Electronic Supplementary Material (ESI) for Dalton Transactions.

Experimental and quantum chemical studies of anionic analogues of N-heterocyclic carbenes

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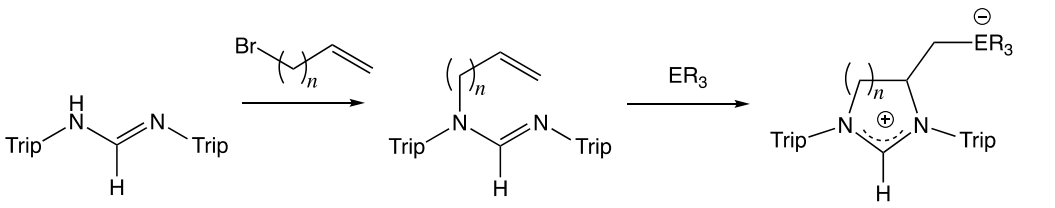
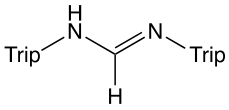
Supporting Information (66 pages)

1. Additional synthetic data



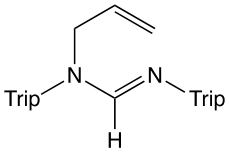
Scheme s1: *Syntheses of zwitterionic WCA-NHC pro-ligands bearing pendant Trip aryl groups [where Trip = 2,4,6-$^{i}Pr_3C_6H_2$; $Ar^f = C_6H_3(CF_3)_2$-3,5 and $R^f = C(CF_3)_3$].*

Precursor s1 and intermediates s2-s4



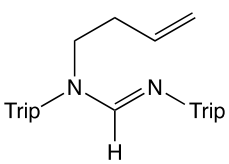
***N,N′*-bis(triisopropylphenyl)formamidine** (**s1**) was prepared using the procedure reported for *N,N′*-bis(diisopropylphenyl)formamidine, by Grubbs *et al.*[1] ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.09–6.89 (4H, overlapping m, aromatic CH of Trip), 3.28 (2H, m, ^{i}Pr CH of Trip), 3.18 (2H, sept, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 2.85 (2H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 1.36–1.09 (36H, overlapping m, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 148.1, 148.0 , 145.5, 143.6, 140.2, 138.6, 131.0, 129.0, 128.2, 125.3, 34.2, 34.1, 34.0, 28.2, 28.1, 24.5, 24.2, 24.1, 24.0, 23.9, 23.6, 22.8, 21.4.

***N,N′*-bis(triisopropylphenyl)-*N*-(1-allyl)formamidine (s2)**, ***N,N′*-bis(triisopropylphenyl)-*N*-(1-butenyl)-formamidine (s3) and *N,N′*-bis(triisopropylphenyl)-*N*-(1-pentenyl)formamidine (s4)**: A common method was used for the synthesis of these three precursors, exemplified here for the allyl system. A mixture of **s1** (0.81 g, 1.8 mmol), allylbromide (0.22 g, 0.17 mL, 1.8 mmol) and K_2CO_3 (0.2 g, 0.90 mmol) was suspended in acetonitrile (15 mL). The reaction mixture was then refluxed in a closed system in the dark for 7 d. After cooling, volatiles were removed under vacuum and the residue dissolved in dichloromethane (30 mL). The resulting solution was filtered through a pad of silica gel, and the solvent then removed under vacuum. Recrystallisation of the crude product from acetonitrile at −30 °C produced colourless crystals of *N,N′*-bis(triisopropylphenyl)-*N*-(1-allyl)formamidine (**s2**) in 29% yield (0.25 g, 0.51 mmol). The corresponding syntheses of *N,N′*-bis(triisopropylphenyl)-*N*-(1-butenyl)formamidine (**s3**) from 4-bromo-1-butene and *N,N′*-bis(triisopropylphenyl)-*N*-(1-pentenyl)formamidine (**s4**) from 5-bromo-1-pentene produced colourless crystals in yields of 54% and 78%, respectively.



s2

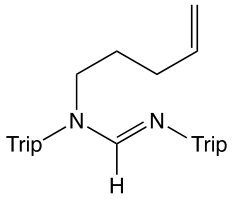
Spectroscopic data for **s2**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.19 (1H, s, NCHN), 7.06–6.82 (4H, overlapping m, aromatic CH of Trip), 6.20 (1H, m, alkene CH), 5.14 (2H, m, alkene CH_2), 4.34 (2H, d, $^3J_{HH}$ = 6.7 Hz, NCH_2), 3.24 (2H, overlapping m, ^{i}PrCH of Trip), 3.17 (2H, overlapping m, ^{i}Pr CH of Trip), 2.89 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.85 (1H, sept, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Trip), 1.34–1.05 (36H, overlapping m, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 151.1 , 148.7, 147.7, 145.1, 142.2, 139.3, 136.2, 133.6, 122.0, 120.4, 117.6, 52.8 , 34.1, 33.9 , 28.3, 27.9, 25.2, 24.3, 23.9, 23.6.



s3

Spectroscopic data for **s3**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.18 (1H, s, NCHN), 7.01 (2H, s, aromatic CH of Trip), 6.99 (2H, s, aromatic CH of Trip), 5.93 (1H, m, alkene CH), 5.15–4.98 (2H, m, alkene CH_2), 3.79 (2H, m, NCH_2), 3.64 (4H, overlapping m, ^{i}Pr CH of Trip), 2.90 (1H, sept, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Trip), 2.85 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.55 (2H, m, $NCH_2C\underline{H}_2$), 1.43–1.08 (36H, overlapping m, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C

151.2, 148.7, 147.5 , 145.1, 142.3 , 139.3, 136.7, 135.9, 122.1, 120.5, 116.2, 49.6, 34.1, 34.0, 31.9, 28.3, 27.9, 25.4, 24.3, 24.1, 24.0, 23.6, 22.8.

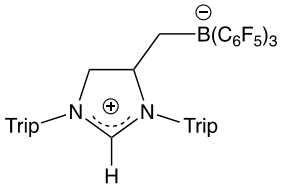


s4

Spectroscopic data for **s4**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.17 (1H, s, NCHN), 7.00 (2H, s, aromatic CH of Trip), 6.92 (2H, s, aromatic CH of Trip), 5.82 (1H, m, alkene CH), 4.98 (2H, m, alkene CH_2), 3.71 (2H, m, NCH_2), 3.21 (4H, overlapping m, ^{i}Pr CH of Trip), 2.90 (1H, sept, $^{3}J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Trip), 2.85 (1H, sept, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 2.11 (2H, m, $C\underline{H}_2CH=CH_2$), 1.85 (2H, m, $NCH_2C\underline{H}_2$), 1.37–1.06 (36H, overlapping m, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 151.3, 148.6, 147.5 , 145.2, 142.2 , 139.3, 138.1, 136.7 , 122.1, 120.5 , 114.7 , 49.8 34.1, 34.0, 31.5, 28.3, 27.9, 26.4, 25.4, 24.3, 24.2, 24.0, 23.6.

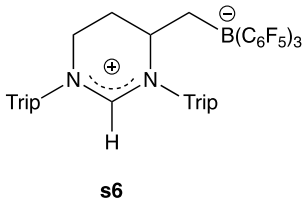
WCA-NHC pro-ligands s5-s9

s5, s6 and s7: The three compounds were prepared via a common approach, illustrated here for **s5**. A solution of $B(C_6F_5)_3$ (0.15 g, 0.3 mmol) in toluene (3 mL) was added to a stirred solution of **s2** (0.12 g, 0.3 mmol) also in toluene (5 mL). The reaction mixture was stirred for 2 h, concentrated and stored at -30°C, resulting in the formation of X-ray quality crystals in 32% yield (0.08 g). **s6** and **s7** were synthesized from **s3/s4** in similar fashion and isolated as X-ray quality crystals in yields of 43% and 38%, respectively.



s5

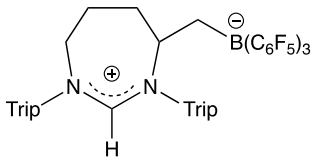
Spectroscopic data for **s5**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.32 (1H, s, NCHN), 7.29–7.05 (4H, m, aromatic CH of Trip), 4.43 (1H, m, NCH), 3.95 (1H, apparent t, $^{2}J_{HH}/^{3}J_{HH}$ = 11.9 Hz, NCH_2), 3.76 (1H, apparent t, $^{2}J_{HH}/^{3}J_{HH}$ = 11.6 Hz, NCH_2), 3.30 (1H, sept, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 3.01–2.87 (3H, overlapping m, ^{i}Pr CH of Trip), 2.77 (1H, sept, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.61 (1H, sept, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 2.35–2.21 (1H, m, CH_2B), 1.65 (1H, m, CH_2B), 1.49 (3H, d, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH_3 of Trip), 1.38 (3H, d, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH_3 of Trip), 1.34–1.22 (18H, overlapping m, ^{i}Pr CH_3 of Trip), 1.22–1.11 (12H, overlapping m, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 155.8 (NCHN), 152.6, 152.2, 149.2 (CF), 147.2, 146.1 (NC of Trip), 145.7, 145.7 (ortho-C of Trip), 127.0, 125.1 (para-C of Trip), 123.2, 123.0, 122.9, 122.8 (meta-CH of Trip), 70.9 (NCH), 58.8 (NCH_2), 34.3 (CH_2B), 29.4, 29.3, 29.3, 29.0, 26.4, 25.1, 25.1 (^{i}Pr CH of Trip), 24.9,23.9, 23.8, 23.7, 23.6, 23.2, 22.8, 22.7 (^{i}Pr CH_3 of Trip). ^{11}B NMR (128 MHz, $CDCl_3$, 298 K): δ_B −15 (s). ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ_F −131.2 (d, $^{3}J_{FF}$ = 23.2 Hz, ortho-CF), −161.6 (t, $^{3}J_{FF}$ = 20.4 Hz, para-F), −165.3 (m, meta-F). Accurate mass ($C_{52}H_{52}N_2{}^{11}BF_{15}{}^{23}Na$): 1023.38818 (meas.), 1023.38762 (calc.). Crystallographic data for **s5**: $C_{125}H_{128}B_2F_{30}N_4$, M_r = 2277.98, triclinic, *P*-1, a = 12.1720(5); b = 16.2564(7) Å, c = 17.7217(5) Å, α = 68.934(3)°, β = 72.219(3)°, γ = 70.185(4)°, V = 3010.5(2) Å^3, Z = 1, T = 150 K, λ = 1.54180 Å. 12520 reflections collected, 11057 independent [R(int) = 0.0502] used in all calculations; R_1 = 0.0456, wR_2 = 0.1180 for observed unique reflections [I > 2σ(I)] and R_1 = 0.0502, wR_2 = 0.1230 for all unique reflections. Max. and min. residual electron densities 0.58 and −0.36 e Å^{-3}. CCDC ref: 1838448.



s6

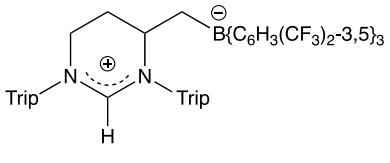
Spectroscopic data for **s6**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.37 (1H, s, NCHN), 7.13 (1H, d, $^{4}J_{HH}$ = 2.0 Hz, aromatic CH of Trip), 7.08 (1H, d, $^{4}J_{HH}$ = 1.7 Hz, aromatic CH of Trip), 7.03 (1H, d, $^{4}J_{HH}$ = 2.0 Hz, aromatic CH of Trip), 6.96 (1H, d, $^{4}J_{HH}$ = 2.0 Hz, aromatic CH of Trip), 4.20 (1H, m, NCH_2), 3.47 (1H, m, NCH_2), 3.22 (1H, m, NCH) 3.09 (2H, overlapping m, ^{i}Pr CH of Trip), 2.93 (1H, sept, $^{3}J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Trip), 2.88 (1H, sept, $^{3}J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 2.76 (1H, sept, $^{3}J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Trip), 2.46 (2H, overlapping m, ^{i}Pr CH of Trip and CH_2B), 2.34 (1H, m, CH_2B), 2.28 (1H, m, $NCH_2C\underline{H}_2$), 1.48 (3H, d, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.37 (3H, d, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.31 (6H, overlapping m, ^{i}Pr CH_3 of Trip), 1.26 (6H, overlapping m, $CH_3{}^{i}$Pr), 1.22 (6H, overlapping m, ^{i}Pr CH_3 of Trip), 1.17 (3H, d, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.13 (3H, d, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.09 (3H, d, $^{3}J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.07 (3H, d,

$^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 0.89 (1H, m, $NCH_2C\underline{H}_2$). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 152.8 (NCHN), 152.1, 152.4, 151.7 (CF), 146.1, 145.7 (NC of Trip), 144.6, 137.9, 133.4, 132.2 (ortho-C of Trip), 129.0 (para-C of Trip), 128.2, 125.3, 123.0, 122.6 (meta-CH of Trip), 63.0 (NCH), 46.5 (NCH_2), 29.2, 29.0, 26.9, 25.7, 25.5, 24.8 (^{i}Pr CH of Trip), 24.3, 24.2, 23.9 (^{i}Pr CH_3 of Trip), 23.8 (CH_2B), 23.6, 23.2, 22.1 (^{i}Pr CH_3 of Trip), 21.4 ($NCH_2\underline{C}H_2$). ^{11}B NMR (128 MHz, $CDCl_3$, 298 K): δ_B -15 (s). ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ_F −131.5 (d, $^3J_{FF}$ = 21.8 Hz, ortho-F), −163.1 (t, $^3J_{FF}$ = 20.4 Hz, para-F), −166.4 (m, meta-F). Accurate mass ($C_{53}H_{54}N_2{}^{11}BF_{15}{}^{23}Na$): 1037.40417 (meas.), 1037.40327 (calc.). Crystallographic data for **s6**: $C_{53}H_{54}BF_{15}N_2{\cdot}2CH_3CN$, M_r = 1096.91, monoclinic, I 2/c, a = 23.1811(5) Å, b = 11.0911(3) Å, c = 43.6034(12) Å, α = 90°, β = 92.608(2)°, γ = 90°, V = 11199.0(5) Å^3, Z = 8, T = 150 K, λ = 1.54180 Å. 33193 reflections collected, 11506 independent [R(int) = 0.0712] used in all calculations; R_1 = 0.0712, wR_2 = 0.1649 for observed unique reflections [I > 2σ(I)] and R_1 = 0.0713, wR_2 = 0.1651, for all unique reflections. Max. and min. residual electron densities 0.77 and −0.58 e Å^{-3}. CCDC ref: 1838453.



s7

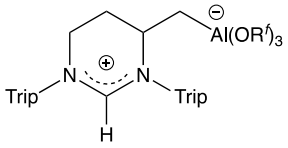
Spectroscopic data for **s7**: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.17 (1H, s, NCHN), 7.05 (3H, overlapping m, aromatic CH of Trip), 6.97 (1H, apparent d, $^4J_{HH}$ = 2.0 Hz, aromatic CH of Trip), 4.08 (1H, m, NCH_2), 3.99 (1H, m, NCH_2), 3.78 (1H, m, NCH) 3.16 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 3.01-2.84 (4H, overlapping m, ^{i}Pr CH of Trip), 2.51 (2H, overlapping m, ^{i}Pr CH of Trip and CH of CH_2B), 2.37 (1H, m, CH_2B), 2.28 (1H, m, $NCHCH_2$), 2.16 (2H, m, $NCHCH_2$), 1.46 (3H, d, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr CH_3 of Trip), 1.31-1.21 (24H, overlapping m, ^{i}Pr CH_3 of Trip), 1.16 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.11 (3H, d, $^3J_{HH}$ = 6.6 Hz, ^{i}Pr CH_3 of Trip), 0.99 (3H, d, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr CH_3 of Trip), 0.87 (1H, br m, $NCH_2C\underline{H}_2$). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 158.0 (NCHN), 151.7, 151.4 (CF), 145.4, 145.0 (NC of Trip), 144.4, 143.6 (ortho-C of Trip), 136.8, 133.9 (para-C of Trip), 123.4, 122.9, 122.8, 122.6 (meta-CH of Trip), 69.7 (NCH), 55.9 (NCH_2), 34.2, 34.2 ($NCHCH_2$), 29.3, 29.0 (NCH_2CH_2), 26.0, 25.3, 25.2 (^{i}Pr CH of Trip), 24.1, 23.9, 23.8, 23.7, 23.0, 22.8 (^{i}Pr CH_3 of Trip). ^{11}B NMR (128 MHz, $CDCl_3$, 298 K): δ_B −14 (s). ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ_F −130.0 (d, $^3J_{FF}$ = 20.4 Hz, ortho-F), −162.2 (t, $^3J_{FF}$ = 20.4 Hz, para-F), −165.7 (m, meta-F). Accurate mass ($C_{54}H_{56}N_2{}^{11}BF_{15}{}^{23}Na$): 1051.42004 (meas.), 1051.41892 (calc.). Crystallographic data for **s7**: $C_{54}H_{56}BF_{15}N_2$, M_r = 1028.83, orthorhombic, P 2_1 2_1 2_1, a = 12.7458(2) Å, b = 15.9989(2) Å, c = 24.8594(5) Å, α = 90°, β = 90°, γ = 90°, V = 5069.30(14) Å^3, Z = 4, T = 150 K, λ = 1.54180 Å. 17800 reflections collected, 9447 independent [R(int) = 0.0560] used in all calculations; R_1 = 0.0521, wR_2 = 0.1327 for observed unique reflections [I > 2σ(I)] and R_1 = 0.0560, wR_2 = 0.1392 for all unique reflections. Max. and min. residual electron densities 0.35 and −0.29 e Å^{-3}. CCDC ref: 1838450.



s8

s8: A solution of B{$C_6H_3(CF_3)_2$-3,5}$_3$ (0.09 g, 0.14 mmol) in toluene (3 mL) was added to a stirred solution of **s3** (0.07 g, 0.14 mmol) also in toluene (5 mL). The reaction mixture was stirred for 2 h, concentrated and stored at 5°C to give crystalline material in 45% yield. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.70 (6H, br s, ortho-CH of $C_6H_3(CF_3)_2$-3,5), 7.51 (3H, s, para-CH of $C_6H_3(CF_3)_2$-3,5), 7.39 (1H, s, NCHN), 7.12 (1H, d, $^4J_{HH}$ = 1.8 Hz, aromatic CH of Trip), 7.10 (1H, d, $^4J_{HH}$ = 1.8 Hz, aromatic CH of Trip), 7.06 (1H, d, $^4J_{HH}$ = 1.8 Hz, CH Trip), 6.94 (1H, d, $^4J_{HH}$ = 1.8 Hz, aromatic CH of Trip), 3.91 (1H, m, NCH), 3.25 (3H, m, NCH_2CH_2, ^{i}Pr CH of Trip), 3.08 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.90 (2H, overlapping m, ^{i}Pr CH of Trip), 2.66 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.29 (1H, sept, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr CH of Trip), 2.04-1.93 (2H, br m, NCH_2), 1.70 (1H, m, $NCHCH_2$), 1.54 (3H, d, $^3J_{HH}$ = 6.7 Hz, ^{i}Pr CH_3 of Trip), 1.46 (4H, overlapping m, ^{i}Pr CH_3 of Trip, $NCHCH_2$), 1.41 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip) 1.30-1.18 (19H, overlapping d, ^{i}Pr CH_3 of Trip, BCH_2), 1.15 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 1.04 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 0.75 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 153.0 (NCHN), 152.3, 151.8 (NC of Trip), 145.9, 145.2 (ipso-C of $C_6H_3(CF_3)_2$-3,5), 144.7 (ortho-C of $C_6H_3(CF_3)_2$-3,5), 133.4 (meta-C of $C_6H_3(CF_3)_2$-3,5), 133.1, 132.0 (ortho-C of Trip), 129.6, 129.2 (para-C of Trip), 128.4 (para-C of $C_6H_3(CF_3)_2$-3,5),

125.6 (CF_3 of $C_6H_3(CF_3)_2$-3,5), 123.2, 123.1, 123.0, 122.9 (meta-C of Trip), 62.6 (NCH), 46.2 (NCH_2), 34.3, 34.2 (CH_2B), 29.4, 29.2, 29.0, 26.7, 25.3, 25.0, 24.7 (^{i}Pr CH of Trip), 24.3, 24.1, 24.0, 23.8, 23.7, 23.5 (^{i}Pr CH_3 of Trip), 22.8 (NCH_2CH_2). ^{11}B NMR (128 MHz, $CDCl_3$, 298 K): δ_B -11 (s). ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ_F –62.6 (s). Accurate mass ($C_{59}H_{63}N_2{}^{11}BF_{18}{}^{23}Na$): 1175.47021 (meas.), 1175.46891 (calc.).



s9

s9: A solution of Al(OR^f)$_3$ (0.32 g, 0.39 mmol) in toluene (3 mL) was added to a stirred solution of **s3** (0.19 g, 0.39 mmol) also in toluene (5 mL). The reaction mixture was stirred for 2 h, concentrated and stored at 5°C to yield X-ray quality crystals of **s9** in 58% yield (0.28 g, 0.23 mmol). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ_H 7.35 (1H, s, NCHN), 7.10 (2H, m, aromatic CH of Trip), 7.08 (2H, m, aromatic CH of Trip), 4.00 (1H, m, NCH), 3.89 (1H, m, NCH_2), 3.54 (1H, m, NCH_2), 3.04-2.81 (5H, overlapping m, ^{i}Pr CH of Trip), 2.76 (1H, sept, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH of Trip), 2.62 (1H, m, NCH_2CH_2), 2.53 (1H, m, NCH_2CH_2), 1.41–1.29 (15H, overlapping m, ^{i}Pr CH_3 of Trip), 1.28–1.16 (18H, overlapping d, ^{i}Pr CH_3 of Trip), 1.14 (3H, d, $^3J_{HH}$ = 6.9 Hz, ^{i}Pr CH_3 of Trip), 0.58 (1H, m, $AlCH_2$), 0.17 (1H, apparent t, $^2J_{HH}$ = 13.5 Hz, $AlCH_2$). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K): δ_C 152.4 (NCHN), 152.1, 151.5 (CF), 145.8, 145.2 (NC of Trip), 144.8, 137.9, 133.6, 132.4 (ortho-C of Trip), 129.0 (para-C of Trip), 128.2, 125.3, 123.0, 122.8 (meta-C of Trip), 119.8, 116.9, 61.2 (NCH), 47.3 (NCH_2), 34.4, 34.3 (CH_2B), 29.2, 29.1, 29.0, 26.7, 26.2, 25.3 (^{i}Pr CH of Trip), 24.9, 24.5, 24.2, 23.8, 23.3, 22.9 (^{i}Pr CH_3 of Trip), 21.4 (NCH_2CH_2). ^{27}Al NMR (104 MHz, $CDCl_3$, 298 K): δ_{Al} 69 (br s). ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ_F –75.4 (s). Accurate mass ($[C_{47}H_{53}AlF_{27}N_2O_3]^{3-}$): 1233.3 (meas.), 1233.3457 (calc.). Crystallographic data: $C_{54}H_{62}Al_1F_{27}N_2O_3$, M_r = 1327.02, triclinic, *P*-1, a = 10.7821(3), b = 15.9984(4), c = 19.1481(3), α = 76.2420(18), β = 76.8789(18), γ = 79.594(2), V = 3096.33(13), Z = 2, T = 150 K, λ = 1.54180 Å. 12876 reflections collected, 12828 independent [R(int) = 0.1083] used in all calculations; R_1 = 0.1037, wR_2 = 0.2394 for observed unique reflections [I > 2σ(I)] and R_1 = 0.1083, wR_2 = 0.2420, for all unique reflections. Max. and min. residual electron densities 1.20 and −0.74 e Å^{-3}. CCDC ref: 1838452.

(η^6-toluene)Li[(5-c')^{Dipp}]: To H(**5-c'**)^{Dipp} (1.53 g, 1.7 mmol) was added toluene (15 mL), the resulting suspension was then cooled to -78°C and *n*-BuLi added (1.2 mL of a 1.6 M solution in hexanes, 1.9 mmol). After warming to room temperature and stirring for 30 min, the suspension was left to stand overnight. The precipitate was filtered and dried *in vacuo* to yield a white powder. Toluene (15 mL) was then added, and the resulting suspension cooled to -78°C before a second portion of *n*-BuLi was added (1.2 mL of a 1.6 M solution in hexanes, 1.9 mmol). After warming to room temperature and stirring for 30 min, the suspension was left to stand overnight. The precipitate was filtered and dried *in vacuo* to yield the product as a white powder (1.34 g, 79 %). ^{1}H NMR (400 MHz, thf-d_8, 298 K): δ_H 7.20-7.02 (11H, overlapping m, aromatic CH of Dipp and toluene), 3.79 (1H, overlapping m, NCH), 3.77 (1H, overlapping sept, ^{i}Pr CH of Dipp), 3.37 (1H, overlapping sept, ^{i}Pr CH of Dipp), 3.32 (1H, overlapping dd , $^{2/3}J_{HH}$ = 10.8 Hz, NCH_2), 3.21 (1H, overlapping dd, $^{2/3}J_{HH}$ = 10.0 Hz, NCH_2), 3.18 (1H, overlapping sept, ^{i}Pr CH of Dipp), 2.93 (1H, sept, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr CH of Dipp), 2.30 (3H, s, CH_3 of toluene), 2.05 (1H, dd, $^{2/3}J_{HH}$ = 12.8 Hz, CH_2B), 1.38 (3H, d, $^3J_{HH}$ = 6.6 Hz, ^{i}Pr CH_3 of Dipp), 1.26 (3H, d, $^3J_{HH}$ = 6.8 Hz, ^{i}Pr CH_3 of Dipp), 1.19 (3H, overlapping d, $^3J_{HH}$ = 6.8 Hz, ^{i}Pr CH_3 of Dipp), 1.17 (3H, overlapping d, ^{i}Pr CH_3 of Dipp), 1.16 (1H, overlapping m, CH_2B), 1.15 (3H, overlapping d, ^{i}Pr CH_3 of Dipp), 1.09 (6H, m, ^{i}Pr CH_3 of Dipp), 1.06 (3H, overlapping d, ^{i}Pr CH_3 of Dipp).^{13}C NMR (101 MHz, thf-d_8, 298 K): δ_c 242.7 (s, NCLiN), 150.0 (NC of Dipp), 149.3 (dm, $^1J_{CF}$ = 228.9 Hz, ortho-CF), 148.6 (NC of Dipp), 148.3, 148.0, 141.2, 139.6 (ortho-C of Dipp), 139.4 (dm, $^1J_{CF}$ = 243.4 Hz, para-CF), 138.6 (ipso-C of toluene), 137.5 (dm, $^1J_{CF}$ = 246.1 Hz, meta-CF), 129.8 (ortho-CH of toluene), 129.1 (meta-CH of toluene), 127.8, 127.6 (para-CH of Dipp), 126.2 (para-CH of toluene), 124.2, 123.8, 123.6, 123.5 (meta-CH of Dipp), 69.0 (NCH), 59.6 (NCH_2), 29.8, 29.4, 29.3, 29.0 (^{i}Pr CH of Dipp), 26.0, 25.8, 25.6, 25.3, 24.4, 23.9, 23.2, 23.0 (^{i}Pr CH_3 of Dipp), 21.6 (CH_3 of toluene) (CH_2B not observed). ^{11}B NMR (128 MHz, thf-d_8, 298 K): -14 (s). ^{19}F NMR (282 MHz, thf-d_8, 298 K): δ_F -130.5 (d, $^3J_{FF}$ = 20.4 Hz, ortho-F), -166.0 (t, $^3J_{FF}$ = 20.4 Hz, para-F), -168.3 (m, meta-F). ^{7}Li NMR (156 MHz, thf-d_8, 298K): -0.5 (s).

Crystallographic data: $C_{53}H_{47}B_1F_{15}LiN_2$, M_r = 1014.67, triclinic, *P*-1, a = 12.2770(5), b = 12.9302(6), c = 17.4766(8), α = 84.133(4), β = 85.803(4), γ = 62.488(5), V = 2446.6(2) Å^3, Z = 2, T = 150 K, λ = 1.54180 Å. 23480 reflections collected, 9980 independent [R(int) = 0.0293] used in all calculations; R_1 = 0.0613, wR_2 = 0.1509 for observed unique reflections [I > 2σ(I)] and R_1 = 0.0856, wR_2 = 0.1728, for all unique reflections. Max. and min. residual electron densities 0.77 and −0.39 e Å^{-3}. CCDC ref: 1838449.

(5-c')^{Dipp}Au(tht): (**5-c'**)^{Dipp}Au(tht) can be isolated in low yield from the reaction between (η^6-toluene)Li[(**5-c'**)^{Dipp}] and (tht)AuCl in toluene and characterized by X-ray crystallography. $C_{51}H_{49}Au_1B_1Cl_2F_{15}N_2S$, M_r = 1285.66, monoclinic, *C*2/*c*, a = 45.7252(11), b = 9.8319(2), c = 26.8014(7), β = 121.195(3)°, V = 10306.8(5) Å^3, Z = 8, T = 150 K, λ = 1.54180 Å. 10583 reflections collected, 10583 independent [R(int) = 0.0425] used in all calculations; R_1 = 0.0460, wR_2 = 0.1215 for observed unique reflections [I > 2σ(I)] and R_1 = 0.0568, wR_2 = 0.1298, for all unique reflections. Max. and min. residual electron densities 1.82 and −1.50 e Å^{-3}. CCDC ref: 1838451.

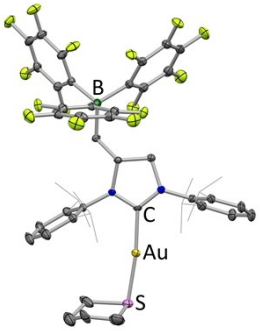


Figure s1: *Molecular structure of (**5-c'**)^{Dipp}Au(tht) as determined by X-ray crystallography. Isopropyl groups shown in wireframe format and hydrogen atoms omitted for clarity; thermal ellipsoids shown at the 35% probability level.*

2. DFT Run files

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12 8 9 1.5
13 8 16 1.5
14 9 10 1.5
15 9 17 1.0
16 10 11 1.0
17 10 12 1.5
18 19 20 1.0
```

```
19 12 14 1.5
20 14 15 1.0
21 14 16 1.5
22 16 27 1.0
23 17 18 1.0
24 24 25 1.0
25 36 37 1.0
26 19 21 1.5
27 21 22 1.0
28 29 30 1.5
29 13 23 1.0
30 34 36 1.5
31 36 35 1.5
32 27 28 1.0
33 35 24 1.0
34 26 29 1.0
35 29 35 1.5
36 26 32 1.0
37 30 31 1.5
38 30 13 1.0
39 31 33 1.0
40 31 34 1.5
41 38 12 1.0
42 39 34 1.0
43 40 39 1.0
44 41 39 1.0
45 42 39 1.0
46 43 13 1.0
47 44 13 1.0
48 45 17 1.0
49 46 17 1.0
50 47 24 1.0
51 48 24 1.0
52 49 27 1.0
53 50 27 1.0
54 51 38 1.0
55 52 38 1.0
56 53 38 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13
```

```
NumericalQuality Good

NOPRINT LOGFILE

eor



#! /bin/sh

# ==============================
# Ligand (I-c)Mes
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 N       3.790576000000       4.611453000000       1.454312000000
2 N       3.045391000000       6.586674000000       1.286635000000
3 C       3.194055000000       5.580847000000       2.207201000000
4 C       3.539787000000       6.249664000000       0.045655000000
5 C       4.000193000000       5.003114000000       0.146925000000
6 C       4.197859000000       3.351891000000       2.022092000000
7 C       5.545035000000       3.130687000000       2.247045000000
8 C       5.902097000000       1.941390000000       2.888703000000
9 C       4.962757000000       1.021442000000       3.298766000000
10 C       3.632820000000       1.268670000000       3.041439000000
11 C       3.221851000000       2.431943000000       2.393971000000
12 C       6.595863000000       4.124804000000       1.845283000000
13 C       5.368056000000      -0.253734000000       4.002679000000
14 C       1.761846000000       2.688279000000       2.124192000000
15 C       2.422915000000       7.846236000000       1.607878000000
16 C       1.094344000000       8.041416000000       1.268373000000
17 C       0.500062000000       9.246327000000       1.651873000000
18 C       1.197352000000      10.214420000000       2.340015000000
19 C       2.538819000000       9.993216000000       2.640507000000
20 C       3.172686000000       8.802618000000       2.270288000000
21 C       0.301721000000       6.999155000000       0.537896000000
22 C       0.529465000000      11.506512000000       2.780791000000
23 C       4.615622000000       8.568402000000       2.595682000000
24 H       4.366196000000       4.454008000000      -0.537066000000
25 H       3.532288000000       6.784457000000      -0.659089000000
26 H       6.812762000000       1.794355000000       3.082113000000
27 H       2.927158000000       0.690937000000       3.292955000000
28 H       6.811653000000       4.005094000000       1.037609000000
29 H       7.447990000000       3.933528000000       2.328394000000
30 H       6.244854000000       5.035644000000       2.012131000000
31 H       5.578295000000      -1.034454000000       3.210776000000
32 H       4.692974000000      -0.494456000000       4.625244000000
33 H       6.063895000000      -0.097590000000       4.493261000000
34 H       1.461517000000       3.255602000000       2.759209000000
35 H       1.156476000000       1.835993000000       2.354127000000
36 H       1.653054000000       2.957628000000       1.182874000000
37 H      -0.393153000000       9.397266000000       1.430240000000
38 H       3.072321000000      10.660732000000       3.167612000000
39 H       0.573326000000       6.949709000000      -0.345316000000
40 H      -0.669200000000       7.150094000000       0.586871000000
41 H       0.553815000000       6.162483000000       0.929697000000
42 H       0.948841000000      12.192244000000       2.168187000000
```

```
43 H       0.837561000000      11.803185000000       3.772745000000
44 H      -0.335057000000      11.489596000000       2.608133000000
45 H       4.768921000000       7.894380000000       3.237339000000
46 H       5.075612000000       9.403772000000       2.973371000000
47 H       5.239784000000       8.567101000000       1.837812000000
END

GUIBONDS
1 1 3 1.0
2 1 5 1.0
3 1 6 1.0
4 2 3 1.0
5 2 4 1.0
6 2 15 1.0
7 4 25 1.0
8 4 5 2.0
9 5 24 1.0
10 6 7 1.5
11 6 11 1.5
12 7 8 1.5
13 7 12 1.0
14 8 26 1.0
15 8 9 1.5
16 9 10 1.5
17 9 13 1.0
18 10 27 1.0
19 10 11 1.5
20 11 14 1.0
21 12 28 1.0
22 12 30 1.0
23 12 29 1.0
24 13 33 1.0
25 13 32 1.0
26 13 31 1.0
27 14 34 1.0
28 14 36 1.0
29 14 35 1.0
30 15 20 1.5
31 15 16 1.5
32 16 17 1.5
33 16 21 1.0
34 17 37 1.0
35 17 18 1.5
36 18 19 1.5
37 18 22 1.0
38 19 38 1.0
39 19 20 1.5
40 20 23 1.0
41 21 39 1.0
42 21 41 1.0
43 21 40 1.0
44 22 44 1.0
45 22 42 1.0
46 22 43 1.0
47 23 45 1.0
48 23 47 1.0
49 23 46 1.0
END

BASIS
type TZP
```

```
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13
FULLSCF
BeckeGrid
    Quality Good
End

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# Ligand (B-c)Mes
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 C      -0.631900785100       1.344814492000      -0.000000000236
2 C      -1.858783345000       0.669511152000      -0.001638580236
3 C      -1.887393815000      -0.730652368000      -0.002956710236
4 C      -0.689121715100      -1.455512408000      -0.002636280236
5 C       0.537760784900      -0.780209038000      -0.000997700236
6 C       0.566371264900       0.619954432000       0.000320439764
7 H      -2.774307065000       1.223330852000      -0.001883420236
8 H      -2.824777005000      -1.246608948000      -0.004208630236
9 H       1.503754475000       1.135910982000       0.001572379764
10 N     -0.754644344700      -2.994115164000      -0.005524853648
11 C      0.774214944500      -3.178705319000       0.005233803084
12 N      1.586712751000      -1.870494005000       0.010753988440
13 C      2.769764229000      -1.791645777000      -0.858194892000
14 C      2.941750142000      -2.719675638000      -1.892825030000
15 C      4.068833179000      -2.644557575000      -2.720665161000
16 C      5.023930184000      -1.641409640000      -2.513875080000
17 C      4.851944228000      -0.713379827400      -1.479244956000
18 C      3.724861239000      -0.788497885300      -0.651404842200
19 C      2.212020990000      -3.486117355000      -2.050820165000
20 H      4.200236807000      -3.353606365000      -3.511160515000
21 C      5.885062921000      -1.584016644000      -3.146375247000
22 H      5.581673362000       0.053061901380      -1.321249811000
23 C      3.593457652000      -0.079449089520       0.139090517500
```

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24 C      -1.748549929000      -4.040196381000      -0.286177265500
25 C      -3.110643622000      -3.717839864000      -0.331621195100
26 C      -4.057528932000      -4.714432520000      -0.598996339200
27 C      -3.642320448000      -6.033381594000      -0.820927547300
28 C      -2.280226780000      -6.355738049000      -0.775483607700
29 C      -1.333341497000      -5.359145439000      -0.508108464100
30 C      -3.427878017000      -2.710114436000      -0.162057631200
31 H      -5.098218448000      -4.468140420000      -0.633717170700
32 C      -4.365775475000      -6.794814919000      -1.025211965000
33 H      -1.962992364000      -7.363463467000      -0.945047178300
34 C      -0.292651986300      -5.605437577000      -0.473387620200
35 H      -0.609837011400       2.424588615000       0.001016519309
36 H       0.023533784140      -5.688302222000       0.555961693400
37 H      -0.131586321100      -6.545667541000      -0.979772323100
38 H       2.613720384000      -4.227322106000      -2.725840989000
39 H       1.323867165000      -3.049311430000      -2.483004579000
40 H       1.966504640000      -3.949562943000      -1.106712168000
41 H       6.695490750000      -1.119638920000      -2.604194407000
42 H       5.648686210000      -0.991372763300      -4.017753054000
43 H       6.174789822000      -2.578774396000      -3.451195419000
44 H       4.424800761000      -0.151554673300       0.824706605900
45 H       2.674517855000      -0.296173148000       0.663476188700
46 H       3.549247100000       0.917098394300      -0.274840080000
47 H      -2.691447116000      -2.201279944000       0.442224577400
48 H      -4.375784747000      -2.716914508000       0.355462021000
49 H      -3.534611084000      -2.202110005000      -1.109126557000
50 H      -3.957201683000      -7.491928022000      -1.741801651000
51 H      -5.256621220000      -6.340219152000      -1.432810478000
52 H      -4.609180904000      -7.314848450000      -0.110488551400
53 H       0.274140125500      -4.829391684000      -0.966235947000
END

GUIBONDS
1 1 2 1.5
2 2 3 1.5
3 3 4 1.5
4 4 5 1.5
5 5 6 1.5
6 6 1 1.5
7 7 2 1.0
8 8 3 1.0
9 9 6 1.0
10 10 4 1.0
11 11 10 1.0
12 12 11 1.0
13 12 5 1.0
14 13 14 1.5
15 14 15 1.5
16 15 16 1.5
17 16 17 1.5
18 17 18 1.5
19 18 13 1.5
20 19 14 1.0
21 20 15 1.0
22 21 16 1.0
23 22 17 1.0
24 23 18 1.0
25 13 12 1.0
26 24 25 1.5
27 25 26 1.5
28 26 27 1.5
```

```
29 27 28 1.5
30 28 29 1.5
31 29 24 1.5
32 30 25 1.0
33 31 26 1.0
34 32 27 1.0
35 33 28 1.0
36 34 29 1.0
37 24 10 1.0
38 35 1 1.0
39 36 34 1.0
40 37 34 1.0
41 38 19 1.0
42 39 19 1.0
43 40 19 1.0
44 41 21 1.0
45 42 21 1.0
46 43 21 1.0
47 44 23 1.0
48 45 23 1.0
49 46 23 1.0
50 47 30 1.0
51 48 30 1.0
52 49 30 1.0
53 50 32 1.0
54 51 32 1.0
55 52 32 1.0
56 53 34 1.0
END

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh
```

```
# ==============================
# Ligand (5-c)Mes
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 N      -3.483929000000       9.325456000000      11.526849000000
2 N      -1.678686000000       7.940764000000      11.591751000000
3 C      -3.107402000000       7.963556000000      11.853065000000
4 C      -1.278053000000       9.146836000000      10.915409000000
5 C      -2.305485000000      10.130509000000      11.357764000000
6 C      -4.690808000000       9.832411000000      12.083636000000
7 C      -5.778994000000      10.001164000000      11.224545000000
8 C      -6.984859000000      10.461699000000      11.735217000000
9 C      -7.135918000000      10.767085000000      13.065698000000
10 C      -6.061385000000      10.590930000000      13.912834000000
11 C      -4.833162000000      10.121494000000      13.434612000000
12 C      -5.635031000000       9.686008000000       9.760845000000
13 C      -8.459946000000      11.280078000000      13.598574000000
14 C      -3.707029000000       9.935591000000      14.445709000000
15 C      -1.056705000000       6.672372000000      11.364596000000
16 C      -0.166991000000       6.213748000000      12.336410000000
17 C       0.414107000000       4.978764000000      12.175864000000
18 C       0.140527000000       4.164743000000      11.093034000000
19 C      -0.748535000000       4.648083000000      10.150254000000
20 C      -1.354222000000       5.879079000000      10.266394000000
21 C       0.143985000000       7.063477000000      13.549044000000
22 C       0.796597000000       2.814056000000      10.961523000000
23 C      -2.335652000000       6.298076000000       9.178440000000
24 H      -2.386458000000       7.243367000000       9.132325000000
25 H      -2.014543000000       5.967758000000       8.329596000000
26 H      -1.348058000000       9.023875000000       9.970921000000
27 H      -0.421928000000       9.420838000000      11.224545000000
28 H      -2.054035000000      10.498087000000      12.201483000000
29 H      -2.459900000000      10.773378000000      10.672882000000
30 H      -7.727042000000      10.557917000000      11.152812000000
31 H      -6.147103000000      10.797074000000      14.831702000000
32 H      -5.132132000000      10.364051000000       9.330446000000
33 H      -6.493297000000       9.619754000000       9.359481000000
34 H      -5.180297000000       8.847861000000       9.660077000000
35 H      -8.595436000000      12.170364000000      13.335552000000
36 H      -8.469073000000      11.214036000000      14.549893000000
37 H      -9.167507000000      10.731162000000      13.250155000000
38 H      -3.608863000000       9.016325000000      14.647246000000
39 H      -3.917505000000      10.414722000000      15.243315000000
40 H      -2.896197000000      10.271860000000      14.081919000000
41 H       1.036926000000       4.672882000000      12.838543000000
42 H      -0.944277000000       4.116992000000       9.397055000000
43 H       0.762666000000       7.742151000000      13.301393000000
44 H       0.530470000000       6.515228000000      14.221970000000
45 H      -0.652691000000       7.455289000000      13.866719000000
46 H       1.735894000000       2.893471000000      10.970063000000
47 H       0.535665000000       2.421914000000      10.109264000000
48 H       0.507724000000       2.233011000000      11.649821000000
49 H      -3.186248000000       5.931442000000       9.344109000000
END

GUIBONDS
1 1 6 1.0
2 1 5 1.0
```

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

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END
```

```
GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

Eor



#! /bin/sh

# ==============================
# Ligand (6-c)Mes
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 C     -11.281062000000       0.756670000000      -2.415005000000
2 C     -10.317491000000      -1.002365000000      -0.973920000000
3 H      -9.405430000000      -1.383371000000      -0.908992000000
4 H     -10.968962000000      -1.747463000000      -0.927995000000
5 C     -10.553838000000      -0.057863000000       0.166279000000
6 H      -9.847825000000       0.638273000000       0.178948000000
7 H     -10.517477000000      -0.550144000000       1.024596000000
8 C     -11.908293000000       0.583081000000      -0.004751000000
9 H     -12.617336000000      -0.095251000000       0.123522000000
10 H     -12.032527000000       1.293461000000       0.673034000000
11 C      -9.699350000000      -0.816313000000      -3.369922000000
12 C     -10.305370000000      -1.728768000000      -4.232990000000
13 C      -9.538755000000      -2.239743000000      -5.270254000000
14 H      -9.920547000000      -2.886028000000      -5.853023000000
15 C      -8.217631000000      -1.828471000000      -5.482458000000
16 C      -7.641912000000      -0.950734000000      -4.582967000000
17 H      -6.732882000000      -0.697027000000      -4.692236000000
18 C      -8.375196000000      -0.432637000000      -3.520365000000
19 C     -11.744668000000      -2.138260000000      -4.093632000000
20 H     -11.917383000000      -2.423124000000      -3.171971000000
21 H     -11.935564000000      -2.879797000000      -4.706489000000
22 H     -12.323417000000      -1.378030000000      -4.313754000000
23 C      -7.417685000000      -2.399979000000      -6.628991000000
24 H      -6.496534000000      -2.068825000000      -6.581483000000
25 H      -7.820688000000      -2.123127000000      -7.479390000000
26 H      -7.414655000000      -3.378309000000      -6.571981000000
27 C      -7.732815000000       0.543022000000      -2.568615000000
28 H      -8.314594000000       1.323727000000      -2.457763000000
29 H      -6.866207000000       0.829666000000      -2.929679000000
30 H      -7.596461000000       0.111275000000      -1.699214000000
31 C     -12.896106000000       2.296716000000      -1.531351000000
32 C     -12.408259000000       3.559910000000      -1.290642000000
33 C     -13.293049000000       4.637942000000      -1.387242000000
34 H     -12.974888000000       5.518350000000      -1.227298000000
```

```
35 C     -14.617202000000       4.448329000000      -1.708715000000
36 C     -15.059597000000       3.184245000000      -1.943089000000
37 H     -15.974687000000       3.060508000000      -2.174297000000
38 C     -14.232380000000       2.056362000000      -1.857575000000
39 C     -10.935631000000       3.795813000000      -0.992923000000
40 H     -10.687163000000       3.323117000000      -0.171030000000
41 H     -10.775036000000       4.756339000000      -0.878904000000
42 H     -10.393243000000       3.460207000000      -1.737220000000
43 C     -15.553503000000       5.632295000000      -1.822735000000
44 H     -15.568654000000       6.118345000000      -0.972337000000
45 H     -16.456473000000       5.316274000000      -2.036522000000
46 H     -15.238373000000       6.229620000000      -2.533776000000
47 C     -14.768707000000       0.654297000000      -2.080864000000
48 H     -14.308132000000       0.246585000000      -2.844164000000
49 H     -15.729249000000       0.697027000000      -2.264562000000
50 H     -14.611142000000       0.113946000000      -1.277973000000
51 N     -10.465965000000      -0.294656000000      -2.256644000000
52 N     -12.014347000000       1.165272000000      -1.366655000000
END

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

```
41 33 35 1.5
42 35 36 1.5
43 35 43 1.0
44 36 37 1.0
45 36 38 1.5
46 38 47 1.0
47 39 40 1.0
48 39 42 1.0
49 39 41 1.0
50 43 44 1.0
51 43 45 1.0
52 43 46 1.0
53 47 49 1.0
54 47 48 1.0
END

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# Lignad (7-c)Mes
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 C       1.067402000000       3.563476000000      -3.784850000000
2 C      -1.123920000000       4.687722000000      -2.963422000000
3 H      -1.008831000000       5.771551000000      -2.793939000000
4 H      -1.733641000000       4.306647000000      -2.132728000000
5 C      -1.827339000000       4.400825000000      -4.291608000000
6 H      -2.902440000000       4.603650000000      -4.174272000000
7 H      -1.729326000000       3.325752000000      -4.501898000000
```

```
8 C      -1.263526000000       5.213574000000      -5.468299000000
9 H      -1.516725000000       4.722952000000      -6.419897000000
10 H      -1.723782000000       6.214620000000       -5.500221000000
11 C       0.249527000000       5.380851000000       -5.346009000000
12 H       0.680369000000       5.770024000000       -6.277540000000
13 H       0.490136000000       6.105523000000       -4.551682000000
14 C       1.861710000000       3.601678000000       -6.020382000000
15 C       1.441725000000       2.533825000000       -6.834532000000
16 C       2.312658000000       2.072370000000       -7.828376000000
17 H       1.995626000000       1.241814000000       -8.465380000000
18 C       3.580594000000       2.638890000000       -8.021704000000
19 C       3.975512000000       3.683954000000       -7.178424000000
20 H       4.969670000000       4.123012000000       -7.298948000000
21 C       3.134875000000       4.177680000000       -6.171306000000
22 C       0.102239000000       1.881194000000       -6.608702000000
23 H       0.006169000000       1.559380000000       -5.561223000000
24 H      -0.028028000000       1.007592000000       -7.259995000000
25 H      -0.727875000000       2.576650000000       -6.802613000000
26 C       4.499283000000       2.108726000000       -9.095476000000
27 H       5.411438000000       2.713738000000       -9.182600000000
28 H       4.003308000000       2.100387000000      -10.077702000000
29 H       4.804062000000       1.072715000000       -8.880480000000
30 C       3.591471000000       5.262759000000       -5.232088000000
31 H       2.990829000000       6.179028000000       -5.340576000000
32 H       4.642251000000       5.525382000000       -5.406836000000
33 H       3.475096000000       4.928569000000       -4.189527000000
34 C       0.474093000000       3.491622000000       -1.505466000000
35 C       1.151915000000       4.326129000000       -0.600389000000
36 C       1.387005000000       3.851152000000        0.696340000000
37 H       1.916246000000       4.492321000000        1.406789000000
38 C       0.971586000000       2.575783000000        1.101109000000
39 C       0.305133000000       1.767633000000        0.170294000000
40 H      -0.021562000000       0.767095000000        0.467227000000
41 C       0.043687000000       2.204957000000       -1.133910000000
42 C       1.648385000000       5.680175000000       -1.038546000000
43 H       2.193240000000       6.184679000000       -0.230662000000
44 H       0.824268000000       6.337145000000       -1.354470000000
45 H       2.319383000000       5.579458000000       -1.905344000000
46 C       1.271694000000       2.070730000000        2.491363000000
47 H       0.541521000000       1.315378000000        2.813113000000
48 H       1.266483000000       2.886803000000        3.227427000000
49 H       2.267654000000       1.601054000000        2.532702000000
50 C      -0.640662000000       1.318623000000       -2.139002000000
51 H      -0.900606000000       0.345283000000       -1.704254000000
52 H       0.021220000000       1.163471000000       -3.005508000000
53 H      -1.563413000000       1.778307000000       -2.525351000000
54 N       0.197598000000       3.980513000000       -2.838276000000
55 N       0.964866000000       4.117765000000       -5.012543000000
END

GUIBONDS
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10 5 8 1.0
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31 22 25 1.0
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45 38 39 1.5
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53 46 47 1.0
54 46 49 1.0
55 46 48 1.0
56 50 51 1.0
57 50 52 1.0
END

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END
```

```
GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor
#! /bin/sh

# ==============================
# Ligand [(5-c')Mes]-
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 F      13.773445000000       2.057145000000      12.054389000000
2 C      13.528770000000       1.511099000000      13.264462000000
3 C      12.275167000000       1.706116000000      13.855110000000
4 C      12.157167000000       1.074262000000      15.084204000000
5 F      11.009215000000       1.155501000000      15.812637000000
6 C      13.161340000000       0.328742000000      15.681924000000
7 F      12.974119000000      -0.224659000000      16.894679000000
8 C      14.372493000000       0.190559000000      15.050550000000
9 C      14.561825000000       0.793439000000      13.829504000000
10 F      15.747009000000       0.677877000000      13.205446000000
11 F      15.364113000000      -0.512503000000      15.626566000000
12 B      11.101024000000       2.493982000000      12.993525000000
13 C       9.679369000000       2.791522000000      13.805605000000
14 C       9.583431000000       4.110948000000      14.559644000000
15 N       8.250373000000       4.328363000000      15.235402000000
16 C       8.438061000000       4.941161000000      16.379142000000
17 N       9.697461000000       5.084805000000      16.705438000000
18 C      10.532866000000       4.319337000000      15.742647000000
19 C      10.152559000000       5.733485000000      17.911364000000
20 C      10.275971000000       4.981279000000      19.073639000000
21 C      10.042610000000       3.483552000000      19.086564000000
22 C       9.268370000000       2.999911000000      20.315902000000
23 C      11.370640000000       2.741375000000      18.994382000000
24 C      10.668858000000       5.668851000000      20.231523000000
25 C      10.917539000000       7.029509000000      20.193236000000
26 C      10.810674000000       7.728225000000      19.025840000000
27 C      10.417413000000       7.106401000000      17.845764000000
28 C      10.307088000000       7.888696000000      16.547167000000
29 C      11.652815000000       7.968931000000      15.821660000000
30 C       9.764217000000       9.310645000000      16.763478000000
31 C       6.943345000000       4.024026000000      14.699380000000
32 C       6.366783000000       4.918873000000      13.793655000000
33 C       5.069770000000       4.625791000000      13.360302000000
34 C       4.398253000000       3.521441000000      13.817310000000
35 C       5.006906000000       2.643309000000      14.688894000000
36 C       6.306190000000       2.858385000000      15.143952000000
37 C       6.973706000000       1.879959000000      16.090647000000
38 C       6.461851000000       2.044887000000      17.525809000000
39 C       6.821789000000       0.443523000000      15.613885000000
40 C       7.086499000000       6.162521000000      13.285191000000
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41 C	6.493172000000	7.435143000000	13.859743000000
42 C	7.102694000000	6.239414000000	11.779306000000
43 C	11.596057000000	3.982794000000	12.455552000000
44 C	10.816367000000	4.701569000000	11.549827000000
45 F	9.736784000000	4.109499000000	10.982346000000
46 C	11.022851000000	6.023224000000	11.206705000000
47 F	10.198927000000	6.644379000000	10.342437000000
48 C	12.066787000000	6.713025000000	11.780526000000
49 F	12.268528000000	8.008046000000	11.476910000000
50 C	12.881825000000	6.063342000000	12.665766000000
51 C	12.630511000000	4.738344000000	12.988647000000
52 F	13.463128000000	4.224503000000	13.928758000000
53 F	13.910438000000	6.714585000000	13.241294000000
54 C	10.752483000000	1.417491000000	11.775648000000
55 C	11.065143000000	1.516671000000	10.423889000000
56 F	11.771466000000	2.567643000000	9.956882000000
57 C	10.693121000000	0.581706000000	9.470853000000
58 F	11.008923000000	0.759004000000	8.170793000000
59 C	9.985280000000	-0.536017000000	9.840801000000
60 F	9.589596000000	-1.433873000000	8.923614000000
61 C	9.692071000000	-0.717661000000	11.167686000000
62 C	10.078415000000	0.235134000000	12.085361000000
63 F	9.757378000000	-0.040229000000	13.373958000000
64 F	9.009465000000	-1.814434000000	11.561045000000
65 H	9.495291000000	2.072747000000	14.429663000000
66 H	8.967946000000	2.820496000000	13.117653000000
67 H	9.695355000000	4.870955000000	13.922417000000
68 H	7.725009000000	5.275475000000	16.926870000000
69 H	11.321935000000	4.836409000000	15.497804000000
70 H	10.778682000000	3.465722000000	16.141615000000
71 H	9.514888000000	3.257333000000	18.292530000000
72 H	9.075004000000	2.034858000000	20.228841000000
73 H	9.787768000000	3.144780000000	21.118958000000
74 H	8.424281000000	3.499153000000	20.389794000000
75 H	11.211629000000	1.766292000000	18.924148000000
76 H	11.899759000000	2.889587000000	19.799633000000
77 H	11.891557000000	3.048944000000	18.216931000000
78 H	10.764968000000	5.182981000000	21.026289000000
79 H	11.177790000000	7.478604000000	20.992147000000
80 H	11.010161000000	8.660961000000	19.019256000000
81 H	9.677740000000	7.406169000000	15.968469000000
82 H	11.554344000000	8.494919000000	15.002752000000
83 H	12.286472000000	8.409111000000	16.429379000000
84 H	11.977734000000	7.065169000000	15.595351000000
85 H	9.632120000000	9.724080000000	15.883115000000
86 H	10.423813000000	9.827717000000	17.270723000000
87 H	8.920478000000	9.239325000000	17.243898000000
88 H	4.645718000000	5.219756000000	12.759168000000
89 H	3.483388000000	3.371000000000	13.537106000000
90 H	4.557336000000	1.889988000000	14.985681000000
91 H	7.936143000000	2.111750000000	16.097719000000
92 H	6.916098000000	1.409691000000	18.126700000000
93 H	6.620435000000	2.959793000000	17.812110000000
94 H	5.509063000000	1.855443000000	17.526785000000
95 H	7.322835000000	-0.152670000000	16.195266000000
96 H	5.890003000000	0.183873000000	15.627054000000
97 H	7.141085000000	0.359945000000	14.695479000000
98 H	8.022295000000	6.101231000000	13.573686000000
99 H	6.968294000000	8.200722000000	13.522474000000
100 H	6.543899000000	7.406169000000	14.827167000000
101 H	5.562512000000	7.478604000000	13.585880000000

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102 H       7.644734000000       7.006107000000      11.520319000000
103 H       7.482750000000       5.415887000000      11.432526000000
104 H       6.185362000000       6.357538000000      11.473984000000
END

GUIBONDS
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27 17 18 1.0
28 18 70 1.0
29 18 69 1.0
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35 21 23 1.0
36 21 22 1.0
37 22 73 1.0
38 22 74 1.0
39 22 72 1.0
40 23 76 1.0
41 23 77 1.0
42 23 75 1.0
43 24 78 1.0
44 24 25 1.5
45 25 79 1.0
46 25 26 1.5
47 26 80 1.0
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49 27 28 1.0
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52 28 30 1.0
53 29 82 1.0
54 29 83 1.0
55 29 84 1.0
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68 35 36 1.5
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93 46 48 1.5
94 48 49 1.0
95 48 50 1.5
96 50 53 1.0
97 50 51 1.5
98 51 52 1.0
99 54 55 1.5
100 54 62 1.0
101 55 56 1.0
102 55 57 1.5
103 57 58 1.0
104 57 59 1.5
105 59 60 1.0
106 59 61 1.5
107 61 64 1.0
108 61 62 1.5
109 62 63 1.0
END

BASIS
type TZP
core None
createoutput None
END
```

```
XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# Ligand [(6-c')Mes]-
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 F       8.959916190000      20.063592600000      19.243064570000
2 C       8.145324480000      20.212785180000      18.168828040000
3 C       8.560180320000      19.778255510000      16.913724710000
4 F       9.779907450000      19.200667370000      16.774188990000
5 C       7.728936220000      19.926458400000      15.797912880000
6 F       8.207372330000      19.452525060000      14.624029800000
7 C       6.442885150000      20.528350550000      15.921604020000
8 C       6.050297340000      20.960058610000      17.217155440000
9 C       6.894521350000      20.801961680000      18.319540250000
10 F       6.496545560000      21.232674390000      19.542828860000
11 F       4.862980410000      21.577977670000      17.424718710000
12 B       5.398153560000      20.728781360000      14.671290250000
13 C       4.288984580000      19.691443430000      14.951063560000
14 C       3.041510350000      19.991073490000      15.562945040000
15 F       2.753118740000      21.217688930000      16.062832090000
16 C       2.057363850000      19.006466180000      15.708396050000
17 F       0.853936770000      19.338985300000      16.239429500000
18 C       2.297584200000      17.683671670000      15.339366700000
19 F       1.320420260000      16.755122250000      15.490763980000
20 C       3.556640820000      17.293051680000      14.894641800000
21 C       4.575757300000      18.232490690000      14.753343960000
22 F       5.832051860000      17.770860580000      14.534733280000
23 F       3.809156310000      15.981883960000      14.655348310000
24 C       6.128474960000      20.463056740000      13.204900050000
25 C       5.370425790000      20.819538570000      11.880458510000
26 N       6.282411170000      21.009103170000      10.703761260000
27 C       6.431252930000      19.733268920000      10.199610890000
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28	N	6.031130840000	18.414069430000	10.147808990000
29	C	5.909141310000	17.907768330000	8.795703770000
30	C	6.726032540000	16.805753240000	8.452071360000
31	C	7.637566600000	16.184679660000	9.478191930000
32	H	4.396796230000	18.333619880000	5.744382070000
33	H	5.297141600000	23.181300090000	10.087852890000
34	C	6.696718410000	16.280212370000	7.153564280000
35	C	5.865030090000	16.832999270000	6.179235080000
36	C	5.046556020000	17.918472050000	6.505949090000
37	C	5.047238620000	18.467193900000	7.801102280000
38	C	4.106155640000	19.613666610000	8.071299100000
39	H	10.800545590000	21.735835800000	11.836044290000
40	H	8.255943590000	25.124334200000	11.280877320000
41	C	4.800074300000	18.341573990000	10.992695380000
42	C	4.251652020000	19.732849720000	11.557281410000
43	C	7.482063710000	21.805072030000	10.929070020000
44	C	8.774769350000	21.260206480000	11.242031060000
45	C	9.096818500000	19.784137140000	11.221804850000
46	H	5.042379810000	17.702731400000	11.867215950000
47	H	8.420829200000	19.220939650000	11.892389430000
48	C	9.823085890000	22.132324990000	11.585565520000
49	C	9.637822460000	23.514470190000	11.616451020000
50	C	8.396552000000	24.049367360000	11.273738650000
51	C	7.329950980000	23.217376300000	10.913479010000
52	C	6.033120680000	23.884303570000	10.526879270000
53	H	3.977598090000	17.811967530000	10.464319410000
54	H	3.573936450000	20.179480880000	10.803558370000
55	C	4.926798190000	22.299985830000	14.605365620000
56	C	3.688026840000	22.700802370000	14.031458170000
57	F	2.828759900000	21.797091950000	13.495714220000
58	C	3.343421610000	24.052289780000	13.935144060000
59	F	2.147458910000	24.408138510000	13.403061350000
60	C	4.235278950000	25.037450750000	14.349451840000
61	F	3.899140210000	26.346977980000	14.241020620000
62	C	5.491885140000	24.677740440000	14.828344870000
63	C	5.850456350000	23.330321720000	14.932721790000
64	F	7.126200950000	23.052180200000	15.303858460000
65	F	6.383997420000	25.642049350000	15.166627360000
66	H	7.037338690000	21.088504250000	13.266012890000
67	H	6.465642660000	19.421579500000	13.097902970000
68	H	4.854885490000	21.782534590000	12.011072770000
69	H	3.610074740000	19.540818790000	12.436647330000
70	H	8.367568430000	16.939481060000	9.837827920000
71	H	4.643933630000	20.488028560000	8.484872450000
72	H	7.326336370000	15.436481540000	6.895420940000
73	C	10.778918330000	24.409097810000	12.004783230000
74	C	5.855927020000	16.251777300000	4.795173210000
75	H	5.148454070000	16.789804880000	4.128912550000
76	H	5.552204660000	15.184688030000	4.840771260000
77	H	8.205291230000	15.325580770000	9.061659600000
78	H	7.038105640000	15.819197150000	10.338561030000
79	H	3.300152300000	19.282901210000	8.753132660000
80	H	3.608556930000	19.963290220000	7.141781570000
81	H	10.131946460000	19.578090790000	11.568033150000
82	H	9.023230490000	19.397287650000	10.184543130000
83	H	6.229075870000	24.665834600000	9.762434130000
84	H	5.582000820000	24.362795650000	11.421788200000
85	H	11.114847330000	24.159052230000	13.033208930000
86	H	10.486007770000	25.480406390000	11.982439870000
87	H	11.624992390000	24.261690070000	11.300921100000
88	H	6.873116300000	16.320648300000	4.355207610000

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END

GUIBONDS
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25 20 21 1.5
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39 29 37 1.5
40 29 30 1.5
41 30 34 1.5
42 30 31 1.0
43 31 70 1.0
44 51 52 1.0
45 55 63 1.5
46 60 62 1.5
47 48 39 1.0
48 48 49 1.5
49 49 50 1.5
50 50 40 1.0
51 50 51 1.5
52 34 72 1.0
53 34 35 1.5
54 62 63 1.5
55 35 36 1.5
56 36 32 1.0
57 36 37 1.5
58 37 38 1.0
```

```
59 38 71 1.0
60 56 57 1.0
61 52 33 1.0
62 62 65 1.0
63 60 61 1.0
64 55 56 1.5
65 56 58 1.5
66 58 59 1.0
67 58 60 1.5
68 41 46 1.0
69 41 53 1.0
70 41 42 1.0
71 42 69 1.0
72 42 54 1.0
73 43 44 1.5
74 43 51 1.5
75 44 48 1.5
76 44 45 1.0
77 45 47 1.0
78 73 49 1.0
79 74 35 1.0
80 75 74 1.0
81 76 74 1.0
82 77 31 1.0
83 78 31 1.0
84 79 38 1.0
85 80 38 1.0
86 81 45 1.0
87 82 45 1.0
88 83 52 1.0
89 84 52 1.0
90 85 73 1.0
91 86 73 1.0
92 87 73 1.0
93 88 74 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE
```

```
eor



#! /bin/sh

# ==============================
# Ligand [(7-c')Mes]-
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 F       1.168353730000       7.074794440000      11.746101380000
2 C       0.618141690000       8.143076920000      11.112912300000
3 C       0.731583700000       8.302543110000       9.703256090000
4 C       0.214193330000       9.500409550000       9.137701840000
5 F       0.409076310000       9.829393790000       7.837448500000
6 C      -0.458617700000      10.433578280000       9.933772310000
7 F      -0.949970640000      11.567486270000       9.374162560000
8 C      -0.599896870000      10.224536030000      11.303476650000
9 C      -0.052986230000       9.088334580000      11.892739950000
10 F      -0.158765260000       8.906704450000      13.232827580000
11 F      -1.243082780000      11.142282290000      12.067451220000
12 B       1.609739720000       7.215141620000       8.846005610000
13 C       3.166057860000       7.373138020000       9.422730910000
14 C       3.695702420000       8.788779750000       9.826548400000
15 N       4.885832630000       8.679494120000      10.718516900000
16 C       5.337380670000       9.961969780000      10.976302980000
17 N       5.477044980000      11.339680500000      10.964279530000
18 C       4.280487060000      11.855416020000      10.270494330000
19 C       4.146913970000      11.294015330000       8.823281840000
20 C       3.869339930000       9.755814810000       8.599611940000
21 C       5.691749370000      11.892641200000      12.287340990000
22 C       6.864629390000      12.664126790000      12.462134570000
23 C       7.169053520000      13.220911970000      13.710672190000
24 C       6.327177880000      13.022375830000      14.804262450000
25 C       5.166632800000      12.258564670000      14.651790170000
26 C       4.825274000000      11.684013980000      13.413279080000
27 C       3.542120250000      10.882218610000      13.366192020000
28 H       6.724686380000       4.553777530000      11.547706720000
29 C       8.536982310000       4.364570340000       9.525001180000
30 C       7.803506170000      12.893330270000      11.305918940000
31 H       8.068738400000      13.812383810000      13.836105320000
32 H       4.519030570000      12.115812110000      15.509126250000
33 C       5.910833690000       7.690503450000      10.434703060000
34 C       6.880834040000       7.792132390000       9.383898830000
35 C       7.170037390000       9.027928930000       8.570257990000
36 H       6.646880200000       9.931049860000       8.902658160000
37 H       8.421994980000       6.746509400000       8.291154370000
38 C       7.702355050000       6.687775540000       9.100863290000
39 C       7.637831100000       5.518969450000       9.859229740000
40 C       6.756434380000       5.449309940000      10.937505830000
41 C       5.907214400000       6.520250020000      11.240061710000
42 C       4.997573690000       6.365839850000      12.434794590000
43 H       3.681376960000       9.897189900000      12.886259200000
44 H       4.379130460000       7.263668600000      12.634859800000
45 C       1.164922260000       5.756643680000       9.100705370000
```

```
46 C      -0.074581910000       5.379449040000       9.686894080000
47 F      -1.039187420000       6.283218430000       9.991832970000
48 C      -0.373252820000       4.034205110000       9.931598710000
49 F      -1.551785720000       3.709292080000      10.520120540000
50 C       0.508449220000       3.017726240000       9.565321760000
51 F       0.185611140000       1.724777430000       9.818545520000
52 C       1.693253640000       3.313733000000       8.897799990000
53 C       2.034653970000       4.635503720000       8.619615090000
54 F       3.135801640000       4.862878450000       7.860659610000
55 F       2.503709340000       2.306650120000       8.486432310000
56 C       1.423436570000       7.400679410000       7.226630630000
57 C       0.105588900000       7.336417480000       6.693913420000
58 F      -0.972795670000       7.181623160000       7.501706730000
59 C      -0.129949480000       7.469326210000       5.323118110000
60 F      -1.400054350000       7.429095250000       4.848255840000
61 C       0.931216800000       7.645743040000       4.442205320000
62 F       0.696374650000       7.774919190000       3.112556070000
63 C       2.235583760000       7.671326110000       4.925703590000
64 C       2.491359620000       7.535011110000       6.294898350000
65 F       3.790973380000       7.489852850000       6.657354640000
66 F       3.268772220000       7.809552790000       4.057211740000
67 H       3.190790820000       6.766440130000      10.349978760000
68 H       3.916535380000       6.878194920000       8.789044100000
69 H       2.913691730000       9.260997110000      10.451619090000
70 H       8.182210310000      11.918441200000      10.932099420000
71 H       4.356921020000      12.962954440000      10.203895830000
72 H       3.343192480000      11.625853940000      10.808338430000
73 H       5.064910930000      11.574589650000       8.263330850000
74 H       3.324440730000      11.861596660000       8.334445840000
75 H       2.938734040000       9.699805380000       8.003152160000
76 H       4.645726710000       9.350856880000       7.929860770000
77 C       6.678330020000      13.631776110000      16.130615920000
78 H       7.662192340000      13.244705480000      16.470093010000
79 H       5.920352020000      13.391519130000      16.906323060000
80 H       6.738515290000      14.735930170000      16.029407320000
81 H       4.315118220000       5.504757730000      12.273273950000
82 H       5.608518180000       6.171562110000      13.341433550000
83 H       2.741483800000      11.459170010000      12.864717880000
84 H       3.165477540000      10.663329350000      14.388072190000
85 H       9.597834660000       4.684076740000       9.598882780000
86 H       8.332900370000       4.021463040000       8.488886650000
87 H       8.378838480000       3.508716460000      10.215301160000
88 H       8.676558130000      13.515023390000      11.597837730000
89 H       7.266361840000      13.414113860000      10.485265320000
90 H       6.922201450000       8.838645060000       7.504561710000
91 H       8.253518540000       9.264612650000       8.636076930000
END

GUIBONDS
1 1 2 1.0
2 2 9 1.5
3 2 3 1.5
4 3 4 1.5
5 3 12 1.0
6 4 5 1.0
7 4 6 1.5
8 6 7 1.0
9 6 8 1.5
10 8 11 1.0
11 8 9 1.5
12 9 10 1.0
```

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13 12 56 1.0
14 12 13 1.0
15 12 45 1.5
16 13 67 1.0
17 13 68 1.0
18 13 14 1.0
19 14 69 1.0
20 14 20 1.0
21 14 15 1.0
22 15 16 1.0
23 15 33 1.0
24 64 65 1.0
25 16 17 1.0
26 17 21 1.0
27 17 18 1.0
28 18 71 1.0
29 18 72 1.0
30 18 19 1.0
31 19 73 1.0
32 19 74 1.0
33 19 20 1.0
34 20 75 1.0
35 20 76 1.0
36 21 26 1.5
37 21 22 1.5
38 22 23 1.5
39 22 30 1.0
40 23 31 1.0
41 23 24 1.5
42 29 39 1.0
43 24 25 1.5
44 25 32 1.0
45 25 26 1.5
46 26 27 1.0
47 27 43 1.0
48 41 42 1.0
49 45 53 1.0
50 42 44 1.0
51 40 41 1.5
52 45 46 1.5
53 46 47 1.0
54 46 48 1.5
55 48 49 1.0
56 30 70 1.0
57 61 62 1.0
58 57 58 1.0
59 57 59 1.5
60 59 60 1.0
61 59 61 1.5
62 61 63 1.5
63 63 66 1.0
64 63 64 1.5
65 33 34 1.5
66 33 41 1.5
67 34 38 1.5
68 34 35 1.0
69 35 36 1.0
70 48 50 1.5
71 52 53 1.5
72 53 54 1.0
73 56 64 1.5
```

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74 56 57 1.5
75 50 51 1.0
76 50 52 1.5
77 52 55 1.0
78 38 37 1.0
79 38 39 1.5
80 40 28 1.0
81 39 40 1.5
82 77 24 1.0
83 78 77 1.0
84 79 77 1.0
85 80 77 1.0
86 81 42 1.0
87 82 42 1.0
88 83 27 1.0
89 84 27 1.0
90 85 29 1.0
91 86 29 1.0
92 87 29 1.0
93 88 30 1.0
94 89 30 1.0
95 90 35 1.0
96 91 35 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# Ligand [(I-c')Mes]-
# ==============================
```

```
"$ADFBIN/adf" <<eor

ATOMS
1 C       3.920437000000      12.772364000000       4.375612000000
2 B       4.380384000000      10.151484000000       4.712887000000
3 N       6.596246000000       9.031989000000       3.536984000000
4 N       7.449543000000      10.641415000000       2.441234000000
5 F       2.925026000000       9.334934000000       2.331219000000
6 F       1.628834000000       7.053020000000       1.889430000000
7 F       1.576738000000       5.096254000000       3.794419000000
8 F       2.889870000000       5.496167000000       6.158485000000
9 F       4.170435000000       7.750590000000       6.631864000000
10 F       2.553128000000      10.031212000000       6.958608000000
11 F       3.039799000000      10.588834000000       9.527302000000
12 F       5.524601000000      11.394849000000      10.317210000000
13 F       7.502594000000      11.644616000000       8.456385000000
14 F       7.074277000000      11.052683000000       5.931382000000
15 F       1.309874000000      10.317661000000       4.214205000000
16 F      -0.045116000000      12.460135000000       3.576746000000
17 F       1.149330000000      14.909969000000       3.458873000000
18 F       3.799185000000      15.119999000000       4.053583000000
19 F       5.208051000000      12.993669000000       4.736933000000
20 C       7.688041000000       9.340933000000       2.772693000000
21 C       5.678262000000      10.113850000000       3.708607000000
22 C       6.251987000000      11.099893000000       2.973549000000
23 H       5.890495000000      11.968391000000       2.843103000000
24 C       6.348497000000       7.642249000000       3.848483000000
25 C       6.764977000000       7.090164000000       5.061792000000
26 C       6.509950000000       5.733981000000       5.291409000000
27 H       6.785424000000       5.346878000000       6.113693000000
28 C       5.866136000000       4.935221000000       4.353609000000
29 C       5.486985000000       5.515188000000       3.142030000000
30 H       5.045405000000       4.981567000000       2.492626000000
31 C       5.739928000000       6.855179000000       2.862120000000
32 C       7.483820000000       7.900310000000       6.103006000000
33 H       6.837003000000       8.243387000000       6.753352000000
34 H       7.944726000000       8.650978000000       5.672061000000
35 H       8.140161000000       7.335086000000       6.561611000000
36 C       5.612011000000       3.472781000000       4.620632000000
37 H       6.412543000000       3.068558000000       5.015114000000
38 H       5.398831000000       3.018885000000       3.778231000000
39 H       4.859795000000       3.380458000000       5.241431000000
40 C       5.450124000000       7.409495000000       1.489761000000
41 H       6.282894000000       7.457502000000       0.974419000000
42 H       5.065565000000       8.307273000000       1.574787000000
43 H       4.813759000000       6.823623000000       1.027855000000
44 C       8.357877000000      11.456581000000       1.677729000000
45 C       8.465985000000      11.241753000000       0.301913000000
46 C       9.404905000000      11.992954000000      -0.408313000000
47 H       9.496387000000      11.852557000000      -1.343755000000
48 C      10.210890000000      12.941165000000       0.216415000000
49 C      10.040673000000      13.155724000000       1.579030000000
50 H      10.572567000000      13.813830000000       2.010132000000
51 C       9.113890000000      12.436054000000       2.333733000000
52 C       7.594588000000      10.232375000000      -0.395897000000
53 H       7.880945000000       9.327413000000      -0.150878000000
54 H       7.673820000000      10.348368000000      -1.365758000000
55 H       6.661231000000      10.363705000000      -0.125731000000
56 C      11.247899000000      13.727929000000      -0.552904000000
57 H      11.543163000000      13.207792000000      -1.329610000000
```

```
58 H      12.016230000000      13.911019000000       0.028290000000
59 H      10.857576000000      14.574153000000      -0.854974000000
60 C       8.960513000000      12.721140000000       3.804477000000
61 H       9.729228000000      13.241220000000       4.117706000000
62 H       8.914513000000      11.876102000000       4.298445000000
63 H       8.137712000000      13.231954000000       3.954255000000
64 C       3.576519000000       8.713471000000       4.528848000000
65 C       2.927363000000       8.420077000000       3.333927000000
66 C       2.253337000000       7.243982000000       3.075078000000
67 C       2.223053000000       6.247938000000       4.030322000000
68 C       2.878101000000       6.459188000000       5.222728000000
69 C       3.532933000000       7.662593000000       5.441501000000
70 C       4.790310000000      10.455500000000       6.294746000000
71 C       3.813158000000      10.401815000000       7.289125000000
72 C       4.031499000000      10.692077000000       8.623922000000
73 C       5.284331000000      11.101007000000       9.027991000000
74 C       6.280363000000      11.214090000000       8.088777000000
75 C       6.020889000000      10.897913000000       6.762624000000
76 C       3.404352000000      11.472224000000       4.362725000000
77 C       2.029338000000      11.459209000000       4.126507000000
78 C       1.272197000000      12.577860000000       3.816893000000
79 C       1.864299000000      13.816903000000       3.763300000000
80 C       3.203433000000      13.914978000000       4.062227000000
END

GUIBONDS
1 78 79 1.5
2 79 80 1.5
3 80 1 1.5
4 77 78 1.5
5 2 21 1.0
6 2 64 1.5
7 2 70 1.5
8 2 76 1.5
9 3 20 1.0
10 3 21 1.0
11 3 24 1.0
12 4 20 1.0
13 4 22 1.0
14 4 44 1.0
15 5 65 1.0
16 6 66 1.0
17 7 67 1.0
18 8 68 1.0
19 9 69 1.0
20 10 71 1.0
21 11 72 1.0
22 12 73 1.0
23 13 74 1.0
24 14 75 1.0
25 15 77 1.0
26 16 78 1.0
27 17 79 1.0
28 18 80 1.0
29 19 1 1.0
30 21 22 2.0
31 22 23 1.0
32 24 25 1.5
33 24 31 1.5
34 25 26 1.5
35 25 32 1.0
```

```
36 26 27 1.0
37 26 28 1.5
38 28 29 1.5
39 28 36 1.0
40 29 30 1.0
41 29 31 1.5
42 31 40 1.0
43 32 33 1.0
44 32 35 1.0
45 32 34 1.0
46 36 39 1.0
47 36 37 1.0
48 36 38 1.0
49 40 42 1.0
50 40 41 1.0
51 40 43 1.0
52 44 45 1.5
53 44 51 1.5
54 45 46 1.5
55 45 52 1.0
56 46 47 1.0
57 46 48 1.5
58 48 49 1.5
59 48 56 1.0
60 49 50 1.0
61 49 51 1.5
62 51 60 1.0
63 52 54 1.0
64 52 53 1.0
65 52 55 1.0
66 56 59 1.0
67 56 57 1.0
68 56 58 1.0
69 60 61 1.0
70 60 62 1.0
71 60 63 1.0
72 64 65 1.5
73 64 69 1.0
74 65 66 1.5
75 66 67 1.5
76 67 68 1.5
77 68 69 1.5
78 70 75 1.5
79 70 71 1.0
80 71 72 1.5
81 72 73 1.5
82 73 74 1.5
83 74 75 1.5
84 76 77 1.5
85 76 1 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
```

```
GGA Becke88 Perdew86
DISPERSION Grimme3
END



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# complex [(I-b)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 Au      -0.874154858400       0.562479185700      -0.206996189200
2 B        0.638099496500      -0.662966304600      -0.367781956700
3 Cl      -2.618535387000       1.976033743000      -0.021527697440
4 H        2.543519718000       2.836327166000       1.242523377000
5 H       -1.169929911000      -1.386705311000      -7.240825519000
6 H        1.295083282000      -3.079877940000       2.106293612000
7 H        2.716191074000       0.608177444700      -2.255948270000
8 H        0.563483060200      -1.497609652000      -7.618668299000
9 H        2.921139572000       1.344606126000       0.349598320000
10 H       1.340066178000       2.085180503000       0.171299418200
11 H       0.916670683500       0.859407911900       6.631846230000
12 N       1.143719453000      -1.378287309000      -1.426203128000
13 C       2.284708686000      -2.086021972000      -1.049416884000
14 C       2.525942627000      -1.799791114000       0.254687677000
15 N       1.509979152000      -0.937636703500       0.666713512700
16 C       0.773048968300      -1.275007261000      -2.824948224000
17 C       1.454534972000      -0.335904617400       1.978105178000
18 C       1.279158356000      -1.135939222000       3.121858377000
19 C       1.177784687000      -0.487067957000       4.363977504000
20 C       1.257888099000       0.900698178000       4.490982348000
21 C       1.521678186000       1.653497003000       3.334387393000
22 C       1.662342693000       1.061392928000       2.076742750000
23 C       1.678567853000      -0.624007422800      -3.687692813000
24 C       1.339116905000      -0.544643195000      -5.040265958000
25 C       0.142645369500      -1.075692950000      -5.543152943000
26 C      -0.732991800600      -1.695647201000      -4.646441279000
27 C      -0.437573686000      -1.808407697000      -3.281930338000
28 C       1.239732217000      -2.646374630000       3.109671920000
29 C       2.133962366000       1.878327566000       0.900912001000
```

```
30 C       1.123642964000       1.579058657000       5.830373227000
31 C      -1.419056894000      -2.439195174000      -2.336302032000
32 C       2.930315595000       0.042244950250      -3.173866989000
33 C      -0.183340498000      -0.965511280500      -7.010969697000
34 H      -0.175392075800       0.085036664340      -7.336245857000
35 H       2.820430704000      -2.707612177000      -1.755868820000
36 H       3.319886055000      -2.108786781000       0.922829503300
37 H       1.031202772000      -1.098121498000       5.257765349000
38 H       1.676957546000       2.731381524000       3.425223448000
39 H       2.046188113000       2.119450054000       6.088537865000
40 H       2.021645680000      -0.030435179960      -5.720806317000
41 H      -1.675095579000      -2.107628254000      -5.014931013000
42 H       2.090973946000      -3.041873154000       3.682752720000
43 H       0.327379419400      -3.020565838000       3.595088047000
44 H       0.310841764100       2.320106632000       5.817657905000
45 H      -2.217794786000      -2.959623196000      -2.877701584000
46 H      -0.924698377200      -3.155651722000      -1.666392067000
47 H      -1.877764253000      -1.657100590000      -1.708558298000
48 H       3.727020725000      -0.680864045700      -2.946223871000
49 H       3.322530281000       0.742729558300      -3.920265582000
END

GUIBONDS
1 1 2 1.0
2 1 3 3
3 28 6 1.0
4 33 8 1.0
5 33 34 1.0
6 2 15 1.0
7 2 12 1.0
8 23 32 1.0
9 24 40 1.0
10 23 24 1.5
11 29 9 1.0
12 30 11 1.0
13 30 39 1.0
14 24 25 1.5
15 25 26 1.5
16 25 33 1.0
17 26 41 1.0
18 29 4 1.0
19 26 27 1.5
20 27 31 1.0
21 28 43 1.0
22 28 42 1.0
23 30 44 1.0
24 31 47 1.0
25 31 45 1.0
26 31 46 1.0
27 32 7 1.0
28 32 49 1.0
29 29 10 1.0
30 32 48 1.0
31 33 5 1.0
32 12 13 1.0
33 12 16 1.0
34 13 35 1.0
35 13 14 2.0
36 14 36 1.0
37 14 15 1.0
38 15 17 1.0
```

```
39 16 23 1.5
40 16 27 1.5
41 17 22 1.5
42 17 18 1.5
43 18 19 1.5
44 18 28 1.0
45 19 37 1.0
46 19 20 1.5
47 20 21 1.5
48 20 30 1.0
49 21 38 1.0
50 21 22 1.5
51 22 29 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor









#! /bin/sh

# ==============================
# complex [(5-b)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor
```

```
ATOMS
1 B      11.498254040000       0.945563983300       2.620862591000
2 C      13.852288550000      -1.189093518000       2.590122756000
3 N      11.479366570000       2.304571067000       2.095957958000
4 C      12.323391930000       3.280073272000       2.851180468000
5 H      11.711972780000       3.974793034000       3.458079954000
6 H      12.937380870000       3.889517930000       2.166957867000
7 C      13.178200610000       2.377365174000       3.750384760000
8 H      14.202807800000       2.255903949000       3.346686078000
9 H      13.272136730000       2.781268082000       4.771531677000
10 N      12.451333580000       1.070180049000       3.718191674000
11 C      10.659679610000       2.762895060000       1.040310574000
12 C      10.961400950000       2.388369903000      -0.293606321300
13 C      10.174775130000       2.881858532000      -1.342093604000
14 H      10.416336120000       2.582930254000      -2.367765474000
15 C       9.096678014000       3.749440801000      -1.119667757000
16 C      12.640544260000       0.120618580400       5.971742413000
17 C       8.802916711000       4.100923523000       0.204561638200
18 H       7.943147844000       4.749110931000       0.408367335700
19 C       9.555688316000       3.619661468000       1.283310821000
20 C      12.103314640000       1.445589813000      -0.553727935700
21 H      13.049011640000       1.856554174000      -0.167786774700
22 C      13.800791690000      -2.006181127000       6.331386665000
23 C       8.261717178000       4.278843134000      -2.263692120000
24 C      14.025378850000      -2.081152085000       4.947545485000
25 C      13.105967010000      -0.894931591600       6.820398614000
26 H      14.564550840000      -2.943590860000       4.540559335000
27 C      13.592569950000      -1.084374090000       4.067222599000
28 C      11.828683300000       1.263027651000       6.526144237000
29 H      12.887453360000      -1.117389107000       2.050811337000
30 C       9.147397224000       3.933212735000       2.699498259000
31 H       9.302477670000       3.043563816000       3.330079674000
32 H      12.895630090000      -0.825166594800       7.893438017000
33 H      12.443332720000       2.162051200000       6.702715187000
34 C      12.880821530000       0.035154718770       4.577913607000
35 C      14.309717800000      -3.087607574000       7.256883421000
36 H      14.068101350000      -4.092339934000       6.875861662000
37 H      13.870660060000      -2.994286062000       8.261000144000
38 H      15.406474040000      -3.041250194000       7.370217096000
39 H      14.378159350000      -2.122479514000       2.339133314000
40 H      14.449995600000      -0.335399672200       2.233981058000
41 H      12.212501050000       1.231595707000      -1.627482355000
42 H      11.934467570000       0.511742436000       0.014088871270
43 H       8.632086210000       3.910942472000      -3.231413970000
44 H       8.272358904000       5.380774357000      -2.298809321000
45 H       7.207393267000       3.970058069000      -2.171619929000
46 H      11.360313120000       0.988894080600       7.482645337000
47 H      11.049790390000       1.546841469000       5.802275334000
48 H       8.091214351000       4.235219934000       2.748066363000
49 H       9.748712711000       4.747544544000       3.136573082000
50 Au      10.359769150000      -0.513809569800       2.086320398000
51 Cl       8.923780081000      -2.354532917000       1.412100156000
END

GUIBONDS
1 34 16 1.5
2 1 3 1.0
3 1 10 1.0
4 3 11 1.0
5 3 4 1.0
6 4 6 1.0
```

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

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END
```

```
RELATIVISTIC Scalar ZORA


GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# complex [(I-c)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 Au      -0.874154858400       0.562479185700      -0.206996189200
2 C        0.638099496500      -0.662966304600      -0.367781956700
3 Cl      -2.618535387000       1.976033743000      -0.021527697440
4 H        2.543519718000       2.836327166000       1.242523377000
5 H       -1.169929911000      -1.386705311000      -7.240825519000
6 H        1.295083282000      -3.079877940000       2.106293612000
7 H        2.716191074000       0.608177444700      -2.255948270000
8 H        0.563483060200      -1.497609652000      -7.618668299000
9 H        2.921139572000       1.344606126000       0.349598320000
10 H       1.340066178000       2.085180503000       0.171299418200
11 H       0.916670683500       0.859407911900       6.631846230000
12 N       1.143719453000      -1.378287309000      -1.426203128000
13 C       2.284708686000      -2.086021972000      -1.049416884000
14 C       2.525942627000      -1.799791114000       0.254687677000
15 N       1.509979152000      -0.937636703500       0.666713512700
16 C       0.773048968300      -1.275007261000      -2.824948224000
17 C       1.454534972000      -0.335904617400       1.978105178000
18 C       1.279158356000      -1.135939222000       3.121858377000
19 C       1.177784687000      -0.487067957000       4.363977504000
20 C       1.257888099000       0.900698178000       4.490982348000
21 C       1.521678186000       1.653497003000       3.334387393000
22 C       1.662342693000       1.061392928000       2.076742750000
23 C       1.678567853000      -0.624007422800      -3.687692813000
24 C       1.339116905000      -0.544643195000      -5.040265958000
25 C       0.142645369500      -1.075692950000      -5.543152943000
26 C      -0.732991800600      -1.695647201000      -4.646441279000
27 C      -0.437573686000      -1.808407697000      -3.281930338000
28 C       1.239732217000      -2.646374630000       3.109671920000
29 C       2.133962366000       1.878327566000       0.900912001000
30 C       1.123642964000       1.579058657000       5.830373227000
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31 C      -1.419056894000      -2.439195174000      -2.336302032000
32 C       2.930315595000       0.042244950250      -3.173866989000
33 C      -0.183340498000      -0.965511280500      -7.010969697000
34 H      -0.175392075800       0.085036664340      -7.336245857000
35 H       2.820430704000      -2.707612177000      -1.755868820000
36 H       3.319886055000      -2.108786781000       0.922829503300
37 H       1.031202772000      -1.098121498000       5.257765349000
38 H       1.676957546000       2.731381524000       3.425223448000
39 H       2.046188113000       2.119450054000       6.088537865000
40 H       2.021645680000      -0.030435179960      -5.720806317000
41 H      -1.675095579000      -2.107628254000      -5.014931013000
42 H       2.090973946000      -3.041873154000       3.682752720000
43 H       0.327379419400      -3.020565838000       3.595088047000
44 H       0.310841764100       2.320106632000       5.817657905000
45 H      -2.217794786000      -2.959623196000      -2.877701584000
46 H      -0.924698377200      -3.155651722000      -1.666392067000
47 H      -1.877764253000      -1.657100590000      -1.708558298000
48 H       3.727020725000      -0.680864045700      -2.946223871000
49 H       3.322530281000       0.742729558300      -3.920265582000
END

GUIBONDS
1 1 2 1.0
2 1 3 3
3 28 6 1.0
4 33 8 1.0
5 33 34 1.0
6 2 15 1.0
7 2 12 1.0
8 23 32 1.0
9 24 40 1.0
10 23 24 1.5
11 29 9 1.0
12 30 11 1.0
13 30 39 1.0
14 24 25 1.5
15 25 26 1.5
16 25 33 1.0
17 26 41 1.0
18 29 4 1.0
19 26 27 1.5
20 27 31 1.0
21 28 43 1.0
22 28 42 1.0
23 30 44 1.0
24 31 47 1.0
25 31 45 1.0
26 31 46 1.0
27 32 7 1.0
28 32 49 1.0
29 29 10 1.0
30 32 48 1.0
31 33 5 1.0
32 12 13 1.0
33 12 16 1.0
34 13 35 1.0
35 13 14 2.0
36 14 36 1.0
37 14 15 1.0
38 15 17 1.0
39 16 23 1.5
```

```
40 16 27 1.5
41 17 22 1.5
42 17 18 1.5
43 18 19 1.5
44 18 28 1.0
45 19 37 1.0
46 19 20 1.5
47 20 21 1.5
48 20 30 1.0
49 21 38 1.0
50 21 22 1.5
51 22 29 1.0
END

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# complex [(5-c)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 N      -3.456671650000       9.079978932000      11.664226280000
2 N      -1.662170124000       7.905968067000      11.329006230000
3 C      -3.004887867000       7.836162963000      11.417477090000
4 C      -1.137533110000       9.303412050000      11.391056170000
5 C      -2.370182750000      10.081004700000      11.871499850000
6 C      -4.827101685000       9.381320170000      11.956965700000
```

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7 C      -5.575097896000      10.138751650000      11.037417970000
8 C      -6.917391680000      10.410153830000      11.339287520000
9 C      -7.519641754000       9.956136094000      12.518043970000
10 C      -6.738560229000       9.215470427000      13.418510300000
11 C      -5.393819789000       8.922670099000      13.165529510000
12 C      -4.963616853000      10.662300280000       9.761756674000
13 C      -8.958745827000      10.278879800000      12.832911410000
14 C      -4.575474764000       8.143206035000      14.166800500000
15 C      -0.821013760700       6.815713532000      10.934777090000
16 C       0.132932601700       6.328759556000      11.853977310000
17 C       0.965735063400       5.278184494000      11.453896860000
18 C       0.869145266800       4.695620957000      10.182107730000
19 C      -0.095491590360       5.195595652000       9.300371711000
20 C      -0.943392814600       6.257861861000       9.646748339000
21 C       0.251911895300       6.903599576000      13.244014660000
22 C       1.789680880000       3.569734923000       9.783271294000
23 C      -1.955962900000       6.759946084000       8.645652854000
24 H      -2.165398798000       7.829801188000       8.769005110000
25 H      -1.603441053000       6.590182316000       7.620620859000
26 H      -0.803574628100       9.606824164000      10.386969320000
27 H      -0.286286700700       9.375323707000      12.077223400000
28 H      -2.319112203000      10.350617920000      12.937474460000
29 H      -2.562086184000      10.991545190000      11.291780860000
30 H      -7.508493996000      10.993652330000      10.628670090000
31 H      -7.189235525000       8.862428836000      14.349228470000
32 H      -4.577386681000      11.683851770000       9.901589008000
33 H      -5.708686668000      10.710301180000       8.956985828000
34 H      -4.126818037000      10.036375540000       9.425582310000
35 H      -9.020249537000      11.143945780000      13.510953940000
36 H      -9.458997110000       9.438704520000      13.333359200000
37 H      -9.524907265000      10.529962190000      11.926699130000
38 H      -4.327591849000       7.135682954000      13.799742110000
39 H      -5.117200810000       8.034852289000      15.113749050000
40 H      -3.617140801000       8.640158419000      14.374277280000
41 H       1.702937913000       4.892402894000      12.162558180000
42 H      -0.181496291200       4.759557619000       8.301905866000
43 H       0.956088550400       7.749949354000      13.268399870000
44 H       0.632112419500       6.150631054000      13.945594920000
45 H      -0.715802370900       7.268488648000      13.613947410000
46 H       2.812355674000       3.942719613000       9.622189349000
47 H       1.460723221000       3.085497181000       8.855221409000
48 H       1.846998472000       2.804377635000      10.570433900000
49 H      -2.917997653000       6.230770831000       8.745834438000
50 Au      -4.209211949000       6.152273727000      11.093110460000
51 Cl      -5.605784810000       4.199584803000      10.716958630000
END

GUIBONDS
1 1 6 1.0
2 1 5 1.0
3 1 3 1.0
4 2 15 1.0
5 2 4 1.0
6 2 3 1.0
7 23 25 1.0
8 23 24 1.0
9 4 27 1.0
10 4 26 1.0
11 4 5 1.0
12 5 29 1.0
13 5 28 1.0
```

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

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END
```

```
SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# complex [(6-c)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 C     -11.286657270000       0.736729843600      -2.414231088000
2 C     -10.260560510000      -1.021950789000      -0.921862479400
3 H      -9.239989218000      -1.427539358000      -0.905432419500
4 H     -10.955494890000      -1.877317945000      -0.853768710000
5 C     -10.491665320000      -0.044161245500       0.226236811400
6 H      -9.706573697000       0.727510501600       0.205024212200
7 H     -10.435720800000      -0.561401792900       1.193795477000
8 C     -11.855621650000       0.616562373100       0.050924060860
9 H     -12.667273360000      -0.108975919800       0.233134745100
10 H     -11.992918030000       1.446714475000       0.758176483600
11 C      -9.723437328000      -0.816572273600      -3.338385589000
12 C     -10.355201030000      -1.674190580000      -4.257938635000
13 C      -9.602401038000      -2.172980018000      -5.326802656000
14 H     -10.085045720000      -2.837564981000      -6.049094577000
15 C      -8.250318556000      -1.841680669000      -5.497167971000
16 C      -7.656821524000      -0.975964674100      -4.571642751000
17 H      -6.609316541000      -0.689618861800      -4.700752268000
18 C      -8.375300417000      -0.449894004800      -3.488630673000
19 C     -11.819115380000      -2.001890930000      -4.110972526000
20 H     -12.052014480000      -2.374938503000      -3.103165446000
21 H     -12.132445120000      -2.756942398000      -4.843319756000
22 H     -12.419827730000      -1.091372312000      -4.256724615000
23 C      -7.469348235000      -2.395872972000      -6.666066694000
24 H      -6.416624146000      -2.085576716000      -6.630116708000
25 H      -7.891451982000      -2.049161260000      -7.621738752000
26 H      -7.499379647000      -3.495856257000      -6.677004815000
27 C      -7.737754750000       0.521689830900      -2.526553906000
28 H      -8.380874751000       1.403570227000      -2.393732440000
29 H      -6.755765573000       0.849576641500      -2.890456716000
30 H      -7.593258563000       0.075952689010      -1.529373037000
31 C     -12.871390380000       2.266894128000      -1.497718557000
32 C     -12.400446220000       3.573601050000      -1.271938144000
33 C     -13.297653300000       4.638104466000      -1.409399022000
34 H     -12.939644980000       5.658180059000      -1.242942449000
35 C     -14.637975700000       4.430309904000      -1.766976134000
36 C     -15.068971900000       3.118723737000      -1.997563148000
37 H     -16.107105860000       2.940191094000      -2.291044514000
```

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38 C     -14.203100240000       2.023242428000      -1.868302305000
39 C     -10.947836550000       3.803936508000      -0.939316856900
40 H     -10.660065800000       3.305132114000      -0.000861965783
41 H     -10.729192580000       4.874430214000      -0.836954088900
42 H     -10.310726650000       3.382653511000      -1.731367361000
43 C     -15.580609150000       5.602394468000      -1.911179099000
44 H     -15.636881430000       6.182626567000      -0.977760947100
45 H     -16.596235790000       5.272785841000      -2.167210735000
46 H     -15.238379060000       6.288522920000      -2.700891542000
47 C     -14.666971510000       0.618626458100      -2.161403315000
48 H     -14.059253820000       0.180608215400      -2.966769576000
49 H     -15.721572550000       0.605021750500      -2.464642404000
50 H     -14.554154640000      -0.037030915690      -1.285140971000
51 N     -10.464959260000      -0.315902562900      -2.209907011000
52 N     -11.967570560000       1.157797850000      -1.326936915000
53 Au     -11.899681360000       1.338888656000      -4.450331830000
54 Cl     -12.573726090000       2.000995608000      -6.689121255000
END

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

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42 35 36 1.5
43 35 43 1.0
44 36 37 1.0
45 36 38 1.5
46 38 47 1.0
47 39 40 1.0
48 39 42 1.0
49 39 41 1.0
50 43 44 1.0
51 43 45 1.0
52 43 46 1.0
53 47 49 1.0
54 47 48 1.0
55 53 1 1.0
56 54 53 1.0
END

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor




#! /bin/sh

# ==============================
# complex [(7-c)Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 C       1.072096799000       3.560701808000      -3.789847143000
2 C      -1.096388220000       4.715872215000      -2.954114512000
3 H      -0.959758095500       5.797988749000      -2.791804738000
4 H      -1.706859189000       4.347916211000      -2.118108466000
```

```
5 C      -1.812606711000       4.433557688000      -4.277083168000
6 H      -2.885462757000       4.643633394000      -4.153728153000
7 H      -1.722038447000       3.357658436000      -4.486875104000
8 C      -1.248813429000       5.241098534000      -5.457244511000
9 H      -1.517166939000       4.755692338000      -6.407334790000
10 H      -1.694608146000       6.248825210000      -5.480908560000
11 C       0.268172215100       5.389340871000      -5.347700033000
12 H       0.694815791300       5.767887491000      -6.285420951000
13 H       0.523873881100       6.115425746000      -4.559414872000
14 C       1.861833897000       3.595506126000      -6.025500395000
15 C       1.431112343000       2.530808518000      -6.837466583000
16 C       2.295565856000       2.060794417000      -7.833076734000
17 H       1.970166821000       1.231813549000      -8.467843853000
18 C       3.566792237000       2.618133979000      -8.031384823000
19 C       3.971585218000       3.662170729000      -7.191563558000
20 H       4.967934654000       4.094900793000      -7.316842015000
21 C       3.137747605000       4.163456198000      -6.182431023000
22 C       0.087385899450       1.887970431000      -6.603998900000
23 H       0.015830685550       1.521160726000      -5.569308862000
24 H      -0.072947434650       1.045992070000      -7.289234913000
25 H      -0.734288070200       2.605535216000      -6.742260463000
26 C       4.479537793000       2.078570298000      -9.106921128000
27 H       5.381898028000       2.694553346000      -9.216186059000
28 H       3.970667201000       2.044520221000     -10.081673520000
29 H       4.800450749000       1.051745130000      -8.872554099000
30 C       3.603529689000       5.251359836000      -5.249573848000
31 H       3.022133069000       6.177283187000      -5.378262580000
32 H       4.661146841000       5.491033832000      -5.416492558000
33 H       3.470829823000       4.930270455000      -4.205099514000
34 C       0.488664343300       3.492144667000      -1.506276487000
35 C       1.108284887000       4.344163515000      -0.576099026200
36 C       1.333488008000       3.864694399000       0.721306257600
37 H       1.820411547000       4.519219370000       1.449607020000
38 C       0.959942075500       2.570568740000       1.104501053000
39 C       0.345712370600       1.747293831000       0.150835400600
40 H       0.050239724170       0.732307583100       0.430953574500
41 C       0.097796942710       2.186770993000      -1.154956610000
42 C       1.536532942000       5.733698599000      -0.977248499900
43 H       2.196314987000       6.177116016000      -0.220625632300
44 H       0.671174489100       6.403976650000      -1.099334046000
45 H       2.066816324000       5.713049868000      -1.940148765000
46 C       1.249733259000       2.060551084000       2.496186680000
47 H       0.514902959700       1.305863142000       2.809069360000
48 H       1.240011984000       2.874941232000       3.233740856000
49 H       2.244220444000       1.588525119000       2.540467777000
50 C      -0.540931703100       1.286928005000      -2.179066302000
51 H      -0.767857719700       0.299957771000      -1.756794979000
52 H       0.135801965800       1.168386157000      -3.039577562000
53 H      -1.475480261000       1.719530635000      -2.568395554000
54 N       0.213463431700       3.986443204000      -2.837142358000
55 N       0.970385865000       4.118286874000      -5.016010446000
56 Au       2.677020074000       2.409683184000      -3.221231026000
57 Cl       4.574602158000       1.048767864000      -2.548927726000
END

GUIBONDS
1 1 54 1.0
2 1 55 1.0
3 50 53 1.0
4 2 4 1.0
5 2 3 1.0
```

```
6 2 54 1.0
7 2 5 1.0
8 5 7 1.0
9 5 6 1.0
10 5 8 1.0
11 8 9 1.0
12 8 10 1.0
13 8 11 1.0
14 11 13 1.0
15 11 12 1.0
16 11 55 1.0
17 14 15 1.5
18 14 21 1.5
19 14 55 1.0
20 15 16 1.5
21 15 22 1.0
22 16 17 1.0
23 16 18 1.5
24 18 19 1.5
25 18 26 1.0
26 19 20 1.0
27 19 21 1.5
28 21 30 1.0
29 22 23 1.0
30 22 24 1.0
31 22 25 1.0
32 26 28 1.0
33 26 27 1.0
34 26 29 1.0
35 30 33 1.0
36 30 32 1.0
37 30 31 1.0
38 34 41 1.5
39 34 35 1.5
40 34 54 1.0
41 35 36 1.5
42 35 42 1.0
43 36 37 1.0
44 36 38 1.5
45 38 39 1.5
46 38 46 1.0
47 39 40 1.0
48 39 41 1.5
49 41 50 1.0
50 42 45 1.0
51 42 44 1.0
52 42 43 1.0
53 46 47 1.0
54 46 49 1.0
55 46 48 1.0
56 50 51 1.0
57 50 52 1.0
58 56 1 1.0
59 57 56 1.0
END

BASIS
type TZP
core None
createoutput None
END
```

```
XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor
#! /bin/sh

# ==============================
# complex [(5-c')Mes]--AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 F      13.780793710000       2.477641735000      12.325353540000
2 C      13.587488700000       1.840374901000      13.512008270000
3 C      12.299875870000       1.793706307000      14.069373760000
4 C      12.238033130000       1.081616735000      15.270541690000
5 F      11.055420190000       0.893127389900      15.940296320000
6 C      13.346679350000       0.500551208600      15.895998780000
7 F      13.208422330000      -0.164400355600      17.071413570000
8 C      14.603025250000       0.601815716200      15.306857360000
9 C      14.722722450000       1.279887023000      14.093300460000
10 F      15.937207940000       1.385361463000      13.502347960000
11 F      15.687454550000       0.048721323750      15.896653180000
12 B      11.030502410000       2.426326644000      13.208265710000
13 C       9.577839662000       2.505204662000      14.022160020000
14 C       9.424061714000       3.732494272000      14.894734950000
15 N       8.077614337000       3.920260646000      15.563068280000
16 C       8.160470949000       4.676607623000      16.671572400000
17 N       9.483520131000       4.795757253000      16.953911930000
18 C      10.317322950000       3.885892490000      16.116676710000
19 C      10.004573660000       5.493909429000      18.079971560000
20 C       9.628088004000       5.118504108000      19.388221030000
21 C       8.725277554000       3.935869058000      19.645691220000
22 H       7.530748066000       6.208413358000      14.339895280000
23 H       9.848252267000       5.572738695000      21.480120030000
24 C      10.135072910000       5.858240559000      20.464541660000
25 C      11.012471600000       6.935151986000      20.279756280000
26 C      11.393647920000       7.257835521000      18.971920100000
27 C      10.914053530000       6.551911227000      17.860288850000
28 C      11.384772060000       6.920197643000      16.475477140000
29 H      12.088682450000       8.085520988000      18.806833830000
30 H       4.482087975000       1.163745424000      14.865172180000
31 C       6.851718528000       3.603964036000      14.901780330000
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32 C       6.352216485000       4.444099462000      13.890103430000
33 C       5.159152424000       4.076657070000      13.251952340000
34 C       4.474856700000       2.901463331000      13.583508210000
35 C       5.003502684000       2.085272310000      14.594265970000
36 C       6.188851784000       2.414134841000      15.262254360000
37 C       6.745646708000       1.531780692000      16.349345110000
38 H      10.624390010000       6.715007460000      15.710130940000
39 H       6.817202101000       2.076150976000      17.302757450000
40 C       7.090930930000       5.690647419000      13.476114600000
41 H       8.902323520000       3.130051229000      18.921974260000
42 H       4.762301052000       4.723637582000      12.465171890000
43 C      11.284100350000       3.995877530000      12.726026680000
44 C      10.394507540000       4.591670130000      11.819458970000
45 F       9.425406206000       3.839909684000      11.219371510000
46 C      10.376495040000       5.949360115000      11.503991560000
47 F       9.470922334000       6.451618197000      10.626881440000
48 C      11.283949150000       6.808681498000      12.124037260000
49 F      11.278583360000       8.134173956000      11.848132350000
50 C      12.185582600000       6.276529232000      13.040520190000
51 C      12.163488540000       4.905736636000      13.319363770000
52 F      13.049388780000       4.511552458000      14.286717750000
53 F      13.062918440000       7.099230492000      13.670674100000
54 C      10.892889840000       1.372180922000      11.933698090000
55 C      11.316803300000       1.600079600000      10.618320870000
56 F      11.875283970000       2.786733880000      10.251131120000
57 C      11.208749640000       0.657364085500       9.591404737000
58 F      11.625457220000       0.949699696400       8.334847987000
59 C      10.667112160000      -0.597739967400       9.859119752000
60 F      10.552868930000      -1.522659014000       8.877885763000
61 C      10.251553910000      -0.887669773700      11.157399140000
62 C      10.380184080000       0.085795332110      12.148662210000
63 F       9.989511113000      -0.298627649800      13.401047470000
64 F       9.737823252000      -2.110995346000      11.441827400000
65 H       9.396177249000       1.602207190000      14.610401050000
66 H       8.787096018000       2.549893669000      13.257126210000
67 H       9.551100638000       4.637997799000      14.275440310000
68 H      10.460610510000       2.936814243000      16.653325040000
69 H      11.293523070000       4.314143091000      15.880462590000
70 C      11.569637430000       7.690832830000      21.461391910000
71 C       3.212931256000       2.504119399000      12.857444320000
72 H       2.756095339000       3.359172411000      12.341471540000
73 H       2.469742182000       2.078391660000      13.546300900000
74 H       7.660643609000       4.204070213000      19.562615910000
75 H       8.888608394000       3.541066213000      20.656616870000
76 H      12.277676560000       6.342635846000      16.192790720000
77 H      11.664403890000       7.979567777000      16.416553920000
78 H       7.763879616000       1.202205954000      16.099718590000
79 H       6.119121930000       0.643956784700      16.497982070000
80 H       6.430696918000       6.387688125000      12.944507640000
81 H       7.916634369000       5.440926086000      12.793539610000
82 H      12.465824930000       7.187186202000      21.856171010000
83 H      10.841194310000       7.751078593000      22.281635080000
84 H      11.863506050000       8.712227338000      21.184404280000
85 H       3.428944572000       1.737375828000      12.097625360000
86 Au       6.611676178000       5.845295981000      17.417382070000
87 Cl       4.801103663000       7.211523654000      18.289247370000
END

GUIBONDS
1 1 2 1.0
2 2 9 1.5
```

```
3 2 3 1.5
4 3 4 1.5
5 3 12 1.0
6 4 5 1.0
7 4 6 1.5
8 6 7 1.0
9 6 8 1.5
10 8 11 1.0
11 8 9 1.5
12 9 10 1.0
13 12 43 1.5
14 12 54 1.5
15 12 13 1.0
16 13 65 1.0
17 13 66 1.0
18 13 14 1.0
19 14 67 1.0
20 14 15 1.0
21 14 18 1.0
22 15 16 1.0
23 15 31 1.0
24 62 63 1.0
25 16 17 1.0
26 17 19 1.0
27 17 18 1.0
28 18 68 1.0
29 18 69 1.0
30 19 20 1.5
31 19 27 1.5
32 20 24 1.5
33 20 21 1.0
34 21 41 1.0
35 55 56 1.0
36 43 44 1.0
37 44 45 1.0
38 44 46 1.5
39 46 47 1.0
40 55 57 1.5
41 57 58 1.0
42 57 59 1.5
43 24 23 1.0
44 24 25 1.5
45 46 48 1.5
46 25 26 1.5
47 26 29 1.0
48 26 27 1.5
49 27 28 1.0
50 28 38 1.0
51 50 51 1.5
52 59 60 1.0
53 51 52 1.0
54 54 55 1.5
55 54 62 1.0
56 59 61 1.5
57 61 64 1.0
58 61 62 1.5
59 31 32 1.5
60 31 36 1.5
61 32 33 1.5
62 32 40 1.0
63 33 42 1.0
```

```
64 33 34 1.5
65 43 51 1.5
66 34 35 1.5
67 35 30 1.0
68 35 36 1.5
69 36 37 1.0
70 37 39 1.0
71 40 22 1.0
72 48 49 1.0
73 48 50 1.5
74 50 53 1.0
75 70 25 1.0
76 71 34 1.0
77 72 71 1.0
78 73 71 1.0
79 74 21 1.0
80 75 21 1.0
81 76 28 1.0
82 77 28 1.0
83 78 37 1.0
84 79 37 1.0
85 80 40 1.0
86 81 40 1.0
87 82 70 1.0
88 83 70 1.0
89 84 70 1.0
90 85 71 1.0
91 86 16 1.0
92 87 86 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor
```

```
#! /bin/sh

# ==============================
# complex [(6-c')Mes]-AuCl
# ==============================

"$ADFBIN/adf" <<eor

ATOMS
1 F       8.889561775000      18.684204950000      19.033770980000
2 C       8.115940997000      19.106636770000      18.008782910000
3 C       8.297874988000      18.597680290000      16.726152050000
4 F       9.263649372000      17.670542630000      16.504086880000
5 C       7.488134808000      19.047562290000      15.678551830000
6 F       7.779866514000      18.482161390000      14.463773140000
7 C       6.473628423000      19.999846510000      15.825837970000
8 C       6.337924280000      20.475638670000      17.138368450000
9 C       7.122029152000      20.062491310000      18.214939940000
10 F       6.935296191000      20.578904610000      19.452888220000
11 F       5.400417711000      21.420213570000      17.419850110000
12 B       5.428849848000      20.526350450000      14.644887390000
13 C       4.015700090000      19.740474650000      15.011328900000
14 C       2.962725971000      20.261977690000      15.779824980000
15 F       2.994577177000      21.535622530000      16.246494760000
16 C       1.818228892000      19.537376070000      16.127597700000
17 F       0.832499032100      20.110784320000      16.856318360000
18 C       1.686306217000      18.210058490000      15.724231930000
19 F       0.585666054000      17.496071500000      16.048192760000
20 C       2.716320193000      17.629538530000      14.987264760000
21 C       3.840823678000      18.392505130000      14.669880510000
22 F       4.817706798000      17.715831500000      13.981755450000
23 F       2.619932088000      16.334165210000      14.595313430000
24 C       6.034151941000      20.201445640000      13.133915880000
25 C       5.176357090000      20.654664190000      11.952112410000
26 N       6.058212909000      21.066364100000      10.807467220000
27 C       6.393701695000      20.189640550000       9.881298096000
28 N       5.929375868000      18.941678750000       9.822516063000
29 C       6.444179820000      18.030179690000       8.826050917000
30 C       7.575366757000      17.253267100000       9.139616681000
31 C       8.276951194000      17.397607310000      10.466914700000
32 H       5.754542463000      16.906706210000       5.701007193000
33 H       4.159965731000      22.433017490000       9.745145300000
34 C       8.024002290000      16.347579980000       8.172340239000
35 C       7.380893778000      16.204737610000       6.933554898000
36 C       6.262306544000      17.002939150000       6.663524465000
37 C       5.771929872000      17.924914540000       7.597538586000
38 C       4.571072703000      18.786777870000       7.295598800000
39 H       9.530638327000      23.968028050000      11.695266470000
40 H       5.662779445000      25.634837800000      10.841311530000
41 C       4.923152013000      18.443025610000      10.788089900000
42 C       4.186940666000      19.616528690000      11.421571830000
43 C       6.644720517000      22.385873860000      10.873804540000
44 C       8.008246959000      22.535154950000      11.200153070000
45 C       8.953909674000      21.362813260000      11.308713960000
46 H       5.431713172000      17.838496620000      11.551238660000
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```
47 H       8.479860785000      20.490457490000      11.776523240000
48 C       8.483457892000      23.834961020000      11.415112810000
49 C       7.655868007000      24.959472750000      11.313825530000
50 C       6.319987858000      24.767977780000      10.940485340000
51 C       5.787968088000      23.494176140000      10.718763340000
52 C       4.336192236000      23.341701750000      10.335793780000
53 H       4.244523309000      17.780932010000      10.234977230000
54 H       3.521763279000      20.085502800000      10.680696800000
55 C       5.332612116000      22.182727200000      14.591742740000
56 C       4.239800016000      22.894134270000      14.084723000000
57 F       3.095525640000      22.238211960000      13.703559360000
58 C       4.232275559000      24.270455760000      13.849525970000
59 F       3.139449814000      24.881865570000      13.325295050000
60 C       5.381265790000      25.013973720000      14.102179540000
61 F       5.413168108000      26.343432160000      13.847839680000
62 C       6.513588459000      24.356038010000      14.574825010000
63 C       6.468851077000      22.978529460000      14.794783160000
64 F       7.647147050000      22.416475690000      15.190448070000
65 F       7.654112393000      25.058863470000      14.786784950000
66 H       6.976771701000      20.765186340000      13.107074910000
67 H       6.308293941000      19.153311090000      12.989429370000
68 H       4.626954735000      21.563729590000      12.201871870000
69 H       3.565830647000      19.259848000000      12.250788610000
70 H       8.614382844000      18.429983830000      10.635431000000
71 H       4.829632070000      19.856034900000       7.311672806000
72 H       8.900135187000      15.733265160000       8.393754709000
73 C       8.169994599000      26.335975180000      11.646167300000
74 C       7.888683908000      15.204592960000       5.924628771000
75 H       7.322766881000      15.252612840000       4.985877571000
76 H       7.808826571000      14.179873790000       6.317164889000
77 H       9.154535786000      16.743082960000      10.519534590000
78 H       7.617247268000      17.141146310000      11.308219820000
79 H       3.771306158000      18.642875850000       8.037279486000
80 H       4.159839717000      18.553676150000       6.306461245000
81 H       9.828774614000      21.630523360000      11.912772520000
82 H       9.322842612000      21.055053680000      10.317194930000
83 H       4.004618533000      24.205501030000       9.746203818000
84 H       3.688487617000      23.292052740000      11.224235330000
85 H       7.934665183000      26.576585310000      12.693862880000
86 H       7.699034097000      27.103640000000      11.017700120000
87 H       9.258889308000      26.402231590000      11.524221980000
88 H       8.949496642000      15.380916760000       5.694222710000
89 Au       7.636907899000      20.725416920000       8.519761456000
90 Cl       9.210335876000      21.403509630000       6.796562489000
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GUIBONDS
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14 12 24 1.0
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27 24 66 1.0
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34 26 43 1.0
35 63 64 1.0
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63 60 61 1.0
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67 58 60 1.5
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71 42 69 1.0
72 42 54 1.0
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74 43 51 1.5
75 44 48 1.5
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87 82 45 1.0
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89 84 52 1.0
90 85 73 1.0
91 86 73 1.0
92 87 73 1.0
93 88 74 1.0
94 89 27 1.0
95 90 89 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor







#! /bin/sh

# ==============================
```

```
# complex [(7-c')Mes]--AuCl
# ============================

"$ADFBIN/adf" <<eor

ATOMS
1 F       1.506175184000       6.920470113000      11.653500120000
2 C       0.994230493800       8.086423331000      11.160050000000
3 C       1.006370652000       8.328560739000       9.778344246000
4 C       0.502297391300       9.584227328000       9.428480197000
5 F       0.489129345600      10.007275060000       8.127634117000
6 C       0.005176710014      10.514980480000      10.347200570000
7 F      -0.465150721900      11.720855900000       9.932222362000
8 C      -0.001407878267      10.207930800000      11.703887770000
9 C       0.504838890900       8.975348861000      12.114465840000
10 F      0.525692596400       8.669027045000      13.436804850000
11 F     -0.475436467800      11.096560570000      12.612474360000
12 B      1.807814994000       7.282222872000       8.771326055000
13 C      3.399475747000       7.413576764000       9.238544210000
14 C      3.887476792000       8.824807012000       9.571980154000
15 N      5.222314040000       8.841195026000      10.306159860000
16 C      5.595198024000       9.791011344000      11.184064360000
17 N      4.920564577000      10.966446740000      11.187943280000
18 C      4.051709377000      11.612489760000      10.147240630000
19 C      4.435749958000      11.170378400000       8.736483783000
20 C      3.901340013000       9.777352530000       8.375778293000
21 C      5.222828442000      11.813425270000      12.314731880000
22 C      6.435068996000      12.532442270000      12.346654050000
23 C      6.688611437000      13.363457690000      13.442675750000
24 C      5.768555447000      13.504231280000      14.492807650000
25 C      4.571415603000      12.783652610000      14.426603110000
26 C      4.278439729000      11.933438050000      13.349165100000
27 C      2.991153900000      11.151161530000      13.302563030000
28 H      6.413945800000       4.967615151000      12.508420290000
29 C      8.078013215000       3.839449257000      10.660856410000
30 C      7.430930595000      12.373451410000      11.229902310000
31 H      7.630803972000      13.918926760000      13.477511120000
32 H      3.844578835000      12.874312700000      15.238992790000
33 C      5.968781874000       7.607638015000      10.405291710000
34 C      6.808995784000       7.211499771000       9.351814097000
35 C      6.964334938000       8.062068621000       8.117252495000
36 H      6.932484818000       9.130135661000       8.369982086000
37 H      8.152708658000       5.684906057000       8.640597887000
38 C      7.497905459000       5.994312991000       9.460572630000
39 C      7.368122663000       5.170541854000      10.582169760000
40 C      6.529709748000       5.597390608000      11.621441680000
41 C      5.821589082000       6.801585825000      11.555145170000
42 C      4.918583159000       7.229448307000      12.681286890000
43 H      3.168668283000      10.125063710000      12.951248980000
44 H      3.888191984000       7.383724545000      12.327961870000
45 C      1.314469134000       5.700042449000       8.967757670000
46 C      0.137764723000       5.263487750000       9.590183093000
47 F     -0.744083364000       6.143538048000      10.142048780000
48 C     -0.235866792400       3.920343621000       9.697625500000
49 F     -1.386057547000       3.565031959000      10.329528010000
50 C      0.574548049600       2.930788985000       9.148411907000
51 F      0.227639718500       1.621825559000       9.241966521000
52 C      1.742986428000       3.309338297000       8.491334625000
53 C      2.075168410000       4.662536069000       8.409449551000
54 F      3.207437883000       4.940898200000       7.701536887000
55 F      2.533819286000       2.357468626000       7.928277959000
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56 C       1.473421026000       7.531337728000       7.161374088000
57 C       0.136742167500       7.567626141000       6.735920292000
58 F      -0.865527232800       7.485934611000       7.654770894000
59 C      -0.270097729100       7.685711815000       5.408845594000
60 F      -1.587291250000       7.732212122000       5.077204407000
61 C       0.694724378600       7.756583323000       4.404716247000
62 F       0.329546569900       7.870733039000       3.102738826000
63 C       2.037523442000       7.698678223000       4.762615965000
64 C       2.395470653000       7.580726410000       6.110765836000
65 F       3.741700163000       7.507464878000       6.326911027000
66 F       2.989998017000       7.751517502000       3.793169448000
67 H       3.488639449000       6.804126773000      10.148705320000
68 H       4.069819391000       6.953018977000       8.507937318000
69 H       3.199976731000       9.243281922000      10.322493520000
70 H       7.716964048000      11.313195900000      11.141359400000
71 H       4.212679290000      12.694317990000      10.262185230000
72 H       2.983438219000      11.423197680000      10.347313780000
73 H       5.534360161000      11.189020490000       8.665608284000
74 H       4.059184833000      11.913261590000       8.016665160000
75 H       2.870227516000       9.858648987000       8.005096282000
76 H       4.489656918000       9.349967290000       7.556651584000
77 C       6.082699124000      14.395421960000      15.672075820000
78 H       6.890121294000      13.968381030000      16.288156710000
79 H       5.205232382000      14.529618200000      16.319311130000
80 H       6.417976369000      15.391086590000      15.343860480000
81 H       4.896912272000       6.475427738000      13.478902610000
82 H       5.262628308000       8.192274310000      13.089748430000
83 H       2.270333541000      11.605315660000      12.605826770000
84 H       2.510902246000      11.107038780000      14.287856550000
85 H       8.942190241000       3.803635166000       9.982656213000
86 H       7.401549678000       3.016726027000      10.377847000000
87 H       8.434277946000       3.632889774000      11.680728720000
88 H       8.325444970000      12.986721310000      11.401441170000
89 H       6.990868749000      12.658644230000      10.261768350000
90 H       6.148536581000       7.869931700000       7.404179727000
91 H       7.912107171000       7.844078720000       7.606415256000
92 Au       6.947242359000       9.404614198000      12.530741640000
93 Cl       8.634676286000       8.922364167000      14.211486010000
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81 39 40 1.5
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96 91 35 1.0
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98 93 92 1.0
END

CHARGE -1.0

BASIS
type TZP
core None
createoutput None
END

XC
GGA Becke88 Perdew86
DISPERSION Grimme3
END

RELATIVISTIC Scalar ZORA



GEOMETRY
    optim Delocalized
END

SAVE  TAPE21 TAPE13

NumericalQuality Good

NOPRINT LOGFILE

eor
```

3. Reference for supporting information

1. K. M. Kuhn and R. H. Grubbs, *Org. Lett.*, 2008, **10**, 2075.