8.10932
C	34.35914	10.78547	9.00687
C	35.35478	10.77874	3.60228
C	36.7926	10.87548	4.14401
C	31.7887	14.48783	3.02005
C	31.90922	15.93407	3.53366
C	27.79464	11.51896	6.14152
C	33.26774	8.62223	8.23057
C	35.23193	9.61571	2.59735

C	30.85726	14.40292	1.79516
H	30.54158	9.79295	5.21921
H	35.17167	13.09082	5.52629
H	31.36027	14.08003	7.32334
H	28.294	12.05493	9.20641
H	29.53877	12.68994	5.70554
H	31.92844	10.14783	10.46706
H	33.54594	10.39449	7.0679
H	36.22123	14.92503	6.75568
H	32.42632	15.88921	8.57543
H	29.6606	10.994	10.97382
H	27.19482	11.96544	5.33244
H	27.11352	11.28863	6.97647
H	28.19906	10.56256	5.77429
H	27.75915	14.29547	6.19383
H	27.59826	13.71515	7.86038
H	29.08564	14.54621	7.35365
H	34.25623	8.21038	7.97119
H	32.52222	8.16526	7.56044
H	33.03345	8.30031	9.25786
H	35.35292	10.39535	8.73463
H	34.19404	10.54619	10.06949
H	34.38306	11.88161	8.90789
H	36.61134	12.31534	1.73525
H	34.70492	10.5407	4.46012
H	33.66106	15.40106	1.27719
H	31.31528	13.89988	3.8218
H	35.84789	14.41545	0.67524
H	35.87584	9.7823	1.71888
H	35.53998	8.66653	3.06415
H	34.20083	9.49288	2.23014
H	37.06791	9.93983	4.65578
H	36.90921	11.70014	4.86499
H	37.52606	11.03192	3.33766
H	31.24726	14.99308	0.95048
H	30.7353	13.36468	1.44749
H	29.85915	14.79823	2.04318
H	32.55736	15.99642	4.42131
H	32.32475	16.60472	2.76473
H	30.91617	16.32552	3.80664
H	36.9346	15.62198	8.82166
H	33.3366	17.98889	8.41375
H	38.00363	17.47042	10.0655

H	34.40576	19.82307	9.67843
H	36.74747	19.58142	10.50776
H	31.99514	10.49876	2.94393

2 + H

$E_{BP86/def\text{-}SVP}$ = -1621.488587
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.766137

C	36.29128	18.78874	9.95867
C	37.03271	17.64727	9.60884
C	36.42638	16.60383	8.89582
C	35.06146	16.67629	8.52394
C	34.32701	17.8316	8.88745
C	34.93711	18.87765	9.59333
C	34.41787	15.57101	7.77286
C	35.14447	14.79449	6.83476
C	34.5426	13.75489	6.12155
C	33.17542	13.43633	6.32132
C	32.44075	14.20406	7.26068
C	33.05082	15.24657	7.96291
C	32.54048	12.34474	5.57795
N	31.60158	11.46526	6.0533
C	31.2501	10.57645	5.04517
C	31.97452	10.91317	3.93273
N	32.76971	12.00125	4.26988
C	31.07667	11.36261	7.40714
C	29.75752	11.8317	7.65144
C	29.25818	11.67766	8.95972
C	30.03214	11.09044	9.96925
C	31.32472	10.63123	9.68985
C	31.88151	10.74552	8.39992
C	33.63041	12.67244	3.30681
C	34.86647	12.05722	2.97
C	35.65912	12.70569	2.00242
C	35.24291	13.90248	1.40454
C	34.01416	14.4749	1.75404
C	33.16866	13.87329	2.70822
C	28.87602	12.45473	6.56681
C	28.27435	13.80781	6.99777
C	33.27616	10.18302	8.1285
C	34.3464	10.84696	9.01902
C	35.34088	10.73868	3.58487
C	36.77354	10.83029	4.14928
C	31.81511	14.50862	3.02325
C	31.96963	15.94078	3.57593
C	27.76247	11.47643	6.13069
C	33.2915	8.64634	8.2789
C	35.22827	9.58321	2.56593

C	30.88684	14.47717	1.78959
H	30.52269	9.77905	5.21813
H	35.14517	13.18118	5.40616
H	31.37978	13.98934	7.4419
H	28.24075	12.02527	9.19257
H	29.51346	12.65043	5.67824
H	31.91689	10.16245	10.48995
H	33.54042	10.40915	7.07428
H	36.20195	15.02652	6.64217
H	32.45662	15.81006	8.69669
H	29.61987	10.98432	10.98389
H	27.15578	11.91475	5.31251
H	27.0775	11.25052	6.97343
H	28.17126	10.51109	5.77057
H	27.71293	14.26234	6.15697
H	27.56289	13.69358	7.84047
H	29.05434	14.53007	7.31203
H	34.29306	8.24242	8.02695
H	32.54938	8.15985	7.6145
H	33.06071	8.33852	9.31917
H	35.35413	10.46307	8.76186
H	34.17607	10.62907	10.0933
H	34.35621	11.94821	8.89477
H	36.62346	12.26356	1.71131
H	34.66976	10.49631	4.43699
H	33.6951	15.40932	1.26855
H	31.32529	13.90284	3.81394
H	35.88125	14.39094	0.65319
H	35.89025	9.75561	1.6927
H	35.52803	8.62196	3.03007
H	34.19622	9.46708	2.17864
H	37.04653	9.88304	4.65637
H	36.88012	11.6512	4.88704
H	37.52258	10.99981	3.34975
H	31.29597	15.0864	0.958
H	30.74285	13.44603	1.40898

VI

$E_{B3LYP/def\text{-}SVP}$ = -1390.650369
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1390.002156

C	31.29672	11.71647	6.03135
N	32.23328	12.513	5.48205
N	30.99597	10.78994	5.08247
C	31.7205	10.94866	3.88575
C	32.47729	12.05565	4.18235
H	33.18302	12.59365	3.57384
H	31.05874	16.84387	4.24699
C	29.67968	15.58198	6.35605
C	30.74349	15.81433	4.06729
H	29.75204	15.84274	3.61171
H	31.43218	15.37252	3.3467
H	30.38312	13.99715	5.11555
H	29.90511	16.61865	6.61239
H	28.68384	15.56298	5.90997
H	29.646	15.00689	7.28135
C	30.70897	15.00383	5.37352
C	32.8201	13.70325	6.04243
C	32.09679	14.90572	5.98861
C	32.71007	16.05279	6.49244
H	32.17605	16.9933	6.46901
H	34.45304	16.9149	7.391
C	33.99432	16.01181	7.00969
C	34.69608	14.81643	7.03227
H	35.70214	14.80081	7.42914
C	34.12939	13.63711	6.55098
C	34.93966	12.34766	6.55419
H	34.25512	11.52198	6.35893
C	35.97844	12.35117	5.4198
H	35.505	12.47971	4.44739
H	36.52704	11.4079	5.40311
H	36.6998	13.15976	5.55428
C	35.62238	12.07338	7.9029
H	36.39434	12.81107	8.12688
H	36.10465	11.0949	7.88293
H	34.91039	12.07905	8.72934
C	30.11234	9.66842	5.28578
C	29.33632	11.80574	7.56674
C	27.99968	8.60188	4.92371
C	28.44263	7.49313	5.62768
C	29.72855	7.46582	6.14303

C	30.59483	8.54598	5.97582
H	30.06891	6.58657	6.67236
H	27.78666	6.64318	5.76595
C	28.34067	10.89128	3.90248
C	26.8909	11.29698	4.2027
H	26.73048	11.48374	5.26635
H	26.17762	10.53279	3.88996
H	26.6415	12.21032	3.65973
H	27.92981	9.74219	2.09711
C	28.53308	10.5997	2.40413
H	29.58031	10.38762	2.19234
H	28.97649	11.74499	4.14081
H	28.22556	11.46109	1.80695
C	32.03769	8.44899	6.44824
C	32.1855	7.8153	7.83718
C	32.88036	7.70272	5.39894
H	32.43655	9.4607	6.51581
H	33.22569	7.8746	8.1627
H	33.929	7.66957	5.70289
H	32.81732	8.19893	4.43063
H	32.53037	6.67474	5.28211
H	31.90868	6.75973	7.83919
H	31.56966	8.32574	8.57877
H	27.00005	8.60162	4.51112
C	30.72338	11.84253	7.37731
C	31.54492	11.99427	8.50076
C	30.99649	12.10819	9.77075
C	29.61783	12.06635	9.94653
C	28.79161	11.9135	8.83835
H	27.71702	11.88302	8.96092
H	28.68259	11.6978	6.7149
H	31.65039	12.22218	10.62538
H	32.61748	12.0124	8.38149
C	28.82253	9.71142	4.7336
H	29.19161	12.15073	10.93741
H	-3.67639	2.95091	-2.31391

VI

$E_{BP86/def\text{-}SVP}$ = -1390.111714
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1389.481415
$E_{BP86/def2\text{-}TZVPP//BP86/def\text{-}SVP}$ = -1390.636674

C	31.28942	11.70947	6.05696
N	32.24613	12.49605	5.48219
N	30.99285	10.75398	5.1057
C	31.72903	10.87929	3.90947
C	32.49738	12.00558	4.18791
H	33.21849	12.54403	3.56239
H	30.93301	16.917	4.3473
C	29.67726	15.49286	6.45956
C	30.65194	15.86468	4.13251
H	29.63107	15.87321	3.69805
H	31.34736	15.47969	3.36016
H	30.38185	13.97187	5.11058
H	29.89948	16.53216	6.78062
H	28.6499	15.48899	6.04093
H	29.68179	14.85048	7.36237
C	30.6887	14.99495	5.40741
C	32.84344	13.69677	6.01456
C	32.10518	14.90977	5.97444
C	32.73669	16.07333	6.45808
H	32.18701	17.02719	6.44639
H	34.52411	16.96411	7.31126
C	34.05072	16.04125	6.94214
C	34.76559	14.83596	6.94892
H	35.80085	14.82328	7.32263
C	34.18381	13.63852	6.4876
C	34.99728	12.3428	6.48614
H	34.30113	11.51165	6.25219
C	36.06947	12.36434	5.37556
H	35.61816	12.51641	4.37544
H	36.62701	11.40538	5.35223
H	36.80352	13.17974	5.5439
C	35.63636	12.04219	7.8569
H	36.39991	12.79827	8.13336
H	36.14431	11.05631	7.83609
H	34.88232	12.01443	8.66971
C	30.08346	9.64598	5.30625
C	29.34227	11.6225	7.6424
C	27.93039	8.61195	4.91677
C	28.33908	7.49281	5.65417

C	29.62879	7.44371	6.19966
C	30.53276	8.51219	6.03243
H	29.94562	6.55244	6.76019
H	27.64912	6.64687	5.7976
C	28.35658	10.9002	3.86489
C	26.8805	11.29225	4.05744
H	26.62719	11.46444	5.12411
H	26.18846	10.51637	3.66886
H	26.65855	12.22573	3.50077
H	28.11664	9.74046	2.01195
C	28.67996	10.6241	2.37947
H	29.76644	10.4338	2.25917
H	28.97586	11.7704	4.17116
H	28.40005	11.4956	1.75082
C	31.97474	8.40492	6.52837
C	32.12593	7.60373	7.83241
C	32.86698	7.8319	5.40286
H	32.33208	9.43501	6.73722
H	33.1716	7.66349	8.19784
H	33.9306	7.8056	5.72038
H	32.78782	8.44908	4.48431
H	32.5594	6.79509	5.15148
H	31.89916	6.52687	7.68837
H	31.46218	7.98889	8.6329
H	26.92103	8.63342	4.48016
C	30.71932	11.86593	7.40292
C	31.52788	12.25843	8.50092
C	30.97874	12.40678	9.78195
C	29.61328	12.16114	10.00407
C	28.80111	11.76713	8.92731
H	27.72897	11.57408	9.08554
H	28.68862	11.32384	6.81275
H	31.62907	12.71085	10.61641
H	32.59997	12.44043	8.35087
C	28.79047	9.71198	4.7231
H	29.18463	12.27504	11.0114

VI + H

$E_{B3LYP/def\text{-}SVP}$ = -1389.617560
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1388.956014

C	28.85614	9.68545	4.60331
C	30.13157	9.62558	5.21204
C	30.60836	8.48898	5.90176
C	29.73965	7.39098	5.99317
C	28.47245	7.41991	5.41465
C	28.04026	8.55178	4.72409
N	31.01916	10.76955	5.06551
C	31.32686	11.71014	5.99614
N	32.25048	12.53529	5.43798
C	32.52006	12.10965	4.14833
C	31.7577	11.00619	3.91851
C	30.76565	11.81543	7.35207
C	29.38102	11.66724	7.56457
C	28.85237	11.77049	8.85151
C	29.69403	12.0169	9.94111
C	31.07036	12.16263	9.73903
C	31.60606	12.06568	8.45453
C	32.83972	13.73496	6.01381
C	32.07927	14.92516	6.01106
C	32.6912	16.07086	6.54167
C	33.99462	16.03425	7.03268
C	34.72427	14.84619	7.00293
C	34.16861	13.66425	6.49332
C	30.6694	15.02551	5.43255
C	30.65614	15.89506	4.16001
C	35.00934	12.38783	6.44541
C	35.68032	12.06434	7.79273
C	32.00914	8.3913	6.50239
C	32.86671	7.36383	5.73785
C	28.36287	10.89623	3.81019
C	28.40395	10.61724	2.29408
C	29.65223	15.53479	6.46968
C	36.06254	12.4622	5.32143
C	26.95664	11.35588	4.23605
C	31.97307	8.08006	8.00955
H	33.22459	12.6371	3.51242
H	30.94478	16.93519	4.38056
H	29.64644	15.91677	3.71956
H	31.35211	15.51137	3.39706
H	30.34524	14.0166	5.13268

H	29.87078	16.56905	6.77964
H	28.63709	15.5303	6.04157
H	29.64487	14.90642	7.3736
H	32.13803	17.01229	6.56127
H	34.44972	16.94194	7.4367
H	35.74781	14.83776	7.383
H	34.33879	11.54489	6.21075
H	35.60522	12.6444	4.33619
H	36.63167	11.52084	5.26128
H	36.78037	13.27745	5.50613
H	36.43682	12.81632	8.06607
H	36.1955	11.09258	7.73514
H	34.95194	12.01095	8.61744
H	30.06713	6.49227	6.52021
H	27.81671	6.54955	5.49662
H	26.89483	11.55668	5.31744
H	26.18803	10.60571	3.99321
H	26.68453	12.28194	3.70558
H	27.72186	9.79474	2.02523
H	29.41158	10.33321	1.95198
H	29.04825	11.73687	4.0073
H	28.09353	11.5097	1.72766
H	32.50432	9.36829	6.3875
H	32.99393	8.08413	8.42383
H	33.89097	7.34025	6.14319
H	32.93081	7.6046	4.66471
H	32.45094	6.34742	5.82647
H	31.54419	7.08519	8.20907
H	31.3765	8.82148	8.56304
H	27.04814	8.5535	4.26818
H	27.77607	11.66044	9.00277
H	28.71245	11.48549	6.72426
H	31.73311	12.35039	10.58693
H	32.68088	12.17054	8.3135
H	29.27717	12.09542	10.94819
H	31.67633	10.36188	3.04834
H	4.54049	1.75844	-0.10713
H	4.09603	2.77754	-1.49265
H	3.04608	4.44785	0.24987
H	3.48684	3.3282	1.55917
H	1.79665	3.8592	1.37625
H	-1.18696	5.47366	4.16891
H	3.60896	1.06686	-1.45272

H	4.02768	-3.90357	0.72743
H	-1.2435	-2.66002	-1.39643

VI +H

$E_{BP86/def\text{-}SVP}$ = -1390.584058
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1389.940356

C	28.85358	9.68569	4.57521
C	30.1285	9.61965	5.20005
C	30.5954	8.47845	5.90274
C	29.71417	7.38141	5.99068
C	28.44607	7.41521	5.39811
C	28.02571	8.55183	4.69463
N	31.02195	10.76126	5.05917
C	31.32974	11.70721	6.00068
N	32.26151	12.5364	5.43449
C	32.53199	12.10923	4.14137
C	31.76346	10.99863	3.90958
C	30.7697	11.81322	7.35533
C	29.39325	11.567	7.58502
C	28.86306	11.67223	8.87789
C	29.69186	12.01866	9.95867
C	31.05849	12.26273	9.7403
C	31.59747	12.16379	8.45069
C	32.85141	13.73854	6.00843
C	32.08219	14.93086	6.01553
C	32.69798	16.08119	6.54936
C	34.01137	16.04701	7.03297
C	34.7486	14.85616	6.99128
C	34.19101	13.66856	6.47834
C	30.66559	15.02675	5.44994
C	30.62974	15.93468	4.20063
C	35.03425	12.39273	6.4184
C	35.70686	12.06018	7.7659
C	31.99097	8.37705	6.51866
C	32.84106	7.31629	5.78566
C	28.37629	10.89821	3.77253
C	28.4113	10.60231	2.25654
C	29.65198	15.49454	6.51451
C	36.0874	12.48114	5.29144
C	26.9754	11.38076	4.20085
C	31.93243	8.10247	8.03519
H	33.2404	12.64261	3.50217
H	30.90655	16.97936	4.45067
H	29.6096	15.95614	3.76662
H	31.32901	15.58314	3.41557
H	30.35397	14.01234	5.12334

H	29.86949	16.52608	6.85923
H	28.62616	15.49903	6.09417
H	29.65733	14.83332	7.40375
H	32.1358	17.02653	6.5774
H	34.46884	16.96046	7.44172
H	35.78296	14.84816	7.36541
H	34.35714	11.54659	6.17452
H	35.62725	12.67306	4.30133
H	36.66431	11.5368	5.22063
H	36.80725	13.30217	5.48458
H	36.46265	12.82004	8.04937
H	36.2334	11.08674	7.70078
H	34.97323	11.99182	8.59449
H	30.03563	6.47746	6.52925
H	27.77987	6.54342	5.47917
H	26.92329	11.60295	5.28579
H	26.19209	10.62958	3.97482
H	26.70529	12.30615	3.65349
H	27.71262	9.78143	1.99547
H	29.41991	10.29723	1.91238
H	29.08176	11.73487	3.96425
H	28.11029	11.49825	1.67658
H	32.50191	9.35336	6.38193
H	32.95446	8.08961	8.46491
H	33.86868	7.28876	6.20118
H	32.91591	7.52668	4.69979
H	32.40905	6.30113	5.89955
H	31.47306	7.11694	8.25423
H	31.34484	8.8755	8.56885
H	27.03087	8.56064	4.22577
H	27.79124	11.48539	9.04075
H	28.73052	11.30758	6.74943
H	31.7142	12.52924	10.58229
H	32.66899	12.34577	8.29771
H	29.27222	12.09783	10.97271
H	31.68245	10.34752	3.03513

V

$E_{B3LYP/def\text{-}SVP}$ = -1619.883320
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1619.154447

C	1.22943	-0.62642	-2.57111
C	0.26516	-1.12546	-1.67102
C	-0.48141	-2.25741	-2.06184
C	-0.26819	-2.86482	-3.29992
C	0.69165	-2.3581	-4.18157
C	1.43727	-1.23531	-3.81006
C	0.03506	-0.50415	-0.35373
N	-0.07198	0.82252	-0.079
C	-0.33205	0.96803	1.30656
C	-0.3555	-0.2873	1.91338
N	-0.13921	-1.14817	0.83769
C	0.08424	1.87604	-1.05523
C	1.28656	2.62463	-1.06168
C	1.40207	3.65845	-2.00242
C	0.37454	3.94024	-2.90097
C	-0.79929	3.18939	-2.87335
C	-0.9762	2.14607	-1.95267
C	2.44488	2.36262	-0.09657
C	2.70229	3.57119	0.82413
C	-2.29789	1.37803	-1.94062
C	-3.46935	2.27186	-1.48928
C	-0.56004	2.24358	2.01421
C	-1.01806	3.43946	1.42308
C	-1.23838	4.58701	2.19282
C	-1.01439	4.5748	3.57087
C	-0.57011	3.39195	4.17527
C	-0.34724	2.24774	3.41241
C	-0.03454	-2.57558	1.04047
C	1.24694	-3.16208	1.12695
C	1.31692	-4.54467	1.35573
C	0.16254	-5.31018	1.50778
C	-1.09091	-4.70269	1.44453
C	-1.22008	-3.3255	1.21404
C	2.52568	-2.32925	1.07624
C	2.98879	-1.99348	2.50806
C	-2.60091	-2.67244	1.21123
C	-3.05071	-2.36613	2.65349
C	3.64983	-2.98135	0.25634
C	-3.66288	-3.49072	0.45827
C	-2.59757	0.72704	-3.30339

C	3.73923	1.9685	-0.83416
H	1.82865	0.24035	-2.29932
H	2.29324	-5.02858	1.42835
H	2.28712	-1.37441	0.5851
H	-1.98743	-5.31078	1.58276
H	-2.50919	-1.70343	0.6959
H	-0.86264	-3.73906	-3.57775
H	2.19388	-0.82939	-4.48662
H	-1.21617	3.48876	0.35422
H	-0.0098	1.32119	3.87959
H	0.23989	-6.38607	1.68696
H	4.5055	-2.29157	0.17148
H	3.31459	-3.23421	-0.76211
H	2.19278	-1.4739	3.06335
H	3.8803	-1.34405	2.48737
H	3.25077	-2.91073	3.06195
H	-3.34583	-3.7392	-0.56819
H	-4.60222	-2.9181	0.39166
H	-3.90018	-4.43682	0.97155
H	-3.14725	-3.29592	3.23955
H	-4.03141	-1.86101	2.65286
H	-2.31914	-1.70872	3.14653
H	-1.60057	3.42122	-3.57912
H	-2.21192	0.56735	-1.20288
H	2.31679	4.25558	-2.03042
H	2.16411	1.51754	0.54884
H	0.85756	-2.83507	-5.15103
H	-1.59547	5.4974	1.70295
H	-0.39277	3.36161	5.25418
H	0.48836	4.75102	-3.62547
H	-2.77551	1.4841	-4.08506
H	-3.50552	0.1055	-3.23709
H	-1.76938	0.08383	-3.63672
H	-3.30029	2.68757	-0.48441
H	-4.40438	1.68873	-1.45881
H	-3.62518	3.11466	-2.18316
H	4.54049	1.75844	-0.10713
H	4.09603	2.77754	-1.49265
H	3.04608	4.44785	0.24987
H	3.48684	3.3282	1.55917
H	1.79665	3.8592	1.37625
H	-1.18696	5.47366	4.16891
H	3.60896	1.06686	-1.45272

H	4.02768	-3.90357	0.72743
H	-1.2435	-2.66002	-1.39643

V

$E_{BP86/def\text{-}SVP}$ = -1621.013427
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.303971
$E_{BP86/def2\text{-}TZVPP//BP86/def\text{-}SVP}$ = -1622.743721

C	1.18178	-0.57214	-2.62819
C	0.26757	-1.12259	-1.69267
C	-0.43278	-2.30038	-2.06351
C	-0.2243	-2.89854	-3.31348
C	0.68296	-2.34008	-4.22976
C	1.38275	-1.17369	-3.87821
C	0.04545	-0.51294	-0.37223
N	-0.05443	0.82203	-0.08308
C	-0.30897	0.96243	1.30846
C	-0.33321	-0.30528	1.91335
N	-0.12868	-1.16248	0.83158
C	0.09272	1.88046	-1.05674
C	1.30104	2.63232	-1.06992
C	1.40507	3.68025	-2.00597
C	0.36102	3.97323	-2.89285
C	-0.81742	3.2167	-2.85954
C	-0.98369	2.15802	-1.94383
C	2.46974	2.35349	-0.12072
C	2.73382	3.54865	0.82036
C	-2.30193	1.38266	-1.92166
C	-3.47539	2.27654	-1.46673
C	-0.54641	2.23285	2.02029
C	-0.9554	3.45281	1.42366
C	-1.19248	4.59576	2.20622
C	-1.034	4.55648	3.60014
C	-0.63776	3.35045	4.20809
C	-0.39837	2.2097	3.43393
C	-0.03107	-2.59481	1.02594
C	1.25398	-3.19111	1.10302
C	1.31469	-4.58389	1.31133
C	0.14919	-5.34771	1.4543
C	-1.1065	-4.72874	1.40338
C	-1.22778	-3.34093	1.19143
C	2.53037	-2.35143	1.06796
C	2.88512	-1.8929	2.50107
C	-2.60161	-2.67003	1.20018
C	-3.00541	-2.31151	2.64748
C	3.71759	-3.05584	0.38962
C	-3.69404	-3.49838	0.49996

C	-2.60014	0.72295	-3.28342
C	3.75535	1.97197	-0.88494
H	1.74769	0.33205	-2.3719
H	2.29532	-5.07843	1.37088
H	2.3139	-1.43756	0.47555
H	-2.01471	-5.3357	1.53239
H	-2.50506	-1.71105	0.64783
H	-0.78406	-3.80968	-3.57476
H	2.10116	-0.72609	-4.58197
H	-1.10198	3.52152	0.33893
H	-0.09833	1.25906	3.8979
H	0.22088	-6.43438	1.61622
H	4.5738	-2.35681	0.29761
H	3.45741	-3.41327	-0.62713
H	2.03928	-1.34077	2.95929
H	3.77673	-1.23155	2.49351
H	3.11464	-2.76706	3.14607
H	-3.40371	-3.79142	-0.53026
H	-4.63341	-2.91224	0.43464
H	-3.93581	-4.42752	1.05726
H	-3.09049	-3.22749	3.26928
H	-3.98687	-1.79304	2.66165
H	-2.24468	-1.6411	3.09707
H	-1.63411	3.4547	-3.55803
H	-2.20283	0.56978	-1.1745
H	2.32759	4.28014	-2.0382
H	2.19003	1.48963	0.5157
H	0.84435	-2.81182	-5.21102
H	-1.51197	5.52711	1.71287
H	-0.51186	3.29911	5.30101
H	0.46675	4.79731	-3.61495
H	-2.76916	1.48156	-4.07589
H	-3.51859	0.10404	-3.21915
H	-1.76854	0.06811	-3.60962
H	-3.29493	2.71078	-0.46316
H	-4.4132	1.68584	-1.41566
H	-3.64633	3.11392	-2.17499
H	4.57217	1.74173	-0.17086
H	4.1068	2.80096	-1.53367
H	3.06787	4.44354	0.2539
H	3.5336	3.29626	1.54588
H	1.82692	3.82403	1.39196
H	-1.21971	5.45502	4.20846

H	3.61171	1.07992	-1.52738
H	4.07886	-3.92641	0.97622
H	-1.15582	-2.74562	-1.36863

V + H

$E_{B3LYP/def\text{-}SVP}$ =-1620.362604
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1619.619861

C	-1.28857	-3.30223	1.28201
C	-0.08059	-2.58764	1.10569
C	1.19463	-3.18257	1.22674
C	1.23116	-4.55688	1.50732
C	0.06039	-5.29331	1.6753
C	-1.18276	-4.67041	1.56924
N	-0.15661	-1.15661	0.85466
C	0.04423	-0.49611	-0.31135
N	-0.06198	0.83658	-0.04475
C	-0.33689	1.02026	1.31956
C	-0.38746	-0.23854	1.85861
C	0.32152	-1.12191	-1.61567
C	1.3078	-0.60124	-2.47615
C	1.56823	-1.21207	-3.70331
C	0.84888	-2.34603	-4.0938
C	-0.1353	-2.86826	-3.2485
C	-0.39819	-2.26477	-2.01858
C	0.06734	1.90467	-1.026
C	1.24612	2.68895	-1.01962
C	1.33141	3.71995	-1.96684
C	0.3005	3.96168	-2.8727
C	-0.84842	3.17367	-2.8507
C	-1	2.12737	-1.9286
C	-0.50681	2.29787	2.03576
C	-1.18744	3.40294	1.49133
C	-1.36081	4.56642	2.24417
C	-0.86315	4.64754	3.54818
C	-0.18653	3.55489	4.10014
C	-0.00706	2.39176	3.35102
C	2.41211	2.478	-0.05052
C	3.71588	2.10278	-0.78276
C	-2.29273	1.3094	-1.94649
C	-2.50912	0.61875	-3.30669
C	2.50372	-2.40524	1.10691
C	3.41662	-2.97387	0.00552
C	-2.6685	-2.64795	1.20219
C	-3.63131	-3.40158	0.26642
C	2.64062	3.71563	0.83959
C	-3.51916	2.16479	-1.57182
C	3.23395	-2.3422	2.46273

C	-3.28922	-2.49351	2.60522
H	1.88274	0.27549	-2.18517
H	2.197	-5.05714	1.60564
H	2.266	-1.368	0.82416
H	-2.09036	-5.2601	1.71365
H	-2.54372	-1.63496	0.78617
H	-0.70669	-3.74956	-3.54903
H	2.34091	-0.79963	-4.35626
H	-1.5934	3.35794	0.48202
H	0.54685	1.5549	3.78314
H	0.11635	-6.36178	1.89783
H	4.31904	-2.35076	-0.10062
H	2.90583	-3.00431	-0.96919
H	2.59902	-1.89918	3.24656
H	4.14783	-1.73232	2.37934
H	3.53421	-3.34532	2.80557
H	-3.21347	-3.52831	-0.74497
H	-4.57837	-2.84725	0.17188
H	-3.87877	-4.40309	0.65161
H	-3.46097	-3.47673	3.07206
H	-4.26019	-1.97666	2.54382
H	-2.64148	-1.9159	3.28318
H	-1.64952	3.37667	-3.56468
H	-2.21329	0.51647	-1.18671
H	2.22489	4.34742	-1.99425
H	2.16177	1.63758	0.61556
H	1.05433	-2.8216	-5.05598
H	-1.89503	5.41394	1.80803
H	0.21217	3.6112	5.1159
H	0.39249	4.77175	-3.60046
H	-2.68087	1.35442	-4.10858
H	-3.39651	-0.03295	-3.26584
H	-1.64509	0.00217	-3.59505
H	-3.42144	2.61409	-0.57153
H	-4.42954	1.5443	-1.57055
H	-3.67777	2.98177	-2.2937
H	4.5243	1.93369	-0.05376
H	4.04658	2.90691	-1.45911
H	2.97241	4.58083	0.24342
H	3.42672	3.50845	1.58309
H	1.72855	4.00725	1.37924
H	-1.00103	5.56038	4.13279
H	3.61295	1.18457	-1.38174

H	3.75191	-3.99609	0.24282
H	-1.17725	-2.67697	-1.37967
H	-0.585	-0.55507	2.8775

V + H

$E_{BP86/def\text{-}SVP}$ = -1621.486513
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.763814

C	-1.29914	-3.29703	1.30147
C	-0.07768	-2.59356	1.11741
C	1.19782	-3.20658	1.22212
C	1.21904	-4.59033	1.4921
C	0.03549	-5.31761	1.66616
C	-1.20659	-4.67527	1.57772
N	-0.14214	-1.15997	0.87061
C	0.05726	-0.49812	-0.30797
N	-0.05283	0.84351	-0.03673
C	-0.32554	1.02997	1.33193
C	-0.37202	-0.23885	1.87694
C	0.33167	-1.1203	-1.61278
C	1.27796	-0.55834	-2.50483
C	1.53463	-1.1663	-3.74108
C	0.85275	-2.33766	-4.11166
C	-0.09011	-2.90117	-3.23529
C	-0.35024	-2.30239	-1.99548
C	0.07247	1.91025	-1.01979
C	1.24749	2.71155	-1.00277
C	1.3316	3.74272	-1.95956
C	0.30363	3.96887	-2.88287
C	-0.84188	3.164	-2.86914
C	-0.99277	2.115	-1.93935
C	-0.50676	2.31013	2.03905
C	-1.16935	3.42264	1.46813
C	-1.36013	4.59392	2.21618
C	-0.8978	4.67733	3.54008
C	-0.23869	3.57829	4.11733
C	-0.04179	2.40645	3.37463
C	2.40668	2.51268	-0.0218
C	3.71304	2.12331	-0.74811
C	-2.27686	1.282	-1.96199
C	-2.4808	0.58997	-3.32623
C	2.51586	-2.44303	1.09362
C	3.39514	-3.00124	-0.04383
C	-2.67207	-2.62315	1.23809
C	-3.64797	-3.35365	0.29313
C	2.6302	3.765	0.8535
C	-3.51255	2.12941	-1.58715
C	3.27691	-2.42597	2.43749

C	-3.28341	-2.48231	2.65
H	1.82611	0.35077	-2.22763
H	2.18765	-5.10544	1.5752
H	2.28152	-1.38777	0.83971
H	-2.12811	-5.25742	1.72623
H	-2.53282	-1.59801	0.83316
H	-0.63353	-3.8143	-3.52014
H	2.27849	-0.72113	-4.41829
H	-1.55041	3.37397	0.44004
H	0.50075	1.56252	3.82677
H	0.08089	-6.39608	1.87922
H	4.31668	-2.3944	-0.15184
H	2.86173	-2.99298	-1.01514
H	2.66089	-1.99824	3.2539
H	4.20128	-1.81942	2.35246
H	3.57743	-3.44814	2.74601
H	-3.23386	-3.4685	-0.729
H	-4.59723	-2.78724	0.21192
H	-3.90492	-4.36588	0.66574
H	-3.46827	-3.47707	3.1046
H	-4.25323	-1.94698	2.60395
H	-2.61943	-1.92284	3.33888
H	-1.64425	3.35409	-3.59749
H	-2.18659	0.48297	-1.19672
H	2.22606	4.3832	-1.97896
H	2.14629	1.67525	0.65805
H	1.05586	-2.81141	-5.08382
H	-1.88235	5.4477	1.75921
H	0.1338	3.63655	5.15092
H	0.39567	4.78141	-3.61904
H	-2.65242	1.32994	-4.1342
H	-3.37068	-0.07055	-3.29304
H	-1.60573	-0.02613	-3.61071
H	-3.41916	2.58244	-0.57971
H	-4.42537	1.49982	-1.58752
H	-3.67639	2.95091	-2.31391

IPr^{Ph}

$E_{B3LYP/def\text{-}SVP}$ = -1390.679003
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1390.030739

C	31.45229	11.62957	5.90135
C	32.40949	12.55932	5.46817
C	32.90213	12.56643	4.15396
C	32.40813	11.60757	3.26978
C	31.45707	10.68325	3.673
C	30.98518	10.69656	4.97552
N	32.89804	13.53956	6.4011
C	34.03075	13.38387	7.14423
N	34.05745	14.53344	7.88415
C	32.97806	15.39242	7.6021
C	32.25403	14.73877	6.65727
C	35.14222	14.80996	8.79194
C	35.14538	14.19374	10.05483
C	36.21453	14.46422	10.90772
C	37.24032	15.31467	10.5253
C	37.22017	15.90348	9.27204
C	36.17776	15.6603	8.37735
C	34.05827	13.22042	10.48592
C	33.54583	13.47915	11.90991
C	36.22778	16.27145	6.98541
C	37.3356	15.61317	6.14656
C	33.97315	13.54399	3.69702
C	33.61094	14.24865	2.38193
C	30.92954	11.60119	7.32939
C	29.42234	11.89447	7.38851
C	34.54871	11.77132	10.33058
C	36.39047	17.79815	7.01991
C	31.26533	10.27253	8.02394
C	35.33594	12.83969	3.59822
C	32.7076	16.71176	8.18681
H	34.31191	13.28965	12.66354
H	32.70679	12.81633	12.12878
H	33.20172	14.50704	12.03605
H	33.21323	13.34776	9.80921
H	35.40463	11.579	10.98154
H	33.75694	11.06858	10.59874
H	34.84781	11.57739	9.3012
H	36.24826	13.99988	11.88398
H	38.06028	15.51258	11.20368
H	38.03237	16.55452	8.97718

H	35.28139	16.05799	6.49072
H	35.60268	18.26902	7.60834
H	36.3443	18.20352	6.00741
H	37.35056	18.09343	7.44695
H	38.32032	15.79353	6.58244
H	37.33956	16.01939	5.13293
H	37.18864	14.53502	6.08192
H	32.77481	11.58153	2.25238
H	31.08543	9.94841	2.97045
H	32.33952	10.08754	8.01482
H	30.77351	9.42827	7.537
H	30.93323	10.29457	9.06378
H	28.84399	11.13101	6.86458
H	29.18663	12.85833	6.93473
H	31.43631	12.38859	7.88514
H	29.07957	11.91776	8.42471
H	34.06619	14.31443	4.46166
H	36.11434	13.54998	3.31222
H	34.36704	14.99709	2.13776
H	32.64621	14.75346	2.45331
H	33.56112	13.55231	1.54317
H	35.31351	12.04524	2.84899
H	35.6107	12.39784	4.55572
H	30.24686	9.96687	5.28145
H	31.33317	15.01901	6.17842
C	32.18593	17.72495	7.37018
C	31.86849	18.97133	7.89144
C	32.07887	19.24089	9.23958
C	32.60508	18.24868	10.05876
C	32.91225	16.99687	9.54179
H	32.04715	17.5326	6.31464
H	31.46814	19.73719	7.23987
H	31.84	20.21487	9.64579
H	32.77329	18.44498	11.10962
H	33.30734	16.23634	10.19757
H	-3.67639	2.95091	-2.31391

IPr^{Ph}

$E_{BP86/def\text{-}SVP}$ = -1390.1345297
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1389.503653
$E_{BP86/def2\text{-}TZVPP//BP86/def\text{-}SVP}$ = -1389.503653

C	31.31456	11.67104	5.87495
C	32.27694	12.61331	5.43031
C	32.70723	12.679	4.07894
C	32.13796	11.7685	3.16653
C	31.18047	10.83243	3.57968
C	30.77753	10.7835	4.92018
N	32.8273	13.55142	6.38039
C	33.97146	13.32373	7.11386
N	34.07246	14.48005	7.85991
C	33.03236	15.41008	7.59904
C	32.24733	14.79022	6.64869
C	35.18174	14.69204	8.76199
C	35.22872	13.95633	9.98039
C	36.29559	14.2215	10.86173
C	37.28357	15.16643	10.54882
C	37.23755	15.84531	9.32606
C	36.19522	15.61844	8.403
C	34.16316	12.91531	10.33154
C	32.93822	13.56062	11.01437
C	36.23049	16.31238	7.04077
C	37.34591	15.70464	6.16302
C	33.80386	13.64701	3.6379
C	33.57455	14.23857	2.23601
C	30.91922	11.55928	7.34627
C	29.40424	11.38446	7.55746
C	34.70721	11.75114	11.17726
C	36.37182	17.84237	7.15343
C	31.72095	10.42412	8.02017
C	35.1834	12.95915	3.74434
C	32.84856	16.75017	8.18338
H	33.22439	14.04421	11.97269
H	32.16903	12.79343	11.2402
H	32.46236	14.331	10.37546
H	33.82752	12.48469	9.36474
H	34.96996	12.06372	12.20991
H	33.93772	10.95741	11.26849
H	35.60825	11.2988	10.7169
H	36.3574	13.672	11.81205
H	38.10436	15.35923	11.25684

H	38.03427	16.5614	9.07257
H	35.26797	16.10761	6.53093
H	35.56684	18.27939	7.7767
H	36.31945	18.3101	6.14866
H	37.34568	18.13605	7.59839
H	38.3482	15.87798	6.60798
H	37.34257	16.16415	5.15269
H	37.21271	14.61091	6.04608
H	32.45223	11.7917	2.11264
H	30.74641	10.13187	2.8494
H	32.8106	10.59113	7.90564
H	31.47563	9.44104	7.56594
H	31.48637	10.36575	9.10351
H	29.03688	10.41359	7.16479
H	28.82505	12.18964	7.06152
H	31.21384	12.50683	7.84258
H	29.16261	11.40724	8.63983
H	33.80472	14.49337	4.35647
H	35.99533	13.66322	3.46758
H	34.33337	15.01866	2.02227
H	32.57154	14.70276	2.14226
H	33.66946	13.47304	1.43772
H	35.24053	12.08449	3.06265
H	35.36418	12.60576	4.77957
H	30.03091	10.03853	5.2341
H	31.31647	15.11969	6.17724
C	32.21227	17.75412	7.40792
C	31.97364	19.0319	7.93069
C	32.37829	19.34894	9.2393
C	33.01971	18.37027	10.01571
C	33.252	17.08588	9.49941
H	31.92087	17.52913	6.37084
H	31.47891	19.79105	7.30532
H	32.19839	20.35471	9.64861
H	33.34142	18.60432	11.0422
H	33.74469	16.33538	10.13072

IPr^{Ph} + H

$E_{B3LYP/def\text{-}SVP}$ =-1389.618100
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1388.956808

C	32.98193	17.05792	9.4966
C	32.73937	16.73217	8.14892
C	32.20023	17.71715	7.29654
C	31.90826	18.99227	7.78126
C	32.15498	19.30658	9.12176
C	32.69186	18.3373	9.97471
C	32.98643	15.38905	7.59848
N	34.0658	14.54823	7.90676
C	33.96727	13.43427	7.1651
N	32.8772	13.50638	6.39666
C	32.25074	14.71111	6.65081
C	32.43282	12.48859	5.45781
C	31.51247	11.51756	5.91051
C	31.10058	10.55425	4.97811
C	31.58142	10.56298	3.66937
C	32.48638	11.54009	3.2567
C	32.9355	12.53391	4.13856
C	30.95801	11.48543	7.33313
C	31.29547	10.16404	8.04833
C	33.92428	13.59166	3.65278
C	35.28151	12.96531	3.28032
C	35.16867	14.78578	8.82735
C	35.12942	14.16019	10.09505
C	36.21997	14.38536	10.94713
C	37.28634	15.19554	10.55798
C	37.29122	15.79675	9.3007
C	36.23454	15.60615	8.3978
C	33.98608	13.25116	10.54648
C	34.41923	11.77152	10.53394
C	36.29437	16.25459	7.01647
C	36.40183	17.78795	7.10478
C	33.42538	13.64372	11.92537
C	37.43871	15.65982	6.17287
C	33.34852	14.41617	2.48639
C	29.4424	11.76117	7.35079
H	34.16602	13.4981	12.7272
H	32.55271	13.01828	12.17102
H	33.10247	14.69619	11.95339

H	33.15804	13.35891	9.82701
H	35.23305	11.59014	11.25421
H	33.57607	11.11816	10.80937
H	34.7839	11.4548	9.54327
H	36.23494	13.91903	11.93435
H	38.12355	15.35723	11.24149
H	38.13689	16.42373	9.0101
H	35.35438	16.02988	6.48863
H	35.57461	18.21846	7.68948
H	36.37342	18.22998	6.09612
H	37.34779	18.1023	7.57393
H	38.42247	15.86822	6.62298
H	37.43782	16.09783	5.16187
H	37.34595	14.5665	6.07051
H	32.85059	11.53244	2.22706
H	31.24566	9.80035	2.96231
H	32.3806	9.97438	8.06399
H	30.81405	9.30217	7.55963
H	30.93882	10.19151	9.09037
H	28.88328	10.97478	6.81902
H	29.1979	12.72352	6.87363
H	31.43736	12.29382	7.90816
H	29.06924	11.79115	8.38688
H	34.10901	14.29643	4.47929
H	35.99923	13.74806	2.9873
H	34.0511	15.21444	2.1987
H	32.38966	14.8867	2.75583
H	33.17512	13.79324	1.59457
H	35.18558	12.26911	2.43186
H	35.71647	12.40243	4.12201
H	30.38984	9.78291	5.28261
H	31.32402	14.98434	6.155
H	32.02788	17.48969	6.24172
H	31.49479	19.74612	7.10709
H	31.92968	20.30634	9.50089
H	32.88115	18.57552	11.02409
H	33.3841	16.31148	10.18076
H	34.67004	12.60516	7.18528
H	4.54049	1.75844	-0.10713
H	4.09603	2.77754	-1.49265
H	3.04608	4.44785	0.24987
H	3.48684	3.3282	1.55917
H	1.79665	3.8592	1.37625

H	-1.18696	5.47366	4.16891
H	3.60896	1.06686	-1.45272
H	4.02768	-3.90357	0.72743
H	-1.2435	-2.66002	-1.39643

IPr^{Ph} + H

$E_{BP86/def\text{-}SVP}$ = -1390.584060
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1389.940519

C	33.03749	17.06828	9.48662
C	32.75363	16.72676	8.14281
C	32.16649	17.70178	7.29817
C	31.86685	18.98034	7.78691
C	32.15293	19.30966	9.12322
C	32.73863	18.35159	9.96765
C	33.00188	15.3845	7.59277
N	34.08091	14.537	7.90972
C	33.98322	13.41139	7.16819
N	32.88733	13.48787	6.39038
C	32.26264	14.6994	6.63759
C	32.43608	12.47155	5.44933
C	31.50085	11.50544	5.9029
C	31.07276	10.54816	4.96134
C	31.55077	10.55864	3.64468
C	32.47123	11.53099	3.23325
C	32.93891	12.51844	4.12307
C	30.94794	11.47495	7.32734
C	31.24846	10.13365	8.02816
C	33.93674	13.56971	3.63811
C	35.2718	12.92465	3.20959
C	35.18058	14.78171	8.83525
C	35.13512	14.16185	10.11312
C	36.22165	14.40505	10.9769
C	37.28949	15.22549	10.58969
C	37.30027	15.81857	9.32122
C	36.24874	15.61109	8.40534
C	33.995	13.24583	10.56237
C	34.44983	11.76946	10.57533
C	36.31491	16.25158	7.01893
C	36.35709	17.7916	7.10267
C	33.41342	13.65283	11.93153
C	37.50679	15.69923	6.20784
C	33.34096	14.43455	2.50744
C	29.43736	11.79273	7.34637
H	34.1526	13.52796	12.74845
H	32.54157	13.01561	12.18161
H	33.07362	14.70773	11.94117
H	33.17011	13.33583	9.82298
H	35.26446	11.60951	11.31099

H	33.60918	11.10319	10.8556
H	34.83171	11.43994	9.58766
H	36.22903	13.94228	11.97459
H	38.12456	15.4013	11.28407
H	38.14867	16.45506	9.0287
H	35.38951	15.98032	6.4682
H	35.49157	18.19374	7.66498
H	36.3418	18.23349	6.08593
H	37.28166	18.14674	7.6021
H	38.47575	15.96236	6.67883
H	37.50967	16.12803	5.18551
H	37.46912	14.59503	6.11732
H	32.83502	11.52732	2.19501
H	31.19948	9.80044	2.92893
H	32.33331	9.90628	8.03687
H	30.73413	9.2869	7.5297
H	30.89443	10.15969	9.07828
H	28.85519	11.02274	6.80018
H	29.21558	12.7726	6.8775
H	31.45638	12.27109	7.9115
H	29.059	11.81956	8.3882
H	34.15843	14.25253	4.48545
H	36.00143	13.70404	2.91152
H	34.05416	15.23066	2.21262
H	32.39348	14.92051	2.81608
H	33.12704	13.8309	1.60197
H	35.13572	12.24868	2.34099
H	35.72354	12.32788	4.02755
H	30.34846	9.77893	5.26772
H	31.33052	14.97097	6.13503
H	31.96506	17.46295	6.24292
H	31.41644	19.72769	7.11691
H	31.9203	20.31464	9.50577
H	32.96048	18.60183	11.01564
H	33.47856	16.32733	10.16628
H	34.68895	12.57543	7.19222

IPr^{Bp}

$E_{B3LYP/def\text{-}SVP}$ = -1619.913748
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1619.185094

C	33.08501	17.05816	9.52049
C	32.80595	16.74646	8.1758
C	32.24201	17.76306	7.37723
C	31.96	19.02291	7.89962
C	32.23996	19.33714	9.24367
C	32.8101	18.32383	10.03682
C	33.03796	15.4158	7.59101
N	34.09584	14.52331	7.87475
C	34.03475	13.3695	7.13627
N	32.90278	13.55401	6.38965
C	32.28963	14.77547	6.64148
C	32.38702	12.58507	5.45711
C	31.36441	11.70698	5.87845
C	30.86756	10.78402	4.94515
C	31.37035	10.73114	3.64674
C	32.38523	11.60403	3.25504
C	32.91331	12.55022	4.14549
C	30.81156	11.71517	7.30156
C	31.12146	10.39425	8.0293
C	34.05582	13.46415	3.71113
C	35.40303	12.72235	3.8099
C	35.19144	14.77183	8.77957
C	35.18725	14.14366	10.04736
C	36.27063	14.3899	10.90318
C	37.31617	15.23071	10.52232
C	37.30159	15.83376	9.26663
C	36.24651	15.61511	8.3673
C	34.07564	13.18824	10.47573
C	34.50633	11.72596	10.24959
C	36.30093	16.24417	6.97712
C	36.46073	17.77353	7.02823
C	33.60432	13.41467	11.92187
C	37.40641	15.58981	6.12685
C	33.84853	14.06996	2.31349
C	29.30633	12.03523	7.33329
H	34.38247	13.1581	12.65924
H	32.73234	12.77647	12.13944
H	33.30733	14.46142	12.09811
H	33.21072	13.37436	9.82108
H	35.38375	11.47363	10.86898

H	33.69051	11.03484	10.52111
H	34.76566	11.56072	9.19317
H	36.29845	13.91366	11.88575
H	38.14962	15.41124	11.20682
H	38.1317	16.48089	8.97266
H	35.34564	16.03544	6.47507
H	35.65946	18.24223	7.62038
H	36.42312	18.19646	6.01067
H	37.42625	18.07106	7.46993
H	38.40496	15.76521	6.56094
H	37.40802	16.007	5.1058
H	37.25673	14.5017	6.05254
H	32.7757	11.5474	2.23654
H	30.97177	10.00272	2.93518
H	32.20404	10.19481	8.04223
H	30.6246	9.53667	7.5458
H	30.7689	10.43683	9.0734
H	28.71282	11.26077	6.81959
H	29.0885	12.99923	6.846
H	31.32555	12.51324	7.85591
H	28.94534	12.09292	8.37351
H	34.09643	14.30205	4.42333
H	36.23609	13.39181	3.53719
H	34.64103	14.80528	2.09828
H	32.87727	14.58433	2.23232
H	33.89271	13.30805	1.51796
H	35.42734	11.85592	3.12738
H	35.5711	12.36019	4.83544
H	30.07712	10.09056	5.24356
H	31.36681	15.0798	6.15481
H	32.047	17.56733	6.32009
H	31.54829	19.79061	7.24004
C	31.94833	20.68447	9.80026
H	33.01619	18.51772	11.09213
H	33.50534	16.29942	10.18005
C	32.79953	21.27623	10.75404
C	32.52526	22.54162	11.27741
C	31.39238	23.24725	10.85994
C	30.53685	22.67424	9.91373
C	30.81171	21.40885	9.39066
H	33.70225	20.74836	11.07117
H	33.20635	22.98284	12.01032
H	31.17752	24.23781	11.26954

H	29.64328	23.21255	9.58585
H	30.11988	20.96384	8.67125

IPr^{Bp}

$E_{BP86/def\text{-}SVP}$ = -1621.0384007
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.3295031
$E_{BP86/def2\text{-}TZVPP//BP86/def\text{-}SVP}$ = -1622.770797

C	33.14305	17.06272	9.51264
C	32.81501	16.74589	8.17188
C	32.19135	17.75649	7.39642
C	31.89701	19.01176	7.93776
C	32.22293	19.33039	9.27859
C	32.85495	18.32435	10.0468
C	33.05318	15.42242	7.57701
N	34.11645	14.52625	7.85747
C	34.0598	13.36232	7.11903
N	32.91464	13.54928	6.37308
C	32.29773	14.77354	6.62236
C	32.38563	12.57263	5.45124
C	31.30966	11.74819	5.86987
C	30.79296	10.82149	4.9413
C	31.32918	10.71152	3.65282
C	32.39875	11.53024	3.26671
C	32.9482	12.48001	4.15045
C	30.72118	11.81719	7.27872
C	30.89644	10.47861	8.02535
C	34.14254	13.33205	3.72694
C	35.45542	12.54393	3.92872
C	35.22097	14.78928	8.75241
C	35.23702	14.15879	10.02671
C	36.3257	14.43049	10.87899
C	37.35689	15.29584	10.48838
C	37.32248	15.89799	9.22515
C	36.26106	15.65626	8.32838
C	34.14612	13.17892	10.45734
C	34.5872	11.72929	10.15887
C	36.29287	16.28541	6.93569
C	36.37907	17.82333	6.98978
C	33.72008	13.34664	11.92749
C	37.43642	15.68243	6.09279
C	34.02206	13.87431	2.29093
C	29.24504	12.26361	7.26162
H	34.52765	13.06136	12.6336
H	32.85348	12.69101	12.15012
H	33.42319	14.39022	12.15898
H	33.25454	13.38377	9.8282

H	35.50235	11.46905	10.73169
H	33.79066	11.01053	10.44401
H	34.80048	11.60831	9.07789
H	36.36602	13.95377	11.86962
H	38.19598	15.49617	11.17234
H	38.14314	16.56574	8.92032
H	35.34247	16.0261	6.42725
H	35.54444	18.25517	7.57685
H	36.33499	18.25084	5.96666
H	37.33036	18.16687	7.44766
H	38.4293	15.90952	6.53437
H	37.42481	16.09938	5.06439
H	37.34185	14.58094	6.02022
H	32.81677	11.4312	2.25374
H	30.91307	9.97925	2.94365
H	31.9623	10.17859	8.06518
H	30.33168	9.65805	7.53527
H	30.52313	10.56298	9.06681
H	28.60336	11.53422	6.72424
H	29.12214	13.24638	6.763
H	31.29286	12.58093	7.84294
H	28.85134	12.35504	8.29509
H	34.18012	14.20667	4.40875
H	36.33181	13.16396	3.64653
H	34.85327	14.57683	2.07687
H	33.06758	14.41678	2.13346
H	34.08154	13.06672	1.53143
H	35.46815	11.62869	3.30035
H	35.56562	12.24355	4.98986
H	29.95772	10.16849	5.23855
H	31.36613	15.07625	6.13447
H	31.96063	17.55808	6.33869
H	31.43945	19.77794	7.29344
C	31.91544	20.6657	9.85456
H	33.0968	18.52111	11.10232
H	33.61148	16.30564	10.15546
C	32.77474	21.26596	10.80658
C	32.48195	22.5237	11.35388
C	31.32235	23.21419	10.963
C	30.45931	22.63362	10.01821
C	30.75222	21.37576	9.4711
H	33.70144	20.74969	11.10086
H	33.171	22.97276	12.08596

H	31.0915	24.20088	11.39302
H	29.54278	23.16092	9.71084
H	30.05214	20.92057	8.75381

IPr^{Bp} + H

$E_{B3LYP/def\text{-}SVP}$ =-1622.120894
$E+ZPVE_{B3LYP/def\text{-}SVP}$ = -1621.378364

C	30.89147	21.4091	9.2465
C	31.99189	20.67751	9.7073
C	32.81512	21.2551	10.68068
C	32.54749	22.52374	11.17555
C	31.44789	23.23743	10.71223
C	30.62024	22.67488	9.74687
C	32.27609	19.32518	9.18173
C	32.05563	19.0063	7.83509
C	32.32506	17.74114	7.34319
C	32.82381	16.73483	8.18059
C	33.04566	17.04535	9.52631
C	32.77772	18.31431	10.01153
C	33.04369	15.4005	7.62
N	34.09577	14.53015	7.92809
C	33.97673	13.43277	7.17415
N	32.90239	13.54265	6.399
C	32.3066	14.75661	6.66306
C	35.20024	14.73361	8.85457
C	35.13306	14.12145	10.11692
C	36.21975	14.31361	10.9689
C	37.3086	15.07971	10.58229
C	37.34115	15.66819	9.3287
C	36.28849	15.50798	8.42761
C	32.43518	12.54648	5.44959
C	31.50302	11.5968	5.89203
C	31.07111	10.65728	4.95677
C	31.54675	10.67073	3.65507
C	32.46453	11.62791	3.25251
C	32.93319	12.59612	4.13957
C	30.95431	11.56547	7.31
C	29.44872	11.87375	7.33106
C	33.93814	13.63538	3.66731
C	33.3748	14.48419	2.51743
C	33.96238	13.25591	10.56349
C	33.42843	13.64854	11.9494
C	36.37904	16.13633	7.04485
C	37.48251	15.46505	6.21036
C	31.25983	10.23065	8.00677
C	35.27381	12.98342	3.27673
C	34.34586	11.76646	10.53415

C	36.5854	17.65702	7.11723
H	34.16039	13.46252	12.73545
H	32.54191	13.05914	12.18581
H	33.15048	14.70181	11.99381
H	33.1418	13.39926	9.85773
H	35.15472	11.55828	11.23582
H	33.49297	11.14601	10.81192
H	34.68352	11.45089	9.54553
H	36.21395	13.85788	11.94907
H	38.13842	15.21609	11.26261
H	38.20056	16.2572	9.03983
H	35.43464	15.96745	6.52581
H	35.80237	18.13991	7.70123
H	36.5712	18.08421	6.11395
H	37.54576	17.9106	7.5676
H	38.46544	15.61884	6.65736
H	37.50533	15.88495	5.20392
H	37.32415	14.38884	6.12478
H	32.82243	11.62498	2.23225
H	31.19814	9.92995	2.94817
H	32.33024	10.02042	8.01805
H	30.76335	9.3951	7.51206
H	30.90913	10.25712	9.039
H	28.88014	11.11529	6.79162
H	29.22974	12.83936	6.87283
H	31.44862	12.34787	7.88788
H	29.08152	11.89668	8.3577
H	34.14281	14.3178	4.4937
H	35.99674	13.7458	2.98519
H	34.08864	15.25942	2.23676
H	32.44011	14.97044	2.80014
H	33.17912	13.88048	1.63071
H	35.15225	12.30118	2.43445
H	35.69987	12.4135	4.10392
H	30.35173	9.90597	5.25169
H	31.40218	15.05716	6.16824
H	32.17595	17.53864	6.2906
H	31.69874	19.76966	7.15757
H	32.93215	18.51588	11.06246
H	33.40706	16.29101	10.2082
H	33.68708	20.71989	11.03295
H	33.2018	22.95848	11.9193
H	31.23727	24.22466	11.10082

H	29.75737	23.2197	9.38771
H	30.22612	20.97334	8.51292
H	34.64759	12.59375	7.19222

IPr^{Bp} + H

$E_{BP86/def\text{-}SVP}$ =-1621.487890
$E+ZPVE_{BP86/def\text{-}SVP}$ = -1620.765596

C	30.85005	21.42101	9.29644
C	31.99434	20.70526	9.72428
C	32.84862	21.31305	10.67622
C	32.56921	22.59117	11.17991
C	31.42694	23.28682	10.74874
C	30.56818	22.69627	9.8061
C	32.28805	19.3515	9.19131
C	31.96225	18.99649	7.85784
C	32.23656	17.72151	7.35687
C	32.85018	16.73464	8.16927
C	33.18224	17.08166	9.50108
C	32.90524	18.36089	9.99446
C	33.06662	15.39587	7.60748
N	34.12081	14.51437	7.92029
C	33.99537	13.3981	7.16808
N	32.90625	13.51268	6.3859
C	32.3135	14.73836	6.6417
C	35.22432	14.71797	8.85017
C	35.15384	14.09485	10.12525
C	36.24482	14.29775	10.99395
C	37.34085	15.08363	10.61382
C	37.37591	15.6812	9.34787
C	36.32108	15.513	8.42784
C	32.43006	12.51604	5.4369
C	31.46327	11.57649	5.87976
C	31.01288	10.63644	4.93133
C	31.5002	10.63777	3.61803
C	32.45155	11.58429	3.21679
C	32.94224	12.55367	4.114
C	30.89997	11.55718	7.30033
C	29.39926	11.91884	7.31016
C	33.97463	13.57655	3.64107
C	33.41858	14.45625	2.50167
C	33.98139	13.21689	10.56643
C	33.40378	13.64363	11.93122
C	36.41134	16.15915	7.04546
C	37.59164	15.57979	6.23651
C	31.15649	10.20544	7.9985
C	35.29672	12.89371	3.23126
C	34.3875	11.72656	10.58226

C	36.49395	17.69697	7.1388
H	34.1338	13.49807	12.75295
H	32.51144	13.03344	12.17679
H	33.09565	14.70814	11.93631
H	33.16564	13.33418	9.82108
H	35.1914	11.53975	11.32336
H	33.52344	11.08825	10.85672
H	34.76485	11.38485	9.59695
H	36.23311	13.83079	11.98969
H	38.17885	15.22886	11.31179
H	38.24617	16.29	9.06058
H	35.48143	15.9162	6.48944
H	35.63515	18.11826	7.69729
H	36.49736	18.14527	6.12475
H	37.42414	18.02442	7.64689
H	38.56537	15.81485	6.71259
H	37.61014	16.01345	5.21636
H	37.52537	14.47741	6.14026
H	32.82196	11.57413	2.1809
H	31.13226	9.89248	2.89708
H	32.23421	9.94661	8.01403
H	30.62135	9.37556	7.49351
H	30.79607	10.23841	9.04625
H	28.7984	11.16782	6.75776
H	29.20993	12.90611	6.84262
H	31.42727	12.33626	7.89051
H	29.01457	11.95403	8.34945
H	34.2033	14.25412	4.49066
H	36.05136	13.65166	2.94036
H	34.15716	15.23271	2.21746
H	32.48035	14.96792	2.7968
H	33.20169	13.85854	1.59288
H	35.15263	12.21873	2.36314
H	35.72138	12.28726	4.05658
H	30.2632	9.88855	5.22942
H	31.39062	15.03836	6.13866

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