Electronic Supplementary Information

Anion-responsive covalently linked and metal-bridged oligomers

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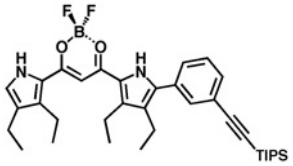
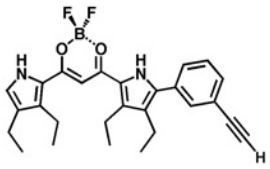
1. Synthetic procedures and spectroscopic data of acyclic anion receptors

General Procedures: Starting materials were purchased from Wako Pure Chemical Industries Ltd., Nacalai Tesque Inc., and Sigma-Aldrich Co. and used without further purification unless otherwise stated. UV-visible spectra were recorded on a Hitachi U-3500 spectrometer. Fluorescence spectra and quantum yields were recorded on a Hitachi F-4500 fluorescence spectrometer and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02, respectively. NMR spectra used in the characterization of products were recorded on a JEOL ECA-600 600 MHz spectrometers. All NMR spectra were referenced to solvent. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus using positive mode. Electrospray ionization mass spectrometric studies (ESI-MS) were recorded on a Bruker microTOF using negative mode ESI-TOF method. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Sumitomo alumina KCG-1525, Wakogel C-200, C-300, and Merck silica gel 60 and 60H.

BF_2 complex of 1-(3,4-diethyl-5-(3-triisopropylsilyl-ethynylphenyl)pyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione, 3m1´. A two-necked round-bottomed flask placed with monoiodo-substituted BF_2 complex of 1,3-bis(3,4-diethylpyrrol-2-yl)-1,3-propanedione[S1] (89.2 mg, 0.183 mmol), 1-(4,4,5,5-tetramethyl-1,3-dioxaborolan-2-yl)-3-[2-(triiso propylsilyl)ethynyl]benzene (93.5 mg, 0.243 mmol), $PdCl_2(PPh_3)_2$ (8.9 mg, 0.0012 mmol), and Cs_2CO_3 (128.5 mg, 0.394 mmol) was flushed with nitrogen and charged with a mixed degassed DMF and water (10:1, 4 mL). The mixture was heated at 80 °C for 16 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1st: CH_2Cl_2, 2nd: $CHCl_3$: hexane = 10:1) and recrystallized from CH_2Cl_2/hexane to afford **3m1´** (65.7 mg, 0.106 mmol, 58%) as an orange solid. R_f = 0.42 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.31(s, 2H, NH), 7.59 (s, 1H, Ar-H), 7.50 (m, 1H, Ar-H), 7.43 (m, 2H, Ar-H), 6.95 (m, 1H, pyrrole-H), 6.52 (s, 1H, CH), 2.83–2.79 (m, 4H, C$\underline{H}_2$CH$_3$), 2.59 (m, 2H, C$\underline{H}_2$CH$_3$), 2.49 (m, 2H, C$\underline{H}_2$CH$_3$), 1.32 (t, J = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.27 (t, J = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.22 (t, J = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.18–1.15 (m, 33H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 475.5 (1.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 506.4 (476.0). MALDI-TOF-MS: *m/z* (% intensity): 617.4 (20), 618.4 (100), 619.4 (37). Calcd for $C_{36}H_{49}BF_2N_2O_2Si$ ([M]$^+$): 618.36.

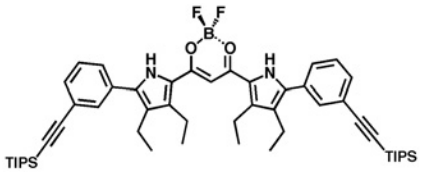


BF_2 complex of 1-(3,4-diethyl-5-(3-ethynylphenyl)-pyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione, 3m1. A solution of **3m1´** (39.0 mg, 0.063 mmol) in THF (8 mL) was treated with TBAF·3H$_2$O (39.7 mg, 0.126 mmol) under nitrogen at room temperature. After 3 h, the solution was washed with water. The organic layer was dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 3:2) and recrystallized from CH_2Cl_2/hexane to afford **3m1** (27.4 mg, 0.028 mmol, 94%) as an orange solid. R_f = 0.10 (CH_2Cl_2:hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.33–9.32 (m, 2H, NH), 7.63 (s, 1H, Ar-H), 7.52–7.43 (m, 3H, Ar-H), 6.95 (m, 1H, pyrrole-H), 6.53 (s, 1H, CH), 3.15 (s, 1H, ethynyl-H), 2.83–2.80 (m, 4H, C$\underline{H}_2$CH$_3$), 2.61 (m, 2H, C$\underline{H}_2$CH$_3$), 2.49 (m, 2H, C$\underline{H}_2$CH$_3$), 1.33–1.18 (m, 12H, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 475.0 (1.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 506.6 (475.0). MALDI-TOF-MS: *m/z* (% intensity): 461.2 (30), 462.2 (100), 463.2 (22). Calcd for $C_{27}H_{29}BF_2N_2O_2$ ([M]$^+$): 462.23. HRMS (ESI-TOF): *m/z* (% intensity): 461.2223. Calcd for $C_{27}H_{28}BF_2N_2O_2$ ([M – H]$^-$): 461.2222.

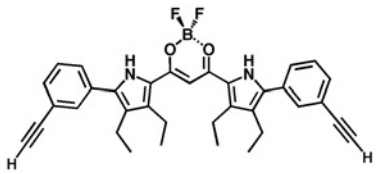


BF_2 complex of 1,3-bis-(3,4-diethyl-5-(3-triisopropylsilylethynylphenyl)pyrrol-2-yl)-1,3-propanedione, 3m2´. A two-necked round-bottomed flask placed with bisiodo-substituted BF_2 complex of 1,3-bis(3,4-diethylpyrrol-2-yl)-1,3-propanedione[S1] (60.7 mg, 0.100 mmol), 1-(4,4,5,5-tetramethyl-1,3-dioxaborolan-2-yl)-3-[2-(triisopropylsilyl)ethynyl]benzene (100.9 mg, 0.262 mmol), $PdCl_2(PPh_3)_2$ (9.5 mg, 0.014 mmol), and Cs_2CO_2 (135.3 mg, 0.415 mmol) was flushed with nitrogen and charged with a mixed degassed DMF and water (10:1, 5 mL). The mixture was heated at 80 °C for 24 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1st: CH_2Cl_2 2nd: 7% EtOAc/hexane) and recrystallized from CH_2Cl_2/MeOH to afford **3m2´** (18.6 mg, 0.022 mmol, 22%) as a red solid. R_f = 0.26 (7%

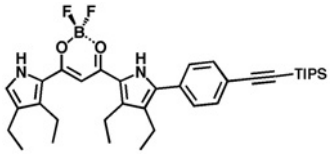
EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.34 (s, 2H, NH), 7.60 (s, 2H, Ar-H), 7.51 (m, 2H, Ar-H), 7.44–7.42 (m, 4H, Ar-H), 6.57 (s, 1H, CH), 2.85–2.86 (m, 4H, C$\underline{H}_2$CH$_3$), 2.61–2.60 (m, 4H, C$\underline{H}_2$CH$_3$), 1.34 (m, 6H, CH$_2$C$\underline{H}_3$), 1.19–1.16 (m, 48H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 499.0 (1.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 506.6 (475.0). MALDI-TOF-MS: *m/z* (% intensity): 873.6 (26), 874.6 (100), 875.6 (40). Calcd for. $C_{53}H_{73}BF_2N_2O_2Si_2$ ([M]$^+$): 874.53.



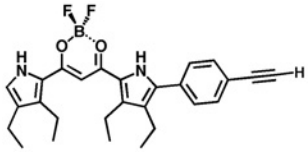
BF_2 complex of 1,3-bis-(3,4-diethyl-5-(3-ethynylphenyl)-pyrrol-2-yl)-1,3-propanedione, 3m2. A solution of **3m2´** (29.7 mg, 0.034 mmol) in THF (10 mL) was treated with TBAF·3H$_2$O (31.6 mg, 0.10 mmol) under nitrogen at room temperature. After 2 h, the solution was washed with water. The organic layer was dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 1:1) and recrystallized from CH_2Cl_2/hexane to afford **3m2** (10.0 mg, 0.0196 mmol, 57%) as a red solid. R_f = 0.23 (2.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.34 (s, 2H, NH), 7.64 (s, 2H, Ar-H), 7.64–7.45 (m, 6H, Ar-H), 6.57 (s, 1H, CH), 3.15 (s, 2H, ethynyl-H), 2.86–2.85 (m, 4H, C$\underline{H}_2$CH$_3$), 2.63–2.61 (q, *J* = 7.8 Hz, 4H, C$\underline{H}_2$CH$_3$), 1.34 (m, 6H, CH$_2$C$\underline{H}_3$), 1.19 (m, 6H, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 497.5 (1.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 535.0 (498.0). MALDI-TOF-MS: *m/z* (% intensity): 561.3 (25), 562.3 (100), 563.3 (38). Calcd for $C_{35}H_{33}BF_2N_2O_2$ ([M]$^+$): 562.26. HRMS (ESI-TOF): *m/z* (% intensity): 561.2536. Calcd for $C_{35}H_{32}BF_2N_2O_2$ ([M – H]$^-$): 561.2536. This compound was further characterized by X-ray diffraction analysis.



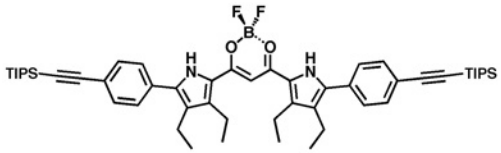
BF_2 complex of 1-(3,4-diethyl-5-(4-triisopropylsilyl-ethynylphenyl)pyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione, 3p1´. A two-necked round-bottomed flask placed with monoiodo-substituted BF_2 complex of 1,3-bis(3,4-diethylpyrrol-2-yl)-1,3-propanedione[S1] (175.3 mg, 0.456 mmol), 1-(4,4,5,5-tetramethyl-1,3-dioxaborolan-2-yl)-4-[2-(triiso propylsilyl)ethynyl]benzene (189.6 mg, 0.388 mmol), $PdCl_2(PPh_3)_2$ (14.3 mg, 0.020 mmol), and Cs_2CO_3 (250.4 mg, 0.769 mmol) was flushed with nitrogen and charged with a mixture degassed DMF and water (10:1, 5 mL). The mixture was heated at 70 °C for 17 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1st: CH_2Cl_2, 2nd: $CHCl_3$: hexane = 4:1) and recrystallized from CH_2Cl_2/hexane to afford **3p1´** (137.4 mg, 0.22 mmol, 57%) as an orange solid. R_f = 0.17 ($CHCl_3$:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.35 (s, 1H, NH), 9.32 (s, 1H, NH), 7.57 (d, *J* = 8.4 Hz, 2H, Ar-*o*-H), 7.46 (d, *J* = 8.4 Hz, 2H, Ar-*m*-H), 6.95 (d, *J* = 3.0 Hz, 1H, pyrrole-H), 6.53 (s, 1H, CH), 2.85–2.78 (m, 4H, C$\underline{H}_2$CH$_3$), 2.61 (q, *J* = 7.8 Hz, 2H, C$\underline{H}_2$CH$_3$), 2.49 (q, *J* = 7.8 Hz, 2H, C$\underline{H}_2$CH$_3$), 1.32 (t, *J* = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.27 (t, *J* = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.22 (t, *J* = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.18–1.15 (m, 24H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 483.5 (1.1). MALDI-TOF-MS: *m/z* (% intensity): 617.3 (24), 618.3 (100), 619.3 (38). Calcd for $C_{36}H_{49}BF_2N_2O_2Si$ ([M]$^+$): 618.36.



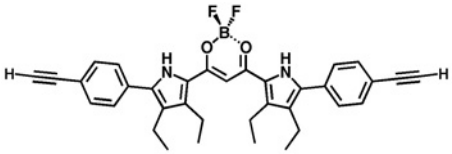
BF_2 complex of 1-(3,4-diethyl-5-(4-ethynylphenyl)-pyrrol-2-yl)-3-(3,4-diethylpyrrol-2-yl)-1,3-propanedione, 3p1. A solution of **3p1´** (112.6 mg, 0.182 mmol) in THF (15 mL) was treated with TBAF·3H$_2$O (112.6 mg, 0.364 mmol) under nitrogen at room temperature. After 1.5 h, the solution was washed with water. The organic layer was dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 2:1) and recrystallized from CH_2Cl_2/hexane to afford **3p1** (69.4 mg, 0.15 mmol, 82%) as an orange solid. R_f = 0.35 (CH_2Cl_2:hexane = 2:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.34 (s, 1H, NH), 9.32 (s, 1H, NH), 7.59 (d, *J* = 8.4 Hz, 2H, Ar-*o*-H), 7.48 (d, *J* = 8.4 Hz, 2H, Ar-*m*-H), 6.96 (d, *J* = 3.0 Hz, 1H, pyrrole-H), 6.53 (s, 1H, CH), 3.19 (s, 1H, ethynyl-H), 2.85–2.78(m, 4H, C$\underline{H}_2$CH$_3$), 2.62 (q, *J* = 7.8 Hz, 4H, C$\underline{H}_2$CH$_3$), 1.32 (t, *J* = 7.8 Hz, 3H, CH$_2$C$\underline{H}_3$), 1.27 (t, *J* = 7.8Hz, 3H, CH$_2$C$\underline{H}_3$), 1.24–1.17 (m, 6H, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 480.0 (1.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 514.0 (480.0). MALDI-TOF-MS: *m/z* (% intensity): 461.2 (17), 462.2 (100), 463.2 (22). Calcd for $C_{27}H_{29}BF_2N_2O_2$ ([M]$^+$): 462.23. HRMS (ESI-TOF): *m/z* (% intensity): 461.2221. Calcd for $C_{27}H_{28}BF_2N_2O_2$ ([M – H]$^-$): 461.2222. This compound was further characterized by X-ray diffraction analysis.



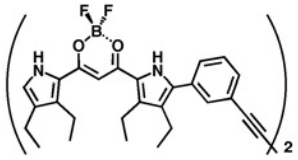
BF_2 complex of 1,3-bis-(3,4-diethyl-5-(4-triisopropylsilylethynyl)phenylpyrrol-2-yl)-1,3-propanedione, 3p2´. A two-necked round-bottomed flask placed with bisiodo-substituted BF_2 complex of 1,3-bis(3,4-diethylpyrrol-2-yl)-1,3-propanedione[S1] (143.2 mg, 0.372 mmol), 1-(4,4,5,5-tetramethyl-1,3-dioxaborolan-2-yl)-4-[2-(triisopropylsilyl)ethynyl]benzene (101.7 mg, 0.168 mmol), $PdCl_2(PPh_3)_2$ (9.5 mg, 0.014 mmol), and Cs_2CO_2 (215.6 mg, 0.662 mmol) was flushed with nitrogen and charged with a mixed degassed DMF and water (10:1, 5 mL). The mixture was heated at 80 °C for 17 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1st: CH_2Cl_2 2nd: 5% EtOAc/hexane) and recrystallized from CH_2Cl_2/MeOH to afford **3p2´** (51.4 mg, 0.059 mmol, 35%) as a red solid. R_f = 0.24 (5% EtOAc/hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.35 (s, 2H, NH), 7.58 (d, J = 8.4 Hz, 4H, Ar-*o*-H), 7.46 (d, J = 8.4 Hz, 4H, Ar-*m*-H), 6.57 (s, 1H, CH), 2.85 (q, J = 7.2 Hz, 4H, C$\underline{H}_2$CH$_3$), 2.62 (q, J = 7.2 Hz, 4H, C$\underline{H}_2$CH$_3$), 1.35 (t, J = 7.2 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.19–1.12 (m, 48H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 514.0 (1.4). MALDI-TOF-MS: *m/z* (% intensity): 874.1 (22), 875.1 (100), 876.1 (67). Calcd for $C_{53}H_{73}BF_2N_2O_2Si_2$ ($[M]^+$): 874.53.



BF_2 complex of 1,3-bis-(3,4-diethyl-5-(4-ethynylphenyl)-pyrrol-2-yl)-1,3-propanedione, 3p2. A solution of **3p2´** (51.4 mg, 0.059 mmol) in THF (15 mL) was treated with TBAF·3H$_2$O (56.8 mg, 0.18 mmol) under nitrogen at room temperature. After 2 h, the solution was washed with water. The organic layer was dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 2:1) and recrystallized from CH_2Cl_2/hexane to afford **3p2** (26.2 mg, 0.047 mmol, 79%) as a red solid. R_f = 0.48 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.36 (s, 2H, NH), 7.60 (d, J = 8.4 Hz, 4H, Ar-*o*-H), 7.48 (d, J = 8.4 Hz, 4H, Ar-*m*-H), 6.57 (s, 1H, CH), 3.19 (s, 2H, ethynyl-H), 2.85 (q, J = 7.8 Hz, 4H, C$\underline{H}_2$CH$_3$), 2.62 (q, J = 7.8 Hz, 4H, C$\underline{H}_2$CH$_3$), 1.34 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.19 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 508.0 (1.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 548.0 (508.0). MALDI-TOF-MS: *m/z* (% intensity): 561.7 (22), 562.7 (100), 563.7 (44). Calcd for $C_{35}H_{33}BF_2N_2O_2$ ($[M]^+$): 562.26. HRMS (ESI-TOF): *m/z* (% intensity): 561.2536. Calcd for $C_{35}H_{32}BF_2N_2O_2$ ($[M - H]^-$): 561.2536. This compound was further characterized by X-ray diffraction analysis.

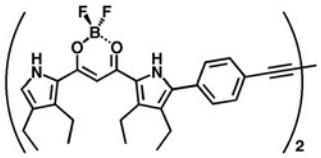


***m*-Ethynyl-bridged dimer, 4m.** A two-necked round-bottomed flask placed with **3m1** (19.7 mg, 0.0426 mmol), $Pd(OAc)_2$ (0.50 mg, 0.0022 mmol), and CuI (0.73 mg, 0.0038 mmol), and DABCO (16.8 mg, 0.150 mmol) was flushed with nitrogen and charged with dried MeCN (1.2 mL). The reaction mixture was stirred for 36 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 0.4% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **4m** (7.2 mg, 0.0078 mmol, 37%) as an orange solid. R_f = 0.35 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.38 (s, 2H, NH), 9.35 (s, 2H, NH), 7.69 (s, 2H, Ar-H), 7.57 (d, J = 7.2 Hz, 2H, Ar-H), 7.52 (d, J = 7.2 Hz, 2H, Ar-H), 7.47 (t, J = 8.4 Hz, 2H, Ar-H), 6.96 (d, J = 3.0 Hz, 2H, pyrrole-H), 6.53 (s, 2H, CH), 2.86–2.78 (m, 8H, C$\underline{H}_2$CH$_3$), 2.62 (q, J = 7.2 Hz, 4H, C$\underline{H}_2$CH$_3$), 2.49 (q, J = 7.2 Hz, 4H, C$\underline{H}_2$CH$_3$), 1.33 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.28 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.24–1.20 (m, 12H, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 477.0 (2.0). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 507.0 (477.0). MALDI-TOF-MS: *m/z* (% intensity): 921.4 (86), 922.4 (100), 923.6 (65), 924.3 (34). Calcd for $C_{54}H_{56}B_2F_4N_4O_4$ ($[M]^+$): 922.44. HRMS (ESI-TOF): *m/z* (% intensity): 921.4368. Calcd for $C_{54}H_{55}B_2F_4N_4O_4$ ($[M - H]^-$): 921.4368. This compound was further characterized by X-ray diffraction analysis.

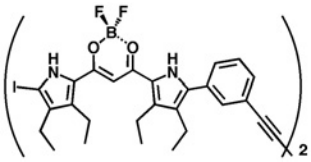


***p*-Ethynyl-bridged dimer, 4p.** A two-necked round-bottomed flask placed with **3p1** (25.2 mg, 0.0545 mmol), $Pd(OAc)_2$ (0.62 mg, 0.0028 mmol), and CuI (0.59 mg, 0.0031 mmol), and DABCO (18.9 mg, 0.168 mmol) was flushed with nitrogen and charged with MeCN (1.2 mL). The reaction mixture was stirred for 22 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 0.4% MeOH/CH_2Cl_2) and recrystallized from THF/hexane to afford **4p** (11.9 mg, 0.013 mmol, 47%) as an orange solid. R_f = 0.18 (0.4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, DMSO-d_6, 20 °C): δ (ppm) 11.8 (s, 2H, NH), 11.73 (s, 2H, NH), 7.76 (d, J = 7.8 Hz, 4H, Ar-*o*-H), 7.65 (d, J = 7.8 Hz, 4H, Ar-*m*-H), 7.19 (s, 2H, pyrrole-H), 6.69 (s, 2H, CH), 2.83–2.78 (m, 8H, C$\underline{H}_2$CH$_3$), 1.20–1.10 (m, 24H,

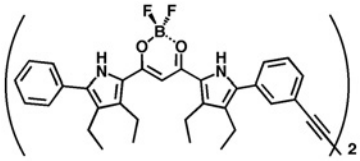
CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 496.5 (2.0). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 529.4 (497.0). MALDI-TOF-MS: *m/z* (% intensity): 921.4 (38), 922.4 (100), 923.4 (93) 922.45 (46). Calcd for $C_{54}H_{56}B_2F_4N_4O_4$ ($[M]^+$): 922.44. HRMS (ESI-TOF): *m/z* (% intensity): 921.4368. Calcd for $C_{54}H_{55}B_2F_4N_4O_4$ ($[M - H]^-$): 921.4368. This compound was further characterized by X-ray diffraction analysis.



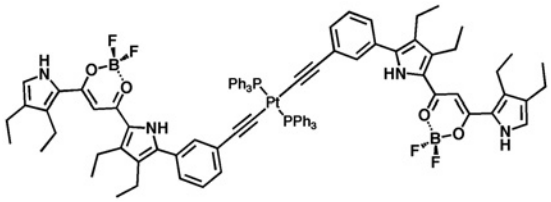
***m*-Ethynyl-bridged bis-iodinated dimer, 4m-I$_2$.** To a CH_2Cl_2 (10 mL) solution of **4m** (30.0mg, 0.0325 mmol) at room temperature was added *N*-iodosuccinimide (29.3 mg, 0.13 mmol). The mixture was stirred at room temperature for 2 h. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **4m-I$_2$** (26.6 mg, 0.023 mmol, 70%) as a red solid. R_f = 0.10 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.42 (s, 2H, NH), 9.36 (s, 2H, NH), 7.69 (t, J = 2.4 Hz, 2H, Ar-H), 7.59–7.57 (m, 2H, Ar-H), 7.53–7.47 (m, 4H, Ar-H), 6.47 (s, 2H, CH), 2.86–2.81 (m, 8H, CH_2CH_3), 2.62 (q, J = 7.8 Hz, 4H, CH_2CH_3), 2.44 (q, J = 7.8 Hz, 4H, CH_2CH_3), 1.37–1.34 (m, 12H, CH_2CH_3) 1.22–1.18 (m, 12H, CH_2CH_3). MALDI-TOF-MS: *m/z* (% intensity): 1173.2 (33), 1174.2 (100), 1175.2 (42), 1176.2 (14). Calcd for $C_{54}H_{54}B_2F_4I_2N_4O_4$ ($[M]^+$):1174.24.



***m*-Ethynyl-bridged dimer, 4m´.** A two-necked round-bottomed flask placed with **4m-I$_2$** (22.0 mg, 0.0187 mmol), phenylboronic acid (6.8 mg, 0.0561 mmol), $Pd(PPh_3)_4$ (0.66 mg, 0.94 μmol), and Cs_2CO_3 (18.3 mg, 0.0561 mmol) was flushed with nitrogen and charged with a mixture degassed DMF and water (10:1, 5 mL). The mixture as heated at reflux for 7 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, 0.5% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **4m´** (0.6 mg, 5.6 μmol, 3%) as an orange solid. R_f = 0.24 (0.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.38 (s, 4H, NH), 7.69 (s, 2H, Ar-H), 7.58 (d, J = 7.8 Hz, 2H, Ar-H), 7.53–7.46 (m, 12H, Ar-H), 7.42 (t, J = 8.4 Hz, 2H, Ar-H), 6.57 (s, 2H, CH), 2.87–2.81 (m, 8H, CH_2CH_3), 2.65–2.61 (m, 8H, CH_2CH_3), 1.37–1.34 (m, 12H, CH_2CH_3) 1.22–1.18 (m, 12H, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 501 (2.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 536 (501). MALDI-TOF-MS: *m/z* (% intensity): 1073.4 (53), 1074.4 (100), 1075.4 (68), 1076.5 (34). Calcd for $C_{66}H_{64}B_2F_4N_4O_4$ ($[M]^+$): 1074.50. HRMS (ESI-TOF): *m/z* (% intensity): 1073.4997. Calcd for $C_{66}H_{63}B_2F_4N_4O_4$ ($[M - H]^-$): 1073.4997.

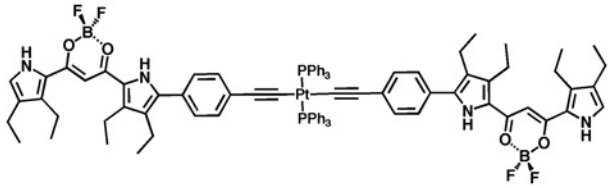


***trans*-Pt-bridged *meta*-dimer, 5m.** A two-necked round-bottomed flask placed with **3m1** (21.2 mg, 0.046 mmol), $PtCl_2(PPh_3)_2$ (17.3 mg, 0.022 mmol), CuI (0.4 mg, 0.0021 mmol) was flushed with nitrogen and charged with a mixed degassed Et_2NH (3 mL). The mixture was heated at reflux for 4 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 0.6% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **5m** (24.2 mg, 0.0147 mmol, 64%) as an orange solid. R_f = 0.21 (0.6% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.36 (s, 2H, NH), 9.07 (s, 2H, NH), 7.83–7.79 (m, 12H, PPh_3), 7.47–7.41 (m, 18H, PPh_3), 7.10–7.09 (m, 2H, Ar-H), 7.02 (t, J = 7.8 Hz, 2H, Ar-H), 6.97 (d, J = 3.0 Hz, 2H, pyrrole-H), 6.50 (s, 2H, CH), 6.34–6.33 (m, 2H, Ar-H), 6.21 (t, J = 1.8 Hz, 8H, Ar-H), 2.52 (q, J = 7.8 Hz, 4H, CH_2CH_3), 2.47 (q, J = 7.8 Hz, 4H, CH_2CH_3), 1.29–1.23 (m, 12H, CH_2CH_3), 1.19 (t, J = 7.8 Hz, 6H, CH_2CH_3), 1.11 (t, J = 7.8 Hz, 6H, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 481.0 (2.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 517.4 (481.0). ESI-TOF-MS: *m/z* (% intensity): 1639.65 (62), 1640.62 (100), 1641.62 (92). Calcd for $C_{90}H_{86}B_2F_4N_4O_4P_2Pt$ ($[M]^+$): 1640.59. HRMS (ESI-TOF): *m/z* (% intensity): 1640.5850. Calcd for $C_{90}H_{85}B_2F_4N_4O_4P_2Pt$ ($[M - H]^-$): 1640.5850.

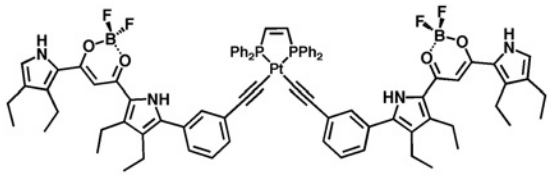


***trans*-Pt-bridged *para*-dimer, 5p.** A two-necked round-bottomed flask placed with **3p1** (20.0 mg, 0.043 mmol), $PtCl_2(PPh_3)_2$ (17.1 mg, 0.022 mmol), CuI (0.4 mg, 0.0021 mmol) was flushed with nitrogen and charged with a mixed degassed Et_2NH (3 mL). The mixture was heated at reflux for 4 h, cooled, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column

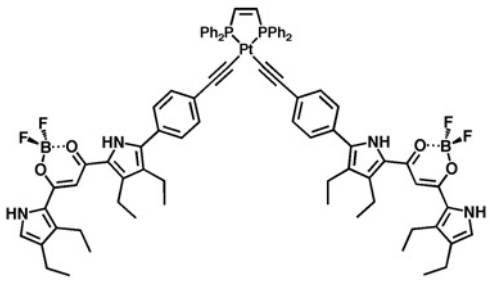
(Wakogel C-300, eluent: 0.6% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **5p** (21.0 mg, 0.0130 mmol, 61%) as an orange solid. R_f = 0.21 (0.6% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 9.32 (s, 2H, NH), 9.24 (s, 2H, NH), 7.83–7.80 (m, 12H, PPh_3), 7.48–7.45 (m, 6H, PPh_3), 7.43–7.41 (m, 12H, PPh_3), 7.10 (d, J = 7.8 Hz, 4H, Ar-H), 6.96 (d, J = 3.0 Hz, 2H, pyrrole-H), 6.46 (s, 2H, CH), 6.33 (d, J = 8.4 Hz, 4H, Ar-H), 2.80–2.77 (m, 8H, $C\underline{H}_2CH_3$), 2.52 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.47 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 1.29–1.23 (m, 12H, $CH_2C\underline{H}_3$), 1.19 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.11 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 503.5 (2.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 560.0 (504.0). ESI-TOF-MS: *m/z* (% intensity): 1639.55 (65), 1640.56 (100), 1641.56 (93). Calcd for $C_{90}H_{86}B_2F_4N_4O_4P_2Pt$ ($[M]^+$): 1640.59. HRMS (ESI-TOF): *m/z* (% intensity): 1640.5850. Calcd for $C_{90}H_{85}B_2F_4N_4O_4P_2Pt$ ($[M - H]^-$): 1640.5850.



***cis*-Pt-bridged *meta*-dimer, 6m.** A flask placed with **5m** (10.2 mg, 6.10 μmol) and *cis*-1,2-bis(diphenylphosphino)ethene (dppee) (2.4 mg, 6.09 μmol) was flushed with nitrogen and charged with CH_2Cl_2 (1.0 mL). The mixture was stirred at room temperature for 9 h, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **6m** (5.0 mg, 3.3 μmol, 54%) as an orange solid. R_f = 0.26 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C; the signals assigned to an ethenyl moiety of dppee ligand cannot be observed): δ (ppm) 9.34 (s, 2H, NH), 9.27 (s, 2H, NH), 7.83–7.80 (m, 8H, PPh_2), 7.53–7.51 (m, 4H, PPh_2), 7.48–7.44 (m, 8H, PPh_2), 7.28–7.24 (m, 8H, Ar-H), 6.96 (d, J = 2.4 Hz, 2H, pyrrole-H), 6.49 (s, 2H, CH), 2.82 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.79 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.55 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.48 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 1.30 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.25 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.20 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.08 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 479.0 (0.96). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 514.0 (479.0). ESI-TOF-MS: *m/z* (% intensity): 1511.56 (69), 1512.56 (100), 1513.55 (90). Calcd for. $C_{80}H_{78}O_4N_4P_2PtB_2F_4$ ($[M]^+$): 1512.53. HRMS (ESI-TOF): *m/z* (% intensity): 1512.5221. Calcd for $C_{80}H_{77}B_2F_4N_4O_4P_2Pt$ ($[M - H]^-$): 1512.5222.

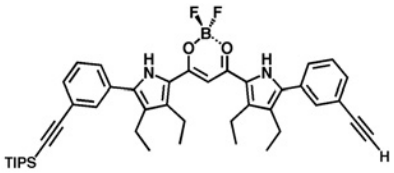


***cis*-Pt-bridged *para*-dimer, 6p.** A flask placed with **5p** (9.8 mg, 6.0 μmol) and *cis*-1,2-bis(diphenylphosphino)ethene (dppee) (2.4 mg, 6.09 μmol) was flushed with nitrogen and charged with CH_2Cl_2 (1.0 mL). The mixture was stirred at room temperature for 9 h, then partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **6p** (5.3 mg, 3.5 μmol, 57%) as an orange solid. R_f = 0.22 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C; the signals assigned to an ethenyl moiety of dppee ligand cannot be observed): δ (ppm) 9.32 (s, 4H, NH), 7.84–7.81 (m, 8H, PPh_2), 7.53–7.51 (m, 4H, PPh_2), 7.48–7.45 (m, 8H, PPh_2), 7.35 (d, J = 2.4 Hz, 8H, Ar-H), 7.25 (d, J = 8.4 Hz, 8H, Ar-H), 6.95 (d, J = 2.4 Hz, 2H, pyrrole-H), 6.49 (s, 2H, CH), 2.82 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.79 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.59 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 2.48 (q, J = 7.8 Hz, 4H, $C\underline{H}_2CH_3$), 1.29 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.25 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.19 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$), 1.15 (t, J = 7.8 Hz, 6H, $CH_2C\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 493.0 (0.96). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 546.9 (493.0). ESI-TOF-MS: *m/z* (% intensity): 1511.56 (64), 1512.56 (100), 1513.55 (86). Calcd for. $C_{80}H_{78}B_2F_4N_4O_4P_2Pt$ ($[M]^+$): 1512.53. HRMS (ESI-TOF): *m/z* (% intensity): 1512.5221. Calcd for $C_{80}H_{77}B_2F_4N_4O_4P_2Pt$ ($[M - H]^-$): 1512.5222.

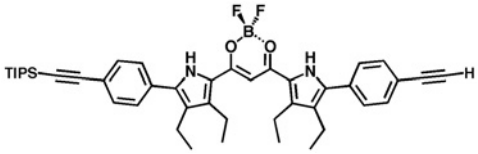


BF_2 complex of 1-(3,4-diethyl-5-(3-triisoprorylsilyl-ethynylphenyl)pyrrol-2-yl)-3-(3,4-diethyl-5-(3-ethynyl phenyl)-pyrrol-2-yl)-1,3-propanedione, m1merSiH. A solution of **3m2´** (268.9 mg, 0.307 mmol) in THF (20 mL) was treated with TBAF·3H_2O (106.7 mg, 0.338 mmol) under nitrogen at room temperature. After 30 min, the solution was washed with water. The organic layer was dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 4:1) to afford **m1merSiH** (106.3 mg, 0.147 mmol, 48%) as a

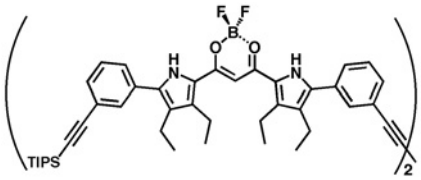
red solid. R_f = 0.57 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.35 (s, 2H, NH), 7.64 (s, 1H, Ar-H), 7.60 (s, 1H, Ar-H), 7.53–7.40 (m, 6H, Ar-H), 6.57 (s, 1H, CH), 3.16 (s, 1H, ethynyl-H), 2.88–2.84 (m, 4H, C$\underline{H}_2$CH$_3$), 2.64–2.59 (m, 4H, C$\underline{H}_2$CH$_3$), 1.34 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.21–1.15 (m, 27H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 498.0 (1.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 573.6 (498). MALDI-TOF-MS: m/z (% intensity): 717.4 (24), 718.4 (100), 719.4 (53). Calcd for $C_{44}H_{53}BF_2N_2O_2Si$ ([M]$^+$): 718.39.



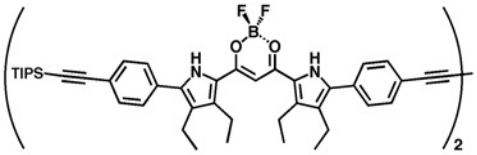
BF_2 complex of 1-(3,4-diethyl-5-(4-triisoprorylsilyl-ethynylphenyl)pyrrol-2-yl)-3-(3,4-diethyl-5-(4-ethynyl phenyl)-pyrrol-2-yl)-1,3-propanedione, p1merSiH. A solution of **3p2´** (387.8 mg, 0.443 mmol) in THF (20 mL) was treated with TBAF·3H$_2$O (153.9 mg, 0.487 mmol) under nitrogen at room temperature. After 30 min, the solution was washed with water. The organic layer was dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 2:1) to afford **p1merSiH** (159.0 mg, 0.221 mmol, 50%) as a red solid. R_f = 0.77 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.35 (s, 2H, NH), 7.61–7.57 (m, 4H, Ar-H), 7.49 (m, 4H, Ar-H), 6.57 (s, 1H, CH), 3.19 (s, 1H, ethynyl-H), 2.87–2.84 (m, 4H, C$\underline{H}_2$CH$_3$), 2.65–2.60 (m, 4H, C$\underline{H}_2$CH$_3$), 1.34 (t, J = 7.8 Hz, 6H, CH$_2$C$\underline{H}_3$), 1.21–1.15 (m, 27H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 511.0 (1.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 555.2 (511). MALDI-TOF-MS: m/z (% intensity): 717.4 (23), 718.4 (100), 719.4 (50). Calcd for $C_{44}H_{53}BF_2N_2O_2Si$ ([M]$^+$): 718.39.



***m*-Ethynyl-bridged dimer, m2merSi2.** A two-necked round-bottomed flask placed with **m1merSiH** (106.3 mg, 0.148 mmol), Pd(OAc)$_2$ (1.7 mg, 0.0076 mmol), and CuI (1.4 mg, 0.0074 mmol), and DABCO (49.8 mg, 0.444 mmol) was flushed with nitrogen and charged with dried MeCN (5 mL). The reaction mixture was stirred for 24 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 4:1) and recrystallized from CH_2Cl_2/MeOH to afford **m2merSi2** (56.3 mg, 0.039 mmol, 53%) as an orange solid. R_f = 0.62 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.37 (s, 4H, NH), 7.70 (s, 4H, Ar-H), 7.61–7.42 (m, 12H, Ar-H), 6.58 (s, 2H, CH), 2.87–2.86 (m, 8H, C$\underline{H}_2$CH$_3$), 2.64–2.60 (m, 8H, C$\underline{H}_2$CH$_3$), 1.35–1.15 (m, 66H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 501.0 (2.3). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 539.4 (501.0). MALDI-TOF-MS: m/z (% intensity): 1433.8 (39), 1434.8 (100), 1435.8 (98), 1436.8 (55). Calcd for $C_{88}H_{104}B_2F_4N_4O_4Si_2$ ([M]$^+$): 1434.77.

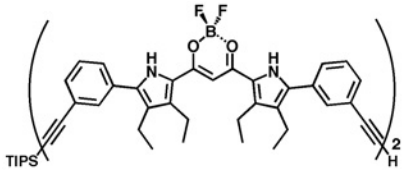


***p*-Ethynyl-bridged dimer, p2merSi2.** A two-necked round-bottomed flask placed with **p1merSiH** (252.0 mg, 0.351 mmol), Pd(OAc)$_2$ (3.9 mg, 0.017 mmol), and CuI (3.3 mg, 0.017 mmol), and DABCO (118.1 mg, 1.053 mmol) was flushed with nitrogen and charged with dried MeCN (10 mL). The reaction mixture was stirred for 14 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 4:1) and recrystallized from CH_2Cl_2/MeOH to afford **p2merSi2** (56.3 mg, 0.039 mmol, 53%) as an orange solid. R_f = 0.62 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.38 (s, 2H, NH), 9.37 (s, 2H, NH), 7.70 (s, 4H, Ar-H), 7.61–7.42 (m, 12H, Ar-H), 6.58 (s, 2H, CH), 2.87–2.86 (m, 8H, C$\underline{H}_2$CH$_3$), 2.64–2.60 (m, 8H, C$\underline{H}_2$CH$_3$), 1.35–1.15 (m, 66H, TIPS, CH$_2$C$\underline{H}_3$). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 526.0 (3.1). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 564.0 (526.0). MALDI-TOF-MS: m/z (% intensity): 1433.6 (43), 1434.7 (100), 1435.7 (99), 1436.7 (69). Calcd for $C_{88}H_{104}B_2F_4N_4O_4Si_2$ ([M]$^+$):1434.77.

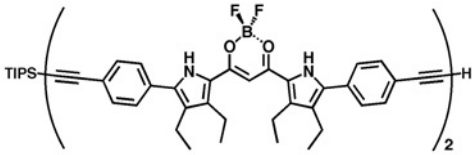


***m*-Ethynyl-bridged dimer, m2merSiH.** A solution of **m2merSi2** (268.9 mg, 0.307 mmol) in THF (20 mL) was treated with TBAF·3H$_2$O (106.7 mg, 0.338 mmol) under nitrogen at room temperature. After 30 min, the solution was washed with water. The organic layer was dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 4:1) to afford **m2merSiH** (106.3 mg, 0.147 mmol, 48%) as a red solid. R_f = 0.57 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.37 (s, 4H, NH), 7.70 (s, 4H, Ar-H), 7.64–7.41 (m, 12H, Ar-H), 6.58 (s, 2H, CH), 3.16 (s, 1H, ethynyl-H), 2.88–2.85 (m, 4H,

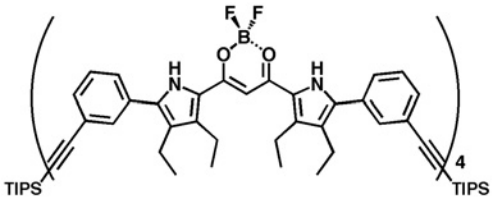
CH_2CH_3), 2.65–2.59 (m, 4H, CH_2CH_3), 1.35 (t, J = 7.8 Hz, 12H, CH_2CH_3), 1.22–1.15 (m, 54H, TIPS, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 501.0 (1.9). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 537 (501). MALDI-TOF-MS: *m*/*z* (% intensity): 1280.6 (27), 1278.6 (100), 1279.6 (82), 1280.7 (39). Calcd for $C_{44}H_{53}BF_2N_2O_2Si$ ($[M]^+$): 1278.64.



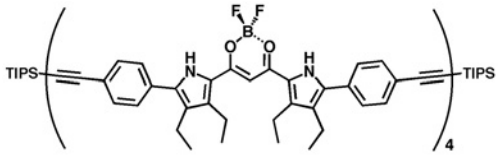
***m*-Et *p*-Ethynyl-bridged dimer, p2merSiH.** A solution of **p2merSi2** (268.9 mg, 0.307 mmol) in THF (20 mL) was treated with TBAF·$3H_2O$ (106.7 mg, 0.338 mmol) under nitrogen at room temperature. After 30 min, the solution was washed with water. The organic layer was dried over anhydrous $NaSO_4$ and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: CH_2Cl_2:hexane = 4:1) to afford **p2merSiH** (106.3 mg, 0.147 mmol, 48%) as a red solid. R_f = 0.57 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.40 (s, 4H, NH), 7.67–7.44 (m, 16H, Ar-H), 6.59 (s, 1H, CH), 6.58 (s, 1H, CH), 3.19 (s, 1H, ethynyl-H), 2.87–2.85 (m, 4H, CH_2CH_3), 2.66–2.61 (m, 4H, CH_2CH_3), 1.35 (t, J = 7.8 Hz, 12H, CH_2CH_3), 1.24–1.15 (m, 54H, TIPS, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 524.5 (2.7). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 564.8 (525). MALDI-TOF-MS: *m*/*z* (% intensity): 1277.6 (54), 1278.6 (100), 1279.6 (65). Calcd for $C_{44}H_{53}BF_2N_2O_2Si$ ($[M]^+$): 1278.64.



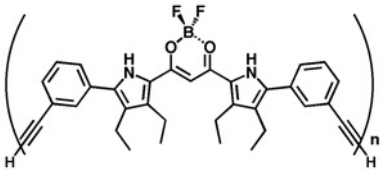
***m*-Ethynyl-bridged tetramer, m4merSi2.** A two-necked round-bottomed flask placed with **m2merSiH** (12.9 mg, 0.010 mmol), $Pd(OAc)_2$ (0.11 mg, 0.49 μmol), and CuI (0.19 mg, 1.00 μmol), and DABCO (3.4 mg, 0.030 mmol) was flushed with nitrogen and charged with dried MeCN (10 mL). The reaction mixture was stirred for 5 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 0.4% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **m4merSi2** (1.9 mg, 0.74 μmol, 15%) as an orange solid. R_f = 0.43 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.38 (s, 4H, NH), 9.37 (s, 4H, NH), 7.70 (s, 8H, Ar-H), 7.60–7.42 (m, 24H, Ar-H), 6.58 (s, 2H, CH), 6.57 (s, 2H, CH), 2.89–2.84 (m, 16H, CH_2CH_3), 2.65–2.59 (m, 16H, CH_2CH_3), 1.34–1.37 (m, 24H, CH_2CH_3) 1.26–1.15 (m, 66H, TIPS, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 501.5 (4.3). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 538.0 (501.0). MALDI-TOF-MS: *m*/z (% intensity): 2554.3 (86), 2555.3 (100), 2556.3 (80), 2557.3 (58). Calcd for $C_{88}H_{104}B_2F_4N_4O_4Si_2$ ($[M]^+$): 2555.26.



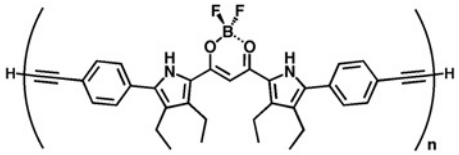
***m*-Ethynyl-bridged tetramer, p4merSi2.** A two-necked round-bottomed flask placed with **p2merSiH** (12.9 mg, 0.010 mmol), $Pd(OAc)_2$ (0.11 mg, 0.49 μmol), and CuI (0.19 mg, 1.00 μmol), and DABCO (3.4 mg, 0.030 mmol) was flushed with nitrogen and charged with dried MeCN (10 mL). The reaction mixture was stirred for 5 h at room temperature. The solution was partioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4 and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300, eluent: 0.4% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **p4merSi2** (1.0 mg, 0.37 μmol, 15%) as an orange solid. R_f = 0.43 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.40 (s, 4H, NH), 9.39 (s, 4H, NH), 7.65 (d, J = 7.8 Hz, 14H, Ar-H), 7.58 (d, J = 8.4 Hz, 4H, Ar-H), 7.52 (d, J = 7.8 Hz, 14H, Ar-H), 7.46 (d, J = 8.4 Hz, 4H, Ar-H), 6.59 (s, 2H, CH), 6.58 (s, 2H, CH), 2.89–2.83 (m, 16H, CH_2CH_3), 2.67–2.61 (m, 16H, CH_2CH_3), 1.33–1.36 (m, 24H, CH_2CH_3) 1.26–1.15 (m, 66H, TIPS, CH_2CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 500.5 (4.5). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 537.0 (501.0). MALDI-TOF-MS: *m*/z (% intensity): 2554.8 (80), 2555.9 (100), 2557.0 (84), 2558.3 (66). Calcd for $C_{88}H_{104}B_2F_4N_4O_4Si_2$ ($[M]^+$): 2555.27.



***m*-Ethynyl-bridged polymer, mpoly.** A two-necked round-bottomed flask placed with **3m2** (10.0 mg, 0.0178 mmol), $Pd(OAc)_2$ (0.20 mg, 0.9 μmol), and CuI (0.17 mg, 0.0009 mmol), and DABCO (6.0 mg, 0.056 mmol) was charged with MeCN (5.0 mL). The reaction mixture was stirred under air for 24 h at room temperature, and, after a few hours, an orange solid was precipitated. The solution was partioned between water and CH_2Cl_2 and evaporated to afford **mpoly**.



***p*-Ethynyl-bridged polymer, ppoly.** A two-necked round-bottomed flask placed with **3p2** (20.0 mg, 0.0356 mmol), $Pd(OAc)_2$ (0.40 mg, 1.8 μmol), and CuI (0.34 mg, 0.0018 mmol), and DABCO (12.5 mg, 0.11 mmol) was charged with MeCN (5.0 mL). The reaction mixture was stirred under air for 12 h at room temperature, and, after a few hours, a red-black solid was precipitated. The solution was partioned between water and CH_2Cl_2 and evaporated to afford **ppoly**.



[S1] H. Maeda and Y. Haketa, *Org. Biomol. Chem.*, 2008, **6**, 3191.

Table 1 Summary of electronic and electrooptical properties of **3m1**,**2**, **3p1**,**2**, and **4m**,**p** (excited at each λ_{max} in CH_2Cl_2).

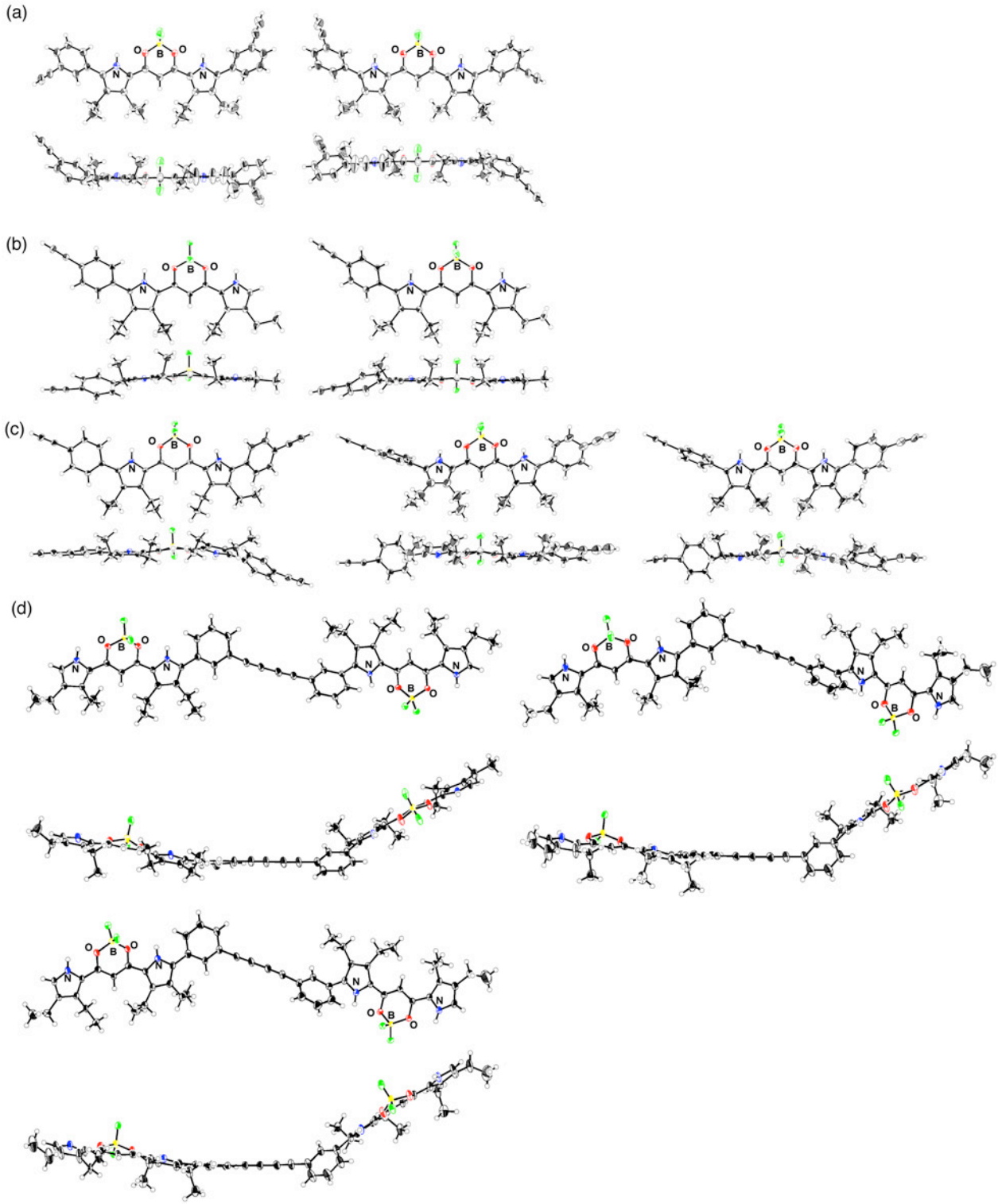
	3m1	**3m2**	**3p1**	**3p2**	**4m**	**4p**
λ_{max} (nm)	457	498	480	508	477	497
λ_{em} (nm)	507	535	516	550	507	529
Quantum yields (Φ_F)	0.83	0.91	0.88	0.87	0.87	0.85

2. X-ray crystallographic data for acyclic anion receptors and their anion complexes

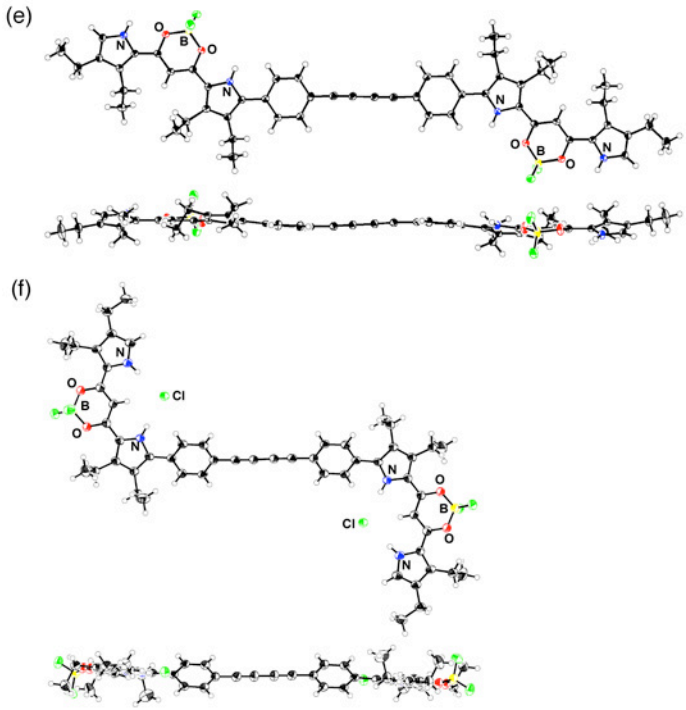
Single-crystal X-ray analysis. A single crystal of **3m2** was obtained by vapor diffusion of hexane into a CH_2Cl_2 solution of **3m2**. The data crystal was a red-colored prism of approximate dimensions 0.60 mm × 0.40 mm × 0.30 mm. Data was collected at 123(2) K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. A single crystal of **3p1** was obtained by vapor diffusion of hexane into a $CHCl_3$ solution of **3p1**. The data crystal was a yellow-colored prism of approximate dimensions 0.60 mm × 0.50 mm × 0.20 mm. Data was collected at 123(2) K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. A single crystal of **3p2** was obtained by vapor diffusion of hexane into a CH_2Cl_2 solution of **3p2**. The data crystal was a red-colored prism of approximate dimensions 0.60 mm × 0.50 mm × 0.40 mm. Data was collected at 123(2) K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. A single crystal of **4m** was obtained by vapor diffusion of hexane into a CH_2Cl_2 solution of **4m**. The data crystal was a red-colored prism of approximate dimensions 0.50 mm × 0.15 mm × 0.15 mm. Data was collected at 90(2) K on a Bruker SMART CCDC diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å), structure was solved by direct method. A single crystal of **4p** was obtained by vapor diffusion of hexane into an acetone solution of **4p**. The data crystal was a red-colored prism of approximate dimensions 0.30 mm × 0.30 mm × 0.20 mm. Data was collected at 123(2) K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. A single crystal of **4p**·$(TBACl)_2$ was obtained by vapor diffusion of hexane into a $CHCl_3$ solution of a 1:2 mixture of **4p** and TBACl. The data crystal was a yellow-colored prism of approximate dimensions 0.50 mm × 0.30 mm × 0.10 mm. Data was collected at 123(2) K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. In each case, the non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation.[S2] The scattering arising from the presence of disordered solvents in the crystals was removed by use of the utility SQUEEZE in the PLATON software package.[S3] CIF files (CCDC-819391–819396) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supporting Table 2 Crystallographic details for compounds **3m2**, **3p1**, **3p2**, **4m**, **4p**, and **4p**·$(TBACl)_2$

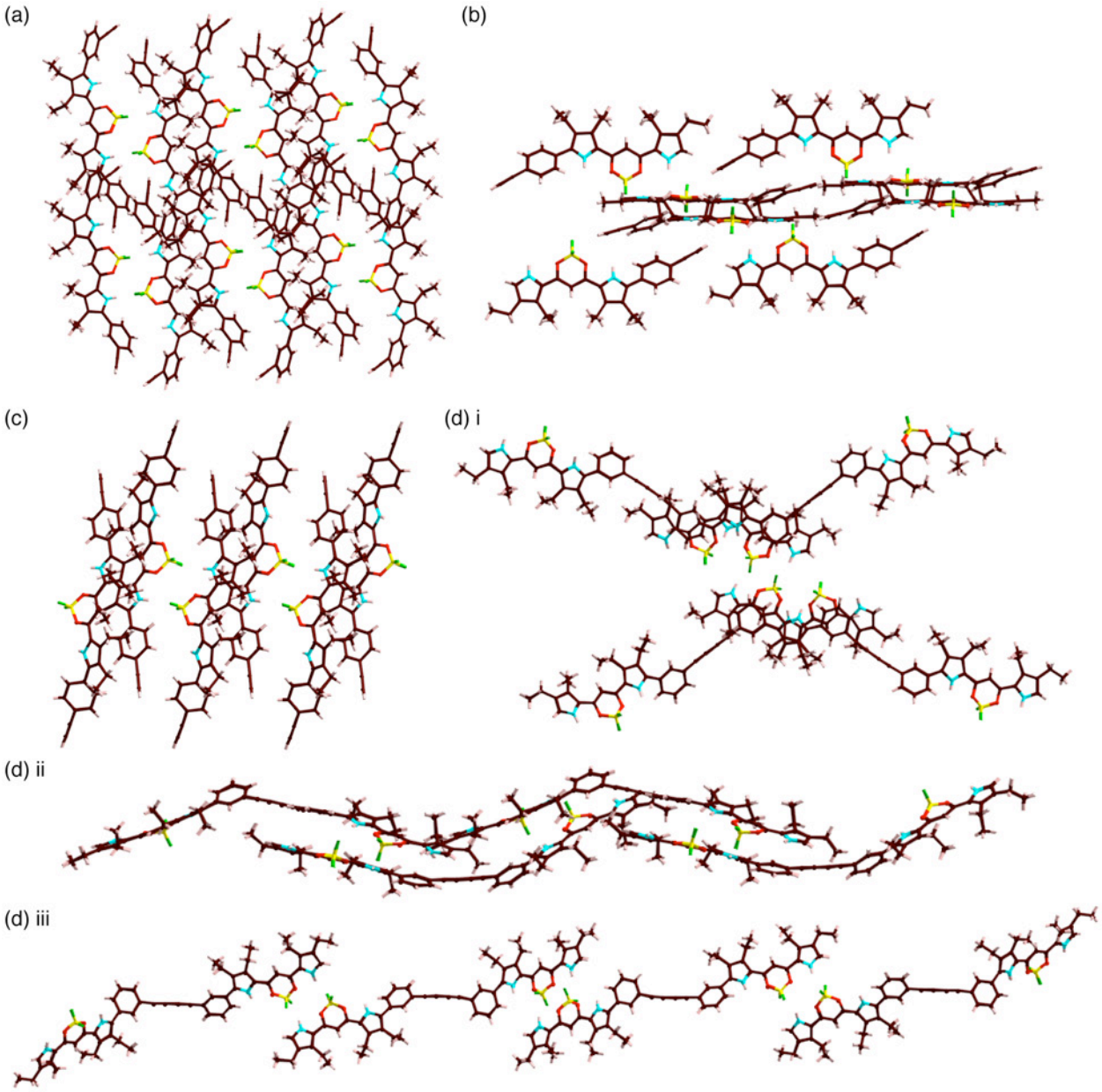
	3m2	**3p1**	**3p2**	**4m**	**4p**	**4p**·$(TBACl)_2$
formula	$C_{35}H_{33}BF_2N_2O_2$	$C_{27}H_{29}BF_2N_2O_2$	$C_{35}H_{33}BF_2N_2O_2$	$C_{54}H_{56}B_2F_4N_4O_4$	$C_{54}H_{56}B_2F_4N_4O_4$· 2acetone	$C_{54}H_{56}B_2F_4N_4O_4$ $2C_{16}H_{36}NCl$ ·0.75water
fw	562.44	462.33	562.44	922.65	1038.80	1490.4
crystal size, mm	0.60 × 0.40 × 0.30	0.60 × 0.50 × 0.20	0.60 × 0.50 × 0.40	0.50 × 0.15 × 0.15	0.30 × 0.30 × 0.20	0.50 × 0.30 × 0.10
crystal system	monoclinic	triclinic	triclinic	monoclinic	orthorhombic	triclinic
space group	$P2_1/n$ (no. 14)	P-1 (no. 2)	P-1 (no. 2)	$P2_1/c$ (no. 14)	*Pbca* (no. 61)	P-1 (no. 2)
a, Å	14.470(4)	12.211(5)	9.380(13)	29.692(5)	14.226(2)	9.681(7)
b, Å	10.780(4)	13.253(5)	9.727(17)	23.863(4)	19.130(3)	9.695(7)
c, Å	19.921(7)	16.614(5)	35.17(4)	16.660(3)	19.557(4)	22.899(14)
α, °	90	102.298(14)	89.33(6)	90	90	95.21(2)
β, °	108.253(15)	97.612(13)	84.28(4)	93.025(3)	90	91.74(2)
γ, °	90	105.900(15)	63.89(6)	90	90	92.92(3)
V, Å^3	2951.2(18)	2473.7(15)	2473.7(15)	11787(4)	5322.4(16)	2136(3)
ρ_{calcd}, gcm^{-3}	1.266	1.241	1.304	1.040	1.296	1.159
Z	4	4	4	8	4	1
T, K	123(2)	123(2)	123(2)	90(2)	123(2)	123(2)
μ(Mo-Kα), mm^{-1}	0.086	0.088	0.089	0.074	0.092	0.137
no. of reflns	23727	23491	24250	60126	46570	16858
no. of unique reflns	6651	11100	11858	20747	6093	9234
variables	403	621	1148	1372	349	525
$\lambda_{Mo\text{-}K\alpha}$, Å	0.71075	0.71075	0.71075	0.71073	0.71075	0.71075
R_1 ($I > 2\sigma(I)$)	0.0687	0.0532	0.0701	0.0663	0.0498	0.0698
wR_2 ($I > 2\sigma(I)$)	0.1607	0.1552	0.1601	0.1642	0.1131	0.1809
GOF	1.050	0.926	1.061	0.916	1.033	0.958



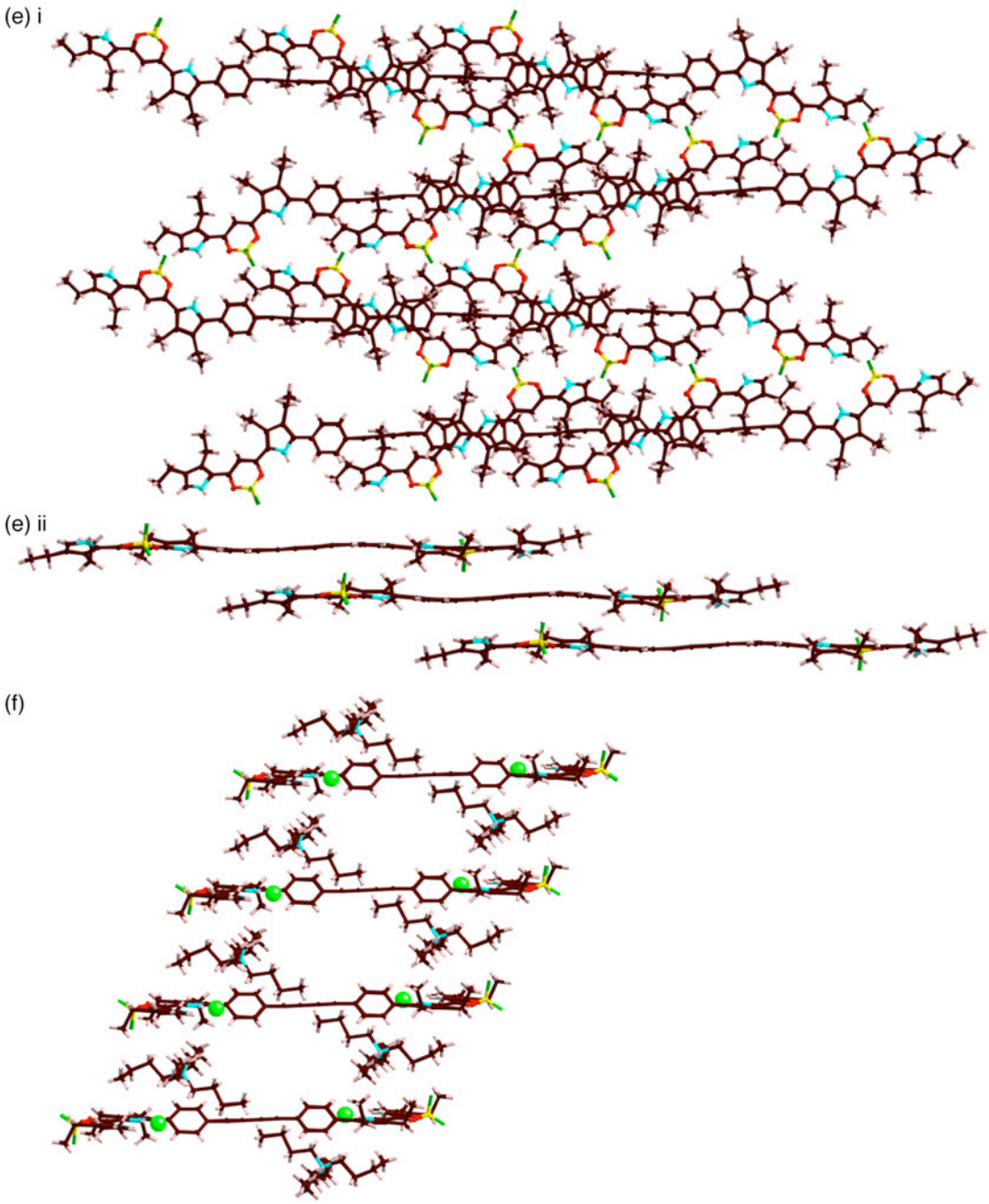
Supporting Figure 1 ORTEP drawings (top and side view) of single-crystal X-ray structures of (a) **3m2**, (b) **3p1**, (c) **3p2**, (d) **4m**, (e) **4p**, and (f) **4p**·$(TBACl)_2$. Distortion of aryl moieties are suggested by the dihedral angles between core 16 atoms' plane and the corresponding aryl plane(s) of 35.6°/39.1° in **3m2**, 29.3° and 37.8° (two independent structures) in **3p1**, 5.7°/39.0°, 28.0°/69.0°, 25.5°/74.6° (three independent structures with one disordered pair) in **3p2**, 19.5°/34.8°, 14.9°/23.2° in **4m** (two independent structures), 2.2° in **4p**, and 40.0° in **4p**·$(TBACl)_2$. Thermal ellipsoids are scaled to the 50% probability level.



Supporting Figure 1 (Continued).



Supporting Figure 2 Solid-state assembled structures of (a) **3m2**, (b) **3p1**, (c) **3p2**, (d) **4m**, (e) **4p**, and (f) **4p**·$(TBACl)_2$. Atom color code: brown, pink, yellow, green, yellow green, blue, and red represent carbon, hydrogen, boron, fluorine, chlorine, nitrogen, and oxygen, respectively.

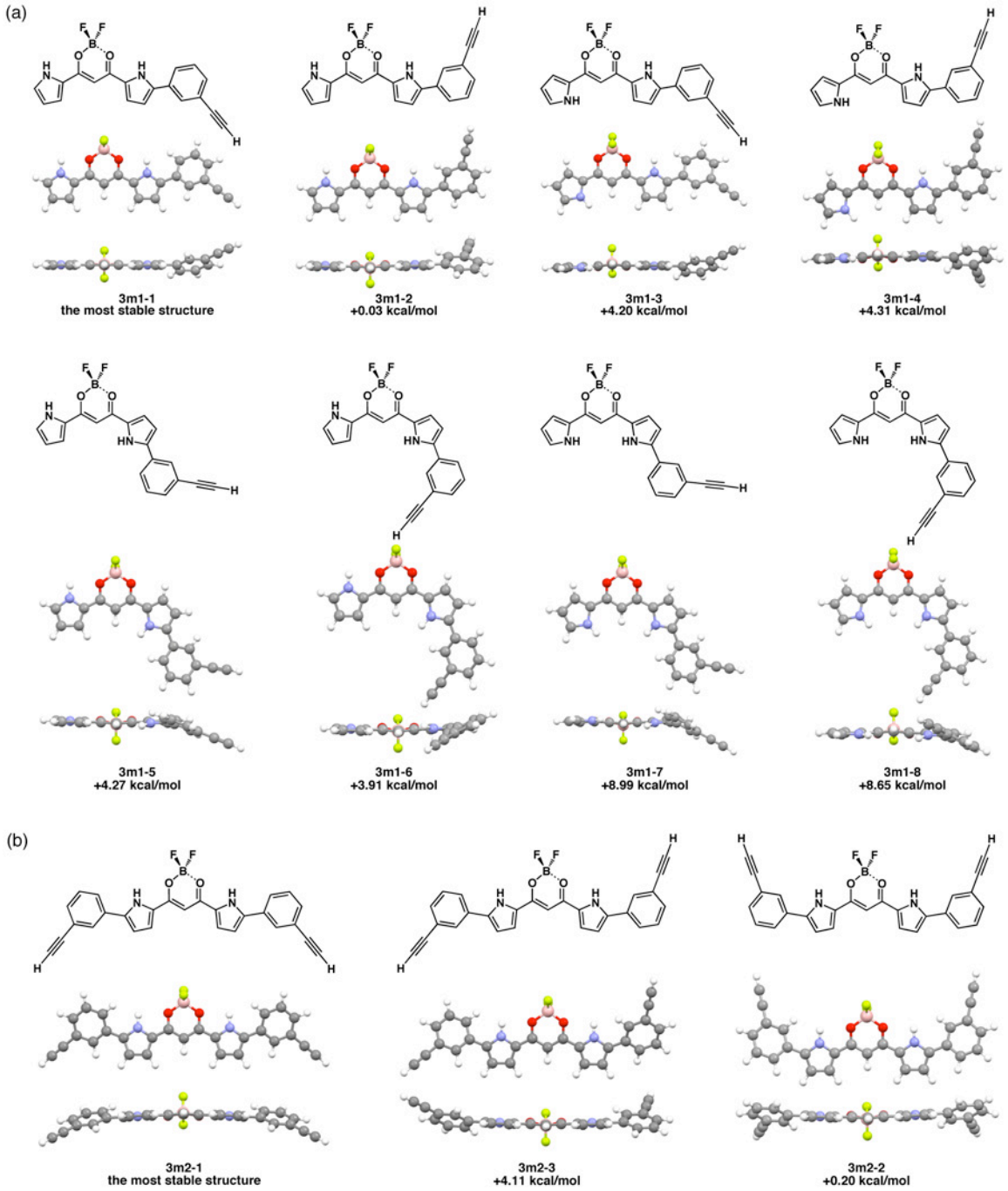


Supporting Figure 2 (Continued).

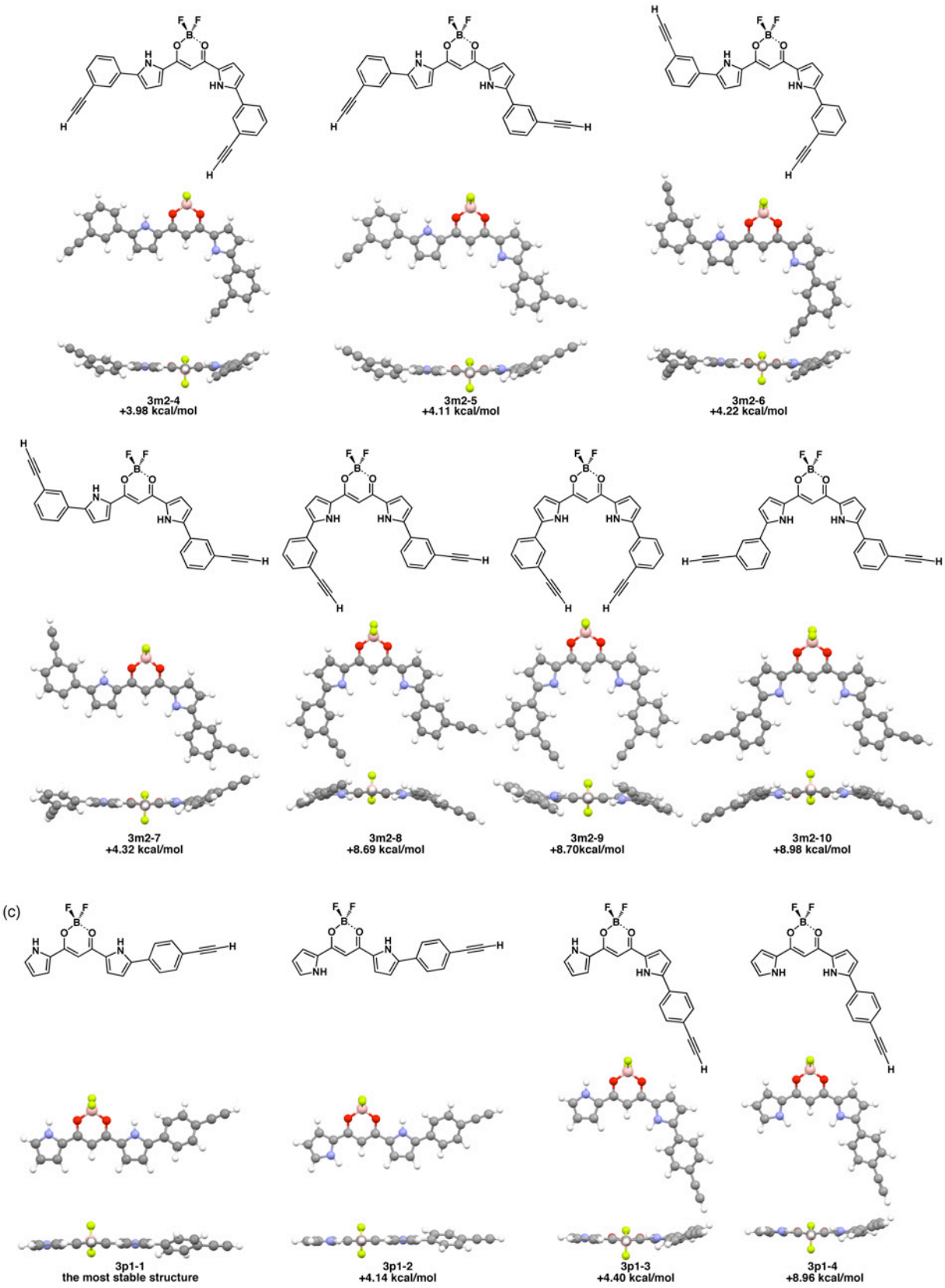
[S2] *CrystalStructure: Crystal Structure Analysis Package* Rigaku and Rigaku/MSC, The Woodlands, 2000.
[S3] (a) Spek, A. L. *PLATON, A Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, 2005. (b) P. van der Sluis and A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194.

3. Optimization of acyclic anion receptors and their anion complexes

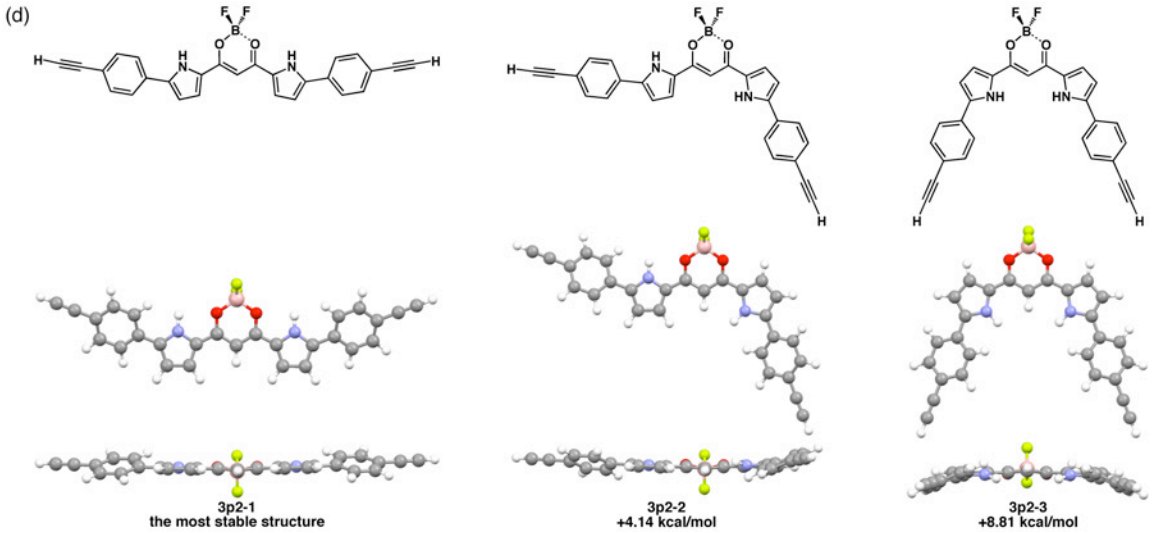
DFT and semi-empirical calculations. Ab initio and semi-empirical calculations of anion receptors and Cl^- binding complexes were carried out by using Gaussian 03 program[S4] and an HP Compaq dc5100 SFF computer. The structures were optimized, and the total electronic energies were calculated at the B3LYP level using a 6-31G** basis set for receptors (monomers and covalently linked dimers) and [1 + 1]-type anion complexes, at AM1 level for Cl^- complexes of covalently linked dimers, and at PM6 level for metal-bridged dimers and their Cl^- complexes.



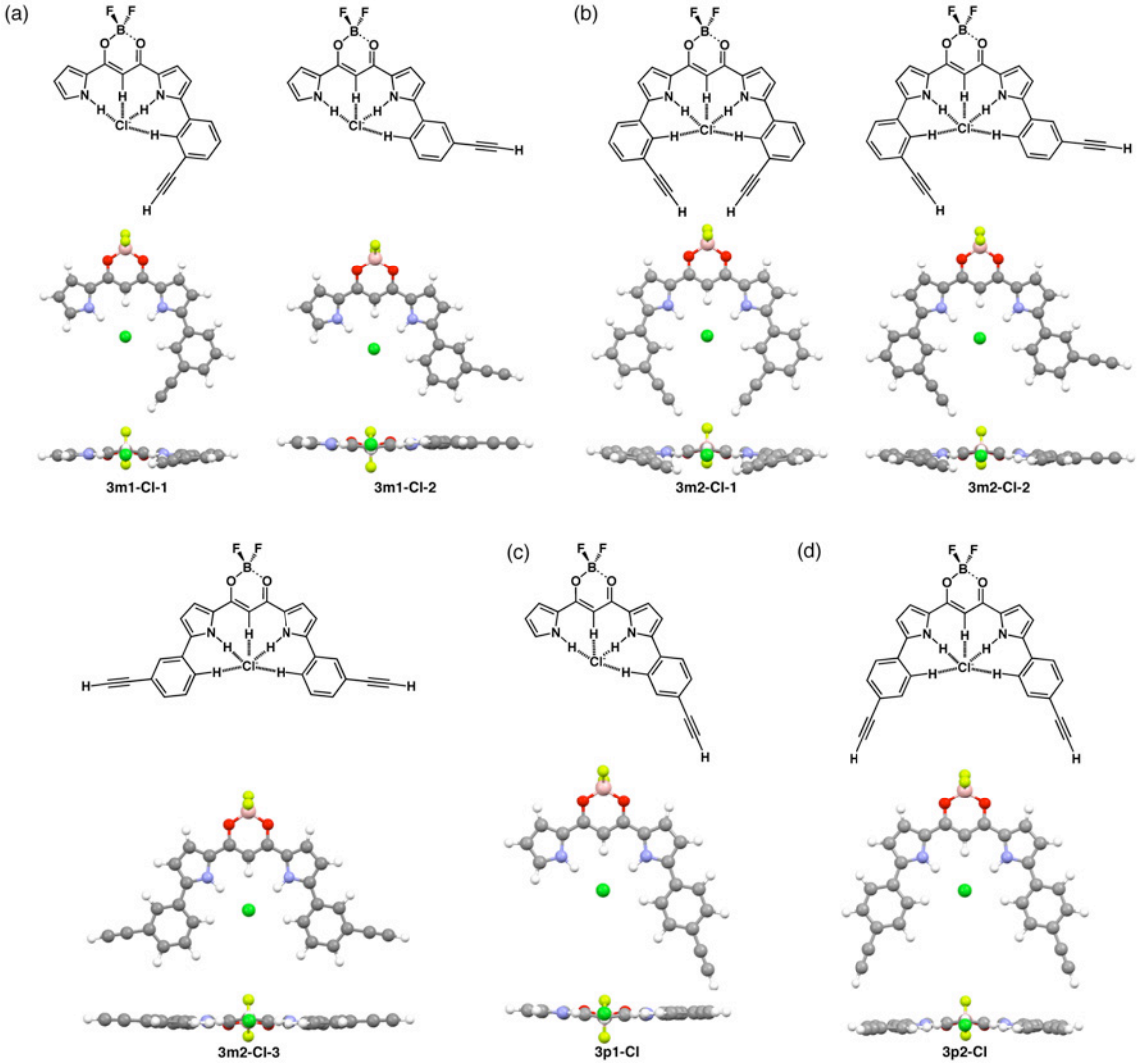
Supporting Figure 3 Optimized structures of (a) **3m1**, (b) **3m2**, (c) **3p1**, and (d) **3p2** (eight, five, four, and three conformations for each compound) at B3LYP/6-31G(d,p) level. Ethyl substituents at β-positions are omitted for facile calculations. In meta-substituted derivatives, the calculations suggest that the orientation of ethynyl moieties does not significantly influence the stabilities of the molecules.



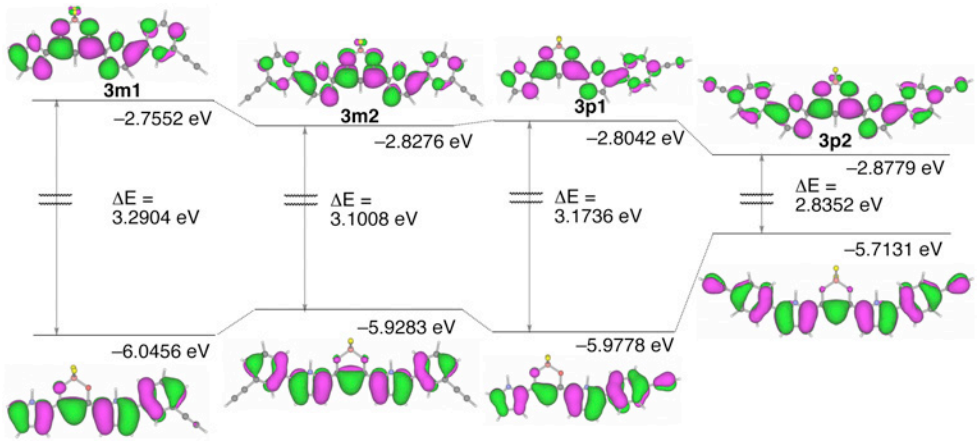
Supporting Figure 3 (Continued).



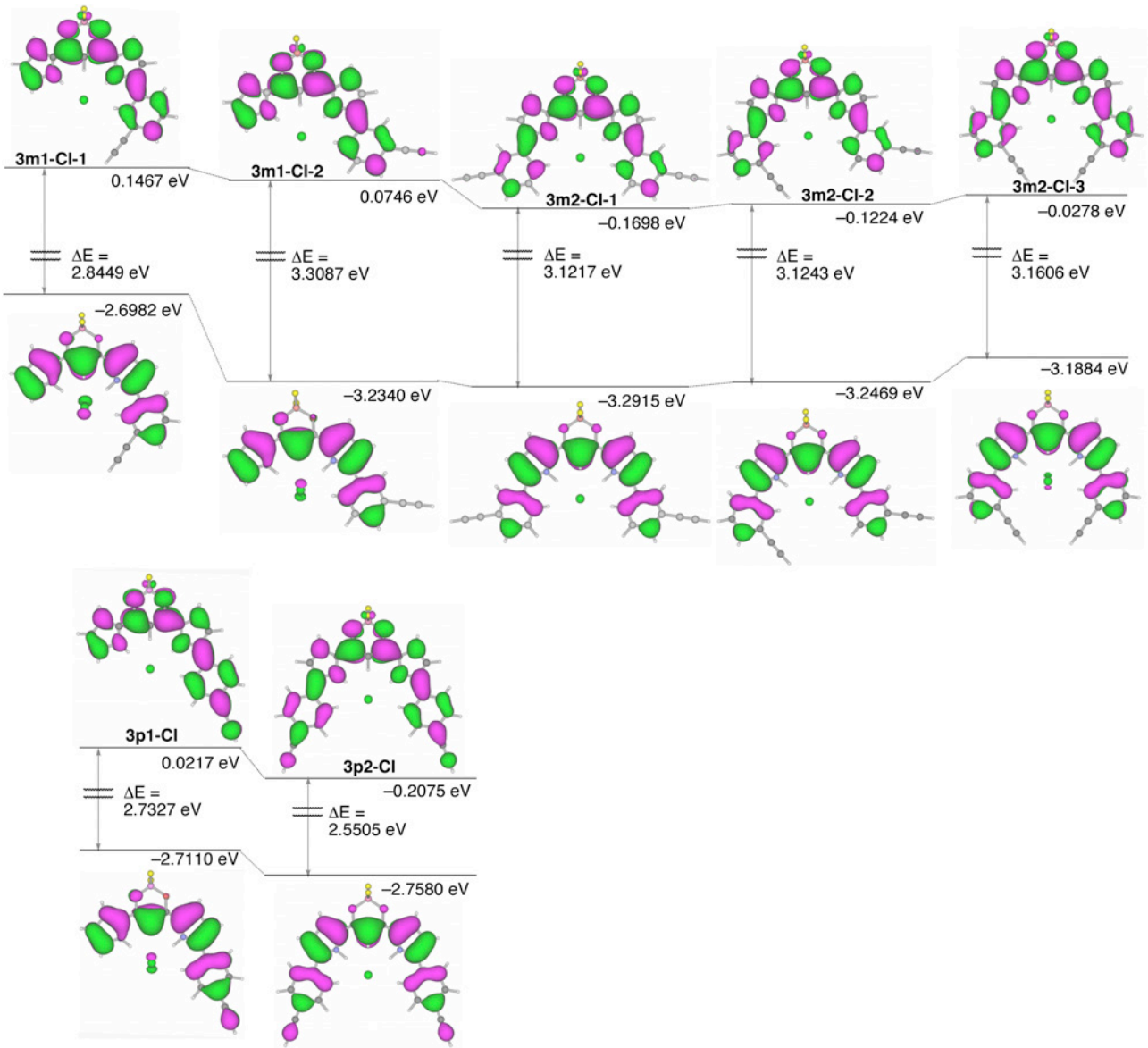
Supporting Figure 3 (Continued).



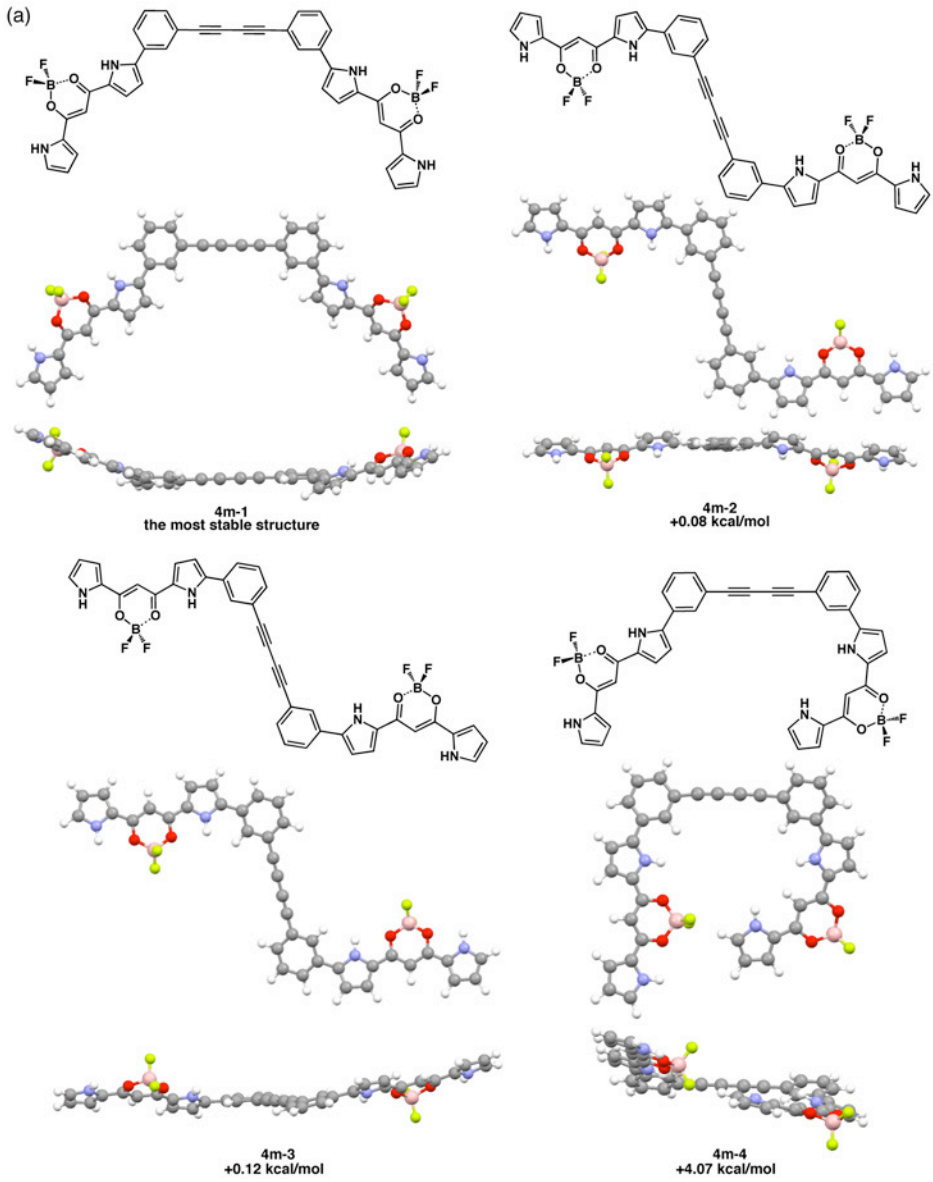
Supporting Figure 4 Optimized structures of anion (Cl^-) complexes of (a) **3m1**, (b) **3m2**, (c) **3p1**, and (d) **3p2** (two, three, one, and one conformations for each complex) at B3LYP/6-31G(d,p) level. Ethyl substituents at β-positions are omitted for facile calculations.



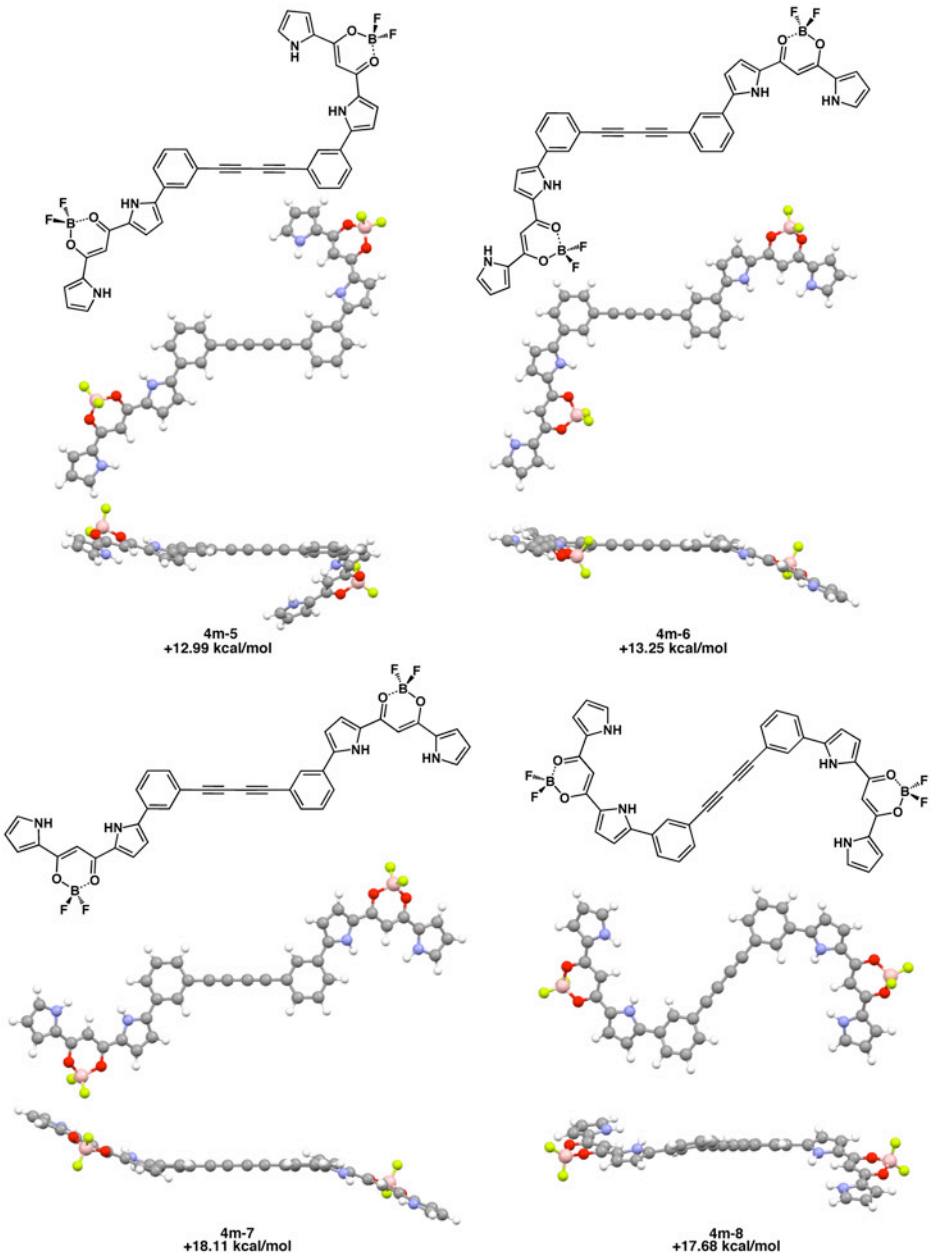
Supporting Figure 5 Molecular orbitals (HOMO and LUMO) of **3m1**, **3m2**, **3p1**, and **3p2** (from left to right) at B3LYP/6-31+G(d,p) level. Ethyl substituents at β-positions are omitted for facile calculations.



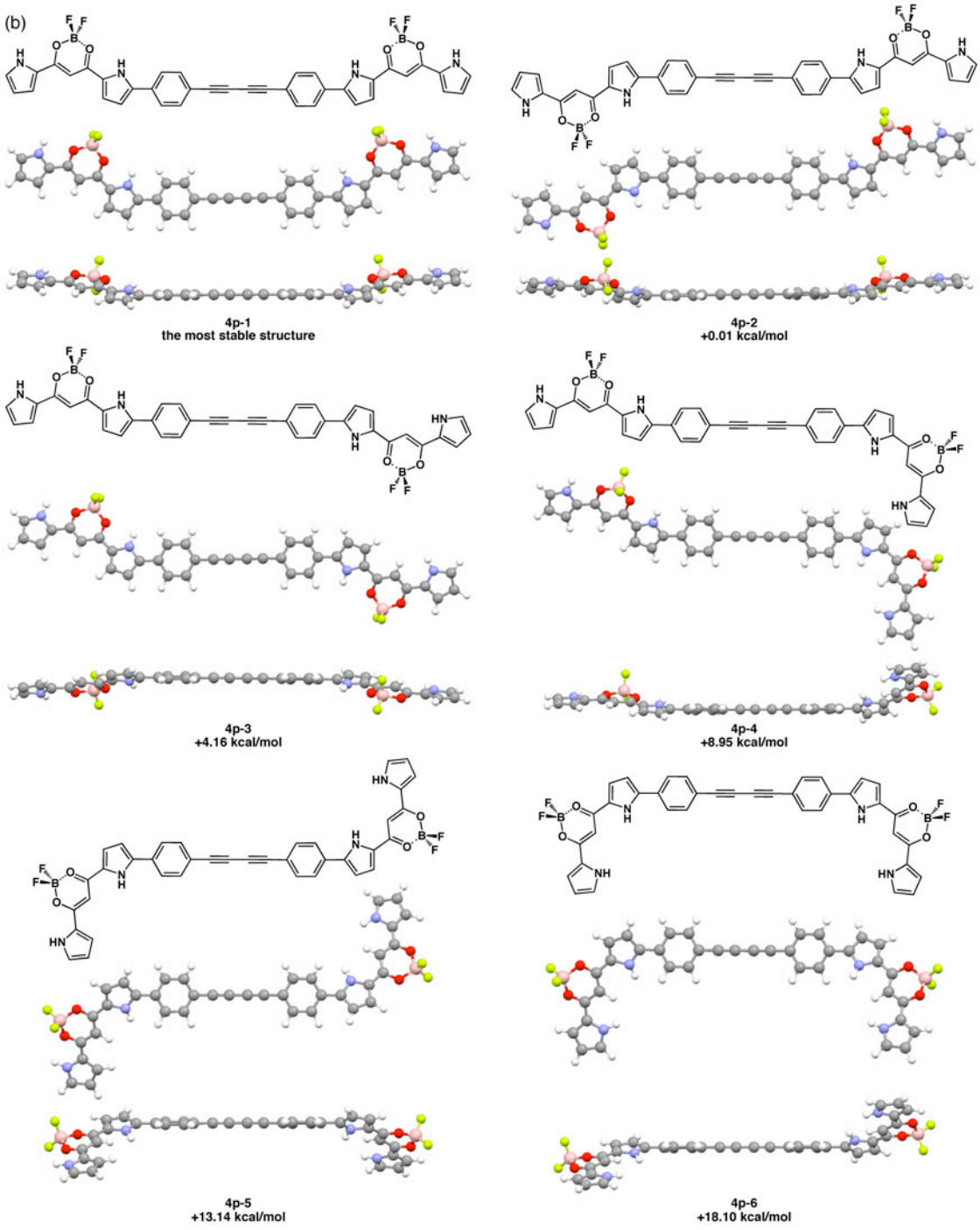
Supporting Figure 6 Molecular orbitals (HOMO and LUMO) of anion (Cl^-) complexes of **3m1** and **3m2** (from left to right in the top) and **3p1** and **3p2** (from left to right in the bottom) at B3LYP/6-31+G(d,p) level. Ethyl substituents at β-positions are omitted for facile calculations. The energies of both HOMO and LUMO in receptor–Cl^- complexes are higher than those of corresponding receptors.



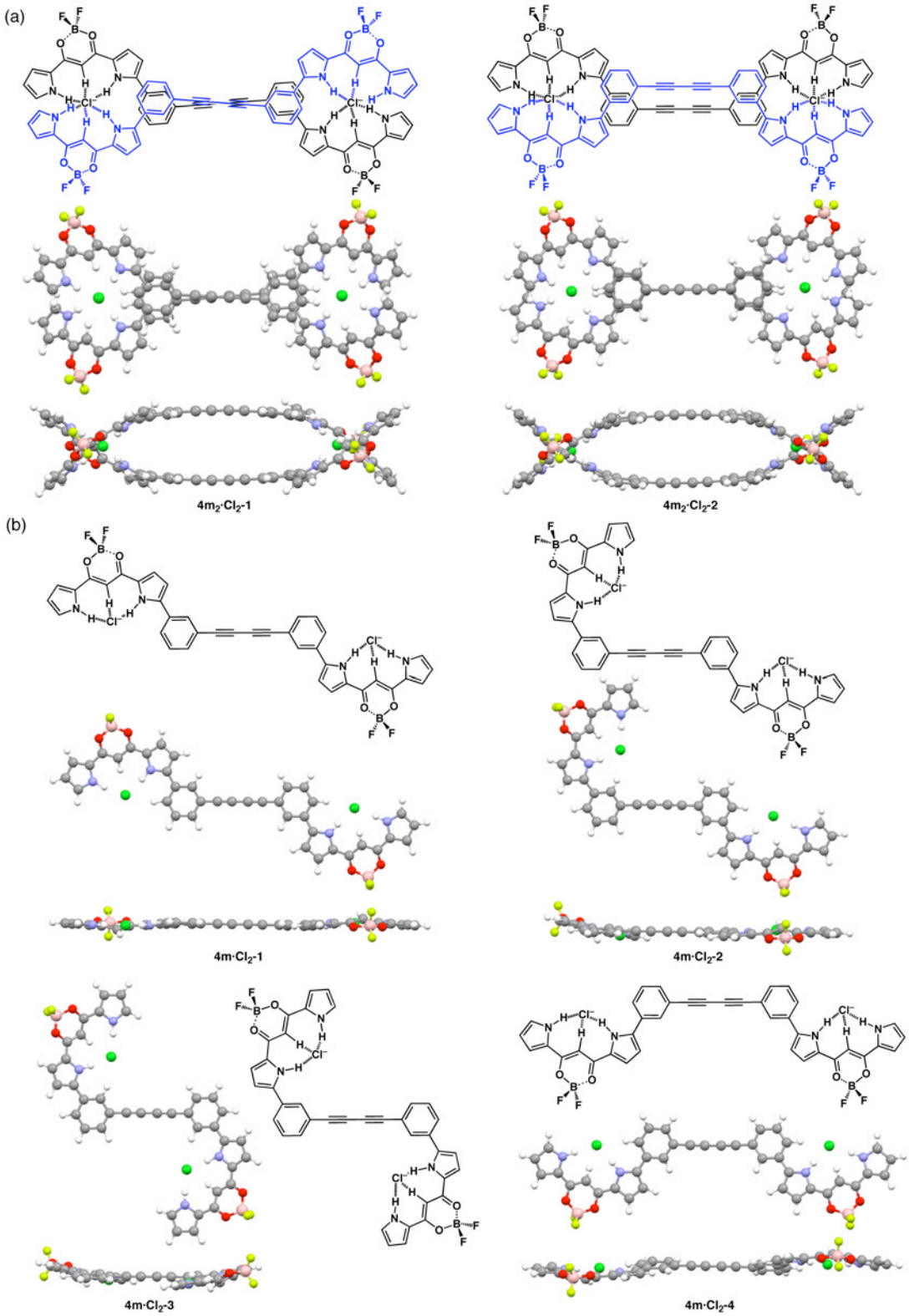
Supporting Figure 7 Optimized structures of (a) **4m** and (b) **4p** (eight and six conformations for each compound) at B3LYP/6-31G(d,p) level. Ethyl substituents at β-positions are omitted for facile calculations. This supporting figure suggests that the conformations without pyrrole inversions are stable although various conformations are theoretically possible in anion-free receptor dimers.



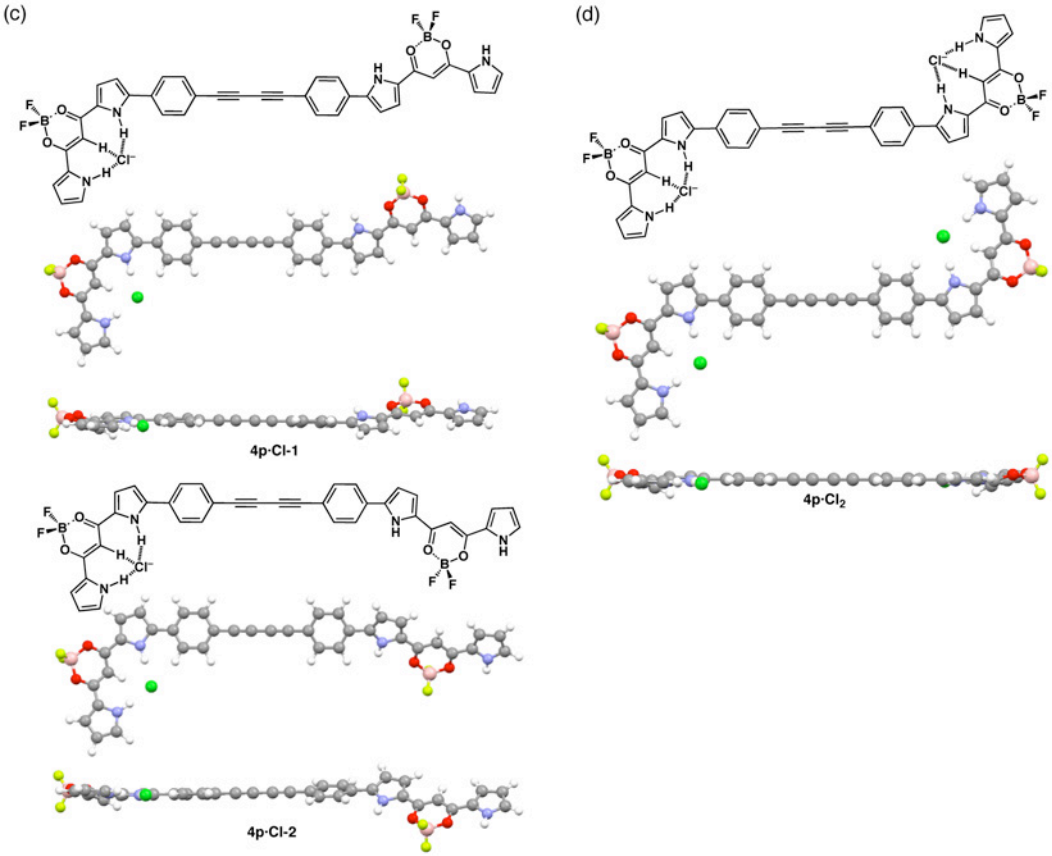
Supporting Figure 7 (Continued)



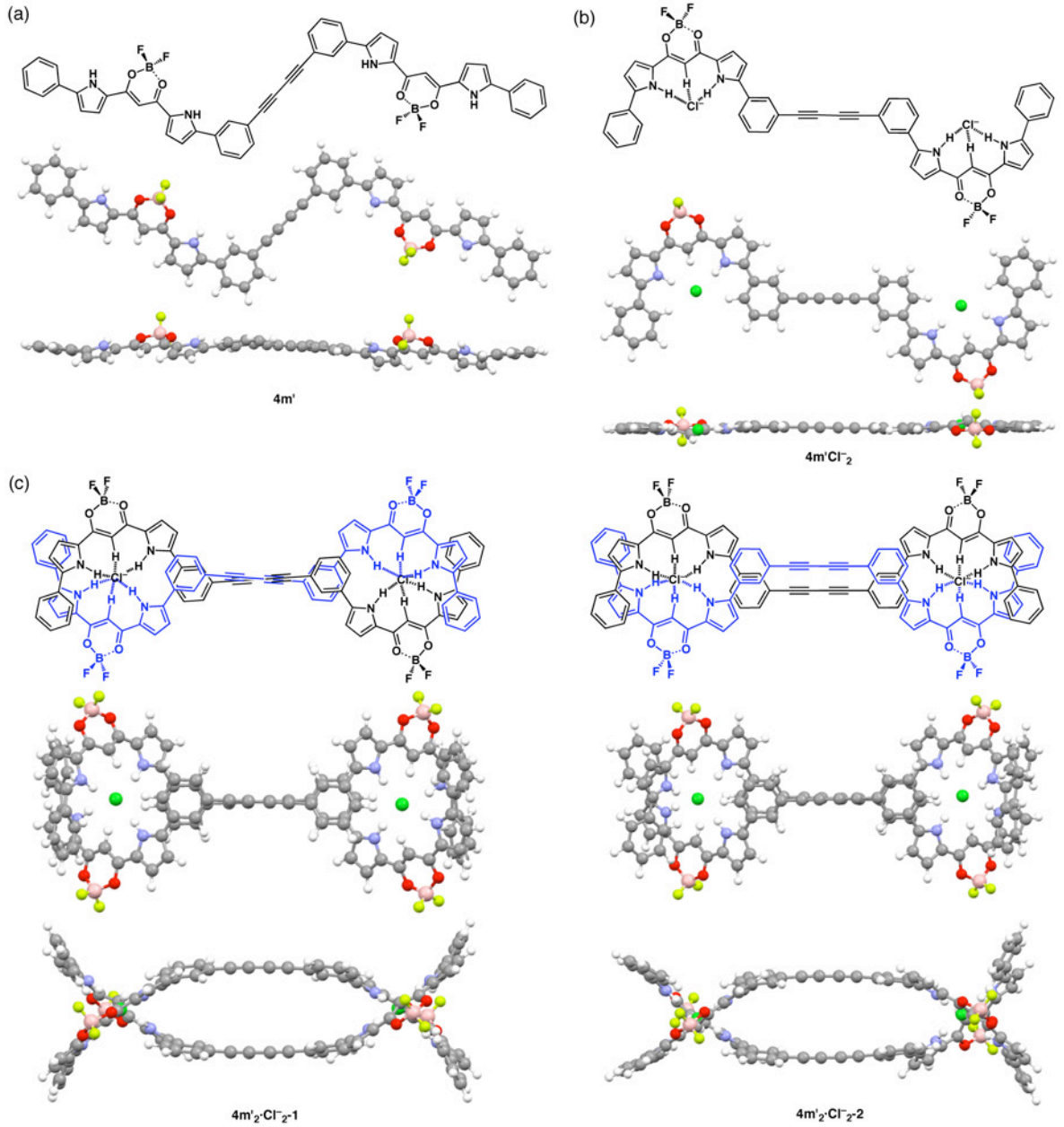
Supporting Figure 7 (Continued)



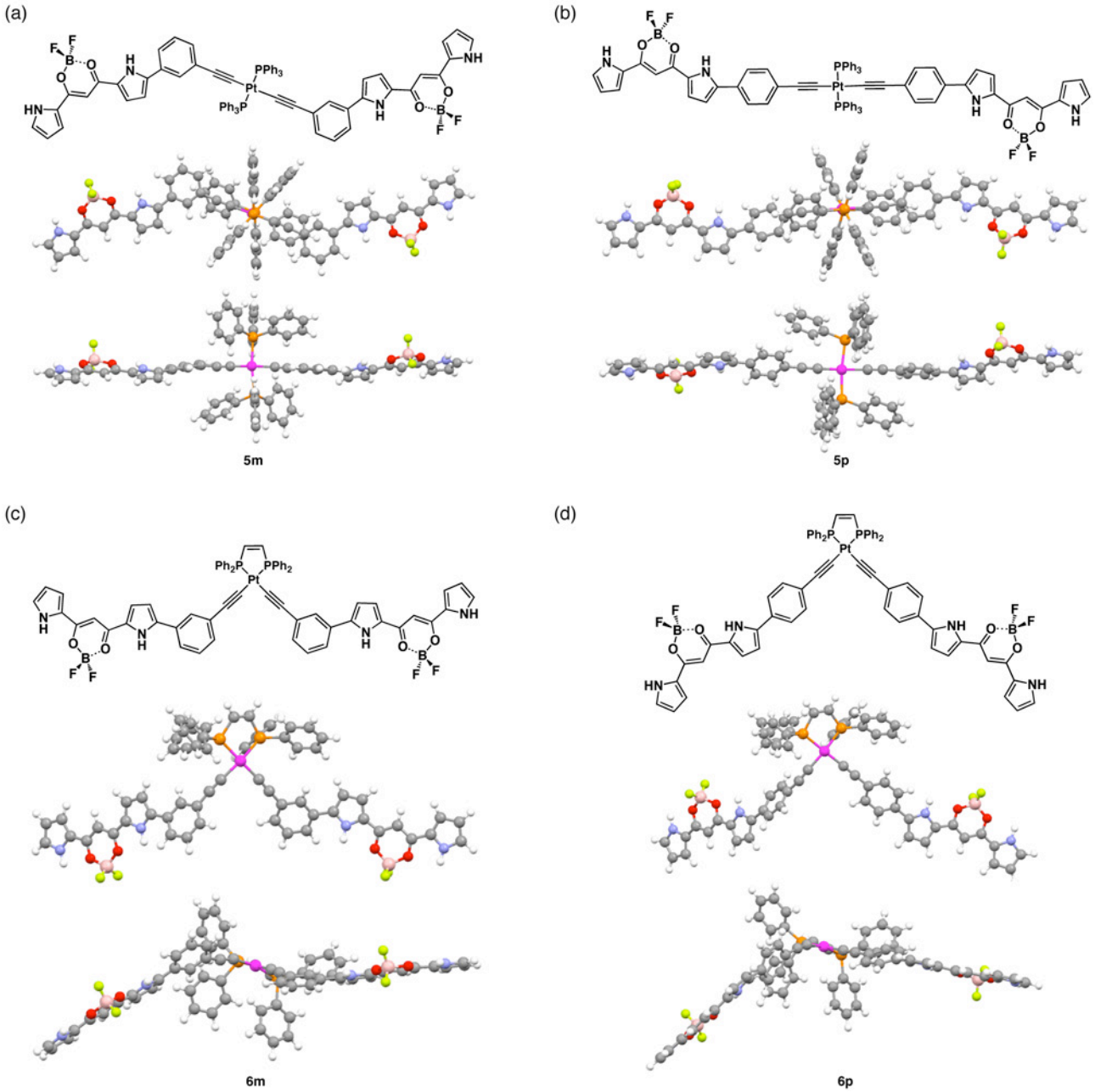
Supporting Figure 8 Optimized structures of anion (Cl^-) complexes of **4m** and **4p**: (a) **4m**$_2$·Cl^-_2 (chiral (*MM*, left) and meso (right) structures), (b) **4m**·Cl^-_2, (c) **4p**·Cl^-, and (d) **4p**·Cl^-_2 (two, four, two, and one conformations as the representatives for each complex) at AM1 level. Ethyl substituents at β-positions are omitted for facile calculations. This supporting figure suggests that various conformations are theoretically possible in anion complexes of receptor dimers. In particular, theoretical study of the [2 + 2]-type complexes of **4m** (**4m**$_2$·Cl^-_2) suggests that formation of two diastereomers seem possible.



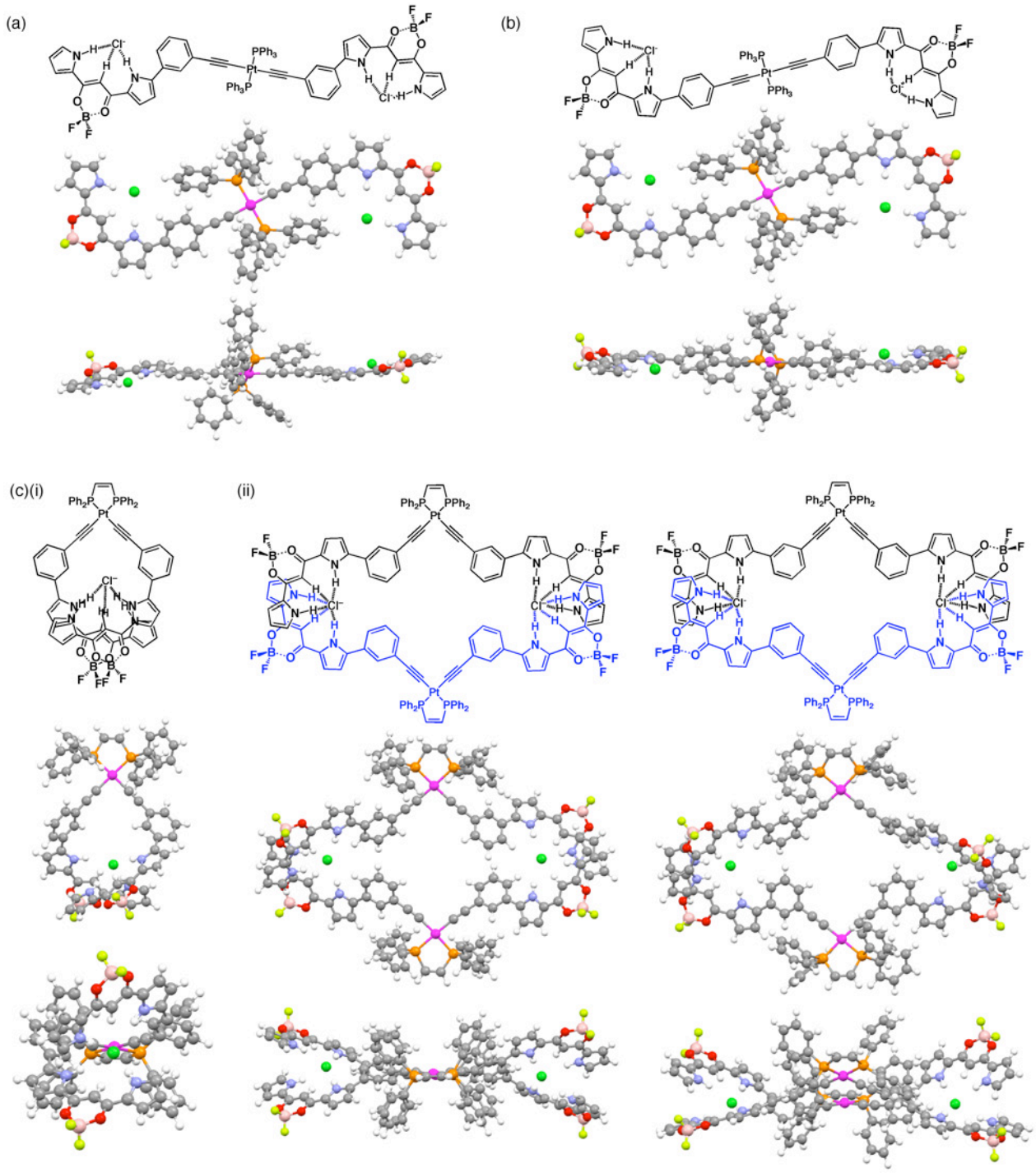
Supporting Figure 8 (Continued)



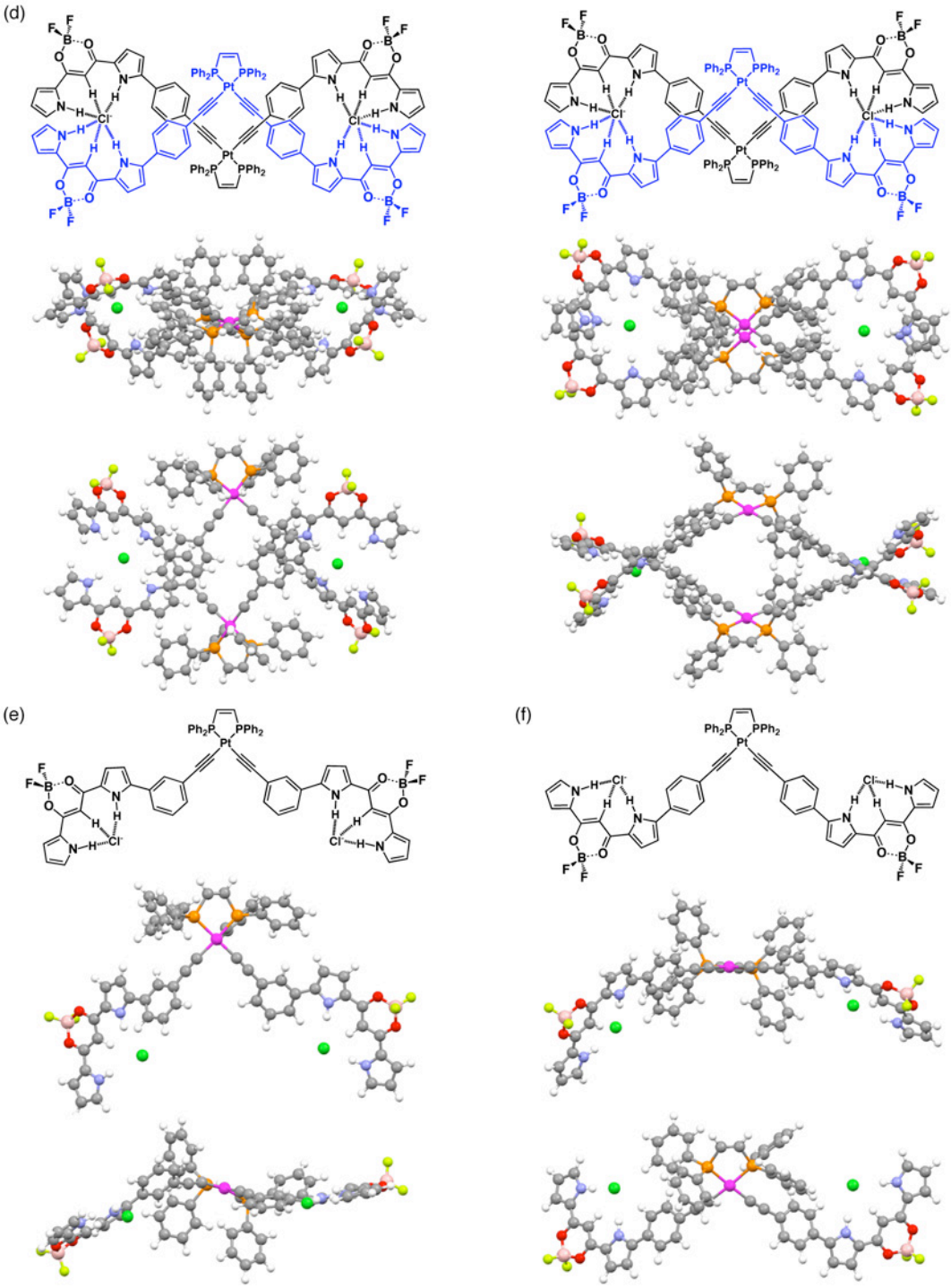
Supporting Figure 9 Optimized structures of anion (Cl^-) complexes: (a) **4m´**, (b) **4m´**$_2$·Cl^-_2 (chiral (*MM*, left) and meso (right) structures), and (c) **4m´**·Cl^-_2 at AM1 level. Ethyl substituents at β-positions are omitted for facile calculations. In the [2 + 2]-type complexes of **4m´** (**4m´**$_2$·Cl^-_2), formation of two diastereomers seem possible in theoretical study.



Supporting Figure 10 Optimized structures of Pt^{II}-bridged dimers (**5m**,**p** and **6m**,**p**) at PM6 level: (a) **5m**, (b) **5p**, (c) **6m**, and (d) **6p**. Ethyl substituents at β-positions are omitted for facile calculations.



Supporting Figure 11 Optimized structures of anion (Cl^-) complexes of Pt^{II}-bridged dimers at PM6 level: (a) **5m**·Cl^-_2, (b) **5p**·Cl^-_2, (c) candidates of the anion complexes with the 1:1 ratio of the dimer **6m** and anion (Cl^-), (i) **6m**·Cl^- as a possible assembly and (ii) **6m**$_2$·Cl^-_2 (chiral (*MM*, left) and meso (right) structures), (d) **6p**$_2$·Cl^-_2, (e) **6m**·Cl^-_2, and (f) **6p**·Cl^-_2. Ethyl substituents at β-positions are omitted for facile calculations. In the [2 + 2]-type complexes of **6p** (**6p**$_2$·Cl^-_2), formation of two diastereomers seem possible in theoretical study.



Supporting Figure 11 (Continued)

Cartesian Coordination of 3m1-1

–1216.4987466 hartree

B,-2.42430582,2.0529178869,0.2291686756
C,8.2201550334,-1.7204174583,0.8488450062
C,-3.5494814953,-0.1619679307,0.0107870524
C,0.1630705134,-0.6494312675,-0.1705766565
C,-1.1495921921,-0.0706961506,-0.0583568304
C,-4.8201258945,-0.8393419463,-0.0252100654
C,0.6198892774,-1.9603406421,-0.3322084965
C,2.021838041,-1.9168284184,-0.361316597
C,2.4164763152,-0.5790078745,-0.2211952678
C,-7.0586829542,-0.9424651256,0.0361536199
C,-6.5919749793,-2.2418065603,-0.1275199509
C,-5.1851883592,-2.1796621665,-0.1665568675
C,3.7529913428,0.016644387,-0.2014361659
C,4.8620214685,-0.7647684213,0.1547540573
C,6.1551300192,-0.220364677,0.1743073408
C,6.3373993082,1.1351711046,-0.1594128207
C,5.2395979184,1.9155343761,-0.5104139697
C,3.959419359,1.3668341534,-0.5381837874
C,7.272850086,-1.0339643088,0.540346182
C,-2.3250917771,-0.8219187394,-0.1032811849
F,-2.4131180695,2.6572500818,1.4562352148
F,-2.4870445549,2.9261158472,-0.8219366766
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H,5.3822262357,2.9584973618,-0.7756521881

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H,-7.2054570196,-3.1272572498,-0.2086130272
H,4.7248623957,-1.801922116,0.439428527
H,1.2053411337,1.1542132446,0.0599674423
H,-5.9878797535,0.8909885046,0.2105990984
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H,-4.5056619778,-3.0114636782,-0.283685343
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H,-2.2879294877,-1.8943869455,-0.2257610076
H,-0.0001515648,-2.8399973948,-0.4278389595
H,2.6894769153,-2.7537770008,-0.5043943711
N,-5.9859578969,-0.1122411846,0.0961343297
N,1.2747587227,0.1619302729,-0.1138985306
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O,-1.160921762,1.2295827282,0.0908884544

Cartesian Coordination of 3m1-2

–1216.4986925 hartree
C,-6.3661564853,3.0813622185,-0.9242130876
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H,-6.8365941027,-2.3019845449,0.9192508079
H,-4.4414748752,-2.9018141652,0.8347297475
H,-2.3174368168,-3.5471379704,-0.1850694695
H,-3.5289070066,1.0373055183,-0.655619038
H,7.9414041343,0.3859991306,-0.3776149131
H,5.6649053539,1.4786354584,-0.1002948853
H,-1.4673798515,0.5644233657,0.2220096977
H,0.3521627818,-3.1972813995,-0.2121629721
H,-6.6748920061,4.0606932787,-1.2087608118
H,2.4644441506,-1.8968294788,-0.0460071718
H,4.8207871115,-2.6294130643,-0.3843277031
H,7.4967091821,-2.2936547109,-0.5696776768
N,-1.3803642713,-0.4310407347,0.0754202695
N,5.8215277607,0.4859056592,-0.1980383572
O,0.8591504724,1.0228591888,0.1214395402
O,3.2984902558,1.331372925,0.0284159558
B,1.9869024582,1.997287099,0.3904644318
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C,4.7883999062,-0.4282296097,-0.1909190859
C,3.4318574135,0.0308339582,-0.0405722931
C,-0.1545637944,-1.0549489826,-0.0017915268
C,5.3588928256,-1.6933324804,-0.3454457248
C,6.7533774813,-1.5200148683,-0.4435473386
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C,-3.804423229,-0.9780544847,0.0899729537
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Cartesian Coordination of 3m1-3

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C,0.1277305023,-0.6080349536,-0.1196887813
C,-1.1708323903,0.0047661121,-0.0166354919
C,-4.8648508306,-0.6742485562,-0.0649565803
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C,-6.133387667,-0.1014396283,0.0029331656
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C,6.3321552423,1.0585744948,-0.2936285247
C,5.2441067561,1.8383706004,-0.6750539875
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C,7.2380360443,-1.0850251653,0.5151086953
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F,-2.4253006965,3.2199112206,-0.4568899089
H,5.4019628082,2.8622592752,-0.9993854626
H,3.1253003336,1.9277096326,-0.9950847784
H,-8.1565178124,-1.0412729725,-0.0948387753
H,4.6755163785,-1.8103313264,0.4871403638
H,1.2058549227,1.1850618226,-0.0047997534
H,-4.3090891099,-2.7161090093,-0.3380854794
H,-6.3176614053,0.9543605164,0.1320105233
H,9.004104503,-2.3738097513,1.1453290749
H,-2.3282526667,-1.8021205723,0.0482697161
H,-0.0781573568,-2.8060728447,-0.2592458391
H,2.6100753259,-2.7748106949,-0.3809668573
H,-6.7269201407,-3.3399195478,-0.3740975223
H,7.3377392547,1.4643198004,-0.3097165226
N,-5.0451928882,-2.0395435739,-0.2187444064
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O,-3.6185684846,1.2752946461,0.039588256

Cartesian Coordination of 3m1-4

–1216.4918766 hartree
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C,6.5136950453,-0.3770911717,0.1991932135
C,5.5923813141,0.5878362646,-0.2476169882
C,4.2275780691,0.2613216932,-0.3003363093

C,6.0373860022,1.8838375336,-0.6556978057
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H,7.568425227,-0.127790066,0.2379037616
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H,-6.0005022974,1.5664928753,-0.0085755815
H,4.3692788441,-2.9283269487,0.8706395265
H,-7.0549474224,-2.5933716343,-0.6784355873
H,-8.1166966072,-0.1045433182,-0.3889348002
H,-2.5022082745,-1.7896740246,0.0311490312
N,-5.1995903699,-1.5819690123,-0.3984840675
N,1.3580005386,-0.4068338763,0.0845054962
O,-3.2804746181,1.455086056,0.0253986715
O,-0.8485267434,1.0956508506,0.1118483257

Cartesian Coordination of 3m1-5

–1216.4919484 hartree
C,-1.4190977322,2.4222626619,-7.8499299755
F,-1.1693509756,1.6609273245,4.1097720092
F,1.0714617706,1.9488999428,4.536290487
H,0.5482011771,-2.2842666451,-5.2896310711
H,-0.2927081044,-0.8542934295,-7.1398398366
H,-0.6980901502,2.4317450704,-4.4019392463
H,-1.7768633092,3.0413300195,-8.6399739906
H,-0.1453779661,-0.5783893273,-1.0686530543
H,0.5359285818,3.3329172032,-2.4333092297
H,0.5964179873,3.3367744547,0.2798812502
H,0.2082382716,-2.006199362,5.5590341252
H,-0.0722403948,-3.7714613557,1.7547285264
H,0.8164793609,-1.3572229553,-3.0218989726
H,0.1145916581,-4.5014270088,6.0278183064
H,-0.0709443619,-5.7376949408,3.6086650044
H,-0.0839802276,-1.4213691724,0.971990844
N,0.1377378379,-2.7249991269,4.8531944984
N,0.1191588109,0.393560206,-1.0666390905
O,0.268974924,-0.18658529,4.0387727731
O,0.3650571504,1.5901745626,2.339664701
B,0.1188922075,1.308558553,3.802400373
C,0.3942945929,2.4862421467,-1.7775734108
C,0.4375461437,2.4930678565,-0.3745038041
C,0.2073030804,0.684328112,1.4148024736
C,0.2532074871,1.1818146793,0.0634022592
C,0.0797383228,-2.4321489455,3.5067620233
C,0.0837799322,-4.0687605257,5.0388895546
C,-0.0111180769,-4.6746520144,3.7912413224
C,-0.0129689664,-3.6478985966,2.8265563448
C,0.1209437267,-1.0573901538,3.0762551212
C,0.035475664,-0.6677096779,1.7374911154
C,0.0629193816,0.6052868356,-3.5401271832
C,0.4076203671,-0.7316152427,-3.8102953508
C,0.273977043,-1.2517832851,-5.0959801748
C,-0.1913955752,-0.4538741434,-6.1371172376
C,-0.5321423684,0.8901068973,-5.8918722254
C,-0.4066271666,1.4049482956,-4.5924847919
C,-1.0133350962,1.7208947756,-6.9515958044
C,0.1859385982,1.1684932485,-2.1950576951

Cartesian Coordination of 3m1-6

–1216.49251 hartree
B,-3.5227224712,-1.9529005834,0.2031621484
C,5.3742653023,3.8218499685,0.8887644015
C,-2.9127312042,3.044706803,-0.168218007
C,-3.5021949106,1.7791722901,-0.1457011725
C,-2.9722945178,0.4426699399,-0.053219719
C,-1.6105768892,0.161936346,0.0853007259
C,-1.1892771058,-1.1728300752,0.0424258522
C,0.1968136374,-1.566305064,0.0385583213
C,0.7415415491,-2.8451819014,0.1451940876
C,2.1394031954,-2.7201675099,0.0940844136
C,2.4454986453,-1.3634153411,-0.0449210937
C,-5.1487873618,3.2914603999,-0.311073934
C,3.7382237733,-0.6861742487,-0.1490938281
C,4.8580590196,-1.3723346878,-0.6530155357
C,6.0912097828,-0.7341452073,-0.7545578087
C,6.235764982,0.5968513914,-0.3698135014
C,5.1295941197,1.3033299413,0.1366526042
C,3.8913723245,0.6502337316,0.2486422169
C,5.2626365982,2.6666594322,0.5468179908
C,-3.9491805963,3.9932120315,-0.2709956577
F,-3.803871014,-2.1621346582,1.5282632174
F,-4.2082864122,-2.7569184815,-0.6561618065
H,6.9456651273,-1.2761034234,-1.1480619706
H,7.1940417146,1.0976569554,-0.45357277
H,3.0585831863,1.1932131439,0.6841711505
H,5.4767159066,4.837403836,1.1946314593
H,-6.166094123,3.6459741842,-0.3858838569
H,-3.8446621733,5.0676006697,-0.3127053498
H,-1.8531796293,3.2506781968,-0.1186525637
H,-5.517131898,1.194038952,-0.2385053025
H,-0.9036579658,0.9737887999,0.1830089366
H,2.8631628133,-3.5165050497,0.1893219212
H,4.7498292002,-2.4002204848,-0.9832574826
H,0.1608597989,-3.7466285179,0.2705045874
H,1.1722180808,0.293495158,-0.3008860135
N,1.2564791606,-0.6809889252,-0.0588038559
N,-4.8659025315,1.9658502683,-0.2360135007
O,-3.8649776309,-0.508430267,-0.1311624695
O,-2.0429472834,-2.156770994,-0.0208496339

Cartesian Coordination of 3m1-7

-1216.4844263 hartree
B,-3.4202352939,-2.2347605897,-0.0046440919
C,8.2126033635,-0.2526285627,1.1102144909
C,2.2827181602,-2.0450646963,-0.2578172536
C,0.9252295563,-2.4012135659,-0.1949496562
C,-1.2511239735,-1.0719468748,-0.0425636189
C,0.1802696031,-1.2257563012,-0.121649986
C,-4.0340767719,1.4530400157,0.1649500567
C,-4.44978848,3.6612838165,0.2127705461
C,-5.6732741014,3.0116293583,0.2751334238
C,-5.4137594334,1.6265716069,0.2484274278
C,-3.2848266125,0.2221830572,0.0962868122
C,-1.9038598161,0.164700918,-0.140321869

C,3.5262234344,0.2370482677,-0.2572420414
C,3.4337716497,1.5434252688,-0.7710357496
C,4.5497366489,2.3775099297,-0.7909210665
C,5.7774024829,1.9278958673,-0.3134705291
C,5.8952800189,0.6206816209,0.1963543327
C,4.765069346,-0.210759063,0.2243452528
C,7.1498637249,0.1465787712,0.6921896534
C,2.3638027507,-0.6510268281,-0.2217707458
F,-3.9126247227,-3.1075170353,0.9153453031
F,-3.7091348636,-2.5470792448,-1.307402284
H,4.4642914181,3.3813659029,-1.1956365943
H,6.6491325751,2.572718071,-0.331857595
H,4.8532386814,-1.2068194815,0.6435398047
H,9.1478885394,-0.6060599499,1.4787121453
H,0.8504706979,0.7864383143,0.0450105578
H,3.1229894709,-2.7159249222,-0.3621672981
H,0.4979247856,-3.3921599251,-0.2244569445
H,-2.4811432528,2.9152112359,0.1420129177
H,-6.1279562785,0.8174196074,0.2721747013
H,2.495943863,1.895050129,-1.191697069
H,-4.2116045773,4.7147735333,0.2174523177
H,-6.6394976519,3.4914248392,0.3305148864
H,-1.3468354187,1.0610975553,-0.3783505879
N,-3.468202545,2.7178614769,0.1394292851
N,1.0792776224,-0.1730778841,-0.1591483936
O,-3.982150905,-0.8580487928,0.2955764468
O,-1.9132147139,-2.1754219855,0.1532909186

Cartesian Coordination of 3m1-8

–1216.484966 hartree
B,3.5406300981,-2.023525007,0.176390204
C,-2.1328935045,-2.7141274624,0.0970675851
C,-5.2600408586,3.8789855482,0.8941342335
C,-0.7359700581,-2.8591741603,0.1397707017
C,-3.7025129994,-0.6569718583,-0.1444968122
C,-3.8324237989,0.6822594821,0.2519712727
C,-5.0594666627,1.3564035027,0.1421140606
C,-6.1786882726,0.6681905477,-0.3607874889
C,-6.0575579832,-0.6656997028,-0.7437647425
C,-4.8351314532,-1.3246427506,-0.6446621658
C,-5.1681885756,2.7223317147,0.5510314056
C,4.9668487707,3.4963652901,-0.2398777606
C,3.6559445582,3.9480446823,-0.2684198108
C,-2.4203411996,-1.3542517559,-0.0433339783
C,4.923323653,2.0898889113,-0.1632973949
C,1.6640559358,0.110013672,0.0973626003
C,1.2196407995,-1.2171031858,0.0260305335
C,3.5844311367,1.7053580324,-0.1419846395
C,3.0323477527,0.3755644528,-0.0569666387
C,-0.1736764431,-1.5891834237,0.0276541239
F,3.7901345032,-2.2349012019,1.5072033693
F,4.2210562408,-2.8428102635,-0.6701008782
H,5.8488419071,4.1193520804,-0.2686688888
H,3.2584117938,4.9503511263,-0.3312468948
H,1.8249797804,2.9072638541,-0.2555802631
H,-1.1247164365,0.2800997382,-0.3234871432
H,-2.8670915999,-3.4999595688,0.1994653166
H,-0.1676886612,-3.7684643976,0.2652848252
H,-5.3475758522,4.8958385672,1.2003929854
H,-2.9895022998,1.2106771656,0.6859529391
H,-7.128582475,1.1849112262,-0.4429151636
H,-6.9220725138,-1.1936282238,-1.1342508405
H,-4.7451690702,-2.3546069665,-0.9738254183
H,0.9593246325,0.91570028,0.2541778523
H,5.7540535735,1.4021850953,-0.1149791081
N,-1.2210339337,-0.688378257,-0.0634001476
N,2.829400681,2.8659371079,-0.2031660278
O,2.0555104252,-2.2101806729,-0.0701579713
O,3.9002580774,-0.5884584431,-0.1582796437

Cartesian Coordination of 3m2-1

–1523.7117827 hartree
B,0.0000104512,2.1771836062,0.1236404488
C,8.7172062253,0.867248429,0.3086212231
C,-2.9065988195,-1.8665859549,-0.7202762775
C,-4.3076733381,-1.8901638417,-0.6541510829
C,-4.7449376803,-0.611583538,-0.2804247928
C,4.7449362479,-0.6116078107,-0.2805131174
C,4.3076549478,-1.8902025628,-0.6541706997
C,2.9065826851,-1.8665987591,-0.7203365918
C,-6.099740417,-0.0956068256,-0.0807859429
C,-7.1449862603,-0.9784071014,0.2281286676
C,-8.454221241,-0.5113979886,0.4193343952
C,-8.7171841889,0.8672870981,0.3088279835
C,-7.6826497205,1.7475909253,0.0050393851
C,-6.3867075762,1.276894221,-0.1942273576
C,-9.5062572878,-1.4276180317,0.7339404296
C,-10.3982852105,-2.2012944373,0.9975093779
C,6.0997467799,-0.0956350197,-0.0809155664
C,6.3867229175,1.2768608014,-0.1943988486
C,9.5062591263,-1.4276468518,0.7338275371
C,10.3981872221,-2.2012205412,0.9980343878
C,7.1449916338,-0.9784353155,0.2280026111
C,-1.2010487737,0.0466579035,-0.2618413207
C,-2.4926041409,-0.5742344199,-0.3850341367
C,2.4926005975,-0.574248873,-0.3850731602
C,-0.0000028015,-0.6173534137,-0.5195664242
C,8.4542303306,-0.5114291814,0.4191904261
C,7.6826728871,1.7475522921,0.0048291164
C,1.2010508436,0.0466506928,-0.2618588973
F,0.000003835,2.9040394365,-1.0392743528
F,0.0000211437,2.9336123969,1.2585685383
H,3.5875381116,1.1165880926,0.1929117236
H,-5.6031236018,1.9770893001,-0.468037662
H,-6.9432935336,-2.0375933808,0.3420389193
H,-9.7276705118,1.2305694366,0.4606553096
H,-7.8882174011,2.8094286817,-0.0884313248
H,-11.1835960578,-2.8821598883,1.2319271539
H,5.6031398877,1.9770551678,-0.4682133678
H,7.8882478394,2.8093855147,-0.0886768726
H,9.7276986074,1.2305263923,0.4604184186
H,6.9432921876,-2.0376169597,0.3419450266
H,11.1834577456,-2.8821425815,1.2324225669
H,-0.000008326,-1.6451715501,-0.8521564148
H,-2.2597722306,-2.6891793795,-0.9891637342
H,-4.9499659994,-2.7277672284,-0.8838049552
H,-3.5875208291,1.1166017055,0.192993094
H,4.9499375665,-2.7278217258,-0.8837954092
H,2.2597473082,-2.6891863433,-0.9892208888
N,-3.6295443162,0.1611066671,-0.1311493476

N,3.629549719,0.1610886794,-0.1312190105
O,1.2294430496,1.2936470274,0.1394064463
O,-1.2294274964,1.2936544001,0.1394246869

Cartesian Coodination of 3m2-2
–1523.7115859 hartree
B,0.2656809456,1.8515495132,-0.3931456282
C,8.5093399751,-1.371888736,-0.4791254313
C,1.2800190845,-0.4030643416,-0.2461855214
C,8.8553582135,-0.1303569103,0.0487472848
C,6.1555760422,-0.9221075082,-0.0744366732
C,-2.9773461358,-2.0185199937,-0.2239898685
C,-4.3744411119,-1.9083361878,-0.159842563
C,-4.6995807161,-0.5453501313,-0.1182753617
C,4.7575878424,-1.3488229302,-0.1448289125
C,4.2064097992,-2.6366237518,-0.2021571385
C,2.809929201,-2.5087691265,-0.2407016366
C,-6.0042071765,0.1151170899,-0.060696757
C,-7.1119339753,-0.5701332445,0.4595542383
C,-8.3752261645,0.037390111,0.5213635598
C,-8.5271114401,1.3596947068,0.0625442667
C,-7.4301490171,2.0446965317,-0.4522312128
C,-6.1805179904,1.4327486635,-0.5208786946
C,-9.4924991463,-0.6780000579,1.0553111719
C,-10.439568659,-1.2816551346,1.5052268868
C,7.1762258673,-1.7671505735,-0.5466119331
C,8.1899261133,2.0063897639,1.0788400604
C,8.4765727631,3.0850235946,1.5457050181
C,6.5090687408,0.3238775192,0.4640318771
C,-1.113633236,-0.2006959958,-0.2489844171
C,-2.4537799172,-0.7225126249,-0.2189986947
C,2.5130099547,-1.1432989611,-0.2127127647
C,0.0236584147,-1.0063413666,-0.3335004806
C,7.8513084418,0.7321750287,0.5256583022
F,0.3023127778,2.2762222098,-1.6962576382
F,0.3500479405,2.8540638035,0.5275083398
H,3.7644919124,0.5383618789,-0.1746332268
H,5.7505999484,0.9851211847,0.8703895219
H,-0.0673116163,-2.0804972711,-0.4033321033
H,9.2854285011,-2.0338364931,-0.85093057
H,-3.3977851166,1.1440104701,-0.0845647495
H,9.8927127135,0.1819878155,0.0981238604
H,-2.4041870143,-2.9328947994,-0.2768323873
H,-5.0867569129,-2.7202295865,-0.1767028353
H,4.7685992083,-3.5587269847,-0.1799275001
H,2.0893141572,-3.3131213074,-0.2733571064
H,-6.9948634011,-1.5785500617,0.8402851276
H,-9.5017550241,1.8325212545,0.1136356213
H,-7.550538471,3.0611779103,-0.8138575039
H,-5.3475661293,1.9724832319,-0.961522499
H,-11.2733978319,-1.8129658809,1.9023074308
H,6.9174029095,-2.7252161973,-0.9853053196
H,8.7256068147,4.0359414606,1.9569464756
N,3.7130435487,-0.4699132414,-0.147197938
N,-3.5225449712,0.1448124318,-0.1609434144
O,-1.0323576933,1.1043064569,-0.1669702506
O,1.4189688824,0.896806638,-0.165055821

Cartesian Coodination of 3m2-3
–1523.7114093 hartree
C,-7.9672946168,2.5270749787,-0.2260885185
C,8.1978794446,3.6975434385,-0.4272067643
C,-8.1978828573,3.6975507757,-0.4270607976
F,-0.0000172303,2.4315935633,1.1902662302
F,0.0000173165,2.2182883226,-1.0980076
H,-5.6146241989,1.3255311846,-0.4756136385
H,-6.9365154769,-2.6096517853,0.6797131817
H,-9.240470318,-1.7512865216,0.9242621774
H,-9.7327747402,0.6512836338,0.5184469852
H,5.6146201465,1.3255243668,-0.4756409517
H,9.7327814825,0.6513097527,0.183931135
H,9.2404813287,-1.7512460448,0.9242982108
H,6.9365224443,-2.6096192344,0.6798076637
H,8.3974161998,4.7288458857,-0.6060304431
H,-8.3974213733,4.7288597159,-0.6058451135
H,0.0000044204,-2.2988383507,-0.5546126326
H,-2.2528196965,-3.3532045258,-0.600034434
H,-4.943021864,-3.3902923529,-0.4950488156
H,-3.5930009063,0.5332044525,0.2656319424
H,3.5929907468,0.5331894467,0.2657738945
H,4.9430218142,-3.3903226354,-0.4948019631
H,2.252827268,-3.3532091093,-0.5999663237
N,3.631119892,-0.446198763,0.0218594992
N,-3.6311255871,-0.4461872885,0.0217309149
O,1.2298491044,0.7076745881,0.20551631
O,-1.2298571863,0.7076771071,0.2054788373
B,-0.0000018452,1.5878044545,0.1192375943
C,1.2010513856,-0.5664503165,-0.0965891482
C,-2.492101462,-1.1968101597,-0.1706692446
C,-1.2010531184,-0.5664475846,-0.0966269133
C,2.4921006312,-1.1968156983,-0.1705922313
C,-2.9021658085,-2.5131714623,-0.399999771
C,-4.3032952424,-2.5351015501,-0.3330959791
C,-4.7442622849,-1.2315645785,-0.0652823065
C,4.7442623541,-1.231562493,-0.0652046116
C,4.3032939413,-2.5351210459,-0.3329108675
C,2.9021693328,-2.5131766669,-0.3999158124
C,-6.1019292915,-0.7078233196,0.0903711154
C,-7.1483809642,-1.5652251545,0.4757621205
C,-8.4440132524,-1.0778416639,0.6228042883
C,-8.7252394492,0.2679541419,0.3998729703
C,-7.6941184817,1.1445161434,0.0151345524
C,-6.3910128777,0.6449537548,-0.1416337338
C,6.1019308411,-0.7078121165,0.0904072032
C,6.391011844,0.6449574182,-0.1416471934
C,7.6941192597,1.1445251564,0.0150880025
C,8.7252447337,0.2679762705,0.3998443371
C,8.4440208491,-1.0778115953,0.6228261227
C,7.1483866426,-1.5652000473,0.4758165569
C,7.9672927874,2.5270755209,-0.2261867775
C,0.0000016043,-1.2485502001,-0.3019403608

Cartesian Coodination of 3m2-4
–1523.7053913 hartree
B,-0.3922257958,-3.5301093177,0.113380859
C,-8.2631859681,2.8815395873,-0.7397268769
C,4.8873254952,-0.6879805552,-0.1911017399
C,0.5690854394,-0.841216809,0.180461734
C,5.8209196936,0.4364985684,-0.2578938104
C,-5.3854941571,0.6518708175,0.148414899

C,-6.124687892,1.765741875,-0.2757697044
C,-7.5273110748,1.7357474263,-0.3028938645
C,-8.1994224929,0.563884451,0.0933793564
C,-7.4699666415,-0.5449104077,0.5128837633
C,-6.077860682,-0.5058689274,0.5474219537
C,7.0871437186,0.271219867,-0.8480419425
C,7.9803991122,1.3369790345,-0.9144597661
C,7.6329312271,2.5875902785,-0.4087281957
C,6.3718474292,2.7766428393,0.1855666965
C,5.4801178066,1.6943705453,0.2610949087
C,1.4605047609,-1.9048484611,-0.006704739
C,2.8898036948,-1.7378534066,-0.0791855826
C,-1.804401171,-0.0598883881,0.1660472306
C,-3.9233543002,0.7117170972,0.1715571138
C,-3.0615192357,1.8135087824,0.2646210801
C,-1.7432795901,1.3330896305,0.262241244
C,-0.8034303771,-1.0919491428,0.1036208525
C,3.8817409984,-2.7169900982,-0.1089189881
C,5.1239058492,-2.06541847,-0.1774846663
C,-8.8880213292,3.8498405919,-1.1081440718
C,5.6900102485,5.1294631095,1.1694268399
C,6.0027442809,4.0506397568,0.719734253
F,-0.5009136749,-3.9585467748,1.4109961483
F,-0.7678082886,-4.4487326808,-0.819695251
H,-5.6120630408,2.6613620731,-0.6084614737
H,3.691778155,-3.7785286388,-0.0590561996
H,-3.3722296062,2.8437523605,0.3586225856
H,-0.8421376244,1.925298615,0.3310479818
H,0.9217847531,0.1671844177,0.3453081166
H,-9.2833014194,0.5375053819,0.0688393102
H,-7.9895076513,-1.4450361033,0.8264204935
H,-5.5308652819,-1.3694214993,0.9141181498
H,7.3570299117,-0.6905169555,-1.2716898047
H,8.9529918368,1.1945799698,-1.3753495138
H,8.3250669494,3.4205588249,-0.4651123943
H,4.529431135,1.8427812682,0.7632662232
H,5.4184348414,6.079697393,1.5678235337
H,-9.4384909886,4.702130786,-1.4334553824
H,3.0710240092,0.374034348,-0.2597286535
H,-3.4398523839,-1.3578363907,-0.0111312951
H,6.0987117007,-2.5309646804,-0.1749977417
N,-3.1375995116,-0.4030105807,0.1189724044
N,3.5299319988,-0.510928397,-0.1127492435
O,-1.2731940126,-2.3018423809,-0.055402742
O,1.0402221234,-3.131090643,-0.151240545

Cartesian Coordination of 3m2-5

–1523.7049982 hartree

B,-0.5033160055,3.3648544491,0.1021927282
C,9.0395830088,-1.7665118088,0.8341335751
C,-9.1844979687,-3.846070028,0.9737206658
C,10.1440709835,-1.7043995053,1.3238504291
C,4.9645500031,1.7069087502,0.0147692369
C,3.7446075337,2.4001991406,0.0714856381
C,1.2939441005,1.6803318136,-0.0213125538
C,2.7178343477,1.4622887957,-0.0275362657
C,-2.0378478817,-0.0359388803,-0.2403537289
C,-4.1805205062,-0.7391189337,-0.2242364565
C,-3.3621875034,-1.8509120735,-0.4680823295
C,-2.0292431288,-1.4129647193,-0.4789819345
C,-0.9999424026,0.9536860205,-0.11866491
C,0.3585516232,0.6710345645,-0.2824657223
C,5.5739870334,-0.8085303634,-0.2209819487
C,-5.6373157638,-0.6391681894,-0.1249126431
C,-6.3078020184,0.5723147455,-0.3729006692
C,-7.6948297819,0.647766462,-0.2669623705
C,-8.4412736642,-0.4761945687,0.0751055879
C,-7.7916338239,-1.7010106187,0.3195531448
C,-6.3934685126,-1.768403561,0.2216874937
C,6.8570658061,-0.7519599013,0.3428665757
C,7.7352205939,-1.842832189,0.2530858949
C,7.3142282677,-3.0150449119,-0.4036658859
C,6.0412362098,-3.0768362605,-0.963044029
C,5.1780396247,-1.9861618588,-0.8810808846
C,-8.5449092116,-2.86356326,0.6747768438
C,4.6797349766,0.345026186,-0.1179043783
F,-0.6421419319,3.9220618046,-1.1426143315
F,-0.8132661403,4.1984445144,1.1337942758
H,5.7229321021,-3.977038454,-1.479806233
H,4.2063540363,-2.0369781571,-1.3640347191
H,-9.7479924491,-4.7108340175,1.238112742
H,11.1164989023,-1.6479562515,1.7558260454
H,-5.8965109021,-2.7073718954,0.4384883596
H,7.9903663843,-3.8603431585,-0.4697358467
H,-5.749647463,1.4523242452,-0.6783454441
H,-8.1976214045,1.589515588,-0.4638385348
H,-9.5214270449,-0.421170847,0.1547022507
H,7.1747726451,0.1380450106,0.8744125228
H,2.8308848207,-0.6610638198,-0.0921991862
H,5.9547593978,2.1385934446,0.0246311312
H,3.5908646923,3.4659279842,0.1491779114
H,-3.6177336877,1.2856192677,0.1432105472
H,-3.7122223249,-2.8564182324,-0.6503253176
H,-1.152837719,-2.0218192596,-0.6484083652
H,0.6684744125,-0.3245722612,-0.5674700921
N,3.3149177126,0.2200677694,-0.1597108114
N,-3.3551173718,0.3404124905,-0.0968808904
O,-1.4205471734,2.1541267061,0.1845665426
O,0.9222527017,2.8958408934,0.271492301

Cartesian Coordination of 3m2-6

–1523.7051792 hartree

B,0.7737040916,3.156739475,0.1867192154
C,-6.4335717597,-3.6663489333,0.6219646236
C,-6.2331453831,-4.79876412,0.9979445576
C,9.0267322966,1.3145121527,0.8663689572
C,-4.8828071469,2.352642352,0.0286606499
C,-3.572199432,2.8543076669,0.0845918356
C,-1.2587131563,1.7669640313,0.0470111851
C,-2.6994029467,1.7690560973,0.0220550258
C,1.7693160444,-0.4497282136,-0.0230238749
C,3.7770657854,-1.466657596,-0.16460756
C,2.7920261468,-2.4615782582,-0.0920056071
C,1.5431399438,-1.828687214,-0.0030028641
C,0.8969144178,0.6941821596,0.0185982696
C,-0.4919102583,0.5990757964,0.1418591472
C,-5.8661735837,-0.0448003142,-0.1612252848
C,5.2327430333,-1.5849617344,-0.2590899225
C,6.0761234583,-0.546656528,0.1626334253
C,7.4722494633,-0.6619544173,0.0637731525

C,8.0298027647,-1.8443565459,-0.4563687202
C,7.196152874,-2.8813484247,-0.8679773157
C,5.8125788387,-2.7572591836,-0.7770432448
C,-7.1238156821,0.2985532305,-0.6898101054
C,-8.1366471238,-0.6524568395,-0.7784848326
C,-7.9200762912,-1.962283799,-0.3566884878
C,-6.6700007103,-2.329031465,0.1744277119
C,-5.656526852,-1.3618692963,0.2734150097
C,8.3140746763,0.4084724744,0.4992887732
C,-4.8071397814,0.9604316187,-0.0697393509
F,0.968253073,3.4802646521,1.5043546484
F,1.2261187183,4.0870733471,-0.6989824013
H,-8.7059101217,-2.7059766001,-0.4304787621
H,-4.7130339833,-1.6469054318,0.7279148215
H,-6.0607314904,-5.7958340702,1.331896399
H,9.6508983253,2.1150777734,1.1902976614
H,5.1731355942,-3.5609608662,-1.1270976898
H,-9.1011364382,-0.3729328193,-1.1911010431
H,5.6640946312,0.3562543257,0.6012956602
H,9.1078291493,-1.9362897765,-0.5306485905
H,7.6285592209,-3.7909924598,-1.2733056561
H,-7.2942916015,1.3081671557,-1.0487760507
H,-3.1276600788,-0.2941420342,-0.2663571698
H,-5.7967365039,2.9248577714,0.0944530629
H,-3.2599518658,3.8827972249,0.1854059268
H,3.542167584,0.6533339396,-0.2041811462
H,2.9781968686,-3.5253773565,-0.0713922677
H,0.5802257871,-2.3125105882,0.0757365488
H,-0.954406418,-0.3698521718,0.2676076016
N,-3.4774301158,0.6267229549,-0.0540091576
N,3.131265974,-0.2651372043,-0.1153859889
O,1.4994439431,1.8490125109,-0.093249659
O,-0.702781951,2.9427022617,-0.0503254037

Cartesian Coodination of 3m2-7

–1523.7048489 hartree

B,-0.8313225272,2.9887614469,-0.0019595871
C,-8.5086326873,0.6502580121,-0.2561580839
C,4.6352960737,0.5153618362,-0.1997559796
C,0.3009219509,0.3804462863,-0.2521070689
C,5.6434096635,-0.5439321306,-0.2507848326
C,-5.5101595983,-1.5506826416,0.2003171516
C,-6.1305753209,-2.7327817109,0.6434073236
C,-7.5142766392,-2.7957240543,0.7827069584
C,-8.3072091454,-1.687532771,0.4946461844
C,-7.7084354122,-0.4939366027,0.0514870354
C,-6.3129982774,-0.4397169302,-0.0970870051
C,6.9226503084,-0.3183599368,0.2783967875
C,7.9077490141,-1.3170344239,0.2398780101
C,7.600190878,-2.5675802654,-0.3295277178
C,6.331813021,-2.7966916592,-0.8548373573
C,5.3613832691,-1.7973158539,-0.8242090772
C,1.1308642139,1.4961818429,-0.0844546434
C,2.5693404804,1.42719099,-0.1231777638
C,-2.0036746573,-0.5694801717,-0.0832399981
C,-4.0549777289,-1.496151952,0.0536377552
C,-3.1274507478,-2.5268933308,-0.1524113469
C,-1.8514165344,-1.9499288924,-0.2385515448
C,-1.0748695043,0.5299500263,-0.0584403082
C,3.4936343303,2.4708481774,-0.1162212726
C,4.7781448157,1.9051537961,-0.1646889637
C,10.3057329641,-0.860367127,1.2445219325
C,-9.1856531728,1.6190629933,-0.514199021
C,9.2061251116,-1.0685413966,0.7850585115
F,-1.0635156614,3.4468140467,-1.2726805235
F,-1.1978193346,3.849740819,0.9874836633
H,-5.5213667647,-3.5937502825,0.8982398199
H,3.2307375675,3.5178249178,-0.1025105398
H,-3.3702307044,-3.5737644695,-0.2615668313
H,-0.9191070945,-2.4707661588,-0.4029688993
H,0.7067911182,-0.5936060412,-0.4864441042
H,-7.9782350631,-3.7141095443,1.1291598312
H,-9.3849218914,-1.7320836088,0.6071787482
H,-5.8703616018,0.4758146351,-0.4758123439
H,7.1543520814,0.6331840915,0.7436807087
H,8.359207896,-3.3417096191,-0.3557014791
H,6.1005634601,-3.7573265233,-1.3047853811
H,4.3925560516,-1.9797393621,-1.2804114808
H,-9.7786416186,2.474455063,-0.7424409292
H,11.2737243605,-0.6754618276,1.6497404722
H,2.9032750332,-0.6723932458,-0.0535476371
H,-3.7077710668,0.5968244886,0.2757636055
H,5.7173499375,2.4367996436,-0.2122052472
N,-3.3492892985,-0.328215801,0.0855020741
N,3.2905741824,0.2473346773,-0.1926767992
O,-1.6119066321,1.6964380034,0.1864281626
O,0.6406755948,2.6826072498,0.1455956435

Cartesian Coodination of 3m2-8

–1523.6978936 hartree

B,0.4050723082,4.6443961538,-0.1023915805
C,3.6090530879,-4.7378246564,-0.6467381116
C,-3.7382209278,0.3018996622,-0.1993047365
C,0.3370245377,1.801770913,-0.1823925535
C,4.7716785296,-1.292690403,0.2658754901
C,-4.2758278834,-1.0589211916,-0.2025717705
C,6.0207148201,-1.5926089701,0.8393785457
C,6.4654636691,-2.9095957959,0.9160921695
C,5.6781211809,-3.9544445257,0.4376769961
C,4.4252231389,-3.6787231148,-0.1397823529
C,3.9880919448,-2.3469612598,-0.2262401196
C,-5.5710674788,-1.3014090796,0.2780832675
C,-6.1101785942,-2.5970068638,0.2816224337
C,-5.3317814329,-3.669390708,-0.1946680428
C,-4.04542238,-3.4340976077,-0.6712085502
C,-3.5199794102,-2.1437494532,-0.6832679751
C,-0.8579554212,2.529135021,-0.0867553209
C,-2.1643189658,1.9228596383,-0.1424951253
C,2.8265848886,1.7951870526,0.0834537606
C,4.3098401935,0.0932760367,0.1895550197
C,5.0285816306,1.2908531713,0.1551998305
C,4.1055944056,2.348242879,0.0911725176
C,1.5529997636,2.4684856514,0.0207568502
C,-3.4097670379,2.5437685867,-0.2204127847
C,-4.3887640922,1.5371653131,-0.2566126873
C,-8.5513773224,-3.0202223614,1.1923139256
C,2.9186152261,-5.6354148597,-1.0729237867
C,-7.4325217747,-2.8248676871,0.7757438798
F,0.3920642354,5.6562101536,0.8069791483
F,0.4712883101,5.0468488321,-1.410684634

H,6.6294622692,-0.7901012639,1.2426467722
H,-3.555629392,3.6122519812,-0.2708863499
H,6.1056402104,1.372109353,0.136219669
H,4.3126844653,3.4058901729,0.0279491973
H,0.3218753645,0.7437251488,-0.4076556897
H,7.4306554012,-3.1251103273,1.3639028226
H,6.0201633632,-4.9815037525,0.5022544761
H,3.0409829769,-2.1448306671,-0.7163711471
H,-6.1629895541,-0.4828144457,0.6719291512
H,-5.7458690085,-4.6716601304,-0.1881064368
H,-3.4516135449,-4.2604173514,-1.0497719999
H,-2.5326436806,-1.9732703745,-1.1029548624
H,2.3174453755,-6.4294574917,-1.4517084003
H,-9.5370878753,-3.1903681891,1.5595710056
H,-1.6977360579,-0.1424360433,0.0611941281
H,2.2338890076,-0.23450698,0.3029204204
H,-5.4553688682,1.6760394882,-0.3568852131
N,2.9789305909,0.4197688098,0.1246557546
N,-2.3913616245,0.5568820117,-0.1498934467
O,1.6013467078,3.7581606295,0.1894280072
O,-0.8544471378,3.8196020149,0.084124363

Cartesian Coordination of 3m2-9

–1523.6978701 hartree
B,0.0003143161,-4.7689409032,0.0004134861
C,5.8680794753,1.2813638556,0.6604795926
C,-4.7230051368,-1.5329513048,0.0746994452
C,-4.0535628545,-0.3149832755,-0.0674486009
C,3.7593169805,-2.5530159996,-0.1211682458
C,4.0536189421,-0.3144713318,0.0667989143
C,4.7231612902,-1.5323152458,-0.0759423602
C,-2.5039698755,-1.9583393718,0.0058402181
C,-4.5724824523,1.0495863562,-0.1642224231
C,4.5724077149,1.0501330493,0.1637769289
C,-5.8679698889,1.2808143732,-0.6614054781
C,-6.3689492541,2.5765493295,-0.7523915237
C,-5.5940556509,3.666896828,-0.3634107655
C,-4.2954983594,3.4599923976,0.1366172269
C,-3.8002566633,2.1496695995,0.2370303239
C,3.7998745475,2.150249506,-0.2367918666
C,4.2949946294,3.4606020152,-0.1361652578
C,5.5937400594,3.6675077913,0.3633732563
C,-2.8091577318,5.5009341103,0.9073292167
C,2.8080610663,5.5016068265,-0.905565059
C,3.4901141297,4.5664405727,-0.5531645059
C,1.207870598,-2.5915654022,-0.0062504851
C,2.5042058448,-1.9580037255,-0.0063645252
C,-3.7590452779,-2.5535382861,0.120059738
C,0.0001118027,-1.8817972627,0.0002593856
C,-3.4909382576,4.5657966612,0.5543253767
C,6.3689364174,2.5771314028,0.7516686898
C,-1.2075528256,-2.5917323556,0.0060243495
F,0.0156410765,-5.5072070709,1.1498774879
F,-0.0148898356,-5.509446615,-1.1475766473
H,3.9217563628,-3.6130509262,-0.2448718838
H,6.4700514218,0.4418626628,0.9923670811
H,-2.2131741482,6.3257069208,1.2233993447
H,2.211834217,6.3264077978,-1.2211023766
H,0.0000319707,-0.8003207405,0.0005524633
H,-3.9213932005,-3.6136227058,0.2434597061
H,-5.792242142,-1.6493940981,0.1754086796
H,-2.0062536201,0.0835862161,-0.3370889591
H,2.0063585476,0.0837727294,0.3372809551
H,7.3697194931,2.7399460018,1.1396365336
H,-5.9808945281,4.6772350019,-0.438457816
H,-2.8153505894,2.0016604742,0.6684358291
H,2.8148015204,2.0022596539,-0.667822787
H,5.9804835612,4.6778703179,0.438583537
H,5.7923749997,-1.648596452,-0.1770830981
H,-6.4696939867,0.4413438343,-0.993819535
H,-7.3695865885,2.7393647149,-1.1407348604
N,-2.7104973211,-0.5925628326,-0.0888557686
N,2.7105964519,-0.592226222,0.0886233847
O,1.2363902978,-3.8913679376,-0.0168266439
O,-1.2359084945,-3.8915429388,0.0159215792

Cartesian Coodination of 3m2-10

–1523.6974202 hartree
C,8.6969249767,-3.4222287285,1.2617003093
C,-7.6058667345,-3.1721301692,0.8021217423
C,-8.6969040288,-3.4224876047,1.2608890634
F,-0.0000247748,5.4810890786,1.0677627957
F,-0.0000118849,5.0432948994,-1.1911511085
H,-5.9318166171,-4.9079994192,-0.3682121967
H,-6.3946296104,-0.7974789473,0.7930566346
H,9.6581634521,-3.6409792916,1.6662344226
H,-9.6581444477,-3.6413006311,1.6653848879
H,2.8298754652,-2.0740939302,-1.2583840159
H,-3.6952919435,-4.382777347,-1.3147817459
H,6.3946177241,-0.7973162489,0.7935084281
H,5.9318137006,-4.9080198809,-0.3671125848
H,3.6953132071,-4.3829397674,-1.3138182145
H,-2.8298456084,-2.0739472265,-1.2589579633
H,-1.9777471511,-0.3027137452,0.0020303833
H,-5.7904491458,1.4415702563,-0.1376791108
H,-3.9332379424,3.4164326192,-0.0045374638
H,1.9777520819,-0.3026759592,0.002148792
H,5.7904519617,1.4416044493,-0.1377443717
H,3.9332358972,3.4164695528,-0.0046994668
H,0.0000222572,0.6715850934,-0.5066902481
N,-2.6952181767,0.3906263718,-0.1369491493
N,2.6952244513,0.3906486019,-0.1369029907
O,1.2290999043,3.6697682149,0.258207779
O,-1.229114015,3.6697506252,0.2581970194
B,-0.0000146621,4.5414597985,0.0839689858
C,-4.717547933,1.3239343237,-0.0922035585
C,-3.7611400025,2.3510159916,-0.0312258135
C,-1.2070456036,2.3953407844,-0.0058066393
C,-2.4997442984,1.7587059106,-0.047886889
C,2.499751083,1.7587292146,-0.0478453775
C,4.0371088875,0.1049870904,-0.1442760596
C,4.7175530147,1.3239676991,-0.092214504
C,3.7611421544,2.3510494887,-0.0312802688
C,1.2070470489,2.3953554571,-0.0057783333
C,0.0000072037,1.7109614611,-0.2063218578
C,4.5437008627,-1.2660016545,-0.2125798688
C,-4.5436924337,-1.2660116294,-0.2130633259
C,5.8064405,-1.5726021458,0.31543836
C,6.3163780918,-2.8787542628,0.2589868191
C,5.5406655234,-3.8973658703,-0.3269676389

C,4.2862205891,-3.5986065119,-0.8507207664
C,3.790245995,-2.2973753147,-0.8023186886
C,-3.7902272772,-2.2972948494,-0.8029484461
C,-4.2862062914,-3.5985159842,-0.8515714046
C,-5.5406649825,-3.8973535942,-0.3278959521
C,-6.3163849824,-2.8788333811,0.2582071616
C,-5.806445274,-1.572691429,0.3148759359
C,7.6058488124,-3.1719678897,0.802972715
C,-4.0371000797,0.1049652801,-0.1445149951

Cartesian Coordination of 3p1-1

–1216.4997438 hartree
B,-2.268006413,2.0529626547,0.2053878137
C,8.8910897304,1.0545382401,-0.0848777946
C,-3.6045089722,-0.0229674677,-0.0158670839
C,0.0400519376,-0.8953760689,0.0064097495
C,-1.207990429,-0.1803087379,0.0306699782
C,-7.1695821951,-0.44104992,-0.2033911356
C,-6.8356950518,-1.7907123155,-0.1945861439
C,-5.4314297235,-1.8743610412,-0.1231534526
C,0.3644837963,-2.2551337558,-0.0026267523
C,1.7631583737,-2.35381666,-0.0095260942
C,2.2902757117,-1.053420884,-0.0102450293
C,-4.9345057812,-0.5697486159,-0.0884590813
C,3.6772191406,-0.5971889569,-0.030826452
C,4.7123575063,-1.4539813476,0.3880812343
C,6.0358598026,-1.0387308386,0.3714904274
C,6.3766146465,0.2580641442,-0.0599756237
C,5.3445255757,1.1185992154,-0.4792051647
C,4.0224099214,0.6954633389,-0.4679643061
C,7.7371853706,0.6891538967,-0.0733310986
C,-2.4538463289,-0.8093126845,0.0693221826
F,-2.1828594575,3.067427418,-0.7025268017
F,-2.2675173667,2.4642297337,1.512964664
H,6.8212381995,-1.7101293881,0.7019392371
H,5.5929572027,2.116987537,-0.8228678011
H,3.2546267941,1.3721610034,-0.8315475766
H,9.9064540601,1.3771918868,-0.0947653892
H,-2.5256537545,-1.8865212444,0.1057811064
H,-5.922013693,1.2841488705,-0.1270205685
H,-8.1342817516,0.0421060197,-0.2491421608
H,-7.5340825664,-2.613822319,-0.2359747365
H,-4.8386529666,-2.7774632485,-0.1012786368
H,2.3435635357,-3.2639916771,-0.0469721018
H,4.4705517253,-2.448398459,0.7488403286
H,-0.3398988621,-3.0742836466,-0.0150919547
H,1.2541169545,0.8109068067,0.0556132757
N,1.2266535313,-0.1965836514,-0.0061074923
N,-6.0205397372,0.2793091735,-0.1397013402
O,-3.5465428305,1.2842917619,-0.0568424966
O,-1.0914991873,1.1237137781,-0.0080776508

Cartesian Coordination of 3p1-2

–1216.4927387 hartree
B,2.2454505866,2.1617567909,0.0875923254
C,-8.8951396282,0.9312823174,0.0414097709
C,1.2259341328,-0.1120157927,-0.0061868798
C,4.9720348577,-0.4278558566,-0.020784804
C,3.6269013124,0.0917939993,0.0021434205
C,-0.0090266053,-0.85247007,-0.0393171422
C,6.1760487529,0.2733413479,0.0025500187
C,7.2238239662,-0.6678383217,-0.0361724782
C,6.644330428,-1.9272770644,-0.0823313754
C,-2.2559205188,-1.0524355248,-0.0321611104
C,-1.7054769717,-2.3417824847,-0.0806375885
C,-0.3084875337,-2.2167595773,-0.0873641882
C,-3.6514109163,-0.6218938429,-0.0213739169
C,-4.0264264623,0.675293189,-0.418342687
C,-5.3562315357,1.0735162359,-0.3998306012
C,-6.3660776355,0.1825738607,0.0099564039
C,-5.9952894185,-1.1187393949,0.4012062396
C,-4.6642185053,-1.5091822233,0.3882757247
C,-7.7345407877,0.5878784865,0.0270046117
C,2.4841718831,-0.7166858886,-0.0336096176
F,2.1768318539,2.857987709,1.2616122466
F,2.176297314,2.941244583,-1.0332804467
H,-5.6279552759,2.0758644827,-0.7128585515
H,-6.7633087022,-1.8134267489,0.7241823146
H,-4.3988458712,-2.5080869296,0.718819364
H,-2.2696912318,-3.2609118734,-0.140249868
H,-3.2763670801,1.3757246311,-0.7738552308
H,7.0951994759,-2.9079955455,-0.1204400713
H,4.6275368545,-2.5332298888,-0.0973416013
H,-1.2530363222,0.8279626578,0.0808009151
H,0.4094021066,-3.0230397461,-0.1322185754
H,-9.9164101601,1.2346720925,0.0542198016
H,2.5546529098,-1.7940579077,-0.0831176101
H,6.2522675281,1.349372948,0.0428788423
H,8.2841670558,-0.4617239117,-0.0314351817
N,-1.2081205812,-0.1765627793,-0.0132808258
N,5.2901280749,-1.7755775702,-0.0733413885
O,1.0810565755,1.184609924,0.0525273519
O,3.5430594156,1.3900804805,0.0596501887

Cartesian Coordination of 3p1-3

–1216.4931495 hartree
B,-3.7858567566,-1.7084661381,0.0650802014
C,8.4679026873,1.6429284897,-0.0804409721
C,-2.994209589,3.2757855403,-0.0422165667
C,-3.6258889599,2.0320159806,-0.1023766646
C,-3.144835975,0.6749301493,-0.0547387787
C,-1.80010608,0.3394861297,0.1224635262
C,-1.4226843086,-1.0060302281,0.0294854482
C,-0.051471146,-1.447246279,0.0575118928
C,0.4463472522,-2.7482670956,0.1210784014
C,1.8478178286,-2.6698895614,0.1263934211
C,2.2049791009,-1.3187788669,0.0654744701
C,-5.2133647886,3.6072158524,-0.2575750559
C,3.520235158,-0.6853294515,0.0430432884
C,4.6431260809,-1.3967218642,-0.4195932419
C,5.8998276376,-0.8097701558,-0.4471907663
C,6.0818839313,0.5200968559,-0.0193963221
C,4.9619370762,1.2350340061,0.4451340651
C,3.7081319715,0.6396841317,0.4795249168
C,7.3728499573,1.1279957233,-0.0529504249
C,-3.9935842947,4.2638473429,-0.1390410211
F,-4.1241040461,-1.9676092707,1.3678303755
F,-4.4649878693,-2.4479959644,-0.8549487514
H,6.7544043174,-1.370209051,-0.810945888
H,5.0904536311,2.2552652616,0.790642576

H,2.8713705289,1.2015027498,0.8850483488
H,9.4320777621,2.0957448826,-0.1050277233
H,-6.2145385214,4.0003628814,-0.3536533225
H,-3.8519461668,5.3346938578,-0.1258126477
H,-1.9311912634,3.4419949573,0.0571208065
H,-5.6540182015,1.5230379382,-0.2986347848
H,-1.0703807389,1.1197549329,0.2871523518
H,2.5401062445,-3.4950686161,0.2086906014
H,4.5193193784,-2.4127287392,-0.7798938467
H,-0.1681745721,-3.6338173235,0.181435436
H,0.994837415,0.3904806552,-0.1583564739
N,1.039493662,-0.5957622406,0.0427958358
N,-4.9779409312,2.2704921459,-0.2346492328
O,-4.064786663,-0.2394036671,-0.214042847
O,-2.3058932303,-1.9547545971,-0.1139152745

Cartesian Coordination of 3p1-4

–1216.4854589 hartree
C,8.3111659662,2.1170498403,-0.0534078284
F,-4.0044843728,-2.2299877283,1.3442301944
F,-4.3707204623,-2.7289790457,-0.8720987038
H,4.6079698318,-2.1518336831,-0.8260536749
H,2.7525669599,1.3252800436,0.9094664483
H,4.9061097807,2.510952183,0.8335021799
H,6.7778124197,-0.9786825207,-0.8384279647
H,9.2471030856,2.6260450485,-0.0701224338
H,-1.1809530674,1.0076431805,0.3547942886
H,-5.9672559145,1.4653315105,-0.1248384806
H,-6.0894550398,4.1857227209,-0.1346177847
H,-3.5080312346,5.0452299931,-0.0908475003
H,-2.0536229921,3.0148000627,-0.0943954783
H,0.9292185505,0.4253147479,-0.1776013315
H,2.6938690904,-3.3661429676,0.1599173009
H,-0.0024189579,-3.660209564,0.1204640321
N,-3.0582896118,2.9612594728,-0.0627807924
N,1.0284568731,-0.5564775694,0.0244740363
O,-2.2290751876,-2.105768318,-0.1822052732
O,-4.0887814141,-0.5008669101,-0.2370548377
B,-3.7223830033,-1.9477984677,0.0332166462
C,-3.2361904859,0.4647770428,-0.0542414314
C,-0.0115752258,-1.4700274496,0.022662057
C,-1.4080375568,-1.1116991059,-0.0026338344
C,-5.1434992317,2.1630015027,-0.1166274765
C,-5.2013035867,3.5710977897,-0.118296253
C,-3.8954112867,4.0369963145,-0.0906795417
C,-3.8012769809,1.7914989296,-0.0831146801
C,2.2343492016,-1.2119111234,0.0409962943
C,1.955515041,-2.5812458332,0.0839872728
C,0.5603196129,-2.7401792704,0.071890243
C,3.5102693484,-0.5022911726,0.0298972118
C,3.620550928,0.8229256536,0.4915604486
C,4.8369112687,1.491942378,0.4679009955
C,5.9962673934,0.8533757921,-0.0110030468
C,5.8922361682,-0.4766436054,-0.4637241024
C,4.6723970229,-1.1372661277,-0.4466926408
C,7.2489490346,1.5371037455,-0.033783928
C,-1.8703819638,0.2048032079,0.1295972296

Cartesian Coordination of 3p2-1

–1523.7135253 hartree
B,0.00000036,-1.7702605121,0.4157219325
C,-7.1974227601,1.2758826911,0.2443743232
C,-10.0695097337,-1.0828819722,-0.1324147572
C,-11.1972903818,-1.5223981327,-0.1410536345
C,-1.2010142584,0.3692353688,0.0753947324
C,2.4916105799,0.9976154704,-0.0149131437
C,1.2010142499,0.3692351374,0.0753906552
C,-4.7464849941,1.0074855419,-0.0812833688
C,-4.3035578552,2.3370727407,-0.152852453
C,-2.9020952284,2.3303894887,-0.1149809727
C,2.9020950065,2.3303893265,-0.114986448
C,4.303556803,2.3370707529,-0.1528876
C,4.7464848563,1.0074857124,-0.0812844179
C,-2.4916107806,0.9976158709,-0.0149049565
C,6.1009052705,0.4623431767,-0.0976915762
C,7.1974224727,1.2758862743,0.244377352
C,8.4914018371,0.7761867979,0.2299022819
C,8.7395289236,-0.5650197495,-0.121699024
C,7.6458617117,-1.3825769823,-0.463711344
C,6.3536473787,-0.8754712608,-0.4551458948
C,10.069508664,-1.0828842112,-0.1323793852
C,11.197294392,-1.5223863712,-0.1410685076
C,-6.100905493,0.4623433549,-0.0977027305
C,-6.3536477889,-0.8754665845,-0.4551742358
C,-7.6458625063,-1.3825711903,-0.4637494896
C,-8.7395297784,-0.5650178889,-0.1217278106
C,-8.4914025668,0.7761845464,0.2298894375
C,0.0000001122,1.0810033805,0.0980519815
F,0.0000023252,-2.0786669917,1.7514241987
F,-0.0000009913,-2.8544637658,-0.4117336613
H,-7.8230640198,-2.4149226276,-0.745599236
H,-9.3249899492,1.4154602267,0.5004948907
H,-7.0270913477,2.304891128,0.5436527153
H,-12.1897195732,-1.9099673823,-0.1486604636
H,0.0000001956,2.1609005678,0.0709601407
H,5.5365457045,-1.5233910736,-0.7584429358
H,-5.5365462923,-1.5233835355,-0.758477633
H,7.0270912927,2.3048987207,0.5436419767
H,9.3249889647,1.4154653396,0.5005016897
H,7.8230631418,-2.4149321335,-0.7455474027
H,12.1897247221,-1.909952844,-0.1486783946
H,-3.594901208,-0.7779704049,0.1191461363
H,-4.9397635774,3.2036312766,-0.2574791576
H,-2.2513791092,3.1913837057,-0.1662866782
H,2.2513787079,3.1913835758,-0.1662891619
H,4.9397615104,3.2036277072,-0.2575336383
H,3.5949009445,-0.7779709704,0.1191353906
N,-3.6305689946,0.2235410507,-0.0046077966
N,3.6305686931,0.2235404281,-0.00461917
O,1.2303146459,-0.939984489,0.113098849
O,-1.2303147206,-0.9399842586,0.1131026447

Cartesian Coordination of 3p2-2

–1523.7069345 hartree
B,-0.7024693293,3.3150436873,-0.0506392174
C,8.7366559098,-3.2803158219,0.0854442294
C,-10.8504497198,-1.4466283792,0.2910181079
C,9.5790907356,-4.1492528658,0.102891099
F,-0.8775368874,3.7561500798,-1.3365738089
F,-1.1110807478,4.189808699,0.9098467863

C,4.9056293611,2.223907925,0.0407290938
C,3.6217463014,2.7909811811,0.0257387771
C,1.2583378885,1.8188127424,-0.0267810194
C,2.6969676356,1.7476011515,-0.0024659015
C,-1.8776350361,-0.2414136334,-0.14027423
C,-3.9376989141,-1.159280463,-0.0899556482
C,-3.0038863339,-2.1958483084,-0.2391855087
C,-1.7236701256,-1.6246463196,-0.2716594846
C,-0.9479878591,0.8557847187,-0.0859726721
C,0.4347651466,0.7018943847,-0.2159725818
C,-5.3953124502,-1.2064966814,-0.0143663254
C,5.7711364974,-0.2238929764,0.0304298623
C,-6.0473463374,-2.3956010087,0.3621020606
C,-7.4310482453,-2.4602247957,0.436367475
C,-8.2194870737,-1.3306506581,0.1423313015
C,-7.5714349723,-0.1390796473,-0.2341678498
C,-6.1866726845,-0.0818232516,-0.3142934041
C,5.5012732917,-1.5041190998,-0.4889138297
C,6.4645618556,-2.5038000221,-0.4684482148
C,7.7431124147,-2.2557659811,0.0654794323
C,8.0204179447,-0.972638724,0.5766629352
C,7.0512971912,0.0199505248,0.5622085691
C,-9.6431450884,-1.3932744103,0.2228247512
C,4.7634374608,0.8324838243,0.022887754
H,9.0008585841,-0.7699923986,0.994271524
H,7.2760140445,0.993148544,0.9862856734
H,-11.9132258805,-1.4924238797,0.3511806277
H,10.321634554,-4.9132563638,0.1177230842
H,-5.7198490274,0.8423788486,-0.6421828217
H,6.2422823503,-3.4834040327,-0.8780280208
H,-5.4585640304,-3.2703559786,0.6183797117
H,-7.9179693327,-3.3831576071,0.7327844014
H,-8.1665386636,0.7358790836,-0.4726444975
H,4.5387238383,-1.7119427642,-0.9478052127
H,3.0230327154,-0.3497048327,0.1173704992
H,5.8459949809,2.7552378748,0.0228424383
H,3.3598314579,3.8381699453,0.0104496697
H,-3.5896757088,0.9355688239,0.1233022424
H,-3.2442369794,-3.2433891426,-0.3467074711
H,-0.7867914238,-2.1507254757,-0.385654978
H,0.8491633259,-0.275305232,-0.420713925
N,3.4183879986,0.566502311,-0.0219953572
N,-3.2283631241,0.0064777273,-0.0386556816
O,-1.4930026565,2.0264355107,0.1202948786
O,0.7608923657,3.009012795,0.1658914898

Cartesian Coordination of 3p2-3

–1523.6994832 hatree
C,0.0000452775,-1.9816407139,-0.1606052871
F,-0.0004070807,-5.25419637,-1.3352166349
F,0.0002097495,-5.8180429071,0.8957878232
H,6.4360364532,0.4552988614,0.8921252787
H,1.9768246765,0.0142985794,0.1679861631
H,-1.9767170868,0.0145450717,0.1670080589
H,-6.8620324918,7.097340759,0.10468121
H,6.8618700606,7.0973697315,0.1080473937
H,-3.9332728701,-3.6959838459,-0.0663537152
H,-5.7894925492,-1.7182776572,-0.0872539412
H,3.9334329997,-3.6959388671,-0.0693452792
H,5.7895376186,-1.7181331338,-0.0899052357
H,-6.4353058357,0.4559535084,0.8940296067
H,-7.3186387518,2.7586870252,0.907556305
H,-3.6566043838,4.1794275938,-0.838003491
H,-2.7943600057,1.8774357744,-0.9145510463
H,2.7935768581,1.8781790365,-0.9123073159
H,3.6558020228,4.180128254,-0.8345249868
H,7.3192923788,2.7580562162,0.906887287
H,0.0000647775,-0.9269446997,-0.4016316324
N,-2.6945060055,-0.6679413538,-0.0163978652
N,2.694550687,-0.6679903474,-0.0163983727
O,1.2294441728,-3.9643754225,0.1884009994
O,-1.2292725762,-3.9642794681,0.1891151973
C,4.0367034933,-0.3808615144,-0.0107869453
C,4.5435797119,0.9882450336,0.0010034616
C,-5.8305157108,1.2655030327,0.4987309866
C,-6.3263383989,2.561109701,0.5163990276
C,-5.547950495,3.6356939557,0.0430842821
C,-4.2608251899,3.3629756312,-0.4570414893
C,-3.7731206847,2.063258904,-0.4810357767
C,3.7726882208,2.0636626285,-0.4794403205
C,4.2603630196,3.363377461,-0.4547449479
C,5.547878867,3.6357224286,0.044573507
C,6.3266865859,2.5607688027,0.5163593784
C,5.8308976014,1.265160043,0.4980012097
C,4.7169976947,-1.6022400643,-0.0335577004
C,-6.0536260774,4.9701865751,0.0669775018
C,-2.4995031172,-2.0385082321,-0.0079732203
C,-4.5435887716,0.9882196171,0.000931526
C,-1.2069471706,-2.6766964787,-0.0009092862
C,3.7613472177,-2.6308628517,-0.0314382496
C,1.2070620083,-2.6767690872,-0.0013810743
C,-3.7612258611,-2.6308713834,-0.0293246479
C,-4.7169239094,-1.6022983665,-0.0316306249
C,-4.0366666157,-0.3808751511,-0.0101238295
C,2.4996198382,-2.0385711148,-0.0088038203
C,6.4828176658,6.1017113254,0.0898130457
C,-6.4829488456,6.1016844622,0.0869846388
C,6.0535261661,4.970212624,0.0691856893
B,-0.0000237113,-4.8248622572,-0.0339246938

Cartesian Coordination of 3m1-Cl-1

–1676.8233252 hartree
B,-3.7575233243,-2.0795440476,-0.0186641287
C,5.2016919685,2.3348612062,0.1450792845
C,-4.5999422005,3.6288439233,0.0695230265
C,-3.2311452005,3.8812432553,0.0027788249
C,2.2239357479,-1.6533273628,0.0331690991
C,-4.7593683341,2.2302707668,0.0681280456
C,-1.7657539494,-0.0981389762,-0.241521423
C,-1.3994506482,-1.4207109852,-0.020048084
C,-3.4842385738,1.6647549851,-0.0057408311
C,-3.0938286934,0.2784040174,-0.0390362382
C,-0.0166102755,-1.8323597368,0.0257738154
C,3.7318573264,0.3619840767,0.0827135688
C,5.0236885111,0.9167294326,0.0665567873
C,6.149820158,0.0781609861,-0.0230534362
C,5.972943325,-1.3003218583,-0.1006641418
C,4.6947837889,-1.8492947647,-0.0876420553
C,3.551175296,-1.0308114939,0.0083102388
C,0.5011026108,-3.1249849374,0.1270887569

C,5.3780490126,3.5300766733,0.2121937326
C,1.8967123868,-3.0160873716,0.1282426766
Cl,0.6536926249,2.3317972704,-0.1001094416
F,-4.4726393977,-2.7768548904,0.9225334439
F,-4.086947263,-2.4260171254,-1.3136378625
H,-5.6783766483,1.6639151988,0.1045874106
H,-1.0102580654,0.6503734234,-0.436638849
H,4.5789976732,-2.9252769675,-0.1624255349
H,-5.3807307247,4.3756172376,0.1126250655
H,-2.6890036847,4.8157650225,-0.0082626957
H,-0.0985614683,-4.0210032245,0.1856500374
H,2.8809423275,1.0364631217,0.1503308059
H,7.1427598384,0.515714192,-0.0338998858
H,6.8378238287,-1.9539839331,-0.1761935227
H,2.6022559011,-3.8308687126,0.2037705269
H,0.9647594384,0.0741325023,-0.0676784887
H,-1.5365609442,2.6098070716,-0.0551558651
H,5.4846134614,4.587779926,0.2678922411
N,-2.5683338732,2.7015894375,-0.0453273341
N,1.0492036635,-0.9547983101,-0.0278721399
O,-4.0342331698,-0.6078494792,0.1760940093
O,-2.2915369627,-2.3569891434,0.2028817541

Cartesian Coordination of 3m1-Cl-2

–1676.8264616 hartree
B,3.5120962078,-2.4422867182,-0.0629471898
C,-2.2220238318,-2.3060824293,0.1180657724
C,5.2995612957,1.6001324868,0.0979335337
C,3.2975492952,-0.0018926595,-0.0323456248
C,3.9408665558,1.2862290784,0.0177821509
C,1.3170418343,-1.358238975,-0.0265060668
C,-8.2931414546,-0.9105520196,-0.019094725
C,-3.349304212,1.3748302178,0.0588478656
C,1.9208071997,-0.1212351839,-0.2245634678
C,-5.8975868015,0.2043563254,0.0202366046
C,-5.7653745711,1.6057802967,0.0359968434
C,-4.4938010232,2.1707828866,0.0538912296
C,-0.87228381,-2.6785361802,0.1043790747
C,-3.4596838754,-0.0301487439,0.0439104385
C,-4.7458749423,-0.5961792001,0.0230375192
C,-7.1943549121,-0.401520186,-0.0012504178
C,-0.1177289751,-1.506510748,0.0226551623
C,-2.2838321629,-0.9047139904,0.0504384314
C,4.1106921621,3.5106536678,0.0576518663
C,5.4070031734,3.0034708769,0.1193439967
Cl,-0.0033796912,2.7426968383,-0.0636590357
F,4.0918901387,-3.2789390326,0.8568986087
F,3.7613539362,-2.8160520484,-1.3678873286
H,6.0949941642,0.8700125743,0.1263019295
H,-4.3815339931,3.2509690205,0.0648412249
H,-0.454798396,-3.6736804281,0.140358503
H,-2.375103921,1.8592329997,0.0737256489
H,-9.2572616286,-1.361565469,-0.0354397968
H,-0.7181502655,0.550504989,-0.0291890878
H,2.2078176728,2.5833097265,-0.0202135153
H,6.3145575906,3.588797174,0.1726257427
H,3.7548149061,4.5307974515,0.0593392997
H,-3.0700957849,-2.9730378395,0.1762008545
H,-4.8667285301,-1.6732131307,0.0038100964
H,1.3173753658,0.758756126,-0.3992776842
H,-6.6549439127,2.2272856632,0.0326566864
N,-0.9974998917,-0.442147624,-0.0080443878
N,3.2372120147,2.477902165,-0.005830471
O,4.0581749997,-1.0514496092,0.1567101257
O,2.0215329054,-2.447512478,0.1688850021

Cartesian Coordination of 3m2-Cl-1

–1984.0374425 hartree
B,0.0000914358,4.9180792842,0.0289343181
C,1.1996893078,2.7786362907,-0.0024230774
C,5.5058146774,-3.5990274007,-0.1161225684
C,3.5940174815,-2.1023025963,0.0880647094
C,-3.594051945,-2.1021752313,0.0871912777
C,-4.1232253941,-3.4044088803,0.0558060305
C,-5.5060071436,-3.5987874732,-0.1163669188
C,2.5609863261,-5.5154003687,0.3362825388
C,-2.5609026489,-5.515393772,0.3332254078
C,-3.2636892629,-4.5388690856,0.2052963117
C,-1.1995920912,2.778683863,-0.0023376546
C,-2.4693721072,2.0952899061,0.0212831377
C,3.7493455005,2.6471659559,0.1088793177
C,0.0000274459,2.1008757664,-0.2035703604
C,3.2636948086,-4.5389423811,0.2074164863
C,4.1231453801,-3.4045587197,0.0568590616
C,-6.3412519333,-2.4948444779,-0.2611808789
C,-4.6627156778,1.5874419621,0.0868417443
C,2.4694401923,2.0951860082,0.0211268389
C,4.4371688601,-0.9856716027,-0.052653159
C,-4.4372648962,-0.9854687745,-0.0525714313
C,5.8173238986,-1.2067227378,-0.2333850383
C,6.3409887987,-2.4951598841,-0.2619176789
C,-3.933222666,0.390492018,-0.0090592541
C,-3.7492436808,2.6473321978,0.1091208686
C,3.9331982105,0.3903172272,-0.0092400461
C,4.662763879,1.5872270363,0.0865789815
C,-5.817542836,-1.2064302413,-0.2324870445
Cl,-0.0000099991,-1.3030176583,-0.100101554
F,0.0000513595,5.4265258516,-1.2538108579
F,0.0001486143,5.8930994415,0.9943110756
H,-0.0000005323,1.0360265474,-0.3916344566
H,-1.8227926567,0.052642088,-0.0893628312
H,1.8227612733,0.05255429,-0.08950211
H,-6.4824661073,-0.3595230096,-0.3643182492
H,5.7382531512,1.6662374157,0.1525013868
H,-3.9553349188,3.7050796945,0.1762283128
H,-5.7381986544,1.6665301625,0.1527589411
H,6.4821592156,-0.3598692197,-0.366013
H,7.4086889278,-2.6387274384,-0.4041774706
H,5.9045561076,-4.6079717991,-0.1375861858
H,2.5207677749,-1.9829500017,0.2172764167
H,-2.5207179309,-1.9829108873,0.2158029107
H,-5.904780377,-4.6077160991,-0.1379780832
H,1.9055337771,-6.3467484826,0.4462339662
H,-1.9053699752,-6.3467904098,0.4423281214
H,3.9554918514,3.704903968,0.175968671
H,-7.4090494081,-2.6383312182,-0.4027905629
N,2.6073468482,0.7219831827,-0.0471707094
N,-2.607353433,0.7220973659,-0.0470574862
O,1.2346563727,4.070999049,0.2157305826
O,-1.2344910336,4.0710470839,0.2158280234

Cartesian Coordination of 3m2-Cl-2

–1984.0407901 hartree

B,0.8585357987,4.744677093,-0.0262337942
C,5.273035117,-4.387747649,-0.0426702335
C,-5.6507592632,-0.6644662011,-0.0126599179
C,-6.3110918449,-1.901898402,-0.0232741939
C,-5.554978096,-3.0891904999,-0.0039573549
C,2.0937791766,-5.9145545155,0.3235491866
C,-8.9509778244,-2.0020561025,-0.0835967827
C,-7.7412245638,-1.95367632,-0.0562211212
C,-0.5990342708,2.7725804197,-0.017622267
C,-1.943128428,2.2513763589,0.0219274266
C,4.2963427536,2.0309041559,0.0894580815
C,0.5064289361,1.9472270021,-0.2127212558
C,2.9208744648,-5.0380239058,0.2154115043
C,3.9208834904,-4.0219256093,0.0883644211
C,-4.1658896504,-3.0133600401,0.0253882978
C,-4.1814929599,2.007339068,0.1063212697
C,2.9586116613,1.638237797,0.0073427358
C,4.5359939857,-1.6609937744,-0.0200676711
C,-4.248294995,-0.5828546423,0.0200911117
C,5.8827708056,-2.0529805398,-0.1581760692
C,6.2426422157,-3.3967058525,-0.1664712419
C,-3.5991951061,0.7309741,0.0349322232
C,-3.1487261716,2.9522289726,0.1018982409
C,4.2040798573,-0.2331154383,0.0026972816
C,5.0737246576,0.8673521516,0.0834175635
C,-3.5102704104,-1.7832500451,0.038636531
C,3.5576566787,-2.6638492356,0.0999639447
C,1.7823112942,2.4725504254,-0.0240549418
Cl,0.0986765163,-1.4491716946,-0.0812388708
F,0.9854901934,5.7311152026,0.9185790672
F,0.9155120772,5.2218686718,-1.3194868834
H,1.3342588447,-6.654731999,0.4160776631
H,4.6303718798,3.0563067382,0.1420698109
H,-5.240198441,2.2156942224,0.1614812623
H,6.6519791878,-1.2964698616,-0.2709942624
H,7.2880564704,-3.672527952,-0.2751766261
H,-3.2293419922,4.0281637242,0.1431976511
H,6.1510000921,0.8164333715,0.1475988401
H,-2.422951387,-1.7706330239,0.0623867708
H,0.3738597992,0.8887019209,-0.3888304992
H,-3.573858128,-3.9237008835,0.0389480823
H,2.068527423,-0.3114097077,-0.0754026484
H,-1.5435691373,0.1475809584,-0.0407923884
H,5.5442385106,-5.4383888239,-0.0490048141
H,2.5045657955,-2.4123474667,0.2001626466
H,-6.249032819,0.2391555179,-0.035621087
H,-6.063716542,-4.0476227322,-0.0135318944
H,-10.0145458786,-2.0407109834,-0.1081774802
N,-2.2434915205,0.903811718,-0.0172328791
N,2.9283077338,0.2576300695,-0.0426017067
O,-0.4713484794,4.0618236039,0.181176787
O,1.9779751744,3.7533467556,0.1759995355

Cartesian Coordination of 3m2-Cl-3

–1984.0437617 hartree

B,0.0002158212,4.7047589031,-0.066217833
C,5.4223756819,-3.8484710186,0.0436930988
C,-5.8053715574,-1.4521188843,-0.0059932419
C,-6.3141833227,-2.759176532,-0.0018018909
C,-5.4229839643,-3.8476399806,0.0505045604
C,8.9227494874,-3.1733860389,-0.0784210899
C,-8.9223566074,-3.1723457018,-0.0965265853
C,-7.7273789337,-2.9808309472,-0.053493161
C,-1.2002195156,2.5648773056,-0.0260201114
C,-2.4713404811,1.884816063,0.0172372524
C,3.7527504758,2.4372099902,0.078050118
C,-0.00003061,1.8793489408,-0.2014619127
C,7.727545271,-2.9817819916,-0.0426922685
C,6.3140707929,-2.7600252284,0.0002611315
C,-4.053306715,-3.6066442763,0.0969456767
C,-4.6650891197,1.3764960383,0.0987414099
C,2.4716060138,1.8845456816,0.0133178879
C,4.4230981882,-1.2042975057,0.0389037086
C,-4.4231952539,-1.2037324605,0.0448412468
C,3.547878535,-2.3078944294,0.0813778244
C,4.0524849744,-3.6073031335,0.0821028021
C,-3.9347848529,0.1779366575,0.0448359326
C,-3.7522838169,2.4376108428,0.0850056635
C,3.9348917707,0.1774487202,0.0391774313
C,4.6654289005,1.3759818979,0.0906845297
C,-3.5484533345,-2.3073294083,0.0960480782
C,5.8055432751,-1.4528622631,-0.0033559158
C,1.2004958995,2.5647657362,-0.0279977958
Cl,-0.0004516944,-1.5600270866,-0.0349605623
F,0.0010630685,5.7086580823,0.8684930335
F,-0.0008766602,5.17168629,-1.3641666062
H,9.97401855,-3.3380368564,-0.1104954138
H,3.9610080109,3.4963088349,0.104641621
H,-5.7412001248,1.4576026533,0.1502225506
H,2.4701277828,-2.1655704442,0.112791324
H,3.3568978943,-4.4407260927,0.1140596253
H,-3.9603149211,3.496713749,0.1131812007
H,5.7416865188,1.4571358691,0.1388126638
H,-2.4709160208,-2.1649849115,0.133779464
H,-0.0001759809,0.8096027126,-0.3584574078
H,-3.3581246607,-4.4401254252,0.1354961941
H,1.8248925072,-0.1574016259,-0.021384955
H,-1.8250806316,-0.157304276,-0.02150705
H,5.813267314,-4.8607353854,0.0452844626
H,6.5065272226,-0.6271387324,-0.0452861343
H,-6.5057682796,-0.626327376,-0.0558342475
H,-5.8140757851,-4.8598271747,0.0523625336
H,-9.9734187909,-3.3369179453,-0.1351227443
N,-2.6088982569,0.5105683066,-0.0056046783
N,2.6089198682,0.5102650686,-0.0086261106
O,-1.2341793377,3.8634450468,0.1479196924
O,1.2349009691,3.8633395735,0.1458011122

Cartesian Coordination of 3p1-Cl

–1676.8276294 hartree

Cl,0.3827204378,2.4854813215,0.0679316184
F,-4.1553853351,-2.4689331553,1.3302747042
F,-4.5293222194,-2.8662960564,-0.9002396266
H,-0.0961323081,-3.9214633058,-0.1232932233
H,4.7988910321,2.3553193409,0.076504706
H,-5.7382486381,4.2473876971,-0.1812187433
H,-3.0690522421,4.8063706757,-0.0555681514

H,2.592790303,-3.6098649075,-0.1388553343
H,2.6134467287,1.2729376174,0.0526565909
H,6.7488037323,-1.4754908326,-0.0767152899
H,4.5589065151,-2.5850301574,-0.0993939174
H,-1.209919069,0.7184607666,0.4089341339
H,9.2452238413,2.1926456867,0.0391346805
H,-1.8215810721,2.6547164969,0.0179398212
H,0.7771137198,0.221441882,0.0171034273
H,-5.9170440595,1.5257541875,-0.1469420742
N,0.9093114558,-0.8020419213,0.0105022296
N,-2.8558532197,2.7000016229,0.0024386894
O,-2.3661823152,-2.348399043,-0.1897791576
O,-4.178781563,-0.6715785072,-0.1846870424
C,1.8507873226,-2.8255561461,-0.0975273086
C,0.4619075747,-2.99761693,-0.0919018138
C,3.4046487973,-0.7561184281,-0.024365553
C,3.5049478634,0.6497246667,0.0255587973
C,4.7465746515,1.2720666239,0.038373176
C,5.9384396721,0.5237807417,0.0023390592
C,5.8410714416,-0.8806599747,-0.0482746406
C,4.6017965572,-1.5015804716,-0.0612013636
C,7.2134618573,1.1665655714,0.0163862711
C,-1.9329303684,-0.0633784713,0.2214184529
C,-5.0238295346,2.1320893252,-0.1130612911
C,-4.9257235044,3.536008561,-0.1281019522
C,-3.569533039,3.8488477023,-0.0594432036
C,-3.7253535405,1.6234781722,-0.0295911159
C,2.1163740366,-1.4466209416,-0.0372216278
C,-1.5136688924,-1.3730641411,0.0182839547
C,-0.1144220033,-1.7271817694,-0.0215698398
C,-3.2763842052,0.2557654412,0.0180855959
C,8.2969702765,1.7092136207,0.0283654513
B,-3.8424768682,-2.1279562263,0.0300794083

Cartesian Coordination of 3p2-Cl

–1984.0458827 hartree

C,-0.0002674977,-2.1516372458,-0.2060988262
Cl,0.000189591,1.2771674252,-0.056487572
F,-0.0008385674,-5.9755371212,0.8827094101
F,-0.0005823593,-5.4497609759,-1.352659314
H,-6.5097760625,0.3471476027,-0.0208700018
H,-1.8242406353,-0.113087435,-0.0287665362
H,1.8242191119,-0.1135417335,-0.0290698094
H,6.7759508356,7.0336158971,0.0192584177
H,-6.7741024698,7.0353818331,0.0191462267
H,3.9587175348,-3.7689415527,0.1049320086
H,5.740946073,-1.7320959325,0.1301991411
H,-3.9597221785,-3.7679535006,0.1038172913
H,-5.7414321075,-1.7306794479,0.1289976415
H,6.5097452084,0.345466306,-0.0243182176
H,7.3882344353,2.6379320712,-0.0215135782
H,3.3707007867,4.1711339542,0.06261494
H,2.4779539085,1.9010663749,0.0679667622
H,-2.4774136735,1.9017177252,0.0642195751
H,-3.3695581849,4.1720001383,0.0590016176
H,-7.387626378,2.6398353713,-0.0181825004
H,-0.0001250567,-1.0826293016,-0.3687837516
N,2.608315603,-0.7820826252,-0.0152853352
N,-2.6085237498,-0.781418052,-0.0154677018
O,-1.2352555158,-4.1338367278,0.1516148429
O,1.2341629773,-4.1341446259,0.1518240237
C,-3.935175636,-0.4482343424,0.0300748177
C,-4.4260570179,0.928731342,0.02574445
C,5.8142196188,1.177771827,0.0002549981
C,6.3159525893,2.4699639008,-0.0007016119
C,5.4450106107,3.5768782426,0.0222816006
C,4.0589507096,3.3323615933,0.0456077973
C,3.5567883244,2.0374129136,0.0482440129
C,-3.5562429191,2.0383253808,0.0460143147
C,-4.0580611237,3.3334068252,0.0434610676
C,-5.4440874676,3.5782885771,0.0220732013
C,-6.3153575419,2.4715940911,0.0010347309
C,-5.8139718319,1.1792682522,0.0019726906
C,-4.6651585926,-1.6486056596,0.0836651994
C,5.9585759826,4.9092528157,0.0210007125
C,2.4706847784,-2.1554853308,0.0107709558
C,4.4262764504,0.9276021133,0.0260508543
C,1.1997206001,-2.8364472041,-0.0282170083
C,-3.7525796911,-2.7086975607,0.0751413114
C,-1.2004526792,-2.8361443216,-0.0283939259
C,3.7518574128,-2.7096392747,0.0759298291
C,4.664709627,-1.6497802636,0.084410263
C,3.9350396351,-0.4492364766,0.0304660794
C,-2.4712503718,-2.1548591255,0.0104103315
C,-6.396051486,6.0402829362,0.0201208591
C,6.3976335886,6.0386181745,0.0202631777
C,-5.9572960376,4.9107999134,0.0208316928
B,-0.0006337444,-4.9765857432,-0.0571064988

Cartesian Coordination of 4m-1

–2431.8271791 hartree

B,11.3640666436,0.0733277326,0.8183950597
B,-11.2506078253,0.0812032037,1.0973108155
C,-4.020333452,-2.5534380279,-0.2127174977
C,-1.8598382857,-3.680811053,0.056610407
C,-0.6406236347,-3.6651077774,-0.0084222042
C,0.7168963359,-3.6473496365,-0.078675648
C,1.9362819043,-3.631170891,-0.1402950122
C,-3.9603558911,-4.8517704214,0.5729239409
C,-3.2797968006,-3.6968293288,0.1347235213
C,9.1553638905,0.8305891154,-0.0081108789
C,11.477930032,3.766856182,0.1774832284
C,10.916190097,2.4435327861,0.252456947
C,7.8227392892,0.4183359143,-0.3616335621
C,-6.8924971246,0.6092768016,-1.4033508239
C,-6.0776052005,-3.7147400391,0.2948266066
C,9.6445063699,2.1198139867,-0.2252765343
C,-12.2150896019,5.4814427567,-1.2867582783
C,-11.1989632883,4.5073780937,-1.3370786303
C,-5.3493025209,-4.848494796,0.6502397911
C,-5.4200239254,-2.5487786767,-0.1389182873
C,10.9932736067,4.9859908396,-0.3011044992
C,12.0047879926,5.9475815335,-0.1114321087
C,13.0848285521,5.3005755306,0.4787980478
C,-5.8215552617,-0.2969361718,-1.3751442512
C,-6.1662031107,-1.3463401374,-0.5125013985
C,6.1299265625,-1.06332804,-0.513710681
C,5.6774844952,0.1635471109,-1.0183709247
C,6.7313583887,1.085171809,-0.924882448
C,5.4418830999,-2.3494146943,-0.3929962021

C,6.1551603701,-3.5615468557,-0.3467824905
C,5.4822388399,-4.7758033729,-0.2253187259
C,4.0932461399,-4.8128194299,-0.158317502
C,3.3565682595,-3.6113649048,-0.2112085544
C,4.0424801274,-2.3893201625,-0.3230549803
C,-11.5763723627,3.4631049023,-0.4901540111
C,-9.742460515,1.7762278429,-0.6593092673
C,-10.9607559031,2.2115368027,-0.1335315945
C,-7.8859490924,0.1110899707,-0.5560839546
C,-9.1831483999,0.5963764341,-0.1656536663
C,-13.1905334057,5.0165140395,-0.4116637694
F,-12.0339916437,-0.7660290461,0.3571906554
F,12.0549763564,-0.5149252343,-0.2091686285
F,11.6486205483,-0.4356983384,2.0511168654
F,-11.3701183901,-0.0769447894,2.4465733222
H,-3.3913155518,-5.7336264551,0.8458054942
H,-7.9335875388,-1.5995385098,0.6545686551
H,-13.2815397581,3.2076439568,0.7100974736
H,-14.1236556224,5.4626315411,-0.1010976199
H,-12.243131574,6.4190631596,-1.822511516
H,-10.2901716319,4.5521039773,-1.9197960426
H,-5.8724415697,-5.7406812773,0.9800023621
H,-7.1625483391,-3.7481889581,0.3262706158
H,-3.4912144558,-1.6591103965,-0.5220320713
H,9.0283179652,2.8690703035,-0.7004475541
H,10.0174833011,5.1523579915,-0.7341918728
H,11.9618407907,6.995301897,-0.3710191803
H,14.0486854215,5.6808202514,0.7830807334
H,13.3228957311,3.261158071,1.0462318065
H,8.0275716023,-1.5485202875,0.3318639456
H,4.6984895767,0.3442652686,-1.4376052545
H,6.7132391123,2.1192428723,-1.2374226162
H,7.2373985172,-3.5605828582,-0.435772109
H,6.0478818787,-5.7017906935,-0.1935917976
H,3.5668718155,-5.7565241272,-0.0673085098
H,3.4729344655,-1.4668651007,-0.3341424811
H,-9.2149629843,2.3723364342,-1.3895250004
H,-6.9499828373,1.5219036378,-1.9787826055
H,-4.9046279294,-0.2297702531,-1.9422474706
N,-12.7947109208,3.8061050316,0.0586098054
N,-7.4177061703,-1.0765034821,-0.0383995158
N,7.4276989005,-0.8809645429,-0.1311125366
N,12.7551772336,3.9944084221,0.6466958117
O,11.6844239461,1.5536388247,0.8283008507
O,9.8813241073,-0.0987932956,0.5619320095
O,-9.8021509076,-0.1473661391,0.7170251403
O,-11.6224395302,1.5073000268,0.7496737165

Cartesian Coordination of 4m-2

–2431.8270584 hartree

B,-8.5650803245,1.5562940307,1.1220403561
B,8.5650321915,-1.5560624203,1.1225292592
C,-1.2555909689,-1.4263236346,-0.5232143327
C,-0.4487991799,-0.5099281572,-0.5252905943
C,1.2556859112,1.4269713678,-0.5229986825
C,0.4488765348,0.5105915467,-0.5252120589
C,-7.8598036394,-1.8282745945,-0.3311657296
C,-10.0279519981,-0.6297898396,-0.030426093
C,-8.6353189855,-0.6797325779,0.0559715108
C,-12.0949770501,0.7622092715,0.1282616134
C,-10.6761813835,0.5675909554,0.2783555296
C,-13.128502961,-0.0546367525,-0.3348423449
C,-14.3242076242,0.6848247424,-0.2472040741
C,-13.9998775049,1.9360502066,0.2650979712
C,-5.9487907277,-2.9975135335,-0.5856436274
C,-7.0107440769,-3.8049131669,-1.0160746877
C,-8.1994463497,-3.0762503432,-0.8605022104
C,-4.5113912905,-3.2700094668,-0.5486921728
C,-3.5729778179,-2.2287732277,-0.5581402987
C,-2.192212,-2.4959142579,-0.5160593042
C,-1.7507670665,-3.8338736297,-0.4766614837
C,-2.680885067,-4.8693797659,-0.4760660804
C,-4.0462242542,-4.5973789131,-0.5065587492
C,13.9992895542,-1.937383538,0.2634236644
C,5.9490040739,2.997778998,-0.5851234239
C,7.0110431029,3.8051443031,-1.0154109142
C,8.1996672232,3.0763248478,-0.859978666
C,4.5116290038,3.2704009538,-0.5481382785
C,3.5731272762,2.2292455972,-0.5577688981
C,2.1923832207,2.4964944479,-0.5156569058
C,1.7510510897,3.8344842822,-0.4760440813
C,2.6812568852,4.8699117951,-0.4752685128
C,4.0465743289,4.5978024393,-0.5057909937
C,8.6352762896,0.6796210267,0.0561459959
C,12.094648863,-0.763015971,0.1274879219
C,10.6759391367,-0.5681191593,0.2779810713
C,7.8598998234,1.8283110711,-0.3308090675
C,10.0279202392,0.6295668736,-0.0300793964
C,13.1282596267,0.0537269125,-0.3356123935
C,14.3238072721,-0.6860476034,-0.24849327
F,8.5019808373,-1.4164941972,2.4845163797
F,7.9390522824,-2.6683616235,0.6416158187
F,-8.5007280521,1.4182156069,2.4841014421
F,-7.9398803514,2.668319719,0.6394003747
H,-6.0065806383,-1.0309402894,0.2388126982
H,-13.0206993818,-1.0674385429,-0.6954395241
H,-15.3145295239,0.3534318359,-0.523620616
H,-6.9134916712,-4.7980007284,-1.4296922909
H,-9.1964293135,-3.4071865891,-1.1131546779
H,-3.8954214857,-1.1949378101,-0.6262422532
H,-0.6870414269,-4.0423923793,-0.4466751774
H,-2.338862346,-5.8991018212,-0.4403028338
H,-4.7604409126,-5.4135309473,-0.4763855498
H,10.5885535211,1.4831655343,-0.3819744368
H,13.020606235,1.0666583138,-0.695889999
H,15.3141410319,-0.354808799,-0.5250521328
H,14.6257150789,-2.7896596668,0.4811432154
H,12.1134121566,-2.7344931674,0.8527042763
H,6.0065947572,1.0310816302,0.2390470311
H,6.9138905799,4.7983078824,-1.4288697779
H,9.1966814233,3.4071825636,-1.11261147
H,3.8954842488,1.1953948858,-0.6260461361
H,0.6873428257,4.0430892253,-0.4460360767
H,2.339319325,5.899656429,-0.4393413897
H,4.7608599017,5.4138891763,-0.4754771326
H,-10.5884443267,-1.4833057592,-0.3827422107
H,-14.6264599681,2.7880931526,0.4832779371
H,-12.1140129362,2.7335185745,0.8539310871
N,-12.6605130643,1.9688277344,0.4849494242
N,12.6599969807,-1.9698496792,0.4837498445

N,6.4902941963,1.8102889297,-0.1840005844
N,-6.4902022536,-1.8101368992,-0.18434406
O,-10.0224359985,1.6150089518,0.7129588854
O,-7.9308598238,0.3378126062,0.4839470054
O,10.0219931443,-1.615615631,0.7121341854
O,7.9306855524,-0.3380331692,0.4836865668

Cartesian Coordination of 4m-3

–2431.8269958 hartree
C,-2.6721736417,4.8619139422,0.0521846685
C,-1.744410858,3.8319872272,-0.073736851
F,7.9774131216,2.7404586255,0.0262921824
F,-7.9409835661,-2.7331162283,0.4738127345
F,-8.4997128627,-1.6464460923,2.4197860126
F,8.926595829,1.8877825139,-1.8850506893
H,-14.6277050778,-2.830574176,0.318064796
H,-9.19275311,3.4806221728,-0.720682777
H,-6.9074660245,4.8917002535,-0.9125289088
H,-6.002406283,0.9835059798,0.3917394635
H,-12.1149643632,-2.8101022467,0.690358929
H,6.0758882636,-0.9154137742,-0.7058493403
H,6.7577458656,-4.9880318864,0.156554024
H,9.0377717959,-3.6133418245,0.5590611154
H,3.8532082316,-1.2383022448,-0.2164846758
H,0.759042584,-3.8767376399,-1.5951088512
H,2.4234958778,-5.7086102769,-1.8159555755
H,4.8024878194,-5.3026377518,-1.2859703689
H,-10.5857223307,1.4967012507,-0.1759625671
H,-15.3136923524,-0.3188306507,-0.4790049076
H,-13.018567576,1.1091415194,-0.5314536357
H,-3.8961949965,1.2299735463,-0.5072989915
H,-4.7512213629,5.4047413976,0.1286458725
H,-2.3276150007,5.8804074825,0.2022467989
H,-0.6800265108,4.0345533177,-0.0294881249
H,10.4912477611,-1.5973434239,0.574013378
H,12.8053492967,-1.3112472052,1.4406691385
H,15.0476920428,0.0680895145,2.0559883472
H,14.4966152505,2.6840135333,1.5383562482
H,12.1049044486,2.7644040332,0.6864977315
N,6.4964936429,-1.7826772363,-0.4041234792
N,-12.6608868899,-2.0163870973,0.3878037471
N,-6.4863734602,1.7990458888,0.044171007
N,12.5921156516,1.924130983,0.9624076054
O,-10.022085333,-1.6874543262,0.6388101005
O,-7.9292712758,-0.3977664719,0.5203498363
O,7.9913990392,0.4286570811,-0.3066600948
O,10.0549800621,1.6826983369,0.1590265644
C,1.2646825899,-1.3768806424,-0.773898165
C,0.4547244568,-0.4709508213,-0.6558307821
C,-0.4455504847,0.5386804453,-0.5233458049
C,-12.0942523907,-0.7844677826,0.1342070624
C,-10.0258264817,0.6145098546,0.0979550655
C,-10.6751151436,-0.6049420524,0.2994207404
C,-7.8565054698,1.8331342142,-0.0953590022
C,-8.633026529,0.6550797332,0.1868717801
C,-8.1955321785,3.1259098401,-0.5037599707
C,-7.0059681004,3.8643603198,-0.5936731346
C,-5.9443260206,3.0181837902,-0.2452362293
C,-14.00032884,-1.9637703881,0.1723548868
C,-14.3236087628,-0.673378001,-0.2320363162
C,-13.1271934454,0.0696799106,-0.2574117531
C,-1.2534696083,1.4462324215,-0.4037783136
C,-2.1887662146,2.5077836331,-0.2629699734
C,-3.5703055151,2.2485776368,-0.3236986197
C,-4.5061401907,3.2833252807,-0.1881754483
C,-4.0382985707,4.5968312819,0.0009347819
C,13.864448513,1.816022373,1.4236641682
C,5.9165035328,-3.0183773419,-0.3876516614
C,6.905966363,-3.9281920419,0.0096322021
C,8 .091053716,-3.2101648882,0.2296585484
C,4.5081078557,-3.240694663,-0.7178110436
C,3.562308176,-2.2138368384,-0.5922074111
C,2.2091309866,-2.4308193866,-0.9106233474
C,1.8020079009,-3.7058076432,-1.3523836478
C,2.7385846287,-4.7287091127,-1.4708518127
C,4.0780782223,-4.5042474948,-1.163149938
B,-8.5646159434,-1.6661667488,1.0508134699
C,8.6304072858,-0.6752227208,-0.0090449948
C,12.0031672363,0.6778419697,0.9083873838
C,10.6451598294,0.5501693352,0.4474227863
C,7.8226453836,-1.8654938822,-0.0403355571
C,9.98375221,-0.6743418996,0.3345380881
C,12.9513752617,-0.2439887233,1.3568461103
C,14.1199491779,0.4733904883,1.679160948
B,8.7118001879,1.740442902,-0.5391353393

Cartesian Coordination of 4m-4

–2431.8206917 hartree
B,6.4987832248,3.9720211729,-0.4750708679
B,-3.4038922234,1.9558631025,-0.1891256321
C,4.5072895137,1.9383728074,-0.3261593044
C,5.8289583132,1.6070212673,-0.6381709201
C,-6.5394684824,3.9933724074,-0.3458791489
C,-5.7128152967,2.8365712226,-0.1356191421
C,-5.7368587722,-0.8006474728,0.7754927384
C,-6.222445721,1.563465644,0.1291011027
C,2.7842135952,3.7514172162,-0.1018193712
C,4.1303807918,3.2935203698,-0.3128603743
C,2.3343480733,5.062216115,0.0637668769
C,0.9442821028,5.0158219394,0.2730883622
C,0.5584657708,3.6813602499,0.2284780161
C,6.2413145225,-2.0033637374,-0.9665348153
C,7.5795793154,-1.6055938443,-0.970125735
C,7.6160916966,-0.2048434958,-0.8585434064
C,5.6496376063,-3.3374193485,-1.0620327901
C,4.3598086594,-3.5983374193,-0.5797915156
C,2.4686174024,-5.1011310056,-0.2002736445
C,1.3258307564,-5.237597848,0.2074359093
C,-1.1062377556,-5.4223551216,1.048649784
C,0.046221267,-5.3500959732,0.6519447534
C,6.3018036039,0.2483808702,-0.7818636947
C,-5.3558154819,-2.9511998199,1.3391253843
C,-6.7436705745,-2.7503004966,1.3098797288
C,-6.9808000171,-1.4129944759,0.9584207596
C,-4.5684391068,-4.1516020221,1.6219027114
C,-3.2356182096,-4.2478501085,1.2012271096
C,-2.4608084585,-5.3878523632,1.480850095
C,-3.0467334945,-6.4605127561,2.1801886235
C,-4.3755189518,-6.3737200643,2.5889948629
C,-5.131330845,-5.2343972423,2.3224086846

C,-5.3304431908,0.5286665471,0.4107784114
C,-7.9220237377,4.1949005577,-0.322289546
C,-8.1568511322,5.5534040623,-0.6058917412
C,3.7883484897,-4.8802863949,-0.6820541452
C,4.5361074646,-5.9239126663,-1.2607824752
C,5.82275497,-5.6711030953,-1.7300272293
C,6.3745934915,-4.3958716402,-1.6421571944
C,-6.9178509935,6.1563002769,-0.7961494866
F,7.0943023554,4.7485818079,-1.4228513949
F,-2.3703756534,2.3250310943,0.6453162199
F,6.9492207252,4.1863882483,0.8025828913
F,-2.9975565693,1.7129720709,-1.4750466081
H,-2.4560653821,-7.344030608,2.3956778209
H,-4.9581698418,5.329919438,-0.7143846206
H,4.1005283791,-6.9140232017,-1.3371830346
H,6.3974090483,-6.4740115183,-2.1813623385
H,7.3659831232,-4.2076002493,-2.0405301897
H,-6.6655502819,7.1796120214,-1.0315119844
H,-7.4908574532,-3.5084511317,1.49306927
H,-7.9444834218,-0.9395050584,0.8381042712
H,-2.776993246,-3.4511497661,0.6253294596
H,-4.8246633151,-7.1993866,3.1321750188
H,-6.1562490975,-5.1729033874,2.6731728406
H,-7.288837641,1.3949225589,0.1636462511
H,2.9758800941,5.9303276657,0.0437004832
H,0.2840265428,5.8536712644,0.4435671031
H,-0.4150776196,3.2237681217,0.3367766694
H,8.4295897949,-2.271315938,-1.0070441821
H,8.4848846326,0.4337020177,-0.8064702366
H,3.7874894465,-2.818572745,-0.0878445093
H,3.7888120148,1.1634150816,-0.093796969
H,-8.6679040856,3.4400527124,-0.1192008665
H,-9.1151435641,6.0481366359,-0.6665980131
H,4.4858362652,-0.8343349984,-0.9714589409
H,-3.7913779525,-1.5454851124,0.9908450036
H,1.6643471644,1.9305345942,-0.1175818169
N,-5.9576747101,5.210666698,-0.6367951521
N,1.6718930177,2.9293431885,0.0089736233
N,5.4830984582,-0.8656373119,-0.8307547367
N,-4.7775186246,-1.759846328,1.0108936005
O,-4.4219092363,3.0649209685,-0.19352752
O,-4.0298400247,0.709004121,0.3741608624
O,5.008512006,4.2346888723,-0.5109101394
O,6.7387027014,2.5193891955,-0.8312975421

Cartesian Coordination of 4m-5

–2431.8064843 hartree

C,9.6296294118,4.357185611,-1.2507115497
C,8.6238629748,5.2686607927,-1.6291772767
F,12.8692667075,0.5925842497,-0.6174641326
F,-10.5247435555,3.274475247,1.7068335317
F,-10.5034895722,1.2673427293,2.8282280134
F,11.9163728552,1.1154800281,1.410658168
H,-4.8801168785,2.7925335682,0.9492306154
H,-14.2595148722,1.0371720508,0.4119822182
H,-15.9347528393,-0.4014101303,-1.1805607673
H,-14.3290744364,-1.9309198182,-2.7578097718
H,-5.0561623165,-1.1986902801,-1.6565777156
H,-7.7368190923,-1.3793484928,-1.8155186258
H,-3.1162317285,-0.9706827626,-0.1888287713
H,-0.6830381217,2.1194095087,1.5468753495
H,-2.6883644117,3.5730750596,1.7486670247
H,6.4203172153,4.9085338706,-1.86575206
H,8.5790584464,-4.9150000314,0.9872105325
H,10.5546208659,-3.0571054339,0.8827340355
H,4.9448216086,-1.9281207425,0.4723617281
H,2.3548584846,-5.2682836879,-0.2872672001
H,4.3366346526,-6.7545796299,-0.4804283821
H,6.6179172782,-5.8281407197,-0.2588985773
H,7.8257853526,0.7515614706,-0.238256004
H,10.6864322487,4.5451442535,-1.1358849896
H,8.7508912001,6.3131622906,-1.8735402885
H,-11.9674368741,-1.399433941,-2.1456817433
H,6.9739503976,2.5614031407,-1.2192683283
H,6.9777751228,-1.3264459846,-0.4824660517
H,-6.7830162434,1.5267458793,1.0619627389
H,-10.0745403081,-0.8830611179,-1.1157527661
N,-6.6486422437,0.8471152711,0.327045495
N,7.6056221755,-1.9588974288,-0.0125654898
N,-12.7554347242,-0.9823596716,-1.677798666
N,7.6674357746,3.2900952227,-1.2573481339
O,10.9035732583,-0.4859914428,0.0301113737
O,-11.5896532336,1.4265956583,0.7566721172
O,-9.1404508093,1.5562254496,0.9442931216
O,10.9341087703,1.8972794995,-0.5694236862
C,-1.7685679762,0.4831466064,0.6455127818
C,-1.6524112569,1.7711578476,1.2077749831
C,-2.7791583413,2.5789064576,1.3223448341
C,-4.0229038338,2.1292207668,0.8831566288
C,7.4210377464,4.5782175941,-1.6290063778
C,7.30653784,-3.2719028516,0.250773877
C,8.4913381662,-3.8903681792,0.6562983144
C,9.5171188216,-2.9309807364,0.6123402327
C,5.9527018542,-3.8085018735,0.1103334532
C,4.8286079143,-2.9791369023,0.2278903993
C,3.5270142045,-3.4924643918,0.079421924
C,3.3565309049,-4.867893633,-0.1766379224
C,4.4708235247,-5.6959840832,-0.2806512313
C,5.7565547028,-5.1781885317,-0.145840011
C,9.603514139,-0.4562152844,-0.0195547584
C,9.0230586058,3.1239851564,-1.0214994571
C,9.6336550687,1.8862213479,-0.6032807515
C,8.9568740313,-1.7300398695,0.1822760464
C,8.9067809192,0.7318656198,-0.2763005835
C,-12.6827789538,-0.0321517749,-0.6715847195
C,-11.4530195039,0.4514423706,-0.0968009552
C,-13.9922932743,0.3200294084,-0.3493602672
C,-14.8549223721,-0.4283855298,-1.1740486676
C,-14.0602355672,-1.2223246247,-1.9882582458
C,-5.4632489887,0.3513018662,-0.134764594
C,-5.7749661406,-0.6370021959,-1.0780559005
C,-7.1730146675,-0.7242223719,-1.1671859799
C,-4.1647378345,0.8447217213,0.3261337305
C,-3.0284333922,0.0315336607,0.215244618
B,11.7262939221,0.7866411055,0.0942405212
C,-0.628752335,-0.3589349102,0.5245372592
C,0.3454025797,-1.0876211967,0.418986864
C,2.3998326648,-2.6340629135,0.2006935679
C,1.4287318663,-1.9007648336,0.3033962082
C,-7.7090758025,0.2076164028,-0.2749995255

C,-10.1892596749,-0.0546575211,-0.430835711
C,-9.0548418743,0.5701961144,0.0902932012
B,-10.453505989,1.9168315961,1.6228564983

Cartesian Coordination of 4m-6

–2431.8060612 hartree
B,8.2762037277,-2.4482824826,0.2602466599
B,-11.8378166861,1.1786679764,0.1214560879
C,10.3410040652,-0.5162036752,-0.17065381
C,9.0339291158,-0.0987261559,0.0893486397
C,-11.7125078491,-2.518776227,0.6992439776
C,-11.2251427715,-1.1911857938,0.4149897276
C,-8.1545575593,0.8085943457,-0.4359184639
C,-9.9196445019,-0.9188289389,-0.0186965016
C,12.0025964932,-2.3901884518,-0.1253404385
C,10.6639670398,-1.86947482,-0.0042612836
C,12.4276492965,-3.7169353094,-0.0896146416
C,13.8256815034,-3.7262320925,-0.2641319164
C,14.2325384768,-2.4068995139,-0.3993647914
C,7.1190247122,2.9528439462,0.2396209344
C,8.3676923444,3.5224959258,-0.0435359677
C,9.3020382373,2.4814599147,-0.1573552544
C,5.8144904596,3.5866249206,0.4372581475
C,4.6239318556,2.8855970187,0.2010924303
C,2.1755025581,2.7677848071,0.1519915144
C,1.1506912043,2.1381210773,-0.0577678951
C,-1.0101582379,0.8002474164,-0.5023627285
C,0.0114612578,1.4347028211,-0.2916766445
C,8.621005807,1.2809397819,0.0593244709
C,-5.9309376494,0.6168304709,-0.7908268459
C,-6.2817243328,1.9571480562,-0.9679982257
C,-7.664084685,2.0754990182,-0.7457600313
C,-4.6323980355,-0.0498406763,-0.8945270003
C,-3.4547777247,0.6712794296,-0.6533503271
C,-2.1951566803,0.0543997739,-0.7498272827
C,-2.120711878,-1.3143946103,-1.082601658
C,-3.2878438756,-2.0327212026,-1.3205620032
C,-4.5327062218,-1.4116219842,-1.2351565313
C,-9.5090302682,0.4162618396,-0.1339255529
C,-13.013631226,-2.9227229434,0.9900480921
C,-12.9997909907,-4.3196255853,1.1766380912
C,3.3716125788,3.496361659,0.3968477499
C,3.3192807022,4.8378345712,0.8257662547
C,4.5005981954,5.5381805705,1.0526578147
C,5.7366624786,4.9241678347,0.8668899735
C,-11.6916616174,-4.7456034439,1.0023460278
F,7.7774083949,-2.8267087162,-0.9587150801
F,-12.3552945069,2.043666433,1.0353968508
F,7.6808372341,-3.0499247462,1.3277241801
F,-12.3557671522,1.2978167773,-1.1415583055
H,-1.1503021053,-1.7931742077,-1.1526734758
H,-9.9239731664,-3.6763002625,0.5915200778
H,2.3552607535,5.3116233472,0.9744785738
H,4.4582465002,6.5698669368,1.3879144424
H,6.6494993772,5.4725715906,1.0747964994
H,-11.2586027727,-5.7328727908,1.068398787
H,-5.6054356914,2.7442473964,-1.2682089093
H,-8.2738115638,2.9631958375,-0.8214883504
H,-3.5094020032,1.7159531277,-0.3684096887
H,-3.2275718804,-3.082874823,-1.5892846833
H,-5.4293278657,-1.9776897136,-1.4711304772
H,-9.2355958843,-1.7241878561,-0.2509444831
H,11.7699637603,-4.5631483942,0.039792176
H,14.4722538051,-4.5911098104,-0.2919111731
H,15.2166819084,-1.9856762878,-0.5429606937
H,8.5567939543,4.5765717457,-0.185120581
H,10.3544333108,2.5827839457,-0.380052712
H,4.6475996503,1.8648429827,-0.166188947
H,11.0881789713,0.2129345981,-0.4508301577
H,-13.8604871928,-2.2551271065,1.0403645463
H,-13.8431547719,-4.9532546205,1.4092507557
H,6.6155122852,0.9005307717,0.5337378653
H,-7.0956789005,-1.0126335883,-0.1454095231
H,13.1468666197,-0.6027392807,-0.3451053839
N,-10.9236725071,-3.6582628216,0.7079321696
N,13.1306354566,-1.6091914401,-0.3201533995
N,7.3016516127,1.6009427292,0.2907949211
N,-7.0822393055,-0.0658932909,-0.4894791086
O,-12.0854539671,-0.2353569193,0.6113851547
O,-10.3393684946,1.4014328838,0.0498827233
O,9.7549167872,-2.7529396793,0.2980633804
O,8.0888408627,-0.9453159881,0.4029903148

Cartesian Coordination of 4m-7

–2431.7983165 hartree
B,-12.2085401659,-2.3160291254,-0.08685
B,12.2077401661,2.3178791254,0.08115
C,-5.6874198662,1.8682004074,1.29087
C,1.763609958,-0.5857001263,-0.39856
C,0.630799985,-0.2100500452,-0.14091
C,-8.7044500793,-1.1072393764,0.43382
C,-10.838649988,0.1680407765,0.12798
C,14.3439598986,-1.4150810276,0.74777
C,14.6701298007,-2.781361051,0.86058
C,-3.083529927,1.0183602209,0.70331
C,-3.3245298317,2.3496402382,1.10243
C,-4.6216798022,2.7609003311,1.39073
C,10.1206000742,1.035189275,-0.1732
C,13.5004197492,-3.5013009672,0.66884
C,6.5798600293,0.4090895286,-0.76525
C,6.599790129,1.8005195272,-0.88363
C,7.92061016,2.2333094326,-0.67726
C,4.1647299907,-0.1292702984,-0.59021
C,3.0835599268,-1.0214202209,-0.69855
C,3.3248598314,-2.3533302382,-1.09537
C,4.6220298019,-2.7646603311,-1.3835
C,5.6874898659,-1.8713804074,-1.28575
C,-10.1210200741,-1.0347092749,0.17069
C,12.9790599052,-1.3230209298,0.48392
C,12.18250999,-0.1394408727,0.27266
C,8.7038400793,1.1067193765,-0.43564
C,10.838729988,-0.1671907765,-0.12881
C,-12.978089905,1.3257709297,-0.48428
C,-12.1821699899,0.1415208727,-0.27445
C,-14.3428498984,1.4188410275,-0.74854
C,-14.6683598005,2.7854410508,-0.85946
C,-13.4984097489,3.504560967,-0.66616
C,-6.5803900294,-0.4109895286,0.76582
C,-6.6009101291,-1.8026095271,0.88178
C,-7.9217801601,-2.2345494325,0.67395

C,-5.4729499615,0.5380203921,0.88459
C,-4.1649799909,0.1267902984,0.59286
C,-1.7636099583,0.5827201263,0.40307
C,5.4727199613,-0.5405503921,-0.88178
C,-0.6307799852,0.2070700452,0.1455
F,-12.6497801865,-2.6034390938,1.1781
F,12.6483001865,2.6037590939,-1.18437
F,12.5307002325,3.2450391023,1.02266
F,-12.5315502322,-3.2417391022,-1.02976
H,-5.7509401734,-2.420149588,1.13328
H,-3.9795400636,-0.8874297149,0.25757
H,-8.1131599338,0.9235005812,0.21726
H,-11.5200297941,2.8739308253,-0.31314
H,11.5216597942,-2.8721008254,0.31545
H,8.1134499338,-0.9238905812,-0.21529
H,-6.6857798427,2.195730479,1.56645
H,-10.3578399211,1.101430742,0.38908
H,15.0056199594,-0.566141075,0.83068
H,15.6449497705,-3.2034811208,1.05648
H,-2.4923497822,3.0400601786,1.18394
H,-4.803579729,3.7823403441,1.71052
H,13.3194796729,-4.5660309542,0.683
H,5.7494501732,2.4172895881,-1.13571
H,8.3015902323,3.2425194053,-0.71982
H,3.9790800634,0.8854997149,-0.25669
H,2.4928997819,-3.0442101786,-1.17525
H,4.8041597287,-3.7866003442,-1.70151
H,6.6858498425,-2.199040479,-1.56119
H,10.3580899211,-1.101240742,-0.38787
H,-15.0048599591,0.5703210749,-0.83296
H,-15.6429097702,3.2082811206,-1.05512
H,-13.3169796727,4.569230954,-0.67868
H,-8.3031702324,-3.2436794052,0.71457
N,7.8675100004,0.0060894364,-0.51459
N,-7.8677500005,-0.0070694364,0.51514
N,12.4881498124,-2.6182208946,0.43631
N,-12.4866298123,2.6206908945,-0.4345
O,-12.7948700703,-0.9819090834,-0.50838
O,12.7949100705,0.9846290834,0.50426
O,10.6972501563,2.1811192337,0.0454
O,-10.6980001562,-2.1800192336,-0.05027

Cartesian Coordination of 4m-8

–2431.7990097 hartree

C,-8.9451644473,4.6342557856,-2.9297890382
C,-9.7170302184,3.5293253526,-2.5185594521
F,-12.1607492286,-0.141457624,-0.1379705973
F,12.1499909255,-0.4304283754,-0.3692432229
F,-11.0209876547,-1.0256590471,-1.9309723567
F,11.2478249156,0.1783626629,1.6584185363
H,-9.2744359167,5.4713119937,-3.5279082172
H,-10.755712805,3.3289451702,-2.7338869897
H,-9.0737852122,-3.136300844,1.4248174458
H,-7.2141457639,0.8080962486,-0.6266078489
H,-6.8474903156,2.9322072442,-1.2209279967
H,-6.7843422547,5.0725242158,-2.5059032854
H,7.0777389161,4.4023482954,-1.870153657
H,7.1781088686,-0.9798729565,0.4169556227
H,6.6130908441,-3.1236077503,0.671386729
H,6.4141023189,-5.4648816937,1.5159477832
H,8.9235326064,-6.3116700118,2.1403293041
H,10.5716230297,-4.2116438049,1.6043594178
H,-6.0662985988,-0.2321400074,1.0103708855
H,-6.8135106219,-4.029175092,2.6321072934
H,-3.852961648,-0.8583457108,0.7293942836
H,-0.8473477745,-2.0259141042,3.5663433453
H,-2.5487077722,-3.3281970306,4.8250000917
H,-4.904874337,-3.3518149329,4.0790205953
H,0.8621352364,3.1920574219,-2.5352200267
H,2.5944599963,4.4892732634,-3.7558023579
H,4.991704886,4.15153533,-3.2533489083
H,3.9352763922,1.2913950867,-0.2133376135
H,6.0260589274,0.4679025757,-0.8624112166
H,9.3100267233,3.0806880475,-1.070904959
N,-7.639380988,3.2767161084,-1.7381920689
N,7.4041594781,-3.6457153991,1.0103949356
N,6.555087231,1.3244140254,-0.9010157003
N,-6.5063728483,-1.1255769007,1.1621216979
O,-10.4849947204,1.1225256548,-1.1588755267
O,-9.9685506409,-0.8871754238,0.1589982599
O,10.4233800707,-1.7106454746,0.5411210275
O,10.036900381,0.5607430111,-0.3125285649
C,7.1436225817,3.3744958498,-1.5440960948
C,8.755897664,0.346674932,-0.2306171086
C,8.2443794005,-0.8499549891,0.2879682975
C,9.1361227055,-1.8839132386,0.6109015715
C,8.7180945568,-3.2044962003,1.0116679191
C,7.3526740129,-4.9341630768,1.4524933078
C,8.6428601235,-5.3413206219,1.7576264159
C,9.5004232272,-4.2585729843,1.4788788333
C,-5.9530554142,-2.1289334421,1.9172237446
C,-7.8373734517,-1.4030747748,0.9032639967
C,-8.119707032,-2.6352392695,1.4889080926
C,-6.9480891202,-3.0879987989,2.1191265768
C,-8.712765385,-0.5466688472,0.1398622591
C,-8.2704282786,0.584303585,-0.5583528352
C,-9.2207022272,1.4276784069,-1.1535106099
C,-8.8934998285,2.6876993689,-1.7738648249
C,-7.6657138145,4.4533199045,-2.4260944138
C,-1.2839823118,-0.5936141162,1.3442054009
C,8.301746847,2.6985335724,-1.1233096941
C,1.3121431362,1.3962893273,-0.5937912229
C,2.2927831159,2.1367778801,-1.3095314566
C,1.9136799718,3.0568585164,-2.3073902771
C,2.8888544857,3.7829882252,-2.985740506
C,4.2393042925,3.6018485845,-2.6974969521
C,4.6428743269,2.6876381026,-1.706790242
C,3.6584602937,1.9678844074,-1.0155475801
C,6.0633968743,2.4995752683,-1.4109311269
C,7.9262180267,1.4144242648,-0.7347347423
C,-0.4520126947,0.0456358177,0.719159042
C,0.4767458724,0.7567049659,0.0263175134
C,-2.2505082243,-1.3359470969,2.077070052
C,-1.8789616425,-2.0513242225,3.233131903
C,-2.8362736167,-2.7810539733,3.932571363
C,-4.1624709713,-2.80374792,3.5084277788
C,-3.5896878256,-1.3744097798,1.647152552
C,-4.5581337433,-2.0981511804,2.356892358
B,-10.9747093642,-0.2660000614,-0.7917821657
B,11.0355864075,-0.3292983364,0.4036222908

Cartesian Coordination of 4p-1

–2431.8298732 hatree

C,-4.0390490694,-0.5473581559,-0.4393615048
O,-10.1759820339,1.3898890066,0.0680388232
O,12.4676315384,2.2826989926,0.1624987878
C,-0.6788112081,-1.6957458933,-0.037999488
C,1.9011938479,-1.6956757135,-0.0387105372
C,0.6788193091,-1.6957583166,-0.0379569172
C,-12.9185987439,1.0572697122,0.0739659156
C,-12.0598845356,-0.0362104751,-0.0586824665
C,-10.6824576355,0.1852227141,-0.0196769587
C,-14.3511785354,0.9353901619,0.1462279331
C,-9.7085579791,-0.8739173468,-0.0488681544
C,-9.8106642769,-2.2679591322,-0.0796219629
C,-8.507584551,-2.7850629815,-0.0767467018
C,-7.6116204676,-1.7051049767,-0.0475665054
C,-16.4418811031,1.7289951482,0.3012780247
C,-16.5325071111,0.3430421919,0.2337279827
C,-15.2198009103,-0.1581570077,0.136995194
C,12.0599074745,-0.0363480573,-0.057792508
C,-5.4258503742,-0.5507325882,-0.4450825931
C,-6.1528358404,-1.6903654569,-0.0491280093
C,-5.4307789534,-2.8328141645,0.3474023312
C,-4.0450058409,-2.8395112651,0.3492019771
C,-3.3190030511,-1.6937688743,-0.0421521186
C,4.0449690108,-2.8394778426,0.3497713036
C,5.4307424035,-2.8327951936,0.3480984167
C,6.1528495425,-1.6904493577,-0.0486372747
C,5.4259114174,-0.5509059852,-0.4449374188
C,4.0391096409,-0.547514163,-0.439343898
C,3.319014317,-1.6938201937,-0.041920809
C,14.3512160976,0.9353656465,0.1463546125
C,16.5325587452,0.343068595,0.2338485765
C,16.4419291212,1.7290455785,0.3008800382
C,-1.9011851978,-1.6956457628,-0.0388274693
C,8.5075980953,-2.785166524,-0.0756464574
C,9.8106803881,-2.2680675679,-0.0785185216
C,15.2198452795,-0.1581779721,0.1374493052
C,9.7085746508,-0.8740166172,-0.0482126669
C,12.9186240555,1.0572054552,0.0741871694
C,10.6824794827,0.1851301542,-0.0192181038
C,7.6116335915,-1.7051973756,-0.0469142002
F,-10.8948523541,3.0906022487,-1.3750186096
F,10.8942274029,3.0917210296,-1.3741502931
F,-10.626947681,3.5390182504,0.8624943241
F,10.6272172921,3.5383218682,0.8638121834
H,-17.2149062471,2.4788192402,0.38125074
H,-17.44721313,-0.231303499,0.2533330341
H,10.7296182253,-2.8355375427,-0.1070976202
H,3.5045809092,-3.7263491848,0.6629719755
H,5.9672270529,-3.7165718568,0.6774865237
H,5.9480183199,0.3366792269,-0.7900378035
H,3.4956327102,0.3374628227,-0.7522296462
H,-12.4541615219,-1.0389985918,-0.1345556734
H,-10.7296018093,-2.8354154756,-0.1084794763
H,-8.0377311413,0.3846668127,0.0442260014
H,-5.9673063927,-3.7166631917,0.6765268601
H,12.4541786788,-1.0391835236,-0.1330564095
H,14.9287358588,-1.1965495371,0.0706365521
H,17.4472709105,-0.2312631232,0.2535734911
H,17.2149561806,2.4789062295,0.3804897625
H,14.7310640854,2.9978395749,0.2733568719
H,8.0377418735,0.3846006295,0.0442994601
H,8.2295347482,-3.8277278431,-0.1247002499
H,-14.9286872638,-1.1965008954,0.0697698514
H,-5.9479197313,0.3369383589,-0.7900191069
H,-3.504656231,-3.726463708,0.6622386447
H,-3.4955338911,0.3376875883,-0.7519855393
H,-8.22951447,-3.8276088053,-0.1260913554
H,-14.7310281561,2.9978124001,0.2740583724
N,15.1291051698,2.0701862428,0.2477095811
N,8.366786559,-0.5666965495,-0.0360506381
N,-15.1290658156,2.0701662654,0.2480997264
N,-8.3667691803,-0.5666048567,-0.0364544552
O,-12.4675695787,2.2827090321,0.162964154
O,10.1759748976,1.3898254304,0.0677861352
B,11.0165284701,2.6403662771,-0.0858655184
B,-11.0165972185,2.64030443,-0.086300404

Cartesian Coodination of 4p-2

-2431.8298895 hartree

C,1.8683460997,-0.3514766172,-0.4980410788
C,0.6670993154,-0.1251740005,-0.4983071716
F,-11.3853254997,-2.4337816174,2.0388101727
F,-11.5209459654,-3.0582474238,-0.1658899187
F,11.5216309223,3.0575683055,-0.1669335828
F,11.3852372486,2.4345990999,2.0381417148
H,-5.4586537558,3.2177101392,-0.3517249081
H,-3.0396651864,2.75995118,-0.3776593194
H,-3.839704383,-1.4610672063,-0.6220933461
H,-6.2490873008,-1.0097468769,-0.6506280302
H,6.2491391966,1.0101542409,-0.6506084619
H,-17.408172213,1.8974875876,-0.0124405754
H,-10.3356870896,3.0809585028,-0.8188797723
H,-7.7023161389,3.5451268837,-1.1052023676
H,-8.269609149,-0.4472095068,0.1402700085
H,14.7564903257,-2.3324096761,-0.3100540009
H,17.4079516537,-1.8984142627,-0.0117390676
H,17.6710191036,0.701738279,0.753083086
H,15.3226806621,1.6607933478,0.8762801474
H,-12.350411394,1.7224809626,-0.2907489851
H,-15.3225721682,-1.6616089243,0.8752592973
H,-17.671029707,-0.7028794268,0.7517190413
H,-14.7567099451,2.3319462133,-0.3100413746
H,3.8397850838,1.4616045913,-0.6219082017
H,3.0395135546,-2.7594189696,-0.3783152102
H,5.4584774274,-3.2173180327,-0.3525470045
H,12.3503126102,-1.7225274899,-0.2914498225
H,8.26966103,0.4473397384,0.1401203672
H,7.7020844781,-3.5447188746,-1.106108086
H,10.3354895078,-3.0807888911,-0.8197160414
N,15.5456620472,0.7106827438,0.6170545069
N,8.4236239748,-0.4981009152,-0.1793233591
N,-15.5456388477,-0.7114743777,0.6161954875
N,-8.4236383127,0.4982808876,-0.1789950168
O,12.9704341237,1.4149941451,0.6538916782
O,-12.9703319694,-1.4154407375,0.6533924082
O,-10.5506522516,-1.0036966593,0.3872528088
O,10.5507460811,1.0035834247,0.3873224499

C,-16.6128001481,1.1828511055,0.1412211681
C,-15.2309449003,1.4075236717,-0.0134643899
C,-9.5348548516,2.3759376734,-0.6489200288
C,-8.1614782871,2.6202828495,-0.7881391976
C,-7.4759396199,1.4328166581,-0.4880862935
C,-6.0461844481,1.1434619291,-0.4927757193
C,-5.1093265562,2.1932706167,-0.4276637169
C,-3.7470315422,1.9394803911,-0.4331781512
C,-3.2614732538,0.6154397405,-0.497337649
C,-4.1968529115,-0.4386368324,-0.5625473976
C,-5.5585969278,-0.1760364358,-0.5642964929
C,-1.8683706853,0.3520798675,-0.4979196848
C,-0.6671196804,0.1257975927,-0.4982601762
C,6.0461209356,-1.1430740459,-0.493185086
C,5.5586049767,0.1764656397,-0.5644249102
C,4.1968737778,0.439140231,-0.5625827258
C,3.2614375945,-0.6148939197,-0.4975622102
C,3.7469244327,-1.9389768885,-0.4336873935
C,5.1092034271,-2.1928439642,-0.4282654686
C,16.6126500054,-1.1836933299,0.1418963018
C,16.7749416443,0.1406057226,0.5331819075
C,-14.5749417973,0.2120890318,0.2878456743
C,-12.14484505,0.7003806715,-0.0084801979
C,-13.187413962,-0.1723049566,0.3093358212
C,-9.6858214044,1.0415022669,-0.2603246452
C,-10.8330759225,0.2281201779,0.0466778688
C,-16.7749821674,-0.1415651714,0.5321584618
C,10.8330831301,-0.2281545245,0.0463943209
C,13.1874293015,0.1719443453,0.309473156
C,7.4758570295,-1.4325141475,-0.4885809336
C,8.1613154204,-2.6199689033,-0.7888711933
C,9.5347084837,-2.3757427539,-0.6496194853
C,15.2307986415,-1.4081249609,-0.0131638097
C,14.5749062113,-0.212655902,0.2882509132
C,12.1448186105,-0.7004950622,-0.0088839838
C,9.6857687772,-1.04139305,-0.2607696078
B,-11.5941093134,-2.0410352878,0.745567308
B,11.594311583,2.0409439163,0.7452327512

Cartesian Coodination of 4p-3

–2431.8232615 hartree

B,11.6195211426,2.087973668,0.6022913646
B,-11.5936986903,-2.0463596107,0.5954952453
C,5.5651445326,0.2176309114,-0.5832519839
C,4.2035797315,0.4815257284,-0.5857335636
C,-16.736164796,-0.066637947,0.8178396186
C,-16.5826327688,1.2509424508,0.4007012534
C,-15.2103026891,1.4565936401,0.159681161
C,-13.1705752576,-0.1463405058,0.3743975547
C,-12.1414151926,0.6981341185,-0.0481151534
C,-6.0436564555,1.1694864727,-0.5257889901
C,-5.1098213681,2.222169577,-0.4639121228
C,-3.7467902431,1.972345744,-0.4708736046
C,-3.2575500535,0.6495954722,-0.5333934831
C,-4.1899009189,-0.4073320688,-0.5959593443
C,-5.5523882504,-0.1487204653,-0.5961928774
C,-1.8637495077,0.389918288,-0.5343090471
C,-0.6620576424,0.1660443024,-0.5338304133
C,0.6725267977,-0.0829867054,-0.5323912615
C,1.8740434931,-0.3077335937,-0.5303806539
C,3.2670305398,-0.5718250908,-0.5262403644
C,3.751024603,-1.8965015987,-0.4637172246
C,5.1130671337,-2.1515986162,-0.4540109039
C,6.050966875,-1.1024891126,-0.5130830123
C,8.1659577881,-2.5797378391,-0.8085061882
C,-9.6823435056,1.0565393917,-0.2848397989
C,9.5390395033,-2.3376990115,-0.6608273902
C,10.8342978028,-0.19176971,0.0550754027
C,12.1516354263,-0.6475370689,-0.0286713301
C,-7.4742727723,1.4545044638,-0.5184177869
C,-8.1643571374,2.6391120422,-0.8198181017
C,-9.5364933472,2.3908991723,-0.6760651624
C,-10.8252615997,0.2401175107,0.0282072741
C,-14.5513056998,0.2562950646,0.4343939148
C,16.8117639188,-0.3027139413,0.760276154
C,15.6829194622,0.537618868,0.8269416443
C,13.185090348,0.1870393544,0.4176644656
C,9.6900789651,-1.0057828424,-0.2642289591
C,14.5638357753,-0.2252337959,0.4983118349
C,16.3649007756,-1.564513003,0.3959889498
C,7.4805990304,-1.3934834597,-0.5035979453
F,-11.6342838257,-2.8129544495,-0.5401571083
F,-11.3119356226,-2.7426083481,1.7338645732
F,11.6714013988,2.8007040004,-0.5672255848
F,11.3279414516,2.8303735271,1.7063687124
H,-5.462066521,3.2456967437,-0.3891672682
H,-3.0417274561,2.7949483332,-0.4176161088
H,-3.8298307619,-1.4287960664,-0.6544822803
H,-6.2406827734,-0.9844751253,-0.6803509482
H,3.0426178966,-2.7163615087,-0.4126461064
H,-15.2834715048,-1.600771364,1.0897928651
H,-17.3774695435,1.9736042368,0.2869850006
H,-14.7437506486,2.3722376062,-0.1740151932
H,-12.355766372,1.7054531198,-0.3739915408
H,8.2747018672,0.4820743163,0.1387190973
H,7.7069831112,-3.5019549097,-1.1334214213
H,10.3387690685,-3.0445108682,-0.8288863213
H,12.3478085771,-1.6483185147,-0.3869862274
H,-8.2605603249,-0.4267458602,0.115650335
H,-7.7088269699,3.5646996693,-1.1399547712
H,-10.339897377,3.0937269135,-0.8429164433
H,-17.6238229696,-0.6141801157,1.0979489609
H,5.4611713883,-3.1765688623,-0.3792609962
H,6.256828626,1.0507792696,-0.6652555211
H,3.8476755289,1.5044444396,-0.6441432233
H,14.4286557258,-2.2980661291,0.0097239628
H,16.9076397843,-2.4857345574,0.2431052847
H,17.8389857106,-0.0289722316,0.9519145479
H,15.6517008803,1.5881452161,1.0734925612
N,-8.4181293217,0.5177127829,-0.2049942746
N,8.4279454593,-0.4623959641,-0.1844443869
N,15.0128747639,-1.5096861743,0.2354372327
N,-15.5108825467,-0.6507905381,0.8339636521
O,-10.5363429268,-0.9769414273,0.4170314881
O,10.5477220645,1.0185320943,0.4581357871
O,-12.9393826892,-1.3726874345,0.7693157609
O,12.9499627906,1.4051974509,0.8169547695

Cartesian Coordination of 4p-4

–2431.8156192 hartree

B,11.3980576922,-0.7950100892,1.9196544892
B,-13.5095998169,-0.7007052333,0.832100141
C,16.5627331447,0.212140026,0.2702903834
C,-11.1281448495,0.60218016,-0.0163289691
C,-0.8576555822,-0.774428782,-0.3494945943
C,0.4690588656,-0.5498482541,-0.5300617317
C,1.6634762887,-0.345894336,-0.6912147326
C,3.0495385733,-0.1090573503,-0.8728031849
C,4.0104900459,-0.9051728159,-0.2147206842
C,5.365359684,-0.669628463,-0.3936074524
C,5.8198844764,0.3709082175,-1.2272248837
C,4.8575321353,1.1627093975,-1.8836727168
C,3.5020094749,0.9291011447,-1.7156474947
C,7.2420654528,0.6338402257,-1.4173906339
C,7.9075408165,1.3264552724,-2.4406482168
C,9.2823596926,1.286888987,-2.1687768654
C,10.6101970624,0.2257191151,-0.1951918647
C,14.9931285459,1.028084729,-1.126934752
C,12.9704088175,0.1223826724,0.2380197386
C,11.9099829188,0.6038862481,-0.533726729
C,14.3537121584,0.3606835051,-0.0798289643
C,16.3805354692,0.9340159644,-0.9042563897
C,9.4536407521,0.5754385136,-0.9775836305
C,-6.2080095615,-1.6560180949,0.4049434153
C,-5.754413899,-0.6522339218,-0.4730199888
C,-4.3997567621,-0.4252795323,-0.6660065002
C,-3.4376273311,-1.205579971,0.0089963625
C,-3.8893166879,-2.2205110957,0.8805447139
C,-5.2447104282,-2.4352638738,1.0746370901
C,-2.0519443004,-0.9760377211,-0.1846450877
C,-11.0603198469,-0.6628473327,0.5824241696
C,-12.480870526,2.6770535204,-0.4124401266
C,-11.91495965,4.6973971247,-1.2180171924
C,-13.2894412434,4.6992077676,-1.0332421203
C,-13.6452067443,3.4337332912,-0.525387461
C,-12.33338137,1.3172493009,0.0450274877
C,-9.674992661,-2.7442990547,1.1107341122
C,-8.3033066606,-3.039579883,1.061894897
C,-7.6301396573,-1.8944369098,0.6243787957
C,-9.8395866157,-1.421706715,0.702365051
F,11.2502318147,0.1063161612,2.9414424447
F,-14.2525248924,-0.8733734834,1.9584174097
F,11.2717966505,-2.0991964882,2.2970185471
F,-14.0050070279,-1.3197292799,-0.2853880226
H,15.1304556071,-0.6487604123,1.591217188
H,2.774496335,1.552320586,-2.2245513913
H,7.4357110016,1.7751111738,-3.3024684288
H,10.0713286334,1.7142083419,-2.7705945416
H,8.061982853,-0.2936357816,0.3224110999
H,12.0969196063,1.2084962705,-1.4091439061
H,14.5040918902,1.5216188495,-1.9543811048
H,17.1667803139,1.3413711604,-1.5229670909
H,17.4687959053,-0.0756354544,0.782572354
H,-8.3687782578,0.0393585672,0.237924382
H,-7.8406456486,-3.9918045564,1.2766558629
H,-10.4856710819,-3.4037624701,1.3815414661
H,-10.4615575706,3.2223706828,-0.8337207425
H,-11.2528611354,5.4702199656,-1.5799259019
H,-13.9528411237,5.5246035752,-1.2464601735
H,-14.6307334166,3.074093428,-0.2709339913
H,-10.2600628625,1.0227969304,-0.5061061359
H,-6.4703903045,-0.0647817028,-1.0410551079
H,-4.067862616,0.3479903071,-1.3505560247
H,-3.1608078774,-2.8259868352,1.4089762355
H,-5.5693877461,-3.2016508859,1.7707325613
H,3.6787125376,-1.7132174015,0.4282678867
H,6.0775269669,-1.3229707078,0.1017048197
H,5.1812427893,1.9831634248,-2.5155820778
N,8.2026945823,0.1878089879,-0.5539664845
N,15.3399603154,-0.1253981019,0.7534820476
N,-11.4356028994,3.4757877766,-0.8487462267
N,-8.5825587485,-0.932766107,0.3926456031
O,-13.4077284403,0.787135307,0.5521082829
O,-12.1130870612,-1.2302582386,1.0960541847
O,10.352760226,-0.5014577082,0.8634540067
O,12.7705707986,-0.6064977322,1.3066400418

Cartesian Coordination of 4p-5

–2431.8088495 hartree
C,11.0384430277,0.3047367038,-0.131432545
C,9.6151797881,-1.7538136716,-0.0281304977
F,-13.6507280197,1.5947219174,1.3569766091
F,13.696050177,-1.5763167192,-1.2885535765
F,14.1318946626,-1.9658173607,0.9372699184
F,-14.0776073306,1.9802280533,-0.8697375762
H,3.9191253025,0.9858899599,-0.8642070074
H,-10.5970502444,-3.3914630085,0.1326645926
H,-10.0424405519,3.8780665413,0.116466332
H,-7.3505373017,4.2011407161,0.1412560665
H,-5.2100310392,3.4707532793,-0.7824631334
H,-2.8309292262,2.8287527043,-0.7888134791
H,-3.8664788275,-1.032291147,0.8034227581
H,-6.2317401892,-0.3749230746,0.8700498192
H,6.2883141009,0.3363480602,-0.9142513337
H,2.8880040808,-2.8760484767,0.7279826401
H,5.2697587482,-3.5090945253,0.7388516613
H,14.2229380227,5.1533256704,0.1465324315
H,11.515237063,5.3951817895,0.0283671269
H,-10.1347005175,-0.9567553784,0.3152903886
H,-14.7269339146,-4.6640818925,-0.256149673
H,7.4280378578,-4.2283719542,-0.1808600747
H,10.1174111883,-3.8861133209,-0.1132088094
H,14.7294026336,2.4782918074,0.183399211
H,10.1856993027,0.9239900852,-0.3760907704
H,10.5661815589,3.0857888077,0.033251453
H,8.2590904043,-0.1290563581,0.1555882181
H,-14.5879743588,-2.1277474179,-0.2505828332
H,-8.2159801237,0.1025701662,-0.1449328712
H,-12.1750986715,-5.5810664912,-0.0082609359
N,-8.3379733258,1.0861678471,0.0359080195
N,11.5569187919,3.2635909931,0.0296100592
N,-13.796474897,-2.7502777817,-0.1739736668
N,8.3919666257,-1.1070644043,-0.0455980928
O,11.9158982118,-1.8579194026,0.2115238238
O,13.3528785348,0.1337968457,0.2776268703
O,-13.3129432822,-0.1223529577,-0.2013919564
O,-11.8633758664,1.8620715472,-0.138228789
C,4.2182299341,0.0048672324,-0.5108927793
C,3.2297012098,-0.8954885473,-0.0611803226
C,3.6369699518,-2.1747332924,0.3761175948

C,4.9763506766,-2.5308813901,0.3723114376
C,13.5005283685,4.3506385507,0.1213184393
C,12.1235945063,4.5031322974,0.0559992477
C,-12.5032128836,-2.2870877147,-0.049552635
C,-10.983610972,-0.3112372058,0.1389151633
C,-12.2546773821,-0.8687073446,-0.0283747012
C,-9.5565033865,1.7411019801,0.0361456086
C,-10.8352220195,1.075657153,0.0201445031
C,-13.8054851172,-4.1075614494,-0.1702387491
C,10.8909513171,-1.081305328,0.0102356127
C,12.3044673196,0.8752329731,0.0688846647
C,7.3712243499,-2.025463179,-0.0692693657
C,7.9619636916,-3.2925964327,-0.1020474852
C,9.3553581884,-3.1223981843,-0.0756579144
C,13.7678303475,2.9673436345,0.1437273609
C,12.5479820476,2.2963480495,0.0871254717
C,-5.9083500814,1.5969293975,0.0324876174
C,-4.9180629846,2.490771473,-0.4195665951
C,-3.5801651125,2.1296733378,-0.4330581201
C,-3.1749032524,0.848532445,0.000413744
C,-4.1638140508,-0.0492588957,0.4543272103
C,-5.4998736339,0.3228320567,0.4729611468
C,-1.8073038213,0.4746620696,-0.0158623947
C,-0.6281825299,0.1527197684,-0.0280502264
C,5.9663170282,-1.6337211217,-0.0736065953
C,5.5557560192,-0.3623349068,-0.519834413
B,13.3358506525,-1.3604463218,0.0157411159
C,1.8611513486,-0.5249122791,-0.0509268115
C,0.6817781526,-0.2038450539,-0.0406780606
C,-12.4932427237,-4.5492847584,-0.042010907
C,-11.6728735217,-3.406863281,0.0329934383
C,-9.2864750167,3.108673776,0.0728105744
C,-7.892317776,3.2688312333,0.0765864756
C,-7.3110013024,1.9965737285,0.0418739856
B,-13.2813526684,1.3771068528,0.0552962755

Cartesian Coordination of 4p-6

–2431.8010409 hartree

B,13.2211537335,-0.4824887594,0.0339274703
B,-13.2208755197,0.4855040879,0.0337728041
C,10.7570148179,1.8215689394,4.9824664167
C,-10.6107187369,-0.0355051726,1.02908604
C,-0.6751025011,0.0677720185,-1.9512172101
C,0.675184049,-0.0738374151,-1.9511133586
C,1.8908492295,-0.2014159586,-1.9517961594
C,3.3010325776,-0.3490630993,-1.9517402498
C,4.0205412623,-0.4334251297,-3.1636804473
C,5.3995728703,-0.5716951822,-3.1597471141
C,6.1205323049,-0.6395656459,-1.9516697756
C,5.3987932216,-0.5655412301,-0.7443108402
C,4.0195700638,-0.4185077563,-0.7397618743
C,7.5715831468,-0.7859582979,-1.9670528941
C,8.4224533341,-1.3028923688,-2.9491543235
C,9.7397072705,-1.2159625776,-2.4712281552
C,10.7867061963,-0.3612272799,-0.3026220445
C,12.6994222433,1.2873051469,3.9766440674
C,11.7338569628,0.4297746821,1.7726973615
C,10.6106686856,0.0373774442,1.0288769242
C,11.6587768474,0.9913701074,3.0987611966
C,12.1325771403,1.804928308,5.1583358502
C,9.6933599228,-0.6481719733,-1.1991137485
C,-6.1203105083,0.6348413202,-1.9525996574
C,-5.3985580561,0.5627200806,-0.7451339183
C,-4.0193844494,0.415225082,-0.7403683256
C,-3.3009105285,0.3433835235,-1.9522447008
C,-4.0204348255,0.4257875045,-3.1643100206
C,-5.3994193269,0.5645369236,-3.1605778108
C,-1.8907664517,0.1953604203,-1.9520827843
C,-10.7865668937,0.3615168721,-0.3029121636
C,-11.6593902262,-0.9857462227,3.1003761797
C,-10.7580114667,-1.8150446733,4.9846592419
C,-12.1334169874,-1.795431205,5.1614171704
C,-12.7000347989,-1.2784172918,3.9793417806
C,-11.7341866446,-0.4257698943,1.7736062976
C,-9.7392280141,1.2120902576,-2.4729777132
C,-8.4219701907,1.2974499898,-2.9511582185
C,-7.571303751,0.7817997771,-1.968199557
C,-9.6931095675,0.6463715391,-1.1999259046
F,13.4878779517,-1.7741376286,0.4052924711
F,-14.2189589078,-0.1301165777,-0.6547752398
F,14.218593772,0.1330025279,-0.6556628739
F,-13.4863892217,1.7779474471,0.4032267906
H,9.5579993785,1.275675329,3.3391498559
H,3.4789114097,-0.369979851,0.1994199938
H,8.1040786123,-1.7337861984,-3.8871771577
H,10.6448093672,-1.5453107216,-2.9588073275
H,8.0345606715,0.1454101832,-0.1353508519
H,9.6225507432,0.055454417,1.4692225466
H,13.7437832869,1.1220531514,3.758976103
H,12.6585396133,2.1291445534,6.0443785884
H,9.967514635,2.1495912279,5.6425440683
H,-8.0345979495,-0.146005694,-0.1347678787
H,-8.1034253125,1.726551567,-3.8899441853
H,-10.6441890414,1.5410851262,-2.9610560797
H,-9.5590974753,-1.2743827273,3.339525106
H,-9.968727822,-2.1437703725,5.6446459315
H,-12.6594272983,-2.1172980218,6.0482882542
H,-13.7442094728,-1.1113581232,3.7621567665
H,-9.6225962655,-0.0538476788,1.4694117579
H,-5.9184985088,0.6609187652,0.2036928387
H,-3.4787095105,0.3682093435,0.1988810052
H,-3.4814230405,0.3681021322,-4.1038342329
H,-5.9351260101,0.5986323628,-4.1035290184
H,3.4814785013,-0.3776063765,-4.1032881951
H,5.9352579503,-0.6072929938,-4.1026548591
H,5.9188052861,-0.6618452625,0.2046705997
N,8.3612701562,-0.4137439993,-0.9069062671
N,10.4782498773,1.3244644811,3.7440832844
N,-10.4790789034,-1.3201177337,3.7454339066
N,-8.361124584,0.4117554815,-0.9074039509
O,-12.9356675264,-0.3231918145,1.2858445594
O,-11.9720959143,0.4787040269,-0.8273230711
O,11.9722611871,-0.478110589,-0.8270346051
O,12.9353459641,0.3278234165,1.2848066811

Cartesian Coordination of 4m$_2$·Cl$^-$$_2$-1 (AM1)

–1.6411702 hartree

B,1.8168670669,0.7351207419,12.0405139236
B,-1.5049846386,-2.0743518781,-11.926847816
B,10.4597697616,3.2066646163,4.9297967794

B,-10.6138825605,-2.5445678915,-4.9851997016
C,-0.1066868837,-3.159421596,-7.8832895709
C,2.9418797808,-1.1864724912,5.0288749639
C,4.2677632521,-0.8252756784,4.7487873704
C,4.7541430543,-0.9174264119,3.4455991648
C,3.930188939,-1.3495328106,2.4102011723
C,2.5949416809,-1.6982153564,2.6770037136
C,1.7410359083,-2.0797983864,1.6276894404
C,2.1083883074,-1.6248250404,3.9909466822
C,4.71804092,4.0637498758,11.9906452567
C,3.3697098998,2.1706095726,10.8684308943
C,2.9863890873,1.585724327,9.6574804337
C,2.2585425682,0.3926388292,9.6890405193
C,4.3640393272,3.2158522258,10.9101158847
C,2.0856875135,-0.4072493638,8.4991041449
C,5.7534676092,4.9175432679,11.529273466
C,6.0136195298,4.5637751874,10.1818106912
C,2.4068365909,-1.1096357564,6.3781243242
C,1.3824176724,-1.9216069774,6.9450940713
C,1.1891266199,-1.4850753887,8.2775786529
C,0.1655836637,-2.6501155581,-0.2971701953
C,-1.9323198164,-3.1457341421,-4.6611364253
C,-3.291518234,-3.3640437832,-4.3931788619
C,-3.7362292084,-3.4505841107,-3.0748105885
C,-2.8454833339,-3.3049225955,-2.015087941
C,-1.4838659466,-3.0693731366,-2.2722938258
C,-0.5889373131,-2.8636840531,-1.2080538104
C,-1.0303631862,-3.0010190463,-3.5982710447
C,-5.573065778,-0.3982564418,-12.3019378676
C,-3.5731449861,-1.3001398274,-10.942428003
C,-3.0173958749,-1.4552014177,-9.6686366546
C,-1.8387810193,-2.1951204414,-9.536074971
C,-4.9232298962,-0.8196171898,-11.1136773638
C,-1.3766283733,-2.635949224,-8.240796955
C,-6.8947421798,-0.0246557495,-11.9448222743
C,-7.023193219,-0.2363491157,-10.5494082802
C,-0.1381344148,-3.4170799068,-6.4918661181
C,-1.4354645072,-3.0586441212,-6.0242872503
C,1.0038767482,-2.368101427,0.7231996396
C,-8.9018589871,-3.1037717645,-6.5965327201
C,8.0491118243,3.3161227133,4.8112254165
C,7.9693961382,2.8046695411,6.1089245869
C,9.1076285987,2.2197794093,6.6727404381
C,-7.604079757,-0.4398420825,-4.333345515
C,-8.4240897312,-3.9698718371,-7.6469955931
C,2.5804655474,3.4677082112,4.8767117684
C,-0.2811415068,2.8376418788,0.332361626
C,6.8584707371,3.6426068008,4.0613591222
C,9.019192046,1.4128295104,7.8655728827
C,1.1992694867,3.2888067168,4.935402775
C,0.4503616788,3.1617446178,3.7689670827
C,1.0892561442,3.2143023964,2.5181674382
C,0.3484044448,3.0313197594,1.3377099417
C,2.4769285514,3.4116849303,2.4558547728
C,3.2263856071,3.5372964081,3.6336388368
C,6.7570226754,4.276718691,2.7954402281
C,5.3817969153,4.3342915641,2.465752564
C,4.6638166344,3.7289571246,3.5372964192
C,8.0666569531,0.249342263,9.5418398546
C,9.4701189323,0.1437308157,9.7089458669
C,10.0706494393,0.8728378155,8.6502105744
C,-3.6286304388,1.5361268251,-2.87717395
C,-4.3129590816,1.129637695,-4.0309081982
C,-7.838353918,0.3683556688,-3.1901571855
C,-6.6412329194,1.0756350233,-2.9257848739
C,-5.6911390189,0.6836745773,-3.9126207909
C,-6.9962169653,-4.8497121124,-9.1496487609
C,-8.2037274794,-5.5856905283,-9.2446720351
C,-9.1020750535,-5.0345801951,-8.2947183079
C,-8.5018256438,-1.3712880101,-4.9759768712
C,-8.1573758917,-1.9969513227,-6.176753056
C,-0.9792678627,2.5791794272,-0.7942313662
C,-2.3357689447,1.5910408704,-5.3512849044
C,-1.6508654563,1.9941657475,-4.2084847701
C,-2.2938667286,1.960617384,-2.9591396391
C,-1.5921904409,2.3130420202,-1.7932607088
C,-3.6564660188,1.1524857988,-5.270181773
F,2.1189334132,-0.0727057418,12.977363042
F,-11.4698180732,-1.7997967791,-5.5714670815
F,-11.0471483131,-3.307828906,-4.0629785963
F,11.218188817,2.5739199012,4.1265437021
F,10.8795619731,4.334768024,5.3566329667
F,-1.3862899207,-3.0710014422,-12.7104995181
F,0.7073069354,1.3574191457,12.1460922934
F,-0.7785093123,-1.0537058504,-12.1719197637
H,0.8631571891,-2.7268979824,6.4362153945
H,6.7468984317,4.9815436036,9.4891072669
H,6.2596461077,5.6941884635,12.0914419532
H,3.3018386369,2.0234745263,8.6990846287
H,4.2609579819,4.0392799078,12.97608576
H,1.0637856367,-1.8974530922,4.2059033208
H,4.3154827066,-1.4083173483,1.3816790464
H,5.7964817751,-0.6344271391,3.2331153623
H,4.9289514648,-0.4576190188,5.5513347483
H,-6.0686289874,-4.9719171752,-9.7126483967
H,-6.4639423968,1.7904101853,-2.1290490074
H,-8.775590826,0.4107350257,-2.6412925106
H,-4.1359864655,1.5066580012,-1.900674758
H,-0.6049180609,2.3274439162,-4.2763451879
H,-1.827250299,1.6069406585,-6.327328291
H,-6.4176669147,-3.2143939839,-7.8883387831
H,-5.8405646864,-0.702173619,-5.5482971677
H,-4.173162676,0.8145217005,-6.1839079438
H,-5.6414782199,-0.9886412236,-9.0867141924
H,-3.1524065317,-2.287881421,-7.0663874479
H,0.7174455321,-3.3174450738,-8.5740067366
H,0.6626882418,-3.8194678358,-5.8804327661
H,-7.8907820716,-0.0785063839,-9.9056337689
H,-7.6692368973,0.3497035878,-12.6047018402
H,-3.5286980163,-1.0536371056,-8.7815165997
H,-5.115250312,-0.3765916643,-13.28710391
H,-0.6374745452,3.0082453268,3.8212674565
H,0.6991314537,3.2358881662,5.9144668005
H,6.8772468944,1.2389510662,8.0565967124
H,5.3447374399,2.8314190359,5.3673528382
H,3.1583488529,3.5419076493,5.8130023126
H,-10.1210606238,-5.3444781658,-8.0792801527
H,-8.3924090077,-6.4120685239,-9.9206750274
H,-7.2722611203,-1.6681629127,-6.7460364762
H,7.0092348319,2.79877878,6.650778705

H,11.1295953615,1.0114149645,8.4496835702
H,9.9766374092,-0.3957027828,10.5013673414
H,7.2662646037,-0.1754780137,10.1511230163
H,4.9388959712,4.7607442646,1.5718282984
H,7.6004380014,4.6375006228,2.2123931234
H,2.9820103243,3.452002783,1.4785653297
H,0.0350282511,-2.8175713893,-3.8056610761
H,-3.2038818704,-3.3614980238,-0.9767654835
H,-4.8040561232,-3.6242432286,-2.8716021786
H,-4.0165569215,-3.457908879,-5.2189721376
H,5.158365266,3.057903499,8.9108239336
H,3.570482798,0.4926466515,7.2186948943
H,0.4930817317,-1.8762974881,9.014955003
N,5.173861194,3.5443649929,9.8085966479
N,2.8252327149,-0.195487375,7.3266796933
N,5.5665585536,3.3210030426,4.5016962181
N,-5.8355783943,-0.7089429945,-10.0495080362
N,-7.1305791804,-3.8766207698,-8.1913233494
N,-6.2867076842,-0.2278417533,-4.7645908287
N,-2.1772096345,-2.5861457324,-7.0906132389
N,7.7964381124,1.0149881113,8.4354487188
O,-9.6243819048,-1.6601697317,-4.3386624377
O,-2.9155996918,-1.6508343703,-12.0345226125
O,2.8929373972,1.7463878566,12.0263433996
O,1.7529948121,-0.0839255339,10.8140332848
O,9.2075731442,3.4507346995,4.1870400079
O,-1.1335970924,-2.5741126368,-10.5883976629
O,10.2958229243,2.3228546911,6.1014051614
O,-10.0352796072,-3.4421135813,-6.0051364356
Cl,5.0938896215,1.8973193217,7.2190817901
Cl,-5.1368359061,-1.7151855788,-7.2345158302

Cartesian Coordination of $4m_2{\cdot}Cl^-_2$-2 (AM1)
–1.640936 hartree
C,-0.6785623758,-0.9410443714,-6.6936365958
O,-1.5160752725,-0.7733828182,10.3561358339
O,3.3412206634,-0.3671394008,-11.5703202545
O,1.509454287,0.7716234709,-10.358415548
O,-2.1303208848,9.2312066586,7.9397649932
C,0.5244752728,-6.2006311399,-10.989556627
C,0.3792729193,-7.5246883019,-11.4735109043
C,0.8120586229,-8.3948986546,-10.4393576799
C,2.6119852095,-7.4125359783,-5.8986389253
C,1.8385935018,-7.0642796047,-7.0101753946
C,2.800938217,0.1326614801,-0.1637053444
C,3.3760966227,-2.9242486616,-3.9134503875
C,3.2219404173,-2.3509162125,-2.64383907
C,3.2310524323,-0.956158208,-2.4933099876
C,3.5435601883,-2.0967910692,-5.033369376
C,5.6985086029,-3.9572405392,-11.6182579062
C,0.3787434711,-0.2928238594,-8.5808313711
C,4.0089972858,-2.5556707243,-10.9915037539
C,1.2967214349,-0.3523186791,-9.6942771329
C,-3.0827889163,1.4588220577,10.8712185016
C,1.0594457665,1.7527510433,5.5520142509
C,0.4832749754,-0.7682672837,8.2033690419
C,1.1503461595,-0.363267841,7.022582006
C,0.6758074406,0.9393371869,6.6937453042
C,-5.0185937158,4.5111286812,10.5049728963
C,-5.7011708964,3.9586497385,11.6174125031
C,-5.0706138784,2.7241805275,11.9205211793
C,3.415710009,-0.1365582891,-3.6204820652
C,3.5705952096,-0.7116990134,-4.8784294799
C,3.5677331103,-6.6127131536,-3.6377835004
C,3.7715450324,-5.3300866454,-3.0748788195
C,3.3531524064,-4.3718127091,-4.0427281102
C,1.719136261,-7.9815551837,-8.0585944253
C,-1.3020174866,0.3507483207,9.6927658952
C,-1.9920499794,1.5267127198,9.9991369354
C,3.018471643,-0.3763816482,-1.2305640439
C,1.2018126751,-7.5808906225,-9.3451824269
C,1.0016719671,3.1532561935,5.6029199297
C,2.5171694302,0.7166171515,1.0203101326
C,-0.3835001552,0.2910501884,8.57978571
C,-4.0127302559,2.5559102783,10.9903834927
C,1.382712247,3.907509542,4.4943667332
C,1.807532304,3.2836573173,3.324964771
C,1.8543272753,1.8803165554,3.2572632263
C,2.2300218604,1.2466015245,2.0601393567
C,1.487742918,1.1191917798,4.3772600858
C,1.9876087761,-1.5278564941,-10.0003151245
C,3.0779883073,-1.459465506,-10.8728391316
C,5.0665641252,-2.723659946,-11.9220642209
C,-1.8047446385,-3.2842452577,-3.3222190595
C,-2.2293525416,-1.246833401,-2.0587492387
C,-1.8535377507,-1.8809146234,-3.2556327876
C,-1.4888048998,-1.1201901055,-4.3764958833
C,-1.060327386,-1.7540918082,-5.551015523
C,-1.00058159,-3.154552796,-5.6008325284
C,-1.3798069725,-3.9084341413,-4.4913936421
C,-2.5167726825,-0.7165237769,-1.0191602594
C,-3.5623170444,6.6142570915,3.637541747
C,-3.7674080191,5.3318451523,3.0746069667
C,-3.350905999,4.3731168832,4.0428007959
C,-0.5234276335,6.200977447,10.9917794388
C,-0.3761148402,7.5251641063,11.4747251301
C,-3.0120708399,6.4203557978,4.9315066112
C,-1.1983808206,7.5810613394,9.346272593
C,-2.6071321383,7.4131235075,5.8989470329
C,-1.8356690822,7.0639097027,7.0115095498
C,-1.7146641815,7.981715519,8.0592498126
C,-0.8073596562,8.3952738304,10.4398465204
C,-3.2208878857,2.3519221922,2.6442413768
C,-3.0185392478,0.3770289378,1.2313420266
C,-3.2315272,0.9571602131,2.4938495416
C,-3.4180913913,0.1379048105,3.6209584586
C,-3.5733380454,0.7133553528,4.8787261266
C,-0.4895961012,0.7654114777,-8.2050238689
C,-3.5448046301,2.0984367954,5.0335474927
C,-3.3754282753,2.9255655945,3.9136661155
C,-2.8007981567,-0.1322559815,0.1646412538
C,3.0162810086,-6.4194041372,-4.9313172514
C,-1.1554330394,0.3604344037,-7.0235180076
C,5.017066592,-4.5094679767,-10.5049867386
Cl,-1.9084909967,3.9434458685,7.878587976
Cl,1.9087312592,-3.942785362,-7.8768572752
F,-1.628835166,-0.6243450971,12.5720982448
F,-3.6227773086,10.4269122242,6.8649082044
F,3.0801854625,1.8096227308,-11.4854477232
F,-3.0886501063,-1.8106739128,11.4812439818

F,1.6209547606,0.6207606741,-12.574340488
F,3.6314031694,-10.4249259412,-6.8661921615
F,-1.605107335,10.3018488189,6.063432356
F,1.6139668496,-10.301879638,-6.0638309375
H,0.8491448776,-9.4807557126,-10.4510619844
H,0.008651315,-7.8064327664,-12.4526204289
H,0.3086943157,-5.2558204187,-11.4922357821
H,-0.7759146307,2.1994893995,7.6537459526
H,1.2564719206,-5.436032346,-9.1200441275
H,-3.3612768792,3.79338563,9.3471880068
H,2.561897528,-4.6179962003,-6.0276929235
H,-5.2069326189,5.447943112,9.9766673353
H,1.5209476509,0.0199319036,4.3287015898
H,2.0955809451,3.8830891448,2.4489353604
H,1.3353931878,5.0061561717,4.5417905007
H,0.6453139908,3.6665182369,6.5115032345
H,-1.7250148512,2.4770715243,9.50852447
H,4.1765556096,-5.099865194,-2.095049795
H,3.7791627154,-7.5803610371,-3.1903255406
H,-3.0752179818,2.998496514,1.7653553896
H,-0.8425922067,9.4812033839,10.4506563564
H,-1.3830625238,6.0642432978,7.0868589647
H,-0.0051967761,7.807052124,12.4536795205
H,-0.3092797207,5.25619524,11.4952051399
H,-4.1719607933,5.1020422266,2.0944887564
H,-3.7721099904,7.5821612977,3.1898646147
H,-1.3309589597,-5.0070518276,-4.5379467343
H,-0.6441410157,-3.6680310631,-6.5092742195
H,-1.5235799422,-0.0209379006,-4.3288256022
H,-2.0913100737,-3.8833583031,-2.4454868841
H,5.3189635213,-2.0187881103,-12.7095879766
H,6.5426672343,-4.4035534334,-12.1317176126
H,5.2066584244,-5.4456390481,-9.9759838288
H,-1.8968920499,0.9205770514,-6.4634623008
H,-1.256648177,5.4359694346,9.1230221516
H,0.7752416832,-2.1994236192,-7.6528530346
H,3.3597213958,-3.7923994787,-9.3468028252
H,-2.5606180495,4.6184242594,6.0281603183
H,-0.5977314263,1.7017919214,-8.7463016831
H,-3.6456787582,2.5347705931,6.041395143
H,-3.7082847998,0.0699937586,5.7616946122
H,-3.4288988165,-0.9559204077,3.5059304733
H,1.7215364826,-2.4781818322,-9.509185017
H,3.7040677817,-0.0680995508,-5.7614462342
H,3.4253274066,0.9572631303,-3.5053403437
H,-5.3241421152,2.0188878895,12.7073048197
H,-6.5451354905,4.4053847667,12.1308260636
H,1.8910674367,-0.9241201671,6.4622587576
H,0.5895291651,-1.7053547195,8.7437976365
H,3.6440925611,-2.5329155098,-6.0413480527
H,3.0777744829,-2.9977332379,-1.7648840676
H,1.3834391387,-6.0657322061,-7.0842798335
N,-0.2464867556,1.3292142729,7.6470256946
N,-1.0127797019,6.2357070615,9.7099594979
N,0.2438456901,-1.3303461972,-7.6470484933
N,1.0139195048,-6.2355607358,-9.7077906389
N,-4.0016608038,3.6689217639,10.1308422634
N,2.8963032682,-5.041485531,-5.1622257685
N,3.9994686313,-3.667992856,-10.1310463438
N,-2.8939552894,5.0423031975,5.1625722332
O,3.0565344592,-8.6447274885,-5.7195613492
O,-3.0490038468,8.6460891749,5.7186761932
O,2.1375178283,-9.230238917,-7.9401835323
O,-3.3473936901,0.366300543,11.5679029466
B,-2.3839433104,-0.7526441971,11.5501931201
B,2.6003247678,-9.7176042968,-6.6252884467
B,2.376539954,0.7507838126,-11.5530119476
B,-2.5922389654,9.7186025905,6.624575152

Cartesian Coordination of 4m·Cl^-_2-1 (AM1)
–0.9132048 hartree
C,-0.0066395848,-0.0285200806,0.6746092925
Cl,-0.2510387398,0.0867759822,9.5798618901
Cl,0.2467333869,-0.0855695097,-9.5801986497
F,-2.3827143324,-6.0725222329,-11.2569189618
F,2.3884755593,6.068939622,11.2579715501
F,0.2398657645,6.3717596602,11.1714064882
F,-0.2334735352,-6.3712895975,-11.1718745063
H,-0.3342034263,-0.7403893523,13.5503131536
H,1.2012455802,5.347259725,6.8104257789
H,0.3714186164,1.9597026245,3.5458863904
H,-0.1102256322,-1.4474868809,-8.2617810972
H,-0.1057861454,0.6547809448,11.3995032125
H,0.1009932325,-0.6536959301,-11.3997285418
H,0.1084276201,1.4482069342,8.2616946247
H,-0.0826731561,-0.3897867042,7.183753536
H,-0.5319517225,2.2710192498,10.0973811121
H,-0.5919588022,-3.4007479466,-14.6447768606
H,-0.1034719092,-0.9155855447,-15.6932464829
H,-0.4414868594,-2.2846704966,3.3178998036
H,-0.4686953646,-2.4032584678,5.8112853624
H,0.3255527112,0.7421217448,-13.5505750806
H,-0.935192004,-3.6778516456,-4.6661613543
H,-1.1925417678,-5.349325868,-6.8101224476
H,-0.3699096599,-1.9598880665,-3.5458302416
H,0.4360336942,2.2858041116,-3.317907689
H,0.4630596573,2.4044038656,-5.811297576
H,0.0803685184,0.3903193002,-7.1837401003
H,0.5313217555,-2.2691556946,-10.0980597943
H,0.5904756708,3.4008246767,14.6447340404
H,0.0967076329,0.9166540735,15.693109048
H,0.9422342018,3.6759836272,4.666468302
N,0.3181638918,2.2290363566,7.5958761627
N,0.0184361104,-1.0315383395,-12.3771798555
N,-0.0230743088,1.0326019522,12.3769596363
N,-0.3173951473,-2.2289640069,-7.5959456249
O,1.0725191602,4.500459886,12.0456541538
O,-1.0702614298,-4.5015009279,-12.0454006596
O,1.2527885391,5.0929698348,9.6543039226
O,-1.2477537579,-5.0945214793,-9.6539732528
C,0.2637179409,1.381453303,-3.918625728
C,0.2772548597,1.4434234318,-5.3084176036
C,0.0589986942,0.3018686903,-6.0782576756
C,0.6335069857,3.9586943865,9.3623332236
C,-0.276854329,-2.3671468439,-12.6963096114
C,-0.4602169951,-3.3818452206,-11.6864658647
C,-0.6216492864,-3.540305608,-7.9799811389
C,-0.0889713375,-3.1441444603,-10.3599126435
C,0.2746011784,2.3676610863,12.6961622081
C,0.4605607066,3.3819478389,11.6863743732

C,0.3666735479,2.4833864834,14.108873468
C,0.1133835846,1.1972840431,14.6468559837
C,-0.1157507649,0.3281370797,13.5465577734
C,0.4179158233,2.1442455648,6.2210366667
C,0.7890483772,3.4270795428,5.7107298308
C,0.9240580701,4.2970677445,6.8155659034
C,0.178868056,0.9332341871,5.4526818189
C,0.1901005472,0.9991689505,4.051082589
C,-0.0167948151,-0.0795460948,1.8757093106
C,-0.1789855863,-0.9331642477,-5.4526599205
B,1.2319143663,5.5734742963,11.047262927
C,-0.1901241474,-0.9990814028,-4.0510530378
C,0.0149484141,0.0800045743,-1.8757005475
C,0.0048262981,0.0289808808,-0.6746007553
C,0.6250362517,3.5397467772,7.9800054685
C,0.0897867081,3.1448681845,10.3595835483
C,-0.3695791319,-2.4829333319,-14.1089690421
C,-0.119014556,-1.1963160745,-14.6470030982
C,-0.030764488,-0.1516125209,3.2798417075
C,-0.2676683484,-1.3806131195,3.9186267402
C,-0.2812915344,-1.4425821925,5.3084186737
C,-0.6303921129,-3.9591022867,-9.3623567769
C,0.109122904,-0.326816743,-13.5467760998
C,-0.416000236,-2.1446129208,-6.2209789885
C,-0.783656057,-3.4283833485,-5.7105285727
C,-0.9177694549,-4.2985009512,-6.8153787147
C,-0.0611441239,-0.3014010175,6.0782691166
C,0.0288519416,0.1520689076,-3.2798298928
B,-1.2269444584,-5.5748952514,-11.0469590798

Cartesian Coordination of 4m·Cl^-_2-2 (AM1)
–0.9064959 hartree
B,-2.4854127913,2.0145777521,11.4409878923
B,3.153725216,-2.3610680047,-10.9450699644
C,1.8864809122,-0.3121829364,-10.9272263952
C,-3.2819132808,2.2154525826,9.1761071326
C,0.6217973234,-0.8951340054,0.5204577893
C,0.8305248838,-1.3316910728,1.7815064155
C,1.0327635534,-1.7369578684,2.8949298337
C,0.9291297977,-0.7319758853,-2.9875587854
C,2.2469420771,-2.1863231574,-5.2540936519
C,-0.2690892291,2.4263777888,-11.9133197148
C,2.7303809151,-2.5071739581,-6.5417559712
C,0.7424875446,-0.3140860081,-4.3137392827
C,-0.1245104149,0.7590734858,-4.5773963698
C,-0.789771194,1.3921269934,-3.5284816276
C,-0.6093888457,0.9772210158,-2.2124334217
C,0.2568923328,-0.0932481723,-1.9344496396
C,1.4503430858,-1.0054394452,-5.3795052624
C,2.4274775356,-1.4022696901,-8.8573709445
C,0.1607492509,2.0287332184,-13.2078334107
C,1.1327110403,0.6970465005,-11.6321455742
C,2.233032267,-1.5170372016,-7.431428878
C,1.0405643075,0.9323831214,-13.0298857186
C,2.0488672056,-0.2437914851,-9.5411576189
C,-5.3816952616,4.3697330939,7.0319555476
C,1.9228775577,-3.3219467378,6.6799876157
C,1.136159608,-1.8234005094,9.1393890613
C,-4.6956220855,3.5293414863,6.1132425155
C,0.3806552364,-1.0368223875,10.0361812466
C,1.1066523743,-2.1820573643,6.5935404513
C,0.7924621113,-1.6541356526,5.3313922717
C,1.3119690633,-2.2539382355,4.1727556568
C,2.1343073031,-3.3901255243,4.2766439077
C,2.4304478958,-3.9174866053,5.5289127692
C,0.6235831794,-1.5813739947,7.8260436288
C,-1.5831870547,0.6060827293,9.7091775108
C,0.4516381635,-0.5234276434,-0.6100616417
C,-4.0210426923,2.936011265,8.1696281553
C,-0.5832139696,-0.3363200735,9.2617432857
C,-4.9499977148,3.9995627339,8.3289033409
C,-2.5933979961,1.0409610007,8.8513584948
F,4.3838019924,-2.0434991926,-11.0995016736
F,2.7919413641,-3.4799089846,-11.4410458122
F,-3.3437407849,1.3139764951,12.0820979365
F,-1.8643725628,2.9023353359,12.1156586505
H,-0.1368536635,2.4843686853,-14.1445382213
H,1.5605338451,0.3608699387,-13.7926452565
H,1.7799661786,0.67391353,-8.9877757467
H,1.6096238238,-1.5669866873,-2.7633952286
H,-0.9559151979,3.226246803,-11.6341567066
H,3.3622657035,-3.341911616,-6.8309185391
H,-0.290849799,1.119704909,-5.612173836
H,-1.4658232106,2.232065204,-3.7485243462
H,-1.1382699702,1.4804024955,-1.3900480683
H,2.5377392321,-3.8576138427,3.3670254977
H,3.0677173799,-4.8096301927,5.6102229578
H,-6.0945075642,5.1438348949,6.7741328694
H,-5.2509458768,4.4248584972,9.2815065491
H,-2.7684820584,0.5359866811,7.8839856657
H,0.1658909111,1.6579098622,-9.9280263288
H,0.9267036765,0.1911879062,-7.1220557108
H,2.434273894,-2.7317887079,-4.3358455112
H,-3.2250585192,1.9555132718,6.3902124145
H,-0.9656487682,-0.2609354412,7.1174495719
H,2.1594809599,-3.7511423934,7.6647684882
H,1.9618749019,-2.4805653635,9.3870771
H,-4.751462575,3.51474668,5.0236919091
H,0.4887796147,-0.9572637678,11.1138116147
H,0.1301319911,-0.7715514129,5.2325806977
N,-0.4176447125,-0.6806595527,7.9153171293
N,-3.8837194169,2.666980382,6.7970771283
N,0.31806964,1.6291181057,-10.9686857082
N,1.4544757334,-0.6094939664,-6.7021823385
O,-3.2050482978,2.7501897699,10.3854359237
O,2.3377822663,-1.3419488909,-11.6285942469
O,2.893154369,-2.4643942218,-9.4987892054
O,-1.4476489504,1.1032649881,10.9315188598
Cl,-2.0023515695,0.611550462,5.7907367948
Cl,-0.0088238209,1.619921426,-8.027334668

Cartesian Coordination of 4m·Cl^-_2-3 (AM1)
–0.9006835 hartree
B,-8.443413381,0.6330608707,-7.327544101
B,7.6329103187,-1.0072516953,8.1305880741
C,-6.0061281265,1.1280184049,-6.1108934419
C,7.0852015361,-3.262280765,5.211578569
C,5.2662485646,1.1446032677,6.2177534606
C,7.7871795922,-4.485971183,5.380954514
C,6.5257764442,-0.8888372502,5.5956759535

C,-6.7786809572,5.6219513321,-4.9393346865
C,-2.1263903703,-3.8991222436,-4.1452626605
C,-4.7231357332,-3.3677703635,-5.5188422439
C,-5.6714845503,4.9759707285,-4.3250091054
C,-5.7655562893,-2.6807323449,-6.1777984903
C,-2.7670246164,-2.6562637639,-4.0101652545
C,-2.2655125378,-1.7196277273,-3.0935968617
C,-1.1463535476,-2.0389833389,-2.3069019624
C,-0.5213138826,-3.2905438405,-2.4476691108
C,-1.0139941591,-4.2093960616,-3.3685628402
C,-3.9424565027,-2.3907581292,-4.8239619675
C,-6.4202988688,-0.1893646067,-6.3126998466
C,0.8180298826,1.2118550542,1.1859059784
C,-6.7058153399,3.4369467937,-5.5883735125
C,-5.6022100874,-1.2997122149,-5.8845103272
C,-7.4350711631,4.6480309814,-5.7310217589
C,7.0939475443,-2.0850716474,6.0450097251
C,-6.9647950951,2.1442663423,-6.173517575
C,0.3527217191,0.4629667349,0.3691041251
C,-0.1703788091,-0.3779267519,-0.5495242911
C,-0.6349444421,-1.126381197,-1.3671441113
C,2.2958530111,3.977436777,3.9784126489
C,3.9897905107,3.0295881114,6.2464093156
C,6.498559636,-4.5946277907,3.5041733306
C,4.9658756422,2.3118260091,6.9709475932
C,2.7523683728,2.6497452755,4.0253657628
C,2.2731646465,1.7237123648,3.0863846305
C,1.329139526,2.1240584019,2.126193559
C,0.8754629087,3.4545615369,2.0975731537
C,1.3653343501,4.3718013178,3.0215718318
C,3.703080481,2.2804079593,5.0617564244
C,6.1916825014,0.0836318571,6.5393201398
C,7.4228128766,-5.3250872313,4.299630881
F,-8.2111405271,0.7584955984,-8.5803748026
F,-9.6426909197,0.3385150457,-7.0038038646
F,7.3230656941,-1.408142503,9.3023878641
F,8.7966431133,-0.4896152544,8.000010064
H,-7.0570090296,6.6614652432,-4.8145832134
H,5.4204752542,2.5708795295,7.9225618882
H,2.6351793357,0.6772533306,3.0842647316
H,0.1369932547,3.7636938425,1.343376075
H,1.0159455499,5.413887164,2.9951101648
H,7.7712653948,-6.3322453773,4.1051291862
H,8.4683775294,-4.7042966299,6.1976758506
H,6.2429873774,-0.7637025638,4.533936253
H,-2.5033195741,-4.631839814,-4.8738788316
H,-4.5455112607,-4.4371114031,-5.5198492502
H,-4.9323850562,5.3881373952,-3.6365547738
H,-6.5565315415,-3.0949769065,-6.7959409325
H,-2.7353421386,-0.7228326781,-2.9849088937
H,0.3552305399,-3.5358065598,-1.8302307659
H,-0.5213501922,-5.1854794001,-3.4837565388
H,-8.3247844205,4.7700837162,-6.341140335
H,-4.9695977784,1.3504010495,-5.7961743138
H,-4.1716130136,-0.2278496776,-4.6394502088
H,-4.94478951,2.9290621256,-4.4027659362
H,5.6450717522,-2.6061690399,3.7081331185
H,4.4650045361,0.3630184567,4.3488659227
H,2.6798791832,4.7131560277,4.7002641273
H,3.526039694,3.9670558378,6.531247417
H,5.9842516557,-4.9030152643,2.5928544475
N,-4.4844490969,-1.1436583774,-5.0552627841
N,4.4836087559,1.1432004608,5.0563452785
N,6.3004545079,-3.3561970563,4.0499327164
N,-5.6265663727,3.6668286614,-4.718636709
O,-8.1673366328,1.9313808068,-6.6877757162
O,7.5756205229,-2.2045646567,7.2736732856
O,6.6393182766,0.0228480073,7.786626927
O,-7.612041875,-0.4716521197,-6.8225242178
Cl,-3.7706067745,1.4983140969,-3.9406193196
Cl,4.5232671642,-1.1511333426,3.1945240587

Cartesian Coordination of 4m·Cl^-_2-4 (AM1)
–0.9123715 hartree
B,-5.2104310289,0.2011271396,10.4277694577
B,-1.5821076517,-0.3485487008,-11.5429273651
C,0.8054899257,-0.1133986468,-11.7667564456
C,-3.0114128625,0.069453913,11.4043728531
C,2.2486431238,0.0961912288,-0.3133583499
C,2.0308586468,-0.0080111429,1.0155284869
C,1.8661622234,-0.098185103,2.2030828374
C,1.7725160697,0.086686123,-3.8257951003
C,-0.3739306703,-0.2532350199,-5.900519143
C,4.0895628012,0.7407892075,-13.0338371652
C,-1.0235976667,-0.4092283965,-7.1454356604
C,2.0677125132,0.1975015296,-5.1935310324
C,3.3753143434,0.5267233014,-5.5878187638
C,4.3612728289,0.7419447004,-4.6258810194
C,4.0706253746,0.6352027569,-3.2695806764
C,2.7673089923,0.3036040929,-2.8610862659
C,1.0123640906,-0.0289255376,-6.168092905
C,-0.1741917965,-0.3516645135,-9.5878650603
C,3.4030635904,0.6721526605,-14.275686777
C,1.9603333258,0.2028152079,-12.5729926411
C,-0.0282279835,-0.286895109,-8.1521345986
C,2.0571729309,0.3388267742,-13.9834670829
C,0.9470152542,-0.4474303468,-10.4169713262
C,-1.3194102713,-0.6101123767,14.6192558537
C,0.4496382105,-0.043627985,4.1904299111
C,-2.2603819016,0.1842785935,5.4675625049
C,-0.2700211316,-0.6430031771,13.6622092724
C,-3.2798367557,0.3052558029,6.4383028647
C,0.2966713589,-0.1515455016,5.5814265632
C,1.4229017546,-0.425349897,6.375401605
C,2.6730739829,-0.5900410347,5.7807989311
C,2.8269656567,-0.4859199426,4.4020920607
C,1.7091484283,-0.2093729521,3.5959371305
C,-1.0237781647,0.0204721365,6.1659160217
C,-3.253300983,0.276207517,9.0245045743
C,2.474582752,0.1886114193,-1.4906703217
C,-2.1620990468,-0.1989535357,12.5403592382
C,-2.6538085245,0.2226871741,7.711258496
C,-2.5151080043,-0.3383216704,13.9090328303
C,-2.4605055984,0.4151696937,10.1671921194
F,-1.8632858432,-1.569006967,-11.8036841467
F,-2.4687725996,0.5161010467,-11.8482628767
F,-5.6135126518,1.406416849,10.5738193975
F,-6.1092566642,-0.7038386515,10.4419709587
H,3.8372928302,0.8458735976,-15.2528762536
H,1.2345015418,0.2053898895,-14.6793999712

H,1.9414344927,-0.6769463115,-9.9962604524
H,0.7542040426,-0.1749086411,-3.5009398515
H,5.1362780974,0.9786284312,-12.8407810598
H,-2.0789006219,-0.587900472,-7.3316854491
H,3.6476436857,0.6157627073,-6.6597753183
H,5.3811902169,1.0005974241,-4.9482835997
H,4.8528699641,0.8056580326,-2.5163350976
H,3.546940828,-0.8043234505,6.4144315499
H,3.815717584,-0.6160671473,3.9395909638
H,-1.2126249617,-0.7672645669,15.6858157608
H,-3.5219430169,-0.2449583944,14.304626172
H,-1.3945066306,0.6894226054,10.0838468227
H,3.4308363545,0.4647371066,-10.9830649645
H,2.1034570745,0.1185243528,-8.0472553559
H,-0.8347247666,-0.2896715788,-4.9193208549
H,-0.2513854354,-0.3903673912,11.5053630338
H,-0.584976083,-0.0895331818,8.2964018247
H,-0.4217398412,0.1759086128,3.555231094
H,-2.384564643,0.2064867504,4.3902915819
H,0.7929443699,-0.8327025988,13.8158092633
H,-4.3460153957,0.4365888956,6.2761263388
H,1.3413504997,-0.5116816338,7.4785794365
N,-1.2775503176,0.0489516244,7.52328553
N,-0.7767575605,-0.393471461,12.4155691059
N,3.2236911995,0.45441364,-12.013338742
N,1.2070419309,-0.0568014421,-7.5351885083
O,-4.3145908884,-0.1123929068,11.5562503296
O,-0.3876377671,0.0145308166,-12.3275367231
O,-1.395562359,-0.2296739388,-10.0857387072
O,-4.5632807889,0.0985491188,9.1075578111
Cl,0.602734095,-0.3461959982,9.7947540695
Cl,3.69442707,0.4406043136,-9.089141856

Cartesian Coordination of 4p·Cl$^-$ (AM1)
–0.8067266 hartree
C,3.7626773778,1.3410351154,0.092021983
H,3.8776963988,-2.0290437245,0.6785833199
H,-6.130690383,0.4525482479,0.0661165597
H,6.3032730457,-1.5397968446,0.733792204
H,-3.7038086254,0.8823804277,0.0949355951
H,15.97171076,-0.9119841979,-0.5688167797
H,8.3740386974,-0.9237099042,-0.2262113134
H,-8.2043058105,-0.03062689,0.1144623498
H,-9.7422588757,2.7837943901,-0.0840566836
H,17.9720314441,0.6436498333,-0.2215195639
H,-10.1678311751,5.3054433652,-0.3500571515
H,16.9411928421,3.0726701966,0.5319499942
H,-12.8719800067,5.6912204356,-0.5956039789
H,14.2337175066,2.7811742711,0.5855102645
H,-14.0119866825,3.2030852089,-0.4435981111
H,12.2083198931,1.7716486367,0.3979478979
H,-9.9923061129,0.8709575708,0.8217486816
H,-10.1174837944,-3.8881687024,0.0904672022
H,10.2271051919,2.7556861906,0.8038179434
H,-7.415006731,-4.2740825266,0.1457159226
H,7.5292208804,3.0499359164,1.0185368861
H,5.4790897037,2.6453958722,-0.0473685692
N,15.9005375712,0.0354667552,-0.291434503
N,8.4805730382,0.0178845027,0.0616791637
N,-10.6873110039,3.2287664823,-0.1614395641
N,-8.3298397516,-1.0750909516,0.1456639611
O,13.412522779,-1.2314543944,-0.5310144833
O,-11.8932520386,-1.6683632931,-0.3090376172
O,-13.0849683312,0.4902519843,-0.4485142738
O,10.9462644545,-1.2415003889,-0.4136875638
C,5.5942596687,-0.7206429412,0.5411672713
C,-0.5793849867,-0.7348515797,0.2365546925
C,0.7450001559,-0.4797503468,0.2547969501
C,-1.761663773,-0.9572730036,0.2209383571
C,1.9246436458,-0.248402543,0.2718800642
C,-5.4314175384,-0.4099827706,0.1192383305
C,-3.1412984691,-1.2146217425,0.2037193595
C,-4.0639448338,-0.1569503861,0.1355613198
C,4.2316493201,-0.9993132318,0.5178271943
C,3.2997413067,0.0285875751,0.293059185
Cl,-8.0558988276,1.8674243112,0.0697325948
F,12.2181103089,-2.9391637347,0.1817152105
F,-13.8114442585,-1.3810625186,-1.3343345585
F,-13.7516635602,-1.2071454265,0.8306713441
F,12.1161993973,-2.3517361647,-1.9139572019
H,-5.3427215272,-3.8254249785,0.2819829182
H,-2.9066284885,-3.3718592537,0.3095335214
H,3.0396328977,2.1518108403,-0.0855783046
C,14.9658560468,2.0203656983,0.3288092085
C,8.0671124715,2.1558194495,0.7177416888
C,7.4700906275,0.9102295755,0.3733882463
C,-7.3303722572,-2.0306569102,0.1536280927
C,6.0548437605,0.5886906191,0.340465866
C,-5.9111444572,-1.7304515465,0.1705253042
C,-10.8169772498,-1.0060059502,0.0876858931
C,9.7181648694,0.6639977968,0.1980703408
C,-9.5631587976,-1.7293187701,0.1215405643
C,-9.3379350728,-3.1322484757,0.1136582079
C,9.4703666801,2.0002738338,0.6090448225
C,-7.9383668164,-3.3245220567,0.1403516391
C,-4.9843948825,-2.7860685527,0.2393427525
C,5.1249816787,1.6157888741,0.115456789
C,-3.618596539,-2.5354903032,0.2555819959
C,-12.9585794923,3.4592626907,-0.378503757
C,14.6800455568,0.6833403637,-0.0424250371
C,-11.9041042579,2.5257640106,-0.1892395863
C,13.390849922,0.0377266387,-0.1631846793
C,-11.9726543758,1.0915905226,-0.0611910262
C,12.1994535919,0.7200770614,0.0938566657
C,-10.8573715887,0.3593283479,0.3680828379
C,10.9885290742,0.0261321358,-0.0481928162
C,-12.3656405371,4.7430040826,-0.4589629143
C,16.3798931923,2.1728430964,0.3008772974
C,-10.9626003668,4.5585101131,-0.328664792
C,16.9273167798,0.9291939437,-0.0858655268
B,12.1726316988,-2.0155161458,-0.6899748026
B,-13.194237391,-0.9748175463,-0.2959665318

Cartesian Coordination of 4p·Cl$^-$-2 (AM1)
–0.8065137 hartree
C,-2.7746923164,0.8634178144,-12.4909897339
C,-3.0357499667,0.5419431022,16.26764492
Cl,-0.3002747959,0.268456492,-7.9468262048
F,3.1672993058,-0.8531404375,-13.3490737419
F,3.4915014231,1.2932395405,-13.4434848269

F,-5.4553573485,-1.4262707572,10.4495111612
F,-4.1120006279,-3.0888108741,10.8733435447
H,5.5878962771,-0.191863826,-9.5231876004
H,5.748958639,-0.194014636,-6.797642732
H,-2.0438380103,-0.0018127378,5.5826055331
H,0.9476158474,0.2121336752,-5.9097278327
H,0.323347869,0.2870505604,-3.5263815056
H,-1.4149096519,-0.1183894824,3.1908271282
H,-1.7336796665,1.1376848994,14.5336133575
H,1.1466699009,1.9519183593,8.5136511801
H,-0.1440025212,1.5038491273,10.8686540114
H,2.6950726783,0.7885027466,4.216255475
H,5.1297432623,-0.2058383392,-4.7678278533
H,2.0696068185,0.8917058342,6.6234852435
H,4.4814271262,-0.1259640679,-2.3775612991
H,-1.1105863804,0.7009966872,-14.0030379497
H,-1.6401939543,0.6558051035,12.3163078084
H,0.7960738588,-0.6013465015,-9.7758401724
H,-3.6671527288,1.047896469,-13.0772122072
H,-2.6166701979,1.0837292811,17.1096360506
H,-3.520187047,0.8529196886,-10.345568186
H,-4.7753155344,-0.6098889325,17.1584471357
H,-1.0655179154,0.4335021381,-9.706314405
H,-2.0365234866,-0.7773924391,7.8275378073
H,-5.0846377937,-1.4527771007,14.7635063292
H,1.5953962455,0.0982803407,-7.9360729244
N,2.6422570856,-0.0054503626,-7.9738146356
N,-4.3758075628,-0.8224544941,15.0463380539
N,-1.4257012439,0.5138146408,-10.686485636
N,-1.4070865666,-0.1534050721,8.2696441123
O,3.5520749484,0.3059255164,-11.4852521766
O,1.5117573007,0.5528321881,-12.8546954211
O,-3.2986526056,-1.2100106475,10.0583440749
O,-4.2820369764,-1.4301951362,12.3124998779
B,2.9671563699,0.3015665709,-12.8385625062
C,-2.7142112298,0.760355306,-11.0748939361
C,-4.1488904606,-0.3269656472,16.310555394
C,4.8475331542,-0.1395958799,-7.3976717537
C,-0.9947670533,0.1629016836,5.2940229054
C,1.6848105844,0.1751665511,-0.2746982883
C,1.3393894777,0.2242508115,1.0282860588
C,1.9942270073,0.1336312429,-1.4366036215
C,1.0338902495,0.2700019148,2.1901515289
C,1.7468849876,0.1356415828,-5.1408783953
C,2.3592006533,0.0868076997,-2.7910799902
C,1.3843522706,0.1789442363,-3.7987435376
C,-0.6473964551,0.1029104495,3.9483282964
C,0.6808283348,0.3270233956,3.5467197467
C,-2.5747484433,0.5699584732,14.9221959054
C,0.2932008512,1.3009056616,8.6776033982
C,-0.3617547664,0.5310168284,7.6753124972
C,3.5108561276,-0.0480046838,-6.8987387608
C,-0.024610182,0.447758778,6.2657468127
C,3.0966147399,-0.0019245088,-5.5091768174
C,2.7790915367,-0.0158199738,-10.4588154522
C,-1.4390625378,0.160225973,9.6364677598
C,3.394331324,-0.0614845967,-9.1488874195
C,4.7715686457,-0.1412344768,-8.8085754897
C,-0.3813692929,1.0696820421,9.901010346
C,1.6526040045,0.612402039,4.5220836571
C,4.0689920631,-0.0957983548,-4.4973804405
C,1.3020270188,0.671524959,5.8657328246
C,3.7091810692,-0.0518769293,-3.1569503244
C,-1.4554233679,0.6822590312,-12.9733448672
C,-3.4186925406,-0.2848011357,14.1710429591
C,-0.6257468544,0.461448532,-11.8410376107
C,-3.362013144,-0.5930153313,12.7584609867
C,0.7971934324,0.2375918536,-11.7874977379
C,-2.3922928871,-0.03500144,11.9220800477
C,1.405780857,-0.2069835179,-10.6057624068
C,-2.4053501401,-0.3793622966,10.5621876033
B,-4.3396365114,-1.8389585586,10.8955307802

Cartesian Coordination of 4p·Cl⁻₂ (AM1)
–0.9140802 hartree
C,-2.4182718059,-0.2103222803,-4.9475794627
Cl,-2.0596414536,0.2039796823,8.3755354736
Cl,2.038142666,0.1564335433,-8.3809781083
F,-1.4724999532,-1.557093477,-13.8762983332
F,1.6175301217,-0.8969857806,13.9183644626
F,-1.531253015,0.6114532804,-13.7818989475
F,1.4214782391,1.2589206953,13.7492626267
H,-4.0214998357,-0.5295940291,-7.2693550523
H,-0.7462389462,0.0600702699,6.2746718948
H,-1.3111275525,-0.0137607749,3.8755950545
H,4.0411410612,0.1951678027,7.2747896665
H,3.8294588521,0.2696655709,9.9962056773
H,-0.9355709224,0.990223389,10.1471573006
H,-2.9385206805,-0.0102049256,14.4165232377
H,-5.5094395136,-0.2185126612,13.4884693149
H,-3.8146344089,-0.5238738495,-9.9921895222
H,5.3385698952,0.1376692254,-10.7512151971
H,5.5247373912,-0.0319335028,-13.4823735629
H,2.9494095817,-0.1584236186,-14.4129124166
H,0.8324504691,0.7476719906,-10.177845659
H,0.7468311229,-0.073087322,-6.2750011172
H,1.3117607234,0.0018853622,-3.8758765329
H,-2.8887983518,-0.1919674062,-2.8391084011
H,-3.4759966287,-0.2664505955,-5.2445937291
H,-5.3400990006,-0.1217375097,10.7526817668
H,0.1260223549,-0.0172990419,-8.3384873535
H,-2.8587590942,0.1182707144,10.1112618105
H,2.8446100023,0.1066260612,-10.1143909255
H,-0.1399910784,0.2528485322,8.3340242243
H,2.8860600719,0.2390593228,2.8379066495
H,3.4730514735,0.3160682178,5.2433187663
N,-0.9176870386,-0.1144852781,-8.3920885006
N,0.9077557377,0.2805521533,8.3888280314
N,3.2184941307,0.0859139934,-11.0966682754
N,-3.2291249698,0.0872620376,11.0945428414
O,1.7533821962,0.0183917074,11.9291084136
O,0.342376277,-0.4805707725,-13.2758763413
O,-0.3100668255,-0.0622075947,13.2853518585
O,-1.7191545901,-0.5961253623,-11.9194614466
C,-0.3549915387,0.607227264,11.005614031
C,-2.4320992965,0.1252323107,12.250863504
C,-3.2779615837,-0.0025082458,13.3851693397
C,-4.6049536078,-0.1122764123,12.9016493515
C,-3.1170721694,-0.4099563266,-7.8551197967
C,-3.0175260309,-0.4070547322,-9.2638236009

C,-1.0199002742,-0.154845143,-10.8834900804
C,2.4253313524,-0.0093701953,-12.2523416283
C,-1.4159488731,-0.1806243961,-5.9328513486
C,-1.7972010619,-0.2323682596,-7.3334541032
C,4.5311661721,0.0796548607,-11.4823265471
C,4.612612895,-0.0125341022,-12.8980865583
C,3.2830844295,-0.075742647,-13.3829647328
C,0.9841917134,-0.0491369671,-12.2006974485
C,0.3030954489,0.2688442228,-11.0210556487
C,-1.6455571735,-0.2185138815,-9.5824063027
C,-0.0728857742,-0.1029207117,-5.5287562648
C,0.2548094899,-0.059207428,-4.176561026
C,-0.7488088757,-0.0917875825,-3.1946834255
C,-2.0930507153,-0.1674655646,-3.5978364528
B,-1.1320485134,-0.4894418992,-13.266260972
C,-4.5326255688,-0.0596534988,11.4833806542
C,-0.4224883762,-0.0490746556,-1.8290450533
C,-0.1521922447,-0.0131951909,-0.6578796552
C,0.1513779337,0.0271969476,0.6571810396
C,0.421654309,0.0632899434,1.8283443574
C,0.7479642573,0.1057611586,3.1939919188
C,2.0911996772,0.1986742183,3.596886488
C,2.4164478523,0.2403906875,4.9466572316
C,1.4153391661,0.1894142345,5.9322949331
C,0.073047775,0.098534204,5.528375916
C,-0.2547529604,0.0572465722,4.1761306255
C,1.7971808527,0.2307472567,7.3330769703
C,3.1277017438,0.2275100805,7.8578882889
C,3.0256307596,0.2669316715,9.2658635975
C,1.6403693109,0.3036482784,9.5805527897
C,1.0089712363,0.3379677319,10.879983254
C,-0.996147006,0.2529781299,12.1972218079
B,1.1552372653,0.1016794995,13.2726850303

Cartesian Coordination of 4m´ (AM1)
–0.5896319 hartree
C,-1.0945931669,-1.1408369272,1.0207167258
O,-1.2154143517,-0.3195977537,8.3125326865
O,1.9492984708,-1.1507188644,-10.5014805737
O,2.1158099714,-0.5242594677,-8.1194363211
O,-1.1427799374,0.3949748717,10.6744018582
C,2.5414977704,0.6674452069,-8.4964802931
C,2.5100247115,0.3382494891,-12.2278632201
C,2.3792681034,0.0570592521,-10.8164998692
C,2.9355320906,1.5395637531,-12.851156931
C,2.89728683,1.3252436327,-14.2518226887
C,2.4458738512,-0.0057127776,-14.4686773987
C,3.0850064753,2.3996320565,-5.3253244323
C,3.4593747833,3.4369986494,-6.2220206444
C,3.3076138155,2.9361826268,-7.5399575875
C,3.0777568656,2.4450723239,-3.873338509
C,2.1847354386,1.6671137505,-3.1267357153
C,2.1920219042,1.7357403128,-1.7242122476
C,3.0970545608,2.5903238953,-1.0727870372
C,3.9807876719,3.3643314306,-1.8211966048
C,3.9770572609,3.2961098252,-3.2120555045
C,-3.1228545851,0.6403805062,14.3234238708
C,-3.4023916009,-2.1024263546,5.2573388687
C,-4.5979120023,-2.3703184259,5.9779689371
C,-4.4098284249,-1.9035184657,7.3036873216
C,-3.1233267659,-2.4025725477,3.8636332378
C,-2.2344718978,-1.6207157558,3.1161322281
C,-1.9884383458,-1.9267134512,1.767922651
C,-2.6398785691,-3.0189188625,1.1708757051
C,-3.5256700288,-3.79099418,1.9188474458
C,-3.769340845,-3.4909454041,3.2566638327
C,-2.4434126419,-0.7595049712,8.5175572637
C,-2.9558165467,0.0796084389,12.1322354078
C,-2.3724429761,-0.0634526138,10.8179600438
C,-3.1024317499,-1.3588725589,7.3781783286
C,-3.0757116236,-0.6554846433,9.7613453226
C,-4.2481210051,-0.309394865,12.5696513237
C,-4.3531249924,0.0392725892,13.9395669017
C,-1.5084649154,2.6800440952,17.0410321843
C,-1.8302486702,2.1987139607,15.773344778
C,-2.7594171787,1.1579462393,15.6309039664
C,-3.3610377692,0.610565816,16.7747477955
C,-3.0351390038,1.0978523459,18.038089037
C,-2.108239952,2.1315548658,18.1743818656
C,1.128975609,-2.3239359999,-17.122638259
C,1.3024153154,-1.7036984777,-15.8867266917
C,2.2476533995,-0.6779981233,-15.7407631251
C,3.0120796965,-0.2830871634,-16.8496593197
C,2.8320357418,-0.9069486692,-18.0817593034
C,1.8922193124,-1.9285373714,-18.2208964971
C,-0.3299965982,-0.4702296368,0.3808842896
C,2.8453236712,1.5996288427,-7.4332519163
C,2.6925034544,1.0144707159,-9.8434784814
F,0.5823957594,-0.4280644286,9.5803030914
F,0.5228055361,-1.7974602358,-8.9525922008
F,2.5743131831,-2.53093709,-8.9030581234
F,-0.2231821252,1.5168075509,9.0167047037
H,-2.4482033541,-3.2601650655,0.1143733438
H,3.504167152,3.469804799,-8.4662001489
H,1.4604454335,1.0056781566,-3.6260568438
H,3.1041432747,2.6453215703,0.0263313474
H,4.6889483877,4.0333895933,-1.3088802196
H,4.6814246435,3.906231808,-3.7982229122
H,-5.4897715019,-2.8372045535,5.5708582424
H,-5.1282889803,-1.9480667244,8.1180220177
H,-1.7301097183,-0.7532041302,3.5683015218
H,-4.0351725783,-4.6461971146,1.4491309528
H,-4.4664459959,-4.1078700098,3.8443909471
H,-4.0948640145,-1.028118125,9.9058788982
H,-5.0104828502,-0.7846857611,11.9579088934
H,-5.2122626561,-0.1083228806,14.5869947631
H,-0.7794421747,3.4975570018,17.1452180293
H,-1.3585312607,2.6528444217,14.8892253549
H,-4.0887214329,-0.2083809625,16.6687390715
H,-3.5101225651,0.6633382069,18.9302987795
H,-1.8514938501,2.5136289039,19.1733925192
H,0.3847499649,-3.1271963864,-17.2301412298
H,0.6815783368,-2.0181741074,-15.0346202135
H,3.757352396,0.5193716399,-16.7398233119
H,3.4354223717,-0.5926835393,-18.9464053142
H,1.7529799885,-2.4206439446,-19.1947366484
H,1.906592114,-1.5162838833,-13.0647003079
H,-1.359760539,1.0040150724,13.1819037877
H,-1.5839500874,-1.1962596889,5.9048625028
H,2.4185226614,0.4140551541,-5.7258731893

H,3.0474070387,2.0095196393,-10.1304252619
H,3.2319945537,2.451396906,-12.3393017543
H,3.1515766331,2.0397028609,-15.0289644362
H,3.7882098495,4.4314748682,-5.9356297835
N,2.7149851752,1.293416943,-6.072121304
N,-2.5059479274,-1.489473582,6.1169956748
N,2.214976876,-0.5907960382,-13.23528325
N,-2.2870968593,0.6585571694,13.2197594856
C,0.5298013253,0.2828645775,-0.3379137276
C,1.2953386207,0.9525201051,-0.9776180632
B,-0.426532698,0.3182457994,9.385253551
B,1.7644976899,-1.5722725932,-9.098292285

Cartesian Coordination of 4m´$_2$·Cl$^-_2$-1 (AM1)
–1.4831024 hartree
C,-0.6733941136,-0.0258658257,2.8838190151
H,-8.9700916567,2.2870660617,1.0302844987
H,-4.9902903349,3.7758646825,-2.9056186482
H,-6.9261230896,5.4589208618,-1.9393517286
H,7.1494447059,0.3944167331,-2.0560343584
H,5.8307942387,2.4573694832,-2.476333623
H,3.353457252,2.3445399722,-2.7360508773
H,3.5082960742,-1.9559282355,-2.212299291
H,13.1578630487,-3.8984094878,2.7034440205
H,8.973085534,-2.3172936198,0.9428335494
H,13.9210825083,-1.5568421913,3.9010645249
H,4.9865800326,-3.6811236651,-3.0317973178
H,13.2805274287,0.2976108177,5.0253580505
H,13.4198833929,2.6928195597,5.6846003719
H,12.4115284098,4.45497161,4.2278202052
H,11.2533888325,3.8105501442,2.1155356404
H,-11.2493436344,-3.8768273647,2.0078867485
H,-11.078203457,-1.4725719857,1.4263712099
H,11.0805197721,1.4260929592,1.4580309595
H,-13.2697121387,-0.4587452029,5.0331103551
H,-13.4074583859,-2.8737996684,5.6159169359
H,-12.4025156701,-4.5884616002,4.1012568599
H,-10.468534552,0.7565145191,1.5158650773
H,7.801017559,-1.4560334057,-0.6915904378
H,10.4717284277,-0.8043528015,1.4767231578
H,-7.802608547,1.4772774737,-0.6347672626
H,-13.9139201971,1.4301571924,3.96886764
H,-10.7170080832,-0.6769419305,-1.4851308774
H,7.8117537096,1.3870145215,0.8652864487
H,-7.810855069,-1.4134948193,0.8306461422
H,10.7143288402,0.7236265842,-1.4786292873
H,-7.1581443006,0.2270642565,2.3714331786
H,-5.8881301981,2.236777081,3.0832051153
H,-3.4075449174,2.1492823407,3.3248804263
H,-3.4579902809,-2.0305484924,2.1800278925
H,11.5945351473,-1.4015058304,-1.292512257
H,11.9331070701,-3.8052336588,-1.8200720032
H,13.0106796509,-4.4786151763,-3.9621148186
H,13.7578324377,-2.734434139,-5.5894086067
H,13.4247409259,-0.3218227538,-5.0745570666
H,-11.9364739211,3.8601384487,-1.6795627133
H,-13.0174130067,4.601752612,-3.7972023051
N,7.2825847196,2.2032696276,1.1907861617
N,-11.387236352,-1.179847933,-2.0297845942
N,11.2206987945,-1.2814226715,1.981137931
N,-7.3046414156,2.2646951972,-1.0576794666
N,-7.281420769,-2.2394858102,1.1300096327
N,11.3838831368,1.2435514677,-2.0077869975
N,-11.2166265103,1.2170011881,2.0367007069
N,7.3029463284,-2.2295596823,-1.1391425897
O,-11.3447099942,4.6647931216,0.8610514885
O,9.0419348564,5.2566576218,0.1976450686
O,-9.4303679662,5.1870088012,-0.6127270216
O,11.3458081847,-4.6902264984,0.6962825251
O,10.9581347664,4.8112853058,-1.2953490411
O,-10.9601838037,-4.7684234057,-1.4318335373
O,9.4289637843,-5.1649296392,-0.7904749395
O,-9.0416669592,-5.2605084788,0.0437102889
C,9.6688424104,3.0356044642,-0.3779924971
C,8.8284213108,3.9524851485,0.2677898311
C,12.5895261168,2.9929913528,-2.8501747143
C,13.0944481694,1.7928826255,-3.4084834638
C,5.3537157599,-1.3852003511,2.8415537082
C,12.332796086,0.7183426777,-2.8693622643
C,5.7073486596,3.5238329803,2.1854419048
C,6.6859287383,4.3729499125,1.6221602388
C,5.3901040964,0.968508437,2.2740082054
C,3.9963726481,1.0165838358,2.4147758291
C,-12.5937626557,-2.901634704,-2.9261862474
C,-13.0996127537,-1.6843467842,-3.4450678858
C,-12.337386162,-0.6274957224,-2.8727903463
C,-6.0989633153,-2.2396806367,1.8426451987
C,-5.7048329212,-3.5902689256,2.0809751374
C,-6.6839986503,-4.4215024649,1.4925674165
C,-5.3877030803,-1.0389351432,2.2489569543
C,-10.7022317583,-3.4777230743,-1.2805175373
C,-12.076937078,1.7518317173,-2.1715650065
C,-12.4991593181,0.7968730775,-3.108051286
C,6.0665328381,-0.2420716242,2.4828428134
C,3.2797032476,-0.1394292317,2.7593273243
C,3.9692579478,-1.3437779189,2.9807869998
C,7.6582285708,3.5399420607,1.001460678
C,-9.6694777578,-3.022527721,-0.4609175841
C,-8.8281617066,-3.9591679453,0.1545483353
C,10.7003537204,3.5164390263,-1.1844185933
C,-13.1074258993,1.2256395935,-4.2987988981
C,-13.2922516182,2.5837656414,-4.5422769716
C,-12.873701821,3.5284930955,-3.6051113389
C,-12.2669152911,3.110701946,-2.4211047695
C,13.1002979009,-1.0881730607,-4.3553014666
C,13.2845605243,-2.4377895493,-4.6425009974
C,12.8673565564,-3.4120708888,-3.7354487133
C,12.2624626056,-3.0324299083,-2.5377202399
C,12.0730271442,-1.6822356124,-2.2444409053
C,12.4939347053,-0.697769543,-3.1504486302
C,-3.9938053051,-1.0912508962,2.3865558202
C,-1.8742748806,0.0088882921,2.8489108529
C,-3.2767941461,0.0535147614,2.7661531953
C,-3.9661492876,1.2503165766,3.0258595617
C,-5.3507697689,1.2959351815,2.8895947423
C,-11.5299050229,-2.574663207,-2.0476639108
C,-7.6571183257,-3.5696421597,0.8993876476
C,1.8772844438,-0.0973517539,2.8450739722
C,0.6764459861,-0.0636896,2.8824291124
Cl,-9.0161799548,0.067091183,0.2137147926

Cl,9.0155476226,-0.0739055962,0.2018739214
F,-10.1449767869,6.5311230066,1.0071272822
F,-9.9783708597,-6.7266628704,-1.2960136436
F,9.9777640435,6.7647169972,-1.0953368248
F,-11.10119992,-5.9884647139,0.4160372972
F,11.1023699883,5.9712770615,0.5906293293
F,11.3891804175,-6.1334146753,-0.9501608973
F,10.1461345962,-6.5601738177,0.7842880109
F,-11.3907855263,6.1601109246,-0.7381219042
H,-4.8173253805,-3.9007152599,2.6223632438
H,-13.7670440316,2.9105229377,-5.4784490357
H,-13.4329512894,0.4827441247,-5.0417805468
H,-9.4930407931,-1.9388483034,-0.3181413352
H,3.4109230904,-2.2516072217,3.25226759
H,7.1605913247,-0.3007702462,2.3548929376
H,-11.5969704954,1.4408083622,-1.2298445905
H,-6.7191540083,-5.5078931273,1.4732681076
H,-13.9230750568,-1.5626418974,-4.1406636629
H,-12.9331799307,-3.9125398761,-3.1380153226
H,3.4604058102,1.9618909259,2.2382444821
H,6.7212177618,5.4594097924,1.6367641853
H,4.820493859,3.8172642248,2.7372889536
H,5.891215299,-2.3316544867,3.0050834701
H,13.9169505456,1.6933968909,-4.1087368831
H,12.9288000188,4.0101385555,-3.0299270382
H,9.4926943163,1.9479800616,-0.2689548613
H,-7.1530031502,-0.3284912546,-2.0588776358
H,-3.5114810814,2.0249292078,-2.1439196113
H,-3.3583101887,-2.2564753195,-2.8060495084
H,-5.835339491,-2.3771198316,-2.5470155329
H,6.924031434,-5.3938678264,-2.1225917185
H,-13.153180221,3.8090494775,2.8454544625
C,12.6861527157,-2.9227599018,2.6217628008
C,11.526787727,2.6381814524,-1.9811403611
C,4.0190622743,-0.9828239351,-2.2758803226
C,1.8726147945,0.1233832025,-2.5755210067
C,3.2739631201,0.1873677441,-2.4863269263
C,3.9339598286,1.4255362001,-2.5681610986
C,5.3171089508,1.4853404824,-2.4221020815
C,6.0574981165,0.3265602698,-2.1928233864
C,5.4108175759,-0.9157363636,-2.1266039464
C,0.6724432409,0.0709180249,-2.6134692433
C,-6.8378171527,4.3865974291,-1.7862986129
C,-5.840206388,3.5153836874,-2.2836342648
C,-6.1575299134,2.2035456394,-1.8250699576
C,-12.1512732285,0.6135900461,2.8578680453
C,-6.0639414269,0.164487044,2.4962255415
C,6.1010220209,2.1813050573,1.904543954
C,-11.5274152965,2.5818496794,1.9464952677
C,-8.9026157637,4.0209216424,-0.2829129534
C,-9.4812741802,3.1999387686,0.6920735304
C,-10.7558154867,3.5185120262,1.1646471517
C,-12.6813941899,2.8366344271,2.7318692181
C,6.8356751472,-4.3270394977,-1.9350382748
C,-5.3213671758,-1.4074358702,-2.4621581976
C,-3.9383791093,-1.3432338708,-2.6079401157
C,-3.2779945968,-0.1084751471,-2.4870971283
C,-1.8767430641,-0.0418594296,-2.5758923524
C,-4.022565195,1.0544817035,-2.2381605921
C,-6.0612024697,-0.2564991857,-2.1947686112
C,-12.1804135058,-0.8012923249,3.1869816086
C,-7.735850846,3.5983870327,-1.01930001
C,12.9118970606,2.4114702665,4.7511815266
C,12.8353064086,1.0714078246,4.3827849578
C,12.1868831955,0.6988916967,3.1936818915
C,-5.4141435235,0.982898008,-2.0893903285
C,-0.6766122544,0.0117187495,-2.613574945
C,6.1547984469,-2.1440763382,-1.9026678963
C,5.837215665,-3.4405560582,-2.4028134879
C,12.1568340245,-0.7047635064,2.819643485
C,13.0753592182,-1.7115878152,3.2398547027
C,7.7345294967,-3.5636733665,-1.1442366619
C,11.5309734896,-2.6427466948,1.8468061671
C,8.9023819703,-4.0094820162,-0.4234514767
C,9.4830634928,-3.2197013344,0.5757810776
C,10.7579207158,-3.5537677544,1.0365993342
B,-10.5874885987,5.7051423427,0.1417578779
B,10.2996121374,5.7609416415,-0.382471089
C,-13.0693205765,1.6062135195,3.3115626814
B,-10.2998160295,-5.7465031122,-0.5508299352
C,-12.3380159354,-3.5206005001,3.8475128625
C,-12.9016976456,-2.5627565034,4.6907495766
C,-12.82600517,-1.2116132316,4.3651307954
C,11.6086341863,1.6916699749,2.389983851
C,-11.6040587662,-1.7678390229,2.3506358599
C,-11.6905112152,-3.1206166196,2.6795620367
C,11.6960124817,3.0332570863,2.7616948145
C,12.3463197069,3.395754898,3.9402832275
B,10.5873473759,-5.706851067,-0.0548203587

Cartesian Coordination of 4m′$_2$·Cl$^-_2$-2 (AM1)
–1.4825172 hartree
C,-13.2668554624,-2.1374066381,-5.3507867579
C,-13.2029706836,-2.4683347245,-4.0002001125
C,11.3724553552,-2.5971550136,-0.637258096
C,11.5967146703,-2.7307140949,-2.0071111503
C,12.2869155656,-3.8351001816,-2.5042520903
C,12.7537295664,-4.8127258221,-1.6254678852
C,12.5353868002,-4.6858475187,-0.2566534211
Cl,8.799858466,-0.522275896,1.1738226515
Cl,-8.9999079328,0.3554434519,-1.1469069547
F,11.4633265838,0.7850542363,-4.7190658642
F,-8.2898920268,4.2791618282,-6.4649039256
F,8.9139294407,-2.4374117317,7.5013340582
F,10.2812913093,-0.7488604814,7.619821635
F,-9.8882151652,-3.722484823,4.3892587109
F,-11.1483775707,-1.9589531654,4.5686700593
F,-9.5385964819,2.8029028809,-7.4610222485
F,10.3348508159,2.6381959155,-4.8687542898
H,3.1674856964,1.8264307553,2.7318302854
H,7.1104424116,1.9379582095,0.9312870883
H,-6.9152254736,-0.3107846731,4.7015772243
H,-4.9914589077,1.3584786365,3.6875249989
H,-13.5711138808,-4.1027828799,-1.6655055708
H,-12.8218999365,-4.1491213499,0.9665569294
H,3.6660614536,3.2187421791,-1.3433871503
H,6.1242920918,2.8447405397,-1.16196132
H,6.0335277568,0.8721215958,6.5210485717
H,4.411052866,2.2275569364,4.7757514764
H,-9.6780666481,-0.4632161466,0.7204439211

H,-7.133822679,2.5634964076,-0.3686025593
H,-5.7767035331,3.9192174641,-1.9443884052
H,-3.303501565,4.0798876604,-1.6723136474
H,-3.5391148245,1.5423300419,1.8337863529
H,-7.8159840838,0.4876185309,0.5961461089
H,10.041447056,-2.0317691075,1.8338168352
H,-12.2738362317,-1.1704399282,-7.0175601985
H,-14.0339174141,-3.0139983203,-3.5294418592
H,10.8204354927,-1.7153504054,-0.2682839453
H,11.2271681988,-1.9556829004,-2.6968670016
H,12.4612275578,-3.9340425418,-3.5851958983
H,13.2945802159,-5.6877657946,-2.0131709983
H,12.9004062019,-5.4622442927,0.4317154668
H,13.229758347,-4.8056055197,2.5317647694
H,12.2063362327,-4.0147717366,4.9436973541
H,8.3691961014,-1.6924994393,3.2065539234
H,5.0757826598,-1.8761470052,-3.6613547527
H,-10.4432703353,1.8872656404,-1.6427491506
H,7.7874767631,-0.7584658972,-0.5373727884
H,10.6534446664,1.2050629543,0.9862558842
H,-7.4575581274,0.1093319651,-2.5325488661
H,-10.8035535293,1.6348353844,0.52316274
H,-11.6334890149,1.0066757225,2.7615907386
H,-13.8834082386,1.7593490693,3.5385221418
H,-15.3149617254,3.1490105322,2.0341070879
H,-14.5051793401,3.7813129554,-0.2268132036
H,11.24394497,0.4551032902,3.0738536356
H,11.3338456632,0.348066411,5.5538037924
H,12.4701287259,2.1473437382,6.8462961627
H,13.5249621982,4.0723488787,5.6494911535
H,13.4374847281,4.1973255064,3.1657018814
H,-14.1469534374,-2.4268363619,-5.9425852204
H,-10.5181190651,-1.1739753396,-1.0566096673
H,7.4244662348,0.1678924432,2.5343796278
H,-10.1555333621,-1.0805740976,-3.2602825638
H,-10.2876685542,-0.5067974984,-5.6645868351
H,14.0558873894,3.7617268602,1.0304797218
H,9.5766532996,0.3597678825,-0.6341548457
H,13.2664266446,3.3878454766,-1.5659813603
H,3.0076844558,-3.8622659714,1.8882528184
H,3.5286020632,-1.8320165703,-1.9050696325
H,6.9501210957,-2.5982559149,0.6503648937
H,5.4619533985,-3.7023376599,2.3009728063
H,-5.5947268941,0.7269822398,-6.3350715824
H,-4.1055009541,-1.0816720088,-4.9108253928
H,-13.6031814035,4.7530709163,-1.9357861763
H,-8.6319021499,1.8579066258,-2.7528194012
H,-12.1273227771,4.8321195797,-4.2362543187
H,-3.1188983114,-1.3222584377,-2.7495213866
H,-3.9230539017,-3.8292208436,0.694245696
H,-6.3690202632,-3.4658764833,0.3770386199
H,7.137434305,-0.4421377979,-4.7627448866
H,-7.2014070672,-2.0214220516,-1.4645465757
N,-11.0452608435,2.630624666,-1.9803796642
N,-6.7837489874,0.0460209101,-3.2946557693
N,-7.3489313357,0.5142589921,1.4998245525
N,10.6865896865,-2.677112704,2.2940071502
N,-11.1997031431,-1.9066461393,-0.8898472189
N,11.3991661945,1.7977628257,0.6855487374
N,7.3535503618,-0.8591721446,-1.4617503893
N,6.8362260382,0.4915548703,3.3057822799
O,9.3863290901,0.8777861868,-3.9604944168
O,-10.0266455653,3.3948047022,-5.4047043332
O,11.2827438877,2.115919486,-2.9585163531
O,-9.0852052493,-1.7776869371,3.7650047718
O,8.4846812131,-0.5692024123,6.3751014169
O,10.38524978,-2.066990165,5.87476831
O,-10.9153749316,-2.9691941258,2.6031384993
O,-8.0035826079,2.1171370397,-6.0512665361
C,-13.8652101757,3.1779990879,0.4335365548
C,11.7501317557,1.2605206621,3.6298214505
C,11.8008464564,1.1966123878,5.0220374414
C,12.4376520512,2.2022561256,5.7483837442
C,13.0258739179,3.2757591966,5.0794357704
C,12.9793494932,3.3457892376,3.6899694466
C,11.6521979723,-3.4600043166,1.6876046007
C,12.4026342672,-4.1249351954,2.7017977701
C,11.8788153868,-3.7174259019,3.9510535261
C,8.1180668456,-0.6679544171,5.1094012475
C,8.7611145787,-1.5401645802,4.2222490881
C,0.6739775184,2.7866451188,0.4649630751
C,5.1998039505,1.8436752973,1.97164015
C,3.8181584545,2.0560888514,1.8740405569
C,3.2606407889,2.5415968648,0.6813614072
C,6.0249846973,2.1218807271,0.8729497757
C,-10.7059378689,-2.1943538602,1.5508326494
C,-5.4223454565,1.9823730116,0.8483120097
C,-6.8431481585,0.0905777427,3.6938267834
C,-5.8499975589,0.9482125053,3.1659857878
C,-6.1812861004,1.1895140108,1.8008772085
C,-12.0400087041,-2.4776935976,-1.8288422821
C,-12.8257843365,-3.4782257851,-1.1851110662
C,-12.4405545697,-3.5082653706,0.1757477778
C,4.0988551173,2.8347344519,-0.4079519669
C,5.4711005617,2.624077914,-0.3037881582
C,6.0965623235,0.9001310819,5.4364271069
C,5.2611707403,1.5985400969,4.5334064432
C,5.7462740723,1.3357173849,3.2190008022
C,9.9521980752,-2.1453436085,4.6257368268
C,-8.919724955,-1.0421214387,2.6780294656
C,-9.7773158048,-1.1516035618,1.5791909625
C,1.8679212274,2.6947508466,0.568375462
C,10.8110546081,-2.822493575,3.6830282568
C,-6.0444321396,2.6441740089,-0.2197057478
C,-0.6697666599,2.8441410442,0.3443646289
C,-7.7655129745,-0.1769773437,2.6475570207
C,-11.4300919804,-2.5266225186,0.3466328175
C,-5.2819656722,3.4002496778,-1.1090256285
C,-3.900673715,3.4923633359,-0.9596304697
C,-3.2650976606,2.8193661716,0.097395802
C,-1.8664395233,2.8552706133,0.2328481353
C,-4.0325114124,2.0731456167,1.0048357244
C,7.0644243641,0.2091726949,4.6605592716
C,11.8453351881,-3.5730340793,0.2521809283
C,-12.0860412144,-2.1018822244,-3.2313501961
C,-11.0403012011,-1.392275654,-3.8407887238
C,-11.1116304361,-1.0654741409,-5.1943260539
C,-12.2216225164,-1.4362391553,-5.9519872709
B,-10.2896884683,-2.62103597,3.8932209461
B,9.5150463845,-1.4803454907,6.9100997522

C,-13.5219661178,2.0459401742,2.5405956576
C,-14.3203328122,2.8211844543,1.6996515535
C,9.0709808541,0.4440453372,-2.7515188316
C,9.8407171402,0.7704035749,-1.6272252099
C,10.9178785449,1.643754644,-1.7768797993
C,12.8161748747,2.9759946293,-0.6661674672
C,3.6637974997,-3.3868749469,1.1445540279
C,1.7260306622,-2.8925224648,-0.2538865347
C,3.1139685687,-2.8558134019,-0.0345436746
C,3.9554864692,-2.2518192188,-0.981123546
C,5.3344717063,-2.1619103868,-0.7464669638
C,5.8703499425,-2.6814707036,0.4407182066
C,5.0341881154,-3.2956418969,1.3719853059
C,0.5379290085,-2.886295767,-0.4354656777
C,-5.7797737732,0.3528488607,-5.3313405101
C,-5.0131636891,-0.5790215802,-4.5933025589
C,-5.6565756663,-0.7524201109,-3.333429397
C,-12.145115372,3.1641842735,-1.3308841927
C,-12.7336819682,4.1506942297,-2.1753934988
C,-6.8706006458,0.7420893568,-4.5094534846
C,-10.922911401,3.2539761562,-3.229973161
C,-7.9020382352,1.709176428,-4.7973896178
C,-8.7771431959,2.1583883274,-3.8039411985
C,-9.8736486093,2.9407005019,-4.1723470754
C,-11.9706107001,4.2002432415,-3.365927227
C,-3.8347049616,-1.8011016696,-2.0635006644
C,-1.9826554074,-2.7473853634,-0.8090948897
C,-3.3661565898,-2.5968088681,-1.0067777194
C,-4.2855630825,-3.2035326236,-0.1345256452
C,-5.6510145312,-2.9979210125,-0.3138875368
C,6.988105265,-0.7053062068,-3.7185376986
C,-6.1182396104,-2.1922802755,-1.3514643203
C,-5.2099988257,-1.5952290557,-2.2368735212
C,-0.7965185015,-2.8339904973,-0.6353471377
C,5.9260378847,-1.4406751978,-3.1469364334
C,12.3232295142,2.4298852926,1.5016406745
C,6.1747446805,-1.520330782,-1.7439991923
C,13.2174804634,3.1702148881,0.6784482642
C,7.8671232466,-0.3442552001,-2.6594636431
C,11.6850301829,2.1213367129,-0.6481355152
C,12.3418812372,2.3358445903,2.9510840046
C,-12.5970938714,2.7657423932,-0.0090459636
C,-11.8005767634,1.9842774942,0.8414857368
C,-12.2645220697,1.628656217,2.1072894723
B,-8.9540488964,3.1915153647,-6.3980589239
B,10.6459172619,1.6090413873,-4.1859447747

Cartesian Coordination of 4m´·Cl^-_2 (AM1)
–0.8398747 hartree
C,-1.1290542551,0.0178667599,1.500167838
O,-1.1300320975,0.0210346043,10.9257851162
O,2.9878848105,0.0170228876,-12.5525795767
O,1.1291194215,-0.0057837492,-10.9254350887
C,-5.8994179832,-0.2203716165,13.0704661281
C,-7.2830506412,-0.1657640189,12.7889510354
C,1.9834414967,-0.0247948956,-2.6162362543
C,3.3750159597,-0.100626103,-2.4362116194
C,4.2132310572,-0.1108518212,-3.5465609097
C,-1.9975695956,-0.3035381356,9.9799964532
C,-7.430247241,-0.1856896491,11.3672235638
C,-1.7201592938,-0.074538119,6.3635520416
C,-0.3311505183,-0.0177174942,6.6972215556
C,-0.2321360398,-0.0958574152,8.1041492293
C,3.6916277475,-0.0487789642,-4.8379095933
C,-1.9837505873,0.0302638239,2.6165055896
C,8.6734992153,0.1166859225,-10.6174167648
C,8.6889675095,0.0387146436,-9.2147253355
C,9.9025644827,-0.017088474,-8.5311417559
C,11.1106617691,0.0038034383,-9.2262326996
C,11.1026942105,0.0828042276,-10.6183112541
C,9.8958526194,0.1396293685,-11.309918024
C,-8.6735428852,-0.1357271982,10.6166918798
C,-8.6891402723,-0.0579123159,9.2139960298
C,-9.9028741502,-0.0077127757,8.5302171942
C,-11.1109743596,-0.034101667,9.2251126455
C,-11.1028684769,-0.112979122,10.6171997164
C,-0.4062177113,0.008183602,0.5396050744
C,3.804254827,0.3409034702,-11.5608224786
C,5.8993323482,0.2143671664,-13.0706684587
C,7.2827619394,0.153513258,-12.7894223304
C,7.4303093036,0.1723835996,-11.3677191108
C,1.7200979544,0.0857578576,-6.3631565313
C,0.3307902587,0.0360275981,-6.6967136687
C,0.2320303003,0.1148490919,-8.1036250344
C,2.3024677604,0.0252351713,-5.0322153711
C,1.4548675737,0.0390367332,-3.9140749584
C,1.128741237,-0.0124186802,-1.4998977243
C,-2.3026666297,-0.0170304021,5.0325370545
C,-1.455046227,-0.0309328034,3.9144170836
C,1.9983032214,0.3141966824,-9.9796004166
C,-5.2242618134,-0.2828187257,11.8222980363
C,-3.8035319199,-0.3379766398,11.561013427
C,-1.5557262316,-0.2091129255,8.6087605561
C,-3.3219936683,-0.6356187343,10.28477685
C,5.2246840244,0.2794508892,-11.8223626864
C,-3.6919567511,0.0542682567,4.8381750231
C,-4.2136881309,0.1136469016,3.5467482676
C,-3.3754602918,0.1034137768,2.4364074495
C,0.4059081852,-0.0026956414,-0.5393312282
C,1.5561192708,0.2215064602,-8.6083475478
C,3.3242878052,0.6399867045,-10.2843375716
Cl,-5.4058827915,-0.2311115922,7.9238330055
Cl,5.4065329331,0.2264196727,-7.9238382922
F,1.0219829516,-0.877677206,-12.9361764793
F,1.1644108759,1.2810764787,-12.742934261
F,-1.0270500894,0.894027872,12.9362621747
F,-1.1596073905,-1.2654134196,12.7437081814
H,-12.0639834789,0.0061426804,8.6799611622
H,4.3913957345,-0.0561346857,-5.6979779711
H,7.7456985308,0.0227749726,-8.6317019751
H,9.8996521003,-0.0774563369,-7.4326893276
H,12.0635634025,-0.0408390836,-8.6812368589
H,12.0509630411,0.101225534,-11.1736704082
H,9.9016372187,0.2046810464,-12.4076532877
H,-7.7458830897,-0.0376827105,8.6310766319
H,-9.9000603338,0.0525851662,7.4317607659
H,-12.0511305688,-0.1357225818,11.172408861
H,5.4124769687,0.2131129491,-14.0414866422
H,8.0891681476,0.097162932,-13.5116049135
H,-0.4892722728,-0.0521724518,-5.9926133474

H,-0.6668130413,0.0999063921,-8.7134428961
H,0.3646922716,0.1023125061,-4.0493613767
H,-0.3647737576,-0.092298994,4.0498142656
H,-3.9973463835,-1.0275716702,9.5042921469
H,-4.3916855479,0.0614525963,5.6982663785
H,-5.3039985054,0.1685042868,3.4084134008
H,-3.7937978543,0.1511753379,1.4209149189
H,-9.9015513164,-0.2292524205,12.4067353415
H,-3.4889309548,-0.2126372302,7.6218720109
H,-5.946745588,-0.2499758919,9.7739953436
H,3.4893807381,0.2153535951,-7.6216483805
H,5.947409147,0.2428688657,-9.7742268266
H,4.0016421635,1.0281244582,-9.5036383748
H,-5.4127467483,-0.2166677629,14.0413700555
H,-8.089831296,-0.1127880942,13.5109711569
H,3.7932524837,-0.1505246343,-1.4207803393
H,5.3034382707,-0.1679094616,-3.4083007478
H,0.4884751784,0.0746942722,5.9931526894
H,0.6665567401,-0.0762935057,8.7140579552
N,-2.4488414046,-0.1951208566,7.5303633881
N,6.1753347406,0.2529448133,-10.7963052023
N,2.4492560364,0.20277816,-7.5300459471
N,-6.1748289088,-0.2608421812,10.7960614754
O,-2.9888087803,-0.0097270256,12.5526883704
C,-9.8958905062,-0.1642366483,11.3089974219
B,1.5334036318,0.1255589232,-12.3378394357
B,-1.5338229103,-0.111725076,12.3381935261

Cartesian Coordination of 5m (PM6)
–0.33735 hartree
C,6.463,-0.002,1.539
C,7.276,-0.041,0.409
C,3.066,-0.030,-0.008
C,11.384,0.43100,-4.8260
F,13.521,0.72800,-1.6900
F,-13.152,1.3370,2.9460
F,-13.597,-0.79100,2.2120
F,12.839,2.8480,-2.2410
H,9.3680,0.71100,-1.3250
H,8.5140,-0.66900,-5.2000
H,6.3050,-0.96800,-3.6920
H,16.291,1.2810,-7.7030
H,14.387,0.17500,-9.3040
H,12.183,-0.11400,-7.7660
H,4.8530,-0.068000,-1.9810
H,4.4410,0.025000,2.2920
H,6.9160,0.011000,2.5250
H,8.3550,-0.046000,0.53100
H,10.856,0.011000,-5.6700
H,1.3870,4.1220,1.8460
H,3.7690,4.9440,1.8810
H,5.3450,4.3180,0.019000
H,4.5420,2.8680,-1.8790
H,2.1610,2.0450,-1.9150
H,-1.1280,1.0340,2.3710
H,-2.0120,1.8750,4.5780
H,-2.1670,4.3530,5.0100
H,-1.4390,5.9900,3.2380
H,-0.55600,5.1490,1.0330
H,-1.0780,1.0340,-2.5100
H,-1.9560,1.8720,-4.7180
H,-2.1420,4.3490,-5.1410
H,-1.4520,5.9870,-3.3550
H,-0.57400,5.1490,-1.1460
H,-1.2850,-4.2670,1.5140
H,-3.6170,-5.2200,1.4400
H,-5.2030,-4.5250,-0.39000
H,-4.4580,-2.8780,-2.1460
H,-4.8170,0.17300,-2.3470
H,-8.5380,-0.64300,-0.36900
H,-10.565,-1.4680,5.9480
H,15.231,1.5750,-5.4130
H,1.7180,-5.5310,-3.7760
H,0.76800,-4.9300,-1.5200
H,-15.128,-0.57700,6.0930
H,-9.5120,-0.20400,1.6030
H,-8.1890,-1.7460,5.2810
H,-6.0800,-1.6130,3.6140
H,-15.964,-1.1940,8.4110
H,-13.806,-2.1130,9.7930
H,-11.702,-1.9510,8.1040
H,-4.8960,-0.34500,1.9170
H,-7.2730,-0.19800,-2.4310
H,-2.1250,-1.9260,-2.0720
H,1.0480,-1.1050,2.3390
H,1.9480,-2.0780,4.4810
H,2.2360,-4.5720,4.7090
H,1.6240,-6.0900,2.7940
H,0.72300,-5.1160,0.65200
H,1.0580,-0.69300,-2.5250
H,2.0080,-1.2930,-4.7800
H,2.3380,-3.7130,-5.4050
N,-8.8830,-0.57300,2.3010
N,-14.551,-0.94000,6.8380
N,14.761,1.1940,-6.2230
N,8.8450,0.31800,-2.0930
O,11.304,1.0390,-2.5520
O,13.382,1.3380,-3.9430
O,-13.373,-0.39100,4.5060
O,-11.382,-0.27200,2.9690
P,-0.13000,2.4200,-0.059000
P,0.15900,-2.3310,-0.21600
Pt,-0.13000,0.026000,-0.059000
B,12.811,1.5160,-2.5520
C,-3.2530,-0.13000,-0.069000
C,-2.0420,-0.063000,-0.049000
C,1.6190,3.0400,-0.041000
C,2.0730,3.8560,1.0280
C,3.4140,4.3200,1.0490
C,4.3030,3.9670,-0.0020000
C,3.8510,3.1490,-1.0700
C,2.5080,2.6860,-1.0900
C,-0.79600,3.0400,1.5590
C,-1.2060,2.1170,2.5580
C,-1.7030,2.5890,3.8010
C,-1.7910,3.9860,4.0450
C,-1.3810,4.9080,3.0460
C,-0.88300,4.4350,1.8040
C,-0.76100,3.0380,-1.6910
C,-1.1510,2.1150,-2.6980

C,-1.6450,2.5880,-3.9420
C,-1.7510,3.9840,-4.1800
C,-1.3610,4.9060,-3.1740
C,-0.86800,4.4340,-1.9290
C,-1.5540,-3.0440,-0.28000
C,-1.9740,-3.9720,0.71100
C,-3.2880,-4.5080,0.66800
C,-4.1820,-4.1160,-0.36300
C,-3.7620,-3.1890,-1.3530
C,-2.4470,-2.6520,-1.3120
C,0.83700,-3.0480,1.3560
C,1.1830,-2.1910,2.4360
C,1.6900,-2.7410,3.6420
C,1.8530,-4.1460,3.7700
C,1.5070,-5.0010,2.6910
C,1.0000,-4.4530,1.4840
C,0.84400,-2.7730,-1.8830
C,1.9390,0.026000,-0.059000
C,1.1940,-1.7490,-2.8020
C,1.7280,-2.0870,-4.0730
C,1.9150,-3.4500,-4.4250
C,1.5650,-4.4750,-3.5060
C,1.0300,-4.1370,-2.2370
C,-12.568,-0.86800,5.4210
C,-9.3100,-0.91500,3.5650
C,-10.695,-0.74600,3.9210
C,-13.199,-1.1660,6.6800
C,-8.1930,-1.3820,4.2640
C,-7.0920,-1.3020,3.3980
C,-7.5410,-0.79200,2.1730
C,-14.936,-1.2880,8.0920
C,-13.819,-1.7520,8.7750
C,-12.726,-1.6780,7.8900
C,-6.8100,-0.52500,0.93300
C,-5.4240,-0.31000,0.97000
C,-4.6990,-0.062000,-0.20400
C,-5.3770,-0.016000,-1.4370
C,-6.7520,-0.22600,-1.4790
C,-7.4660,-0.48300,-0.31100
C,-11.208,-1.0660,5.1790
C,12.711,0.84600,-4.9510
C,9.3940,0.15600,-3.3460
C,10.755,0.55500,-3.5850
C,13.454,0.75900,-6.1820
C,8.4030,-0.40100,-4.1590
C,7.2520,-0.55900,-3.3720
C,7.5460,-0.10500,-2.0800
C,15.273,1.0120,-7.4680
C,14.282,0.44800,-8.2640
C,13.137,0.28800,-7.4590
C,6.7100,-0.060000,-0.88000
C,5.3130,-0.047000,-1.0000
C,4.4890,-0.019000,0.13600
C,5.0770,0.0070000,1.4140
B,-12.932,-0.0020000,3.1100

Cartesian Coordination of 5p (PM6)
–0.338386 hartree
C,-6.9500,-0.62000,0.13800
C,-3.2470,-0.20500,-0.13200
C,-13.517,0.54300,0.14400
F,-13.226,-1.7890,-2.3550
F,12.303,3.8920,1.5840
F,12.531,3.8460,-0.70100
F,-12.975,-3.2670,-0.79800
H,-16.831,-1.6570,-0.64600
H,-19.123,-0.73300,-0.057000
H,-18.707,1.7090,1.0730
H,-16.031,2.0900,1.0800
H,-11.564,2.6900,1.2300
H,-8.9000,3.0240,1.4000
H,-6.7280,2.7650,0.38200
H,-4.3320,2.2320,0.16400
H,-5.2820,-1.9510,-0.10900
H,-7.6650,-1.4350,0.16300
H,-13.664,1.5260,0.56700
H,1.4610,-4.3880,1.9750
H,3.8440,-4.9220,2.6010
H,5.4180,-3.0690,3.2600
H,4.6120,-0.68100,3.2920
H,2.2320,-0.14700,2.6650
H,-1.0540,-2.8980,-0.77900
H,-1.9350,-5.1510,-1.4790
H,-2.0890,-7.0220,0.20100
H,-1.3620,-6.6400,2.5820
H,-0.48200,-4.3850,3.2860
H,-1.0080,0.94300,2.2360
H,-1.8870,2.1610,4.2600
H,-2.0730,0.96200,6.4690
H,-1.3800,-1.4530,6.6540
H,-0.50200,-2.6710,4.6320
H,-1.2130,1.0520,-4.4180
H,-3.5450,1.6980,-5.1210
H,-5.1330,2.7060,-3.4450
H,-4.3880,3.0700,-1.0650
H,4.6470,-2.3290,-1.3440
H,7.4020,1.0380,1.0310
H,13.781,-0.54000,-0.28300
H,-9.7070,-0.68300,-0.44800
H,1.7840,5.9950,-2.1430
H,0.83700,3.8490,-3.0640
H,9.4810,1.1580,0.15400
H,16.354,3.1700,0.83600
H,18.793,2.4610,0.80200
H,18.821,-0.18700,0.16700
H,16.237,-0.91300,-0.15000
H,11.928,-2.1820,-0.55000
H,9.3610,-2.9700,-0.71100
H,7.1050,-2.4910,-1.4220
H,4.9550,1.2230,1.0570
H,-2.0550,2.4260,-0.36200
H,1.1210,-1.5490,-2.4400
H,2.0250,-2.6310,-4.5290
H,2.3110,-1.2690,-6.6290
H,1.6970,1.1740,-6.6410
H,0.79600,2.2560,-4.5510
H,1.1280,2.0230,0.88900
H,2.0760,4.1680,1.8100
H,2.4050,6.1540,0.29400
N,16.682,2.2380,0.63000

N,9.7400,0.19500,-0.0080000
N,-9.8030,0.19800,0.035000
N,-17.000,-0.76300,-0.21000
O,-12.024,-1.1470,-0.57600
O,-14.463,-1.4730,-0.65600
O,14.043,2.6560,0.63600
O,11.692,1.9640,0.41600
P,-0.058000,-1.8400,1.8140
P,0.23000,1.2180,-1.8260
Pt,-0.058000,-0.36200,-0.069000
B,-13.245,-1.9730,-0.99700
C,2.0120,-0.36100,-0.069000
C,-1.9700,-0.31600,-0.14500
C,1.6930,-2.2350,2.2900
C,2.1480,-3.5800,2.2710
C,3.4900,-3.8820,2.6240
C,4.3770,-2.8370,2.9950
C,3.9220,-1.4910,3.0140
C,2.5810,-1.1920,2.6600
C,-0.72100,-3.4960,1.3010
C,-1.1300,-3.7110,-0.042000
C,-1.6260,-4.9820,-0.43700
C,-1.7130,-6.0360,0.51000
C,-1.3040,-5.8210,1.8520
C,-0.80700,-4.5510,2.2480
C,-0.69000,-0.93900,3.3070
C,-1.0800,0.42200,3.2030
C,-1.5750,1.1090,4.3430
C,-1.6810,0.43300,5.5880
C,-1.2890,-0.92800,5.6920
C,-0.79500,-1.6150,4.5520
C,-1.4830,1.7080,-2.3480
C,-1.9020,1.5010,-3.6880
C,-3.2160,1.8640,-4.0840
C,-4.1110,2.4330,-3.1410
C,-3.6920,2.6390,-1.8000
C,-2.3770,2.2760,-1.4030
C,0.90900,0.42500,-3.3610
C,1.2560,-0.95200,-3.3540
C,1.7650,-1.5610,-4.5310
C,1.9270,-0.79400,-5.7150
C,1.5810,0.58400,-5.7210
C,1.0720,1.1930,-4.5440
C,0.91400,2.8030,-1.1450
C,3.2250,-0.36200,-0.069000
C,1.2630,2.8920,0.22800
C,1.7970,4.1020,0.74900
C,1.9810,5.2210,-0.10600
C,1.6330,5.1310,-1.4790
C,1.0990,3.9230,-1.9980
C,14.401,1.4390,0.31000
C,11.056,-0.19800,-0.10900
C,12.105,0.76400,0.095000
C,17.966,1.7980,0.59600
C,17.952,0.44800,0.27000
C,16.604,0.070000,0.10400
C,11.055,-1.5610,-0.42000
C,9.7160,-1.9700,-0.51300
C,8.9030,-0.85500,-0.25300
C,15.821,1.2020,0.33200
C,7.4490,-0.73900,-0.20900
C,6.6390,-1.6860,-0.86400
C,5.2560,-1.5930,-0.83000
C,4.6240,-0.53900,-0.14200
C,5.4290,0.41200,0.51600
C,6.8130,0.30900,0.48400
C,13.462,0.45600,-0.013000
C,-14.611,-0.27900,-0.13900
C,-11.035,0.75700,0.29400
C,-12.231,0.040000,-0.060000
C,-18.195,-0.21400,0.12700
C,-17.955,1.0290,0.70000
C,-16.559,1.2270,0.70300
C,-10.806,2.0020,0.88700
C,-9.4160,2.1800,0.96700
C,-8.8010,1.0400,0.42700
C,-15.975,0.097000,0.12800
C,-7.3860,0.71000,0.28400
C,-6.4160,1.7290,0.29100
C,-5.0660,1.4340,0.16000
C,-4.6330,0.10400,0.0070000
B,12.622,3.1580,0.47900

Cartesian Coordination of 6m (PM6)
–0.370716 hartree
C,9.2780,-6.8210,-0.23400
F,-0.76200,11.452,-0.27600
F,-2.0750,11.786,-2.1290
F,11.591,-3.7900,-0.46000
F,10.956,-4.3400,-2.5960
H,-5.1330,9.8820,1.1350
H,13.144,-7.6020,-1.1760
H,7.4440,-3.2370,-0.65900
H,6.3390,-7.0510,0.71100
H,4.2040,-5.4240,0.92600
H,14.067,-9.9470,-0.85200
H,12.024,-11.455,0.13300
H,9.8970,-9.7990,0.34100
H,2.8850,-3.6490,-0.096000
H,2.6970,0.64100,-0.19400
H,5.1750,0.74700,-0.037000
H,6.5020,-1.3180,0.13700
H,8.6850,-7.6390,0.14600
H,-3.9270,-4.9090,1.8270
H,-5.6910,-3.7280,0.41800
H,-4.9850,0.48400,4.2090
H,-5.5760,2.6770,3.1870
H,-5.5800,2.9320,0.70900
H,-5.0240,1.0250,-0.74100
H,-4.4570,-1.4600,2.7900
H,-8.9070,-1.1970,-1.7860
H,-8.2860,-1.4880,-4.1800
H,-3.1160,3.3080,-0.39600
H,-0.49700,2.0770,-3.5690
H,-0.32200,4.4370,-4.3310
H,-1.5640,6.2170,-3.1720
H,-2.5190,-6.1080,0.017000
H,-1.0770,-8.0690,-0.37400
H,1.3190,-8.0270,0.29400
H,2.2790,-5.9970,1.3630

H,-3.6300,14.275,0.84700
H,-1.9830,7.6530,-1.4500
H,-5.4570,7.4310,0.90100
H,-4.8630,4.9530,0.034000
H,-5.1970,15.721,2.2250
H,-7.0780,14.051,3.2680
H,-6.4600,11.572,2.3820
H,-5.8910,-1.5910,-4.8450
H,-4.1070,-1.6020,-3.1250
H,-7.1660,-1.2020,-0.050000
H,-1.6920,-0.70000,2.0740
H,-0.88500,0.32800,4.1820
H,-0.39600,-1.0890,6.1700
H,-0.66500,-3.5550,6.0450
H,-1.3380,-4.6350,3.9220
H,0.86900,-4.0120,1.7800
N,12.617,-8.3870,-0.82100
N,-4.4300,13.934,1.3580
N,-2.8010,7.2570,-1.0100
N,6.8770,-3.9640,-0.24600
O,-2.9750,12.156,-0.0020000
O,-2.4200,9.8890,-0.80500
O,9.4110,-4.5400,-0.85100
O,11.360,-6.0430,-1.0440
P,-4.2490,-1.7160,-0.25800
P,-1.9460,-3.4180,1.1960
Pt,-1.9690,-1.6720,-0.27600
C,-4.7850,12.601,1.3710
C,-4.6230,7.1490,0.27400
C,-4.3080,5.8560,-0.16800
C,-3.1610,5.9410,-0.97000
C,-5.3030,14.653,2.1100
C,-6.2500,13.778,2.6280
C,-5.9280,12.487,2.1660
C,-2.4280,4.8960,-1.6880
C,-2.5220,3.5610,-1.2660
C,-1.8350,2.5400,-1.9410
C,-1.0330,2.8660,-3.0500
C,-0.93400,4.1890,-3.4700
C,-1.6260,5.1970,-2.8030
C,-2.0700,0.065000,-1.2060
C,-1.9850,1.2460,-1.4560
C,-4.2840,10.280,0.59900
C,10.617,-7.0140,-0.57900
C,7.3530,-5.2430,-0.061000
C,8.7190,-5.5520,-0.39000
C,11.291,-8.2800,-0.45600
C,6.2950,-6.0050,0.44200
C,5.1800,-5.1600,0.54400
C,5.5610,-3.8850,0.10700
C,13.051,-9.6590,-0.62600
C,11.991,-10.406,-0.12300
C,10.883,-9.5420,-0.016000
C,4.7910,-2.6430,0.023000
C,3.3920,-2.6920,-0.064000
C,2.6300,-1.5150,-0.13800
C,3.2840,-0.27000,-0.13400
C,4.6720,-0.21500,-0.050000
C,5.4230,-1.3860,0.034000
C,-5.5230,-1.4480,-1.4770
C,-6.8640,-1.3010,-1.0980
C,-1.4640,-1.3460,2.9410
C,-1.0170,-0.75200,4.1290
C,-0.73500,-1.5500,5.2430
C,-0.87800,-2.9420,5.1700
C,-1.2710,-3.5470,3.9710
C,-1.5490,-2.7380,2.8690
C,0.42000,-4.8960,1.3130
C,-0.92600,-4.9390,0.94400
C,-1.4740,-6.0670,0.33100
C,-0.66200,-7.1810,0.10200
C,1.2270,-6.0160,1.0780
C,-3.9960,11.645,0.63600
C,-3.6670,8.0190,-0.25500
C,-3.4570,9.4380,-0.14600
C,0.68700,-7.1570,0.47600
C,-5.3370,1.9690,1.1600
C,-5.0300,0.87700,0.34500
C,-4.7340,-0.36000,0.92800
C,-4.6960,-0.50900,2.3130
C,-7.8590,-1.2920,-2.0690
C,-7.5060,-1.4340,-3.4200
C,-6.1630,-1.5170,-3.7910
C,-5.1530,-1.5290,-2.8150
C,-4.6620,-3.3930,0.52000
C,-4.9820,0.60000,3.1250
C,-5.3280,1.8280,2.5500
C,-3.7460,-3.9960,1.2620
C,0.0040000,-1.6720,-0.27600
B,10.866,-4.6280,-1.2610
B,-2.0060,11.345,-0.83600

Cartesian Coordination of 6p (PM6)
–0.350159 hartree
C,-3.6540,-9.7620,-4.3610
F,-5.8700,-7.1240,-6.1950
F,-6.8010,-8.3070,-4.5030
F,9.9790,6.8020,1.5580
F,10.261,5.8700,-0.48100
H,11.659,2.1460,1.6670
H,-3.9350,-6.0690,-2.5400
H,-5.9620,-11.052,-7.5090
H,-5.5060,-13.397,-8.5100
H,-3.3700,-14.394,-7.1720
H,-2.6410,-12.561,-5.3490
H,-1.6840,-9.6230,-1.9720
H,-0.95100,-7.8500,-0.093000
H,-2.0330,-6.0430,1.5850
H,-1.8690,-3.8180,2.6900
H,-2.5060,-1.8870,-1.1170
H,-2.6170,-4.0930,-2.2310
H,-2.9330,-10.462,-3.9450
H,-4.0850,5.5640,1.0160
H,-5.8500,3.8990,1.7960
H,7.2140,3.7100,1.3620
H,-5.1430,1.6760,-3.4170
H,-5.7340,-0.74300,-3.4150
H,-5.7380,-2.0180,-1.2750
H,-5.1820,-0.90000,0.84400
H,-4.6150,2.8420,-1.3120

H,-9.0650,0.67500,2.7280
H,5.1170,-0.30000,0.79100
H,2.6290,-0.27100,0.73200
H,2.6320,3.6580,2.5160
H,5.1070,3.6320,2.5880
H,0.71100,4.7310,0.68000
H,-2.6770,5.8880,3.1620
H,-1.2350,7.5020,4.3430
H,1.1610,7.7450,3.7200
H,2.1210,6.3550,1.8950
H,14.092,6.1460,1.0830
H,16.601,5.5290,1.2650
H,16.698,2.8770,1.8140
H,14.166,1.9870,1.9120
H,9.8320,0.42800,1.9740
H,7.3050,-0.47600,2.0770
H,-8.4440,-0.070000,5.0220
H,-6.0490,-0.25700,5.6670
H,-4.2650,0.47800,4.1130
H,-7.3240,1.4110,1.1550
H,-1.8500,1.8510,-0.98200
H,-1.0430,1.8070,-3.3270
H,-0.55400,3.9290,-4.5330
H,-0.82300,6.1130,-3.3800
H,-1.4960,6.1980,-1.0000
N,-5.2270,-11.681,-7.2180
N,-3.2560,-6.7110,-2.1570
N,7.5230,2.7650,1.5410
N,14.457,5.2240,1.2760
O,11.802,5.4450,1.1600
O,9.4310,4.5960,
O,-4.6440,-7.6060,-4.2680
O,-5.3450,-9.3350,-5.9570
P,-4.4070,1.7890,1.5610
P,-2.1040,3.9460,0.95900
Pt,-2.1270,1.7420,1.5580
C,15.777,4.8460,1.3870
C,15.812,3.4640,1.6680
C,14.483,2.9950,1.7190
C,8.9370,1.0100,1.8550
C,7.6150,0.53600,1.9050
C,6.7410,1.6370,1.7050
C,13.636,4.0950,1.4710
C,5.2810,1.6720,1.6720
C,4.5730,0.56800,1.1630
C,3.1810,0.58300,1.1260
C,2.4690,1.7030,1.6020
C,3.1810,2.8020,2.1270
C,4.5730,2.7840,2.1620
C,1.0560,1.7230,1.5650
C,11.294,3.1580,1.5090
C,-2.2280,-0.22500,1.6700
C,-4.4280,-10.128,-5.4610
C,-3.0490,-8.0150,-2.6590
C,-3.8020,-8.4920,-3.7900
C,-4.9430,-12.933,-7.7180
C,-3.8340,-13.441,-7.0090
C,-3.4500,-12.480,-6.0500
C,-2.0680,-8.6280,-1.8460
C,-1.6830,-7.7010,-0.86200
C,-2.4220,-6.5090,-1.0710
C,-4.3250,-11.381,-6.1790
C,-2.3550,-5.2200,-0.38900
C,-2.1310,-5.1320,0.99300
C,-2.0470,-3.8850,1.6180
C,-2.1850,-2.7090,0.86300
C,-2.4050,-2.8030,-0.53300
C,-2.4790,-4.0410,-1.1520
C,-5.6810,1.0330,2.5530
C,-7.0220,1.0600,2.1470
C,-1.6220,2.8020,-1.4970
C,-1.1750,2.7640,-2.8240
C,-0.89300,3.9570,-3.4970
C,-1.0360,5.1880,-2.8450
C,-1.4290,5.2320,-1.5030
C,-1.7070,4.0340,-0.84400
C,0.26300,5.3350,1.4770
C,-1.0840,5.2180,1.8290
C,-1.6320,5.9830,2.8600
C,0.52900,7.0330,3.1880
C,1.0690,6.2520,2.1620
C,12.195,4.2130,1.3750
C,8.8860,2.4030,1.6210
C,9.9150,3.3960,1.4460
C,-0.81900,6.8980,3.5370
C,-5.4950,-0.95500,-1.2780
C,-5.1880,-0.30800,-0.078000
C,-4.8920,1.0600,-0.087000
C,-4.8540,1.7780,-1.2810
C,-8.0170,0.64200,3.0240
C,-7.6640,0.20100,4.3090
C,-6.3210,0.12000,4.6810
C,-5.3110,0.54200,3.8000
C,-4.8200,3.6380,1.5620
C,-5.1400,1.1150,-2.4840
C,-5.4860,-0.24100,-2.4790
C,-3.9040,4.4970,1.1430
C,-0.15400,1.7420,1.5580
B,-5.7110,-8.0520,-5.2440
B,10.350,5.7290,0.853

Cartesian Coordination of 5m·Cl⁻₂ (PM6)
–0.621463 hartree
C,15.993,-1.3180,-0.089000
Cl,-11.330,-0.073000,-0.16000
Cl,11.203,0.27400,-0.11000
F,12.730,-5.7160,3.1510
F,12.485,-6.4030,1.0180
F,-12.440,6.3730,-2.3560
F,-12.275,6.8580,-0.16000
H,5.9970,-3.5590,1.7550
H,4.7970,-1.9080,0.78700
H,4.6010,2.2530,-0.32500
H,7.0890,2.3960,-0.18600
H,8.4320,0.42500,0.41200
H,15.946,-3.4210,0.64100
H,11.341,-2.2070,0.0030000
H,8.1400,-5.1590,2.0820
H,14.969,0.60600,-0.64800
H,17.026,-1.1070,-0.25000

H,0.65300,-2.5590,-4.0200
H,2.7160,-3.0870,-5.2630
H,4.8760,-3.3760,-4.0630
H,4.9690,-3.1290,-1.5890
H,2.9240,-2.6090,-0.30800
H,-1.6610,-0.55300,-2.8300
H,-3.5050,-1.1640,-4.3570
H,-4.1830,-3.5420,-4.6310
H,-3.0030,-5.3260,-3.3640
H,-1.1560,-4.7580,-1.8290
H,-0.95900,-1.8130,1.5450
H,-1.0980,-3.3080,3.5200
H,-0.15300,-5.6080,3.4330
H,0.94500,-6.4290,1.3600
H,1.1000,-4.9740,-0.63400
H,-0.99200,4.5010,-0.39300
H,-3.1360,5.7180,-0.43100
H,-5.1220,4.8190,0.77200
H,-4.9510,2.6790,2.0240
H,-2.8260,1.4260,2.0810
H,-7.2960,-2.3470,-0.070000
H,-8.5480,-0.27700,-0.51300
H,-15.126,-0.29600,0.17100
H,-17.086,1.5620,-0.0090000
H,9.4720,-1.4280,0.52000
H,12.687,-0.53600,-0.033000
H,1.0080,1.0430,6.4470
H,-0.21800,3.1000,5.7780
H,-0.75800,3.5170,3.4030
H,-9.5080,1.6090,-0.59700
H,-12.778,0.79600,-0.25800
H,-5.9060,3.6960,-1.5000
H,-15.876,3.9100,-0.59200
H,-11.453,2.1460,-1.2670
H,-7.9700,5.4180,-1.7180
H,-4.8000,1.8900,-0.81400
H,-4.8040,-2.3380,0.019000
H,1.2500,2.0270,-1.6220
H,2.9520,3.5640,-2.5580
H,3.8040,5.4730,-1.2090
H,2.9470,5.8550,1.0920
H,1.2390,4.3510,2.0560
H,1.1640,-0.24200,2.3350
H,1.6900,-0.61900,4.7240
N,-8.8440,2.3420,-0.86400
N,13.735,-1.0260,-0.0020000
N,8.8450,-2.1700,0.84900
N,-13.805,1.3280,-0.30200
O,10.974,-4.9160,1.9150
O,-13.266,4.8930,-0.79800
O,-10.771,5.4060,-1.0990
O,13.431,-4.3490,1.4490
P,-0.16700,1.9340,0.91200
P,0.11900,-2.1380,-1.1130
Pt,-0.046000,-0.073000,-0.16000
C,1.1540,0.28300,4.4320
C,0.77200,1.2170,5.3980
C,0.085000,2.3780,5.0220
C,-0.21200,2.6110,3.6750
C,-6.9400,3.4780,-1.3320
C,-15.418,2.9500,-0.45200
C,-12.957,3.6200,-0.83900
C,-14.022,2.6980,-0.55200
C,-7.4660,2.2150,-0.96000
C,-10.585,4.1100,-1.1390
C,-11.641,3.2120,-1.1070
C,-8.0160,4.3790,-1.4530
C,-6.7570,0.96100,-0.69700
C,-5.3540,0.96600,-0.65000
C,-4.6440,-0.21900,-0.38400
C,-5.3510,-1.4200,-0.17900
C,-6.7460,-1.4200,-0.23100
C,-7.4530,-0.24300,-0.48500
C,-9.2000,3.6700,-1.1640
C,-15.018,0.75100,-0.057000
C,-16.042,1.7340,-0.14900
C,7.0130,-3.3190,1.5230
C,6.7020,-0.88800,0.64200
C,5.3020,-0.97000,0.56700
C,4.5400,0.15700,0.21100
C,5.1920,1.3780,-0.057000
C,6.5820,1.4550,0.023000
C,7.3420,0.33300,0.36600
C,3.1290,0.068000,0.10600
C,15.436,-2.5170,0.37100
C,13.012,-3.2710,0.83300
C,14.026,-2.3390,0.42200
C,10.673,-3.8220,1.2600
C,11.640,-3.0460,0.63800
C,8.1310,-4.1560,1.6980
C,9.2700,-3.4420,1.2760
C,7.4700,-2.0830,0.99900
C,0.064000,-3.3150,0.32600
C,-0.62200,-3.6690,2.6090
C,-0.091000,-4.9610,2.5590
C,0.52400,-5.4260,1.3910
C,0.60500,-4.6000,0.26500
C,-1.7580,2.8930,0.86700
C,-1.8440,4.0900,0.15300
C,-3.0580,4.7870,0.12600
C,-4.1720,4.2830,0.80500
C,-4.0760,3.0820,1.5140
C,-2.8660,2.3780,1.5440
C,1.1160,3.1140,0.26800
C,1.5950,2.8810,-1.0230
C,2.5640,3.7410,-1.5560
C,3.0440,4.8110,-0.79600
C,1.5920,4.1740,1.0390
C,0.18400,1.6750,2.7190
C,0.85600,0.50700,3.0810
C,2.5610,5.0280,0.50000
C,-0.54200,-2.8330,1.4880
C,3.9670,-3.1530,-3.5050
C,4.0190,-3.0210,-2.1150
C,2.8550,-2.7260,-1.3940
C,-1.2730,-2.6220,-2.2480
C,-1.9260,-1.6100,-2.9530
C,-2.9750,-1.9480,-3.8180
C,-3.3590,-3.2840,-3.9670
C,-2.6960,-4.2890,-3.2530

C,-1.6480,-3.9590,-2.3860
C,-3.2280,-0.19200,-0.31700
C,1.6480,-2.5630,-2.0780
C,1.5870,-2.6890,-3.4670
C,2.7530,-2.9890,-4.1810
C,-2.0200,-0.15000,-0.26600
C,1.9260,0.0040000,-0.0080000
B,12.416,-5.3760,1.8890
B,-12.198,5.9120,-1.1120

Cartesian Coordination of 5p·Cl^-_2 (PM6)
–0.62902 hartree
F,14.643,3.4820,-0.33100
F,-14.672,-3.4610,-0.20600
H,0.73400,-4.1140,5.4510
H,11.791,-3.3770,-2.0500
H,14.488,-3.3310,-2.2820
H,7.0830,1.3640,-1.8200
H,10.891,-0.96600,-1.6170
H,7.8960,5.8870,-0.56100
H,15.251,-0.75800,-1.9620
H,10.939,0.98700,-0.75300
H,10.583,5.8090,-0.76700
H,-5.8930,-4.8470,-0.42000
H,-3.5880,-3.9320,-0.59300
H,-4.7910,-0.48300,1.7050
H,-7.0910,-1.3680,1.8640
H,-10.868,-1.1630,1.8540
H,9.0970,1.8230,-0.96500
H,-11.818,3.3660,1.9890
H,-14.525,3.3340,2.0370
H,5.9160,4.8330,0.49500
H,3.6100,3.9230,0.68500
H,4.7810,0.48400,-1.6440
H,-3.5250,0.98600,-1.6140
H,-5.9530,0.96800,-1.1440
H,-6.8370,1.8400,1.0060
H,-5.2620,2.7640,2.7020
H,-2.8310,2.8160,2.2710
H,0.63700,1.4080,-2.3050
H,0.86200,2.3890,-4.5640
H,-0.69200,4.1780,-5.3280
H,-2.4960,4.9870,-3.8200
H,-2.7550,4.0340,-1.5550
H,0.63300,1.6020,2.1520
H,1.6180,3.1760,3.7910
H,1.1010,5.6080,3.6760
H,-0.41400,6.4760,1.9070
H,-1.4230,4.9380,0.25800
H,2.8120,-2.8250,-2.1880
H,5.2370,-2.7760,-2.6470
H,6.8310,-1.8470,-0.97200
H,5.9720,-0.96800,1.1860
H,3.5490,-0.98400,1.6820
H,-0.63800,-1.6330,-2.0540
H,-1.6360,-3.2320,-3.6630
H,-1.1200,-5.6610,-3.5110
H,0.40400,-6.5030,-1.7380
H,1.4240,-4.9400,-0.12000
H,-0.62600,-1.3940,2.3970
H,-0.83700,-2.3480,4.6700
H,2.5390,-4.9290,3.9490
H,2.7830,-4.0040,1.6720
H,-9.0980,-1.8390,0.98500
H,-10.901,0.95100,1.6250
H,-15.276,0.76000,1.6910
H,-10.568,-5.8290,0.76000
H,-7.8790,-5.9010,0.60100
N,11.977,-1.2620,-1.7270
N,-9.1130,-2.8610,0.91900
N,9.1180,2.8420,-0.86600
N,-11.990,1.2440,1.7140
O,14.029,1.7460,-1.7130
O,12.589,3.8320,-1.3100
O,-14.066,-1.6900,1.1150
O,-12.619,-3.7820,0.75900
P,-1.1950,1.9390,-0.077000
P,1.2020,-1.9380,0.17100
Pt,0.0030000,0.0000,0.045000
C,11.767,1.6330,-1.0600
C,11.594,3.0130,-1.0780
C,13.084,-0.39000,-1.6950
C,12.961,1.0270,-1.4710
C,14.256,-1.1570,-1.9280
C,8.5030,5.0130,-0.66200
C,2.7650,1.5550,-0.29700
C,6.3270,1.9410,-1.2750
Cl,-9.1890,0.64100,1.5000
Cl,9.1810,-0.64700,-1.4640
F,-14.541,-3.7500,2.0260
F,14.512,3.8220,-2.5560
B,13.971,3.2350,-1.4740
C,-0.058000,2.1990,-2.6200
C,0.073000,2.7470,-3.9050
C,-0.80000,3.7520,-4.3310
C,-1.8120,4.2110,-3.4820
C,-1.9480,3.6730,-2.1980
C,-0.47400,3.1730,1.1140
C,0.37900,2.6710,2.0970
C,0.94500,3.5560,3.0250
C,0.65700,4.9220,2.9560
C,-0.19700,5.4120,1.9620
C,-0.76700,4.5350,1.0300
C,3.0180,-1.9300,-0.21100
C,3.4870,-2.4240,-1.4300
C,4.8600,-2.4020,-1.6970
C,5.7550,-1.8860,-0.75300
C,5.2730,-1.3890,0.46200
C,3.9010,-1.4020,0.73700
C,0.47200,-3.1900,-0.99700
C,-0.38600,-2.7010,-1.9840
C,-0.95800,-3.5990,-2.8950
C,-0.67000,-4.9640,-2.8060
C,0.18800,-5.4410,-1.8080
C,0.76400,-4.5490,-0.89500
C,1.0820,-2.6570,1.8830
C,-2.7580,-1.5580,0.38300
C,0.077000,-2.1760,2.7210
C,-0.046000,-2.7080,4.0130
C,0.83400,-3.7000,4.4500

C,1.8490,-4.1640,3.6030
C,1.9760,-3.6410,2.3120
C,-14.279,1.1550,1.7320
C,-12.965,-1.0440,1.4120
C,-13.097,0.37600,1.6130
C,-9.8950,-4.9950,0.78900
C,-8.4890,-5.0290,0.70000
C,-8.0150,-3.6960,0.78000
C,-11.591,-3.0360,1.0760
C,-6.6500,-3.1760,0.72400
C,-5.6510,-3.8930,0.044000
C,-4.3570,-3.3810,-0.057000
C,-4.0400,-2.1390,0.52700
C,-5.0360,-1.4400,1.2400
C,-6.3280,-1.9460,1.3310
C,-11.738,-1.7150,1.4840
C,-10.284,-3.6470,0.93100
C,-12.466,2.5130,1.8890
C,-13.887,2.4870,1.9100
C,10.291,3.6230,-0.90100
C,8.0250,3.6810,-0.72900
C,6.6580,3.1660,-0.66500
C,5.6670,3.8810,0.028000
C,4.3730,3.3730,0.13800
C,9.9060,4.9750,-0.77400
C,-4.8740,2.3930,1.7550
C,-1.0620,2.6770,-1.7790
C,1.7020,0.99300,-0.16200
C,-3.0160,1.9260,0.28800
C,-3.8870,1.4030,-0.67100
C,-5.2620,1.3870,-0.41200
C,-5.7570,1.8790,0.80100
C,-3.4970,2.4170,1.5020
C,12.443,-2.5240,-1.9710
C,13.857,-2.4900,-2.0950
C,4.0470,2.1350,-0.44900
C,-1.6950,-0.99300,0.25200
B,-14.002,-3.1870,0.92600

Cartesian Coordination of 6m·Cl⁻ (PM6)
–0.540199 hartree
H,4.7370,4.6020,-0.26900
H,2.2560,4.6570,-0.41300
H,2.0420,0.93900,1.7680
H,4.1560,-2.2440,-2.2760
H,6.2130,-3.4010,-5.8690
H,2.3640,-3.1930,-2.9740
H,6.3310,-0.84800,-2.3550
H,7.6880,-1.5260,-4.5980
H,-4.7170,6.5770,0.055000
H,-6.4760,4.7650,0.29800
H,-8.1360,2.0560,-3.1900
H,-7.7960,-0.40700,-3.2220
H,-6.1940,-1.4650,-1.6350
H,-4.9400,-0.092000,-0.018000
H,-6.9040,3.4670,-1.5920
H,-8.3150,1.7140,4.0500
H,-6.5980,1.3470,5.8080
H,-4.1800,1.5840,5.2660
H,-3.4580,2.1920,2.9720
H,-7.6380,2.3210,1.7480
H,-1.6670,3.4070,-1.8670
H,-0.77900,3.8870,-4.1300
H,-0.59700,6.2310,-4.9470
H,-1.2990,8.1190,-3.4920
H,-2.1840,7.6880,-1.2220
H,0.10400,5.3240,1.1980
H,-3.6820,7.3350,1.9880
H,-2.5350,8.8300,3.5720
H,-0.093000,8.6020,3.9800
H,1.2110,6.8450,2.7900
H,0.75800,-3.4720,-1.5970
H,3.9050,-1.0960,1.2260
H,3.2010,-4.5920,-0.15200
H,6.0200,1.7350,3.6040
H,4.5090,-8.0300,1.9960
H,-0.76300,-6.8020,-3.7820
H,-2.5100,-6.1940,-1.8110
H,-2.1220,-5.6540,0.89900
H,-3.3860,-1.9600,2.7290
H,-1.3440,-1.8860,-1.0700
H,4.0170,-3.2610,1.2750
H,2.2190,-6.6120,-1.4180
N,4.8730,-2.2720,-3.0520
N,3.3250,-5.5690,0.12000
N,4.5100,-0.68500,1.9410
N,0.13100,-4.2160,-1.9100
O,1.6600,-5.9330,-4.7410
O,3.9070,-4.8870,-5.3880
O,6.1140,-3.3310,3.8660
O,5.4670,-5.6740,3.0620
P,-2.6480,5.0810,0.26100
P,-4.8880,2.7710,0.54400
Pt,-2.6090,2.8200,0.54300
C,3.7140,-4.0190,-4.4320
C,2.7550,3.8450,0.10700
C,1.9900,2.8150,0.68800
C,2.6380,1.7470,1.3390
C,0.57500,2.8500,0.63500
C,5.9810,-2.8960,-4.9500
C,6.7450,-1.9230,-4.2870
C,6.0420,-1.5580,-3.1120
C,2.5230,-4.0040,-3.6910
C,1.5580,-4.9930,-3.8370
C,4.8100,-3.1140,-4.1820
C,4.1490,3.8090,0.18900
Cl,2.9010,-2.3020,-0.73300
F,7.5140,-5.1440,3.9530
F,5.6790,-5.0900,5.2710
F,3.3560,-7.0820,-5.7650
F,2.2740,-5.4550,-6.9030
H,-3.2070,-4.4400,2.7780
H,3.0160,-8.8410,-0.10600
H,6.7130,-0.75000,4.4170
H,5.8790,2.7390,0.91900
C,-1.8950,6.8470,-1.8530
C,-1.9650,8.0700,3.0420
C,-0.59100,7.9400,3.2730
C,0.14200,6.9570,2.6030
C,2.8270,-6.6760,-0.52700

C,3.2480,-7.8330,0.16600
C,6.0250,-0.48500,3.6350
C,4.0350,1.7300,1.4290
C,0.38900,-5.0930,-2.9840
C,5.6650,0.80600,3.2100
C,4.0270,-7.4130,1.2600
C,-0.68200,-6.0120,-3.0560
C,-1.5890,-5.6950,-2.0300
C,-1.0740,-4.5760,-1.3320
C,4.7470,-5.0940,2.1400
C,4.0750,-6.0000,1.2340
C,5.3500,-2.8610,2.9140
C,-1.6790,-3.8510,-0.21100
C,-2.2040,-4.5690,0.87600
C,-2.8130,-3.8840,1.9290
C,-2.9150,-2.4910,1.9060
C,-2.3920,-1.7670,0.81800
C,-1.7640,-2.4540,-0.23900
C,-2.5600,0.85100,0.70100
C,-2.4950,-0.35500,0.76800
C,4.6520,-3.7010,2.0500
C,5.3100,-1.4130,2.8440
C,4.7220,0.66300,2.1630
C,-2.0010,5.5260,-1.4150
C,-0.49400,6.1000,1.6960
C,-1.8640,6.2460,1.4680
C,-2.6090,7.2180,2.1370
C,-7.2530,0.20800,-2.5060
C,-7.2600,1.8300,3.8100
C,-6.2910,1.6220,4.7990
C,-4.9330,1.7580,4.4970
C,-4.5340,2.1070,3.2000
C,-5.5140,2.3170,2.2270
C,-6.8720,2.1770,2.5110
C,-1.6060,4.4520,-2.2160
C,-1.1000,4.7150,-3.4970
C,-0.99500,6.0310,-3.9520
C,-1.3910,7.0970,-3.1330
C,-6.3570,-0.38600,-1.6130
C,-5.6510,0.40100,-0.69400
C,-5.8590,1.7820,-0.68100
C,-6.7450,2.3890,-1.5730
C,-7.4460,1.5950,-2.4870
C,-5.4040,4.5780,0.31500
C,-4.4880,5.5230,0.20000
C,-0.63400,2.8610,0.60400
B,2.8020,-5.8610,-5.7330
B,6.2140,-4.8260,4.0660

Cartesian Coordination of $6m_2 \cdot Cl^-_2$ (chiral *MM*) (PM6)
–1.07894 hartree
C,-2.4110,0.028000,8.9300
H,-1.2430,-6.0650,-4.9260
H,-0.63500,-7.1250,-7.0940
H,-1.3940,-6.1150,-9.2340
H,-2.7550,-4.0490,-9.2290
H,-1.0980,-1.2990,-7.4680
H,-5.0750,-0.86300,-9.1990
H,-4.1460,0.66600,-10.894
H,-1.7220,1.2170,-10.903
H,-0.21200,0.23200,-9.1830
H,7.4460,-1.7910,-7.1400
H,4.2980,-0.057000,-5.4930
H,2.9330,1.3670,-4.0210
H,0.50300,0.90900,-3.7010
H,0.81700,-2.5080,-6.3120
H,4.1090,-4.7890,-8.9560
H,1.9730,-3.7460,-7.6800
H,11.325,0.60100,-6.1830
H,13.157,-0.71700,-7.6780
H,11.844,-2.6960,-8.9700
H,-8.5160,0.99800,7.3350
H,-7.8810,0.69900,3.6410
H,9.0540,-0.55300,-6.5690
H,5.4050,-1.4320,-6.6760
H,-5.6280,-3.1980,-8.4820
H,-8.5770,-1.6990,6.7170
H,-5.0650,-0.49200,7.1050
H,7.8610,1.6020,-7.8400
H,7.4620,1.8130,-4.1200
H,-3.1050,-0.80200,10.878
H,-1.4190,0.37500,9.1290
H,-10.900,-2.3440,5.8200
H,-12.216,-3.6030,7.8250
H,-10.550,-3.6510,9.9510
H,-1.1620,2.0760,3.0670
H,-3.6240,1.9320,3.4280
H,-4.5360,1.0480,5.5460
H,-6.7860,-1.4810,7.8070
H,-0.50300,0.36400,6.9710
H,10.948,3.7990,-9.7930
H,7.9790,5.8630,1.1770
H,9.6600,4.4450,2.3350
H,6.8860,0.39600,2.1850
H,7.6910,-0.18800,6.4290
H,9.0530,-2.1670,5.8770
H,9.3500,-2.8740,3.5120
H,8.2590,-1.5880,1.6790
H,6.3620,2.2880,0.43400
N,-9.2680,1.2700,7.9700
N,9.9350,-0.83800,-7.0030
N,4.7960,-2.1520,-7.0730
N,-9.2910,-2.1970,7.2540
N,7.8800,2.3000,-3.3220
N,8.4550,1.9850,-8.5800
N,-4.3370,-0.43600,7.8240
N,-8.2790,1.0480,2.7640
O,-5.6530,-1.8340,10.920
O,-11.520,2.5430,3.4810
O,-12.022,2.6070,5.9930
O,6.7900,-4.2920,-9.2420
O,9.2710,-3.6540,-9.2170
O,10.718,4.2520,-4.5090
O,-8.0340,-2.7400,10.630
O,10.982,4.1220,-7.0560
P,-3.7750,-2.3530,-6.9310
P,6.1730,1.7370,4.6940
P,3.8170,2.0370,6.9020
P,-6.2360,-2.1570,-4.8330
Pt,-4.0020,-1.7150,-4.7550

Pt,3.9010,1.5650,4.6740
C,2.7560,-0.59100,9.9230
C,3.4830,4.6210,8.0260
C,2.8480,3.4640,7.5710
C,1.4560,3.3540,7.5730
C,0.68700,4.4200,8.0580
C,1.3110,5.5780,8.5280
C,2.7070,5.6800,8.5100
C,5.6230,2.3560,7.3740
C,6.5830,2.2410,6.4730
C,4.1320,-0.073000,-0.62700
C,4.5860,-0.22200,-1.9380
C,9.5320,2.8720,-8.3710
C,9.0020,3.1500,-3.4010
C,5.6840,0.50700,-2.4040
C,9.9260,3.3530,-7.0650
C,9.2510,3.0200,-5.8890
C,9.6710,3.4810,-4.6390
C,6.2870,4.8940,2.1030
C,5.8590,3.8880,2.9800
C,3.1580,0.57500,9.2630
C,3.3190,0.54600,7.8770
C,3.0810,-0.61300,7.1350
C,9.3780,2.4330,-10.600
C,8.3660,1.7150,-9.9270
C,7.4820,2.2090,-2.0010
C,8.3600,3.0120,-1.2220
C,9.2980,3.5910,-2.0890
C,6.3350,1.4160,-1.5510
C,5.8800,1.5740,-0.23300
C,4.7850,0.82400,0.23800
C,4.3860,0.98500,1.5880
C,8.1420,-1.2720,2.7170
C,8.7510,-1.9950,3.7460
C,8.5860,-1.5950,5.0780
C,7.8150,-0.46900,5.3820
C,7.2220,0.25200,4.3440
C,7.3690,-0.14200,3.0130
C,6.8160,3.0960,3.6170
C,8.1830,3.2840,3.4010
C,8.5990,4.2910,2.5240
C,7.6510,5.0910,1.8740
C,4.1070,1.1540,2.7530
C,10.105,3.1510,-9.6330
C,-1.1880,0.72700,6.2080
C,-2.5750,0.65400,6.4110
C,1.9300,1.4380,4.7110
C,0.72900,1.3500,4.8330
C,-7.9600,-2.3610,9.3820
C,-6.8130,-1.7560,8.8660
C,-5.6870,-1.5070,9.6550
C,-9.1510,-2.6030,8.5970
C,-4.4890,-0.87300,9.1560
C,-3.4520,1.0960,5.4070
C,-2.9380,1.6020,4.2090
C,-1.5600,1.6850,4.0030
C,-0.67400,1.2510,5.0070
C,-10.357,-3.2370,8.9790
C,-11.221,-3.2110,7.8690
C,-10.544,-2.5590,6.8150
C,-3.0770,0.11300,7.6770
C,2.6760,-1.7750,7.8060
C,2.5140,-1.7620,9.1940
Cl,6.9100,0.38200,-6.0090
Cl,-7.0370,-0.098000,5.7640
F,11.422,6.0020,-5.8150
F,8.5050,-5.8130,-9.3510
F,8.1580,-4.3980,-11.078
F,-12.666,4.2410,4.5160
F,-13.597,2.1870,4.3810
F,-6.4460,-3.7140,11.970
F,12.739,4.1780,-5.5860
F,-7.2830,-1.6870,12.522
H,8.9340,2.6580,3.8830
H,10.106,4.2530,-1.8360
H,8.3030,3.1430,-0.16100
H,7.6270,1.0470,-10.341
H,9.5580,2.4190,-11.655
H,3.1850,-0.63500,6.0370
H,3.3260,1.4830,9.8430
H,4.7800,3.7320,3.1310
H,5.5500,5.5090,1.5860
H,8.3560,2.3940,-5.9470
H,6.0240,0.35700,-3.4330
H,4.0770,-0.91300,-2.6130
H,3.2750,-0.64000,-0.26800
H,7.6360,2.4230,6.6780
H,5.7960,2.6250,8.4140
H,3.1890,6.5880,8.8650
H,0.71000,6.4060,8.9020
H,-0.40100,4.3430,8.0570
H,0.93700,2.4650,7.1900
H,4.5670,4.7340,8.0080
H,2.6180,-0.58600,11.002
H,2.1880,-2.6640,9.7110
H,2.4740,-2.6840,7.2390
H,-2.9950,-1.3870,0.46200
H,-3.6320,-0.86500,2.8160
H,-5.8080,0.16800,3.3290
H,-8.9840,1.4070,5.3210
H,-12.247,2.4980,8.7380
H,-10.798,1.6610,10.861
H,-8.4520,0.71800,9.8950
H,-8.4500,1.6080,-0.48100
H,-10.579,2.5300,0.89700
H,-6.7520,0.23400,-0.90100
H,-7.5570,-3.0310,-6.8430
H,-8.3510,-6.5280,-3.6650
H,-8.6730,-5.9180,-1.2760
H,-7.9250,-3.6910,-0.44600
H,-6.8700,-2.0740,-1.9760
H,-7.3020,-4.9400,-5.2310
H,-10.354,0.68200,-4.4950
H,-9.0510,2.7930,-4.3590
H,-6.5630,2.7350,-4.4290
H,-5.3590,0.57700,-4.6330
H,-9.1930,-1.4930,-4.7000
H,-2.6070,-3.9940,-4.8740
C,-2.4450,-4.4870,-8.2800
C,-1.5890,-5.6290,-5.8630

C,-2.3620,-4.4610,-5.8430
C,-8.6060,-0.57500,-4.6590
C,-7.2110,-0.58900,-4.7040
C,-6.4620,0.58600,-4.6240
C,-7.1340,1.8100,-4.5040
C,-8.5310,1.8410,-4.4620
C,-9.2670,0.65100,-4.5400
C,-7.4440,-4.6410,-4.1920
C,-7.0440,-3.3910,-3.7170
C,-7.2060,-3.0400,-2.3750
C,-7.7990,-3.9570,-1.4970
C,-8.2150,-5.2070,-1.9630
C,-8.0360,-5.5500,-3.3080
C,-6.5300,-2.7690,-6.6000
C,-10.357,2.0320,3.7880
C,-3.2860,-0.58200,9.8420
C,-6.0780,-0.015000,-0.084000
C,-6.4340,0.28300,1.2420
C,-9.7190,2.0180,1.2880
C,-8.6130,1.5330,0.57400
C,-7.7230,0.92900,1.5030
C,-9.2760,1.1420,9.3400
C,-10.504,1.6360,9.8320
C,-11.262,2.0700,8.7290
C,-2.0720,-1.2930,-4.7740
C,-9.9800,1.8100,5.1140
C,-10.834,2.0950,6.1820
C,-5.5490,-0.036000,2.2860
C,-9.5130,1.7200,2.6550
C,-10.493,1.8410,7.5640
C,-4.3170,-0.63200,1.9980
C,-3.9570,-0.92800,0.68400
C,-4.8440,-0.62600,-0.36800
C,-4.2640,-1.2340,-2.8570
C,-4.5170,-0.95000,-1.7090
C,-1.6740,-5.6540,-8.2890
C,-1.2460,-6.2220,-7.0820
C,1.2810,-1.6510,-5.8280
C,2.4630,0.52500,-4.5320
C,10.071,-1.9100,-7.9100
C,5.2240,-3.1690,-7.9500
C,3.2370,-0.29200,-5.3610
C,8.9630,-2.7320,-8.3440
C,7.6530,-2.5600,-7.8900
C,6.5990,-3.3410,-8.3660
C,-0.88600,-1.0710,-4.8680
C,-1.2740,-0.020000,-9.1920
C,-2.1220,0.53500,-10.154
C,-3.4870,0.22300,-10.151
C,-4.0060,-0.65000,-9.1880
C,-3.1460,-1.2070,-8.2400
C,-1.7850,-0.89500,-8.2250
C,-2.7820,-3.9100,-7.0560
C,0.50100,-0.81700,-5.0080
C,1.1030,0.27300,-4.3500
C,-5.5260,-2.8470,-7.4570
C,4.0910,-3.9400,-8.2980
C,2.6500,-1.3910,-6.0100
C,12.114,-0.94800,-7.6110
C,11.167,-0.25300,-6.8260
C,3.4320,-2.2790,-6.8740
C,2.9820,-3.3930,-7.6340
C,11.433,-1.9770,-8.2860
B,11.494,4.6630,-5.7400
B,-6.8540,-2.5060,11.546
B,-12.483,2.9110,4.5860
B,8.1890,-4.5680,-9.7440

Cartesian Coordination of $6m_2 \cdot Cl^-_2$ (meso) (PM6)
–1.079713 hartree
C,5.782,-6.971,-0.814
H,3.3310,2.7800,-1.4220
H,2.6900,0.41500,-0.96200
H,6.7910,-0.50000,0.0070000
H,11.016,1.7630,0.44000
H,8.8150,0.20500,0.51100
H,7.8600,10.002,-2.8650
H,10.274,11.225,-2.7320
H,12.034,9.3890,-1.8200
H,-8.0600,-5.6020,5.9240
H,-4.4230,-5.6920,5.0830
H,-6.0680,-6.1710,6.3140
H,-3.9760,-3.9670,3.8150
H,-3.4410,-2.5130,1.8960
H,-1.1920,-2.6010,0.82700
H,-9.5950,-8.0920,9.0260
H,-11.655,-6.7780,7.8730
H,-10.603,-5.2290,5.9140
H,-0.27900,-6.3810,5.7900
H,-1.6980,-7.7640,7.6230
H,0.049000,-5.5700,3.6970
H,-10.009,0.77700,-2.1330
H,-9.5910,2.6680,-3.6940
H,-7.9100,6.7300,-1.8380
H,-5.9880,8.1110,-2.7550
H,6.7170,-7.3890,-1.1800
H,4.7460,-8.7870,-0.40000
H,3.8730,-9.7360,4.2370
H,1.5190,-9.5080,5.0080
H,-0.093000,-8.1320,3.7050
H,0.62200,-6.9900,1.6340
H,4.6300,-8.6120,2.1760
H,0.014000,-9.7300,-2.4130
H,-0.77100,-7.8250,-3.8020
H,0.15500,-5.5440,-3.4360
H,1.8650,-5.1440,-1.6850
H,1.7170,-9.3770,-0.65400
H,5.5330,-3.9800,1.8920
H,7.2420,-3.2680,3.5420
H,9.6660,-3.4410,3.0060
H,10.398,-4.3310,0.80500
H,8.7270,-5.0520,-0.87100
H,6.1610,-6.4370,-3.4110
H,6.8290,-5.5420,-5.6080
H,7.2330,-3.1070,-5.9100
H,6.9530,-1.5490,-3.9870
H,7.7460,3.9670,-1.1770
H,8.1810,7.5810,-2.0610
N,8.2800,3.2060,-0.74700
N,-8.7180,-6.0580,6.5620

N,8.9260,8.2820,-2.1130
N,-3.5440,-6.0290,5.4880
N,-7.4710,-3.4780,1.2050
N,9.0040,6.0260,-4.9150
N,-7.8120,-8.1520,3.6800
N,3.7830,6.5100,-4.1170
O,7.3370,7.6540,-7.7160
O,-6.8610,-8.3050,8.7490
O,-4.3440,-8.2580,8.2550
O,12.057,6.7400,-1.0650
O,11.741,4.2870,-0.39200
O,4.8200,7.9100,-7.3150
O,-9.9200,-8.0200,0.71200
O,-9.7320,-5.7690,-0.49700
P,-6.5210,5.0180,-0.53700
P,-4.0680,6.7840,-1.7050
P,3.1770,-6.8610,0.21700
P,5.6960,-5.0800,-0.76400
Pt,3.6500,-4.6340,0.13500
Pt,-4.2490,4.8360,-0.53700
C,-2.0800,-7.1410,6.8360
C,-1.3460,-6.4280,5.8760
C,-2.2690,-5.7410,5.0410
C,-10.083,-5.8860,6.5920
C,-10.620,-6.7000,7.6150
C,-9.5490,-7.3860,8.2170
C,-0.43600,-4.1140,2.1790
C,-1.4210,-3.2390,1.6790
C,-2.6780,-3.1930,2.2820
C,-2.9760,-4.0100,3.3760
C,-3.4530,-6.8930,6.6000
C,-8.3620,-6.9880,7.5600
C,-4.6030,-7.3740,7.3290
C,-5.9080,-6.9370,7.0790
C,-7.0000,-7.4160,7.8020
C,10.982,9.2570,-1.9910
C,10.062,10.211,-2.4640
C,8.7980,9.5850,-2.5360
C,7.7980,1.9590,-0.39500
C,8.8800,1.2080,0.14200
C,10.025,2.0160,0.11000
C,6.4010,1.5540,-0.56800
C,6.0410,0.21900,-0.31500
C,4.7060,-0.19700,-0.46500
C,3.7260,0.73500,-0.86000
C,4.0900,2.0570,-1.1130
C,10.275,8.0510,-1.7720
C,9.6560,3.2660,-0.44200
C,5.4180,2.4720,-0.97500
C,10.773,6.7770,-1.3010
C,9.9610,5.6570,-1.1180
C,10.471,4.4380,-0.65900
C,4.3570,-1.5520,-0.24100
C,0.83000,-4.2130,1.5500
C,1.9040,-4.3230,1.0060
C,6.7910,-2.6200,-3.8540
C,6.9440,-3.4950,-4.9330
C,6.7190,-4.8660,-4.7630
C,6.3450,-5.3670,-3.5120
C,6.2060,-4.4840,-2.4390
C,6.4170,-3.1130,-2.5970
C,7.0340,-4.5840,0.41600
C,8.3880,-4.6800,0.096000
C,9.3370,-4.2710,1.0390
C,8.9230,-3.7680,2.2790
C,7.5630,-3.6730,2.5830
C,6.6040,-4.0810,1.6460
C,1.3970,-8.5330,-1.2660
C,1.9100,-7.2490,-1.0780
C,1.4790,-6.1660,-1.8460
C,0.51100,-6.3820,-2.8360
C,-0.0100000,-7.6630,-3.0390
C,0.43200,-8.7380,-2.2570
C,3.5890,-8.5070,2.4850
C,2.6710,-7.7500,1.7550
C,1.3490,-7.6040,2.1820
C,0.93700,-8.2440,3.3590
C,1.8440,-9.0140,4.0920
C,3.1680,-9.1440,3.6570
C,4.7590,-7.6990,-0.40100
C,-1.9950,-4.8750,3.8920
C,-0.72500,-4.9180,3.2960
Cl,-6.5610,-5.0080,4.1880
Cl,6.6690,5.7730,-2.3950
F,-5.2350,-8.5130,10.355
F,13.250,5.7030,0.59900
F,13.552,5.0740,-1.5530
F,-11.675,-6.9710,-0.32500
F,-9.9730,-7.7830,-1.5700
F,5.7500,7.4390,-9.3590
F,6.1050,9.4590,-8.4100
F,-5.5060,-10.151,8.8180
H,-4.6290,-0.92200,4.4590
H,-6.1260,-2.4980,3.3030
H,-7.7570,-5.9510,2.1820
H,10.059,7.2140,-7.8210
H,12.011,6.1970,-6.2500
H,10.825,5.3330,-3.9750
H,0.60000,7.2730,-4.5360
H,2.1790,7.9990,-6.6030
H,-0.012000,5.8910,-2.8830
H,0.94400,4.4140,1.0540
H,3.3600,4.8550,0.62400
H,4.1010,5.8350,-1.5130
H,6.3540,6.3070,-4.8280
H,8.3030,5.8100,-4.2040
H,4.6100,6.1530,-3.6300
H,-7.3250,-7.2580,3.7680
H,-7.1410,-3.9250,2.0650
H,-0.26700,9.5240,-0.11300
H,-1.6920,11.377,0.74800
H,-4.1670,11.236,0.55700
H,-5.2310,9.2740,-0.49100
H,-1.2880,7.5430,-1.1660
H,-3.1340,8.6830,-3.8610
H,-1.9010,8.2690,-5.9650
H,-1.2610,5.9570,-6.6120
H,-1.8820,4.0340,-5.1590
H,-3.1200,4.4030,-3.0440
H,-9.2080,5.6000,0.75700

H,-4.9840,5.5620,1.8350
H,-5.5960,6.2920,4.1250
H,-7.9770,6.6760,4.7370
H,-9.7710,6.3280,3.0540
H,-8.0950,4.5180,-3.0460
H,-7.4010,2.5630,0.78600
H,-8.9090,0.73500,0.10000
H,6.2840,-2.4000,-1.7720
H,-9.8710,-10.315,2.2470
H,-8.6970,-11.215,4.5100
H,-7.1020,-9.2250,5.4180
H,-7.7780,-1.0970,-1.0570
H,-9.1940,-3.3230,-1.6200
H,-6.2100,0.14500,-0.13500
H,-3.9410,1.2130,3.3710
H,8.8860,5.7410,-1.3040
H,5.6720,3.5130,-1.1930
C,9.9520,6.7770,-6.8450
C,-5.8870,-0.086000,0.88000
C,-6.2800,-1.2850,1.4960
C,-8.5700,-3.1440,-0.76300
C,-7.8380,-1.9850,-0.46300
C,-7.1600,-2.2020,0.76700
C,-7.7230,-9.2270,4.5350
C,-8.5590,-10.257,4.0510
C,-9.1730,-9.7910,2.8740
C,4.0610,-2.7120,-0.064000
C,-8.4970,-6.2850,1.4490
C,-9.0460,-7.5640,1.5690
C,-5.8290,-1.5750,2.7950
C,-8.3440,-4.0770,0.27500
C,-8.7090,-8.4760,2.6400
C,-4.9870,-0.67800,3.4580
C,-4.6000,0.51800,2.8540
C,-5.0600,0.82800,1.5590
C,-2.2740,4.8360,-0.53700
C,-1.8240,6.1270,-5.6940
C,-2.1820,7.4320,-5.3280
C,-2.8810,7.6590,-4.1390
C,-3.2180,6.5710,-3.3320
C,-1.9410,8.3510,-0.80900
C,-3.3310,8.2920,-0.92100
C,-4.1430,9.3160,-0.43000
C,-3.5460,10.431,0.17000
C,-2.1530,10.508,0.27900
C,-1.3530,9.4710,-0.20600
C,-4.4800,3.1140,0.40300
C,-4.7280,2.0590,0.94200
C,-1.0770,4.9570,-0.66200
C,0.31000,5.1500,-0.87900
C,0.72900,5.6870,-2.1110
C,2.0890,5.9380,-2.3510
C,2.4750,7.5060,-5.6950
C,1.6580,7.1270,-4.6190
C,-8.8680,-5.4190,0.41900
C,2.4840,6.5080,-3.6420
C,10.358,5.7900,-4.8350
C,10.965,6.2460,-6.0260
C,-6.0450,5.7440,2.0850
C,-7.0660,5.5610,1.1500
C,-8.4070,5.7630,1.4790
C,-2.8750,5.2640,-3.6860
C,-2.1720,5.0470,-4.8790
C,4.9990,7.2880,-6.1790
C,6.2580,6.8370,-5.7800
C,7.3990,7.0500,-6.5580
C,3.0350,5.6430,-1.3540
C,3.8010,7.1220,-5.3850
C,8.7260,6.6430,-6.1530
C,2.6170,5.0940,-0.13800
C,1.2650,4.8460,0.10800
C,-5.8600,7.2420,-2.1130
C,-6.8610,6.5180,-1.6410
C,-9.1200,2.6610,-2.7130
C,-9.3540,1.5960,-1.8350
C,-8.7390,1.5740,-0.58000
C,-7.8900,2.6190,-0.19500
C,-7.6740,3.6810,-1.0760
C,-8.2740,3.7100,-2.3360
C,-8.7310,6.1710,2.7770
C,-7.7190,6.3650,3.7250
C,-6.3810,6.1520,3.3830
B,-5.4800,-8.8310,9.0730
B,12.687,5.4480,-0.59400
B,-10.348,-7.1480,-0.44600
B,6.0000,8.1300,-8.2330

Cartesian Coordination of 6p$_2$·Cl$^-_2$ (chiral *MM*) (PM6)
–1.09057 hartree
H,-0.77000,5.3660,4.9440
H,-2.3210,6.8940,6.1480
H,-3.8820,8.3470,4.8720
H,-3.9040,8.2930,2.4000
H,-3.9940,4.6100,-0.62700
H,-4.1890,8.9140,0.029000
H,-6.4910,8.9250,-0.85500
H,-7.5610,6.8110,-1.6190
H,-6.3080,4.6710,-1.5040
H,8.7510,-1.1980,-2.0290
H,5.3820,1.1300,-2.3740
H,3.8540,2.9800,-1.7570
H,0.68000,0.13800,-1.0140
H,2.2060,-1.7190,-1.6270
H,5.6350,-4.5340,-3.6000
H,3.3960,-3.0450,-3.3560
H,12.373,1.1580,-0.34100
H,14.377,-0.64100,-0.64400
H,13.261,-2.9060,-1.6020
H,-9.3730,-3.2440,-0.76600
H,-6.8000,-2.1280,1.5900
H,10.194,0.0070000,-1.0840
H,6.6700,-0.79900,-1.8200
H,-1.9110,9.2040,0.13000
H,-10.251,-0.14000,-0.057000
H,-6.8250,0.43900,-1.2950
H,9.2150,2.8770,-2.4000
H,6.8990,2.3580,0.38900
H,-6.0110,3.6600,-3.9690
H,-3.7410,2.2420,-3.6110
H,-12.337,-1.0690,1.1340

H,-14.382,0.63100,0.62000
H,-13.390,2.6080,-0.93200
H,-0.77400,-0.35600,-0.88500
H,-3.9720,-3.2570,-0.65000
H,-5.5740,-1.5800,-1.5180
H,-8.9200,0.80200,-1.3850
H,-2.3730,1.3300,-1.7520
H,11.304,6.5680,-2.8540
H,-1.4280,-7.4320,-5.0520
H,-2.6880,-8.8750,-3.4690
H,-1.9660,-4.5330,2.0630
H,-2.9040,-8.6490,0.98700
H,-5.0600,-8.4480,2.1850
H,-5.6830,-6.3250,3.3120
H,-4.1300,-4.3770,3.2460
H,1.9940,-0.34300,2.6980
N,-10.017,-4.0290,-0.91500
N,11.120,-0.43100,-1.0960
N,6.1100,-1.5530,-2.2260
N,-11.181,0.29200,-0.079000
N,6.6460,2.7810,1.2860
N,9.8330,3.6010,-2.7870
N,-6.3160,1.0750,-1.9130
N,-6.4560,-2.3390,2.5320
O,-8.5780,3.7470,-2.9080
O,-7.8810,-5.5250,3.5430
O,-9.5800,-6.3850,1.8260
O,8.2940,-4.4090,-2.7990
O,10.732,-3.8750,-2.2120
O,8.1270,6.0970,1.4010
O,-10.942,3.3870,-1.9830
O,9.6400,6.5240,-0.62500
P,-2.2210,6.6820,0.43600
P,-0.67900,-6.6520,0.55900
P,2.3290,-6.4330,1.7230
P,0.65500,6.5980,-1.0360
Pt,-0.77100,5.0320,-0.18500
Pt,0.80700,-4.9510,0.88800
C,3.6880,-6.5390,5.6430
C,4.6730,-7.8880,1.0730
C,3.9750,-6.6850,0.92500
C,4.5030,-5.6300,0.17900
C,5.7580,-5.7830,-0.42600
C,6.4650,-6.9800,-0.28500
C,5.9210,-8.0320,0.46300
C,1.4480,-8.1080,1.6540
C,0.21700,-8.1980,1.1830
C,3.5730,-1.3460,1.6100
C,4.8900,-1.2420,1.1230
C,10.061,4.8610,-2.1990
C,7.1290,4.0250,1.7530
C,5.6270,-0.076000,1.3270
C,9.4470,5.2730,-0.95200
C,8.6880,4.4150,-0.15900
C,8.0160,4.8600,0.98200
C,-0.42800,-6.3210,-3.4960
C,-0.26200,-6.1460,-2.1140
C,3.5560,-6.8270,4.2790
C,2.6010,-6.1380,3.5330
C,1.7880,-5.1580,4.1070
C,11.256,4.7390,-4.1330
C,10.554,3.5250,-3.9560
C,5.7960,2.2510,2.2350
C,5.7430,3.1510,3.3350
C,6.5660,4.2460,3.0330
C,5.0650,1.0000,2.0350
C,3.7560,0.89200,2.5400
C,3.0170,-0.26800,2.3300
C,2.7860,-2.5000,1.3750
C,-3.8510,-5.3150,2.7590
C,-4.7210,-6.4070,2.7930
C,-4.3700,-7.6040,2.1570
C,-3.1520,-7.7100,1.4800
C,-2.2920,-6.6080,1.4490
C,-2.6260,-5.4110,2.0850
C,-0.97200,-6.9710,-1.2400
C,-1.8470,-7.9520,-1.7070
C,-2.0050,-8.1190,-3.0880
C,-1.2950,-7.3030,-3.9780
C,2.0680,-3.4530,1.1740
C,10.946,5.5710,-3.0400
C,-2.7210,0.31800,-1.5350
C,-4.0740,-0.020000,-1.7290
C,-0.53400,-3.6720,0.19600
C,-1.3410,-2.8780,-0.22800
C,-10.517,2.2400,-1.5220
C,-9.2150,1.7950,-1.7400
C,-8.2670,2.5770,-2.4080
C,-11.493,1.4860,-0.75900
C,-6.8900,2.1890,-2.5680
C,-4.5210,-1.3110,-1.3980
C,-3.6240,-2.2580,-0.90400
C,-2.2670,-1.9270,-0.72500
C,-1.8260,-0.62600,-1.0410
C,-12.862,1.7580,-0.53900
C,-13.376,0.72700,0.27100
C,-12.318,-0.16700,0.54400
C,-4.9840,0.99300,
C,1.9280,-4.8770,5.4730
C,2.8740,-5.5660,6.2360
Cl,8.0980,1.1040,-1.3150
Cl,-8.1740,-1.2820,-0.23000
F,8.3500,8.1310,0.37600
F,9.7500,-5.9190,-1.8840
F,10.100,-5.1860,-3.9890
F,-8.1810,-7.7360,3.0370
F,-9.8290,-6.6140,4.1000
F,-9.9560,5.4420,-2.2230
F,10.106,7.2630,1.5000
F,-10.499,4.2540,-4.0640
H,-2.4210,-8.5850,-1.0290
H,3.3130,1.7270,3.0810
H,6.7560,5.1090,3.6440
H,5.1810,2.9970,4.2320
H,10.544,2.6560,-4.5930
H,11.904,4.9730,-4.9500
H,1.0540,-4.5890,3.5120
H,4.2130,-7.5720,3.8300
H,0.41200,-5.3550,-1.7500
H,0.11300,-5.6780,-4.1890

H,8.6120,3.3570,-0.43400
H,6.6410,0.0000,0.92300
H,5.3250,-2.0730,0.56900
H,-0.34600,-9.1260,1.1240
H,2.0170,-8.9550,2.0300
H,6.4760,-8.9620,0.56700
H,7.4430,-7.0900,-0.76000
H,6.1850,-4.9650,-1.0120
H,3.9680,-4.6780,0.049000
H,4.2710,-8.7230,1.6460
H,4.4310,-7.0630,6.2390
H,2.9830,-5.3420,7.2960
H,1.3050,-4.1110,5.9320
H,-5.2640,2.2060,0.59900
H,-1.7240,0.97300,2.7380
H,-2.9760,-0.93900,3.7080
H,-8.5730,-3.2700,1.1880
H,-11.455,-6.9150,-0.16000
H,-12.276,-5.8340,-2.4950
H,-10.914,-3.5130,-2.8100
H,-4.7070,-1.8960,5.2910
H,-6.3080,-4.0690,5.3570
H,-6.5160,0.28400,1.5420
H,0.35100,9.1390,-1.0180
H,5.1550,8.6650,-0.30200
H,5.9090,6.8500,1.2140
H,4.3780,4.9570,1.7470
H,2.1060,4.8630,0.77800
H,2.8890,8.6140,-1.2970
H,2.2290,7.8270,-5.6420
H,0.84000,6.0740,-6.7230
H,-0.58600,4.5770,-5.3380
H,-0.63900,4.8190,-2.8710
H,2.2070,8.1030,-3.1860
H,-0.75900,5.2780,2.4660
C,-3.1980,7.6620,2.9420
C,-1.4430,6.0150,4.3840
C,-1.4380,5.9770,2.9830
C,1.5780,7.3380,-3.6430
C,0.76700,6.4980,-2.8800
C,-0.014000,5.5010,-3.4710
C,0.013000,5.3550,-4.8650
C,0.81600,6.1940,-5.6410
C,1.5980,7.1840,-5.0330
C,3.1950,7.8090,-0.62900
C,2.3490,6.7400,-0.32200
C,2.7560,5.7150,0.53300
C,4.0420,5.7610,1.0880
C,4.8990,6.8210,0.78700
C,4.4740,7.8470,-0.069000
C,-0.19300,8.2550,-0.69600
C,-7.8260,-4.4170,2.8440
C,-5.8720,2.7930,-3.3490
C,-5.4690,0.43800,1.8190
C,-6.1880,-3.3700,4.5500
C,-5.3520,-2.2440,4.5120
C,-5.5220,-1.6170,3.2470
C,-10.851,-4.2140,-1.9940
C,-11.553,-5.4270,-1.8190
C,-11.129,-5.9920,-0.60200
C,-4.8290,-0.45300,2.6980
C,0.50900,3.6150,-0.69600
C,-8.6110,-4.2360,1.7030
C,-9.4350,-5.2440,1.2050
C,-3.4790,-0.24500,3.0360
C,-6.8770,-3.4390,3.3140
C,-10.171,-5.1190,-0.036000
C,-2.7760,0.82700,2.4970
C,-3.4110,1.7180,1.6050
C,-4.7680,1.5190,1.2830
C,-1.9800,3.6530,0.55600
C,-2.6630,2.7790,1.0380
C,-3.1950,7.6920,4.3410
C,-2.3170,6.8710,5.0580
C,2.5620,-0.68800,-1.6820
C,3.4940,1.9530,-1.7430
C,11.379,-1.7520,-1.5110
C,6.6300,-2.7940,-2.6630
C,4.3480,0.90800,-2.0950
C,10.341,-2.6470,-1.9850
C,9.0200,-2.2490,-2.1740
C,8.0200,-3.1520,-2.5520
C,1.2810,2.7370,-1.0060
C,-5.8350,5.5970,-1.1640
C,-6.5400,6.8010,-1.2300
C,-5.9380,7.9910,-0.79800
C,-4.6340,7.9760,-0.29700
C,-3.9400,6.7640,-0.23500
C,-4.5250,5.5730,-0.66600
C,-2.3130,6.8100,2.2820
C,1.7100,0.35300,-1.3300
C,2.1640,1.6870,-1.3610
C,-1.3710,8.2870,-0.097000
C,5.5480,-3.5470,-3.1820
C,3.8860,-0.41900,-2.0780
C,13.344,-0.80100,-0.86500
C,12.307,0.14500,-0.70400
C,4.7500,-1.5370,-2.4530
C,4.3870,-2.7740,-3.0550
C,12.765,-1.9840,-1.3650
B,9.0670,7.0350,0.67800
B,-10.005,4.2340,-2.8140
B,-8.8780,-6.5910,3.1480
B,9.7280,-4.8760,-2.7340

Cartesian Coordination of $6p_2 \cdot Cl^-_2$ (meso) (PM6)
–1.09411 hartree
H,3.0810,2.5150,-1.3660
H,0.80900,6.0500,-0.38100
H,1.5210,7.1010,-2.5200
H,3.0430,7.9320,-7.1270
H,1.4830,7.3870,-4.9930
H,10.534,2.2970,-5.9860
H,11.797,3.1920,-8.2030
H,10.199,5.0660,-9.3210
H,-8.5120,-4.9450,3.7850
H,-7.6590,-1.2830,3.7690
H,-9.0320,-2.8960,3.7130
H,-5.5460,-1.0340,3.8840
H,-3.1270,-0.62500,3.6500

H,-3.8370,3.6200,3.3410
H,-12.590,-6.1850,3.8150
H,-11.018,-8.3830,3.7870
H,-8.4520,-7.5170,3.7770
H,-8.4120,2.9070,3.9390
H,-10.777,1.6140,4.0060
H,-6.2760,3.2260,3.5550
H,-7.0000,-6.2480,-3.5720
H,-6.5780,-4.9760,-5.6660
H,-5.0480,-0.39900,-5.1400
H,-3.1730,0.42900,-6.6380
H,5.0660,0.96500,4.9700
H,3.2800,-0.18500,6.3590
H,0.83200,2.1770,9.7710
H,-1.6360,1.8730,9.8280
H,-2.8370,1.0480,7.8090
H,-1.5990,0.51700,5.7430
H,2.1090,1.6540,7.7290
H,-0.11200,-4.1640,5.6480
H,-0.46300,-4.5110,3.2120
H,-0.074000,-2.6500,1.6110
H,0.67000,-0.42500,2.4240
H,0.62800,-1.9620,6.5050
H,1.9460,4.3960,4.0430
H,2.5260,6.7090,4.7320
H,4.9020,7.4410,4.8230
H,6.7210,5.8590,4.2210
H,6.1880,3.5420,3.5340
H,4.9210,-0.44400,2.6820
H,6.3290,-1.1450,0.78200
H,6.8000,0.42100,-1.0850
H,5.8430,2.7190,-1.0710
H,5.0670,5.1110,-4.6530
H,8.3030,3.5740,-5.8140
N,4.3480,5.7510,-5.0010
N,-9.3390,-5.5470,3.7820
N,8.9920,3.7060,-6.5520
N,-8.1350,-0.37700,3.8020
N,-4.3240,-5.9820,4.7640
N,9.2950,5.4770,-3.1630
N,-8.6260,-3.8630,7.0420
N,8.0980,0.32400,-3.4740
O,12.270,3.3740,-3.1080
O,-12.314,-3.4470,3.8940
O,-11.729,-0.95400,3.9530
O,7.7740,6.2610,-8.8450
O,5.5180,7.2240,-8.1160
O,11.692,0.88300,-3.2790
O,-7.3270,-6.6980,8.9270
O,-5.2420,-7.7060,7.8370
P,-3.6090,-1.6440,-3.4320
P,-1.2160,-0.60300,-5.3570
P,1.2410,0.62300,5.0450
P,3.5250,2.1120,3.2830
Pt,1.2440,1.9960,3.2210
Pt,-1.3330,-1.8250,-3.4320
C,-9.7950,1.1780,3.9420
C,-8.5630,1.8480,3.9040
C,-7.5350,0.87000,3.8150
C,-9.3520,-6.9230,3.7770
C,-10.695,-7.3630,3.7840
C,-11.516,-6.2210,3.8000
C,-4.2200,2.6080,3.4560
C,-3.3170,1.5270,3.4790
C,-3.8190,0.21800,3.6350
C,-5.1880,-0.0050000,3.7580
C,-9.5340,-0.21000,3.8780
C,-10.672,-5.0860,3.7990
C,-10.474,-1.3080,3.8740
C,-10.093,-2.6500,3.8080
C,-11.032,-3.6850,3.8310
C,10.014,4.4960,-8.4290
C,10.841,3.5190,-7.8470
C,10.192,3.0440,-6.6870
C,3.1380,6.0360,-4.3940
C,2.4490,6.9770,-5.2030
C,3.2580,7.2610,-6.3150
C,2.7190,5.4110,-3.1420
C,1.8650,6.1000,-2.2640
C,1.4660,5.5150,-1.0630
C,1.9140,4.2250,-0.72200
C,2.7530,3.5260,-1.6170
C,8.8580,4.6160,-7.6220
C,4.4400,6.4940,-6.1970
C,3.1590,4.1150,-2.8090
C,7.7210,5.4930,-7.7900
C,6.6420,5.5360,-6.9030
C,5.5710,6.4120,-7.0950
C,1.5820,3.6190,0.51100
C,-1.9240,1.7390,3.3580
C,-0.72700,1.8960,3.2640
C,5.6490,2.0390,-0.23200
C,6.1840,0.74800,-0.24500
C,5.9220,-0.13500,0.80900
C,5.1260,0.27100,1.8840
C,4.6080,1.5690,1.8940
C,4.8540,2.4560,0.84300
C,4.0410,3.8220,3.7750
C,5.3770,4.2190,3.8100
C,5.6840,5.5300,4.1940
C,4.6580,6.4210,4.5300
C,3.3230,6.0100,4.4820
C,3.0050,4.7010,4.0980
C,0.49400,-2.1000,5.4320
C,0.71200,-1.0670,4.5200
C,0.51800,-1.2430,3.1480
C,0.098000,-2.4950,2.6800
C,-0.12200,-3.5400,3.5810
C,0.076000,-3.3460,4.9540
C,1.0290,1.5040,7.7300
C,0.34500,1.0270,6.6110
C,-1.0420,0.86600,6.6230
C,-1.7540,1.1730,7.7910
C,-1.0790,1.6380,8.9220
C,0.31000,1.8070,8.8910
C,3.0680,0.44600,5.4980
C,-6.0910,1.0740,3.7220
C,-5.5890,2.3810,3.5760
Cl,-6.6740,-3.5080,4.2110
Cl,6.6640,3.4640,-3.8680

F,-13.526,-1.8220,2.8210
F,6.0950,6.8300,-10.300
F,7.1610,8.4520,-9.1410
F,-6.8110,-8.9320,8.9710
F,-5.5130,-7.4680,10.103
F,13.411,1.7160,-2.0070
F,13.523,1.8420,-4.2640
F,-13.493,-1.8800,5.0820
H,-0.93800,-5.9760,-0.041000
H,-1.5990,-7.1790,2.0270
H,-6.3790,-5.0370,6.1960
H,12.539,6.1070,-2.9220
H,10.969,8.3060,-2.9300
H,8.4090,7.4460,-3.1480
H,8.3510,-2.9640,-3.4470
H,10.724,-1.6920,-3.3250
H,6.1790,-3.2660,-3.5260
H,3.7260,-3.6260,-3.4930
H,3.1010,0.64400,-3.4910
H,5.5350,1.0210,-3.5490
H,8.9860,2.8260,-3.2290
H,8.4700,4.8770,-3.2510
H,7.6320,1.2330,-3.5370
H,-8.0040,-3.6840,6.2530
H,-5.0040,-5.2360,4.5920
H,2.9600,1.9960,-5.9160
H,1.8330,4.2150,-5.7990
H,-0.62400,4.3430,-5.4620
H,-1.9740,2.2880,-5.2670
H,1.6490,-0.088000,-5.7200
H,-0.55500,-0.18300,-8.2890
H,0.10900,-1.7950,-10.045
H,0.35500,-4.2090,-9.5060
H,-0.059000,-5.0220,-7.1920
H,-0.72300,-3.4400,-5.4000
H,-6.3040,-0.88900,-2.2840
H,-2.0780,-0.19400,-1.4640
H,-2.7160,1.1680,0.51300
H,-5.1100,1.5010,1.0920
H,-6.8930,0.48000,-0.30800
H,-5.1190,-2.9870,-5.6490
H,-4.4680,-3.5470,-1.3770
H,-5.9370,-5.5260,-1.4380
H,4.4300,3.4660,0.82300
H,-9.6220,-5.4410,9.7800
H,-11.230,-3.4080,9.0090
H,-10.148,-2.3530,6.7640
H,-1.6780,-7.8700,4.2020
H,-3.0060,-8.5040,6.4620
H,-4.1580,-3.8600,3.1270
H,-3.4870,-2.6750,1.0720
H,6.6310,4.8610,-6.0430
H,3.8330,3.5670,-3.4740
C,11.467,6.1440,-2.9890
C,-3.4420,-4.3330,2.4460
C,-3.2480,-7.7280,5.7580
C,-2.5600,-7.3970,4.5790
C,-3.2400,-6.3080,3.9690
C,-9.7750,-3.1740,7.3580
C,-10.330,-3.7340,8.5290
C,-9.4970,-4.7940,8.9310
C,-2.9040,-5.6020,2.7350
C,1.3650,3.0550,1.5600
C,-6.3560,-5.8170,6.9620
C,-7.3340,-5.8180,7.9610
C,-2.0060,-6.1900,1.8230
C,-4.3460,-6.8460,5.8780
C,-8.4320,-4.8780,8.0030
C,-1.6360,-5.5200,0.65900
C,-2.1630,-4.2450,0.37700
C,-3.0740,-3.6620,1.2830
C,0.64200,-1.8250,-3.4320
C,0.053000,-3.5080,-8.7290
C,-0.087000,-2.1490,-9.0350
C,-0.46600,-1.2420,-8.0390
C,-0.70500,-1.7160,-6.7490
C,1.1270,0.87500,-5.6850
C,-0.25700,0.96300,-5.5180
C,-0.89900,2.2000,-5.4300
C,-0.14000,3.3710,-5.5370
C,1.2450,3.2960,-5.7210
C,1.8780,2.0520,-5.7900
C,-1.5470,-2.9260,-1.8070
C,-1.8110,-3.5490,-0.80300
C,1.8460,-1.7030,-3.4660
C,4.1310,-2.6150,-3.5050
C,5.5080,-2.4080,-3.5210
C,6.0380,-1.1040,-3.5270
C,9.7460,-1.2470,-3.3800
C,8.5090,-1.9060,-3.4420
C,-5.3450,-6.7790,6.9230
C,7.4880,-0.91900,-3.4980
C,9.3080,6.8510,-3.1040
C,10.647,7.2870,-2.9920
C,-3.1440,-0.043000,-1.2320
C,-4.1600,-0.61200,-2.0050
C,-5.5090,-0.43400,-1.6930
C,-0.56200,-3.0670,-6.4250
C,-0.18100,-3.9670,-7.4300
C,10.435,1.2370,-3.2990
C,10.051,2.5800,-3.2390
C,10.987,3.6130,-3.1460
C,5.1550,-0.0070000,-3.5300
C,9.4960,0.14500,-3.3930
C,10.625,5.0120,-3.0950
C,3.7790,-0.21000,-3.5090
C,3.2480,-1.5180,-3.4920
C,-3.0170,-0.17600,-5.7470
C,-3.9940,-0.61300,-4.9710
C,-6.1200,-4.6530,-4.7340
C,-6.3550,-5.3700,-3.5550
C,-5.7610,-4.9650,-2.3570
C,-4.9330,-3.8350,-2.3290
C,-4.7170,-3.1220,-3.5090
C,-5.2940,-3.5230,-4.7150
C,-5.8480,0.33700,-0.57700
C,-4.8420,0.91300,0.21000
C,-3.4960,0.72500,-0.11400
B,-12.804,-2.0170,3.9370
B,6.6380,7.2140,-9.1320

B,-6.2210,-7.7250,8.9890
B,12.763,1.9450,-3.1610

Cartesian Coordination of 6m·Cl^-_2 (PM6)
–0.65093 hartree
H,-2.6500,-0.36300,0.72200
H,-2.6120,2.1150,0.53700
H,-4.5820,3.4420,1.1820
H,7.4000,-3.3350,-1.5790
H,10.150,-4.8820,-4.4260
H,5.9000,-4.6150,-2.1940
H,9.3480,-1.7910,-1.4800
H,11.227,-2.6660,-3.2560
H,-8.5480,-6.9860,1.0260
H,-6.9110,-8.7500,1.8630
H,-4.5130,-8.0450,-3.2710
H,-2.0950,-8.6350,-3.1860
H,-0.89300,-8.6400,-1.0030
H,-2.0830,-8.0840,1.0750
H,-5.7490,-7.5160,-1.2060
H,-3.7210,-11.967,2.9040
H,-3.0550,-11.346,5.2220
H,-2.8900,-8.9510,5.8750
H,-3.5720,-7.1670,4.2950
H,-4.4030,-10.225,1.3080
H,-4.7700,-4.7520,-0.84300
H,-4.6450,-3.9440,-3.1850
H,-6.7250,-3.4550,-4.4620
H,-8.9470,-3.7240,-3.3850
H,-9.1130,-4.3970,-1.0090
H,-7.7030,-2.1900,0.72100
H,-8.9450,-5.5790,3.1610
H,-10.598,-4.1360,4.2860
H,-10.821,-1.7410,3.6550
H,-9.3680,-0.78000,1.8790
H,4.2970,-5.0430,-0.85700
H,-6.1090,4.4410,2.1600
H,-5.1430,7.8430,2.5850
H,-8.6460,1.0430,2.0920
H,-7.8490,10.739,4.1200
H,3.2450,-8.5580,-2.8940
H,1.3090,-7.9660,-1.0950
H,-0.11500,-6.1760,-0.13200
H,-0.0100000,-3.5570,3.2700
H,3.6460,-4.6240,1.2880
H,-6.3840,6.2740,3.1000
H,-3.8780,9.9860,2.5250
N,8.2280,-3.4430,-2.1890
N,-5.5400,8.7350,2.9280
N,-6.9220,3.8200,2.2970
N,3.7600,-5.8620,-1.1090
O,5.7130,-7.5930,-3.6770
O,7.8510,-6.4590,-4.1660
O,-9.6480,5.8320,3.6000
O,-8.9860,8.1880,3.9160
P,-4.7940,-7.3090,1.7000
P,-6.9290,-5.0050,1.0250
Pt,-4.7470,-5.0290,1.7000
C,7.4700,-5.4770,-3.3900
C,-3.5110,0.22400,1.0220
C,-3.4940,1.6120,0.92400
C,-4.6050,2.3630,1.3030
C,-4.6880,-1.8560,1.6230
C,8.4420,-4.4490,-3.1150
C,9.7100,-4.2530,-3.6670
C,10.259,-3.1080,-3.0620
C,9.3170,-2.6370,-2.1510
C,6.2000,-5.4480,-2.8160
C,5.3870,-6.5740,-2.9170
C,-4.6560,-0.43000,1.5130
Cl,-4.3450,5.9000,1.8770
Cl,4.8730,-2.5840,-1.2160
F,-11.227,7.5340,3.8390
F,7.4790,-8.6950,-4.7340
F,6.3490,-7.0540,-5.8750
F,-9.9540,6.9320,5.6520
H,2.4600,-3.3830,3.0500
H,-5.5000,11.967,3.4740
H,-10.084,3.2800,2.8910
H,-6.6370,-0.17500,2.3060
C,-8.0410,-3.9370,-2.8190
C,-9.9670,-3.7220,3.5020
C,-10.091,-2.3720,3.1480
C,-9.2750,-1.8330,2.1490
C,-5.7420,10.916,3.3780
C,-9.0160,3.2360,2.7300
C,-5.7580,1.7320,1.8040
C,4.1670,-6.7270,-2.1000
C,-8.2760,2.0450,2.2510
C,-6.9570,10.289,3.7110
C,3.1600,-7.6830,-2.2480
C,2.1420,-7.3670,-1.3360
C,2.5330,-6.2210,-0.63200
C,-7.7640,7.8550,3.5850
C,-6.8170,8.9290,3.4270
C,-8.4040,5.5620,3.2820
C,1.8510,-5.4880,0.43700
C,0.45700,-5.5820,0.57000
C,-0.22000,-4.8950,1.5890
C,0.51300,-4.0930,2.4840
C,1.8950,-3.9940,2.3540
C,2.5640,-4.6850,1.3460
C,-2.7850,-5.1300,1.8790
C,-1.6000,-5.0450,1.6480
C,-7.4050,6.5290,3.3500
C,-8.1380,4.2220,2.8130
C,-6.9830,2.5000,1.9460
C,-4.8920,9.9240,2.8930
C,-8.1300,-4.3300,-1.4790
C,-6.9560,-4.6090,-0.78000
C,-8.3360,-2.6400,1.4950
C,-8.2310,-3.9850,1.8520
C,-9.0310,-4.5340,2.8570
C,-3.9830,-8.0410,-2.3180
C,-4.6870,-7.7560,-1.1380
C,-3.6980,-10.919,3.2020
C,-3.3000,-10.566,4.5020
C,-3.2330,-9.2230,4.8760
C,-3.6240,-8.2130,3.9810
C,-4.0730,-8.5830,2.7180

C,-4.0850,-9.9240,2.3110
C,-5.7020,-4.5230,-1.3890
C,-5.6190,-4.0760,-2.7140
C,-6.7880,-3.7940,-3.4290
C,-2.6270,-8.3870,-2.2680
C,-1.9550,-8.3970,-1.0430
C,-2.6430,-8.0900,0.13300
C,-4.0090,-7.7940,0.080000
C,-6.6420,-7.7210,1.6380
C,-7.4870,-6.8060,1.1910
C,-4.7470,-3.0550,1.7000
B,6.8500,-7.4780,-4.6610
B,-9.9950,7.1280,4.2870

Cartesian Coordination of 6p·Cl^-_2 (PM6)
–0.59265 hartree
C,-2.8760,-3.9090,3.9280
Cl,-6.6470,-1.8250,5.4170
Cl,6.6930,5.2010,-2.6100
F,13.553,3.5820,-3.0160
F,13.440,3.4410,-0.75900
F,-5.4880,-5.8250,11.283
F,-6.7860,-7.2810,10.140
H,-4.1300,-2.1700,4.3320
H,10.998,10.037,-1.6380
H,-1.6510,-6.1870,5.3800
H,-10.122,-0.68700,7.9760
H,-11.204,-1.7580,10.214
H,-9.5970,-3.7960,10.972
H,-3.1420,2.1850,-5.4040
H,-5.0180,1.3470,-3.9130
H,-6.5480,-3.2270,-4.4700
H,-6.9700,-4.5120,-2.3840
H,-5.9090,-3.8050,-0.24500
H,-4.4390,-1.8260,-0.17100
H,-5.0890,-1.2370,-4.4390
H,-6.8650,2.1930,0.92500
H,-5.0820,3.2050,2.3330
H,-2.6870,2.8760,1.7520
H,-2.0490,1.5270,-0.23400
H,-6.2750,0.83700,-1.0600
H,-0.69300,-1.6920,-4.1910
H,-0.028000,-3.2620,-5.9940
H,-2.9800,-6.8360,7.6350
H,12.569,7.8370,-1.6450
H,-6.3530,-3.3680,7.3920
H,-1.5710,-5.4810,3.2090
H,-0.90900,-4.2640,1.1500
H,-3.4600,-0.97100,2.2850
H,-7.9780,-2.0150,7.4570
H,7.6620,2.9680,-2.2940
H,8.4990,6.6100,-1.9830
H,9.0150,4.5590,-1.9750
H,5.5640,2.7560,-2.3080
H,3.1310,2.3780,-2.2540
H,3.7560,-1.8910,-2.2840
H,6.2090,-1.5310,-2.3130
H,10.753,0.041000,-2.1010
H,8.3800,-1.2300,-2.2320
H,8.4390,9.1780,-1.8630
H,0.38600,-2.4330,-8.3020
H,0.14100,-0.016000,-8.8250
H,-0.52400,1.5850,-7.0590
H,1.6800,1.6620,-4.4880
H,-1.9440,4.0350,-4.0200
H,-0.59400,6.0910,-4.2010
H,1.8630,5.9660,-4.5380
H,2.9900,3.7470,-4.6690
H,-4.9780,-3.5560,5.7870
N,9.3240,7.2090,-1.8910
N,8.1280,2.0580,-2.2370
N,-8.6000,-2.2000,8.2450
N,-4.2980,-4.3020,5.9540
O,-5.2170,-6.0480,9.0150
O,-7.3020,-5.0470,10.111
O,11.722,2.6160,-2.0370
O,12.299,5.1060,-1.8490
P,-3.5800,0.090000,-2.2120
P,-1.1860,1.1440,-4.1290
Pt,-1.3040,-0.090000,-2.2120
B,-6.1960,-6.0750,10.166
C,-2.9860,1.5740,-4.5170
C,-3.9640,1.1320,-3.7450
C,-6.0910,-2.9090,-3.5350
C,-6.3260,-3.6340,-2.3610
C,-5.7320,-3.2380,-1.1610
C,-4.9040,-2.1080,-1.1240
C,-4.6870,-1.3870,-2.3000
C,-5.2640,-1.7800,-3.5080
C,-5.8200,2.0520,0.65600
C,-4.8130,2.6230,1.4470
C,-3.4680,2.4370,1.1220
C,-3.1150,1.6760,-0.0010000
C,-4.1320,1.1130,-0.78000
C,-5.4800,1.2890,-0.46500
C,-0.53100,-1.3120,-5.2140
C,-0.15000,-2.2050,-6.2250
C,0.084000,-1.7380,-7.5210
C,-0.055000,-0.37700,-7.8170
C,-0.43500,0.52300,-6.8150
C,-0.67500,0.041000,-5.5290
C,1.1580,2.6250,-4.4470
C,-0.22700,2.7120,-4.2800
C,-0.86900,3.9480,-4.1830
C,-0.11000,5.1190,-4.2820
C,1.2750,5.0450,-4.4670
C,1.9080,3.8020,-4.5440
C,-1.5180,-1.2020,-0.59500
C,-1.7820,-1.8330,0.40400
C,1.8750,0.032000,-2.2450
C,0.67100,-0.090000,-2.2120
C,-5.3200,-5.1150,8.1070
C,10.464,2.9700,-2.0550
C,10.080,4.3130,-1.9860
C,11.017,5.3450,-1.8860
C,5.1850,1.7280,-2.2960
C,9.5250,1.8790,-2.1570
C,10.655,6.7440,-1.8260
C,3.8090,1.5250,-2.2770
C,3.2770,0.21600,-2.2690

C,4.1610,-0.88000,-2.2890
C,5.5370,-0.67300,-2.3030
C,6.0680,0.63100,-2.3010
C,9.7750,0.48700,-2.1530
C,8.5380,-0.17100,-2.2210
C,7.5170,0.81600,-2.2690
C,9.3380,8.5830,-1.8230
C,10.677,9.0180,-1.7070
C,11.497,7.8750,-1.7120
C,-6.3300,-4.1530,8.1530
C,-7.3080,-4.1610,9.1510
C,-1.9780,-4.4910,3.0130
C,-4.3200,-5.1740,7.0620
C,-8.4070,-3.2210,9.1990
C,-1.6080,-3.8140,1.8530
C,-2.1350,-2.5360,1.5800
C,-3.0460,-1.9600,2.4890
C,-3.4140,-2.6380,3.6480
C,-3.2220,-6.0560,6.9360
C,-2.5330,-5.7170,5.7600
C,-3.2130,-4.6230,5.1580
C,-9.7490,-1.5120,8.5650
C,-10.305,-2.0800,9.7320
B,12.792,3.6780,-1.9120

[S4 (as a complete Ref. 10)] *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

4. Anion-binding properties

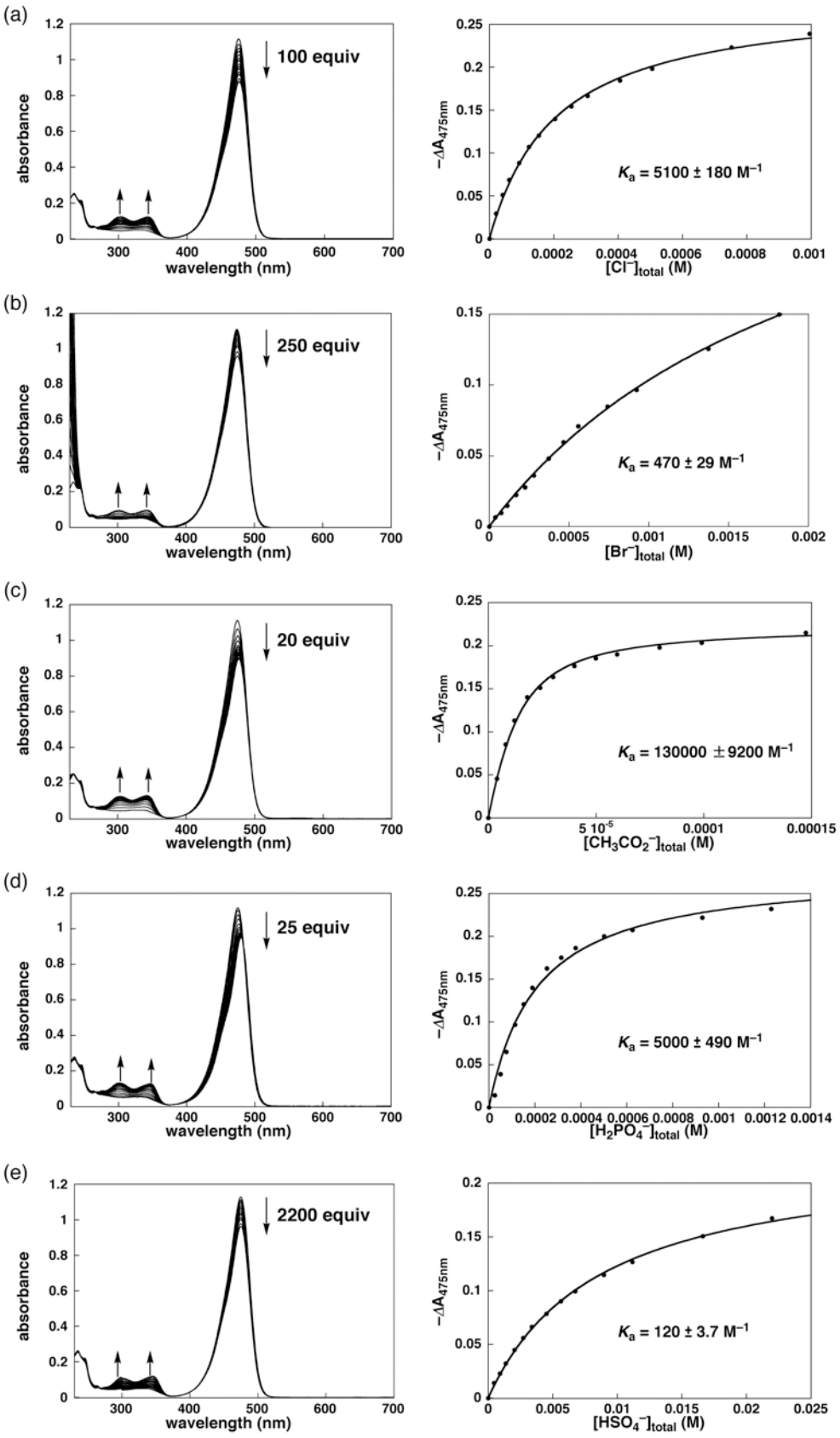
Supporting Table 3 Binding constants (K_a, M^{-1}) of **2a–c** (references), **3m1**,**2**, and **3p1**,**2** with various anions as tetrabutylammonium (TBA) salts in CH_2Cl_2 examined on the basis of the UV/vis absorption spectral changes. The values in the parentheses are the ratios of the K_a values to that of **2a**.

	K_a (**2a**) [a]	K_a (**2b**) [b]	K_a (**2c**) [b]	K_a (**3m1**)	K_a (**3m2**)	K_a (**3p1**)	K_a (**3p2**)
Cl^-	6,800	4,200	2,700	5,100	4,800	1,600	9,100
		(0.61)	(0.40)	(0.75)	(0.71)	(0.24)	(1.34)
Br^-	1,200	600	300	470	370	910	860
		(0.50)	(0.25)	(0.39)	(0.31)	(0.76)	(0.72)
$CH_3CO_2^-$	210,000	98,000	27,000	130,000	76,000	140,000	94,000
		(0.47)	(0.13)	(0.62)	(0.36)	(0.67)	(0.45)
$H_2PO_4^-$	91,000	36,000	2,200	5,000	6,100	62,000	9,900
		(0.40)	(0.024)	(0.055)	(0.067)	(0.68)	(0.11)
HSO_4^-	1,200	–	25	120	270	220	52
			(0.021)	(0.010)	(0.023)	(0.18)	(0.043)

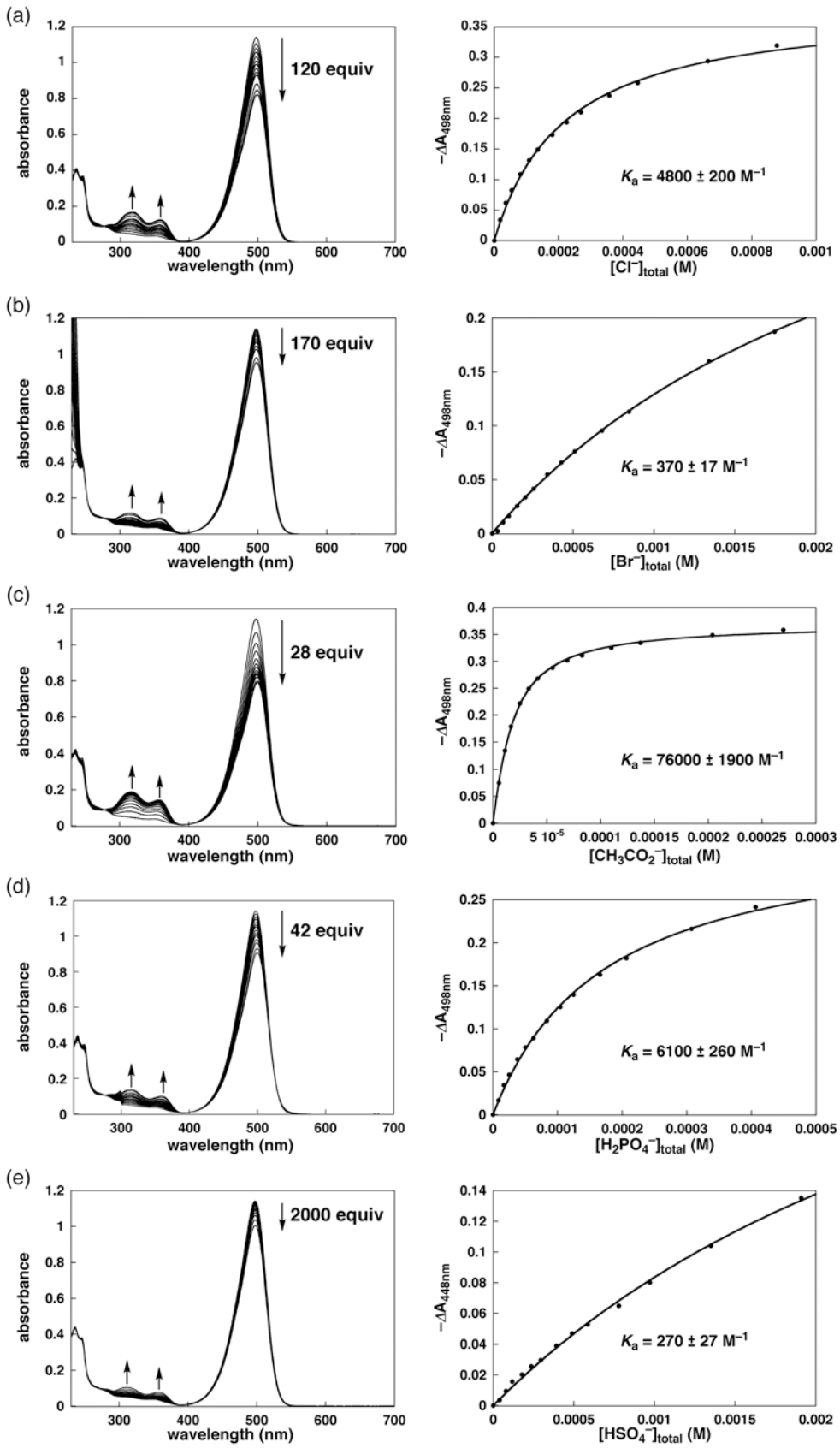
[a] Ref. [S5]. [b] Ref. [S1].

Supporting Table 4 Apparent binding constants (K_{app}, M^{-1}) of each receptor unit of **4m**,**p**, **4m´**, **5m**,**p**, and **6m**,**p** with various Cl^- and Br^- as TBA salts in CH_2Cl_2 at r.t. under diluted conditions.

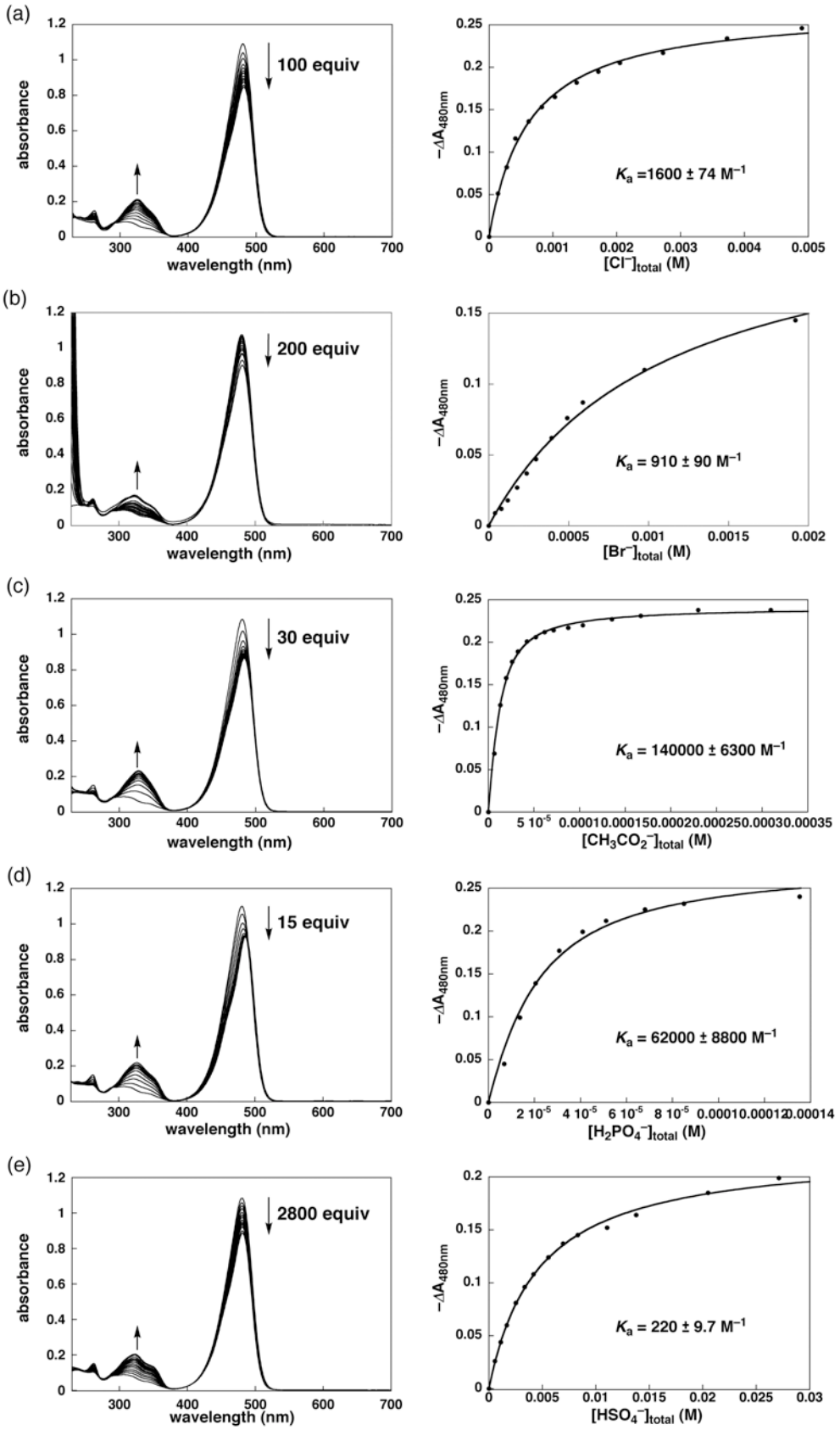
	K_{app} (**4m**)	K_{app} (**4p**)	K_{app} (**4m´**)	K_{app} (**5m**)	K_{app} (**5p**)	K_{app} (**6m**)	K_{app} (**6p**)
Cl^-	6,200	10,000	6,900	7,100	1,900	7,500	7,700
Br^-	1,200	1,200	550	45	300	1,600	750



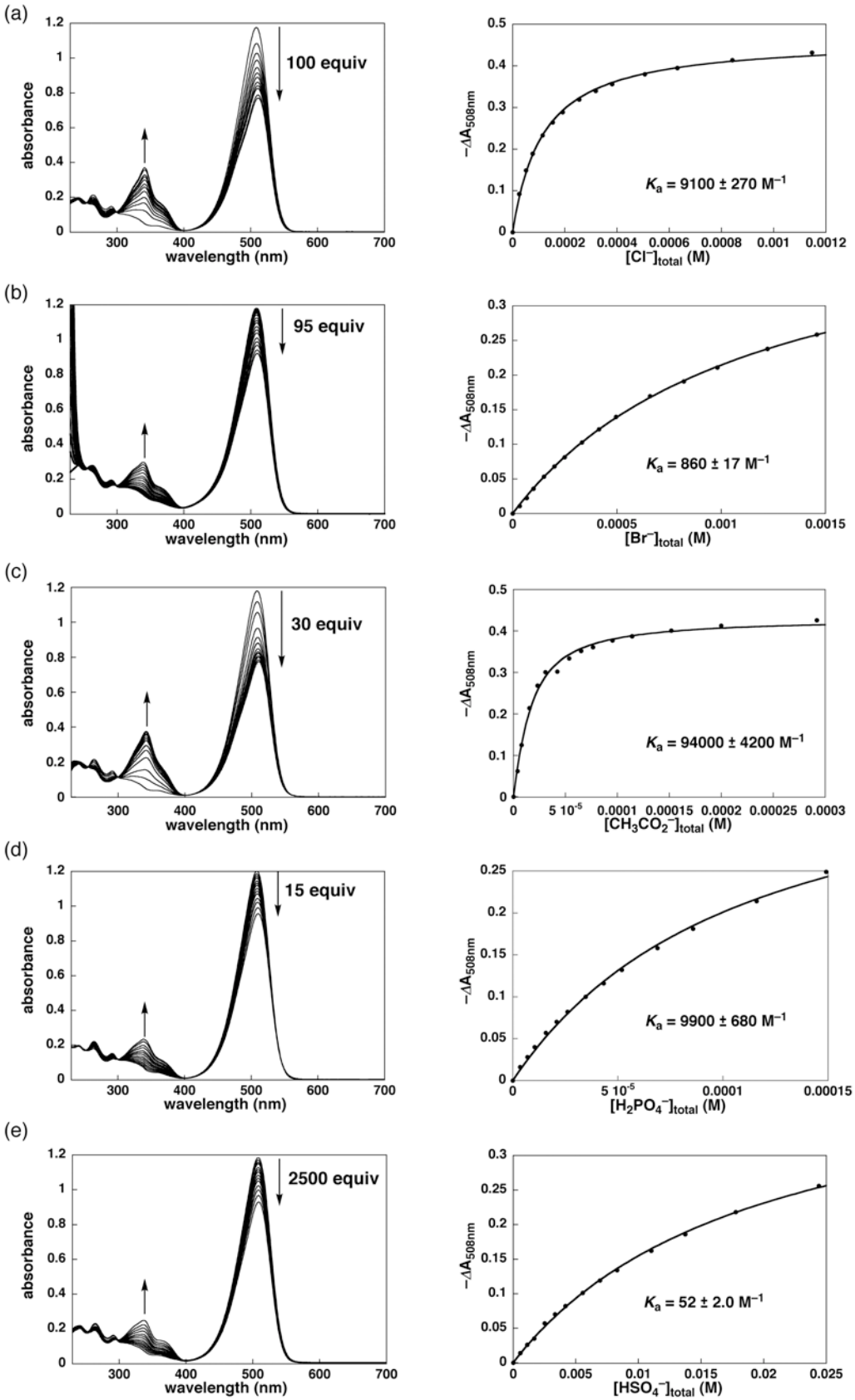
Supporting Figure 12 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3m1** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, (d) $H_2PO_4^-$, and (e) HSO_4^- as TBA salts in CH_2Cl_2



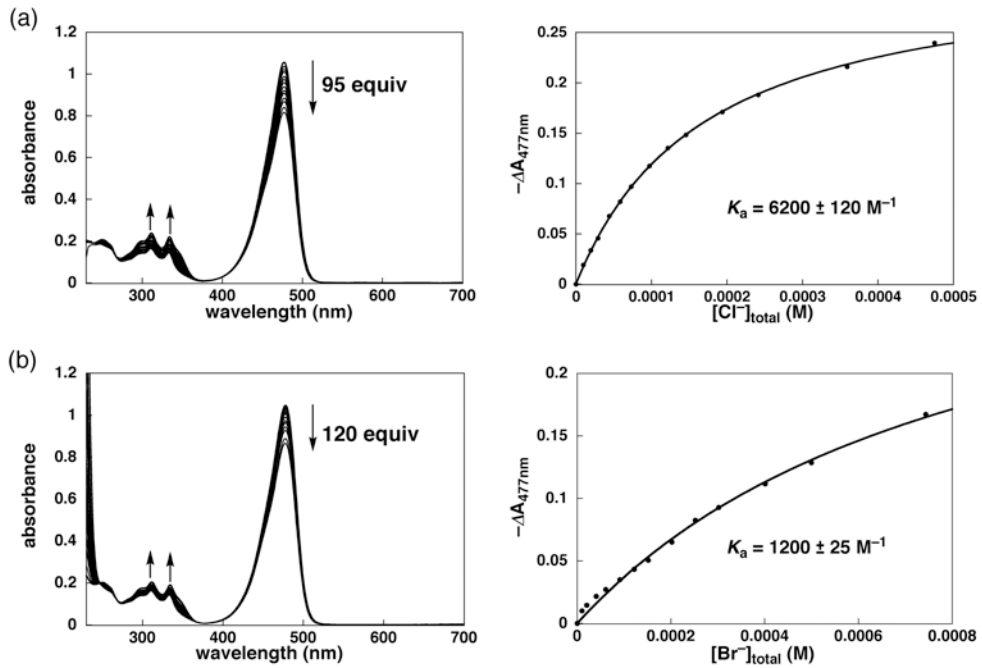
Supporting Figure 13 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3m2** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, (d) $H_2PO_4^-$, and (e) HSO_4^- as TBA salts in CH_2Cl_2.



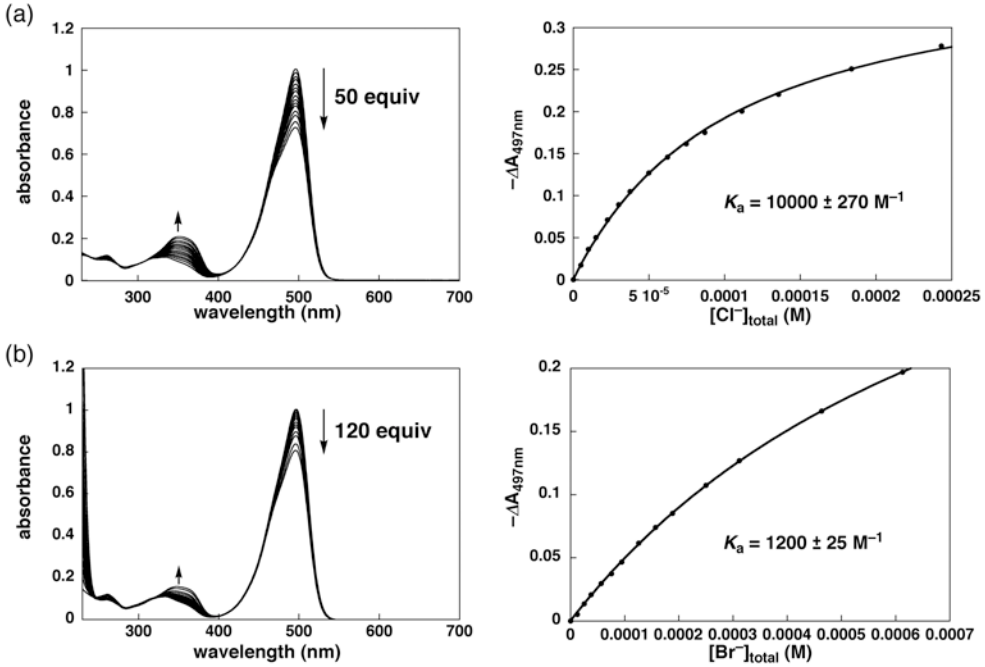
Supporting Figure 14 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3p1** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, (d) $H_2PO_4^-$, and (e) HSO_4^- as TBA salts in CH_2Cl_2.



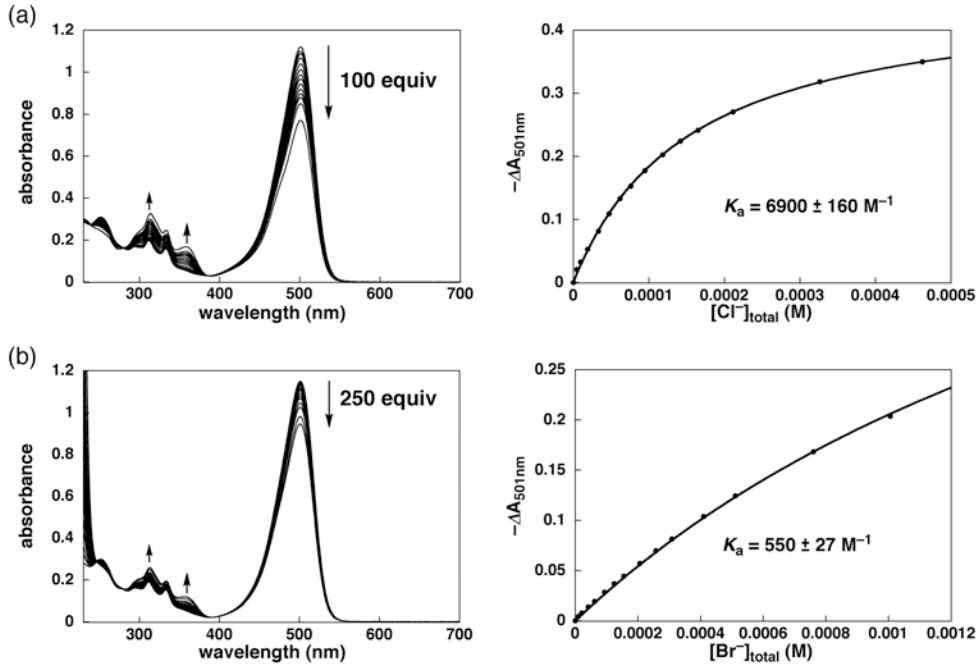
Supporting Figure 15 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3p2** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, (c) $CH_3CO_2^-$, (d) $H_2PO_4^-$, and (e) HSO_4^- as TBA salts in CH_2Cl_2.



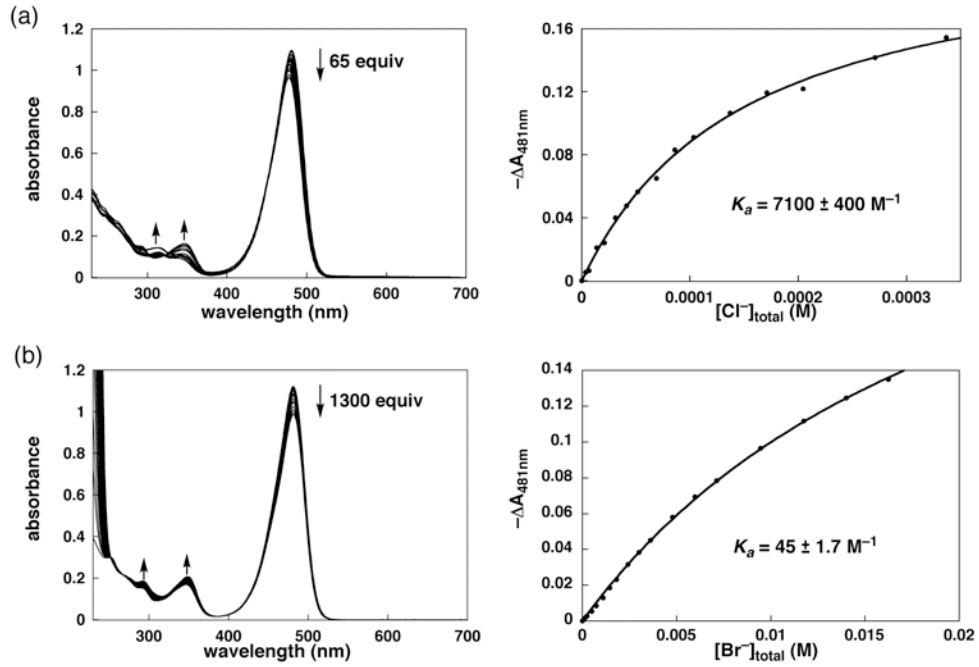
Supporting Figure 16 UV/vis absorption spectral changes of **4m** (5.2×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



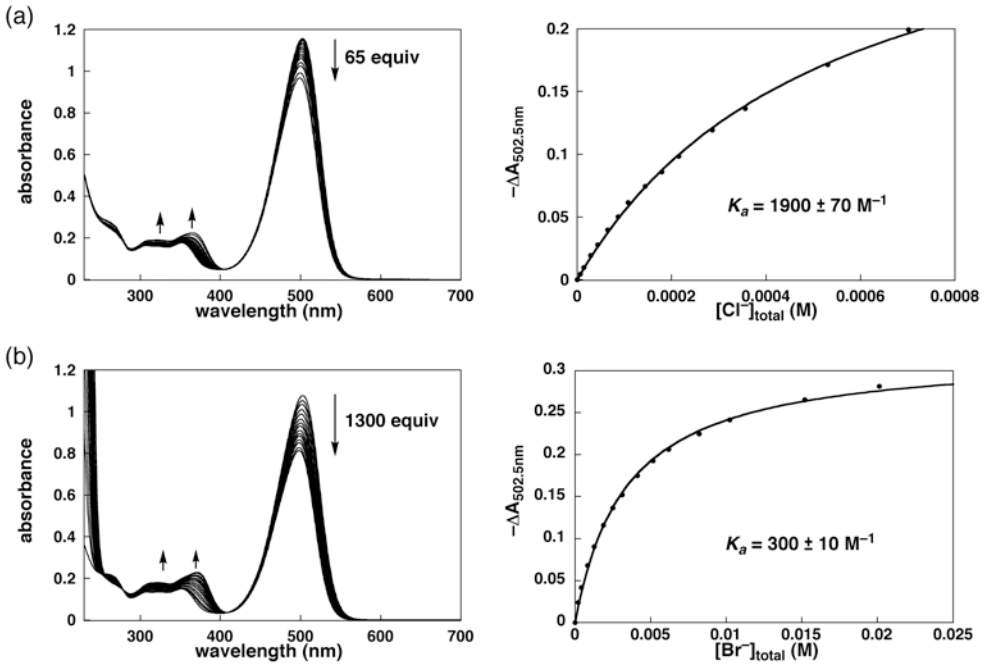
Supporting Figure 17 UV/vis absorption spectral changes of **4p** (5.1×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



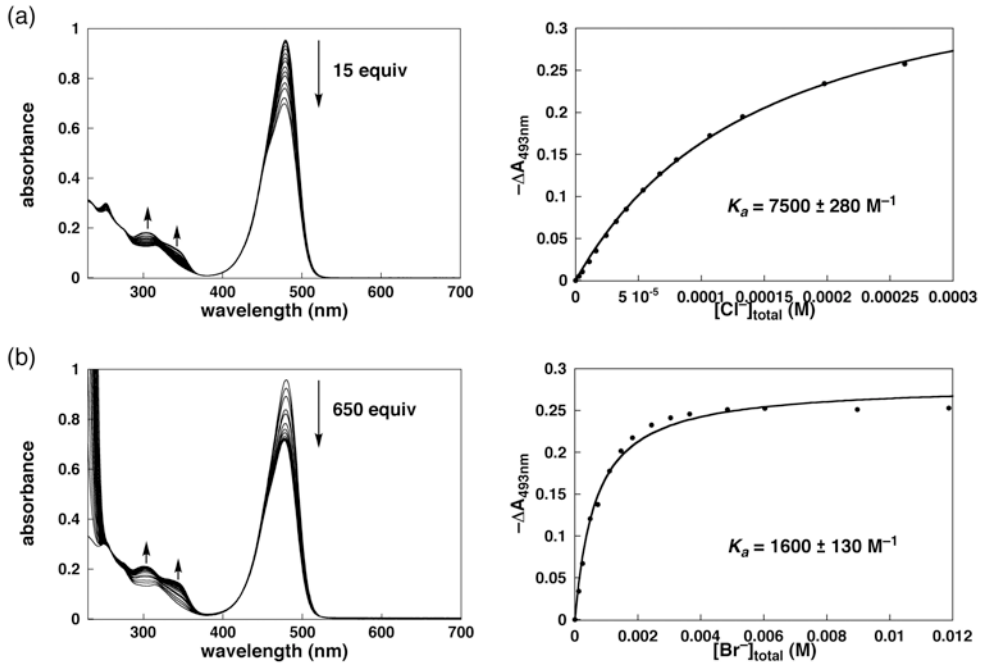
Supporting Figure 18 UV/vis absorption spectral changes of **4m´** (5.1×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



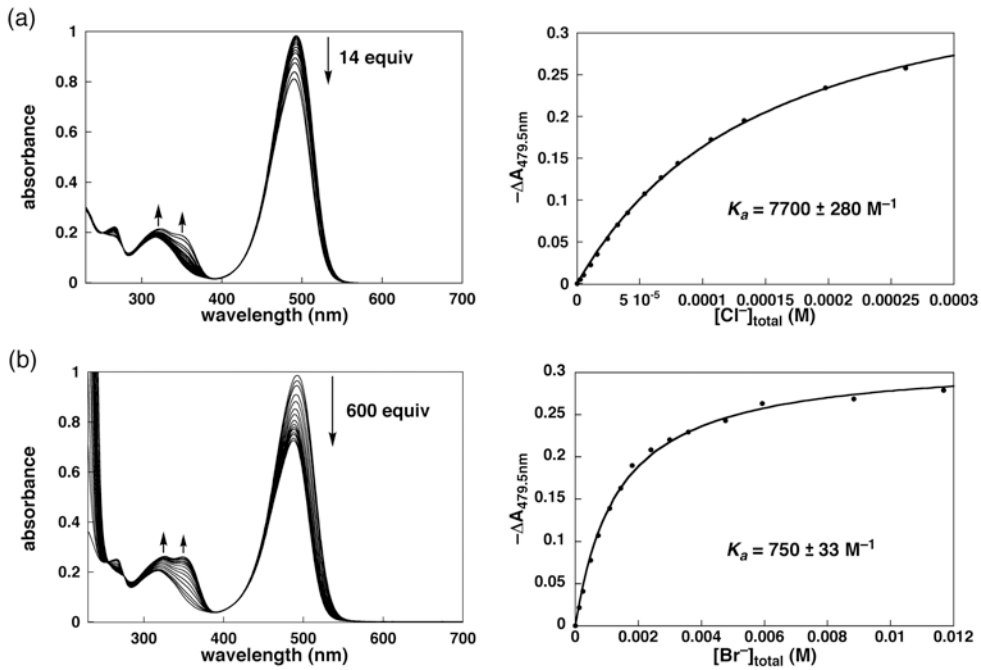
Supporting Figure 19 UV/vis absorption spectral changes of **5m** (5.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



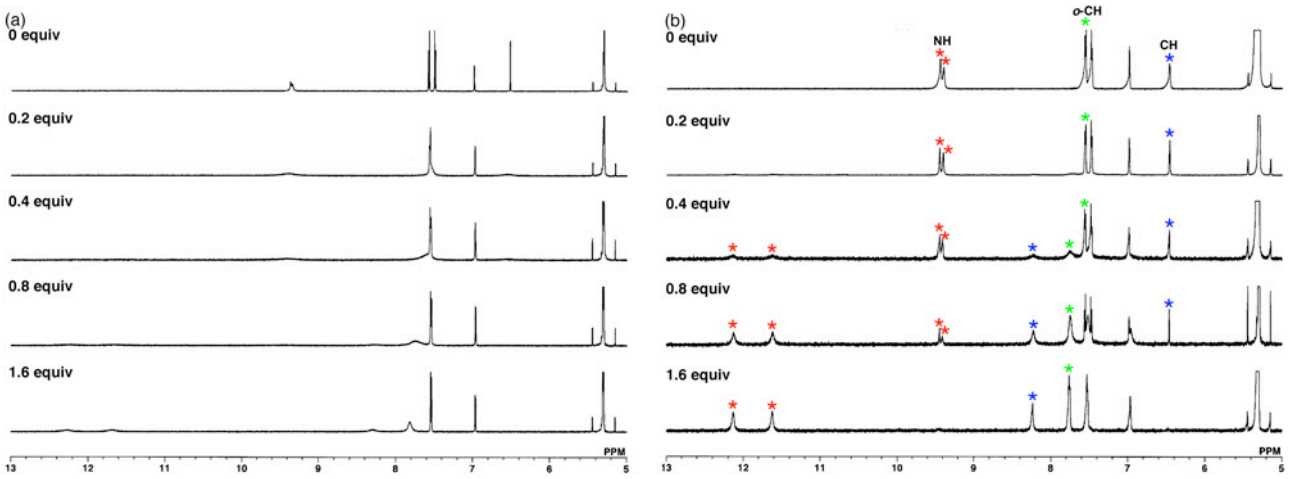
Supporting Figure 20 UV/vis absorption spectral changes of **5p** (5.0×10^{-6} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



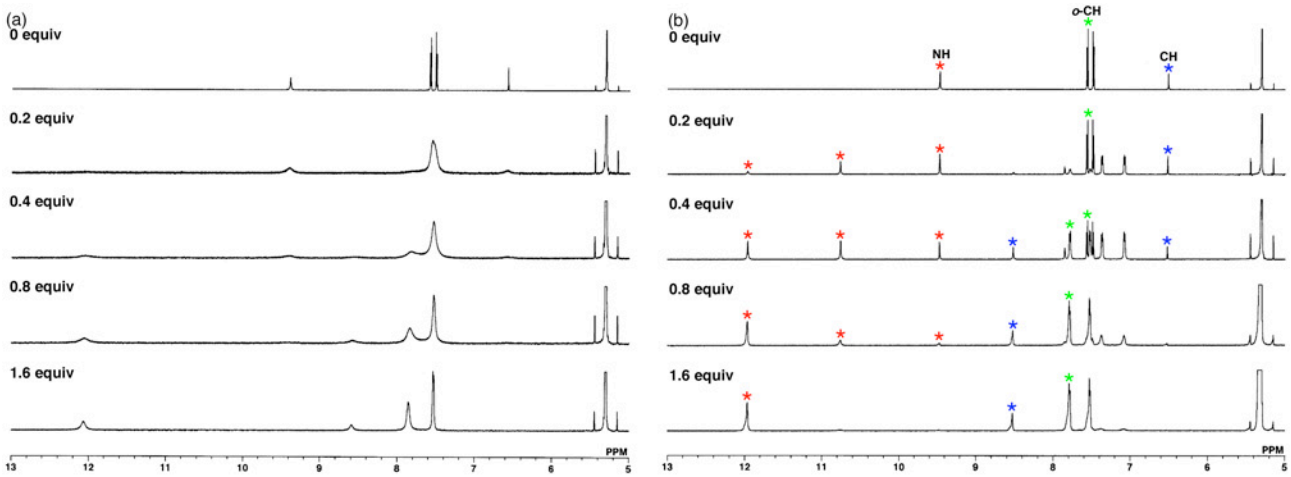
Supporting Figure 21 UV/vis absorption spectral changes of **6m** (1.0×10^{-5} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



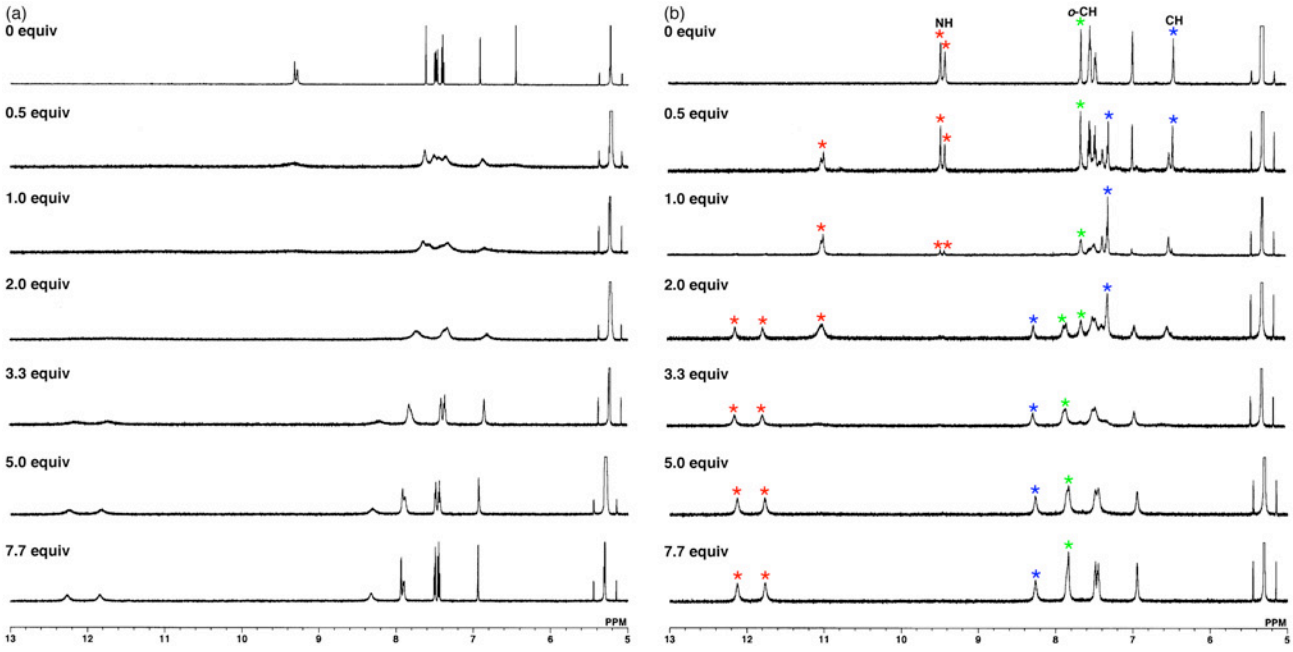
Supporting Figure 22 UV/vis absorption spectral changes of **6p** (1.0×10^{-5} M) upon the addition of (a) Cl^- and (b) Br^- as TBA salts in CH_2Cl_2.



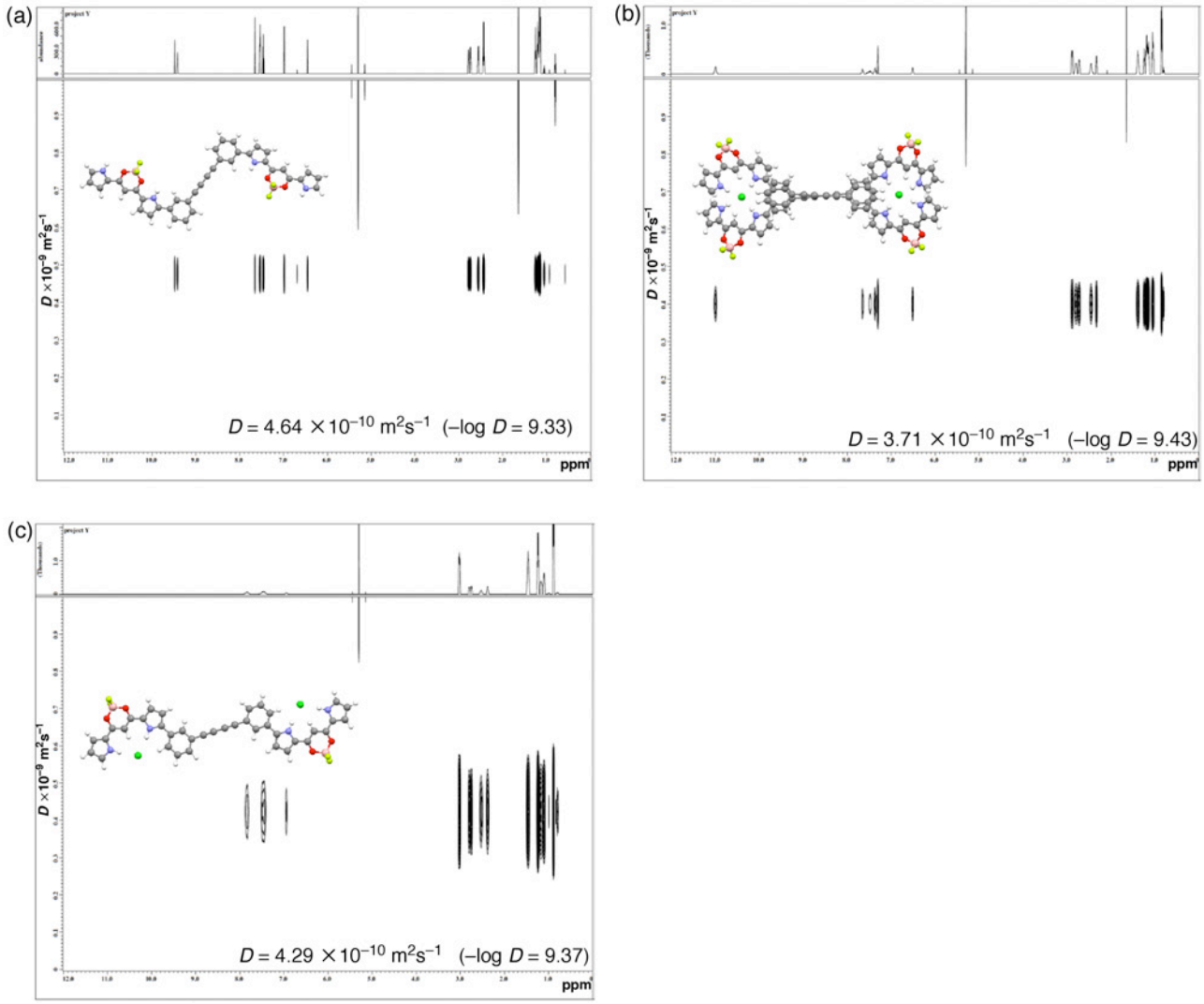
Supporting Figure 23 ^{1}H NMR spectral changes of **3p1** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–1.6 equiv) added as a TBA salt.



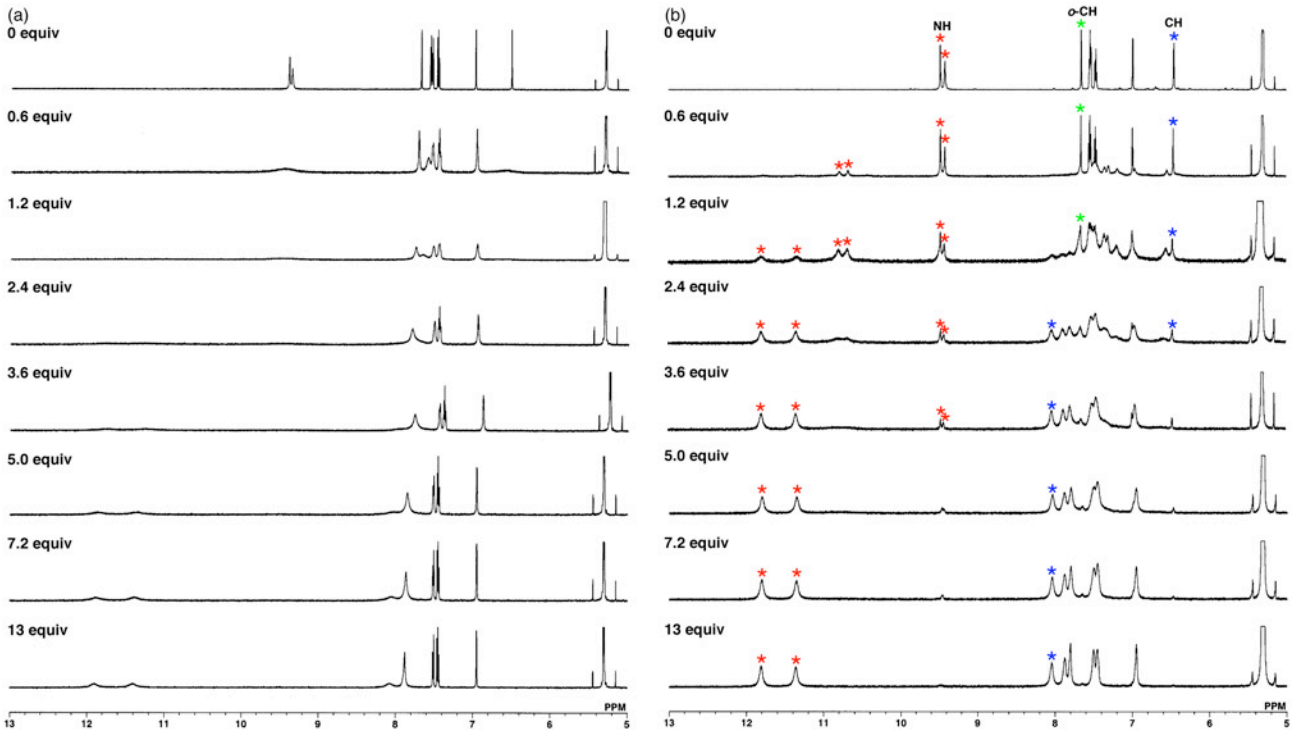
Supporting Figure 24 ^{1}H NMR spectral changes of **3p2** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–1.6 equiv) added as a TBA salt. Intermediate NH signals between those of anion-free receptor and [1 + 1]-type complexes in the presence of 0.2, 0.4, and 0.8 equiv of Cl^- at –50 °C suggest the formation of a [2 + 1]-type complex. This behavior is also observed in α-aryl-substituted receptors.[S6]



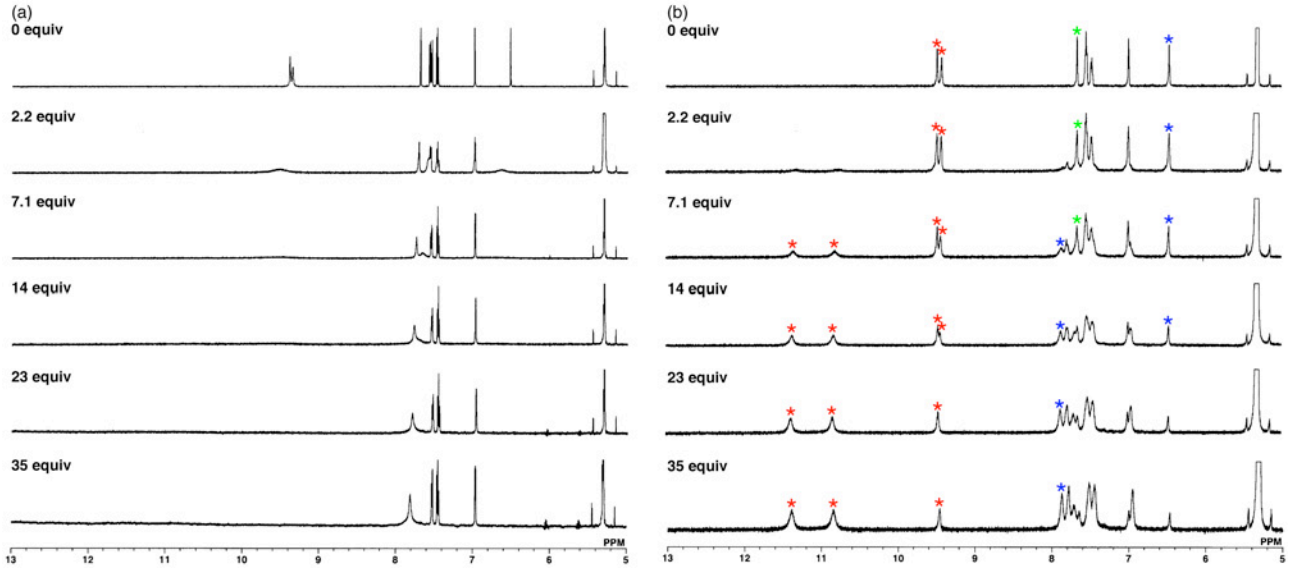
Supporting Figure 25 ^{1}H NMR spectral changes of **4m** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–7.7 equiv) added as a TBA salt. Intermediate NH signals between those of anion-free receptor and [1 + 2]-type complex in the presence of 0.5, 1.0, and 2.0 equiv of Cl^- at –50 °C suggest the formation of a [2 + 2]-type complex, also supported by theoretical study.



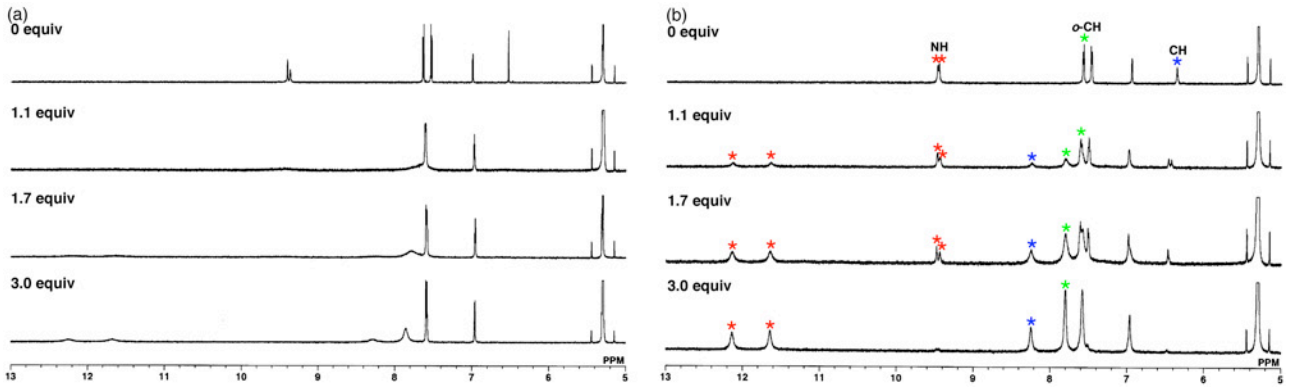
Supporting Figure 26 ^{1}H DOSY of **4m** with (a) 0, (b) 1.0, and (c) 5.0 equiv of Cl^- added as a TBA salt in CD_2Cl_2 (1.0×10^{-3} M) at –50 °C.



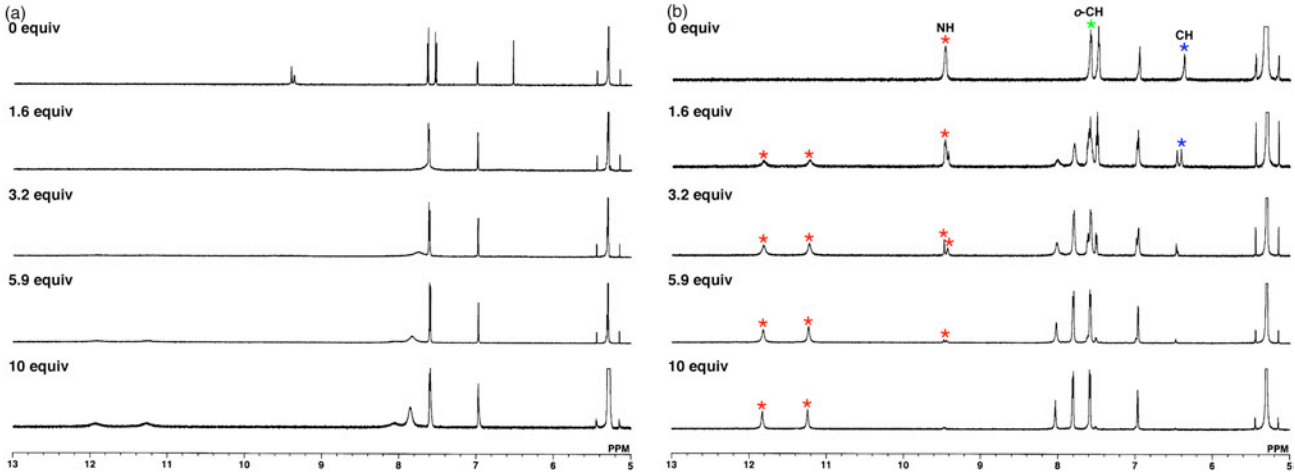
Supporting Figure 27 ^{1}H NMR spectral changes of **4m** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Br^- (0–13 equiv) added as a TBA salt. Intermediate NH signals between those of anion-free receptor and [1 + 2]-type complex in the presence of 0.6, 1.2, and 2.4 equiv of Br^- at –50 °C suggest the formation of a [2 + 2]-type complex.



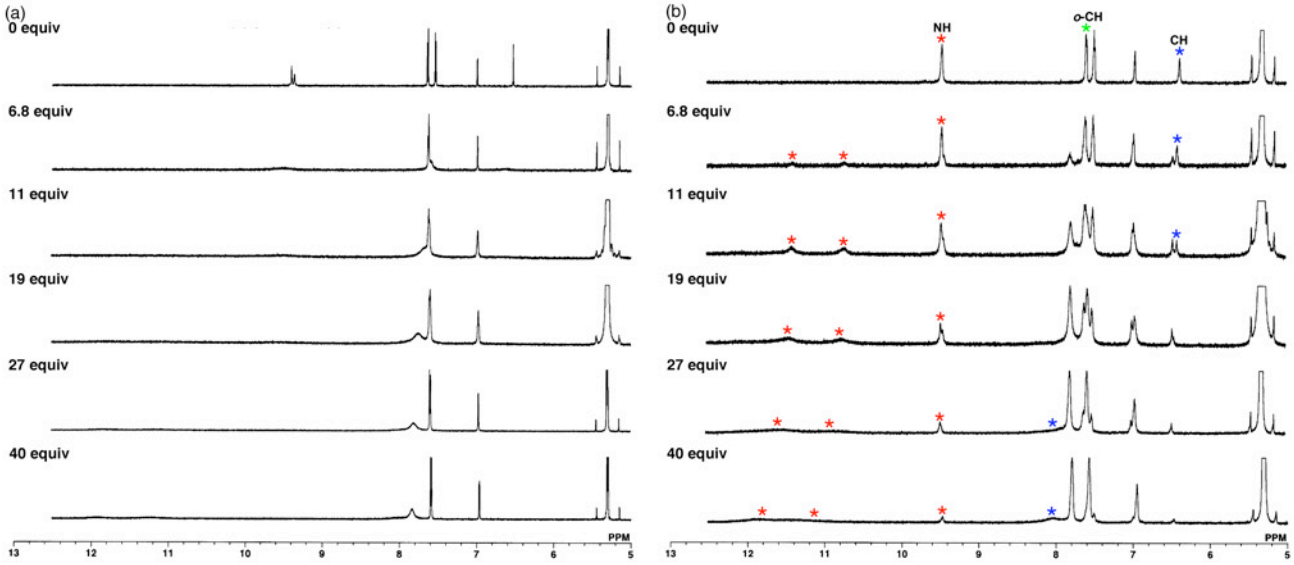
Supporting Figure 28 ^{1}H NMR spectral changes of **4m** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of I^- (0–35 equiv) added as a TBA salt.



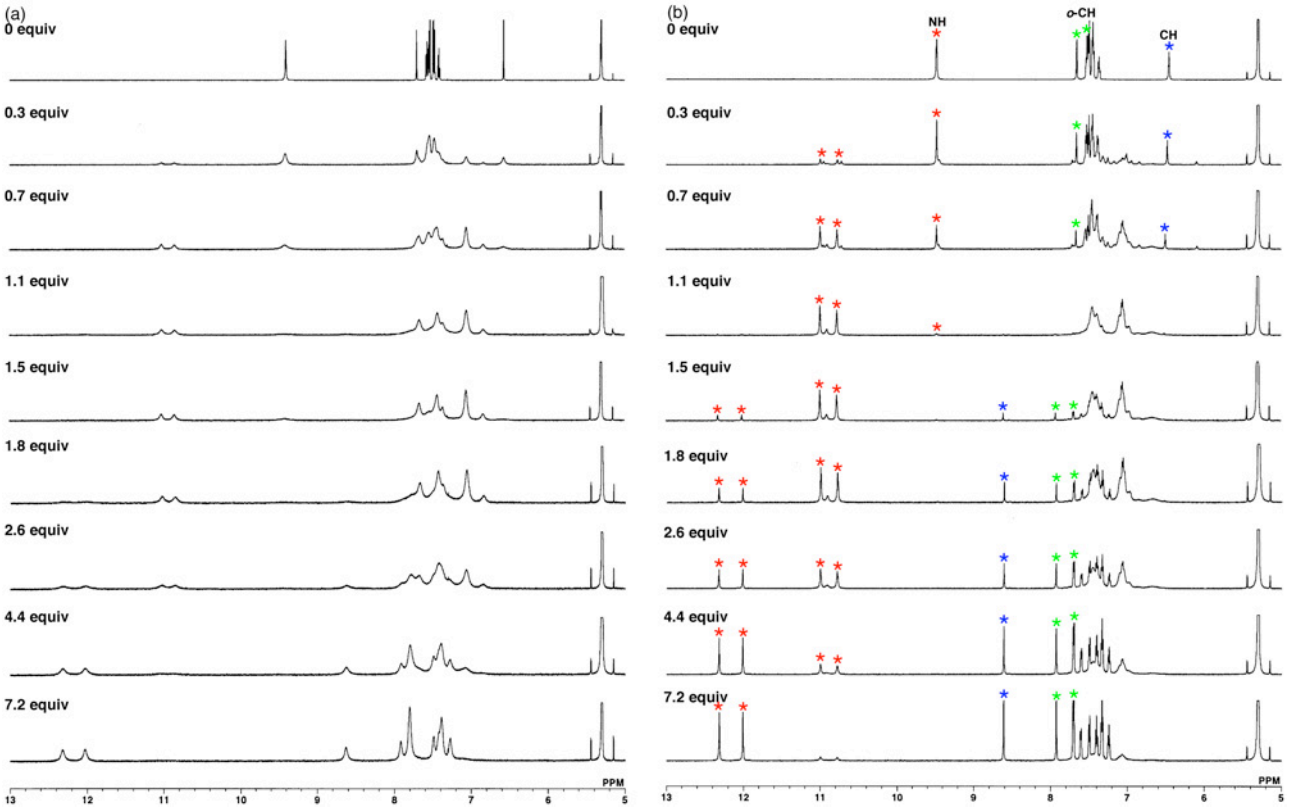
Supporting Figure 29 ^{1}H NMR spectral changes of **4p** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–3.0 equiv) added as a TBA salt.



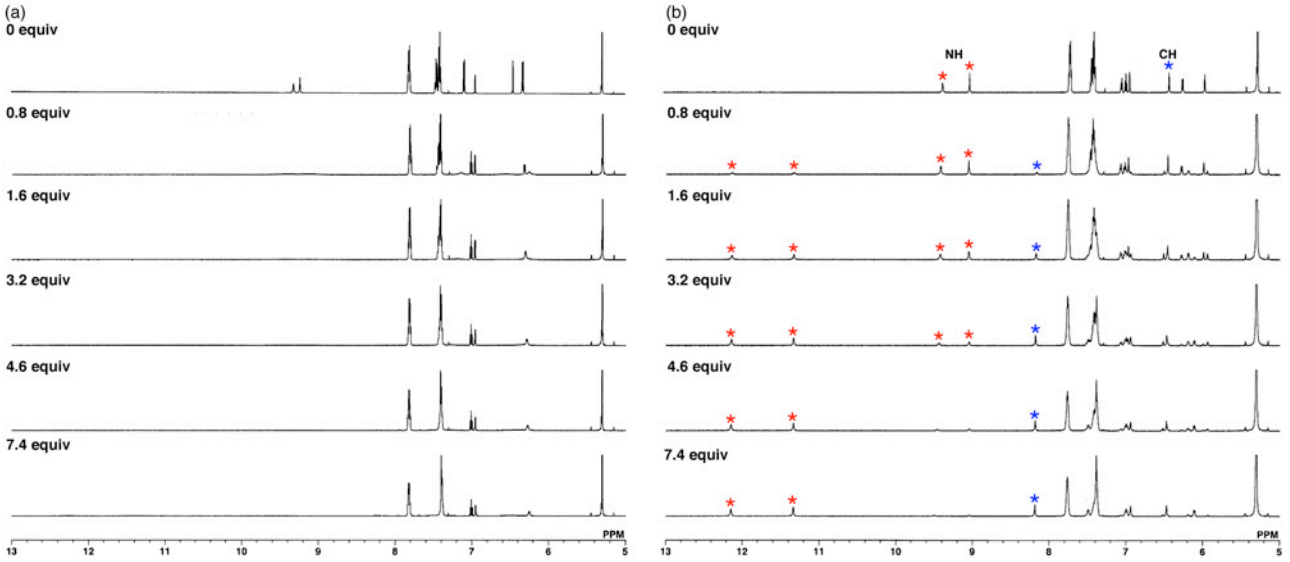
Supporting Figure 30 ^{1}H NMR spectral changes of **4p** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Br^- (0–10 equiv) added as a TBA salt.



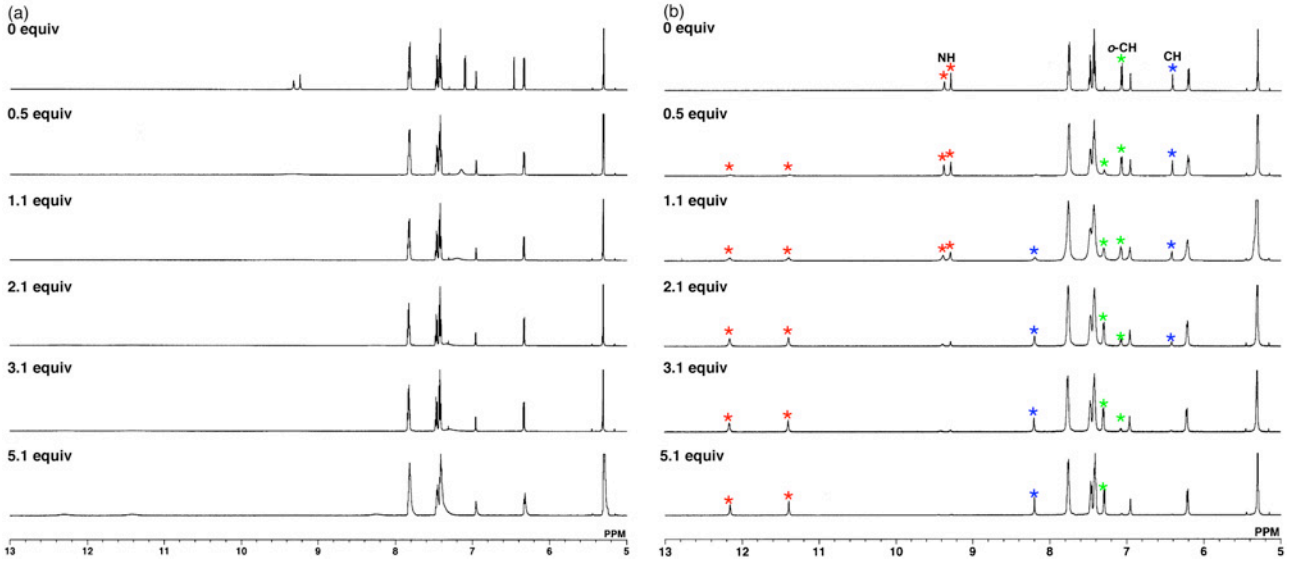
Supporting Figure 31 ^{1}H NMR spectral changes of **4p** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of I^- (0–40 equiv) added as a TBA salt.



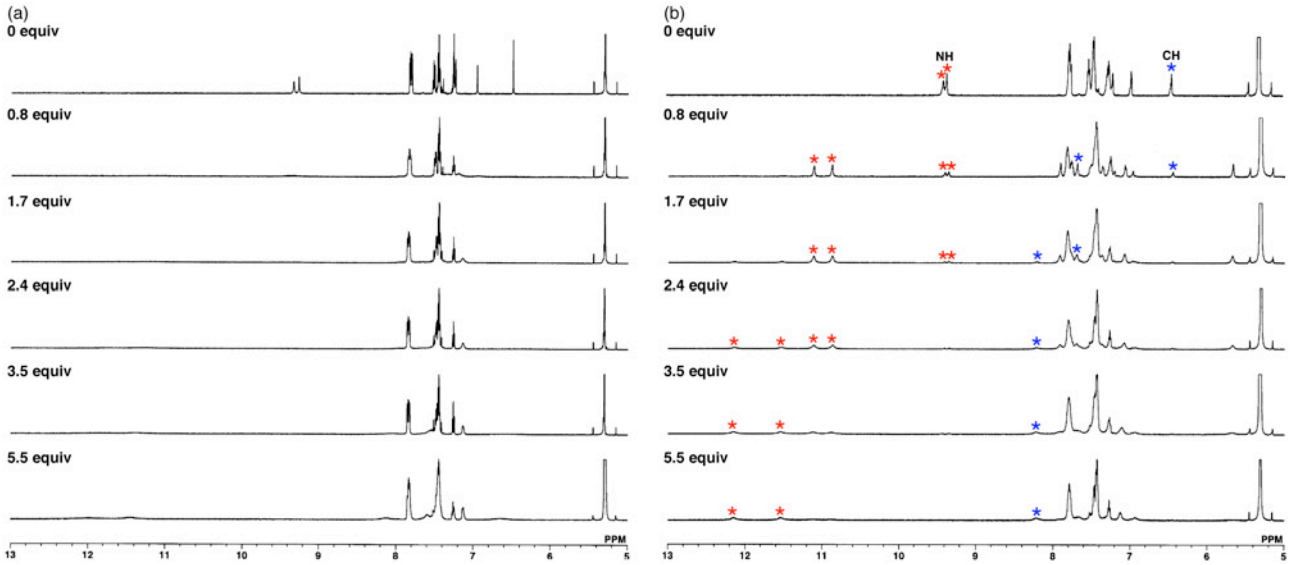
Supporting Figure 32 ^{1}H NMR spectral changes of **4m′** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–7.2 equiv) added as a TBA salt. Intermediate NH signals between those of anion-free receptor and [1 + 2]-type complex in the presence of 0.3–4.4 equiv of Cl^- at –50 °C suggest the formation of a [2 + 2]-type complex, also supported by theoretical study.



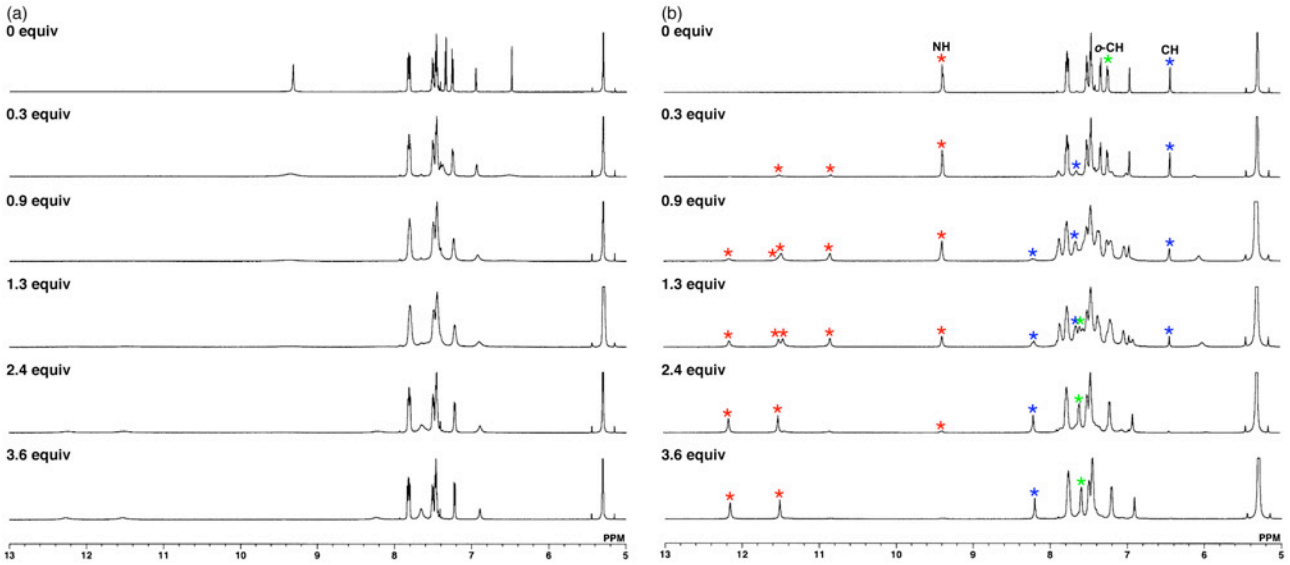
Supporting Figure 33 ^{1}H NMR spectral changes of **5m** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–7.4 equiv) added as a TBA salt.



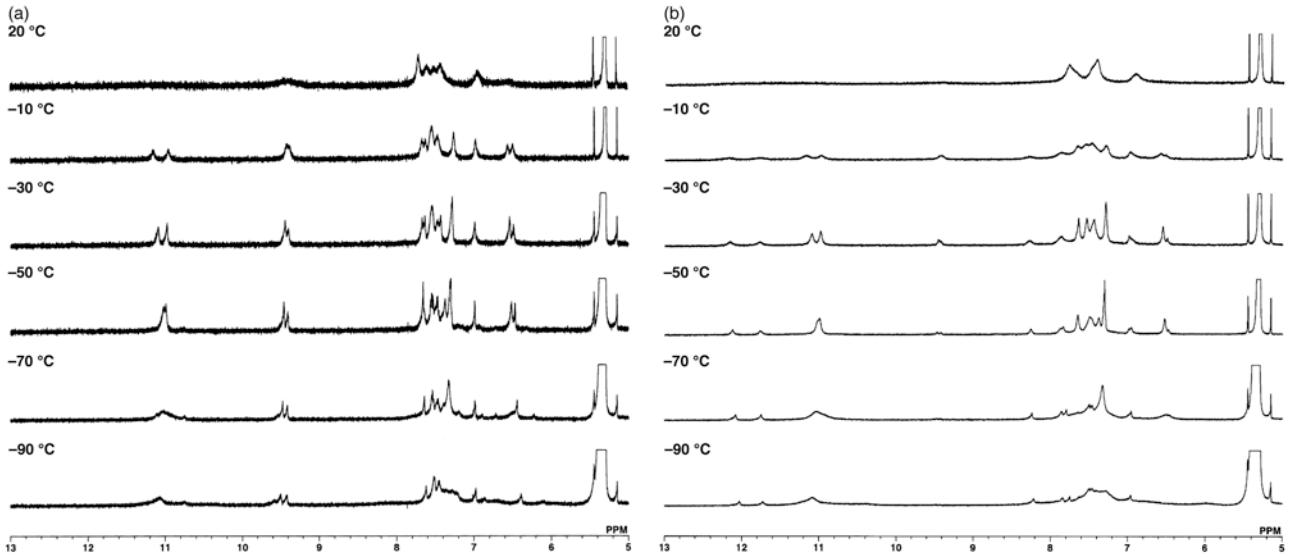
Supporting Figure 34 ^{1}H NMR spectral changes of **5p** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–5.1 equiv) added as a TBA salt.



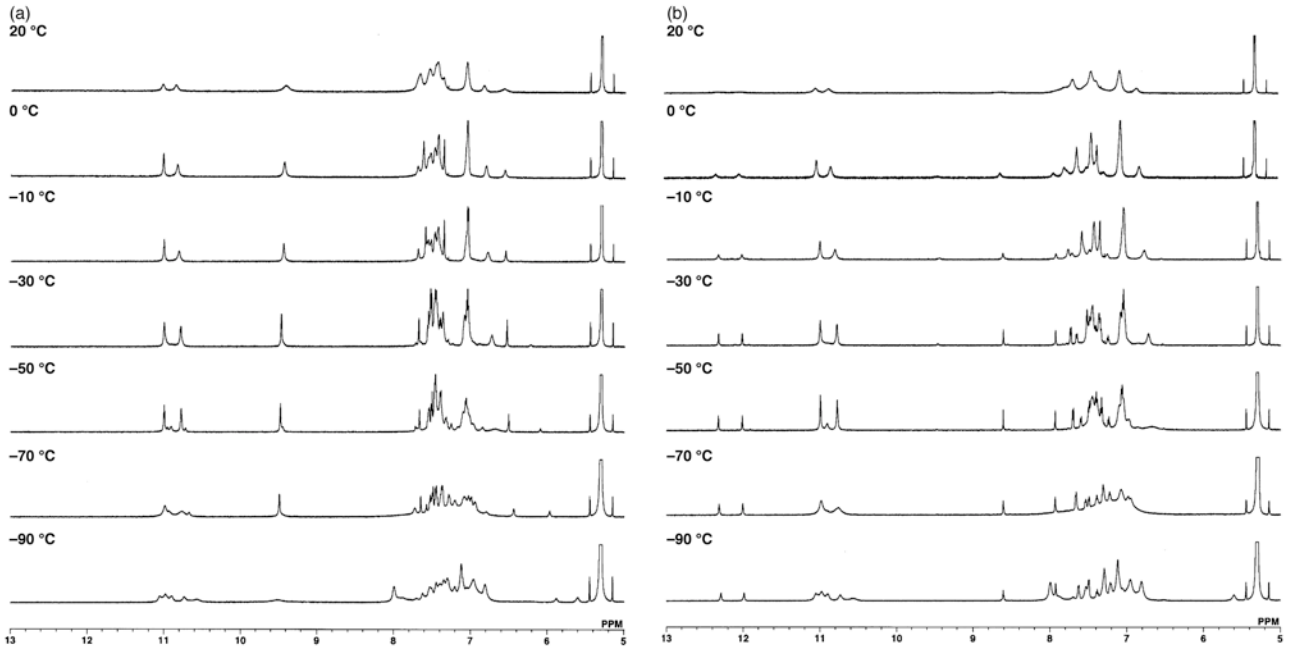
Supporting Figure 35 ^{1}H NMR spectral changes of **6m** in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–5.5 equiv) added as a TBA salt. The dimer **6m** show the slow solubility under these conditions, therefore, it is difficult to discuss the binding behaviors quantitatively. Intermediate NH signals between those of anion-free receptor and [1 + 2]-type complex in the presence of 0.8, 1.7, and 2.4 equiv of Cl^- at –50 °C suggest the formation of a [1 + 1]-type complex, also supported by theoretical study. Formation of a [2 + 2]-type complex may be excluded by the preference of a [1 + 1]-type complex consisting of two components (= a receptor and an anion).



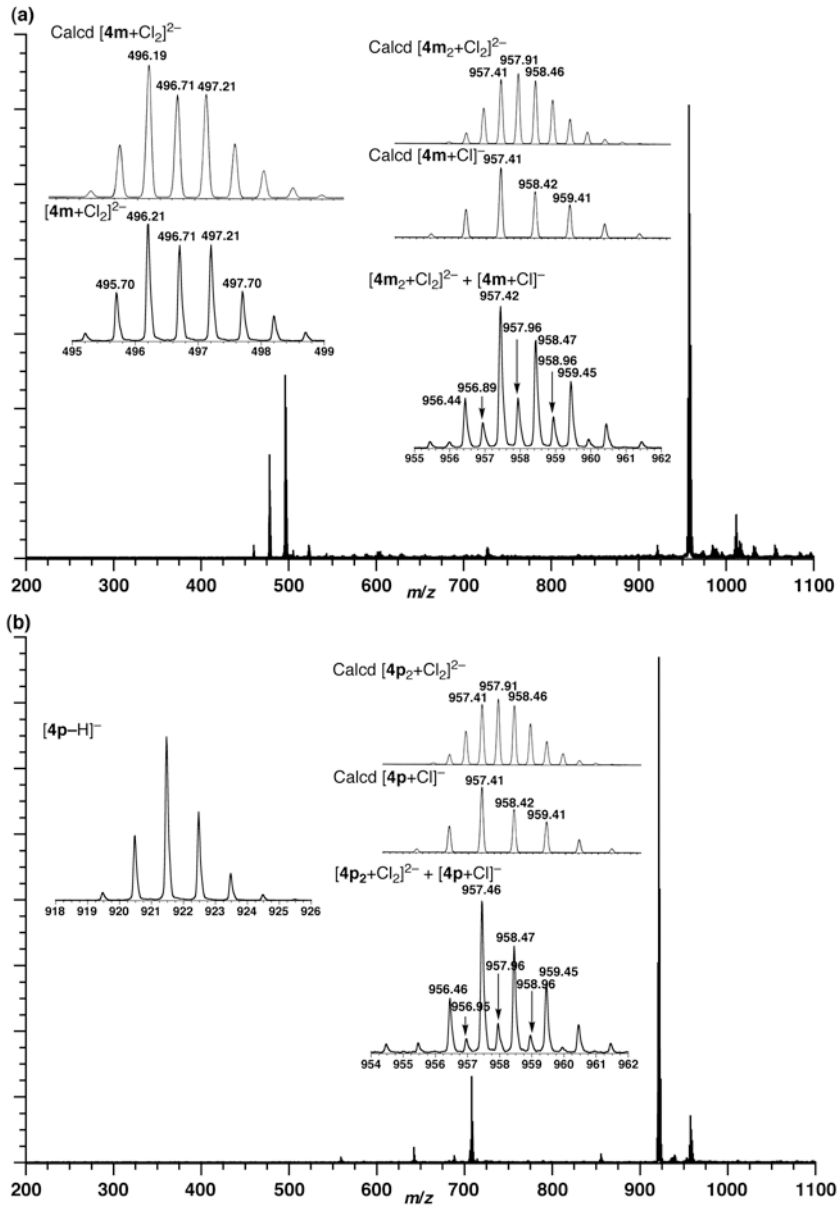
Supporting Figure 36 ^{1}H NMR spectral changes of **6p** (1.0×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- (0–3.6 equiv) added as a TBA salt. Intermediate NH signals between those of anion-free receptor and [1 + 2]-type complex in the presence of 0.3, 0.9, and 1.3 equiv of Cl^- at –50 °C suggest the formation of a [2 + 2]-type complex, also supported by theoretical study.



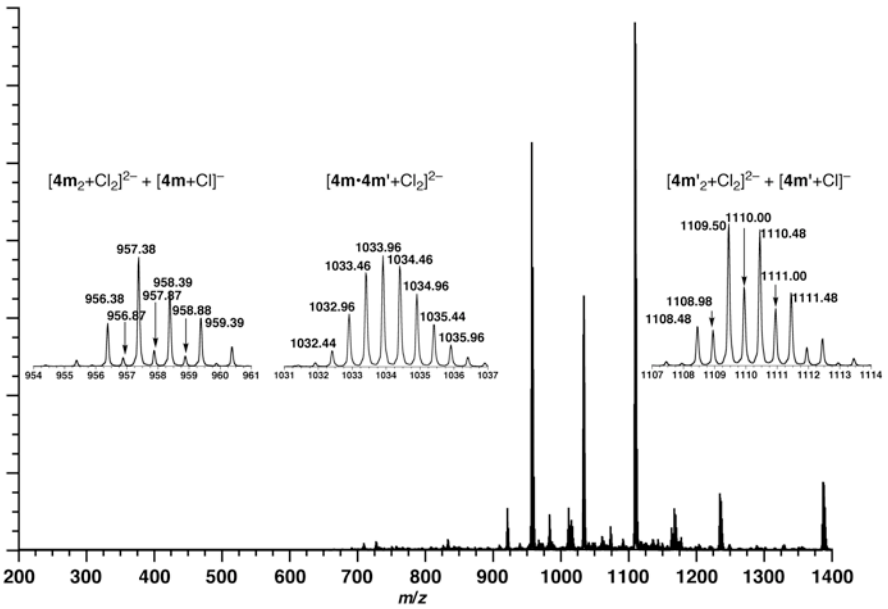
Supporting Figure 37 Variable temperature ^{1}H NMR spectral changes of **4m** (1.0×10^{-3} M) from 20 to –90 °C in CD_2Cl_2 with (a) 0.78 and (b) 1.76 equiv of Cl^- added as a TBA salt. From the ratios of **4m**/**4m**$_2$·Cl^-_2/**4m**·Cl^-_2 by addition of TBACl (1.78 equiv), association constants defined as [**4m**$_2$·Cl^-_2]/[**4m**]^2[Cl^-]^2 (K_{22}), [**4m**·Cl^-_2]/[**4m**][Cl^-]^2 (K_{12}) and [**4m**·Cl^-_2]^2/[**4m**$_2$·Cl^-_2][Cl^-]^2 (K_{12}^2/K_{22}) at –10, –30, –50, and –70 °C are 1.5×10^{10}, 5.9×10^{10}, 1.2×10^{11} and 5.8×10^{11} M^{-3} for K_{22}, 4.7×10^6, 7.3×10^6, 7.9×10^6 and 1.6×10^7 M^{-2} for K_{12}, and 1.5×10^3, 8.7×10^2, 5.1×10^2 and 4.4×10^2 M^{-1} for K_{12}^2/K_{22}, respectively.



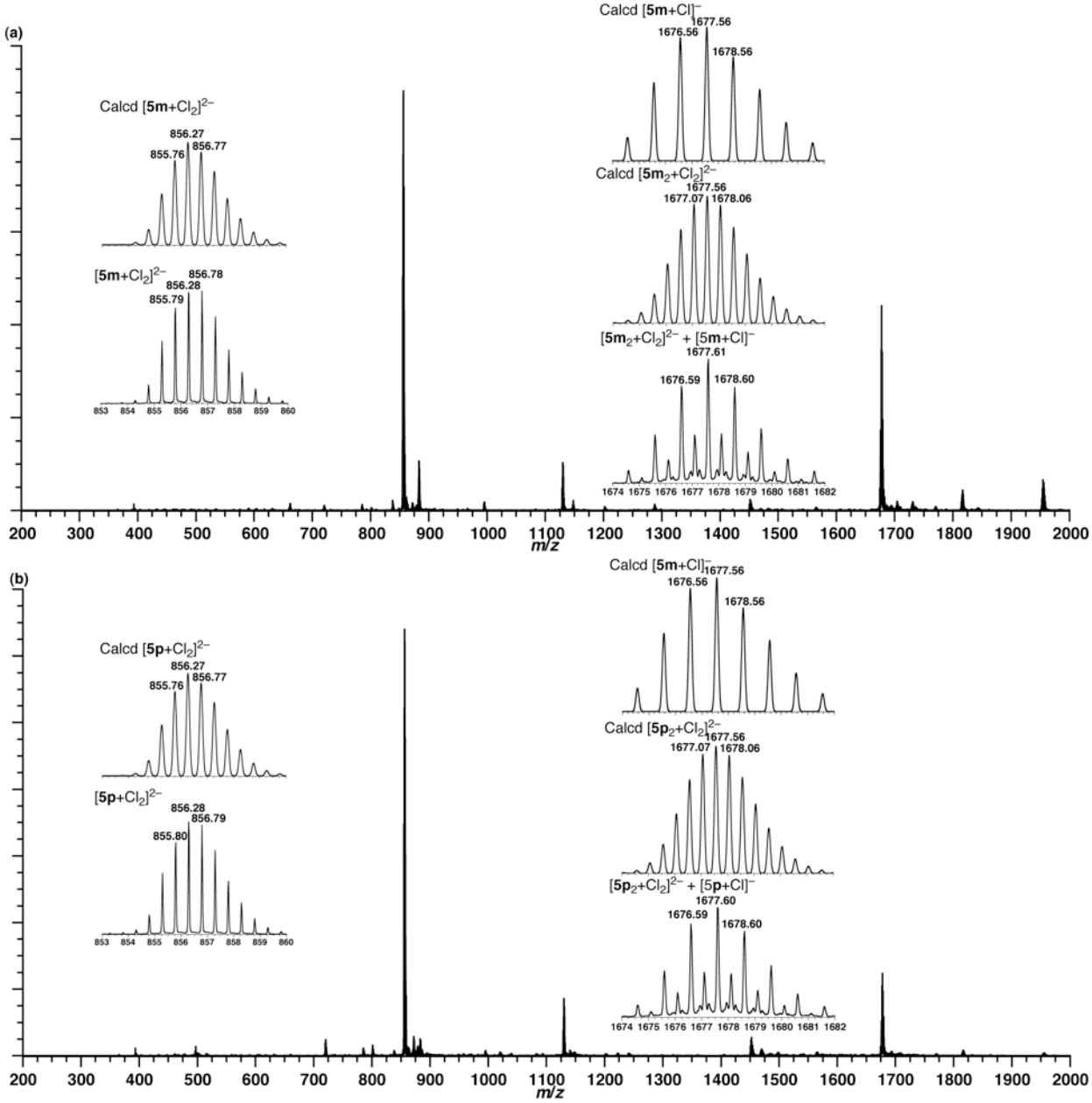
Supporting Figure 38 Variable temperature ^{1}H NMR spectral changes of **4m´** (1.0×10^{-3} M) from 20 to –90 °C in CD_2Cl_2 with (a) 0.70 and (b) 1.50 equiv of Cl^- added as a TBA salt. Complicated NH signals around 11 ppm are presumably derived from stereoisomers of [2 + 2]-type assemblies along with analogs including higher oligomers.



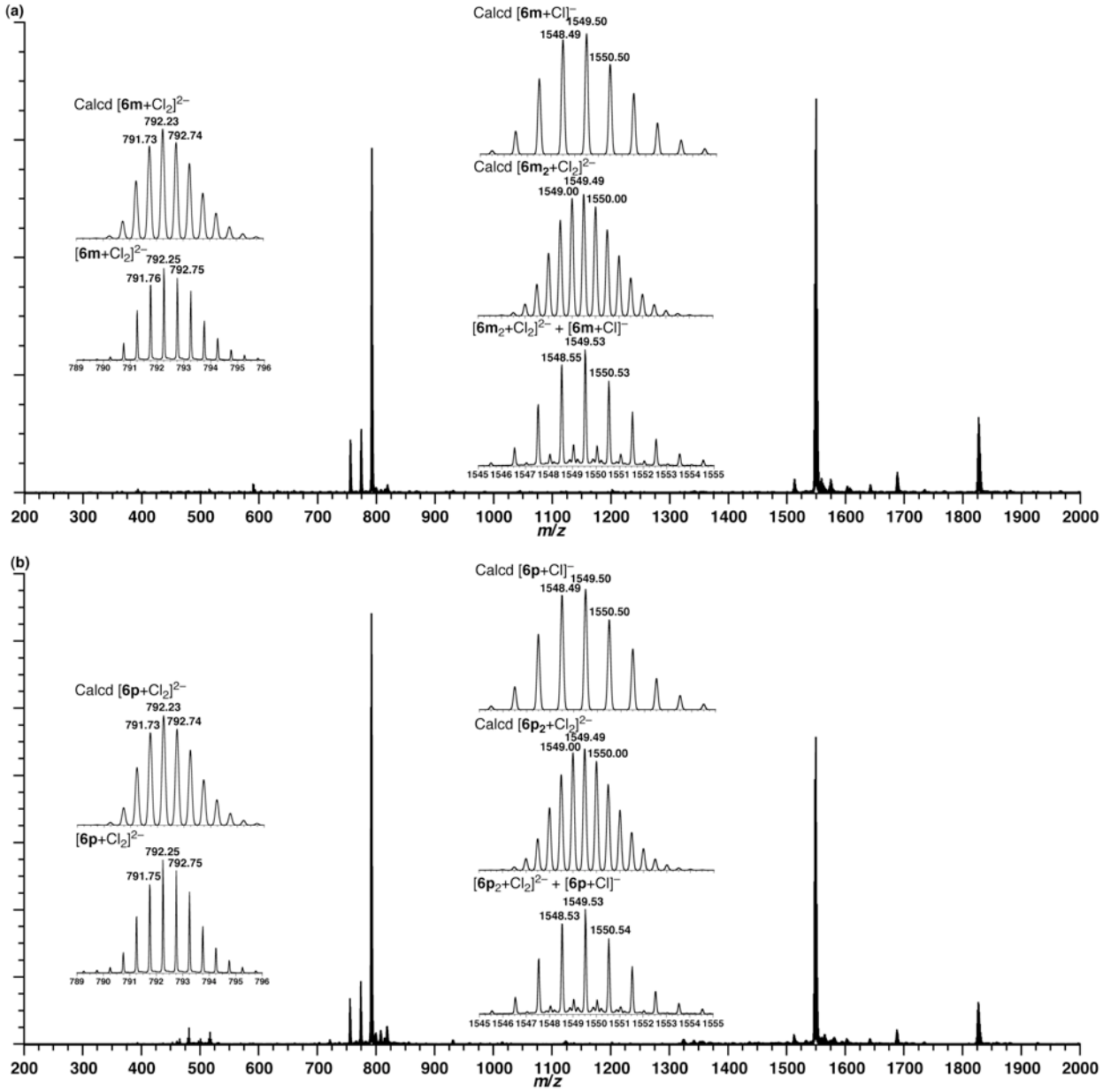
Supporting Figure 39 ESI-TOF-MS at negative mode of (a) **4m** with 1.0 equiv of Cl^- and (b) **4p** with 1.0 equiv of Cl^- as a TBA salt from CH_3CN solutions (1×10^{-6} M). Under the condition for ESI-TOF-MS measurements, a trace amount of [2 + 2]-type complex of **4p** is also observed.



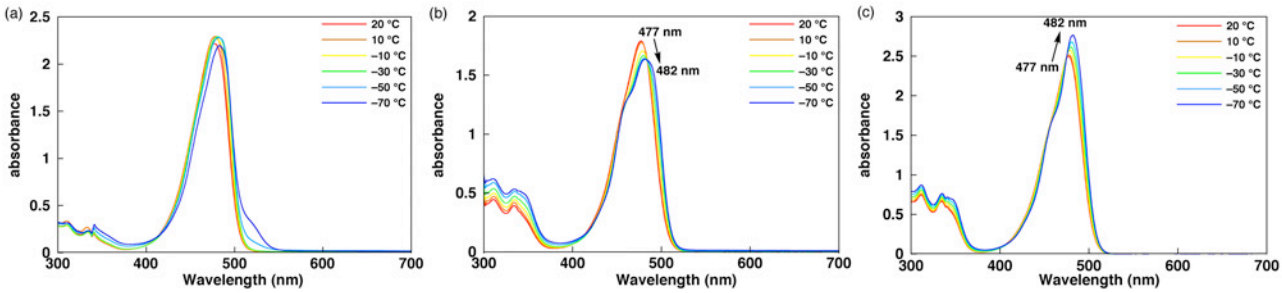
Supporting Figure 40 ESI-TOF-MS at negative mode of (a) **4m** and **4m´** with 1.0 equiv of Cl^- as a TBA salt from CH_3CN solutions (**4m** and **4m´**: 1×10^{-6} M).



Supporting Figure 41 ESI-TOF-MS at negative mode of (a) **5m** with 1.0 equiv of Cl^- and (b) **5p** with 1.0 equiv of Cl^- as a TBA salt from CH_3CN solutions (1×10^{-6} M). Under the condition for ESI-TOF-MS measurements, trace amounts of [2 + 2]-type complexes of **5m** and **5p** are also observed.



Supporting Figure 42 ESI-TOF-MS at negative mode of (a) **6m** with 1.0 equiv of Cl^- and (b) **6p** with 1.0 equiv of Cl^- as a TBA salt from CH_3CN solutions (1×10^{-6} M). Under the condition for ESI-TOF-MS measurements, a trace amount of [2 + 2]-type complex of **6m** is also observed.



Supporting Figure 43 Variable temperature UV/vis absorption spectral changes of **4m** (1.0×10^{-3} M) from 20 to –70 °C in CH_2Cl_2 with (a) **4m**, (b) **4m** with the existence of 1.0 equiv of Cl^-, and (c) **4m** with the existence of 2.0 equiv of Cl^-. Cl^- was added as a TBA salt. The differences in the initial absorbances are within an error. The dimer 4m shows quite different temperature-dependent behaviors in UV/vis absorption spectra in the presences of 1.0 and 2.0 equiv of Cl^-, suggesting that the intermediate species ([2 + 2]-type complex) exists by addition of 1.0 equiv of Cl^-.

[S5] H. Maeda, Y. Kusunose, Y. Mihashi and T. Mizoguchi, *J. Org. Chem.*, 2007, **72**, 2612.
[S6] H. Maeda, Y. Haketa and T. Nakanishi, *J. Am. Chem. Soc.*, 2007, **129**, 13661.