Supporting information

General details of synthetic procedures and instrumentation

Materials: All reactions involving air- or moisture-sensitive compounds were carried out under an inert atmosphere by using Schlenk-type glassware or in a glovebox. Solvents (except for fluorobenzene and 1,2-difluorobenzene) were dried using an MBraun SPS800 prior to use. Fluorobenzene and 1,2-difluorobenzene were distilled from CaH_2. NMR-solvents were dried over molecular sieves (CD_2Cl_2) or potassium (C_6D_6, $C_6D_5CD_3$) and degassed before use when necessary. Solid starting materials were dried on high vacuum before use when necessary. Unless otherwise noted, all starting materials were commercially available and were used without further purification. L^{py} and L^{NHC} were prepared via literature routes.[s1,s2]

Techniques: The following instruments were used for physical characterization of the compounds: IR: Nicolet Magna-IR 560; NMR: Bruker AVC500 (^{1}H: 500 MHz; ^{13}C: 125 MHz); Bruker DRX500 (^{11}B: 160 MHz), Varian Unity500 (^{1}H: 500 MHz; ^{13}C: 126 MHz, ^{11}B: 160 MHz), Varian Mercury VX-300 (^{31}P: 122 MHz, ^{19}F: 282 MHz, ^{11}B: 96 MHz). Mass spectra were measured by the EPSRC National Mass Spectrometry Service Centre, Swansea University. Elemental microanalysis was carried out at London Metropolitan University. For all crystallographic studies, diffaction data were collected at 150 K using an Enraf Nonius Kappa CCD diffractometer;[s3] structures were solved with SIR92,[s4] or SuperFlip,[s5] and refined using the CRYSTALS software suite,[s6] as per the information contained in the CIF.

Synthesis of [L^{py}·BBr_2][BBr_4]: To a solution of BBr_3 (0.12 cm^3, 1.26 mmol) in hexanes (30 cm^3) was added a solution of Mes_2py (0.20 g, 0.63 mmol) also in hexanes (20 cm^3), and the reaction mixture stirred at room temperature for 2 h. The resulting cream suspension was filtered, the precipitate washed with hexanes (2 x 50 cm^3) and dried *in vacuo*. The crude solid was extracted into minimum 1,2-difluorobenzene; layering with pentanes and storage at room temperature yielded [L^{py}·BBr_2][BBr_4] as yellow crystals suitable for X-ray crystallography. Isolated yield: 0.38 g, 73 %. **Spectroscopic and analytical data**: ^{1}H NMR (300 MHz, CD_2Cl_2, 20°C): δ_H 2.07 (s, 12H, *ortho*-CH_3 of Mes), 2.36 (s, 6H, *para*-CH_3 of Mes), 7.03 (s, 4H, *meta*-CH of Mes), 7.86 (d, 2H, $^3J_{HH}$ = 6.8 Hz, β-CH of py), 8.70 (t, 1H, $^3J_{HH}$ = 6.8 Hz, γ-CH of py). ^{13}C NMR (126 MHz, CD_2Cl_2, 20°C): δ_c 20.9 (*para*-CH_3 of Mes), 21.6 (*ortho*-CH_3 of Mes), 128.0 (β-CH of py), 128.7 (*meta*-CH of Mes), 129.6 (γ-CH of py), 136.8 (*para*-C of Mes), 142.3 (*ortho*-C of Mes), 147.8 (α-C of py), 155.5 (*ipso*-C of Mes). ^{11}B NMR (96 MHz, CD_2Cl_2, 20°C): δ_B 42 (br, BBr_2^+), -26 ($[BBr_4]^-$). Elemental microanalysis: calc. (for $C_{23}H_{25}B_2Br_6N$) C 33.80, H 3.09, N 1.71; meas. C 33.72, H 2.86, N 1.74. **Crystallographic data**: $C_{23}H_{25}B_2Br_6N$, M_r = 816.50, orthorhombic, *P* c n n, *a* = 11.8539(2), *b* = 13.1384(3), *c* = 18.3488(4) Å, *V* = 2857.67(10) Å^3, *Z* = 4, ρ_c = 1.898 Mg m^{-3}, *T* = 150 K, λ = 0.71073 Å. 18846 reflections collected, 3257 independent [R(int) = 0.032], which were used in all calculations. R_1 = 0.0356, wR_2 = 0.0676 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0578, wR_2 = 0.0740 for all unique reflections. Max./min. residual electron densities 1.12 and -0.99 e Å^{-3}. CCDC reference: 839372.

Synthesis of [L^{py}·BBr_2][$AlBr_4$]: To a solution of BBr_3 (0.12 cm^3, 1.27 mmol) in fluorobenzene (30 cm^3) was added a solution of Mes_2py (0.40 g, 1.27 mmol) also in fluorobenzene (20 cm^3), and the reaction mixture stirred at room temperature for 2 h. A solution/suspension of $AlBr_3$ (0.34 g, 1.27 mmol) also in fluorobenzene was then added to the resulting orange reaction mixture, which was stirred for a further 12 h. The resulting red solution was filtered and volatiles removed *in vacuo*. The crude solid product was washed with hexanes (2 x 50 cm^3), extracted into minimum fluorobenzene and layered with pentane; storage at room temperature yielded [L^{py}·BBr_2][$AlBr_4$] as yellow crystals suitable for X-ray crystallography. Isolated yield: 0.59 g, 57 %.

Spectroscopic data: ^{1}H NMR (300 MHz, CD_2Cl_2, 20°C): δ_H 2.12 (s, 12H, *ortho*-CH_3 of Mes), 2.37 (s, 6H, *para*-CH_3 of Mes), 7.07 (s, 4H, *meta*-CH of Mes), 8.06 (d, 2H, $^3J_{HH}$ = 9.0 Hz, β-CH), 8.95 (t, 1H, $^3J_{HH}$ = 9.0 Hz, γ-CH). ^{13}C NMR (126 MHz, CD_2Cl_2, 20°C): δ_c 21.8 (*para*-CH_3 of Mes), 21.9 (*ortho*-CH_3 of Mes), 126.0 (β-CH of py), 128.9 (*meta*-CH of Mes), 130.2 (γ-CH of py), 138.6 (*para*-C of Mes), 145.1 (*ortho*-C of Mes), 152.2 (α-C of py), 156.76 (*ipso*-C of Mes). ^{11}B NMR (96 MHz, CD_2Cl_2): δ_B 42 (br). Elemental microanalysis: calc. (for $C_{23}H_{25}AlBBr_6N$) C 33.15, H 3.03, N 1.68; meas. C 33.02, H 3.16, N 1.52.

Crystallographic data: $C_{23}H_{25}AlBBr_6N$, M_r = 832.67, monoclinic, *P* 2_1/n, *a* = 12.4226(10), *b* = 13.3058(10), *c* = 18.0226(10) Å, β = 103.59°, *V* = 2895.56(4) Å^3, *Z* = 4, ρ_c = 1.910 Mg m^{-3}, *T* = 150 K, λ = 0.71073 Å. 49830 reflections collected, 6593 independent [R(int) = 0.021], which were used in all calculations. R_1 = 0.0316, wR_2 = 0.0678 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0400, wR_2 = 0.0715 for all unique reflections. Max./min. residual electron densities 2.04 and -1.51 e Å^{-3}. CCDC reference: 839371.

Synthesis of [L^{py}·Bcat][$AlCl_4$]: To a mixture of BrBcat (0.22 g, 1.11 mmol) and Mes_2py (0.35 g, 1.11 mmol) in dichloromethane (40 cm^3) at -10°C was added a solution/suspension of $AlCl_3$ (0.296 g, 2.22 mmol) also in dichloromethane (10 cm^3). The reaction mixture stirred at room temperature for 12 h, after which it was filtered and volatiles removed *in vacuo*. The crude solid product was washed with hexanes, extracted into minimum dichloromethane and layered with hexanes; storage at room temperature yielded [L^{py}·Bcat][$AlCl_4$] as yellow crystals suitable for X-ray crystallography. Isolated yield 0.49 g, 68 %.

Spectroscopic data: ^{1}H NMR (500 MHz, CD_2Cl_2, 20°C): δ_H 2.12 (s, 12H, *ortho*-CH_3 of Mes), 2.18 (s, 6H, *para*-CH_3 of Mes), 6.92 (s, 4H, *meta*-CH of Mes), 7.10 (s, 4H, CH of cat), 8.12 (d, $^3J_{HH}$ = 8.0 Hz, 2H, β-CH of py), 9.04 (t, $^3J_{HH}$ = 8.0 Hz, 1H, γ-CH of py). ^{13}C NMR (126 MHz, CD_2Cl_2 , 20°C) δ_c 20.9 (*ortho*-CH_3 of Mes), 21.5 (*para*-CH_3 of Mes), 113.7 (2-CH of cat), 125.2 (3-CH of cat), 126.9 (β-C of pyridine), 129.2 (γ-CH of pyridine), 129.6 (*meta*-CH of Mes), 137.7 (*ortho*-C of Mes), 143.7 (*para*-C of Mes), 146.6 (1-C of catechol), 151.2 (α-CH of py) and 159.8 (*ipso*-C of Mes). ^{11}B NMR (96 MHz, CD_2Cl_2, 20°C): δ_B 28 (br).

Crystallographic data: $C_{29}H_{29}BNO_2AlCl_4$, M_r = 603.16, triclinic, P-1, a = 9.2145(3), b = 12.0905(4), c = 14.8659(5) Å, α = 105.339(1), β = 107.565(1), γ = 93.368(1)°, V = 1505.3(1) Å^3, Z = 2, ρ_c = 1.331 Mg m^{-3}, T = 150 K, λ = 0.71073 Å, 25940 reflections collected, 5396 independent [R(int) = 0.028], which were used in all calculations. R_1 = 0.0669, wR_2 = 0.1781 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0546, wR_2 = 0.1672 for all unique reflections. Max./min. residual electron densities 1.09 and -0.90 e Å^{-3}. CCDC reference: 839373.

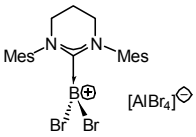
Syntheses of L^{py}·$AlCl_3$ and L^{py}·$GaCl_3$: The two compounds were prepared in similar fashion, exemplified for L^{py}·$AlCl_3$. To a solution/suspension of $AlCl_3$ (0.21 g, 1.59 mmol) in fluorobenzene (30 cm^3) was added a solution of Mes_2py (0.50 g, 1.59 mmol) also in fluorobenzene (20 cm^3), and the reaction mixture stirred at room temperature for 24 h. The resulting olive-green solution was filtered and volatiles removed *in vacuo*. The crude solid product was washed with hexanes, extracted into minimum fluorobenzene and layered with pentane; storage at room temperature yielded L^{py}·$AlCl_3$ as colourless crystals suitable for X-ray crystallography. Isolated yield: 0.56 g, 79 %. L^{py}·$GaCl_3$ was similarly isolated as colourless crystals (isolated yield: 0.40 g, 51 %).

Spectroscopic data: (for L^{py}·$AlCl_3$) ^{1}H NMR (300 MHz, $C_6D_5CD_3$, 20°C): δ_H 2.08 (s, 12H, *ortho*-CH_3 of Mes), 2.13 (s, 6H, *para*-CH_3 of Mes), 6.48 (d, 2H, $^3J_{HH}$ = 9.0 Hz, β-CH), 6.76 (s, 4H, *meta*-CH of Mes), 6.92 (t, 1H, $^3J_{HH}$ = 9.0 Hz, γ-CH). ^{13}C NMR (126 MHz, $C_6D_5CD_3$, 20°C): δ_c 20.3 (*para*-CH_3 of Mes), 21.4 (*ortho*-CH_3 of Mes), 128.7 (β-CH), 129.1 (*meta*-CH of Mes), 133.7 (γ-CH), 137.5 (*para*-C of Mes), 140.6 (*ortho*-C of Mes), 142.2 (α-C), 163.5 (*ipso*-C of Mes). EI-MS (*m/z*): 316.2 {10%, $[Mes_2py]^+$}, 447.1 {100%, $[Mes_2py{\cdot}AlCl_3]^+$}; exact mass: calc. for $[Mes_2py{\cdot}AlCl_3^+]$ 447.0868, meas. 447.0838. Microanalysis: calc. C 61.55, H 5.61, N 3.12; meas. C 61.66, H 5.50, N 3.02. (for L^{py}·$GaCl_3$) ^{1}H NMR

(300 MHz, CD_2Cl_2, 20°C): δ_H 2.51 (s, 12H, *ortho*-CH_3 of Mes), 2.55 (s, 6H, *para*-CH_3 of Mes), 6.85 (d, 2H, $^3J_{HH}$ = 6.0 Hz, β-CH), 7.23 (s, 4H, *meta*-CH of Mes), 7.59 (t, 1H, $^3J_{HH}$ = 6.0 Hz, γ-CH). ^{13}C NMR (126 MHz, CD_2Cl_2, 20°C): δ_c 21.3 (*para*-CH_3 of Mes), 21.4 (*ortho*-CH_3 of Mes), 128.2 (β-CH), 129.2 (*meta*-CH of Mes), 133.2 (γ-C), 137.4 (*para*-C of Mes), 140.7 (*ortho*-C of Mes), 142.2 (α-C), 162.9 (*ipso*-C of Mes). EI-MS (*m/z*): 316.0 {10%, $[Mes_2py^+]$}, 489.0 {100%, $[Mes_2py{\cdot}GaCl_3]^+$}; exact mass: calc. for $[Mes_2py{\cdot}GaCl_3^+]$ 489.0308, meas. 489.0299. Microanalysis: calc. C 56.20, H 5.13, N 2.85; meas. C 56.66, H 5.50, N 3.02.

Crystallographic data: (for $L^{py}{\cdot}AlCl_3$) $C_{23}H_{25}Al_1Cl_1N_1$, M_r = 448.80, monoclinic, $P2_1/c$, a = 9.3044(10), b = 16.4546(2), c = 15.8068(2) Å, β = 106.66(5)°, V = 2318.48(5) Å^3, Z = 4, ρ_c = 1.286 Mg m^{-3}, T = 150 K, λ = 0.71073 Å. 33829 reflections collected, 5275 independent [R(int) = 0.022], which were used in all calculations. R_1 = 0.0428, wR_2 = 0.0915 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0663, wR_2 = 0.1008 for all unique reflections. Max./min. residual electron densities 0.56 and -0.76 e Å^{-3}. CCDC reference: 839365. (for $L^{py}GaCl_3$) $C_{23}H_{25}Cl_{13}Ga_1N_1$, M_r = 491.54, monoclinic, $P2_1/c$, a = 9.3105(2), b = 16.5276(3), c = 15.7099(3) Å, β = 106.67(8)°, V = 2315.81(8) Å^3, Z = 4, ρ_c = 1.410 Mg m^{-3}, T = 150 K, λ = 0.71073 Å. 22059 reflections collected, 5262 independent [R(int) = 0.022], which were used in all calculations. R_1 = 0.0335, wR_2 = 0.0705 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0528, wR_2 = 0.0781 for all unique reflections. Max./min. residual electron densities 0.59 and -0.52 e Å^{-3}. CCDC reference: 839367.

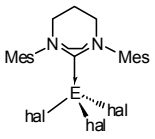
Synthesis of $[L^{NHC}{\cdot}BBr_2][AlBr_4]$: To a stirred solution of $L^{NHC}{\cdot}BBr_3$ (0.30 g, 0.53 mmol) in fluorobenzene (25 cm^3) was added $AlBr_3$ (0.14 g, 0.53 mmol) also in fluorobenzene (15 cm^3), and the reaction mixture stirred for 15 min to give a yellow solution. Volatiles were removed *in vacuo* to give a yellow solid which was washed with toluene (3 x 10 cm^3) and dried *in vacuo*. Dark yellow crystals suitable for X-ray diffraction were obtained from a layering of a concentrated fluorobenzene solution with hexanes at room temperature. Isolated yield: 0.34 g, 76 %



Spectroscopic data: ^{1}H NMR (300 MHz, CD_2Cl_2, 20°C): δ_H 2.30 (s, 6H, *para*-CH_3 of Mes), 2.41 (s, 12H, *ortho*-CH_3 of Mes), 2.62 (quin, $^3J_{HH}$ = 5.7 Hz, 2H, CH_2), 3.84 (t, $^3J_{HH}$ = 5.7 Hz, 4H, NCH_2), 7.01 (s, 4H, *meta*-CH of Mes). ^{13}C NMR (126 MHz, CD_2Cl_2, 20°C): δ_C 18.1 (*ortho*-CH_3 of Mes), 19.2 (CH_2), 21.4 (*para*-CH_3 of Mes), 48.4 (NCH_2), 129.3 (*para*-C of Mes), 131.1 (*meta*-CH of Mes), 136.9 (*ortho*-C of Mes), 143.2 (*ipso*-C of Mes), 165.6 (br, NCN). ^{11}B NMR (96 MHz, CD_2Cl_2, 20°C): δ_B 51.4 (br). Elemental microanalysis: calc. (for $C_{22}H_{28}AlBBr_6N_2$) C 31.52, H 3.37, N 3.34; meas. C 31.27, H 3.26, N 3.11.

Crystallographic data: (for fluorobenzene hemi-solvate) $C_{50}H_{61}Al_2B_2Br_{12}F_4$, M_r = 1771.49, triclinic, P-1, a = 14.9451(2), b = 15.0835(2), c = 15.2202(2) Å, α = 100.901(1), β = 95.178(1), γ = 105.988(1)°, V = 3201.7(1) Å^3, Z = 2, ρ_c = 1.837 Mg m^{-3}, T = 150K, λ = 0.71073 Å, 80911 reflections collected, 14561 independent [R(int) = 0.036], which were used in all calculations. R_1 = 0.0460, wR_2 = 0.0625 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0753, wR_2 = 0.0769 for all unique reflections. Max./min. residual electron densities 1.87 and -1.86 e Å^{-3}. CCDC reference: 839370.

Syntheses of $L^{NHC}{\cdot}BBr_3$ and $L^{NHC}{\cdot}ECl_3$ (E = Al, Ga): All three compounds were prepared in similar fashion: to a solution of L^{NHC} (0.50 g, 1.56 mmol) in hexane (20 cm^3) was added the Group 13 trihalide (1.87 mmol) and the reaction mixture stirred at room temperature overnight. The resulting precipitate was isolated by filtration, dried for 2 h *in vacuo*. Single crystals of each compound were obtained by layering a concentrated dichloromethane solution with hexane. Yields: $L^{NHC}{\cdot}BBr_3$ 0.88 g, 98 %; $L^{NHC}{\cdot}AlCl_3$ 0.68 g, 97%; $L^{NHC}{\cdot}GaCl_3$ 0.76 g, 98%.



E= B; hal = Br
E = Al, Ga; hal = Cl

Spectroscopic data: (for $L^{NHC}{\cdot}BBr_3$) ^{1}H NMR (300 MHz, CD_2Cl_2, 20°C): δ_H 2.29 (s, 6H, *para*-CH_3 of Mes), 2.41 (s, 12H, *ortho*-CH_3 of Mes), 2.62 (quin, $^3J_{HH}$ = 5.7 Hz, 2H, CH_2), 3.61 (t, $^3J_{HH}$ = 5.7 Hz, 4H, NCH_2), 6.90 (s, 4H, *meta*-CH of Mes). ^{13}C NMR (126 MHz, CD_2Cl_2, 20°C): δ_C 18.0 (*ortho*-CH_3 of Mes), 19.0 (CH_2), 20.2 (*para*-CH_3 of Mes), 47.9 (NCH_2), 129.5 (*para*-C of Mes), 130.8 (*meta*-CH of Mes), 134.9 (*ortho*-C of Mes), 141.4 (*ipso*-C of Mes). ^{11}B NMR (96 MHz, CD_2Cl_2, 20°C): δ_B -16. MS (EI): 491 (70 %) (M-HBr)$^+$; MS (CI, NH_3) 569.9 (3 %) (M-H)$^-$. (for $L^{NHC}{\cdot}AlCl_3$) ^{1}H NMR (500 MHz, C_6D_6, 20°C): δ_H 1.29 (quin, $^3J_{HH}$ = 5.7 Hz, 2H, CH_2), 2.08 (s, 6H, *para*-CH_3 of Mes), 2.25 (s, 12H, *ortho*-CH_3 of Mes), 2.50 (t, $^3J_{HH}$ = 5.7 Hz, 4H, NCH_2), 6.78 (s, 4H, *meta*-CH of Mes). ^{13}C NMR (126 MHz, C_6D_6, 20°C): δ_c 18.6 (*ortho*-CH_3 of Mes), 20.0 (CH_2), 21.1 (*para*-CH_3 of Mes), 48.5 (NCH_2), 130.9 (*meta*-CH of Mes), 136.0 (*para*-C of Mes), 140.1 (*ortho*-C of Mes). ^{27}Al (78 MHz, C_6D_6, 20°C) δ_{Al} 102. MS (EI): 418 (8 %) (M-Cl)$^+$; MS (CI-NH_3) 455.1 (1 %) (M)$^-$. (for $L^{NHC}{\cdot}GaCl_3$) ^{1}H NMR (500 MHz, C_6D_6, 20°C): δ_H 1.29 (quin, $^3J_{HH}$ = 6.0 Hz, 2H, CH_2), 2.08 (s, 6H, *para*-CH_3 of Mes), 2.25 (s, 12H, *ortho*-CH_3 of Mes), 2.52 (t, $^3J_{HH}$ = 6.0 Hz, 4H, NCH_2), 6.77 (s, 4H, *meta*-CH of Mes). ^{13}C NMR (126 MHz, C_6D_6, 20°C): δ_c 18.9 (*ortho*-CH_3 of Mes), 20.1 (CH_2), 21.4 (*para*-CH_3 of Mes), 49.1 (NCH_2), 130.4 (*meta*-CH of Mes), 136.1 (*para*-C of Mes), 139.3 (*ortho*-C of Mes). MS (EI): 461 (100 %) (M-HCl)$^+$; MS (CI-NH_3) 496 (67 %) (M-H)$^-$.

Crystallographic data: (for $L^{NHC}{\cdot}BBr_3$) $C_{22}H_{28}Br_3BN_2$, M_r = 571.00, monoclinic, P 2$_1$/n, a = 8.2731(1), b = 16.7816(2), c = 16.7028(3) Å, β = 92.028(1)°, V = 2317.5(1) Å^3, Z = 4, ρ_c = 1.636 Mg m^{-3}, T = 150 K, λ = 0.71073 Å, 16415 reflections collected, 5207 independent [R(int) = 0.0003], which were used in calculations. R_1 = 0.0498, wR_2 = 0.0838 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0334, wR_2 = 0.071 for all unique reflections. Max. and min. residual electron densities 0.88 and -0.89 e Å^{-3}. CCDC reference: 839366. (for $L^{NHC}{\cdot}AlCl_3$) $C_{22}H_{28}Cl_3AlN_2$, M_r = 453.82, monoclinic, P 2$_1$/n, a = 9.374(2), b = 16.2628(4), c = 15.8953(3) Å, β = 106.356(1)°, V = 2318.5(1) Å^3, Z = 4, ρ_c = 1.300Mg m^{-3}, T = 150 K, λ = 0.71073 Å, 10229 reflections collected, 5285 independent [R(int) = 0.142],which were used in calculations. R_1 = 0.0816, wR_2 = 0.1590 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0527, wR_2 = 0.1440 for all unique reflections. Max. and min. residual electron densities 0.68 and -0.53 e Å^{-3}. CCDC reference: 839368. (for $L^{NHC}{\cdot}GaCl_3$) $C_{22}H_{28}Cl_3GaN_2$, M_r = 496.56, monoclinic, P 2$_1$/n, a = 9.3709(1), b = 16.2052(2), c = 15.8875(3) Å, β = 106.271(1)°, V = 2316.0(1) Å^3, Z = 4, ρ_c = 1.424 Mg m^{-3}, T = 150 K, λ = 0.71073 Å, 30498 reflections collected, 5271 independent [R(int) = 0.0004],which were used in calculations. R_1 = 0.0795, wR_2 = 0.1220 for observed unique reflections [$F^2 > 2\sigma(F^2)$] and R_1 = 0.0402, wR_2 = 0.0846 for all unique reflections. Max. and min. residual electron densities 1.16 and -1.08 e Å^{-3}. CCDC reference: 839369.

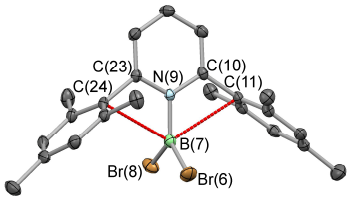
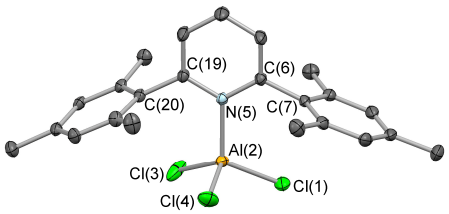


Figure S1: Molecular structure of the cationic component of $[L^{py}{\cdot}BBr_2][AlBr_4]$. Hydrogen atoms omitted for clarity and thermal ellipsoids set at the 40 % probability level. Key bond bond lengths [Å] and angles [°]: Br(6)-B(7) 1.872(4), B(7)-Br(8) 1.880(3), B(7)-N(9) 1.528(4), B(7)···C(11) 2.786(5), B(7)···C(24) 2.754(5), Br(6)-B(7)-Br(8) 120.4(2), Br(6)-B(7)-N(9) 121.3(2), Br(8)-B(7)-N(9) 118.3(2).



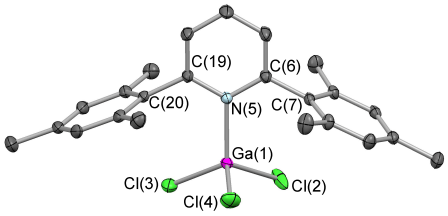


Figure S2: Molecular structures of (upper) $L^{py}{\cdot}AlCl_3$ and (lower) $L^{py}{\cdot}GaCl_3$. Hydrogen atoms omitted for clarity and thermal ellipsoids set at the 40 % probability level. Key bond bond lengths [Å] and angles [°]: (for $L^{py}{\cdot}AlCl_3$) Cl(1)-Al(2) 2.124(1), Al(2)-Cl(3) 2.106(1), Al(2)-Cl(4) 2.108(1), Al(2)-N(5) 2.009(2), Cl(1)-Al(2)-Cl(3) 102.7(1), Cl(1)-Al(2)-Cl(4) 108.4(1), Cl(3)-Al(2)-Cl(4) 112.9(1), Cl(1)-Al(2)-N(5) 116.3(1), Cl(3)-Al(2)-N(5) 112.5(1), Cl(4)-Al(2)-N(5) 104.3(1); (for $L^{py}{\cdot}GaCl_3$) Ga(1)-Cl(2) 2.164(1), Ga(1)-Cl(3) 2.146(1), Ga(1)-Cl(4) 2.149(1), Ga(1)-N(5) 2.043(2), Cl(2)-Ga(1)-Cl(3) 102.0(1), Cl(2)-Ga(1)-Cl(4) 108.6(1), Cl(3)-Ga(1)-Cl(4) 112.2(1), Cl(2)-Ga(1)-N(5) 116.5(1), Cl(3)-Ga(1)-N(5) 113.6(1), Cl(4)-Ga(1)-N(5) 104.3(1).

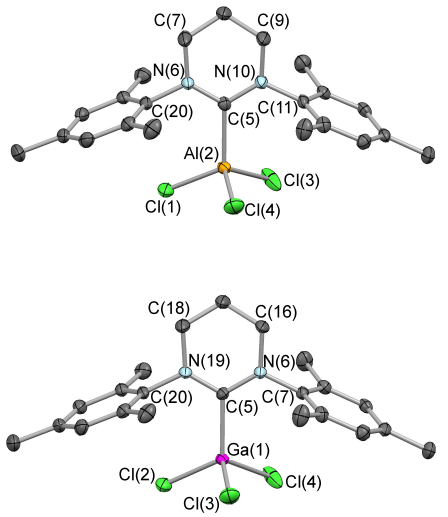


Figure S3: Molecular structures of (upper) $L^{NHC}{\cdot}AlCl_3$ and (lower) $L^{NHC}{\cdot}GaCl_3$. Hydrogen atoms omitted for clarity and thermal ellipsoids set at the 40 % probability level. Key bond bond lengths [Å] and angles [°]: (for $L^{NHC}{\cdot}AlCl_3$) Cl(1)-Al(2) 2.147(1), Al(2)-Cl(3) 2.119(1), Al(2)-Cl(4) 2.130(1), Al(2)-C(5) 2.077(2), Cl(1)-Al(2)-Cl(3) 103.4(1), Cl(1)-Al(2)-Cl(4) 107.2(1), Cl(3)-Al(2)-Cl(4) 111.6(1), Cl(1)-Al(2)-C(5) 116.6(1), Cl(3)-Al(2)-C(5) 112.5(1), Cl(4)-Al(2)-C(5) 105.7(1); (for $L^{NHC}{\cdot}GaCl_3$) Ga(1)-Cl(2) 2.191(1), Ga(1)-Cl(3) 2.178(1), Ga(1)-Cl(4) 2.166(2), Ga(1)-C(5) 2.065(3), Cl(2)-Ga(2)-Cl(3) 105.6(1), Cl(2)-Ga(1)-Cl(4) 102.0(1), Cl(3)-Ga(1)-Cl(4) 109.5(1), Cl(2)-Ga(1)-C(5) 117.9(1), Cl(3)-Ga(1)-C(5) 107.0(1), Cl(4)-Ga(1)-C(5) 114.3(1).

Details of DFT calculations

Geometry optimizations on the molecules L^{py}, $[L^{py}{\cdot}BBr_2]^+$, L^{NHC} and $[L^{NHC}{\cdot}BBr_2]^+$, and single point calculations on L^{py} and L^{NHC} (geometries obtained from the optimized $[L^{py}{\cdot}BBr_2]^+$ and $[L^{NHC}{\cdot}BBr_2]^+$ structures with the $[BBr_2]^+$ fragment removed) were performed using the Vosko-Wilk-Nusair local density approximation with exchange from Becke[s7] and correlation corrections from either Perdew[s8] or Lee-Yang-Parr,[s9] respectively giving BP or BLYP. Slater-type orbitals (STOs)[s10] were used for the triple zeta basis set with an additional set of polarization functions (TZP). The large frozen core basis set approximation was applied with no molecular symmetry. The general numerical integration was 6.0. Initial coordinates of compounds used for DFT calculations were obtained directly from the X-ray crystal structures. The DFT calculations were performed using the Amsterdam Density Functional (ADF) Package Software 2010.[s11] The run files corresponding to the geometry optimizations are provided below.

References for Supporting Information

s1 (a) E. Bosch and C. L. Barnes, *Inorg. Chem.*, 2001, **40**, 3234.
s2 M. Iglesias, D.J. Beestra, J.C. Knight, L.-L. Ooi, A. Stasch, S. Coles, L. Male, M.B. Hursthouse, K.J. Cavell, A. Dervisi and I.A. Fallis, *Organometallics*, 2008, **27**, 3279-3289.
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s5 L. Palatinus and G. Chapuis, *J. Appl. Cryst.*, 1997, **40**, 786-790.
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s11 (a) G. te Velde, F. M. Bickelhaupt, S. J. A. van Gisbergen, C. Fonseca Guerra, E. J. Baerends, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931-967. (b) C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Acc.*, 1998, **99**, 391-403. (c) E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo and A.L. Yakovlev, ADF2010, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

ADF Run Files

Complete output for all calculations herein provided upon request. Below are run files for the geometry optimization and single point calculations presented.

Calculations done at GGA:BP level:

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4 C      -8.848260000000     7.150280000000    14.457100000000
5 N      -7.924240000000     6.671460000000    13.612000000000
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9 C      -7.691640000000     2.999360000000    12.937600000000
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SAVE  TAPE21 TAPE13

INTEGRATION 6

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44 H	1.831720000000	8.039350000000	11.097600000000
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GGA Becke Perdew
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SAVE  TAPE21 TAPE13

INTEGRATION 6

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4 C      2.490000000000     7.899340000000    12.945400000000
5 C      3.146730000000     8.952870000000    12.077000000000
6 C      3.195080000000     7.410850000000    14.053900000000
7 C      2.666320000000     6.428330000000    14.896200000000
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11 C     3.428900000000     5.946760000000    16.108800000000
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13 C    -0.662066000000     9.688810000000    10.310800000000
14 C    -0.981514000000     8.780970000000     9.303380000000
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core Large
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XC
GGA Becke Perdew
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GEOMETRY
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SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

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# ==============================
# LPy·BBr2+ Geometry Optimization
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 Br      1.491040000000     -0.738571000000     12.341600000000
2 N       0.000000000000     -0.000000000000      9.843540000000
3 C      -0.536407000000     -1.082190000000      9.175410000000
4 C      -0.535615000000     -1.076360000000      7.782630000000
5 C       0.000000000000     -0.000000000000      7.078830000000
6 C      -1.102280000000     -2.219910000000      9.953980000000
7 C      -2.490220000000     -2.240940000000     10.245200000000
8 C      -3.422480000000     -1.141310000000      9.794260000000
9 C      -3.009550000000     -3.354180000000     10.910400000000
10 C     -2.212810000000     -4.451420000000     11.265600000000
11 C     -2.803880000000     -5.626480000000     12.001400000000
12 C     -0.858102000000     -4.423840000000     10.914100000000
13 C     -0.282528000000     -3.337630000000     10.246700000000
14 C      1.158830000000     -3.417490000000      9.802530000000
15 B      0.000000000000     -0.000000000000     11.385600000000
16 H     -0.963913000000     -1.936460000000      7.268600000000
17 H      0.000000000000     -0.000000000000      5.988560000000
18 H     -4.346140000000     -1.147510000000     10.385300000000
19 H     -2.977420000000     -0.141726000000      9.881290000000
20 H     -3.709470000000     -1.283130000000      8.739930000000
21 H     -4.075640000000     -3.367680000000     11.150300000000
22 H     -2.151510000000     -6.506040000000     11.947400000000
23 H     -2.949780000000     -5.382830000000     13.064900000000
24 H     -3.787190000000     -5.897770000000     11.594400000000
25 H     -0.226311000000     -5.281820000000     11.155800000000
26 H      1.706920000000     -4.162830000000     10.391000000000
27 H      1.688270000000     -2.460680000000      9.899010000000
28 H      1.224210000000     -3.723900000000      8.746220000000
29 Br    -1.491040000000      0.738571000000     12.341600000000
30 C      0.536407000000      1.082190000000      9.175410000000
31 C      0.535615000000      1.076360000000      7.782630000000
```

32 C	1.102280000000	2.219910000000	9.953980000000
33 C	2.490220000000	2.240940000000	10.245200000000
34 C	3.422480000000	1.141310000000	9.794260000000
35 C	3.009550000000	3.354180000000	10.910400000000
36 C	2.212810000000	4.451420000000	11.265600000000
37 C	2.803880000000	5.626480000000	12.001400000000
38 C	0.858102000000	4.423840000000	10.914100000000
39 C	0.282528000000	3.337630000000	10.246700000000
40 C	-1.158830000000	3.417490000000	9.802530000000
41 H	0.963913000000	1.936460000000	7.268600000000
42 H	4.346140000000	1.147510000000	10.385300000000
43 H	2.977420000000	0.141726000000	9.881290000000
44 H	3.709470000000	1.283130000000	8.739930000000
45 H	4.075640000000	3.367680000000	11.150300000000
46 H	2.151510000000	6.506040000000	11.947400000000
47 H	2.949780000000	5.382830000000	13.064900000000
48 H	3.787190000000	5.897770000000	11.594400000000
49 H	0.226311000000	5.281820000000	11.155800000000
50 H	-1.706920000000	4.162830000000	10.391000000000
51 H	-1.688270000000	2.460680000000	9.899010000000
52 H	-1.224210000000	3.723900000000	8.746220000000

END

GUIBONDS
1 1 15 3
2 2 3 1.5
3 2 30 1.0
4 2 15 1.0
5 3 4 1.5
6 3 6 1.0
7 4 16 1.0
8 4 5 1.5
9 5 17 1.0
10 5 31 1.5
11 6 7 1.5
12 6 13 1.5
13 7 8 1.0
14 7 9 1.5
15 8 18 1.0
16 8 20 1.0
17 8 19 1.0
18 9 10 1.5
19 9 21 1.0
20 10 11 1.0
21 10 12 1.5
22 11 22 1.0
23 11 24 1.0
24 11 23 1.0
25 12 13 1.5
26 12 25 1.0
27 13 14 1.0
28 14 26 1.0
29 14 28 1.0
30 14 27 1.0
31 15 29 1.5
32 30 31 1.5
33 30 32 1.5
34 31 41 1.0
35 32 39 1.5
36 32 33 1.5
37 33 34 1.0
38 33 35 1.5
39 34 43 1.0
40 34 44 1.0
41 34 42 1.0
42 35 36 1.5
43 35 45 1.0
44 36 38 1.5
45 36 37 1.0
46 37 46 1.0
47 37 48 1.0
48 37 47 1.0
49 38 39 1.5
50 38 49 1.0
51 39 40 1.0
52 40 50 1.0
53 40 51 1.0
54 40 52 1.0
END

```
CHARGE 1.0

BASIS
type TZP
core Large
createoutput None
END

XC
GGA Becke Perdew
END
```

```
GEOMETRY
   optim Delocalized
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# LNHC·BBr2+ - BBr2+ Single Point
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 H    -12.333000000000    10.131000000000    19.839400000000
2 H    -12.564600000000    11.534000000000    18.772300000000
3 H    -13.566200000000    10.092300000000    18.560100000000
4 C     -8.847440000000     7.148920000000    14.455900000000
5 N     -7.923160000000     6.670360000000    13.610900000000
6 C     -8.089060000000     5.368540000000    12.974300000000
7 C     -7.553730000000     4.225430000000    13.600000000000
8 C     -6.800540000000     4.282620000000    14.907300000000
9 C     -7.688420000000     2.998560000000    12.935500000000
10 C     -8.293190000000     2.892830000000    11.679100000000
11 C     -8.414750000000     1.563010000000    10.978800000000
12 C     -8.766800000000     4.065520000000    11.069800000000
13 C     -8.665160000000     5.315590000000    11.684000000000
14 C     -9.122770000000     6.557060000000    10.957100000000
15 C     -6.676830000000     7.414420000000    13.307900000000
16 C     -6.888990000000     8.910720000000    13.493700000000
17 C     -7.497970000000     9.176860000000    14.863700000000
18 N     -8.695630000000     8.328540000000    15.074600000000
19 C     -9.695400000000     8.816560000000    16.017800000000
20 C    -10.700800000000     9.691400000000    15.544200000000
21 C    -10.776800000000    10.120100000000    14.098700000000
22 C    -11.615700000000    10.191500000000    16.472900000000
23 C    -11.542400000000     9.875630000000    17.838900000000
24 C    -10.503900000000     9.044800000000    18.270300000000
25 C     -9.553320000000     8.514840000000    17.386500000000
26 C     -8.401690000000     7.707040000000    17.934900000000
27 C    -12.551600000000    10.435200000000    18.809300000000
28 H     -6.915000000000     3.342830000000    15.460700000000
29 H     -7.137560000000     5.097520000000    15.558200000000
```

30 H	-5.722920000000	4.420300000000	14.724700000000
31 H	-7.295600000000	2.099640000000	13.416100000000
32 H	-9.458140000000	1.357340000000	10.701400000000
33 H	-8.059180000000	0.740480000000	11.610100000000
34 H	-7.826500000000	1.556610000000	10.049200000000
35 H	-9.224360000000	4.006480000000	10.079300000000
36 H	-9.659060000000	6.287860000000	10.040100000000
37 H	-9.792960000000	7.175390000000	11.568700000000
38 H	-8.268240000000	7.186130000000	10.661400000000
39 H	-5.876960000000	7.038780000000	13.965600000000
40 H	-6.398930000000	7.167820000000	12.275600000000
41 H	-5.929490000000	9.436040000000	13.405000000000
42 H	-7.553210000000	9.295960000000	12.706800000000
43 H	-7.820940000000	10.220000000000	14.969900000000
44 H	-6.776570000000	8.969330000000	15.669900000000
45 H	-11.705200000000	10.671500000000	13.911200000000
46 H	-9.942510000000	10.789600000000	13.835300000000
47 H	-10.747500000000	9.267180000000	13.408100000000
48 H	-12.407200000000	10.856700000000	16.119400000000
49 H	-10.417800000000	8.805750000000	19.332800000000
50 H	-8.715590000000	7.134780000000	18.816100000000
51 H	-7.584920000000	8.372500000000	18.256400000000
52 H	-7.990960000000	6.999760000000	17.205400000000

END

GUIBONDS

1 27 1 1.0
2 27 2 1.0
3 27 3 1.0
4 4 18 1.0
5 4 5 1.5
6 5 6 1.0
7 5 15 1.0
8 6 13 1.5
9 6 7 1.5
10 7 9 1.5
11 7 8 1.0
12 8 28 1.0
13 8 29 1.0
14 8 30 1.0
15 9 10 1.5
16 9 31 1.0
17 10 11 1.0
18 10 12 1.5
19 11 34 1.0
20 11 32 1.0
21 11 33 1.0
22 12 35 1.0
23 12 13 1.5
24 13 14 1.0
25 14 36 1.0
26 14 37 1.0
27 14 38 1.0
28 15 40 1.0
29 15 39 1.0
30 15 16 1.0
31 16 42 1.0
32 16 17 1.0
33 16 41 1.0
34 17 18 1.0
35 17 43 1.0
36 17 44 1.0
37 18 19 1.0
38 19 20 1.5
39 19 25 1.5
40 20 21 1.0
41 20 22 1.5
42 21 47 1.0
43 21 45 1.0
44 21 46 1.0
45 22 23 1.5
46 22 48 1.0
47 23 24 1.5
48 23 27 1.0
49 24 49 1.0
50 24 25 1.5
51 25 26 1.0

```
52 26 52 1.0
53 26 50 1.0
54 26 51 1.0
END

BASIS
type TZP
core Large
createoutput None
END

XC
GGA Becke Perdew
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# LPy·BBr2+ - BBr2+ Single Point
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 H     -1.706370000000     4.164230000000    10.386900000000
2 N      0.000000000000     0.000000000000     9.847210000000
3 C     -0.537394000000    -1.081550000000     9.179170000000
4 C     -0.534722000000    -1.076810000000     7.786340000000
5 C      0.000000000000     0.000000000000     7.082440000000
6 C     -1.102750000000    -2.219640000000     9.957350000000
7 C     -2.490830000000    -2.241470000000    10.247400000000
8 C     -3.421880000000    -1.138910000000     9.800670000000
9 C     -3.011230000000    -3.357790000000    10.906500000000
10 C    -2.215460000000    -4.457830000000    11.255300000000
11 C    -2.808360000000    -5.637950000000    11.981700000000
12 C    -0.859784000000    -4.427800000000    10.907700000000
13 C    -0.282943000000    -3.337800000000    10.247800000000
14 C     1.158420000000    -3.415520000000     9.802600000000
15 H    -1.687990000000     2.459310000000     9.904070000000
16 H    -0.962071000000    -1.937230000000     7.272040000000
17 H     0.000000000000     0.000000000000     5.992200000000
18 H    -4.346980000000    -1.148630000000    10.389300000000
19 H    -2.976560000000    -0.140053000000     9.894800000000
20 H    -3.705930000000    -1.274430000000     8.744680000000
21 H    -4.078310000000    -3.373870000000    11.141800000000
22 H    -2.156510000000    -6.517550000000    11.921700000000
23 H    -2.955030000000    -5.402120000000    13.046800000000
24 H    -3.791340000000    -5.905290000000    11.571400000000
25 H    -0.228869000000    -5.287780000000    11.144400000000
26 H     1.706370000000    -4.164230000000    10.386900000000
27 H     1.687990000000    -2.459310000000     9.904070000000
28 H     1.223050000000    -3.716370000000     8.744570000000
29 H    -1.223050000000     3.716370000000     8.744570000000
30 C     0.537394000000     1.081550000000     9.179170000000
```

31 C	0.534722000000	1.076810000000	7.786340000000
32 C	1.102750000000	2.219640000000	9.957350000000
33 C	2.490830000000	2.241470000000	10.247400000000
34 C	3.421880000000	1.138910000000	9.800670000000
35 C	3.011230000000	3.357790000000	10.906500000000
36 C	2.215460000000	4.457830000000	11.255300000000
37 C	2.808360000000	5.637950000000	11.981700000000
38 C	0.859784000000	4.427800000000	10.907700000000
39 C	0.282943000000	3.337800000000	10.247800000000
40 C	-1.158420000000	3.415520000000	9.802600000000
41 H	0.962071000000	1.937230000000	7.272040000000
42 H	4.346980000000	1.148630000000	10.389300000000
43 H	2.976560000000	0.140053000000	9.894800000000
44 H	3.705930000000	1.274430000000	8.744680000000
45 H	4.078310000000	3.373870000000	11.141800000000
46 H	2.156510000000	6.517550000000	11.921700000000
47 H	2.955030000000	5.402120000000	13.046800000000
48 H	3.791340000000	5.905290000000	11.571400000000
49 H	0.228869000000	5.287780000000	11.144400000000

END

GUIBONDS
1 40 15 1.0
2 2 3 1.5
3 2 30 1.0
4 40 1 1.0
5 3 4 1.5
6 3 6 1.0
7 4 16 1.0
8 4 5 1.5
9 5 17 1.0
10 5 31 1.5
11 6 7 1.5
12 6 13 1.5
13 7 8 1.0
14 7 9 1.5
15 8 18 1.0
16 8 20 1.0
17 8 19 1.0
18 9 10 1.5
19 9 21 1.0
20 10 11 1.0
21 10 12 1.5
22 11 22 1.0
23 11 24 1.0
24 11 23 1.0
25 12 13 1.5
26 12 25 1.0
27 13 14 1.0
28 14 26 1.0
29 14 28 1.0
30 14 27 1.0
31 40 29 1.0
32 30 31 1.5
33 30 32 1.5
34 31 41 1.0
35 32 39 1.5
36 32 33 1.5
37 33 34 1.0
38 33 35 1.5
39 34 43 1.0
40 34 44 1.0
41 34 42 1.0
42 35 36 1.5
43 35 45 1.0
44 36 38 1.5
45 36 37 1.0
46 37 46 1.0
47 37 48 1.0
48 37 47 1.0
49 38 39 1.5
50 38 49 1.0
51 39 40 1.0
END

BASIS
type TZP
core Large
createoutput None
END

XC	INTEGRATION 6
GGA Becke Perdew	
END	NOPRINT LOGFILE
SAVE TAPE21 TAPE13	eor

Calculations done at GGA:BLYP level:

```
#! /bin/sh

# ==============================
# LNHC·BBr2+ Geometry Optimization
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 Br    -10.208500000000     4.975260000000    16.196700000000
2 B     -10.188100000000     6.267170000000    14.749100000000
3 Br    -11.780600000000     6.492280000000    13.661600000000
4 C      -8.860920000000     7.144050000000    14.454000000000
5 N      -7.931090000000     6.663980000000    13.606100000000
6 C      -8.078370000000     5.351840000000    12.958800000000
7 C      -7.525400000000     4.210640000000    13.581400000000
8 C      -6.767450000000     4.264750000000    14.896600000000
9 C      -7.637690000000     2.981870000000    12.908500000000
10 C     -8.236060000000     2.871090000000    11.646700000000
11 C     -8.334990000000     1.535850000000    10.935700000000
12 C     -8.724640000000     4.041850000000    11.039300000000
13 C     -8.645930000000     5.294120000000    11.660100000000
14 C     -9.116200000000     6.534090000000    10.920100000000
15 C     -6.671680000000     7.413390000000    13.304600000000
16 C     -6.878310000000     8.917180000000    13.490100000000
17 C     -7.497540000000     9.184000000000    14.862600000000
18 N     -8.707950000000     8.330270000000    15.073100000000
19 C     -9.702430000000     8.837050000000    16.030400000000
20 C    -10.705000000000     9.725170000000    15.562700000000
21 C    -10.796000000000    10.160400000000    14.110500000000
22 C    -11.605300000000    10.242700000000    16.501100000000
23 C    -11.521700000000     9.934170000000    17.871000000000
24 C    -10.485800000000     9.092840000000    18.296400000000
25 C     -9.548830000000     8.544310000000    17.403700000000
26 C     -8.393820000000     7.728480000000    17.958500000000
27 C    -12.519700000000    10.515000000000    18.853200000000
28 H     -6.861580000000     3.315000000000    15.433400000000
29 H     -7.117870000000     5.059360000000    15.561200000000
30 H     -5.694900000000     4.427190000000    14.714100000000
31 H     -7.232670000000     2.089400000000    13.386000000000
32 H     -9.373560000000     1.313890000000    10.658300000000
33 H     -7.966230000000     0.717753000000    11.562700000000
```

34 H	-7.746730000000	1.544010000000	10.008000000000
35 H	-9.172110000000	3.980180000000	10.046900000000
36 H	-9.623270000000	6.252910000000	9.992040000000
37 H	-9.813310000000	7.136710000000	11.512300000000
38 H	-8.269890000000	7.180260000000	10.644800000000
39 H	-5.878600000000	7.036980000000	13.965800000000
40 H	-6.391330000000	7.166690000000	12.276100000000
41 H	-5.915390000000	9.435150000000	13.411900000000
42 H	-7.531500000000	9.308090000000	12.699600000000
43 H	-7.818420000000	10.224900000000	14.966700000000
44 H	-6.781590000000	8.973590000000	15.669500000000
45 H	-11.716500000000	10.727300000000	13.940800000000
46 H	-9.956180000000	10.816000000000	13.837100000000
47 H	-10.793000000000	9.312530000000	13.417200000000
48 H	-12.389700000000	10.915900000000	16.153700000000
49 H	-10.389700000000	8.860870000000	19.357400000000
50 H	-8.706220000000	7.178680000000	18.852600000000
51 H	-7.568240000000	8.390410000000	18.258800000000
52 H	-7.997740000000	7.003090000000	17.242700000000
53 H	-12.292300000000	10.216900000000	19.881700000000
54 H	-12.521200000000	11.612100000000	18.807800000000
55 H	-13.538900000000	10.180000000000	18.618900000000

END

GUIBONDS

1 1 2 3
2 2 3 1.5
3 2 4 1.5
4 4 18 1.0
5 4 5 1.5
6 5 6 1.0
7 5 15 1.0
8 6 13 1.5
9 6 7 1.5
10 7 9 1.5
11 7 8 1.0
12 8 28 1.0
13 8 29 1.0
14 8 30 1.0
15 9 10 1.5
16 9 31 1.0
17 10 11 1.0
18 10 12 1.5
19 11 34 1.0
20 11 32 1.0
21 11 33 1.0
22 12 35 1.0
23 12 13 1.5
24 13 14 1.0
25 14 36 1.0
26 14 37 1.0
27 14 38 1.0
28 15 40 1.0
29 15 39 1.0
30 15 16 1.0
31 16 42 1.0
32 16 17 1.0
33 16 41 1.0
34 17 18 1.0
35 17 43 1.0
36 17 44 1.0
37 18 19 1.0
38 19 20 1.5
39 19 25 1.5
40 20 21 1.0
41 20 22 1.5
42 21 47 1.0
43 21 45 1.0
44 21 46 1.0
45 22 23 1.5
46 22 48 1.0
47 23 24 1.5
48 23 27 1.0
49 24 49 1.0
50 24 25 1.5
51 25 26 1.0
52 26 52 1.0
53 26 50 1.0

```
54 26 51 1.0
55 27 55 1.0
56 27 53 1.0
57 27 54 1.0
END

CHARGE 1.0

BASIS
type TZP
core Large
createoutput None
END

XC
GGA BLYP
END

GEOMETRY
   optim Delocalized
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# Free LNHC Geometry Optimization
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 C      4.816710000000     9.480180000000    10.650600000000
2 N      5.437320000000     9.002630000000     9.541810000000
3 C      5.674860000000     9.935300000000     8.447940000000
4 C      6.795490000000    10.791800000000     8.496660000000
5 C      7.024180000000    11.662000000000     7.417870000000
6 C      6.175050000000    11.703600000000     6.302510000000
7 C      5.066480000000    10.844100000000     6.287350000000
8 C      4.796020000000     9.958190000000     7.343430000000
9 C      3.561580000000     9.075340000000     7.292580000000
10 C     6.423060000000    12.678300000000     5.163520000000
11 C     7.721210000000    10.806900000000     9.698040000000
12 C     5.929740000000     7.601080000000     9.336740000000
13 C     6.167290000000     6.929400000000    10.695100000000
14 C     4.937710000000     7.124610000000    11.590600000000
15 N     4.584860000000     8.579200000000    11.638800000000
16 C     3.870960000000     9.036640000000    12.822600000000
17 C     2.465080000000     9.154970000000    12.788400000000
18 C     1.683380000000     8.880440000000    11.517500000000
19 C     1.798130000000     9.574600000000    13.950900000000
20 C     2.485030000000     9.873910000000    15.137000000000
21 C     3.883090000000     9.761070000000    15.133700000000
22 C     4.593710000000     9.349500000000    13.993900000000
23 C     6.110500000000     9.299210000000    14.021500000000
24 C     1.735270000000    10.291400000000    16.390800000000
25 H     7.889460000000    12.326100000000     7.455190000000
26 H     4.384530000000    10.866500000000     5.435230000000
```

27 H	2.901390000000	9.383660000000	6.474160000000
28 H	2.999900000000	9.132890000000	8.232470000000
29 H	3.818010000000	8.018950000000	7.128840000000
30 H	6.161050000000	12.237500000000	4.193470000000
31 H	5.815650000000	13.587600000000	5.283890000000
32 H	7.474040000000	12.988400000000	5.124190000000
33 H	8.543900000000	11.514300000000	9.544670000000
34 H	7.168380000000	11.097300000000	10.600800000000
35 H	8.155590000000	9.816990000000	9.893120000000
36 H	6.855750000000	7.641910000000	8.749400000000
37 H	5.193840000000	7.026870000000	8.752020000000
38 H	7.045090000000	7.377770000000	11.180300000000
39 H	6.372770000000	5.860080000000	10.556400000000
40 H	5.130980000000	6.775800000000	12.611800000000
41 H	4.083070000000	6.546000000000	11.203400000000
42 H	0.608909000000	9.011050000000	11.687800000000
43 H	2.000780000000	9.565370000000	10.720800000000
44 H	1.846740000000	7.858520000000	11.149800000000
45 H	0.711648000000	9.674920000000	13.923200000000
46 H	4.441690000000	10.013800000000	16.036700000000
47 H	6.490610000000	9.645820000000	14.988900000000
48 H	6.533740000000	9.935120000000	13.233600000000
49 H	6.496820000000	8.283630000000	13.857000000000
50 H	2.358570000000	10.918600000000	17.039600000000
51 H	0.826170000000	10.853700000000	16.144700000000
52 H	1.428400000000	9.413600000000	16.979000000000

END

GUIBONDS

1 1 15 1.5
2 1 2 1.5
3 2 12 1.0
4 2 3 1.0
5 3 8 1.5
6 3 4 1.5
7 4 11 1.0
8 4 5 1.5
9 5 6 1.5
10 5 25 1.0
11 6 7 1.5
12 6 10 1.0
13 7 8 1.5
14 7 26 1.0
15 8 9 1.0
16 9 27 1.0
17 9 28 1.0
18 9 29 1.0
19 10 30 1.0
20 10 31 1.0
21 10 32 1.0
22 11 34 1.0
23 11 35 1.0
24 11 33 1.0
25 12 37 1.0
26 12 36 1.0
27 12 13 1.0
28 13 14 1.0
29 13 39 1.0
30 13 38 1.0
31 14 41 1.0
32 14 15 1.0
33 14 40 1.0
34 15 16 1.0
35 16 17 1.5
36 16 22 1.5
37 17 18 1.0
38 17 19 1.5
39 18 42 1.0
40 18 44 1.0
41 18 43 1.0
42 19 45 1.0
43 19 20 1.5
44 20 24 1.0
45 20 21 1.5

```
46 21 22 1.5
47 21 46 1.0
48 22 23 1.0
49 23 48 1.0
50 23 49 1.0
51 23 47 1.0
52 24 51 1.0
53 24 52 1.0
54 24 50 1.0
END

BASIS
type TZP
core Large
createoutput None
END
```

```
XC
GGA BLYP
END

GEOMETRY
   optim Delocalized
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# Free LPy Geometry Optimization
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 N      0.107191000000     7.005650000000    10.516900000000
2 C      0.425827000000     7.889810000000    11.492000000000
3 C      1.199970000000     7.371880000000    12.677400000000
4 C      2.525130000000     7.815390000000    12.912400000000
5 C      3.235190000000     8.780490000000    11.971900000000
6 C      3.219190000000     7.331730000000    14.033900000000
7 C      2.639020000000     6.430020000000    14.936300000000
8 C      1.329890000000     5.998310000000    14.679600000000
9 C      0.599930000000     6.445680000000    13.567000000000
10 C    -0.815148000000     5.933800000000    13.352200000000
11 C     3.395550000000     5.954840000000    16.165100000000
12 C     0.047454000000     9.243710000000    11.422100000000
13 C    -0.656794000000     9.694280000000    10.303600000000
14 C    -0.974649000000     8.784420000000     9.293210000000
15 C    -0.586115000000     7.439250000000     9.437460000000
16 C    -0.921757000000     6.427790000000     8.371160000000
17 C     0.114558000000     5.838310000000     7.602450000000
18 C    -0.222069000000     4.927170000000     6.590280000000
19 C    -1.551360000000     4.567490000000     6.320830000000
20 C    -2.557340000000     5.151640000000     7.100390000000
21 C    -2.270320000000     6.077730000000     8.118360000000
22 C    -3.424300000000     6.655360000000     8.927630000000
23 C    -1.881680000000     3.553880000000     5.238420000000
24 C     1.576530000000     6.181750000000     7.837260000000
25 H     4.313640000000     8.779880000000    12.167700000000
```

26 H	2.878560000000	9.812500000000	12.097500000000
27 H	3.078060000000	8.512970000000	10.920000000000
28 H	4.245520000000	7.665090000000	14.198400000000
29 H	0.858843000000	5.289460000000	15.362900000000
30 H	-1.130010000000	5.307160000000	14.194300000000
31 H	-1.531620000000	6.761320000000	13.256800000000
32 H	-0.884532000000	5.343720000000	12.430400000000
33 H	3.059510000000	4.960150000000	16.482100000000
34 H	3.240330000000	6.639630000000	17.012300000000
35 H	4.475270000000	5.907390000000	15.977000000000
36 H	0.302823000000	9.923480000000	12.233300000000
37 H	-0.952650000000	10.739200000000	10.220300000000
38 H	-1.511900000000	9.103670000000	8.401730000000
39 H	0.580322000000	4.488920000000	5.993840000000
40 H	-3.598560000000	4.879690000000	6.918130000000
41 H	-4.330020000000	6.055450000000	8.782040000000
42 H	-3.660690000000	7.685890000000	8.627140000000
43 H	-3.197730000000	6.677920000000	10.000300000000
44 H	-2.935180000000	3.615610000000	4.940820000000
45 H	-1.264670000000	3.708820000000	4.343980000000
46 H	-1.695610000000	2.527850000000	5.588730000000
47 H	2.209740000000	5.710390000000	7.077120000000
48 H	1.746620000000	7.266420000000	7.798370000000
49 H	1.905720000000	5.842690000000	8.827080000000

END

GUIBONDS

1 1 15 1.5	25 12 13 1.5
2 1 2 1.5	26 12 36 1.0
3 2 3 1.5	27 13 14 1.5
4 2 12 1.5	28 13 37 1.0
5 3 9 1.5	29 14 38 1.0
6 3 4 1.5	30 14 15 1.5
7 4 5 1.0	31 15 16 1.0
8 4 6 1.5	32 16 21 1.5
9 5 26 1.0	33 16 17 1.5
10 5 27 1.0	34 17 18 1.5
11 5 25 1.0	35 17 24 1.0
12 6 7 1.5	36 18 19 1.5
13 6 28 1.0	37 18 39 1.0
14 7 8 1.5	38 19 23 1.0
15 7 11 1.0	39 19 20 1.5
16 8 9 1.5	40 20 40 1.0
17 8 29 1.0	41 20 21 1.5
18 9 10 1.0	42 21 22 1.0
19 10 32 1.0	43 22 41 1.0
20 10 30 1.0	44 22 42 1.0
21 10 31 1.0	45 22 43 1.0
22 11 33 1.0	46 23 44 1.0
23 11 34 1.0	47 23 46 1.0
24 11 35 1.0	48 23 45 1.0
	49 24 49 1.0

```
50 24 48 1.0
51 24 47 1.0
END

BASIS
type TZP
core Large
createoutput None
END

XC
GGA BLYP
END
```

```
GEOMETRY
   optim Delocalized
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# LPy·BBr2+ Geometry Optimization
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 Br      1.505900000000     -0.727349000000     12.387300000000
2 N       0.000000000000      0.000000000000      9.868750000000
3 C      -0.541229000000     -1.085720000000      9.191650000000
4 C      -0.537477000000     -1.076790000000      7.795980000000
5 C       0.000000000000      0.000000000000      7.089890000000
6 C      -1.116430000000     -2.241390000000      9.952410000000
7 C      -2.513920000000     -2.276240000000     10.217300000000
8 C      -3.454360000000     -1.169580000000      9.768340000000
9 C      -3.042310000000     -3.407690000000     10.850400000000
10 C     -2.247360000000     -4.512450000000     11.197800000000
11 C     -2.852840000000     -5.712590000000     11.897800000000
12 C     -0.883524000000     -4.471030000000     10.874600000000
13 C     -0.297516000000     -3.366170000000     10.240000000000
14 C      1.158510000000     -3.446460000000      9.811240000000
15 B      0.000000000000      0.000000000000     11.418000000000
16 H     -0.964364000000     -1.933270000000      7.279620000000
17 H      0.000000000000      0.000000000000      6.001670000000
18 H     -4.391000000000     -1.206160000000     10.333900000000
19 H     -3.028150000000     -0.168646000000      9.894030000000
20 H     -3.711040000000     -1.287030000000      8.704860000000
21 H     -4.111260000000     -3.432230000000     11.065400000000
22 H     -2.191790000000     -6.584050000000     11.845600000000
23 H     -3.031840000000     -5.490940000000     12.959400000000
24 H     -3.819020000000     -5.984130000000     11.455400000000
25 H     -0.254981000000     -5.330780000000     11.107800000000
26 H      1.695320000000     -4.192940000000     10.405500000000
27 H      1.689390000000     -2.494350000000      9.913910000000
28 H      1.233920000000     -3.753640000000      8.757340000000
```

29 Br	-1.505900000000	0.727349000000	12.387300000000
30 C	0.541229000000	1.085720000000	9.191650000000
31 C	0.537477000000	1.076790000000	7.795980000000
32 C	1.116430000000	2.241390000000	9.952410000000
33 C	2.513920000000	2.276240000000	10.217300000000
34 C	3.454360000000	1.169580000000	9.768340000000
35 C	3.042310000000	3.407690000000	10.850400000000
36 C	2.247360000000	4.512450000000	11.197800000000
37 C	2.852840000000	5.712590000000	11.897800000000
38 C	0.883524000000	4.471030000000	10.874600000000
39 C	0.297516000000	3.366170000000	10.240000000000
40 C	-1.158510000000	3.446460000000	9.811240000000
41 H	0.964364000000	1.933270000000	7.279620000000
42 H	4.391000000000	1.206160000000	10.333900000000
43 H	3.028150000000	0.168646000000	9.894030000000
44 H	3.711040000000	1.287030000000	8.704860000000
45 H	4.111260000000	3.432230000000	11.065400000000
46 H	2.191790000000	6.584050000000	11.845600000000
47 H	3.031840000000	5.490940000000	12.959400000000
48 H	3.819020000000	5.984130000000	11.455400000000
49 H	0.254981000000	5.330780000000	11.107800000000
50 H	-1.695320000000	4.192940000000	10.405500000000
51 H	-1.689390000000	2.494350000000	9.913910000000
52 H	-1.233920000000	3.753640000000	8.757340000000

END

GUIBONDS

1 1 15 3
2 2 3 1.5
3 2 30 1.0
4 2 15 1.0
5 3 4 1.5
6 3 6 1.0
7 4 16 1.0
8 4 5 1.5
9 5 17 1.0
10 5 31 1.5
11 6 7 1.5
12 6 13 1.5
13 7 8 1.0
14 7 9 1.5
15 8 18 1.0
16 8 20 1.0
17 8 19 1.0
18 9 10 1.5
19 9 21 1.0
20 10 11 1.0
21 10 12 1.5
22 11 22 1.0
23 11 24 1.0
24 11 23 1.0
25 12 13 1.5
26 12 25 1.0
27 13 14 1.0
28 14 26 1.0
29 14 28 1.0
30 14 27 1.0
31 15 29 1.5
32 30 31 1.5
33 30 32 1.5
34 31 41 1.0
35 32 39 1.5
36 32 33 1.5
37 33 34 1.0
38 33 35 1.5
39 34 43 1.0
40 34 44 1.0
41 34 42 1.0
42 35 36 1.5
43 35 45 1.0
44 36 38 1.5
45 36 37 1.0
46 37 46 1.0
47 37 48 1.0
48 37 47 1.0
49 38 39 1.5

```
50 38 49 1.0
51 39 40 1.0
52 40 50 1.0
53 40 51 1.0
54 40 52 1.0
END

CHARGE 1.0

BASIS
type TZP
core Large
createoutput None
END
```

```
XC
GGA BLYP
END

GEOMETRY
   optim Delocalized
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# LNHC·BBr2+ - BBr2+ Single Point
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 H    -12.292600000000    10.212600000000    19.881300000000
2 H    -12.523800000000    11.607600000000    18.807600000000
3 H    -13.539700000000    10.174100000000    18.619100000000
4 C     -8.860540000000     7.143970000000    14.452200000000
5 N     -7.930190000000     6.664080000000    13.604800000000
6 C     -8.076860000000     5.351930000000    12.957400000000
7 C     -7.525630000000     4.210550000000    13.581100000000
8 C     -6.769330000000     4.264590000000    14.897400000000
9 C     -7.638990000000     2.981410000000    12.909100000000
10 C     -8.236180000000     2.870440000000    11.646800000000
11 C     -8.336500000000     1.534740000000    10.936900000000
12 C     -8.722540000000     4.041400000000    11.038000000000
13 C     -8.643130000000     5.293990000000    11.658100000000
14 C     -9.111150000000     6.534000000000    10.916700000000
15 C     -6.670610000000     7.413620000000    13.304200000000
16 C     -6.877390000000     8.917380000000    13.489800000000
17 C     -7.497460000000     9.183840000000    14.862000000000
18 N     -8.707990000000     8.330040000000    15.071600000000
19 C     -9.702800000000     8.836020000000    16.028900000000
20 C    -10.705500000000     9.724380000000    15.561800000000
21 C    -10.796700000000    10.160500000000    14.109900000000
22 C    -11.605900000000    10.241000000000    16.500700000000
23 C    -11.522500000000     9.930970000000    17.870300000000
24 C    -10.486700000000     9.089200000000    18.295000000000
25 C     -9.549700000000     8.541510000000    17.401900000000
26 C     -8.395330000000     7.724140000000    17.955800000000
```

27 C	-12.520800000000	10.510500000000	18.852900000000
28 H	-6.864860000000	3.315120000000	15.434400000000
29 H	-7.119950000000	5.059730000000	15.561200000000
30 H	-5.696410000000	4.426110000000	14.716100000000
31 H	-7.236790000000	2.088570000000	13.388400000000
32 H	-9.375370000000	1.313490000000	10.660000000000
33 H	-7.968370000000	0.716799000000	11.564500000000
34 H	-7.748480000000	1.541620000000	10.009000000000
35 H	-9.168940000000	3.979590000000	10.045000000000
36 H	-9.617250000000	6.252800000000	9.988110000000
37 H	-9.808470000000	7.137680000000	11.507600000000
38 H	-8.263820000000	7.179190000000	10.642100000000
39 H	-5.877900000000	7.037130000000	13.965800000000
40 H	-6.389620000000	7.167140000000	12.275800000000
41 H	-5.914440000000	9.435400000000	13.412300000000
42 H	-7.530160000000	9.308430000000	12.699100000000
43 H	-7.818360000000	10.224700000000	14.966300000000
44 H	-6.781970000000	8.973160000000	15.669300000000
45 H	-11.716800000000	10.728200000000	13.940800000000
46 H	-9.956490000000	10.815600000000	13.836400000000
47 H	-10.794700000000	9.313050000000	13.416100000000
48 H	-12.390500000000	10.914300000000	16.153900000000
49 H	-10.391100000000	8.855720000000	19.355700000000
50 H	-8.707710000000	7.174810000000	18.850200000000
51 H	-7.568540000000	8.384930000000	18.255400000000
52 H	-8.000880000000	6.998140000000	17.239600000000

END

GUIBONDS

1 27 1 1.0
2 27 2 1.0
3 27 3 1.0
4 4 18 1.0
5 4 5 1.5
6 5 6 1.0
7 5 15 1.0
8 6 13 1.5
9 6 7 1.5
10 7 9 1.5
11 7 8 1.0
12 8 28 1.0
13 8 29 1.0
14 8 30 1.0
15 9 10 1.5
16 9 31 1.0
17 10 11 1.0
18 10 12 1.5
19 11 34 1.0
20 11 32 1.0
21 11 33 1.0
22 12 35 1.0
23 12 13 1.5
24 13 14 1.0
25 14 36 1.0
26 14 37 1.0
27 14 38 1.0
28 15 40 1.0
29 15 39 1.0
30 15 16 1.0
31 16 42 1.0
32 16 17 1.0
33 16 41 1.0
34 17 18 1.0
35 17 43 1.0
36 17 44 1.0
37 18 19 1.0
38 19 20 1.5
39 19 25 1.5
40 20 21 1.0
41 20 22 1.5
42 21 47 1.0
43 21 45 1.0
44 21 46 1.0
45 22 23 1.5

```
46 22 48 1.0
47 23 24 1.5
48 23 27 1.0
49 24 49 1.0
50 24 25 1.5
51 25 26 1.0
52 26 52 1.0
53 26 50 1.0
54 26 51 1.0
END

BASIS
type TZP
core Large
```

```
createoutput None
END

XC
GGA BLYP
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# LPy·BBr2+ - BBr2+ Single Point
# ==============================

"$ADFBIN/adf" <<eor
ATOMS
1 H     -1.695510000000     4.191270000000    10.407000000000
2 N      0.000000000000    -0.000000000000     9.869210000000
3 C     -0.541894000000    -1.085460000000     9.191890000000
4 C     -0.536857000000    -1.077060000000     7.796300000000
5 C      0.000000000000    -0.000000000000     7.090310000000
6 C     -1.117140000000    -2.241390000000     9.952300000000
7 C     -2.515090000000    -2.277780000000    10.215000000000
8 C     -3.456840000000    -1.173990000000     9.761650000000
9 C     -3.042900000000    -3.409030000000    10.848900000000
10 C    -2.247180000000    -4.512650000000    11.198300000000
11 C    -2.852150000000    -5.712660000000    11.898900000000
12 C    -0.883377000000    -4.470820000000    10.874900000000
13 C    -0.297756000000    -3.365710000000    10.240500000000
14 C     1.158650000000    -3.444860000000     9.812700000000
15 H    -1.688840000000     2.492450000000     9.916170000000
16 H    -0.963046000000    -1.933820000000     7.279940000000
17 H     0.000000000000    -0.000000000000     6.002120000000
18 H    -4.395160000000    -1.212200000000    10.324300000000
19 H    -3.033540000000    -0.171873000000     9.887490000000
20 H    -3.709910000000    -1.293310000000     8.697520000000
21 H    -4.112100000000    -3.434620000000    11.062500000000
22 H    -2.190980000000    -6.584030000000    11.846700000000
23 H    -3.030740000000    -5.490680000000    12.960500000000
24 H    -3.818480000000    -5.984520000000    11.456900000000
25 H    -0.254329000000    -5.329960000000    11.109100000000
26 H     1.695510000000    -4.191270000000    10.407000000000
27 H     1.688840000000    -2.492450000000     9.916170000000
```

28 H	1.234990000000	-3.751520000000	8.758730000000
29 H	-1.234990000000	3.751520000000	8.758730000000
30 C	0.541894000000	1.085460000000	9.191890000000
31 C	0.536857000000	1.077060000000	7.796300000000
32 C	1.117140000000	2.241390000000	9.952300000000
33 C	2.515090000000	2.277780000000	10.215000000000
34 C	3.456840000000	1.173990000000	9.761650000000
35 C	3.042900000000	3.409030000000	10.848900000000
36 C	2.247180000000	4.512650000000	11.198300000000
37 C	2.852150000000	5.712660000000	11.898900000000
38 C	0.883377000000	4.470820000000	10.874900000000
39 C	0.297756000000	3.365710000000	10.240500000000
40 C	-1.158650000000	3.444860000000	9.812700000000
41 H	0.963046000000	1.933820000000	7.279940000000
42 H	4.395160000000	1.212200000000	10.324300000000
43 H	3.033540000000	0.171873000000	9.887490000000
44 H	3.709910000000	1.293310000000	8.697520000000
45 H	4.112100000000	3.434620000000	11.062500000000
46 H	2.190980000000	6.584030000000	11.846700000000
47 H	3.030740000000	5.490680000000	12.960500000000
48 H	3.818480000000	5.984520000000	11.456900000000
49 H	0.254329000000	5.329960000000	11.109100000000

END

GUIBONDS
1 40 15 1.0
2 2 3 1.5
3 2 30 1.0
4 40 1 1.0
5 3 4 1.5
6 3 6 1.0
7 4 16 1.0
8 4 5 1.5
9 5 17 1.0
10 5 31 1.5
11 6 7 1.5
12 6 13 1.5
13 7 8 1.0
14 7 9 1.5
15 8 18 1.0
16 8 20 1.0
17 8 19 1.0
18 9 10 1.5
19 9 21 1.0
20 10 11 1.0
21 10 12 1.5
22 11 22 1.0
23 11 24 1.0
24 11 23 1.0
25 12 13 1.5
26 12 25 1.0
27 13 14 1.0
28 14 26 1.0
29 14 28 1.0
30 14 27 1.0
31 40 29 1.0
32 30 31 1.5
33 30 32 1.5
34 31 41 1.0
35 32 39 1.5
36 32 33 1.5
37 33 34 1.0
38 33 35 1.5
39 34 43 1.0
40 34 44 1.0
41 34 42 1.0
42 35 36 1.5
43 35 45 1.0
44 36 38 1.5
45 36 37 1.0
46 37 46 1.0
47 37 48 1.0
48 37 47 1.0
49 38 39 1.5
50 38 49 1.0
51 39 40 1.0
END

```
BASIS
type TZP
core Large
createoutput None
END

XC
GGA BLYP
END

SAVE  TAPE21 TAPE13

INTEGRATION 6

NOPRINT LOGFILE

eor
```