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Supporting Information

Heteroatom Cycloaddition at the $(BN)_2$ Bay Region of Dibenzoperylene

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Supporting Information (SI)

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1. General

Experimental details. All reactions were done under inert conditions by flaming the glassware with a heat gun (630 °C) under vacuum, following purging with argon. Molecular sieve was dried under vacuum and with a temperature profile from 150 °C to 300 °C over 5 hours. Chemicals and solvents were purchased from commercial suppliers in anhydrous form or were dried by known methods. Column chromatography were done using a medium pressure liquid chromatography (MPLC) system (PuriFlash 430 evo, Interchim) with Si-IR 20 μm columns in size of 12 g up to 120 g. Pre-coated polyester sheets (40 x 80 mm) from Machery-Nagel (POLYGAM®SIL G/UV254) with 0.2 mm silica gel 60 with fluorescent indicator were used for thin layer chromatography (TLC). For visualization, UV light source (254 nm and 366 nm) was used. Nuclear magnetic resonance spectroscopy (NMR) was done on a Bruker Avance III HDX 600 equipped with a dual ($^{1}H/^{13}C$) probe head. Chemical shifts (δ) are given in ppm, coupling constants in Hertz (Hz) and the multiplicities of the signals are designated as follows: s = singlet, br s = broad singlet, d = doublet, dd = doublet of doublet, t = triplet and m = multiplet. The signals of NMR solvents were calibrated ($^{1}H/^{13}C$): CD_2Cl_2 5.32/53.84 ppm and thf-d_8 3.58/67.21 ppm. Reference for ^{1}H and ^{13}C were tetramethyl silane (TMS), for ^{11}B $BF_3{\cdot}OEt_3$ in $CDCl_3$ and $CFCl_3$ for ^{19}F. High resolution mass spectrometry was done on a maXis 4G Bruker system with an APCI source combined with a direct inlet probe (DIP) system. Optical spectra were recorded on a PerkinElmer Lambda 1050 spectrometer with a PerkinElmer 3D WB Det Module. Excitation and emission spectra were recorded on a Cary Variant SPVF spectrometer using Hellma Analytics quartz cuvettes. All measurements were done in spectroscopy grade solvents. The fluorescence quantum yields were measured with an excitation wavelength λ_{ex} = 370 nm (diphenylanthracene in ethanol as reference).

X-Ray crystallography. X-ray data were collected with a Bruker Smart APEX II diffractometer with graphite-monochromated Mo K_α radiation. The programs used were

Bruker's APEX2v2011.8-0, including SADABS for absorption correction, SAINT for data reduction and SHELXS for structure solution, as well as the WinGX suite of programs version 1.70.01 or the GUI ShelXle, including SHELXL for structure refinement.[1]

Cyclic voltammetry. Cyclic voltammetry (CV) was carried out using a CHI760E Bipotentiostat (CH-Instruments) controlled by the CHI760E software (version 20.04). The full-glass electrochemical measurement cell was placed in a faraday cage in a nitrogen filled glovebox. A platinum disc electrode (3 mm diameter, Metrohm part no. 6.1204.310) served as the working electrode and a coiled platinum wire (30 cm length, 3 mm diameter) as the counter electrode. As a reference electrode, a Haber-Luggin double-reference system, consisting of a Ag/Ag^+ redox couple (a silver wire placed in a 0.01 M $AgClO_4$ solution in 0.1 M tetrabutylammonium hexafluorophosphate (TBAHFP)/acetonitrile (MeCN)) capacitively connected to a platinum wire immersed in the electrolyte of the sample compartment, is employed.[2] The reference electrode chamber is further separated from the Haber-Luggin capillary by a spacer frit filled with 0.1 M TBAHFP/MeCN. In this way, contamination of the sample compartment and vice versa of the Ag/Ag^+ reference electrode chamber can be prevented. The sample chamber was filled with 0.1 M TBAHFP in tetrahydrofuran (THF).
CV measurements were performed at scan rates between 20 mV/s and 5 V/s. The voltage drop, caused by the resistance of the electrolyte, was corrected by positive feedback iR-compensation. If not stated otherwise, all cyclic voltammograms are corrected by the capacitive background currents. All potentials are given versus the formal potential of the ferrocene/ferrocenium (Fc/Fc^+) couple, which was determined by cyclic voltammetry to be at 185 ± 2 mV vs. the Ag/Ag^+ reference system.

All chemicals were handled under inert conditions and stored inside a nitrogen filled glovebox. THF (HPLC-grade) was distilled from Na three times, degassed via freeze-pump-thaw and stored over activated 4 Å molecular sieve. Acetonitrile (HPLC-grade) was subsequent

distilled from P_2O_5, CaH_2 and again P_2O_5, followed by degassing via freeze-pump-thaw and storing over activated 3 Å molecular sieve. Prior to use, both solvents were run through a column filled with activated neutral alumina. The electrolyte TBAHFP (98%, Alfa Aesar) was recrystalized five times in 3:1 EtOH/H_2O, followed by drying 7 d at 105 °C and 2-3 mbar. Ferrocene (98%, Acros Organics) and $AgClO_4$ (≥ 97%, anhydrous, Alfa Aesar) were used as received.

Computational Details. Geometry optimizations were performed using the M062X functional[3] as implemented in Gaussian 16[4] in conjunction with the 6-311+G** basis set.[5] Harmonic vibrational frequencies were computed to confirm the nature of stationary points as minima or first-order saddle points, and to obtain Gibbs free energies at T = 298.15 K and T = 339 K. The influence of THF solvent was considered during geometry optimization and harmonic vibrational frequency computations using the polarizable continuum model with the integral equation formalism implemented in Gaussian 16.[6] The NICS values were computed using the GIAO[7] method at the M062X/6-311+G** level of theory.

2. Syntheses

General synthesis of cycloaddition reactions

In a dried flask equipped with a Soxhlet extractor filled with 3 Å molecular sieve, 145 mg $(BN)_2$ dibenzoperylene **1** (0.3 mmol, 1 equiv.) were dissolved in dry thf (30 mL). 5 mL of a *p*-toluenesulfonic acid solution (0.6 M in thf, 10 equiv., stored over 3 Å molecular sieve) and 10 equiv. of the benzaldehyde derivative were added, and the mixture stirred under reflux (95 °C oil bath temperature) for 5 days. After cooling down to room temperature, the reaction mixture was quenched with sat. $NaHCO_3$ solution (20 mL) and extracted with ethylacetate (3 x 20 mL). All combined organic layers were washed with brine (3 x 20 ml) and dried over $MgSO_4$. All volatiles were removed under reduced pressure. Column chromatography yielded the desired compound.

Synthesis of 3a (with BA-H):

Column Chromatography: n-hexane/DCM 4:1, R_f = 0.13, colorless solid, yield: 115 mg (0.20 mmol, 67 %).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.30 (d, *J* = 8.0 Hz, 1H, H-4), 8.17-8.12 (m, 3H, H-22, H-16, H-14), 8.12-8.09 (m, 2H, H-10, H-8), 8.05 (dd, *J* = 7.3 Hz, *J* = 1.4 Hz, 1H, H-1), 7.76 (t, *J* = 7.8 Hz, 1H, H-15), 7.69-7.66 (m, 1H, H-3), 7.45-7.42 (m, 1H, H-2), 7.39-7.36 (m, 2H, H-28, H-26), 7.24-7.21 (m, 3H, H-30, H-29, H-25), 7.09 (dd, *J* = 8.5 Hz, *J* = 2.0 Hz, 1H, H-24), 7.02 (s, 1H, H-31), 6.86 (d, *J* = 8.5 Hz, 1H, H-19), 2.80 (t, *J* = 7.9 Hz, 2H, H-32), 2.71-2.68 (m, 2H, H-36), 1.80-1.75 (m, 2H, H-33), 1.71-1.66 (m, 2H, H-37), 1.52-1.47 (m, 2H, H-34), 1.47-1.41 (m, 2H, H-38), 1.02 (t, *J* = 7.4 Hz, 3H, H-35), 0.99 (t, *J* = 7.4 Hz, 3H, H-39).

^{11}B NMR (CD_2Cl_2, 193 MHz): δ = 28.3.

^{13}C NMR (CD_2Cl_2, 151 MHz): δ = 141.8 (C-5), 141.1 (C-27), 139.8 (C-13), 139.2 (C-17), 136.8 (C-20), 136.0 (C-9), 135.5 (C-23), 133.7 (C-12), 132.5 (C-1), 132.3 (C-15), 132.1 (C-3), 129.1 (C-30), 129.1 (C-29, C-25), 129.0 (C-24), 127.2 (C-6), 126.7 (C-2), 126.5 (C-28, C-26), 124.7 (C-8), 124.7 (C-10), 124.7 (C-22), 124.6 (C-11), 124.5 (C-7), 124.4 (C-18), 123.8 (C-21), 122.9 (C-4), 120.1 (C-16)*, 119.8 (C-14)*, 116.1 (C-19), 84.0 (C-), 36.1 (C-), 35.5 (C-), 34.6 (C-), 34.3 (C-), 22.9 (C-), 14.3 (C-), 14.2 (C-). C*s belong to the multipet in the ^{1}H-NMR (8.17-8.12 ppm) and can be interchanged.

HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{39}H_{37}B_2N_2O$: 571.30993; found: 571.30996.

UV/Vis (dichloromethane) λ (log ε): 383 (4.31), 364 (4.34), 348 (4.13), 334 (3.77), 299 (4.13), 287 (4.27), 261 (4.78), 256 (4.75), 233 (4.83).

Fluorescence quantum yield: 88 %.

Synthesis of 3b (with BA-OH)

Column Chromatography: n-hexane/DCM 1:3, R_f = 0.29, colorless solid, yield: 130 mg (0.22 mmol, 74 %).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.33 (d, *J* = 8.3 Hz, 1H, H-4), 8.20 (d, *J* = 8.0 Hz, 2H, H-14, H-16), 8.17-8.15 (m, 3H, H-8, H-10, H-22), 8.08 (dd, *J* = 7.4 Hz, *J* = 1.3 Hz, 1H, H-1), 7.81 (t, *J* = 8.0 Hz, 1H, H-15), 7.70-7.67 (m, 1H, H-3), 7.46-7.42 (m, 1H, H-2), 7.28-7.26 (m, 2H, H-26, H-28), 7.12 (dd, *J* = 8.4 Hz, *J* = 1.9 Hz, 1H, H-24), 7.08 (s, 1H, H-32), 6.92 (d, *J* = 8.4 Hz, 1H, H-19), 6.69-6.66 (m, 2H, H-25, H-29), 4.93 (s, 1H, H-31), 2.83 (t, *J* = 7.9 Hz, 2H, H-33), 2.71-2.68 (m, 2H, H-37), 1.81-1.75 (m, 2H, H-34), 1.71-1.65 (m, 2H, H-38), 1.52-1.46 (m, 2H, H-35), 1.46-1.39 (m, 2H, H-39), 1.02 (t, *J* = 7.4 Hz, 3H, H-36), 0.98 (d, *J* = 7.4 Hz, 3H, H-40).

^{11}B NMR (CD_2Cl_2, 193 MHz): δ = 29.2.

^{13}C NMR (CD_2Cl_2, 151 MHz): δ = 156.4 (C-30), 141.8 (C-5), 139.9 (Cq), 139.3 (Cq), 136.9 (C-20), 136.1 (C-9), 135.5 (C-23), 133.9 (C-27), 133.8 (Cq), 132.6 (C-1), 132.4 (C-15), 132.2 (C-3), 129.1 (C-24), 128.1 (C-26, C-28), 127.3 (C-6), 126.8 (C-2), 124.8 (C-8), 124.8 (C-10), 124.7 (C-22), 124.6 (Cq), 124.6 (Cq), 124.4 (C-18), 123.8 (C-21), 122.9 (C-4), 120.1 (C-16)*, 119.9 (C-14)*, 116.2 (C-), 115.8 (C-25, C-29), 83.7 (C-32), 36.1 (C-33), 35.5 (C-37), 34.6 (C-34), 34.3 (C-38), 22.9 (C-39, C-35), 14.3 (C-36), 14.2 (C-40).
C*s belong to the duplet in the ^{1}H-NMR at 8.20 ppm and can be interchanged, Cq cannot completely assigned due to the multiplet signal in the ^{1}H NMR.
HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{39}H_{37}B_2N_2O_2$: 587.30485; found: 571.30405.
UV/Vis (dichloromethane) λ (log ε): 383 (4.28), 364 (4.31), 348 (4.11), 334 (3.75), 229 (4.10), 286 (4.26), 262 (4.76), 256 (4.74), 233 (4.82).
Fluorescence quantum yield: 80 %

Synthesis of 3c (with BA-NO_2)

Column Chromatography: n-hexane/DCM 1:1, R_f = 0.25 yellow solid, yield: 137 mg (0.22 mmol, 73 %).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.31 (d, *J* = 8.2 Hz, 1H, H-4), 8.18-8.14 (m, 3H, H-14, H-16, H-22), 8.11 (s, 2H, H-8, H-10), 8.07-8.03 (m, 3H, H-1, H-25, H-29), 7.79 (t, *J* = 7.7 Hz, 1H, H-15), 7.71-7.67 (m, 1H, H-3), 7.56-7.53 (m, 2H, H-26, H-28), 7.46-7.43 (m, 1H, H-2), 7.10 (dd, *J* = 8.5 Hz, *J* = 2.0 Hz, 1H, H-24), 7.08 (s, 1H, H-31), 6.72 (d, *J* = 8.5 Hz, 1H, H-19), 2.82 (t, *J* = 7.9 Hz, 2H, H-32), 2.71-2.68 (m, 2H, H-36), 1.79-1.74 (m, 2H, H-33), 1.71-1.65 (m, 2H, H-37), 1.52-1.46 (m, 2H, H-34), 1.46-1.40 (m, 1H, H-38), 1.02 (t, *J* = 7.4 Hz, 3H, H-35), 0.98 (t, *J* = 7.4 Hz, 3H, H-39).

^{11}B NMR (CD_2Cl_2, 193 MHz): δ = 28.9.

^{13}C NMR (CD_2Cl_2, 151 MHz): δ = 148.5 (C-30), 147.9 (C-27), 141.9 (C-5), 139.9 (C-13), 139.2 (C-17), 136.3 (C-20), 136.3 (C-9), 136.0 (C-23), 133.4 (C-), 132.6 (C-15), 132.5 (C-1), 132.4 (C-3), 129.1 (C-24), 127.7 (C-26, C-28), 126.8 (C-2), 125.0 (C-22), 124.9 (C-8/10), 124.8 (C-8/10), 124.6 (C-7/11), 124.5 (C-7/11), 124.4 (C-25, C-29), 124.1 (C-18), 123.9 (C-21), 123.0 (C-4), 120.3 (C-14/16), 120.0 (C-14/16), 115.9 (C-19), 82.9 (C-31), 36.1 (C-32), 35.5 (C-36), 34.6 (C-33), 34.3 (C-37), 22.9 (C-34), 22.9 (C-38), 14.3 (C-35), 14.2 (C-39).
HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{39}H_{36}B_2N_3O_3$: 616.29501; found: 616.29395.
UV/Vis (dichloromethane) λ (log ε): 381 (4.18), 362 (4.27), 348 (4.11), 332 (3.79), 298 (4.17), 284 (4.40), 261 (4.78), 255 (4.76), 233 (4.78).
Fluorescence quantum yield: 7 %.

Synthesis of 3d (with BA-F)

Column Chromatography: n-hexane/DCM 85:15, R_f = 0.21, colorless solid, yield: 141 mg (0.24 mmol, 80 %).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.33-8.30 (m, 1H, H-4), 8.19-8.16 (m, 2H, H-14, H-16), 8.16 (d, *J* = 1.7 Hz, 1H, H-22), 8.13 (s, 2H, H-8, H-10), 8.06 (dd, *J* = 7.4 Hz, *J* = 1.4, 1H, H-1), 7.79 (t, *J* = 7.9 Hz, 1H, H-15), 7.70-7.67 (m, 1H, H-3), 7.46-7.43 (m, 1H, H-2), 7.39-7.35 (m, 2H, H-26, H-28), 7.11 (dd, *J* = 8.4 Hz, *J* = 1.7 Hz , 1H, H-24), 7.06 (s, 1H, H-32), 6.93-6.90 (m, 2H, H-29, H-25), 6.84 (d, *J* = 8.4 Hz, 1H, H-19), 2.81 (t, *J* = 7.9 Hz, 2H, H-33), 2.72-2.68 (m, 2H, H-37), 1.80-1.74 (m, 2H, H-34), 1.71-1.66 (m, 2H, H-38), 1.52-1.46 (m, 2H, H-35), 1.46-1.40 (m, 2H, H-39), 1.02 (t, *J* = 7.4 Hz, 3H, H-36), 0.98 (t, *J* = 7.4 Hz, 3H, H-40).

^{11}B NMR (CD_2Cl_2, 193 MHz): δ = 28.5

^{13}C NMR (CD_2Cl_2, 151 MHz): δ = 163.1 (d, *J* = 246 Hz, C-30), 141.8 (C-5), 139.9 (C-13), 139.2 (C-17), 137.4 (d, *J* = 3 Hz, C-27), 136.6 (C-20), 136.2 (C-9), 135.6 (C-23), 133.6 (C-12), 132.5 (C-1), 132.4 (C-15), 132.2 (C-3), 129.1 (C-24), 128.5 (d, *J* = 9 Hz, C-28, C-26), 127.1 (C-6), 126.8 (C-2), 124.8 (C-8), 124.8 (C-10), 124.8 (C-22), 124.6 (C-7), 124.5 (C-11), 124.3 (C-18), 123.8 (C-21), 122.9 (C-4), 120.2 (C-16)*, 119.9 (C-14)*, 116.1 (C-19), 116.0 (d, *J* = 22 Hz, C-29, C-25), 83.3 (C-32), 36.1 (C-33), 35.5 (C-37), 34.6 (C-34), 34.3 (C-38), 22.9 (C-35, C-39), 14.3 (C-36), 14.2 (C-40).

C*s belong to the multiplet in the ^{1}H-NMR (8.19-8.16 ppm) and can be interchanged.

^{19}F NMR (CD_2Cl_2, 564 MHz): δ = -113.84.

HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{39}H_{36}B_2FN_2O$: 589.30051; found: 589.29964.

UV/Vis (dichloromethane) λ (log ε): 382 (4.32), 363 (4.34), 348 (4.13), 334 (3.78), 299 (4.12), 286 (4.28), 262 (4.77), 255 (4.74), 233 (4.83).

Fluorescence quantum yield: 78 %.

Synthesis of 3e (with Mesitaldehyde)

Column Chromatography: n-hexane/DCM 84:16, R_f = 0.3, colorless solid, yield: 74.0 mg (0.12 mmol, 40 %).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.26-8.24 (m, 1H, H-4), 8.07-8.01 (m, 4H, H-8, H-14, H-16, H-22), 7.98 (d, *J* = 1.3 Hz, 1H, H-10), 7.88 (dd, *J* = 7.3 Hz, *J* = 1.3 Hz, 1H, H-1), 7.69 (t, *J* = 7.9 Hz, 1H, H-15), 7.67-7.64 (m, 1H, H-3), 7.39-7.36 (m, 1H, H-2), 6.97 (s, 2H, H-29, H-34), 6.95 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H, H-24), 6.48-6.46 (m, 2H, H-19, H-25), 2.79-2.75 (m, 2H, H-35), 2.72 (s, 3H, H-32), 2.68-2.64 (m, 2H, H-39), 2.17 (s, 3H, H-33), 1.79-1.73 (m, 2H, H-36), 1.70-1.65 (m, 2H, H-40), 1.62 (s, 3H, H-31), 1.54-1.48 (m, 2H*, H-41), 1.48-1.41 (m, 2H, H-37), 1.03 (t, *J* = 7.4 Hz, 3H, H-38), 0.99 (t, *J* = 7.4 Hz, 3H, H-42).

*signal overlaps with water

^{11}B NMR (CD_2Cl_2, 193 MHz): δ = 28.4.

^{13}C NMR (CD_2Cl_2, 151 MHz): δ = 141.8 (C-5), 139.7 (C-13), 139.1 (C-17), 138.1 (C-q), 137.1 (C-q), 136.3 (C-20), 135.8 (C-q), 135.7 (C-9), 135.2 (C-23), 134.8 (C-q), 133.6 (C-12), 132.5 (C-1), 132.1 (C-15), 132.0 (C-25), 131.9 (C-3), 130.3 (C-29), 128.6 (C-24), 127.1 (C-6), 126.6 (C-2), 124.6 (C-7), 124.6 (C-10), 124.5 (C-8), 124.5 (C-22), 124.4 (C-11), 124.2 (C-18), 123.7 (C-21), 122.7 (C-4), 120.0 (C-16*), 119.6 (C-14*), 115.5 (C-19), 82.6 (C-34), 36.2

(C-35), 35.5 (C-39), 34.6 (C-36), 34.2 (C-40), 23.0 (C-41), 23.0 (C-37), 21.1 (C-31), 20.9 (C-33), 20.6 (C-32), 14.3 (C-38), 14.2 (C-42).

All C-q's are quaternary carbons of the mesityl group and cannot completely assigned. C-16 and C-14 can be interchanged due to the proton mulitplet at 8.07-8.01 ppm.

HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{42}H_{43}B_2N_2O$: 613.35697; found: 613.35570.
UV/Vis (dichloromethane) λ (log ε): 384 (4.29), 365 (4.32), 349 (4.11), 336 (3.74), 300 (4.08), 287 (4.24), 262 (4.73), 255 (4.71), 235 (4.74).

Fluorescence quantum yield: 84 %.

Synthesis of 3f (with Pivalaldehyde)

Column Chromatography: n-hexane/DCM 4:1, R_f = 0.2 , colorless solid, yield: 24.8 mg (45.0 µmol, 15 %) with impurities.

^{1}H NMR (CD_2Cl_2, 600 MHz): δ = 8.46-8.41 (m, 1H), 8.30-8.22 (m, 5H), 8.17 (d, *J* = 2 Hz, 1H), 7.93-7.87 (m, 1H), 7.80-7.73 (m, 1H), 7.58-7.50 (m, 1H), 7.31-7.27 (m, 2H), 6.52 (s, 1H), 2.90-2.84 (m, 2H), 2.78-2.72 (m, 2H), 1.86-1.66 (m, 4H), 1.52-1.39 (m, 4H)*, 1.04-0.95 (m, 6H)*, 0.93 (s, 9H).

Signals which overlap with impurities are marked with * and are given with correct proton numbers.

Synthesis of 3g (with Cinnamaldehyde)

Column Chromatography: n-hexane/DCM 85:15, R_f = 0.18, colorless solid, yield: 137 mg (0.23 mmol, 77 %).

^{1}H NMR (THF-d_8, 600 MHz): δ = 8.48-8.46 (d, *J* = 8.4 Hz, 1H, H-4), 8.35-8.28 (m, 5H, H-8, H-10, H-14, H-16, H-22), 8.23 (dd, *J* = 7.4 Hz, *J* = 1.4 Hz, 1H, H-1), 7.84 (t, *J* = 8.0 Hz, 1H, H-15), 7.74-7.67 (m, 1H, H-3), 7.49-7.44 (m, 1H, H-2), 7.44-7.39 (m, 1H, H-19), 7.32-7.27 (m, 3H, H-24, H-29, H-33), 7.17-7.06 (m, 3H, H-30, H-31, H-32), 7.03 (d, *J* = 5.4 Hz, 1H, H-25), 6.84 (d, *J* = 15.9 Hz, 1H, H-27), 6.53 (dd, *J* = 15.9 Hz, *J* = 5.4 Hz, 1H, H-26), 2.87 (t, *J* = 7.7 Hz, 2H, H-34), 2.74 (t, *J* = 7.7 Hz, 2H, H-38), 1.84-1.66 (m, 4H, H-35, H-39), 1.53-1.39 (m, 4H, H-36, H-40), 1.03-0.95 (m, 6H, H-37, H-41).

^{11}B NMR (THF-d_8, 193 MHz): δ = 28.6.

^{13}C NMR (THF-d_8, 151 MHz): δ = 142.6 (C-5), 140.3 (C-q), 139.9 (C-q), 137.5 (C-20), 136.7 (C-28), 136.4 (C-9), 135.5 (C-23), 134.3 (C-q), 133.0 (C-27), 132.9 (C-1), 132.6 (C-15), 132.5 (C-3), 129.5 (C-24), 128.9 (C-30, C-32), 128.7 (C-26), 128.5 (C-31), 127.5 (C-29, C-33), 127.0 (C-2), 125.2 (C-m), 125.2 (C-m), 125.2 (C-q), 125.1 (C-m), 124.4 (C-q), 123.4 (C-4), 120.5 (C-m), 120.3 (C-m), 116.0 (C-19), 82.6 (C-25), 36.4 (C-34), 35.8 (C-38), 35.0 (C-35), 34.8 (C-39), 23.2 (C-36), 23.1 (C-40), 14.2 (C-37), 14.2 (C-41). The "C-m" signals belongs to the mulitplet CHs at 8.35-8.28 ppm in the proton NMR and cannot completely assigned. Due to this mulitplet, all quaternary "C-q" cannot completely assigned.

HR-MS (APCI-DIP): m/z $[M+H]^+$ calcd. for $C_{41}H_{39}B_2N_2O$: 597.32564; found: 571.32546.

UV/Vis (dichloromethane) λ (log ε): 383 (4.26), 364 (4.30), 349 (4.09), 335 (3.74), 299 (4.13), 286 (4.31), 261 (4.85), 254 (4.83), 233 (4.80).

Fluorescence quantum yield: 80 %.

3. Spectra

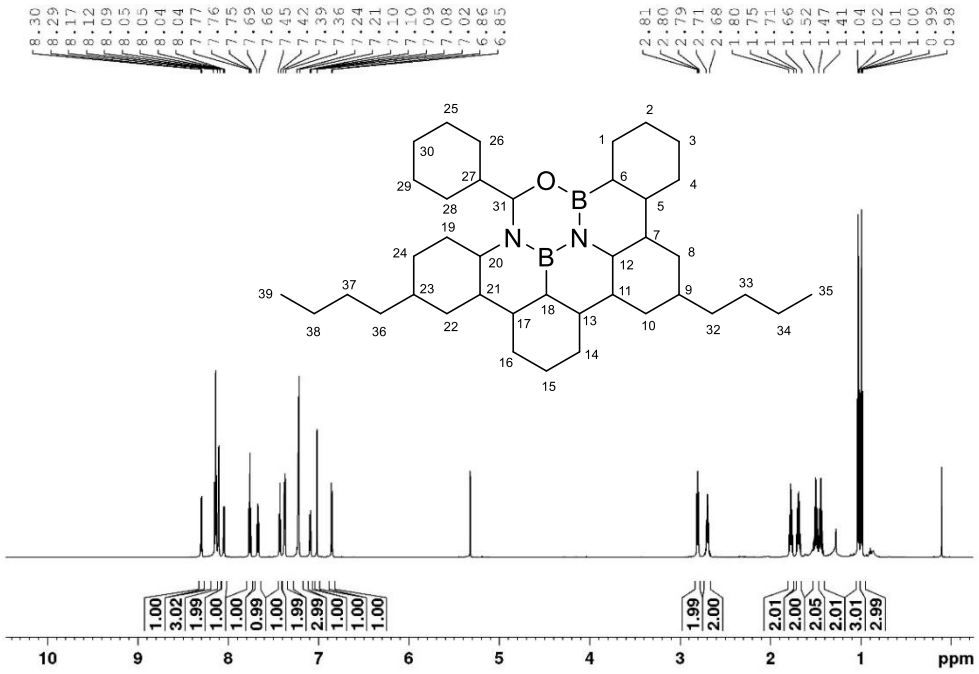


Figure S1: ^{1}H-NMR of **3a** in CD_2Cl_2.

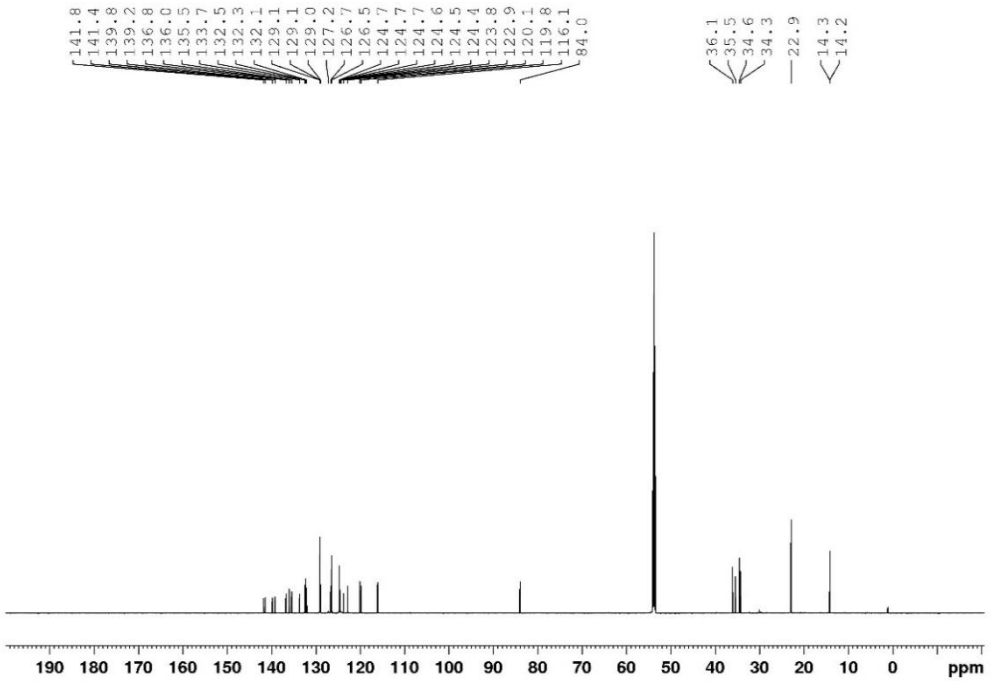


Figure S2: ^{13}C-NMR of **3a** in CD_2Cl_2.

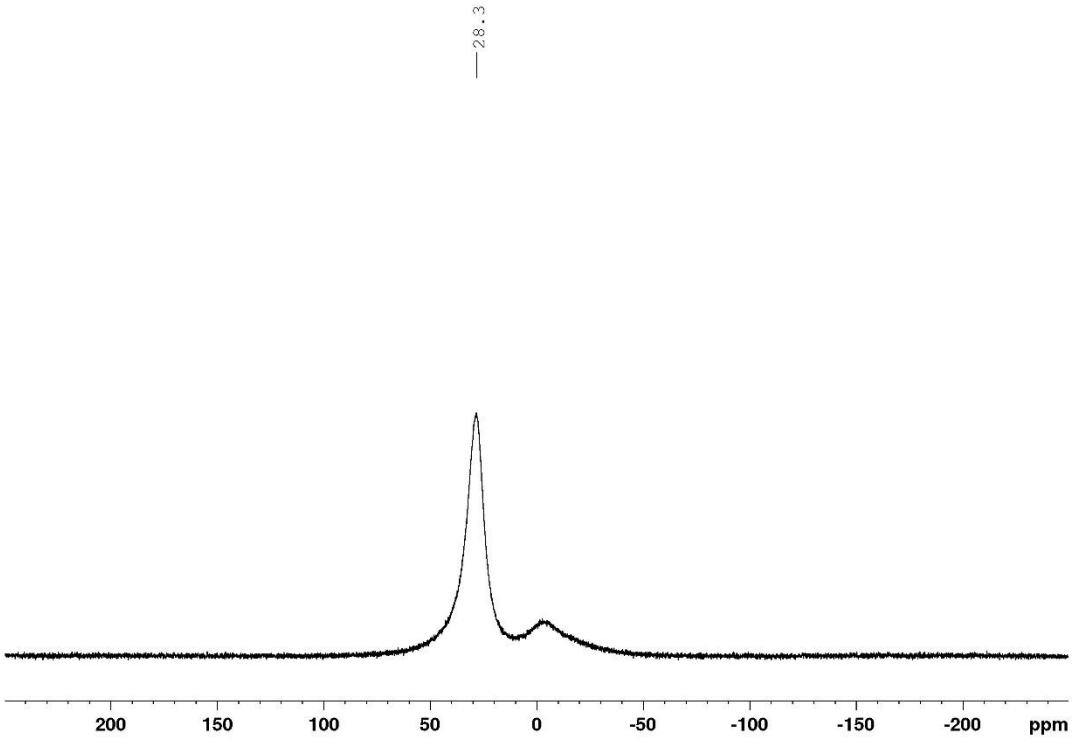


Figure S3: 11B-NMR of **3a** in CD_2Cl_2.

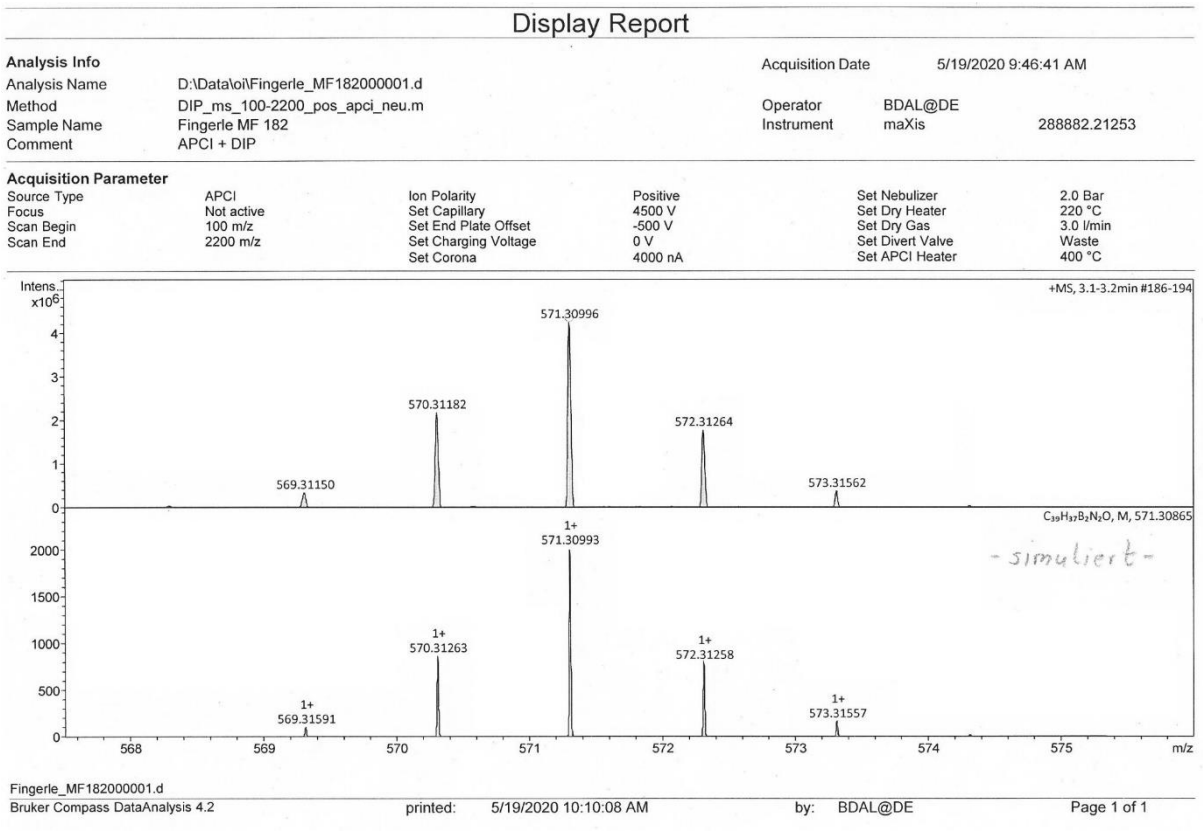


Figure S4: High resolution MS of **3a**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

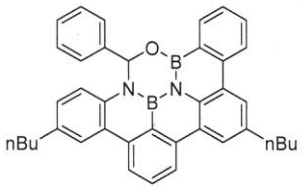
Datum: 11.05.2020

Probenbezeichnung: MF182 nominelle Masse: 570.30

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt): $C_{39}H_{36}B_2N_2O$

Strukturformel (falls bekannt):



Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M+H]^+_{(theor.)}$ = 571,30993

Gemessen = 571,30996

Relative Massenabweichung = 0,05 ppm

Figure S5: Data sheet high resolution MS of **3a**.

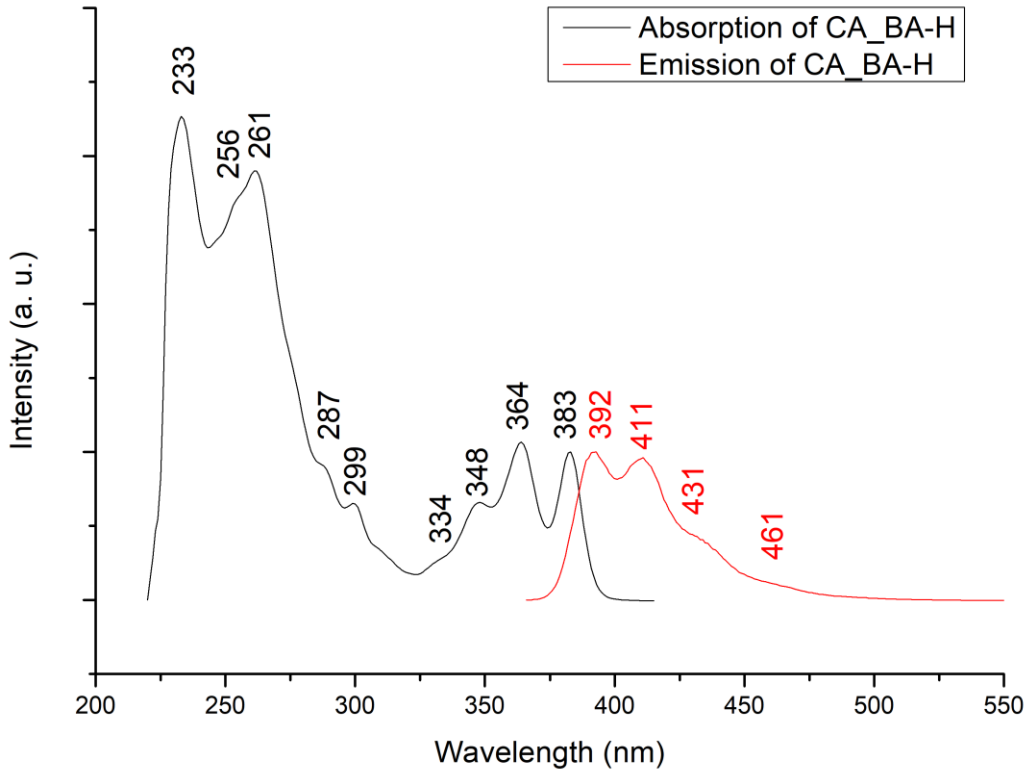


Figure S6: Absorption and emission spectra of **3a** (10^{-5} mol/L) in CD_2Cl_2.

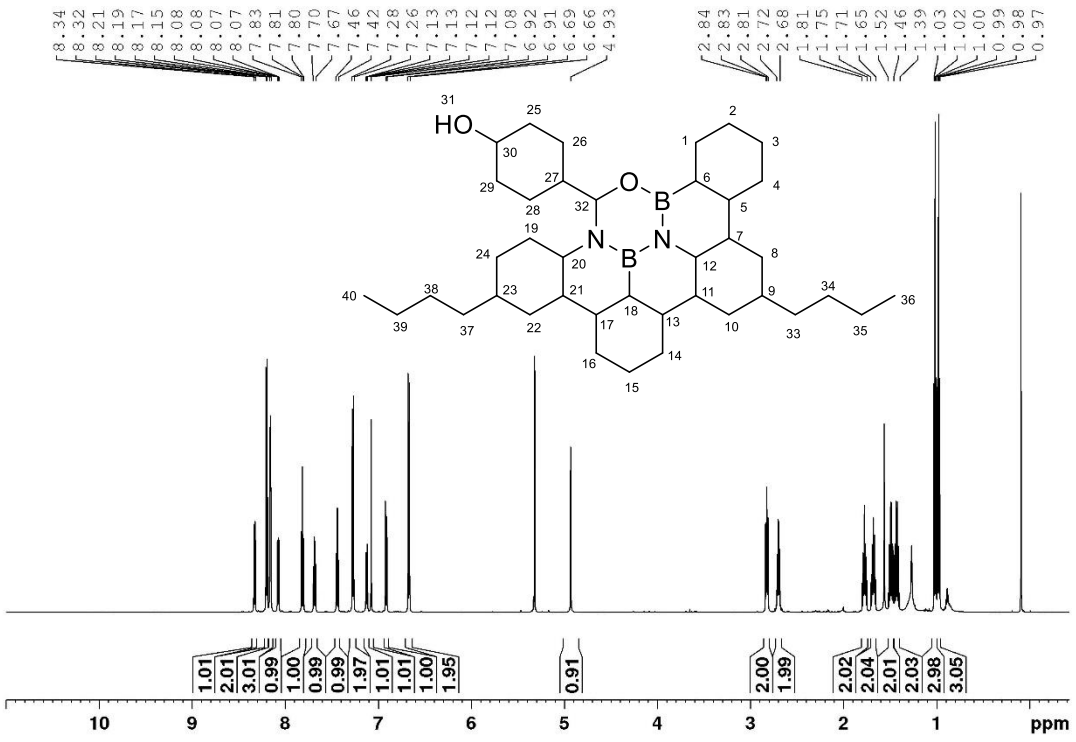


Figure S7: ^{1}H-NMR of **3b** in CD_2Cl_2.

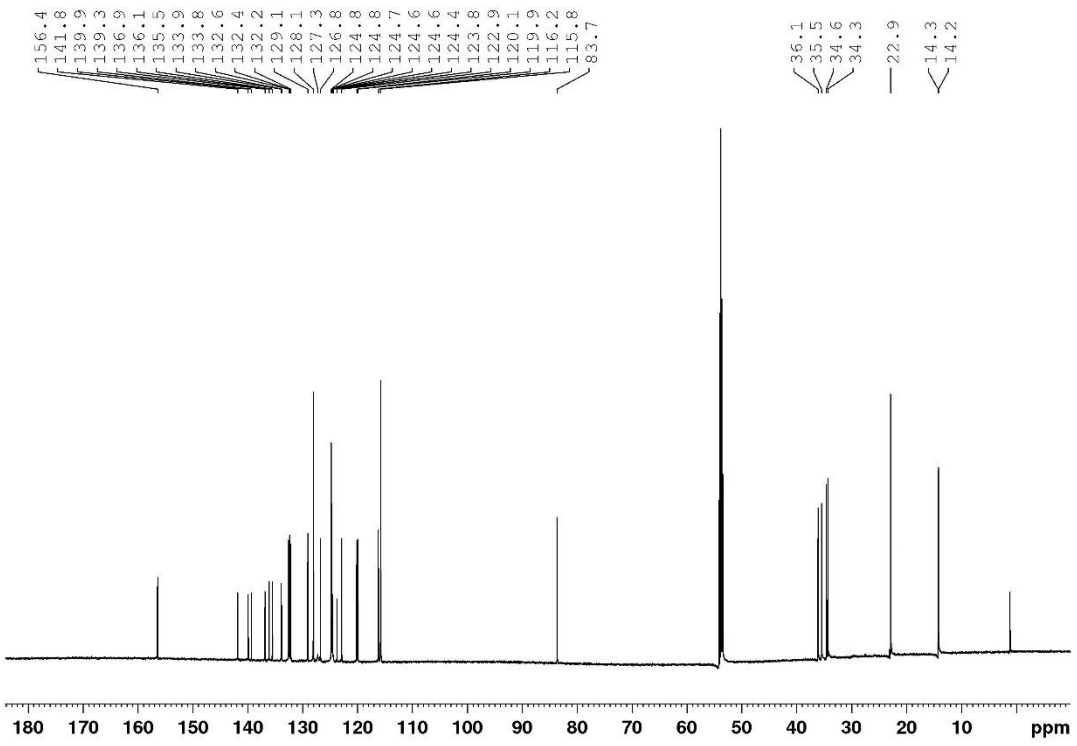


Figure S8: ^{13}C-NMR of **3b** in CD_2Cl_2.

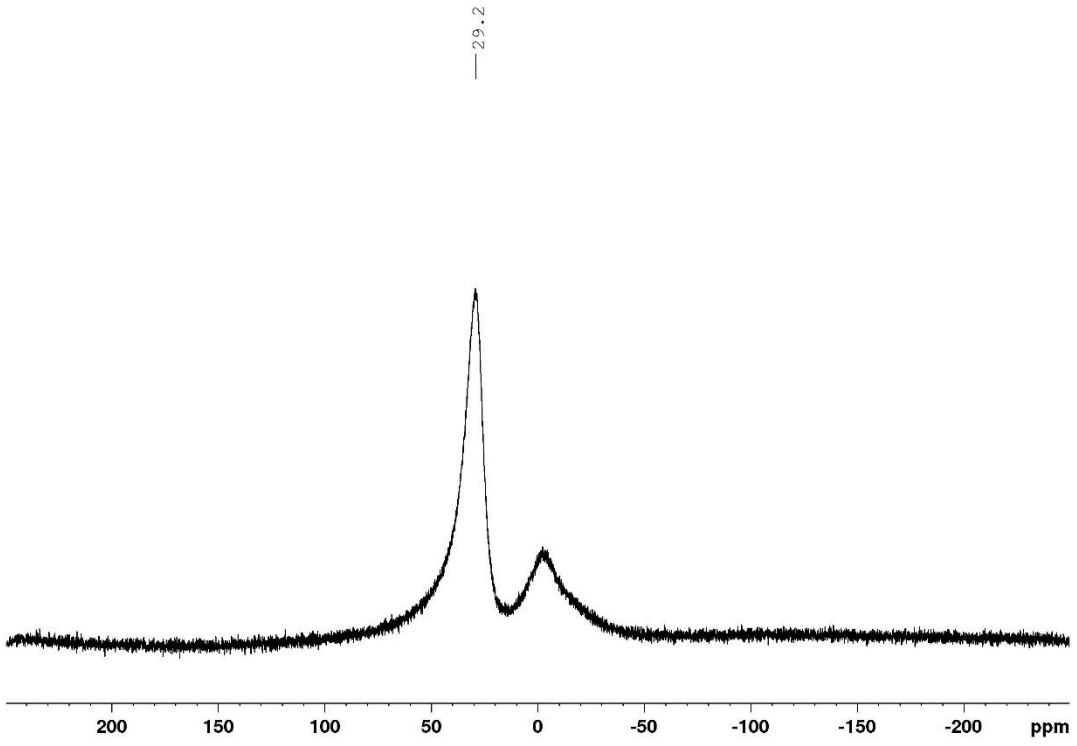


Figure S9: ^{11}B-NMR of **3b** in CD_2Cl_2.

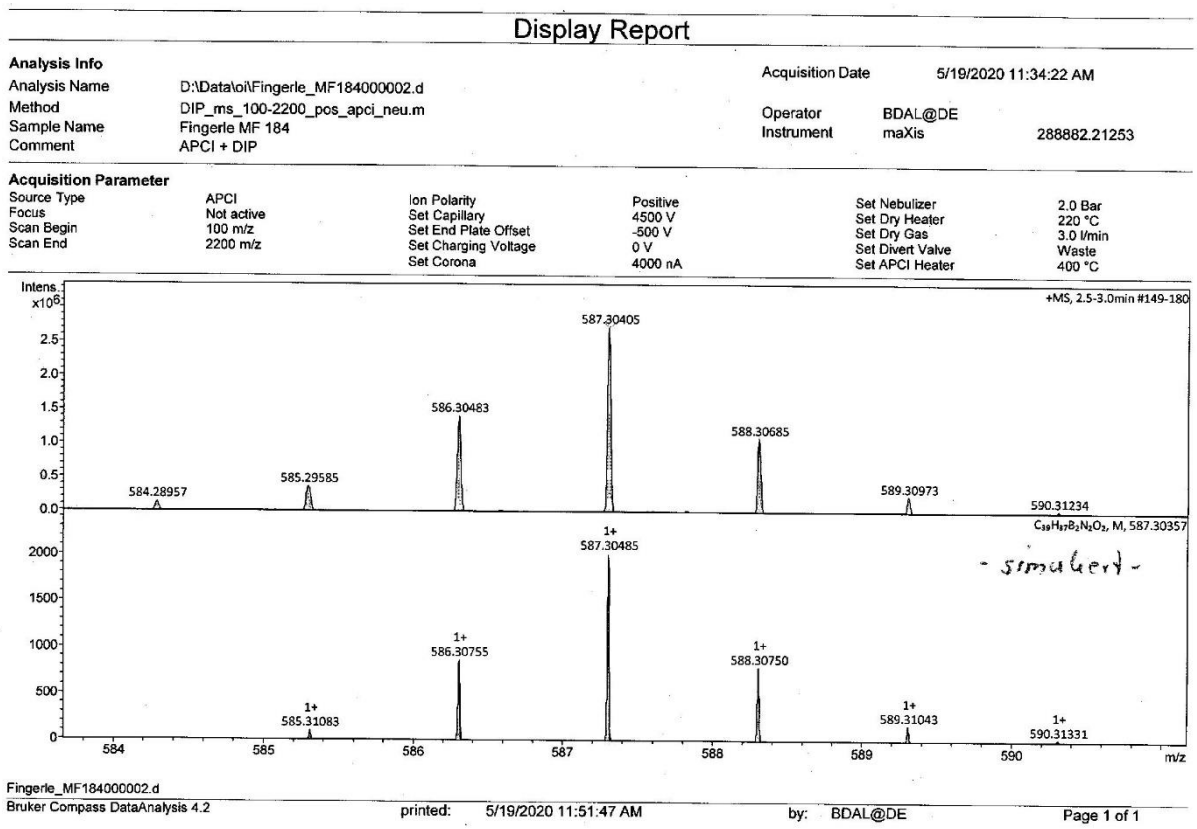


Figure S10: High resolution MS of **3b**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

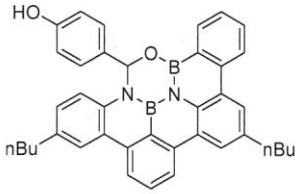
Datum: 11.05.2020

Probenbezeichnung: MF184 nominelle Masse: 586.30

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt): $C_{39}H_{36}B_2N_2O_2$

Strukturformel (falls bekannt):



Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M+H]^+_{(theor.)}$ = 587,30485

Gemessen = 587,30405

Relative Massenabweichung = 1,37 ppm

Figure S11: Data sheet high resolution MS of **3b**.

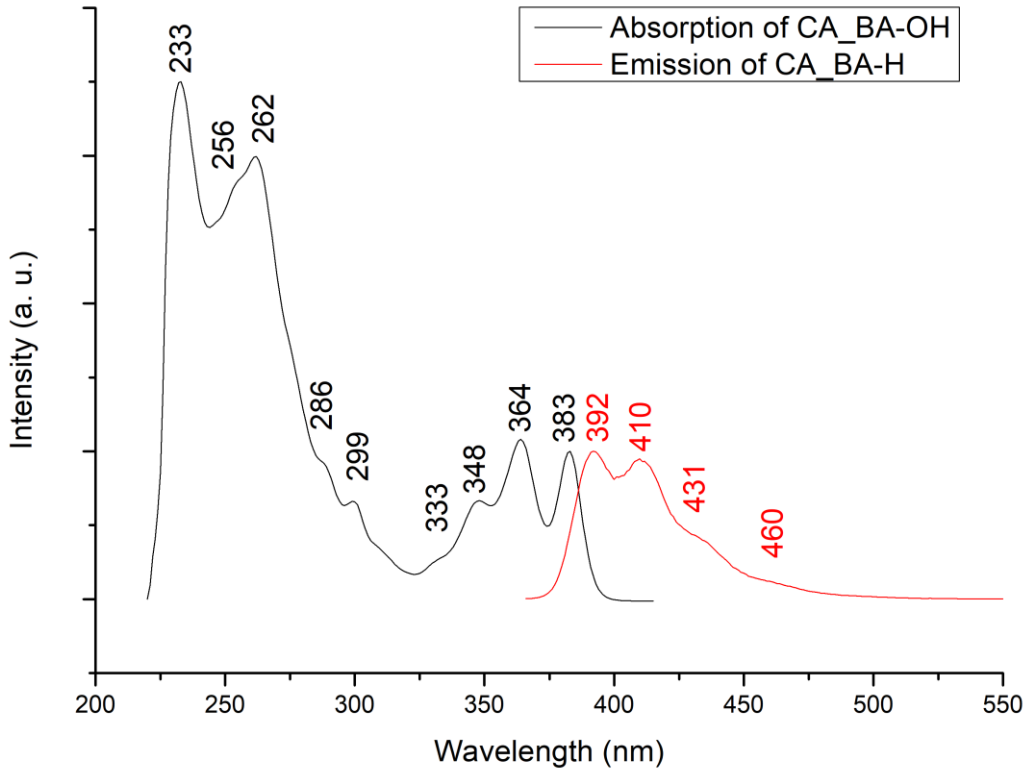


Figure S12: Absorption and emission spectra of **3b** (10^{-5} mol/L) in CD_2Cl_2.

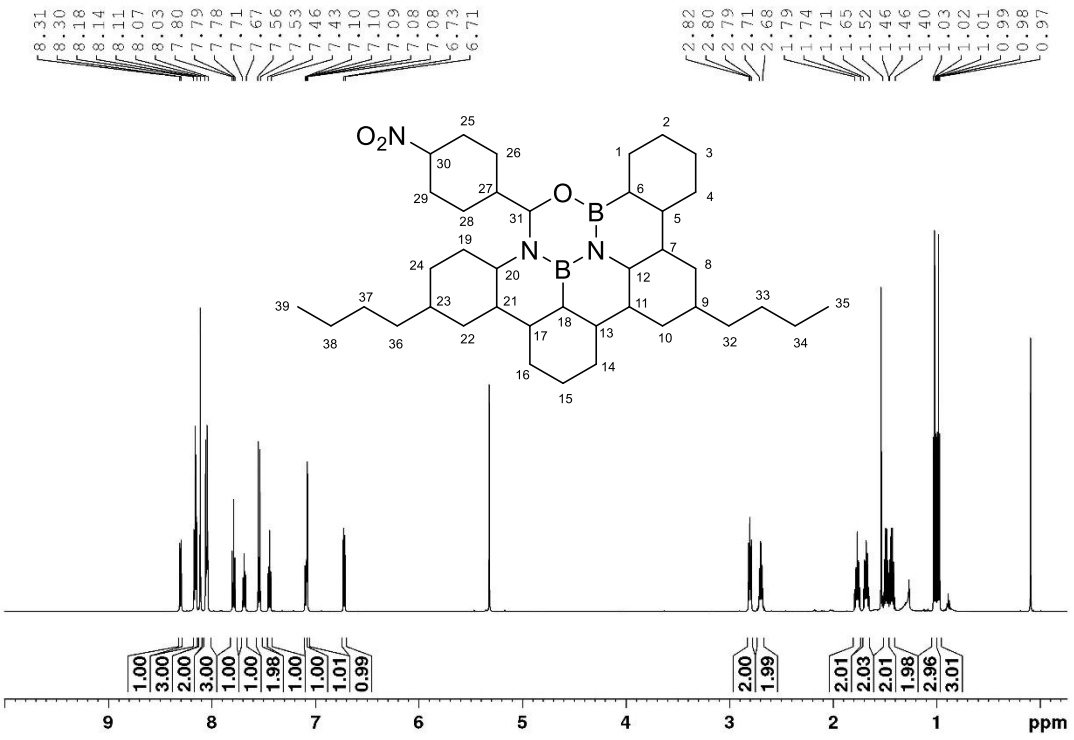


Figure S13: ^{1}H-NMR of **3c** in CD_2Cl_2.

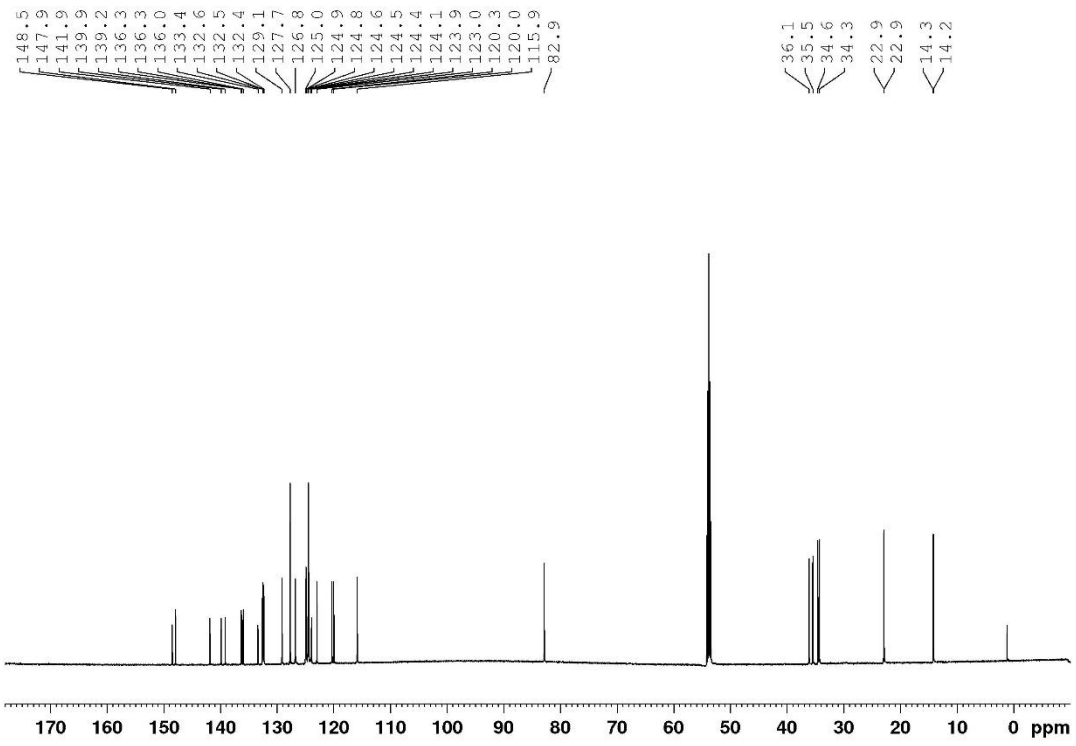


Figure S14: ^{13}C-NMR of **3c** in CD_2Cl_2.

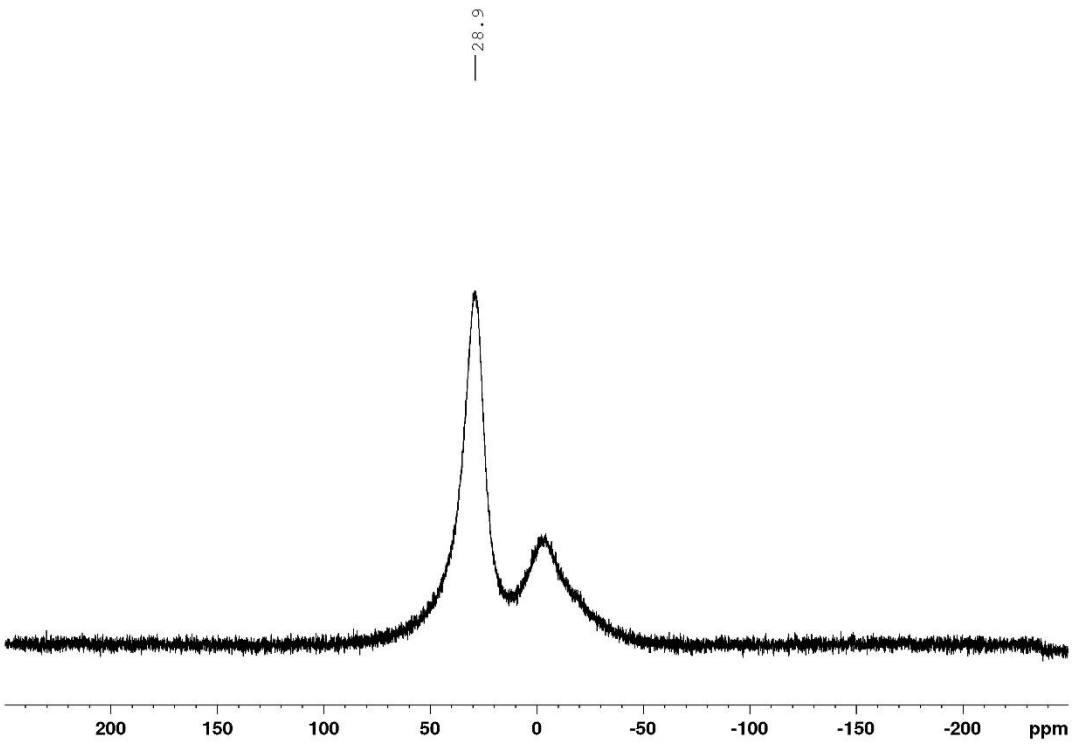


Figure S15: ^{11}B-NMR of **3c** in CD_2Cl_2.

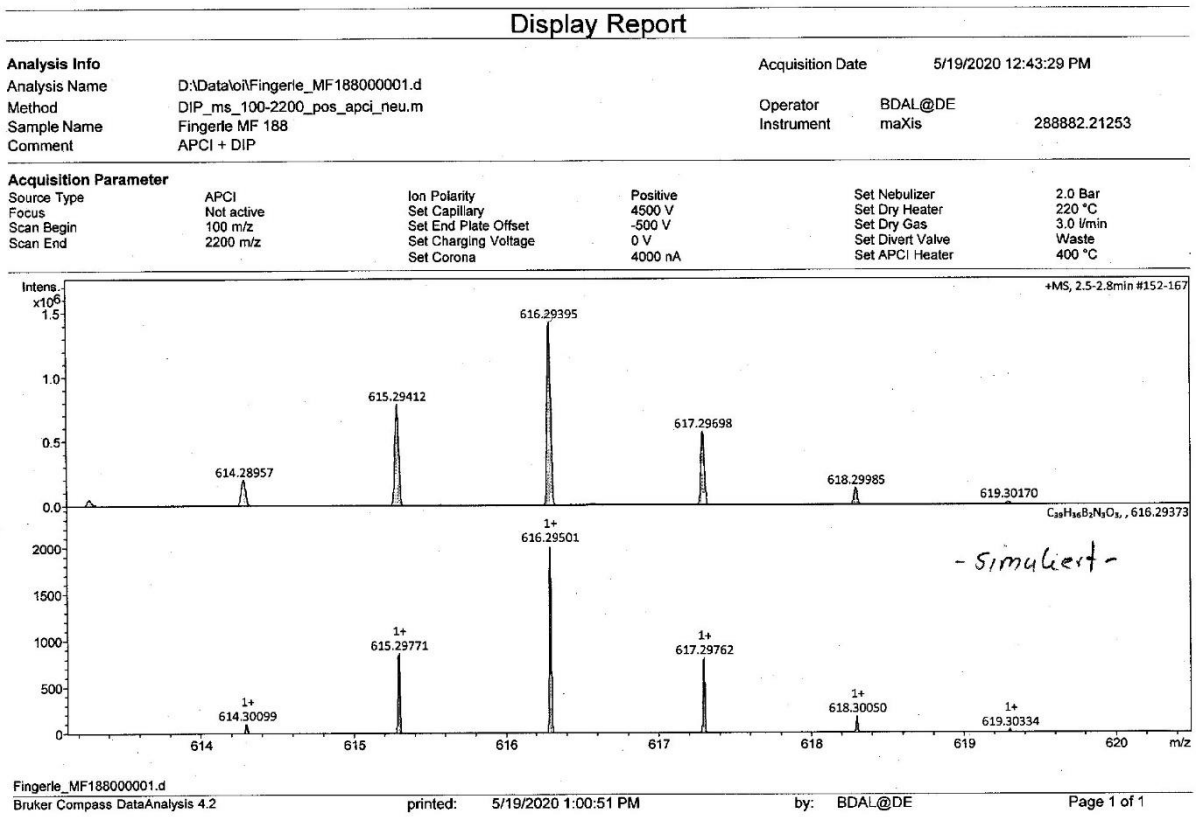


Figure S16: High resolution MS of **3c**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

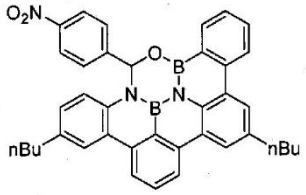
Datum: 11.05.2020

Probenbezeichnung: MF188 nominelle Masse: 615.29

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt): $C_{39}H_{35}B_2N_3O_3$

Strukturformel (falls bekannt):



Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M + H]^+_{(theor.)}$ = 616,29501

Gemessen = 616,29395

Relative Massenabweichung = 1,73 ppm

Figure S17: Data sheet high resolution MS of **3c**.

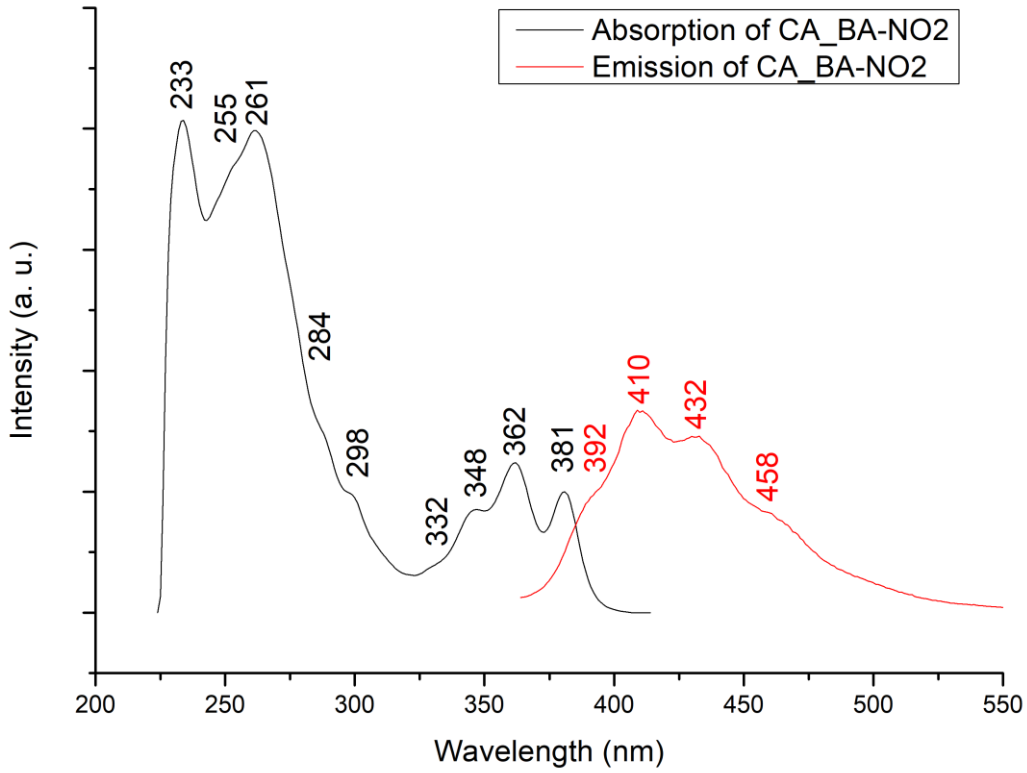


Figure S18: Absorption and emission spectra of **3c** (10^{-5} mol/L) in CD_2Cl_2.

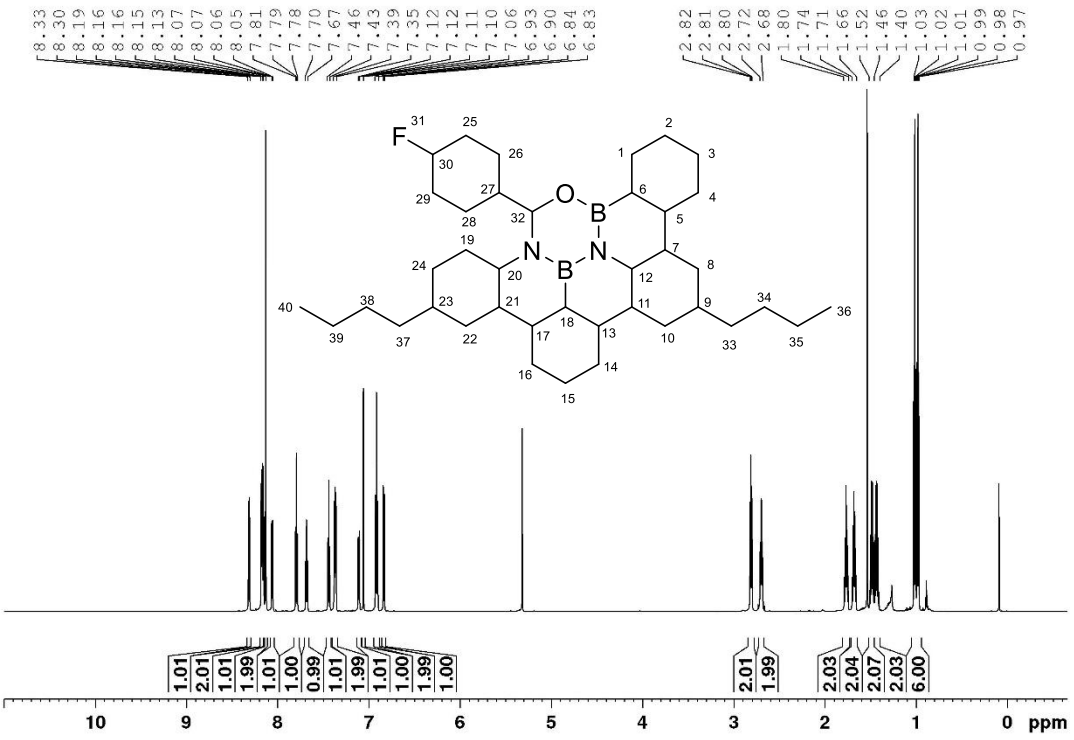


Figure S19: ^{1}H-NMR of **3d** in CD_2Cl_2.

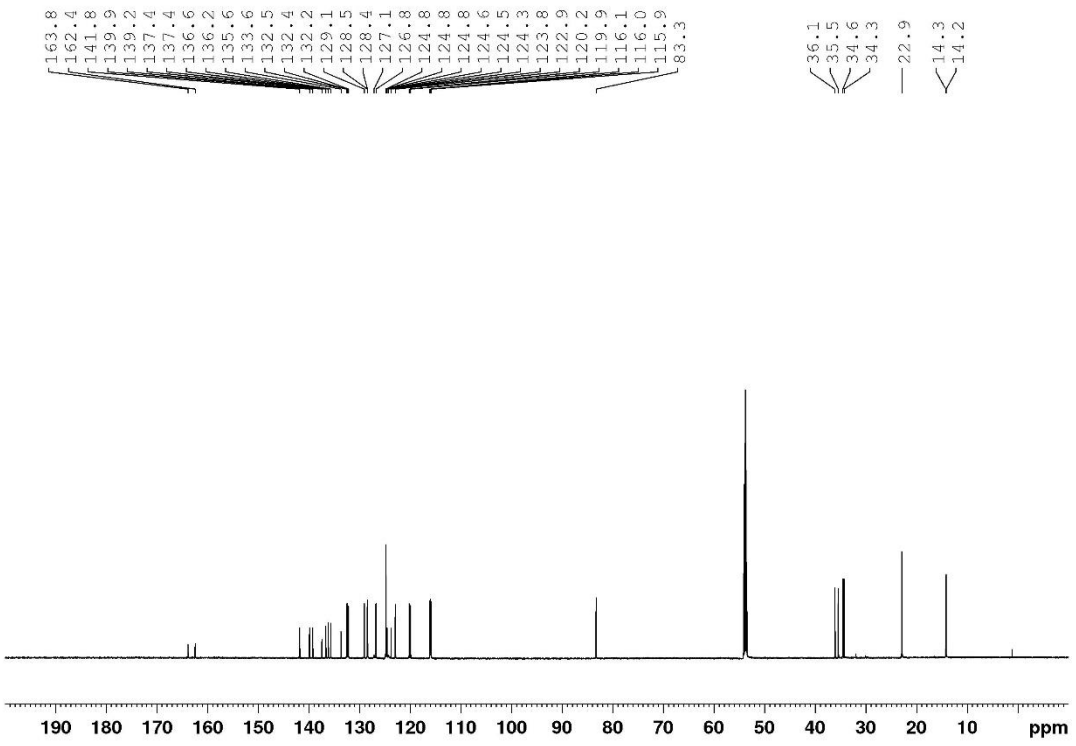


Figure S20: ^{13}C-NMR of **3d** in CD_2Cl_2.

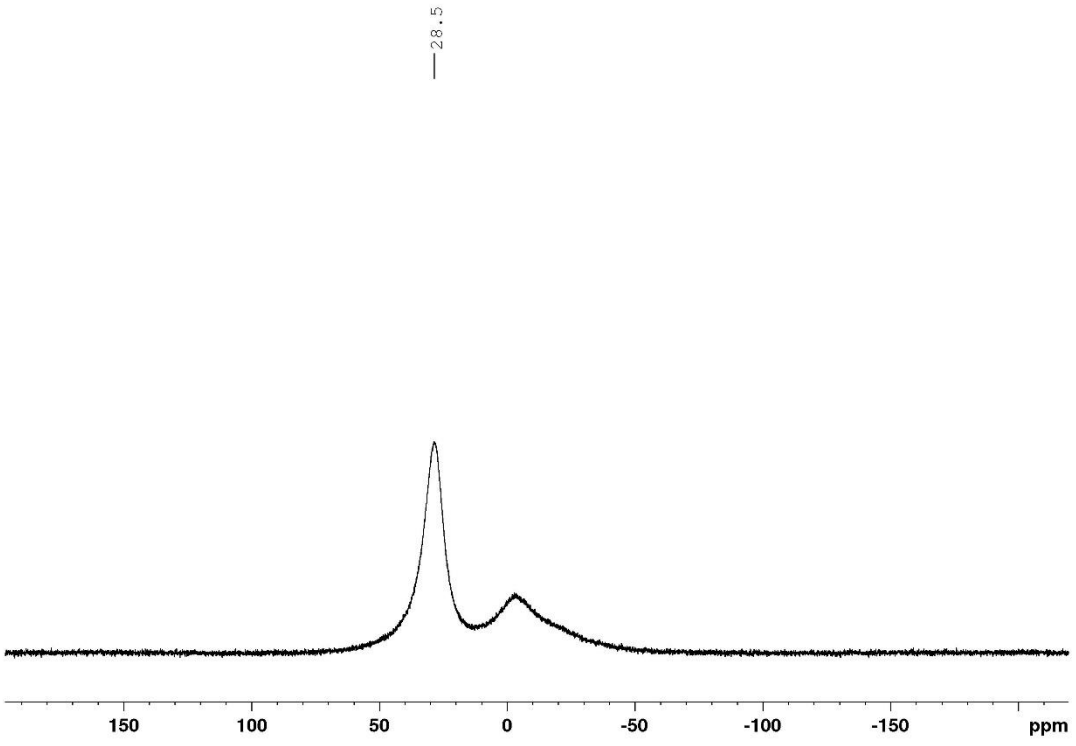


Figure S21: ^{11}B-NMR of **3d** in CD_2Cl_2.

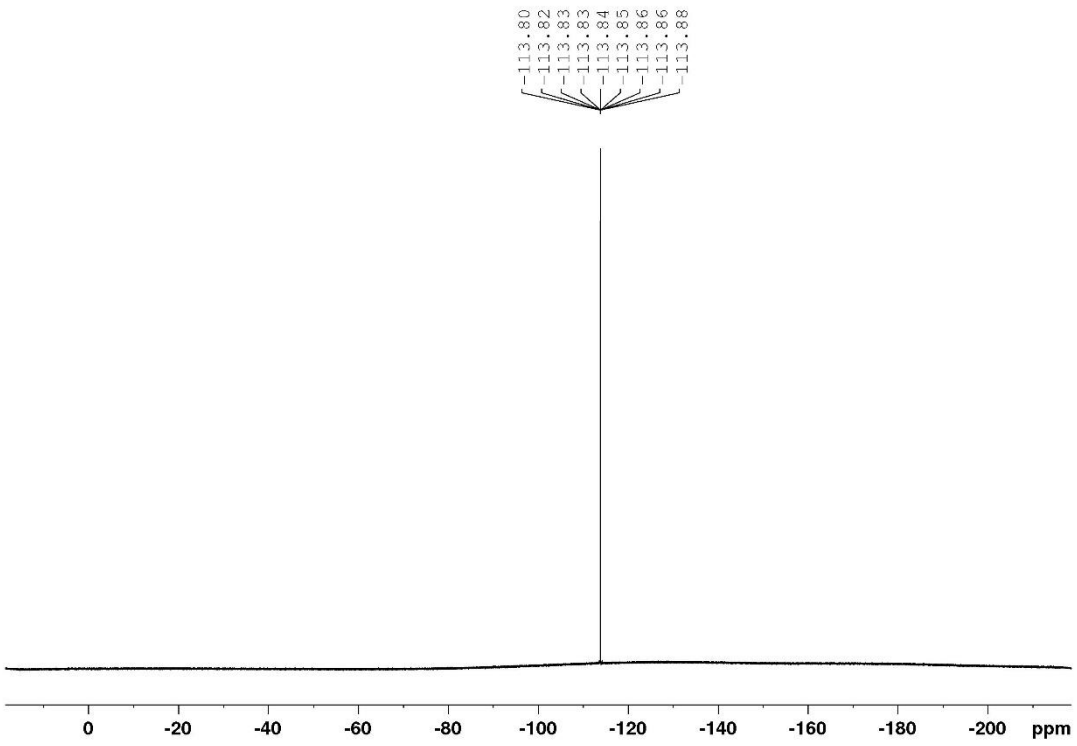


Figure S22: ^{19}F NMR of **3d** in CD_2Cl_2.

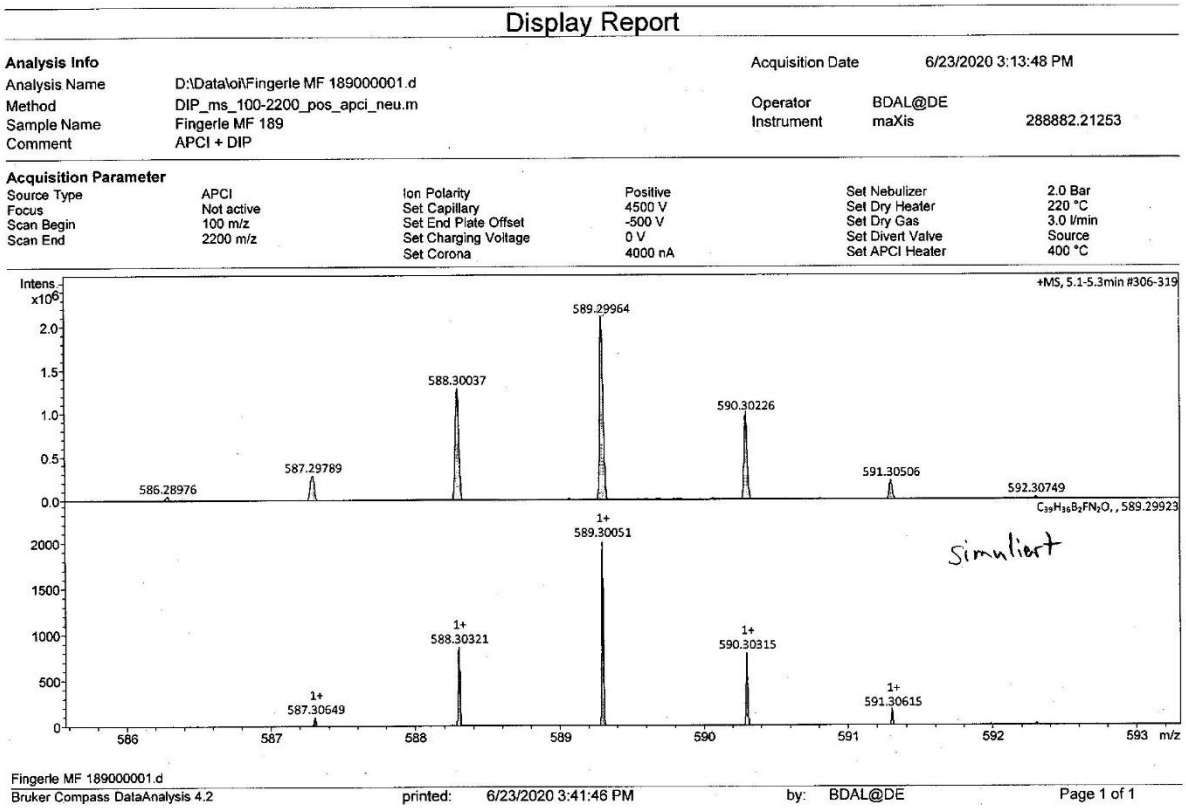


Figure S23: High resolution MS of **3d**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

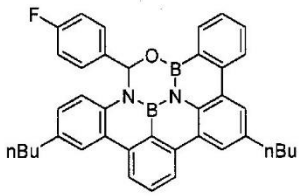
Datum: 17.07.2020

Probenbezeichnung: MF189 nominelle Masse:

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt):

Strukturformel (falls bekannt):



Chemical Formula: $C_{39}H_{35}B_2FN_2O$
Exact Mass: 588,29

Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M+H]^+_{(theor.)}$ = 589,30051

Gemessen = 589,29964

Relative Massenabweichung = 1,48 ppm

Figure S24: Data sheet high resolution MS of **3d**.

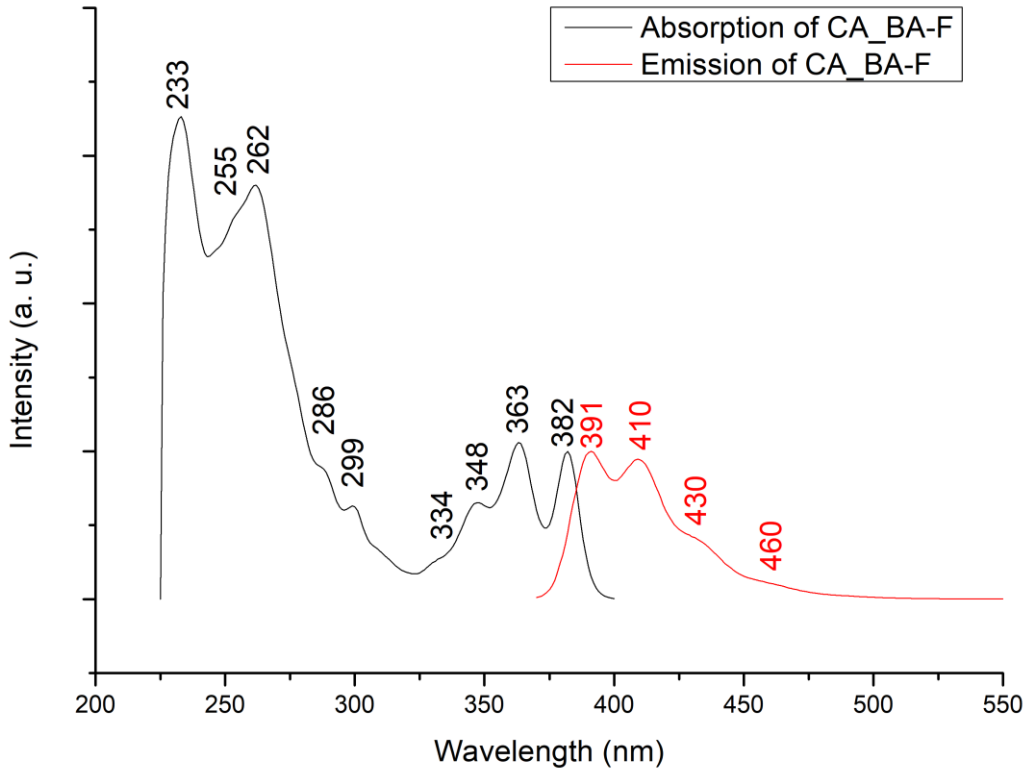


Figure S25: Absorption and emission spectra of **3d** (10^{-5} mol/L) in CD_2Cl_2.

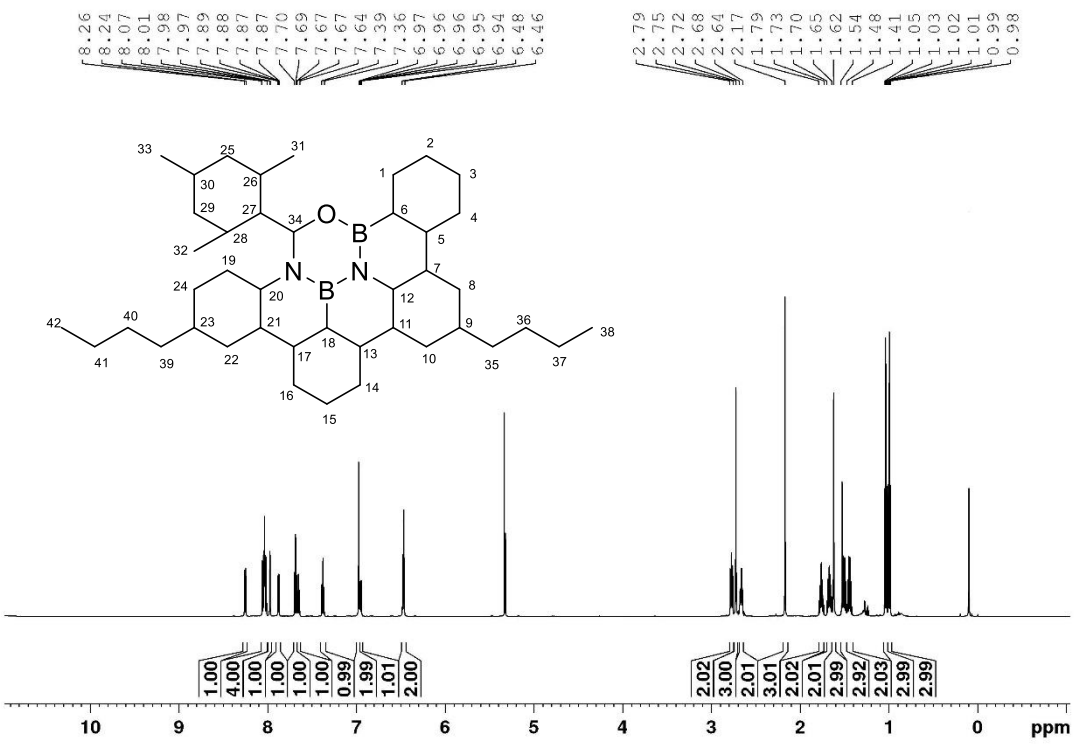


Figure S26: ^{1}H-NMR of **3e** in CD_2Cl_2.

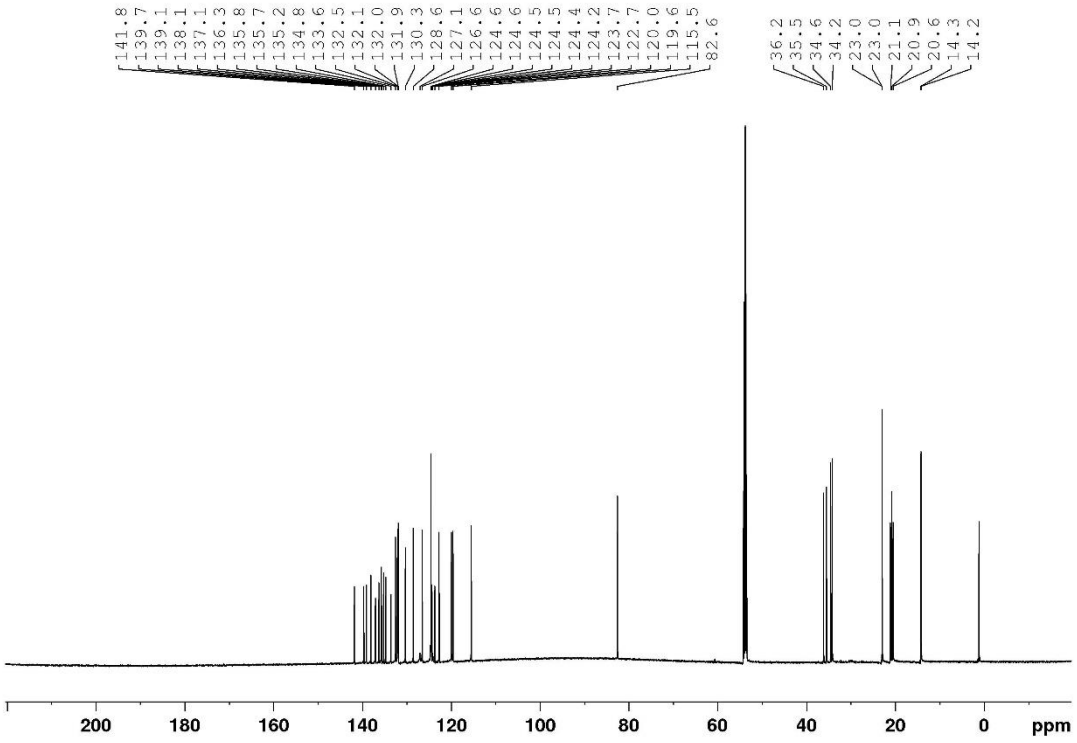


Figure S27: ^{13}C-NMR of **3e** in CD_2Cl_2.

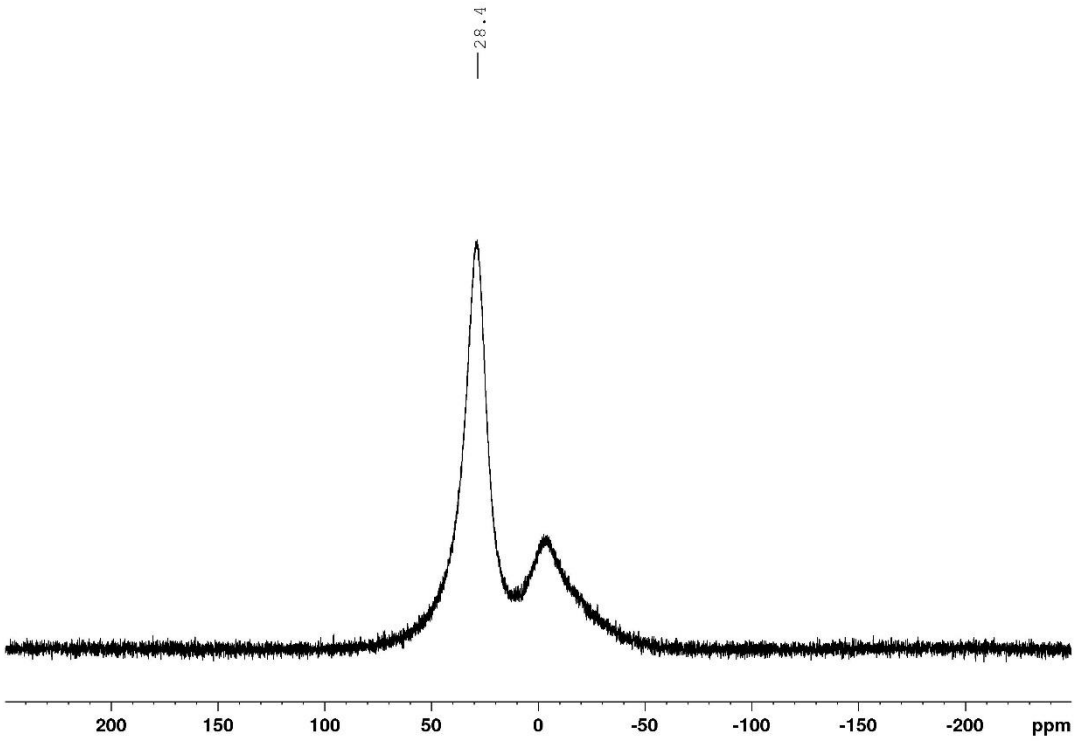


Figure S28: ^{11}B-NMR of **3e** in CD_2Cl_2.

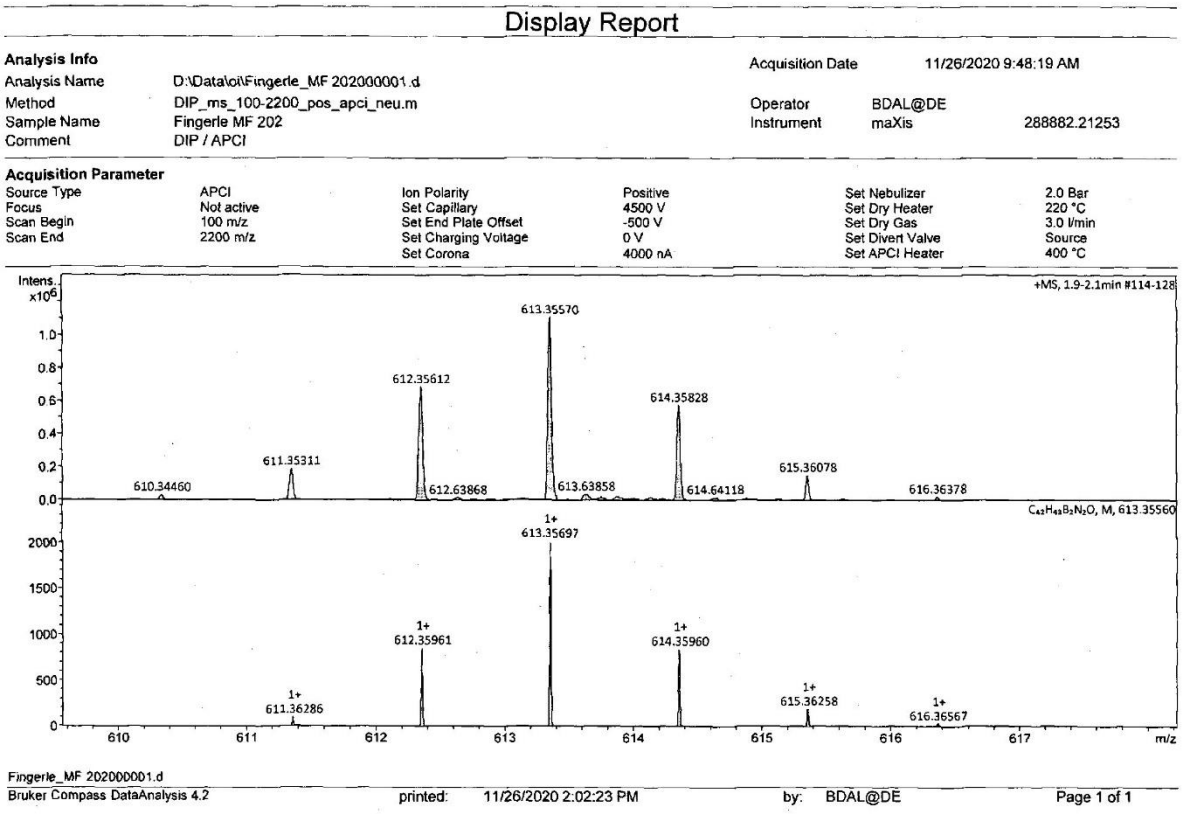


Figure S29: High resolution MS of **3e**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

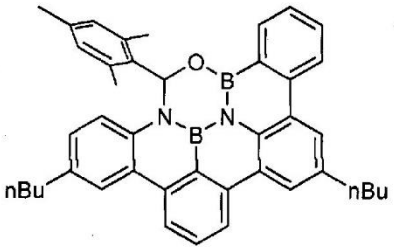
Datum: 12.11.2020

Probenbezeichnung: MF202 nominelle Masse:

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt):

Strukturformel (falls bekannt):



Chemical Formula: $C_{42}H_{42}B_2N_2O$
Exact Mass: 612,35

Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M+H]^+_{(theor.)}$ = 613,35697

Gemessen = 613,35570

Relative Massenabweichung = 2,0 ppm

Figure S30: Data sheet high resolution MS of **3e**.

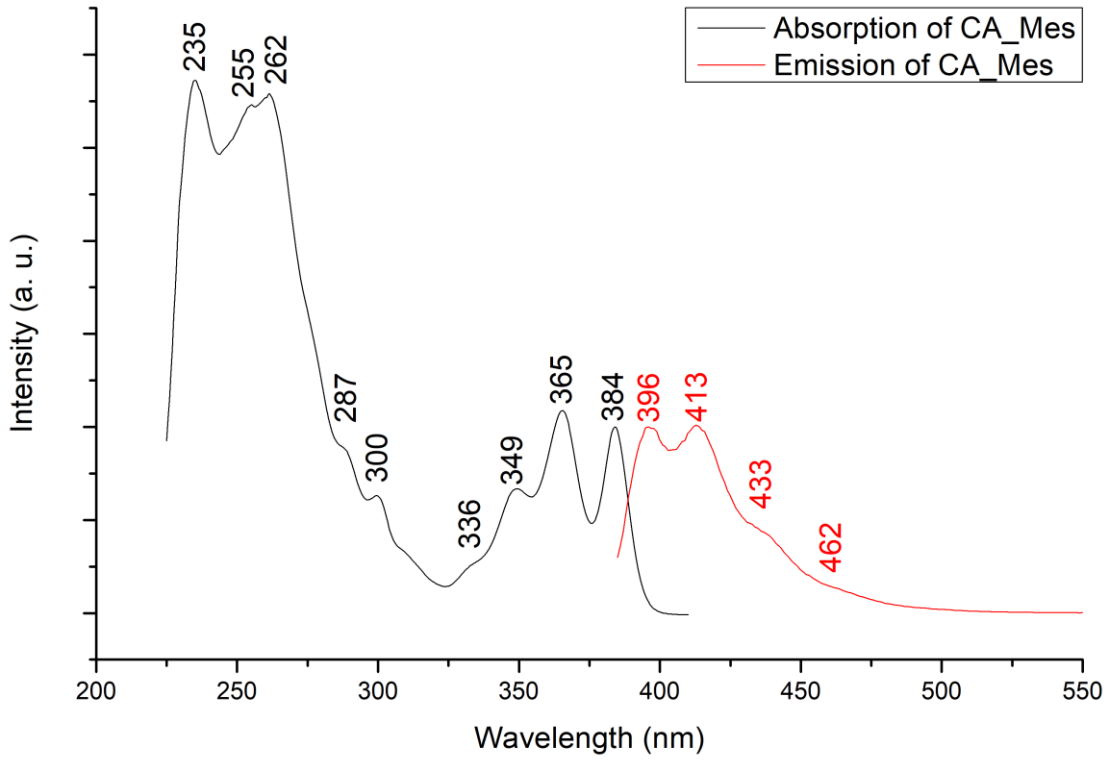


Figure S31: Absorption and emission spectra of **3e** (10^{-5} mol/L) in CD_2Cl_2.

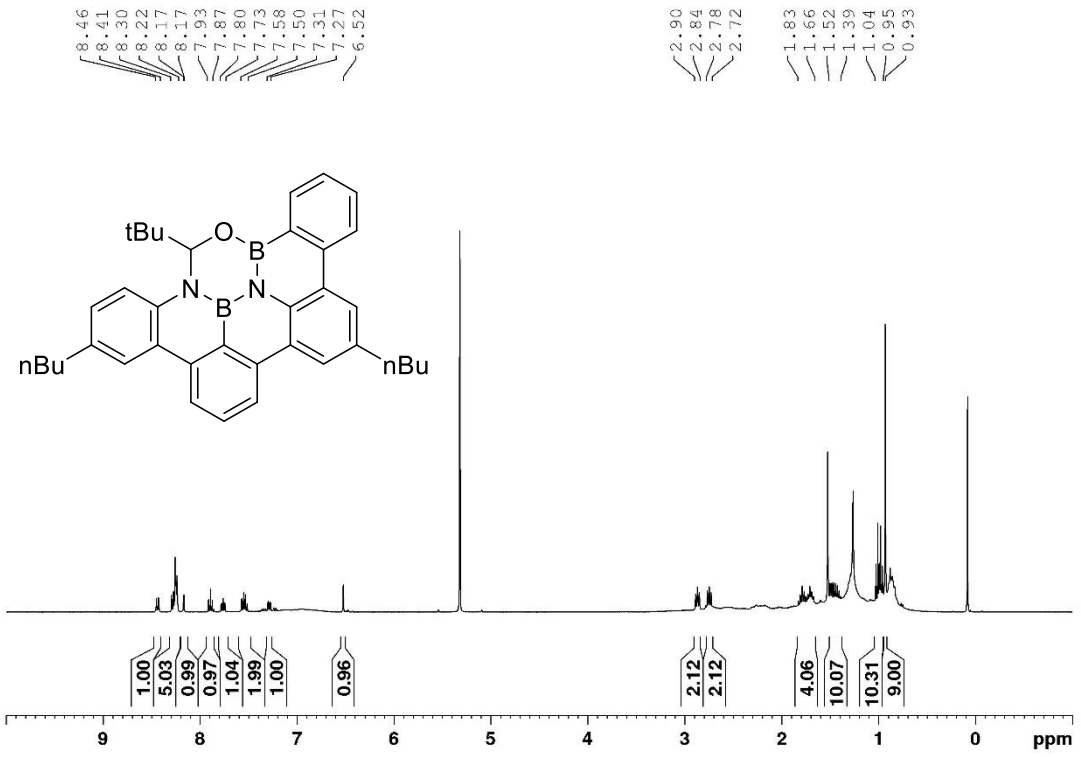


Figure S32: ^{1}H-NMR of **3f** in CD_2Cl_2.

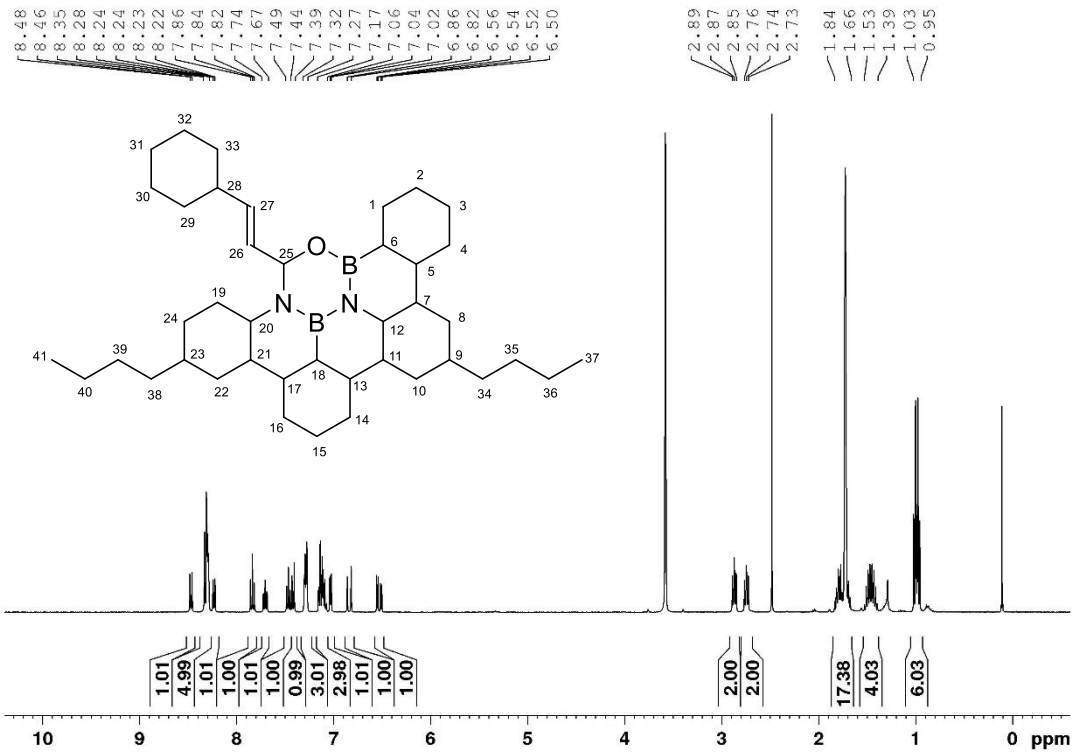


Figure S33: ^{1}H-NMR of **3g** in CD_2Cl_2.

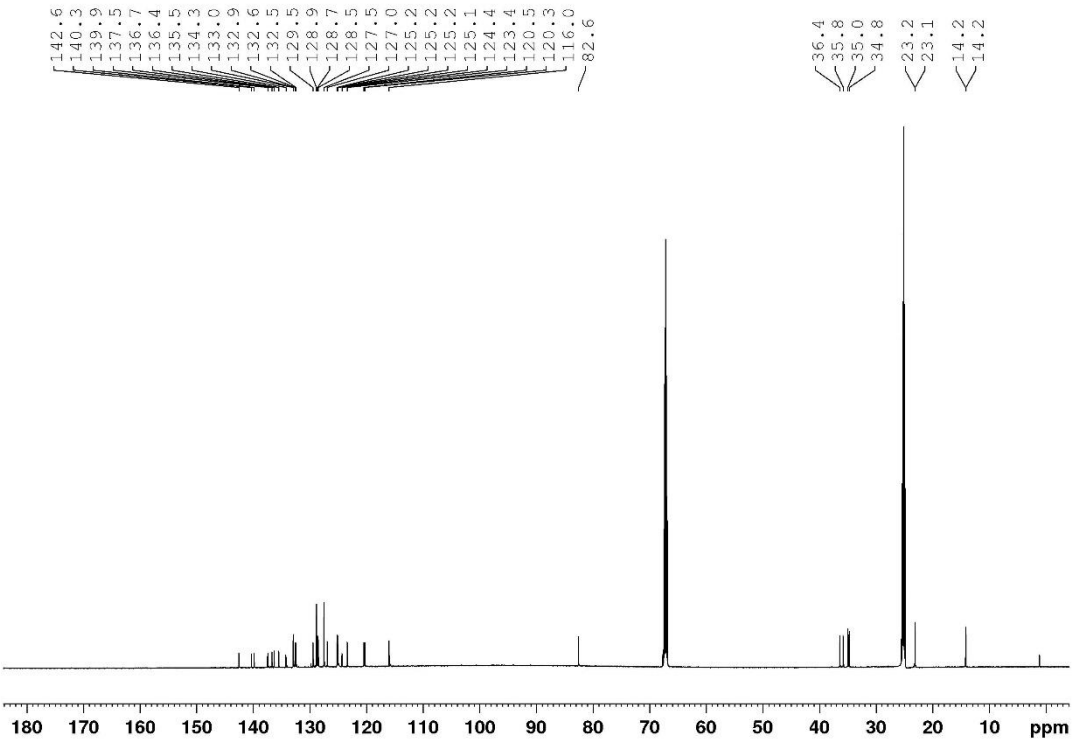


Figure S34: ^{13}C-NMR of **3g** in CD_2Cl_2.

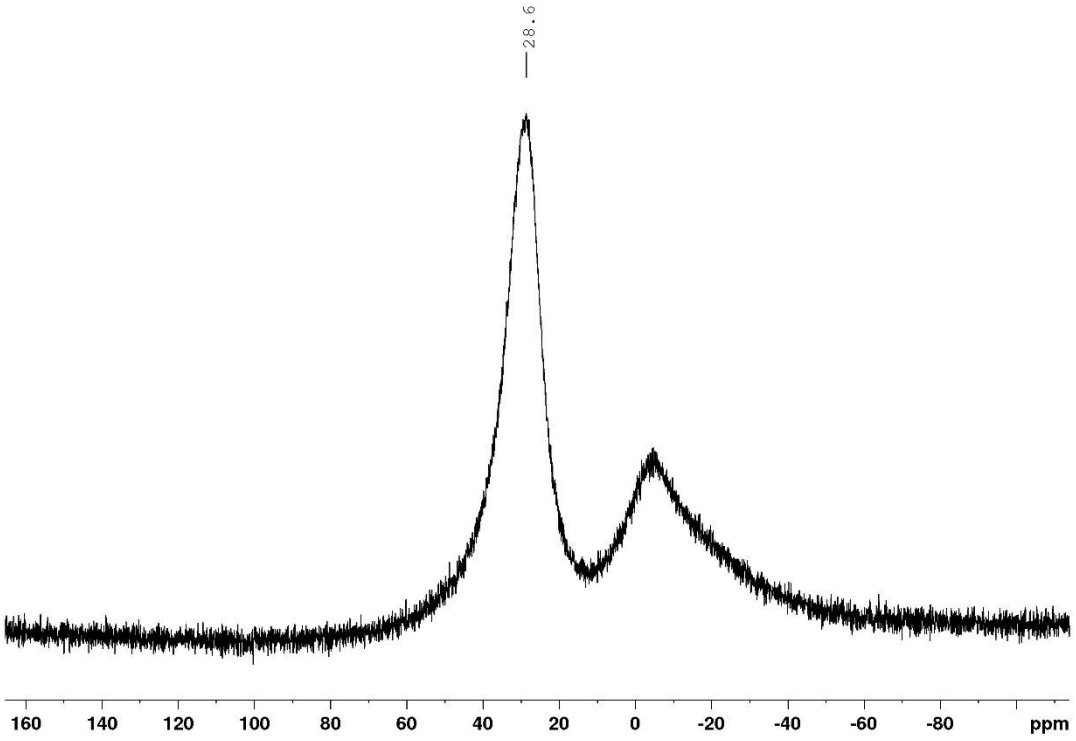


Figure S35: ^{11}B-NMR of **3g** in CD_2Cl_2.

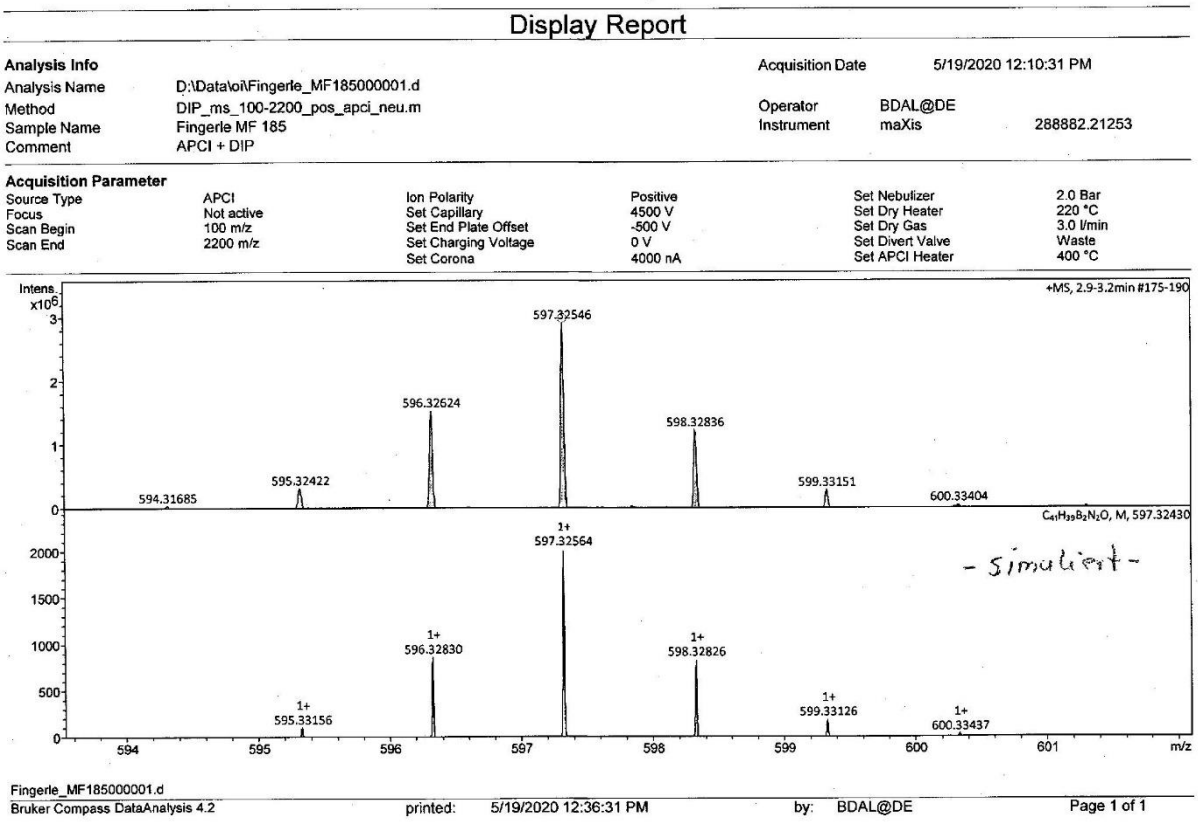


Figure S36: High resolution MS of **3g**.

High Resolution MS DIP-APCI

☐ **FT-ICR-MS**

☐ **ESI- oder APCI-TOF-MS** (MS/MS möglich)

☐ **egal (je nach freien Kapazitäten)**

Name: Michael Fingerle AK: Bettinger

Tel. 76250 email:

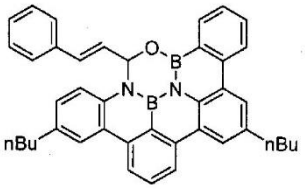
Datum: 11.05.2020

Probenbezeichnung: MF185 nominelle Masse:

Falls Masse nicht bekannt, welcher Massenbereich soll gemessen werden:

Summenformel (falls bekannt):

Strukturformel (falls bekannt):



Chemical Formula: $C_{41}H_{38}B_2N_2O$
Exact Mass: 596,32

Einwaage (zwischen 0,1mg und 2 mg):

Löslich in:

Falls schon gelöst, in welchem Lösemittel und in welcher Konzentration:

Hinweise bezüglich Zersetzlichkeit:

Hinweise bezüglich Toxizität (wenn bekannt):

Hohe Massengenauigkeit erwünscht? ja/nein

Massenanalyse erwünscht?

Wenn ja, welche Elemente sollen berücksichtigt werden?

MS/MS erwünscht?:

Ergebnis:

$[M+H]^+_{(theor.)}$ = 597,32564

Gemessen = 597,32546

Relative Massenabweichung = 0,30 ppm

Figure S37: Data sheet high resolution MS of **3g**.

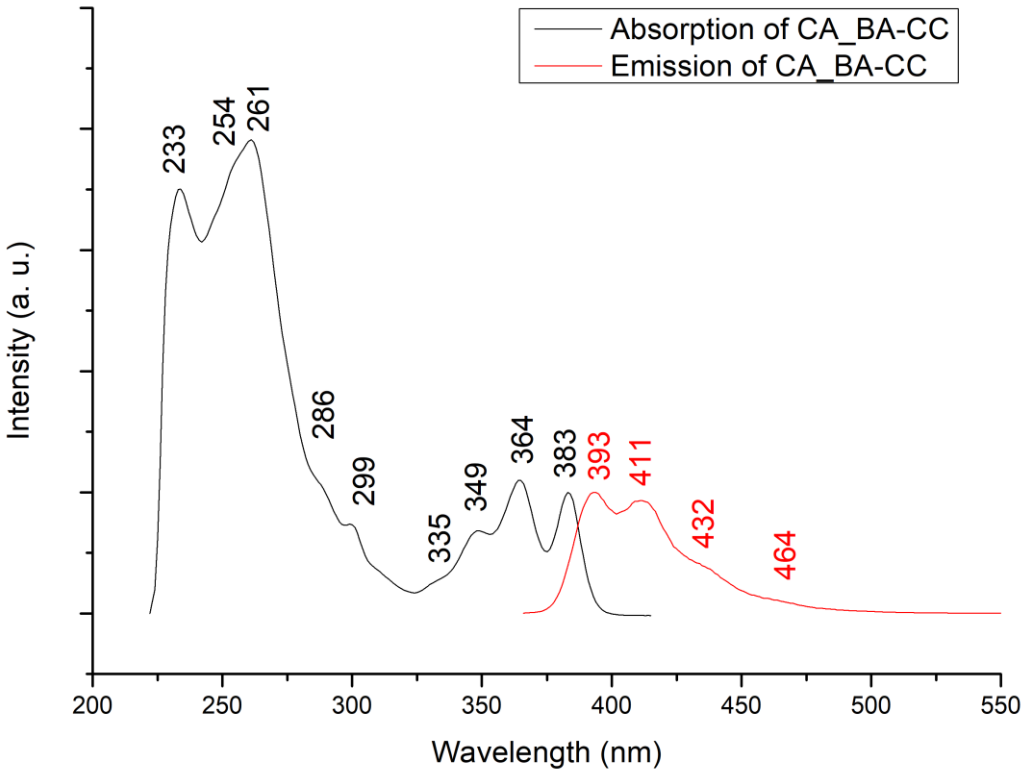


Figure S38: Absorption and emission spectra of **3g** (10^{-5} mol/L) in CD_2Cl_2.

4. X-Ray Crystallographic Data

Empirical formula	$C_{39}H_{36}B_2N_2O$
Formula weight / [g/mol]	570.32
Temperature / [K]	100(2)
Radiation wavelength / [Å]	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.1035(3) Å; α = 107.688(2) ° b = 12.5038(5) Å; β = 108.360(2) ° c = 12.9042(4) Å; γ = 107.158(2) °
Volume / [$Å^3$]	1460.95(9)
Z	2
Radiation	MoKα
Density / [mg m^{-3}]	1.296
Absorption coefficient	0.076
F(000)	604
Crystal size / [mm]	0.16 x 0.14 x 0.12
Theta range for data collection / [°]	2.162-24.845
Limiting indices	-13≤h≥13 -14≤k≥11 -15≤l≥15
Reflections collected	13539
Independent reflects	4971
R_{int}	0.05
Completeness / [%]	98.2
Absorption correction	Multi-scan
Trans. (max., min.)	0.7451, 0.6696
Goodness-of-fit on F^2	1.014
Parameters / restrain	399/0
R_1, wR_2 / [l>2σ(*I*)]	0.0491, 0.1029
R_1, wR_2 / [all data]	0.0944, 0.1214
$\Delta\rho_{max,min}$ / [e·$Å^{-3}$]	0.252, -0.206

5. Computational Investigations

5.1 Cycloaddition-dehydration with other dienophiles

The computational investigation (M062X/6-311+G**) of the cycloaddition-dehydration sequence with other hetero dienophiles are summarized in Figure S39. The reaction with nitrile, isonitrile, and CO_2 are strongly endergonic, while those with imine and iminium ion are exergonic. Note, however, that the cycloaddition product **B** does not correspond to a stationary point for the reaction with imine, indicating that the sequence **A** → **B** → **C** is not feasible for this reagent. Most exergonic is the reaction with the iminoborane yielding the borazine core.

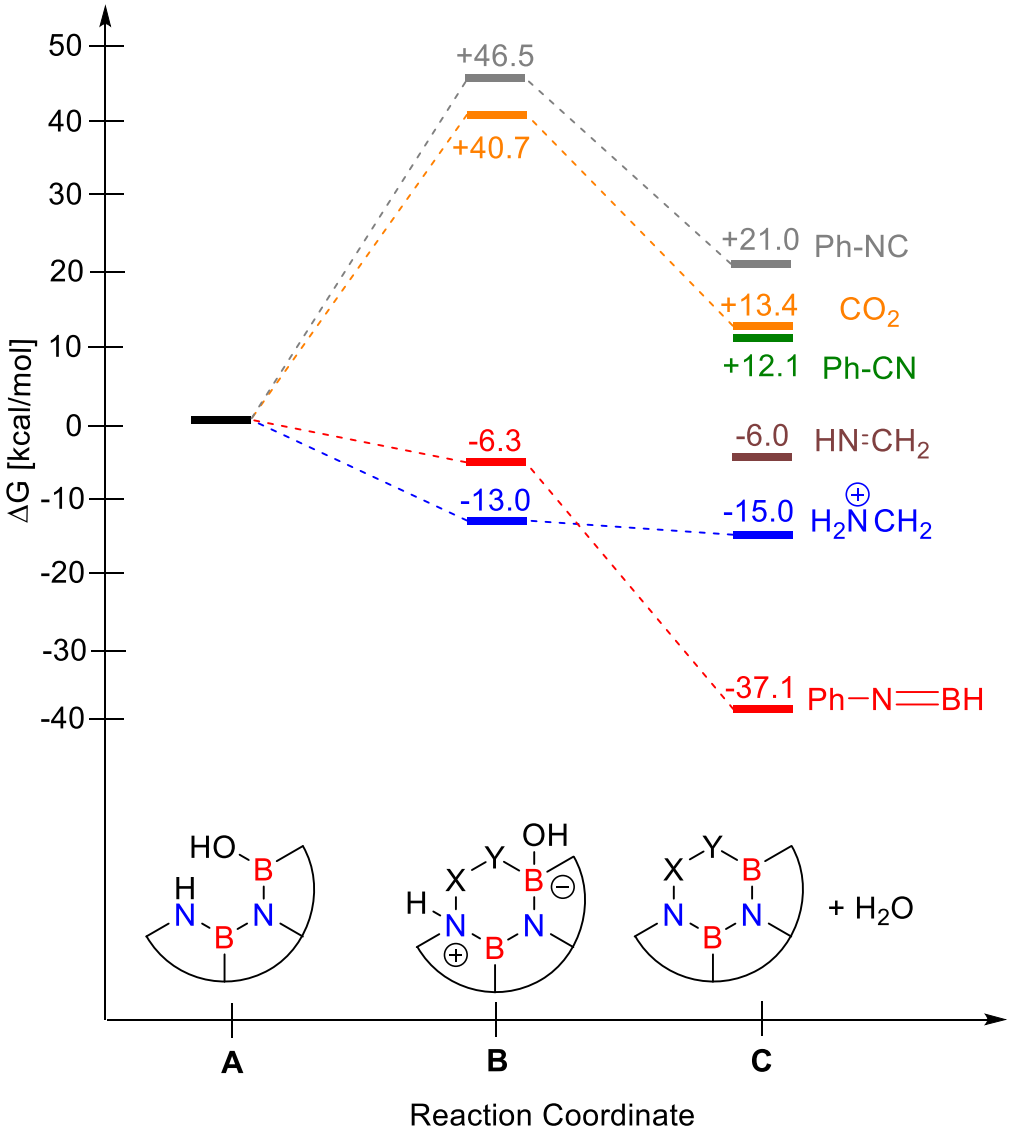


Figure S39: Gibbs free enthalpies for reaction of **A** with other hetero dienophiles.

5.2 NICS computations for 3a

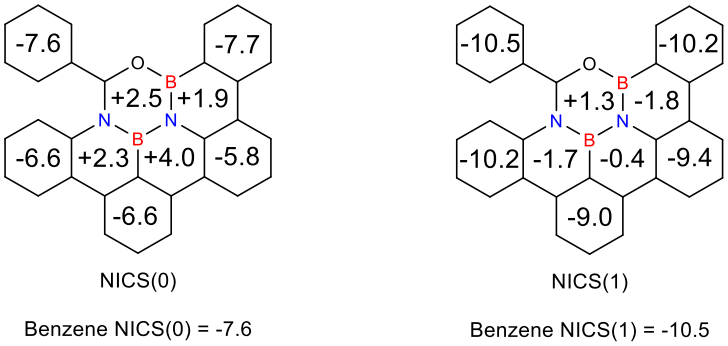


Figure S40. NICS(0) and NICS(1) computed for **A** at the M062X/6-311+G** level of theory. The values for benzene computed at the same level of theory are given for comparison.

6. Cyclic Voltammetry

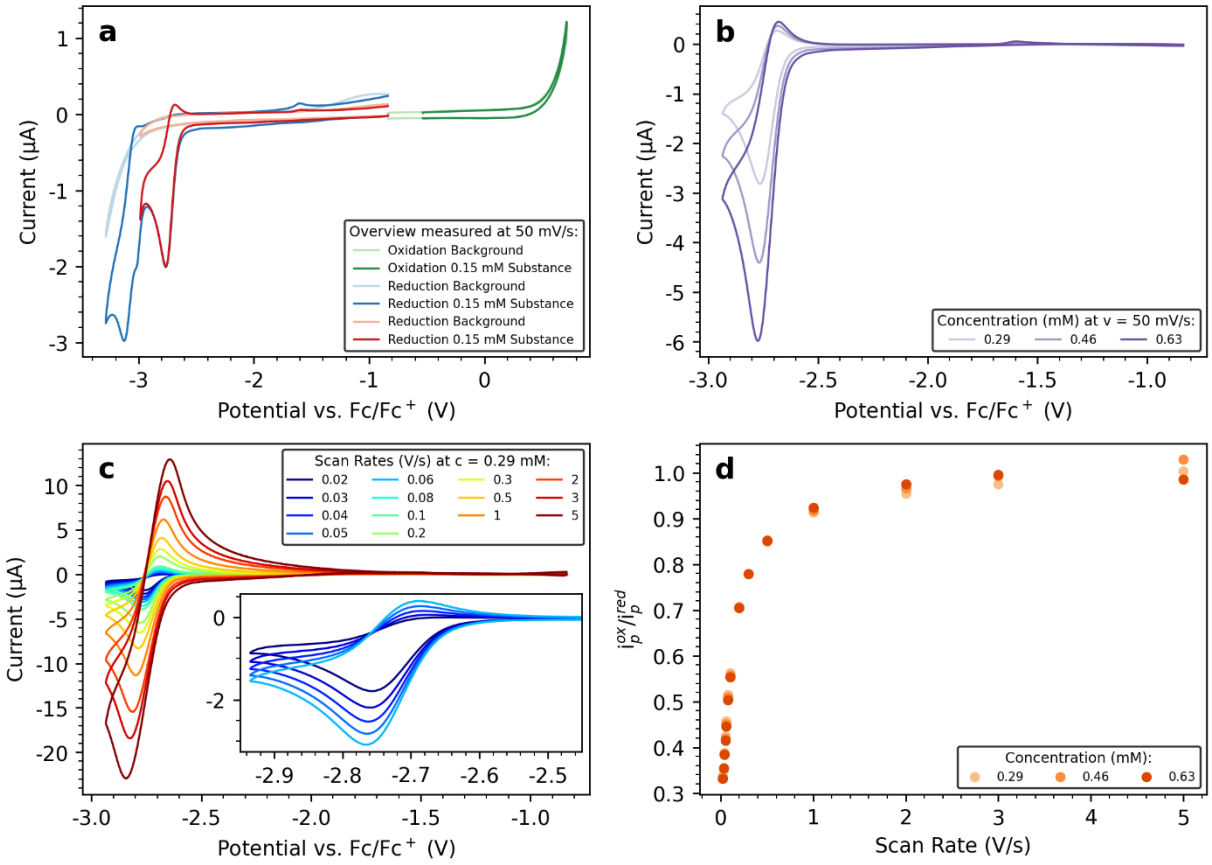


Figure S41. Cyclovoltammetry of the **3a** in 0.1 M TBAHFP/THF. **(a)** Electrolyte background scans (light colours) and measurements of **3a** (dark colours) in oxidative and reductive direction. **(b)** Concentration-dependent CV with 50 mV/s scan rate. **(c)** Scan rate-dependent CV at a fixed concentration of 0.29 mM. The inset shows CV measurements recorded at slower scan rates. **(d)** Scan rate-dependent peak current height ratios for all three substance concentrations.

In Figure S41 (a), an overview of the electrochemical response of a 0.15 mM solution of **3a** (dark colours) in 0.1 TBAHFP/THF is shown. The measurements were carried out with a scan rate of 50 mV/s and are displayed without background correction. The respective background electrolyte scans are depicted in light colours. In the oxidative direction, no electrochemical reaction of the Dibenzoperylene occurs within the electrochemical measurement window. In the reductive direction, three consecutive signals at approx. -2.7, -3.0 and -3.1 V vs. Fc/Fc^+ (dark blue curve) can be observed in the forward scan. When reversing the potential scan direction at approx. -2.9 V vs. Fc/Fc^+, a reverse peak of the first reduction can be seen (dark red curve). Only the first reduction wave was analyzed in more detail.

Figure S41 (b) shows concentration-depended CV measurements of the first reduction of **3a** at a fixed scan rate of 50 mV/s. With increasing concentration, a small shift of the peak potential of the reduction towards more negative potentials can be observed, indicating an incomplete iR-compensation. Additionally, a small oxidative feature at around -1.6 V vs. Fc/Fc^+ can be observed in the backward scan. Scan rate-dependent CV measurements of the first reduction at a constant concentration of 0.29 mM are displayed in figure S41 (c). The scans at slow scan rates are magnified in the inset for a better overview. With increasing scan rate, the oxidative backward peak becomes more pronounced. This indicates a transition of an EC mechanism to a quasi-reversible electron transfer with E^0 of -2.724 ± 0.007 V vs. Fc/Fc^+. Simultaneously, the additional oxidative feature at approx. -1.6 V vs. Fc/Fc^+ disappears with increasing scan rate, suggesting that it is related to a follow-up reaction after the first reduction. However, this was not further investigated.

We calculate the scan rate-dependent peak/current ratios of the redox wave at -2.724 V vs. Fc/Fc^+ by using the empirical formula found by Nicholson[8]

$$\frac{i_p^{ox}}{i_p^{red}} = \left|\frac{i_p^{ox}}{i_p^{red}}\right| + 0.485 \cdot \left|\frac{i^{rev}}{i_p^{red}}\right| + 0.086$$

with i_p^{ox} and i_p^{red} as peak currents of the oxidative and reductive wave, and i^{rev} as the current at the potential where the scan direction is reversed. Figure S41 (d) displays the results for measurements made with all three concentrations of Dibenzoperylene **3a** used in Figure S41 (b). We find that a peak/current ratio of approx. one is achieved for scan rates greater than 2 V/s for all three concentrations. No further kinetic studies for the electrochemical reaction mechanisms were made.

7. Cartesian Coordinates of Stationary Points in Å

7.1 Calculations without solvent

$(BN)_2$ dibenzoperylene (C_1), S_0

```
45
Scf done: -1158.72276779

6       -3.590187000     -2.791290000     -0.137170000
6       -2.923373000     -1.557607000     -0.070342000
6       -3.662402000     -0.361717000      0.030880000
6       -5.063268000     -0.460483000      0.054090000
6       -5.715052000     -1.677198000     -0.013034000
6       -4.968187000     -2.853993000     -0.108245000
7       -1.537492000     -1.541444000     -0.101030000
5       -0.765721000     -0.355723000     -0.063365000
6       -1.548239000      0.952106000      0.016809000
6       -0.836611000      2.161998000      0.054572000
6       -1.544773000      3.353107000      0.234082000
6       -2.930761000      3.330298000      0.330726000
6       -3.638935000      2.142037000      0.254052000
6       -2.957944000      0.928481000      0.101179000
6        0.636862000      2.128605000     -0.086949000
6        1.324082000      3.332386000     -0.250568000
6        2.701349000      3.383349000     -0.360140000
6        3.420706000      2.209202000     -0.270514000
6        2.793623000      0.969683000     -0.109837000
6        1.372717000      0.910670000     -0.079086000
6        3.626163000     -0.242787000      0.019377000
6        3.011538000     -1.502997000      0.010959000
6        3.798765000     -2.658617000      0.130749000
6        5.172480000     -2.587632000      0.259716000
6        5.780719000     -1.331082000      0.287671000
6        5.023742000     -0.179934000      0.175197000
7        0.703603000     -0.337817000     -0.060303000
5        1.473477000     -1.556284000     -0.084872000
1        4.496655000      2.257621000     -0.353220000
1        3.206680000      4.328741000     -0.511462000
1        0.767910000      4.255995000     -0.320005000
8        0.808966000     -2.760850000     -0.178517000
1       -4.717079000      2.173649000      0.331566000
1       -1.041675000      4.305622000      0.321533000
1       -3.467220000      4.261521000      0.472927000
1        3.337132000     -3.642665000      0.137301000
1        5.767226000     -3.488043000      0.352469000
1        6.854874000     -1.252819000      0.408963000
1        5.536133000      0.769886000      0.231358000
1       -5.660291000      0.439189000      0.122052000
1       -6.796937000     -1.714726000      0.006244000
1       -5.465353000     -3.815175000     -0.161698000
1       -3.000136000     -3.698601000     -0.213552000
1       -1.091657000     -2.446008000     -0.151313000
1        1.402365000     -3.512037000     -0.219530000
```

Compound tetramethylethylene (TME) (C_2), S_0

```
18
scf done: -235.788685613

6        0.669805000      0.000034000     -0.000040000
6       -0.669795000      0.000057000      0.000031000
6        1.512002000      1.252679000      0.034065000
1        2.332309000      1.122145000      0.746563000
1        1.972169000      1.437138000     -0.942783000
1        0.960720000      2.143218000      0.327531000
6        1.511796000     -1.252733000     -0.034093000
1        1.971361000     -1.437597000      0.943071000
1        0.960524000     -2.143087000     -0.328148000
1        2.332614000     -1.122151000     -0.745975000
6       -1.511850000     -1.252673000      0.034095000
1       -2.332322000     -1.122229000      0.746404000
```

```
1       -1.971879000     -1.437259000     -0.942949000
1       -0.960497000     -2.143153000      0.327652000
6       -1.511936000      1.252711000     -0.034083000
1       -2.331699000      1.122567000     -0.747277000
1       -1.972972000      1.436527000      0.942570000
1       -0.960461000      2.143434000     -0.326503000
```

Compound tetracyanoethylene (TCNE) (D_{2h}), S_0

```
10
scf done: -447.474600814

6        0.000000000      0.000000000      0.676823000
6        0.000000000      0.000000000     -0.676823000
6        0.000000000      1.223271000      1.420850000
7        0.000000000      2.200576000      2.024438000
6        0.000000000     -1.223271000      1.420850000
7        0.000000000     -2.200576000      2.024438000
6        0.000000000      1.223271000     -1.420850000
7        0.000000000      2.200576000     -2.024438000
6        0.000000000     -1.223271000     -1.420850000
7        0.000000000     -2.200576000     -2.024438000
```

Compound methoxyethene (C_1), S_0

```
10
scf done: -193.080751986

6        0.737628000     -0.566341000      0.000049000
6        1.432581000      0.569956000      0.000043000
1        1.221463000     -1.536134000      0.000101000
1        0.977202000      1.550266000     -0.000097000
1        2.511578000      0.514972000      0.000124000
8       -0.603656000     -0.714765000     -0.000045000
6       -1.364982000      0.475174000     -0.000035000
1       -1.151453000      1.071697000     -0.892500000
1       -2.409376000      0.172914000     -0.000070000
1       -1.151528000      1.071675000      0.892461000
```

Compound benzaldehyde (C_s), S_0

```
14
scf done: -345.515805225

6       -1.323799000     -1.324811000     -0.000029000
6        0.044055000     -1.099668000     -0.000031000
6       -2.208294000     -0.245599000     -0.000031000
1        0.754511000     -1.918267000     -0.000027000
1       -3.276953000     -0.425492000     -0.000028000
6        0.529193000      0.209556000     -0.000041000
6       -1.727255000      1.059461000     -0.000037000
1       -2.417715000      1.893947000     -0.000038000
6       -0.355388000      1.286014000     -0.000045000
1        0.033812000      2.299479000     -0.000050000
1       -1.707527000     -2.337857000     -0.000025000
6        1.990039000      0.466280000     -0.000032000
8        2.830717000     -0.394492000      0.000188000
1        2.276829000      1.536723000      0.000145000
```

Compound H_2O (C_{2v}), S_0

```
3
scf done: -76.4208334206

8        0.000000000      0.000000000      0.116605000
```

```
1        0.000000000      0.761605000     -0.466419000
1        0.000000000     -0.761605000     -0.466419000
```

Compound **B** with TME (C_1), S_0

```
63
scf done: -1394.47271134

6       -2.790707000     -1.064292000     -0.598554000
6       -3.534750000      0.115192000     -0.400621000
6       -4.906864000      0.056626000     -0.672639000
6       -5.515638000     -1.096661000     -1.143273000
6       -4.750567000     -2.228591000     -1.397859000
6       -3.389398000     -2.202801000     -1.130244000
6       -2.885668000      1.406308000     -0.054713000
6       -1.488422000      1.488656000     -0.206269000
6       -0.773926000      2.681263000     -0.012504000
6       -1.515090000      3.824862000      0.348103000
6       -2.883589000      3.739251000      0.526297000
6       -3.581983000      2.540805000      0.333619000
6        0.691667000      2.657013000     -0.128401000
6        1.431909000      3.839617000      0.028331000
6        2.808844000      3.824185000      0.042325000
6        3.485870000      2.615161000     -0.102720000
6        2.815565000      1.416522000     -0.312432000
6        1.393285000      1.432769000     -0.335547000
6        3.571425000      0.144088000     -0.468890000
6        2.919761000     -1.093788000     -0.325039000
6        3.683375000     -2.262703000     -0.448212000
6        5.048315000     -2.231822000     -0.698449000
6        5.677770000     -1.002109000     -0.871008000
6        4.943513000      0.168830000     -0.767585000
5        1.324101000     -1.194832000     -0.215009000
8        0.807498000     -2.179238000     -1.215339000
7        0.703172000      0.238202000     -0.500957000
5       -0.674500000      0.245064000     -0.427155000
7       -1.361152000     -1.115105000     -0.310190000
6        0.640325000     -1.602031000      1.250827000
6       -0.918086000     -1.818479000      1.076086000
1        4.565011000      2.618031000     -0.028982000
1        3.364142000      4.742651000      0.186840000
1        0.918805000      4.782978000      0.157533000
1       -4.651668000      2.523510000      0.500041000
1       -1.031942000      4.777092000      0.519822000
1       -3.432061000      4.623802000      0.829205000
1        3.181973000     -3.221742000     -0.359971000
1        5.613597000     -3.153160000     -0.781560000
1        6.735778000     -0.954921000     -1.101827000
1        5.449496000      1.108209000     -0.950226000
1       -5.504971000      0.950493000     -0.552731000
1       -6.579299000     -1.098410000     -1.347682000
1       -5.203050000     -3.120889000     -1.811833000
1       -2.776809000     -3.070076000     -1.344211000
1       -0.864345000     -1.720089000     -0.995220000
1        1.341026000     -2.160424000     -2.012937000
6       -1.299601000     -3.290094000      0.925855000
1       -2.378059000     -3.405719000      0.818315000
1       -0.785986000     -3.751121000      0.079828000
1       -1.011265000     -3.823349000      1.830947000
6        1.311272000     -2.871933000      1.798331000
1        0.879252000     -3.193681000      2.753843000
1        1.266315000     -3.707296000      1.097185000
1        2.365305000     -2.652762000      1.982047000
6       -1.775694000     -1.201380000      2.175866000
1       -2.831388000     -1.441444000      2.028877000
1       -1.464253000     -1.627000000      3.132184000
1       -1.667990000     -0.117968000      2.237861000
6        0.956283000     -0.483219000      2.263569000
1        0.456660000      0.463935000      2.047042000
1        0.696015000     -0.770983000      3.287666000
1        2.032418000     -0.286068000      2.244017000
```

Compound **B** with TCNE (C_1), S_0

```
55
scf done: -1606.16401315

6       -2.804478000     -0.854241000     -0.786853000
6       -3.510160000      0.338272000     -0.546437000
6       -4.887962000      0.301890000     -0.787994000
6       -5.525417000     -0.841744000     -1.244319000
6       -4.794055000     -1.992865000     -1.510360000
6       -3.425480000     -1.993447000     -1.285586000
6       -2.835684000      1.604407000     -0.163678000
6       -1.436849000      1.672568000     -0.305821000
6       -0.698396000      2.837297000     -0.040560000
6       -1.420415000      3.971367000      0.378570000
6       -2.791415000      3.901054000      0.541082000
6       -3.511489000      2.728898000      0.280194000
6        0.767851000      2.796550000     -0.149448000
6        1.522322000      3.962237000      0.049749000
6        2.899027000      3.927194000      0.058699000
6        3.562465000      2.718774000     -0.131118000
6        2.877557000      1.535157000     -0.379248000
6        1.460102000      1.579339000     -0.399082000
6        3.617372000      0.257219000     -0.565763000
6        2.942093000     -0.974778000     -0.516158000
6        3.675363000     -2.161809000     -0.637331000
6        5.051702000     -2.150297000     -0.812188000
6        5.711432000     -0.928425000     -0.901895000
6        5.002504000      0.257503000     -0.787209000
5        1.365024000     -1.017242000     -0.503037000
8        0.778099000     -1.950806000     -1.470384000
7        0.741443000      0.398367000     -0.616936000
5       -0.635744000      0.443821000     -0.581786000
7       -1.352775000     -0.931086000     -0.546356000
6        0.618732000     -1.553587000      1.014058000
6       -0.946270000     -1.669947000      0.769331000
1        4.641046000      2.709928000     -0.059804000
1        3.465806000      4.832580000      0.235817000
1        1.022459000      4.906715000      0.214068000
1       -4.580220000      2.720784000      0.450208000
1       -0.920574000      4.900667000      0.613955000
1       -3.325076000      4.775908000      0.893521000
1        3.156124000     -3.114106000     -0.585981000
1        5.602522000     -3.079833000     -0.891229000
1        6.781840000     -0.897285000     -1.068376000
1        5.544545000      1.187827000     -0.891635000
1       -5.470073000      1.202119000     -0.643406000
1       -6.594329000     -0.824634000     -1.417875000
1       -5.276860000     -2.881467000     -1.895641000
1       -2.840576000     -2.879572000     -1.499113000
1       -0.872450000     -1.504542000     -1.275834000
1        1.408756000     -2.229654000     -2.137383000
6       -1.345880000     -3.078541000      0.625881000
7       -1.673500000     -4.170699000      0.506351000
6        1.194479000     -2.832672000      1.396554000
7        1.685195000     -3.839751000      1.651969000
6       -1.741253000     -1.075447000      1.854877000
7       -2.370111000     -0.603402000      2.689644000
6        0.926321000     -0.537318000      2.011422000
7        1.178485000      0.315208000      2.739568000
```

Compound **B** with methoxyethene (C_1), S_0

```
55
scf done: -1351.76975761

6       -2.704788000     -1.154437000     -0.517468000
6       -3.400539000      0.066947000     -0.445566000
6       -4.790241000      0.002163000     -0.618516000
6       -5.452972000     -1.192908000     -0.851928000
6       -4.736454000     -2.381204000     -0.949529000
6       -3.360491000     -2.352004000     -0.784936000
6       -2.712140000      1.370315000     -0.235878000
6       -1.304954000      1.381511000     -0.222853000
```

```
6       -0.549302000      2.556666000     -0.078104000
6       -1.262935000      3.764504000      0.051608000
6       -2.645687000      3.758128000      0.052893000
6       -3.382598000      2.576048000     -0.084948000
6        0.919358000      2.462819000     -0.037821000
6        1.696609000      3.619320000      0.127289000
6        3.068340000      3.547853000      0.227235000
6        3.704585000      2.310901000      0.154230000
6        3.002556000      1.127177000     -0.040683000
6        1.583587000      1.203414000     -0.128575000
6        3.717752000     -0.180079000     -0.132460000
6        3.004373000     -1.391842000     -0.145226000
6        3.718186000     -2.594981000     -0.203464000
6        5.103975000     -2.627428000     -0.251126000
6        5.805441000     -1.424478000     -0.266279000
6        5.120255000     -0.220887000     -0.214695000
5        1.412851000     -1.436382000     -0.191585000
8        0.902095000     -2.217106000     -1.364472000
7        0.847216000      0.037120000     -0.277513000
5       -0.529476000      0.102713000     -0.299561000
7       -1.269099000     -1.234528000     -0.289879000
6        0.655773000     -2.086084000      1.115003000
1        4.779245000      2.287139000      0.267359000
1        3.652546000      4.447954000      0.373307000
1        1.218756000      4.587163000      0.193898000
1       -4.462909000      2.634918000     -0.067674000
1       -0.752849000      4.711527000      0.163211000
1       -3.176918000      4.696189000      0.165990000
1        3.159390000     -3.526443000     -0.225478000
1        5.634260000     -3.572128000     -0.291376000
1        6.887678000     -1.422336000     -0.327331000
1        5.701399000      0.690539000     -0.256762000
1       -5.370217000      0.914417000     -0.582524000
1       -6.528815000     -1.193152000     -0.977563000
1       -5.240061000     -3.316825000     -1.157241000
1       -2.779925000     -3.265175000     -0.864450000
1       -0.787389000     -1.804279000     -1.020277000
6       -0.864426000     -1.989432000      1.045521000
1        1.422152000     -2.039749000     -2.151397000
1       -1.357832000     -2.960542000      0.940744000
1        0.929633000     -3.137960000      1.230408000
8       -1.383581000     -1.284867000      2.113467000
6       -2.680263000     -1.639199000      2.577938000
1       -3.470019000     -1.155476000      1.999429000
1       -2.817877000     -2.724744000      2.542362000
1       -2.735207000     -1.305322000      3.612755000
1        0.965151000     -1.556532000      2.018165000
```

Compound **B** with benzaldehyde (C_1), S_0

```
59
scf done: -1504.22394411

6       -2.518907000     -1.274742000     -1.018431000
6       -3.244690000     -0.073249000     -0.916656000
6       -4.635306000     -0.173891000     -1.056519000
6       -5.271461000     -1.385248000     -1.279506000
6       -4.527290000     -2.554809000     -1.394825000
6       -3.148605000     -2.489978000     -1.265654000
6       -2.586052000      1.246442000     -0.714088000
6       -1.181167000      1.298693000     -0.757280000
6       -0.449533000      2.484671000     -0.581689000
6       -1.186735000      3.666738000     -0.379681000
6       -2.568949000      3.622909000     -0.336562000
6       -3.280392000      2.427737000     -0.492935000
6        1.022493000      2.423892000     -0.555560000
6        1.783246000      3.600344000     -0.495865000
6        3.157934000      3.553075000     -0.405986000
6        3.807729000      2.323214000     -0.329495000
6        3.118153000      1.116575000     -0.382605000
6        1.707956000      1.174386000     -0.560752000
6        3.822034000     -0.189203000     -0.203159000
6        3.113052000     -1.402860000     -0.247639000
6        3.791691000     -2.599633000      0.003726000
6        5.152004000     -2.627649000      0.272420000
```

```
6         5.856994000     -1.427108000      0.297700000
6         5.199654000     -0.228196000      0.070986000
5         1.575086000     -1.436420000     -0.629286000
8         1.250703000     -2.088652000     -1.909889000
7         0.992480000     -0.000646000     -0.721426000
5        -0.377600000      0.040562000     -0.851984000
7        -1.076153000     -1.313648000     -0.841752000
8         0.771685000     -2.143499000      0.462452000
1         4.883406000      2.326725000     -0.224888000
1         3.734223000      4.469521000     -0.377491000
1         1.291957000      4.563519000     -0.532746000
1        -4.359857000      2.453884000     -0.422238000
1        -0.694035000      4.617240000     -0.224575000
1        -3.119468000      4.539977000     -0.160721000
1         3.227903000     -3.528815000      0.000508000
1         5.659045000     -3.565979000      0.465652000
1         6.920740000     -1.422163000      0.505762000
1         5.783917000      0.680474000      0.122042000
1        -5.237017000      0.723398000     -1.003050000
1        -6.349534000     -1.413486000     -1.380303000
1        -5.011570000     -3.503587000     -1.588180000
1        -2.546098000     -3.388019000     -1.355598000
1        -0.619669000     -1.901152000     -1.561256000
6        -0.569177000     -2.017240000      0.527113000
1        -1.086172000     -2.983439000      0.499337000
1         1.863123000     -2.798031000     -2.110037000
6        -1.071564000     -1.171367000      1.678936000
6        -2.397753000     -1.266512000      2.100478000
6        -0.211335000     -0.266760000      2.299310000
6        -2.872286000     -0.433368000      3.107792000
6        -0.687901000      0.565748000      3.305023000
6        -2.019489000      0.490634000      3.703208000
1        -3.064025000     -1.989668000      1.640121000
1         0.826813000     -0.228761000      1.990134000
1        -3.904292000     -0.509001000      3.429017000
1        -0.017389000      1.272261000      3.779381000
1        -2.388917000      1.142196000      4.486375000
```

Compound **C** with TME (C_1), S_0

```
60
scf done: -1318.04344173

6         3.463295000     -2.079976000     -0.929595000
6         2.777034000     -0.964492000     -0.413914000
6         3.504856000      0.251476000     -0.309787000
6         4.863270000      0.267436000     -0.655600000
6         5.527773000     -0.855176000     -1.108448000
6         4.805949000     -2.033599000     -1.260282000
7         1.409332000     -1.025385000     -0.053102000
5         0.677327000      0.201220000     -0.019344000
6         1.431795000      1.527039000      0.010278000
6         0.713372000      2.719269000      0.204841000
6         1.419517000      3.882047000      0.522394000
6         2.805653000      3.847420000      0.625796000
6         3.518188000      2.681950000      0.384647000
6         2.833445000      1.507287000      0.054012000
6        -0.755878000      2.692461000      0.055937000
6        -1.479506000      3.882412000     -0.008867000
6        -2.860761000      3.887503000     -0.124161000
6        -3.538666000      2.686160000     -0.211961000
6        -2.860524000      1.462618000     -0.197329000
6        -1.456487000      1.462852000     -0.034829000
6        -3.591570000      0.194946000     -0.366920000
6        -2.966607000     -1.033184000     -0.051188000
6        -3.695878000     -2.219354000     -0.262274000
6        -4.989499000     -2.208859000     -0.751502000
6        -5.594833000     -0.990484000     -1.056828000
6        -4.902347000      0.191432000     -0.874463000
7        -0.774410000      0.240664000      0.085655000
5        -1.465314000     -0.990526000      0.345333000
1        -4.617758000      2.700514000     -0.279845000
1        -3.403234000      4.824317000     -0.147306000
1        -0.956612000      4.828339000      0.030203000
1         4.595906000      2.696662000      0.478918000
```

1	0.908150000	4.814167000	0.721077000
1	3.339287000	4.750262000	0.900204000
1	-3.236306000	-3.175436000	-0.064134000
1	-5.520768000	-3.139655000	-0.910100000
1	-6.601639000	-0.966576000	-1.457725000
1	-5.378870000	1.117065000	-1.167192000
1	5.403691000	1.203091000	-0.599394000
1	6.576698000	-0.805083000	-1.371769000
1	5.281712000	-2.922938000	-1.656583000
1	2.943894000	-3.005213000	-1.102791000
6	-0.553465000	-2.077005000	1.092821000
6	0.764335000	-2.345062000	0.276903000
6	0.379880000	-3.075937000	-1.028536000
6	-0.242086000	-1.436857000	2.471253000
6	1.718418000	-3.182125000	1.156965000
6	-1.291989000	-3.391071000	1.403246000
1	0.262181000	-4.147715000	-0.855597000
1	1.125159000	-2.936531000	-1.808641000
1	-0.567145000	-2.692735000	-1.421231000
1	2.440140000	-3.762953000	0.590680000
1	2.272559000	-2.535805000	1.839676000
1	1.149228000	-3.894452000	1.750445000
1	0.233337000	-2.163189000	3.135958000
1	0.410465000	-0.565226000	2.397598000
1	-1.169416000	-1.114907000	2.955404000
1	-2.253437000	-3.164702000	1.868802000
1	-1.480174000	-4.003324000	0.521049000
1	-0.741649000	-4.005147000	2.118836000

Compound **C** with TCNE (C_1), S_0

```
52
scf done: -1529.74174007
```

6	3.744839000	-2.028855000	-0.178351000
6	3.003460000	-0.834833000	-0.078021000
6	3.634067000	0.394191000	-0.387157000
6	4.969648000	0.377003000	-0.820347000
6	5.672713000	-0.809530000	-0.912861000
6	5.065125000	-2.021381000	-0.582555000
5	1.509926000	-0.763988000	0.215511000
7	0.797503000	0.454222000	0.044565000
6	1.496772000	1.679951000	-0.064566000
6	0.803397000	2.910559000	0.050380000
6	1.533355000	4.094512000	-0.032037000
6	2.910623000	4.088469000	-0.187611000
6	3.579585000	2.885001000	-0.287025000
6	2.896954000	1.662585000	-0.249335000
6	-0.663244000	2.957297000	0.227728000
6	-1.350208000	4.124898000	0.566785000
6	-2.735809000	4.106755000	0.676368000
6	-3.469384000	2.956577000	0.419147000
6	-2.806687000	1.776221000	0.073993000
6	-1.402750000	1.780810000	0.028113000
6	-3.507822000	0.539350000	-0.309698000
6	-2.808055000	-0.679082000	-0.459004000
6	-3.473097000	-1.791203000	-0.986774000
6	-4.822005000	-1.734094000	-1.297743000
6	-5.532668000	-0.555845000	-1.107448000
6	-4.868649000	0.562622000	-0.637298000
5	-0.656571000	0.463755000	-0.030690000
7	-1.429794000	-0.745249000	-0.103000000
1	-4.546585000	2.988788000	0.512560000
1	-3.254939000	5.012903000	0.966181000
1	-0.825369000	5.046778000	0.776616000
1	4.655993000	2.896761000	-0.380071000
1	1.018778000	5.043934000	0.021213000
1	3.458139000	5.021494000	-0.229170000
1	-2.953999000	-2.717548000	-1.188167000
1	-5.307735000	-2.613046000	-1.702460000
1	-6.585642000	-0.501115000	-1.352544000
1	-5.413191000	1.493322000	-0.550516000
1	5.466225000	1.290879000	-1.114333000
1	6.700914000	-0.794261000	-1.255257000
1	5.616198000	-2.950312000	-0.659032000

```
1        3.282990000     -2.979412000      0.042766000
6       -0.809250000     -2.051352000      0.034400000
6        0.546064000     -1.937629000      0.842129000
6        1.118086000     -3.283391000      0.941009000
7        1.517098000     -4.356552000      1.015814000
6        0.247252000     -1.465052000      2.203795000
7        0.037820000     -1.047990000      3.252543000
6       -1.663182000     -2.995367000      0.796711000
7       -2.249538000     -3.739263000      1.442890000
6       -0.477120000     -2.630122000     -1.293922000
7       -0.183178000     -3.024082000     -2.330629000
```

Compound **C** with methoxyethene (C_1), S_0

```
52
scf done: -1275.36408994

6       -2.801068000     -1.150527000     -0.371196000
6       -3.478364000      0.094429000     -0.349971000
6       -4.859332000      0.108602000     -0.595762000
6       -5.579703000     -1.043939000     -0.842453000
6       -4.907135000     -2.262331000     -0.874371000
6       -3.542965000     -2.311334000     -0.653043000
6       -2.746790000      1.349064000     -0.104611000
6       -1.340064000      1.322161000     -0.114038000
6       -0.578401000      2.487278000      0.077772000
6       -1.252264000      3.689110000      0.313412000
6       -2.641221000      3.714594000      0.343197000
6       -3.391845000      2.567196000      0.133958000
6        0.898640000      2.394039000      0.035421000
6        1.658442000      3.563431000      0.051168000
6        3.041509000      3.534426000      0.014913000
6        3.689881000      2.316911000     -0.045068000
6        2.988162000      1.106994000     -0.078736000
6        1.568863000      1.142337000     -0.043594000
6        3.727814000     -0.168733000     -0.171381000
6        3.015613000     -1.378873000     -0.256108000
6        3.718625000     -2.590107000     -0.372362000
6        5.099313000     -2.622917000     -0.399905000
6        5.804219000     -1.421274000     -0.298738000
6        5.134430000     -0.217001000     -0.185721000
5        1.480712000     -1.335688000     -0.205067000
7        0.833324000     -0.059241000     -0.095426000
5       -0.622433000     -0.016675000     -0.150893000
7       -1.411204000     -1.211367000     -0.156979000
6        0.574543000     -2.624834000     -0.325567000
1        4.769319000      2.314400000     -0.080071000
1        3.608756000      4.456640000      0.024484000
1        1.163670000      4.523849000      0.075310000
1       -4.470035000      2.633351000      0.186976000
1       -0.719598000      4.610567000      0.501791000
1       -3.148314000      4.651297000      0.544731000
1        3.164746000     -3.519683000     -0.441178000
1        5.629825000     -3.563020000     -0.491278000
1        6.888211000     -1.427486000     -0.307546000
1        5.727572000      0.682861000     -0.106862000
1       -5.380077000      1.056678000     -0.613535000
1       -6.644700000     -0.993750000     -1.030350000
1       -5.441491000     -3.178666000     -1.095371000
1       -3.051814000     -3.269017000     -0.738467000
6       -0.773409000     -2.437922000      0.333635000
1       -1.429988000     -3.288890000      0.152808000
1        0.421845000     -2.849305000     -1.388982000
8       -0.535442000     -2.351318000      1.721911000
6       -1.707494000     -2.215159000      2.498489000
1       -2.193330000     -1.249082000      2.325083000
1       -2.423102000     -3.016258000      2.274503000
1       -1.404760000     -2.282026000      3.541996000
1        1.050574000     -3.499561000      0.121254000
```

Compound **C** with benzaldehyde (C_1), S_0

```
56
scf done: -1427.82426909

6       -2.731716000     -0.113255000     -0.768070000
6       -3.232502000      1.196785000     -0.546169000
6       -4.611364000      1.405533000     -0.687772000
6       -5.489279000      0.387143000     -1.009081000
6       -4.993539000     -0.900479000     -1.184795000
6       -3.637929000     -1.147341000     -1.060787000
6       -2.339016000      2.304742000     -0.154198000
6       -0.962255000      2.047867000     -0.034359000
6       -0.041116000      3.037451000      0.357750000
6       -0.532599000      4.318393000      0.623525000
6       -1.892839000      4.580279000      0.504022000
6       -2.796039000      3.598060000      0.123972000
6        1.398247000      2.691795000      0.457964000
6        2.322766000      3.650627000      0.875883000
6        3.677087000      3.372813000      0.942113000
6        4.137588000      2.121756000      0.571543000
6        3.267332000      1.113591000      0.149354000
6        1.877438000      1.399257000      0.117911000
6        3.793268000     -0.208063000     -0.269643000
6        2.909861000     -1.205753000     -0.719454000
6        3.397479000     -2.453556000     -1.129878000
6        4.751987000     -2.729217000     -1.105419000
6        5.633765000     -1.743089000     -0.657158000
6        5.167403000     -0.506506000     -0.246000000
5        1.409275000     -0.892872000     -0.702058000
7        0.972970000      0.396524000     -0.259995000
5       -0.440900000      0.659323000     -0.333165000
7       -1.354323000     -0.375256000     -0.684868000
8        0.489960000     -1.816305000     -1.125392000
1        5.200952000      1.934346000      0.612789000
1        4.373580000      4.133331000      1.272057000
1        1.985013000      4.638111000      1.157013000
1       -3.843101000      3.858438000      0.054817000
1        0.119996000      5.128045000      0.918518000
1       -2.257013000      5.579532000      0.714098000
1        2.688111000     -3.202499000     -1.464817000
1        5.127616000     -3.694200000     -1.423808000
1        6.698632000     -1.944024000     -0.627996000
1        5.892401000      0.220178000      0.092961000
1       -5.011757000      2.398964000     -0.539001000
1       -6.547842000      0.591192000     -1.108533000
1       -5.662823000     -1.721277000     -1.412841000
1       -3.293615000     -2.165191000     -1.172484000
6       -0.895356000     -1.750163000     -0.864089000
1       -1.372153000     -2.165035000     -1.755798000
6       -1.206303000     -2.638678000      0.334369000
6       -1.095950000     -4.019100000      0.171160000
6       -1.549521000     -2.119084000      1.577844000
6       -1.322426000     -4.873681000      1.242144000
6       -1.774813000     -2.975403000      2.652657000
6       -1.662156000     -4.350657000      2.487448000
1       -0.822462000     -4.420523000     -0.799665000
1       -1.652559000     -1.047580000      1.708365000
1       -1.235222000     -5.945278000      1.107617000
1       -2.043238000     -2.564874000      3.618718000
1       -1.841620000     -5.014747000      3.324546000
```

Compound **3a** (C_1), S_0

```
56
scf done: -1428.37106587

6       -2.741927000     -0.038606000     -0.759391000
6       -3.205985000      1.293732000     -0.549170000
6       -4.574415000      1.550609000     -0.746108000
6       -5.476166000      0.564908000     -1.110533000
6       -5.018539000     -0.740085000     -1.280750000
6       -3.675735000     -1.035228000     -1.102944000
6       -2.289276000      2.368765000     -0.129568000
6       -0.913734000      2.074128000     -0.009896000
6        0.032535000      3.045895000      0.388279000
6       -0.433975000      4.337339000      0.670410000
```

```
6       -1.790188000      4.631818000      0.559935000
6       -2.715781000      3.672522000      0.167566000
6        1.463207000      2.671998000      0.476350000
6        2.415759000      3.611960000      0.889186000
6        3.766572000      3.305635000      0.941319000
6        4.199871000      2.046122000      0.559022000
6        3.305130000      1.053248000      0.137026000
6        1.914753000      1.366396000      0.125625000
6        3.801511000     -0.272302000     -0.298507000
6        2.888506000     -1.263030000     -0.727229000
6        3.357519000     -2.517321000     -1.153281000
6        4.711623000     -2.808851000     -1.165850000
6        5.619010000     -1.832255000     -0.740975000
6        5.175461000     -0.589577000     -0.315334000
5        1.395499000     -0.924024000     -0.676292000
7        0.984663000      0.379703000     -0.239978000
5       -0.428796000      0.672503000     -0.297785000
7       -1.374604000     -0.350035000     -0.623231000
8        0.448340000     -1.838868000     -1.063933000
1        5.259701000      1.836205000      0.590266000
1        4.481721000      4.050862000      1.269177000
1        2.100379000      4.605713000      1.175268000
1       -3.758287000      3.953896000      0.104931000
1        0.239347000      5.127388000      0.973531000
1       -2.132243000      5.636186000      0.785893000
1        2.635546000     -3.260764000     -1.472248000
1        5.066598000     -3.778401000     -1.496591000
1        6.682797000     -2.044508000     -0.742926000
1        5.916165000      0.131921000      0.001653000
1       -4.943615000      2.558302000     -0.610860000
1       -6.522402000      0.808210000     -1.252376000
1       -5.705970000     -1.534545000     -1.548092000
1       -3.362481000     -2.061789000     -1.218358000
6       -0.946830000     -1.743178000     -0.808452000
1       -1.422765000     -2.135897000     -1.710418000
6       -1.286370000     -2.655182000      0.369552000
6       -1.370081000     -4.031667000      0.141135000
6       -1.458123000     -2.169067000      1.665774000
6       -1.616282000     -4.910812000      1.192208000
6       -1.703128000     -3.047979000      2.720098000
6       -1.782246000     -4.419183000      2.486745000
1       -1.235604000     -4.416982000     -0.864882000
1       -1.411912000     -1.103124000      1.854301000
1       -1.680353000     -5.976370000      1.002122000
1       -1.836766000     -2.659135000      3.723335000
1       -1.976558000     -5.100826000      3.307131000
```

Compound **3c** (C_1), S_0

```
58
scf done: -1632.93383773

6       -1.152413000      2.321813000     -1.124785000
6       -0.543452000      3.517313000     -0.641650000
6       -1.221199000      4.730262000     -0.856683000
6       -2.449680000      4.799219000     -1.492455000
6       -3.050551000      3.622140000     -1.932485000
6       -2.412710000      2.404928000     -1.746545000
6        0.748313000      3.489282000      0.068468000
6        1.421330000      2.254810000      0.197847000
6        2.662591000      2.139525000      0.864407000
6        3.223167000      3.303158000      1.409080000
6        2.560980000      4.521834000      1.289934000
6        1.341146000      4.629031000      0.632716000
6        3.320840000      0.815183000      0.948833000
6        4.542917000      0.674118000      1.618149000
6        5.202994000     -0.543085000      1.680159000
6        4.659246000     -1.651972000      1.051981000
6        3.439237000     -1.587678000      0.364808000
6        2.751131000     -0.340422000      0.340283000
6        2.899718000     -2.781399000     -0.325656000
6        1.670598000     -2.701724000     -1.020508000
6        1.163139000     -3.829639000     -1.688108000
6        1.848624000     -5.033051000     -1.682822000
```

```
6        3.063870000     -5.117506000     -0.994565000
6        3.580245000     -4.016347000     -0.329152000
5        0.922822000     -1.367378000     -0.984877000
7        1.500330000     -0.251246000     -0.295208000
5        0.793512000      1.005419000     -0.371696000
7       -0.502220000      1.078719000     -0.976639000
8       -0.287363000     -1.216709000     -1.623665000
1        5.201027000     -2.585977000      1.099082000
1        6.145267000     -0.624979000      2.208867000
1        4.992893000      1.530413000      2.100852000
1        0.867282000      5.599607000      0.575875000
1        4.172386000      3.283935000      1.926644000
1        3.009263000      5.410263000      1.721589000
1        0.217179000     -3.743237000     -2.210967000
1        1.451883000     -5.898998000     -2.200432000
1        3.612533000     -6.053023000     -0.978662000
1        4.523734000     -4.132116000      0.186517000
1       -0.768578000      5.651450000     -0.515503000
1       -2.935809000      5.756557000     -1.636854000
1       -4.018961000      3.645947000     -2.418833000
1       -2.918863000      1.512728000     -2.083877000
6       -1.182065000     -0.131355000     -1.445003000
1       -1.597694000      0.060633000     -2.437457000
6       -2.310012000     -0.601825000     -0.521649000
6       -3.266461000     -1.480167000     -1.042401000
6       -2.380208000     -0.229861000      0.821536000
6       -4.278822000     -1.987883000     -0.239038000
6       -3.386332000     -0.730202000      1.642203000
6       -4.320649000     -1.603084000      1.097805000
1       -3.214436000     -1.774874000     -2.084892000
1       -1.654194000      0.460957000      1.231063000
1       -5.026340000     -2.666621000     -0.625546000
1       -3.456455000     -0.452369000      2.684732000
7       -5.396828000     -2.134327000      1.963069000
8       -6.212908000     -2.892585000      1.453830000
8       -5.407974000     -1.785084000      3.136572000
```

Phenyl isocyanide (C_{2v}), S_0

```
13
scf done: -324.406124755

6        0.000000000      0.000000000      3.188287000
7        0.000000000      0.000000000      2.018364000
6        0.000000000      0.000000000      0.628139000
6        0.000000000     -1.213512000     -0.055930000
6        0.000000000      1.213512000     -0.055930000
6        0.000000000     -1.205330000     -1.444553000
6        0.000000000      1.205330000     -1.444553000
6        0.000000000      0.000000000     -2.140044000
1        0.000000000     -2.139445000      0.504504000
1        0.000000000      2.139445000      0.504504000
1        0.000000000     -2.144736000     -1.983501000
1        0.000000000      2.144736000     -1.983501000
1        0.000000000      0.000000000     -3.223048000
```

CO_2 ($D_{\infty h}$), S_0

```
3
scf done: -188.574879675

6        0.000000000      0.000000000      0.000000000
8        0.000000000      0.000000000      1.154787000
8        0.000000000      0.000000000     -1.154787000
```

Benzonitrile (C_{2v}), S_0

```
13
scf done: -324.437625172
```

```
6        0.000000000      0.000000000      2.040818000
7        0.000000000      0.000000000      3.191068000
6        0.000000000      0.000000000      0.602978000
6        0.000000000      1.213045000     -0.089553000
6        0.000000000     -1.213045000     -0.089553000
6        0.000000000      1.206868000     -1.477769000
6        0.000000000     -1.206868000     -1.477769000
6        0.000000000      0.000000000     -2.170997000
1        0.000000000      2.144453000      0.462450000
1        0.000000000     -2.144453000      0.462450000
1        0.000000000      2.145166000     -2.018489000
1        0.000000000     -2.145166000     -2.018489000
1        0.000000000      0.000000000     -3.254328000
```

Imine H_2CNH (C_s), S_0

```
5
scf done: -94.6103969974

7       -0.665447000     -0.154636000      0.000005000
6        0.584402000      0.028847000     -0.000031000
1        1.068884000      1.010185000      0.000058000
1        1.242915000     -0.839866000      0.000075000
1       -1.160078000      0.739046000      0.000021000
```

Iminium ion $H_2CNH_2^+$ (C_{2v}), S_0

```
6
scf done: -94.9506168492

6        0.000000000      0.000000000     -0.673213000
7        0.000000000      0.000000000      0.598478000
1        0.000000000      0.943814000     -1.210293000
1        0.000000000     -0.943814000     -1.210293000
1        0.000000000      0.867598000      1.135260000
1        0.000000000     -0.867598000      1.135260000
```

Phenyl iminoborane (C_{2v}), S_0

```
14
scf done: -311.818143001

7        0.000000000      0.000000000      3.310134000
5        0.000000000      0.000000000      2.071590000
1        0.000000000      0.000000000      4.303607000
6        0.000000000      0.000000000      0.543339000
6        0.000000000      1.205716000     -0.169980000
6        0.000000000     -1.205716000     -0.169980000
6        0.000000000      1.205216000     -1.559642000
6        0.000000000     -1.205216000     -1.559642000
6        0.000000000      0.000000000     -2.255184000
1        0.000000000      2.147817000      0.366167000
1        0.000000000     -2.147817000      0.366167000
1        0.000000000      2.144446000     -2.099735000
1        0.000000000     -2.144446000     -2.099735000
1        0.000000000      0.000000000     -3.338824000
```

Compound **B** with phenyl isocyanide (C_1), S_0

```
58
scf done: -1483.07993988

6       -2.766840000     -1.766538000     -0.491598000
6       -3.847499000     -0.959391000     -0.095683000
6       -5.103130000     -1.581301000     -0.039603000
6       -5.278707000     -2.919464000     -0.350471000
6       -4.189030000     -3.695089000     -0.732661000
```

6	-2.934475000	-3.111773000	-0.797571000
6	-3.693093000	0.482388000	0.242816000
6	-2.417450000	1.063230000	0.117723000
6	-2.154286000	2.412908000	0.409445000
6	-3.240465000	3.200908000	0.831700000
6	-4.497432000	2.636340000	0.956996000
6	-4.738759000	1.288339000	0.673588000
6	-0.774822000	2.919867000	0.286854000
6	-0.476191000	4.248762000	0.616528000
6	0.814296000	4.729547000	0.547347000
6	1.848323000	3.884723000	0.156998000
6	1.626729000	2.554869000	-0.188034000
6	0.289688000	2.074125000	-0.140080000
6	2.755142000	1.664142000	-0.588366000
6	2.526857000	0.322711000	-0.942254000
6	3.606651000	-0.473220000	-1.346560000
6	4.902199000	0.014522000	-1.377874000
6	5.131152000	1.337929000	-1.005610000
6	4.075333000	2.148640000	-0.624066000
5	1.064124000	-0.283614000	-0.957113000
8	0.676015000	-0.905708000	-2.229328000
7	0.022469000	0.759554000	-0.496239000
5	-1.253589000	0.245798000	-0.348944000
7	-1.409761000	-1.243207000	-0.603204000
7	0.789396000	-1.534197000	0.081480000
1	2.848680000	4.292143000	0.128544000
1	1.026973000	5.759450000	0.805431000
1	-1.263825000	4.915499000	0.939608000
1	-5.742443000	0.905787000	0.800865000
1	-3.120543000	4.249118000	1.068638000
1	-5.322049000	3.256689000	1.289012000
1	3.414972000	-1.504685000	-1.628292000
1	5.725055000	-0.621064000	-1.683163000
1	6.136722000	1.742491000	-1.018168000
1	4.301197000	3.171176000	-0.355112000
1	-5.968860000	-1.002445000	0.251720000
1	-6.267693000	-3.357484000	-0.293626000
1	-4.313042000	-4.743653000	-0.972166000
1	-2.062512000	-3.695333000	-1.067835000
1	-1.035904000	-1.394268000	-1.558808000
6	-0.366646000	-2.073962000	0.282550000
1	0.990174000	-0.389297000	-2.973827000
6	1.890371000	-2.148789000	0.774971000
6	2.214026000	-3.476156000	0.528096000
6	2.640393000	-1.385491000	1.663779000
6	3.304645000	-4.046347000	1.177506000
6	3.725089000	-1.962317000	2.310538000
6	4.061906000	-3.291433000	2.066021000
1	1.612704000	-4.044104000	-0.170885000
1	2.375766000	-0.348167000	1.833533000
1	3.561501000	-5.081232000	0.985595000
1	4.311027000	-1.370852000	3.003479000
1	4.912731000	-3.736148000	2.567955000

Compound **B** with CO_2 (C_1), S_0

48
scf done: -1347.25435785

6	-2.814565000	-1.263949000	-0.203676000
6	-3.526289000	-0.058826000	-0.059469000
6	-4.924399000	-0.160868000	-0.062881000
6	-5.576908000	-1.374581000	-0.202375000
6	-4.845510000	-2.547497000	-0.353906000
6	-3.462202000	-2.484366000	-0.352362000
6	-2.861105000	1.269556000	0.051390000
6	-1.458130000	1.320772000	-0.038215000
6	-0.720956000	2.516711000	0.030056000
6	-1.451998000	3.707431000	0.196502000
6	-2.831354000	3.664680000	0.292623000
6	-3.546882000	2.464007000	0.223930000
6	0.749962000	2.463649000	-0.047120000
6	1.509627000	3.642500000	-0.038192000
6	2.886916000	3.602129000	-0.083234000
6	3.547376000	2.376058000	-0.098525000
6	2.859058000	1.167819000	-0.092366000

```
6        1.439876000      1.220898000     -0.120140000
6        3.580309000     -0.137280000     -0.026516000
6        2.883537000     -1.355055000     -0.124159000
6        3.587475000     -2.560691000     -0.040256000
6        4.961512000     -2.587988000      0.142531000
6        5.651113000     -1.382436000      0.248826000
6        4.970737000     -0.177734000      0.169424000
5        1.324472000     -1.376384000     -0.360215000
7        0.717730000      0.039421000     -0.214446000
5       -0.658858000      0.068478000     -0.183614000
7       -1.353016000     -1.297159000     -0.228012000
8        0.595461000     -2.199017000      0.763861000
6       -0.665427000     -2.207604000      0.897357000
8       -1.387096000     -2.739778000      1.670779000
1        4.628124000      2.381663000     -0.118513000
1        3.458149000      4.521951000     -0.095097000
1        1.015696000      4.604103000     -0.006458000
1       -4.624149000      2.499734000      0.313568000
1       -0.958412000      4.667029000      0.267120000
1       -3.377718000      4.590618000      0.430550000
1        3.033372000     -3.491683000     -0.112441000
1        5.491460000     -3.530747000      0.211078000
1        6.723900000     -1.379848000      0.403529000
1        5.543386000      0.732998000      0.280297000
1       -5.520376000      0.735812000      0.036352000
1       -6.659618000     -1.403467000     -0.198650000
1       -5.344347000     -3.501552000     -0.466117000
1       -2.870965000     -3.387058000     -0.449620000
1       -1.006170000     -1.741888000     -1.097851000
8        0.848058000     -2.022505000     -1.577833000
1        1.484575000     -1.967566000     -2.291324000
```

Compound **B** with iminium ion ($H_2CNH_2^+$) (C_1), S_0

```
51
scf done: -1253.72155028

6        2.856054000     -1.402711000      0.112325000
6        3.580593000     -0.204931000      0.000184000
6        4.976680000     -0.332310000      0.030700000
6        5.606255000     -1.559285000      0.165488000
6        4.857197000     -2.723904000      0.295962000
6        3.474474000     -2.637569000      0.270836000
6        2.930580000      1.130517000     -0.086203000
6        1.530470000      1.203650000      0.057079000
6        0.817155000      2.415991000      0.023094000
6        1.565994000      3.593968000     -0.153327000
6        2.938856000      3.526394000     -0.302766000
6        3.632164000      2.310380000     -0.277063000
6       -0.652912000      2.394757000      0.125494000
6       -1.378928000      3.594186000      0.155082000
6       -2.756632000      3.592448000      0.192388000
6       -3.450921000      2.387971000      0.160743000
6       -2.795206000      1.160874000      0.126296000
6       -1.378040000      1.173239000      0.164629000
6       -3.560827000     -0.114923000      0.031636000
6       -2.900590000     -1.355878000      0.086345000
6       -3.642697000     -2.541420000      0.013253000
6       -5.020755000     -2.526615000     -0.135476000
6       -5.672089000     -1.298141000     -0.209168000
6       -4.955720000     -0.114298000     -0.124991000
5       -1.345024000     -1.413643000      0.255924000
8       -0.791519000     -2.321181000      1.241858000
7       -0.677359000     -0.041219000      0.225431000
5        0.705281000     -0.027853000      0.192093000
7        1.378058000     -1.417453000      0.086586000
7       -0.626062000     -2.128853000     -1.151728000
1       -4.530646000      2.425294000      0.170239000
1       -3.300766000      4.527221000      0.233045000
1       -0.859124000      4.541895000      0.158526000
1        4.704891000      2.325183000     -0.413783000
1        1.091015000      4.564013000     -0.195549000
1        3.497566000      4.442749000     -0.451353000
1       -3.130569000     -3.498194000      0.091228000
1       -5.582465000     -3.450877000     -0.191002000
1       -6.747933000     -1.261058000     -0.330780000
```

```
1       -5.508015000      0.812377000     -0.191965000
1        5.589498000      0.556044000     -0.034070000
1        6.687887000     -1.604571000      0.186769000
1        5.340255000     -3.683570000      0.425684000
1        2.872536000     -3.532531000      0.395482000
1        1.010442000     -1.974565000      0.878609000
6        0.854894000     -2.088317000     -1.165640000
1        1.265125000     -3.093815000     -1.210223000
1       -1.378271000     -2.466863000      1.987453000
1        1.221796000     -1.503947000     -2.007778000
1       -0.958967000     -3.091831000     -1.176385000
1       -1.012137000     -1.647800000     -1.962524000
```

Compound **B** with phenyl iminoborane (C_1), S_0

```
59
scf done: -1470.57784969

6       -2.445139000      0.277425000     -1.112429000
6       -2.781876000      1.589784000     -0.738066000
6       -4.104466000      1.988946000     -0.981869000
6       -5.036311000      1.144718000     -1.562920000
6       -4.670689000     -0.144398000     -1.937369000
6       -3.373307000     -0.570118000     -1.707456000
6       -1.793663000      2.532166000     -0.143894000
6       -0.450000000      2.119286000     -0.049357000
6        0.575275000      2.951765000      0.434896000
6        0.205939000      4.242343000      0.859622000
6       -1.115683000      4.643750000      0.792470000
6       -2.121158000      3.808197000      0.294448000
6        1.954294000      2.438424000      0.489407000
6        3.001688000      3.268105000      0.916021000
6        4.295867000      2.801856000      0.989747000
6        4.573208000      1.476666000      0.663965000
6        3.585092000      0.593055000      0.244705000
6        2.258144000      1.095362000      0.117274000
6        3.907925000     -0.835583000     -0.047528000
6        2.925413000     -1.711003000     -0.541812000
6        3.270867000     -3.038952000     -0.819150000
6        4.551423000     -3.524265000     -0.602196000
6        5.518639000     -2.661172000     -0.092723000
6        5.200718000     -1.340049000      0.178780000
5        1.435196000     -1.233575000     -0.816085000
7        1.255919000      0.266558000     -0.358318000
5       -0.043132000      0.730599000     -0.438604000
7       -1.112262000     -0.272524000     -0.885769000
7        0.341693000     -2.021659000     -0.019930000
5       -0.949343000     -1.573317000      0.020309000
1        5.597807000      1.142531000      0.743420000
1        5.095936000      3.459002000      1.306982000
1        2.801750000      4.296366000      1.184746000
1       -3.136253000      4.181089000      0.266184000
1        0.935177000      4.935823000      1.255310000
1       -1.382553000      5.636959000      1.135102000
1        2.507896000     -3.697494000     -1.225853000
1        4.797952000     -4.556429000     -0.823088000
1        6.524941000     -3.017665000      0.094921000
1        5.982449000     -0.710700000      0.581452000
1       -4.410339000      2.993157000     -0.721771000
1       -6.046559000      1.496696000     -1.732140000
1       -5.387456000     -0.812783000     -2.397239000
1       -3.070326000     -1.578130000     -1.969975000
1       -0.713620000     -0.633411000     -1.779517000
8        0.997626000     -1.339346000     -2.229284000
1        1.658147000     -0.973018000     -2.820848000
1        0.621836000     -2.806807000      0.550482000
6       -2.160850000     -2.158598000      0.810294000
6       -2.323135000     -3.547958000      0.882880000
6       -3.071344000     -1.351597000      1.506506000
6       -3.362489000     -4.114216000      1.613835000
6       -4.101331000     -1.912515000      2.251758000
6       -4.252467000     -3.295624000      2.300955000
1       -1.631513000     -4.193621000      0.350865000
1       -2.974393000     -0.270530000      1.475179000
1       -3.476459000     -5.191346000      1.649154000
1       -4.788612000     -1.271870000      2.791650000
```

```
1       -5.061382000     -3.733016000      2.874504000
```

Compound **C** with phenyl isocyanide (C_1), S_0

```
55
scf done: -1195.54253095

6        2.818901000     -1.506528000     -0.000036000
6        3.548698000     -0.297517000      0.000042000
6        4.950609000     -0.385580000      0.000093000
6        5.613945000     -1.596498000      0.000049000
6        4.875916000     -2.777628000     -0.000058000
6        3.494544000     -2.732209000     -0.000098000
6        2.886957000      1.028063000      0.000053000
6        1.482557000      1.079157000      0.000016000
6        0.765567000      2.289996000      0.000013000
6        1.498640000      3.481433000      0.000057000
6        2.886391000      3.439026000      0.000091000
6        3.585566000      2.237123000      0.000085000
6       -0.716002000      2.258470000     -0.000033000
6       -1.453171000      3.444331000     -0.000092000
6       -2.837480000      3.433732000     -0.000145000
6       -3.520640000      2.229492000     -0.000115000
6       -2.846773000      1.005591000     -0.000036000
6       -1.429614000      1.033219000     -0.000028000
6       -3.594388000     -0.275169000      0.000023000
6       -2.899071000     -1.500281000     -0.000032000
6       -3.596700000     -2.716142000      0.000002000
6       -4.978726000     -2.736551000      0.000095000
6       -5.673998000     -1.524792000      0.000176000
6       -4.999420000     -0.316148000      0.000144000
5       -1.374743000     -1.440718000     -0.000057000
7       -0.721915000     -0.178318000     -0.000028000
5        0.703845000     -0.210456000     -0.000023000
7        1.380108000     -1.495078000     -0.000052000
8       -0.588861000     -2.588594000     -0.000078000
6        0.744004000     -2.711150000     -0.000063000
1       -4.600910000      2.252333000     -0.000173000
1       -3.386317000      4.367120000     -0.000214000
1       -0.943508000      4.397475000     -0.000111000
1        4.666011000      2.270542000      0.000103000
1        1.014042000      4.447717000      0.000068000
1        3.441215000      4.370276000      0.000120000
1       -3.029795000     -3.640681000     -0.000042000
1       -5.518511000     -3.675640000      0.000119000
1       -6.757955000     -1.525631000      0.000273000
1       -5.585997000      0.591906000      0.000236000
1        5.538905000      0.521391000      0.000176000
1        6.696628000     -1.621219000      0.000094000
1        5.376664000     -3.738257000     -0.000109000
1        2.909693000     -3.639573000     -0.000170000
```

Compound **C** with CO_2 (C_1), S_0

```
45
scf done: -1270.85710948

6        2.819258000     -1.296350000     -0.091740000
6        3.510191000     -0.061253000     -0.057871000
6        4.898334000     -0.076325000     -0.256666000
6        5.599390000     -1.244651000     -0.483014000
6        4.904022000     -2.446988000     -0.541175000
6        3.533011000     -2.472838000     -0.353792000
6        2.809511000      1.229824000      0.105434000
6        1.409205000      1.241795000      0.013216000
6        0.659725000      2.429726000      0.088414000
6        1.350333000      3.628258000      0.292222000
6        2.734090000      3.618283000      0.414544000
6        3.468760000      2.442307000      0.321442000
6       -0.814548000      2.366259000     -0.031778000
6       -1.567546000      3.535295000     -0.152246000
6       -2.948318000      3.496687000     -0.245757000
6       -3.606844000      2.279379000     -0.220094000
```

```
6       -2.912325000      1.070781000     -0.118087000
6       -1.498647000      1.125673000     -0.034381000
6       -3.637995000     -0.222205000     -0.097035000
6       -2.925093000     -1.429431000      0.033449000
6       -3.600311000     -2.657162000      0.070801000
6       -4.978190000     -2.707258000     -0.025856000
6       -5.691031000     -1.513529000     -0.161748000
6       -5.038193000     -0.293379000     -0.196323000
5       -1.404814000     -1.337771000      0.119449000
7       -0.765022000     -0.069385000      0.048626000
5        0.666581000     -0.072731000      0.006230000
7        1.394138000     -1.321358000      0.062869000
8       -0.615857000     -2.463207000      0.271449000
6        0.730903000     -2.513465000      0.399530000
1       -4.685349000      2.278218000     -0.286484000
1       -3.512316000      4.416085000     -0.340261000
1       -1.069787000      4.494534000     -0.187319000
1        4.542441000      2.489293000      0.441480000
1        0.829430000      4.570975000      0.388355000
1        3.253852000      4.552144000      0.595531000
1       -3.020749000     -3.567748000      0.176947000
1       -5.500996000     -3.655449000      0.002638000
1       -6.771832000     -1.537624000     -0.240769000
1       -5.637741000      0.599772000     -0.302947000
1        5.438472000      0.860475000     -0.261847000
1        6.671220000     -1.215972000     -0.634394000
1        5.425454000     -3.375002000     -0.741558000
1        3.015846000     -3.415898000     -0.405220000
8        1.248765000     -3.522130000      0.773307000
```

Compound **C** with benzonitrile ($C_{\infty v}$), S_0

```
55
scf done: -1406.72651510

6       -2.410493000      0.630403000     -0.678177000
6       -2.519040000      2.027728000     -0.488906000
6       -3.705862000      2.654151000     -0.895482000
6       -4.741661000      1.954491000     -1.486786000
6       -4.590989000      0.591878000     -1.731372000
6       -3.432261000     -0.056744000     -1.343823000
6       -1.380693000      2.829030000      0.009612000
6       -0.114650000      2.221014000      0.029435000
6        1.051890000      2.919822000      0.379154000
6        0.919350000      4.260810000      0.760466000
6       -0.335285000      4.856772000      0.778340000
6       -1.482537000      4.163837000      0.402208000
6        2.351438000      2.212643000      0.330476000
6        3.545617000      2.922543000      0.465468000
6        4.772827000      2.283666000      0.414096000
6        4.829836000      0.915635000      0.207858000
6        3.673835000      0.147777000      0.043225000
6        2.421729000      0.809289000      0.120298000
6        3.759600000     -1.311171000     -0.204478000
6        2.584474000     -2.084549000     -0.265076000
6        2.663603000     -3.470065000     -0.464638000
6        3.885034000     -4.097556000     -0.624946000
6        5.051454000     -3.329594000     -0.585673000
6        4.993773000     -1.962361000     -0.377903000
5        1.228957000     -1.375818000     -0.125500000
7        1.241721000      0.063407000     -0.012301000
5       -0.018064000      0.720596000     -0.128578000
7       -1.229153000     -0.052320000     -0.272901000
7       -0.032507000     -2.062346000     -0.033018000
1        5.800570000      0.441801000      0.175877000
1        5.686899000      2.853104000      0.527507000
1        3.521004000      3.995415000      0.599905000
1       -2.438405000      4.670122000      0.440360000
1        1.774265000      4.845943000      1.071562000
1       -0.423220000      5.889139000      1.097024000
1        1.739703000     -4.037852000     -0.487155000
1        3.942335000     -5.168273000     -0.780670000
1        6.016371000     -3.805666000     -0.718069000
1        5.924358000     -1.411899000     -0.361602000
1       -3.800217000      3.725851000     -0.777728000
1       -5.642181000      2.472349000     -1.792506000
```

```
1       -5.367498000      0.035294000     -2.241640000
1       -3.313803000     -1.108313000     -1.565179000
6       -1.146835000     -1.429910000     -0.010248000
6       -2.365041000     -2.157861000      0.454869000
6       -2.538514000     -3.488333000      0.077352000
6       -3.269849000     -1.564455000      1.336738000
6       -3.628492000     -4.210029000      0.548194000
6       -4.345000000     -2.295684000      1.825168000
6       -4.533129000     -3.614970000      1.422727000
1       -1.807118000     -3.942414000     -0.580040000
1       -3.129726000     -0.534354000      1.644666000
1       -3.766858000     -5.239700000      0.240872000
1       -5.037533000     -1.834684000      2.519021000
1       -5.378610000     -4.180160000      1.796681000
```

Compound **C** with imine (H_2CNH) (C_1), S_0

```
47
scf done: -1176.92918138

6       -2.842305000     -1.441313000      0.000011000
6       -3.575979000     -0.226544000     -0.000016000
6       -4.974763000     -0.300611000     -0.000005000
6       -5.658775000     -1.502803000      0.000021000
6       -4.933839000     -2.688447000      0.000041000
6       -3.549728000     -2.657516000      0.000038000
6       -2.888141000      1.077211000     -0.000044000
6       -1.481567000      1.097160000     -0.000009000
6       -0.756310000      2.303573000     -0.000013000
6       -1.473512000      3.503869000     -0.000071000
6       -2.862291000      3.487088000     -0.000119000
6       -3.573541000      2.296786000     -0.000104000
6        0.724304000      2.261495000      0.000038000
6        1.453782000      3.452217000      0.000104000
6        2.836235000      3.458649000      0.000154000
6        3.520083000      2.256118000      0.000118000
6        2.854249000      1.028716000      0.000040000
6        1.433013000      1.030263000      0.000029000
6        3.629482000     -0.235952000     -0.000017000
6        2.960573000     -1.472259000      0.000011000
6        3.703319000     -2.661032000     -0.000012000
6        5.085722000     -2.652526000     -0.000076000
6        5.749970000     -1.425384000     -0.000131000
6        5.036746000     -0.240489000     -0.000104000
5        1.415586000     -1.454876000      0.000025000
7        0.732574000     -0.183549000      0.000015000
5       -0.709785000     -0.211291000      0.000010000
7       -1.440263000     -1.440436000      0.000012000
7        0.639567000     -2.630100000      0.000022000
1        4.599838000      2.285152000      0.000167000
1        3.378920000      4.395501000      0.000221000
1        0.936426000      4.400770000      0.000128000
1       -4.653636000      2.341197000     -0.000146000
1       -0.976227000      4.463222000     -0.000089000
1       -3.402023000      4.427249000     -0.000171000
1        3.191620000     -3.618601000      0.000020000
1        5.645330000     -3.580080000     -0.000091000
1        6.833410000     -1.395090000     -0.000200000
1        5.597980000      0.682914000     -0.000166000
1       -5.551082000      0.614215000     -0.000014000
1       -6.741314000     -1.514426000      0.000029000
1       -5.442743000     -3.644981000      0.000062000
1       -3.024400000     -3.600647000      0.000057000
6       -0.798626000     -2.749837000      0.000042000
1       -1.128812000     -3.307089000     -0.886556000
1       -1.128797000     -3.307038000      0.886678000
1        1.104762000     -3.523425000     -0.000001000
```

Compound **C** with iminium ion ($H_2CNH_2^+$) (C_1), S_0

```
48
scf done: -1177.28204005
```

```
6        2.847339000     -1.445747000     -0.133627000
6        3.572247000     -0.240210000      0.026434000
6        4.971140000     -0.313876000     -0.020733000
6        5.645655000     -1.501288000     -0.236290000
6        4.918694000     -2.667341000     -0.441565000
6        3.534357000     -2.637182000     -0.396784000
6        2.889602000      1.060646000      0.170344000
6        1.488332000      1.102219000      0.064898000
6        0.764854000      2.308518000      0.097405000
6        1.472176000      3.492299000      0.299283000
6        2.856610000      3.455501000      0.441484000
6        3.568887000      2.267336000      0.369527000
6       -0.706694000      2.272750000     -0.084162000
6       -1.421124000      3.453812000     -0.268989000
6       -2.802610000      3.455841000     -0.399641000
6       -3.501839000      2.268258000     -0.336825000
6       -2.843591000      1.041070000     -0.172999000
6       -1.431937000      1.056022000     -0.073629000
6       -3.614611000     -0.213467000     -0.077804000
6       -2.957306000     -1.434645000      0.206646000
6       -3.699381000     -2.623493000      0.351671000
6       -5.069201000     -2.626834000      0.209414000
6       -5.718375000     -1.424527000     -0.095301000
6       -5.011907000     -0.245649000     -0.236359000
5       -1.458638000     -1.349091000      0.261443000
7       -0.737712000     -0.172731000      0.058579000
5        0.725474000     -0.189714000      0.005334000
7        1.428069000     -1.430097000     -0.044366000
7       -0.565036000     -2.588336000      0.593753000
1       -4.578721000      2.302138000     -0.410922000
1       -3.331573000      4.389593000     -0.540422000
1       -0.894553000      4.396541000     -0.320134000
1        4.643686000      2.302893000      0.478825000
1        0.971983000      4.448199000      0.369960000
1        3.392601000      4.381949000      0.610119000
1       -3.204195000     -3.564035000      0.580175000
1       -5.636798000     -3.541554000      0.322569000
1       -6.794197000     -1.415497000     -0.223501000
1       -5.565031000      0.650356000     -0.477509000
1        5.551207000      0.590682000      0.097126000
1        6.727306000     -1.513663000     -0.268415000
1        5.423803000     -3.602376000     -0.648934000
1        3.009147000     -3.559313000     -0.603595000
6        0.712952000     -2.668550000     -0.192903000
1        1.277027000     -3.506004000      0.209940000
1        0.432253000     -2.876013000     -1.231124000
1       -1.095548000     -3.451397000      0.458311000
1       -0.325431000     -2.549101000      1.590902000
```

Compound **C** with phenyl iminoborane (C_1), S_0

```
56
scf done: -1394.18651355

6       -2.404151000      0.826968000     -0.638288000
6       -2.437765000      2.219722000     -0.406936000
6       -3.608324000      2.921497000     -0.732098000
6       -4.710305000      2.295558000     -1.283580000
6       -4.645418000      0.933154000     -1.566682000
6       -3.502370000      0.217413000     -1.260996000
6       -1.238169000      2.936456000      0.065015000
6       -0.006747000      2.257871000      0.027056000
6        1.197436000      2.901479000      0.351185000
6        1.146592000      4.234645000      0.775241000
6       -0.073602000      4.892093000      0.853754000
6       -1.260755000      4.264070000      0.495957000
6        2.461807000      2.143973000      0.246459000
6        3.680776000      2.819076000      0.330703000
6        4.887370000      2.146147000      0.271413000
6        4.889898000      0.771475000      0.119950000
6        3.705714000      0.039448000     -0.001980000
6        2.469446000      0.736951000      0.052773000
6        3.760109000     -1.430437000     -0.171590000
6        2.568636000     -2.175859000     -0.173065000
6        2.622721000     -3.570525000     -0.312178000
6        3.826587000     -4.235919000     -0.448139000
```

```
6        5.008793000     -3.493679000     -0.460179000
6        4.977941000     -2.117191000     -0.328230000
5        1.235095000     -1.409077000     -0.090377000
7        1.255492000      0.033324000     -0.067569000
5        0.002034000      0.748868000     -0.165936000
7       -1.255294000      0.054428000     -0.318243000
7       -0.044249000     -2.044232000     -0.022734000
5       -1.298982000     -1.370072000     -0.034247000
1        5.842071000      0.261675000      0.098994000
1        5.821329000      2.688944000      0.345003000
1        3.688927000      3.895289000      0.434048000
1       -2.190082000      4.811986000      0.579455000
1        2.039143000      4.764263000      1.078951000
1       -0.100754000      5.916743000      1.206628000
1        1.702304000     -4.145696000     -0.327305000
1        3.854619000     -5.313506000     -0.555204000
1        5.961919000     -3.995704000     -0.579917000
1        5.918668000     -1.586010000     -0.360145000
1       -3.639973000      3.992583000     -0.580956000
1       -5.596351000      2.868385000     -1.527633000
1       -5.477514000      0.430574000     -2.044864000
1       -3.451686000     -0.831454000     -1.516978000
1       -0.067521000     -3.035310000      0.171193000
6       -2.585262000     -2.183023000      0.363302000
6       -2.792759000     -3.483798000     -0.109632000
6       -3.512652000     -1.660572000      1.274685000
6       -3.893685000     -4.233397000      0.296214000
6       -4.602065000     -2.410278000      1.699972000
6       -4.798352000     -3.697707000      1.205851000
1       -2.095684000     -3.915471000     -0.822691000
1       -3.381094000     -0.650780000      1.651115000
1       -4.043341000     -5.233202000     -0.094557000
1       -5.302706000     -1.990423000      2.412267000
1      -5.653328000     -4.279771000      1.529472000
```

7.2 Calculations in thf solution

Compound **A** - $(BN)_2$ dibenzoperylene (C_1), S_0

```
45
scf done: -1158.73325543

6       -3.588456000     -2.795389000     -0.115398000
6       -2.922500000     -1.559510000     -0.059776000
6       -3.662792000     -0.363251000      0.036631000
6       -5.064579000     -0.462308000      0.071028000
6       -5.715245000     -1.681122000      0.015933000
6       -4.967002000     -2.858566000     -0.077703000
7       -1.536895000     -1.542541000     -0.097272000
5       -0.763418000     -0.356140000     -0.063965000
6       -1.547956000      0.952313000      0.012756000
6       -0.837795000      2.164446000      0.040430000
6       -1.550121000      3.358158000      0.193644000
6       -2.937267000      3.334850000      0.281455000
6       -3.643837000      2.143653000      0.221845000
6       -2.959036000      0.928944000      0.091424000
6        0.638037000      2.131237000     -0.082737000
6        1.327968000      3.337958000     -0.222557000
6        2.706691000      3.388510000     -0.315572000
6        3.424690000      2.211628000     -0.233954000
6        2.795211000      0.970360000     -0.094300000
6        1.373058000      0.911854000     -0.075871000
6        3.627848000     -0.244716000      0.026009000
6        3.013079000     -1.505073000     -0.001946000
6        3.799120000     -2.663590000      0.105690000
6        5.172920000     -2.591848000      0.243723000
6        5.781459000     -1.335413000      0.291036000
6        5.024974000     -0.181683000      0.188386000
7        0.703999000     -0.336576000     -0.068178000
5        1.475517000     -1.559438000     -0.105195000
1        4.501568000      2.262265000     -0.302228000
1        3.214799000      4.335449000     -0.446596000
```

```
1        0.776495000      4.264984000     -0.281834000
8        0.803962000     -2.753809000     -0.215368000
1       -4.722613000      2.176403000      0.290664000
1       -1.052367000      4.314854000      0.262673000
1       -3.475798000      4.267850000      0.401817000
1        3.337762000     -3.646754000      0.093132000
1        5.767513000     -3.493278000      0.327202000
1        6.855023000     -1.258407000      0.417899000
1        5.539376000      0.766395000      0.255424000
1       -5.663073000      0.436442000      0.139665000
1       -6.797008000     -1.719774000      0.043912000
1       -5.463404000     -3.820680000     -0.122040000
1       -2.998149000     -3.702550000     -0.189222000
1       -1.090970000     -2.447961000     -0.149489000
1        1.378103000     -3.521709000     -0.255152000
```

H_2O (C_{2v}), S_0

```
3
scf done: -76.4274369894

8        0.000000000      0.000000000      0.117430000
1        0.000000000      0.760525000     -0.469718000
1        0.000000000     -0.760525000     -0.469718000
```

Compound **4** (C_1), S_0

```
42
scf done: -1082.15382441

6       -2.444431000     -2.870788000      0.217995000
6       -2.084606000     -1.536002000      0.406305000
6       -2.984915000     -0.488501000      0.013946000
6       -4.227772000     -0.876314000     -0.502172000
6       -4.579146000     -2.207806000     -0.668980000
6       -3.675560000     -3.209673000     -0.322268000
7       -0.867005000     -1.217140000      1.040941000
5       -0.627202000      0.179017000      1.224820000
6       -1.361267000      1.289346000      0.578003000
6       -0.640651000      2.474079000      0.330884000
6       -1.358711000      3.500251000     -0.287947000
6       -2.673184000      3.256135000     -0.705660000
6       -3.283732000      2.003712000     -0.618283000
6       -2.599489000      0.959389000      0.020982000
6        0.860068000      2.397415000      0.424515000
6        1.686091000      3.359846000     -0.164431000
6        2.998031000      3.057005000     -0.521348000
6        3.470909000      1.749150000     -0.429798000
6        2.694773000      0.758804000      0.177615000
6        1.478528000      1.160503000      0.757399000
6        2.945712000     -0.708392000      0.023141000
6        1.875628000     -1.654219000      0.134424000
6        2.093958000     -2.988102000     -0.218175000
6        3.343558000     -3.424879000     -0.641604000
6        4.395280000     -2.515378000     -0.705094000
6        4.197997000     -1.176787000     -0.382840000
7        0.774765000      0.192961000      1.463685000
5        0.609715000     -1.129540000      0.844406000
1        4.418593000      1.500527000     -0.891939000
1        3.615456000      3.817895000     -0.982303000
1        1.284534000      4.333187000     -0.421391000
1       -4.252850000      1.863682000     -1.080557000
1       -0.909593000      4.460615000     -0.511025000
1       -3.213811000      4.059248000     -1.193865000
1        1.276807000     -3.696701000     -0.133581000
1        3.502194000     -4.463967000     -0.902882000
1        5.379775000     -2.848205000     -1.012889000
1        5.036177000     -0.493790000     -0.450492000
1       -4.938668000     -0.111246000     -0.789924000
1       -5.550999000     -2.462432000     -1.073311000
1       -3.935601000     -4.252675000     -0.457730000
1       -1.741320000     -3.637042000      0.523720000
```

Benzaldehyde (C_s), S_0

```
14
scf done: -345.521814275

6        1.327734000     -1.325082000      0.000035000
6       -0.041126000     -1.103602000      0.000004000
6        2.208943000     -0.241875000      0.000054000
1       -0.743702000     -1.928833000     -0.000011000
1        3.278067000     -0.418838000      0.000079000
6       -0.530078000      0.205798000     -0.000008000
6        1.724269000      1.062705000      0.000043000
1        2.412371000      1.899011000      0.000058000
6        0.351396000      1.286516000      0.000011000
1       -0.040019000      2.298783000      0.000002000
1        1.714883000     -2.336729000      0.000045000
6       -1.986892000      0.466661000     -0.000043000
8       -2.834493000     -0.394412000     -0.000087000
1       -2.271119000      1.535175000     -0.000056000
```

Compound **B** with benzaldehyde (C_1), S_0

```
59
scf done: -1504.24080983

6       -2.549287000     -1.242652000     -1.020096000
6       -3.264987000     -0.038204000     -0.893871000
6       -4.658962000     -0.126719000     -1.010370000
6       -5.305708000     -1.332250000     -1.236832000
6       -4.570118000     -2.504716000     -1.377807000
6       -3.188540000     -2.451890000     -1.270618000
6       -2.596141000      1.275943000     -0.687337000
6       -1.190286000      1.321665000     -0.731404000
6       -0.454599000      2.504798000     -0.551425000
6       -1.183704000      3.691125000     -0.345733000
6       -2.566943000      3.653062000     -0.303063000
6       -3.283974000      2.461404000     -0.462726000
6        1.018631000      2.437470000     -0.526429000
6        1.782401000      3.611076000     -0.445134000
6        3.158164000      3.560378000     -0.355018000
6        3.804877000      2.328047000     -0.295825000
6        3.109629000      1.124069000     -0.367698000
6        1.700108000      1.185786000     -0.552257000
6        3.811317000     -0.184984000     -0.202282000
6        3.103668000     -1.397528000     -0.291511000
6        3.784080000     -2.600633000     -0.070850000
6        5.140395000     -2.634477000      0.220799000
6        5.841497000     -1.432661000      0.300876000
6        5.184798000     -0.228206000      0.097988000
5        1.566110000     -1.419392000     -0.692823000
8        1.271146000     -2.010523000     -2.012099000
7        0.981507000      0.014133000     -0.738714000
5       -0.393551000      0.061130000     -0.851470000
7       -1.097882000     -1.290936000     -0.869632000
8        0.765562000     -2.186304000      0.355113000
1        4.880566000      2.327985000     -0.189797000
1        3.735818000      4.475290000     -0.310433000
1        1.293962000      4.576129000     -0.462115000
1       -4.363254000      2.494661000     -0.395910000
1       -0.688480000      4.640298000     -0.191182000
1       -3.113610000      4.572153000     -0.126764000
1        3.229084000     -3.533633000     -0.125198000
1        5.647415000     -3.577901000      0.388001000
1        6.900856000     -1.431647000      0.530484000
1        5.765335000      0.679746000      0.189692000
1       -5.256092000      0.771856000     -0.934293000
1       -6.385409000     -1.353016000     -1.318393000
1       -5.062904000     -3.448640000     -1.572680000
1       -2.598731000     -3.355657000     -1.380890000
1       -0.665309000     -1.851052000     -1.622905000
6       -0.580995000     -2.036322000      0.451676000
```

1	-1.104451000	-2.996431000	0.415352000
1	1.698556000	-2.865913000	-2.104191000
6	-1.041017000	-1.223545000	1.645982000
6	-2.356811000	-1.327882000	2.099062000
6	-0.160518000	-0.345709000	2.277892000
6	-2.800337000	-0.530509000	3.149491000
6	-0.605080000	0.450364000	3.327968000
6	-1.926932000	0.366407000	3.758144000
1	-3.038191000	-2.031683000	1.631353000
1	0.869702000	-0.295046000	1.944647000
1	-3.824072000	-0.613661000	3.494282000
1	0.081720000	1.134445000	3.812023000
1	-2.272102000	0.989021000	4.575139000

Transition state with benzaldehyde (C_1), S_0

59
scf done: -1504.22286991

6	-2.390439000	-0.892724000	-1.292048000
6	-3.064694000	0.315474000	-1.030219000
6	-4.457533000	0.304701000	-1.181367000
6	-5.148503000	-0.829546000	-1.578248000
6	-4.456836000	-2.003470000	-1.862111000
6	-3.079215000	-2.027448000	-1.717077000
6	-2.330153000	1.555739000	-0.667299000
6	-0.921121000	1.525285000	-0.667865000
6	-0.136331000	2.639950000	-0.330972000
6	-0.809790000	3.834302000	-0.015494000
6	-2.193370000	3.871625000	-0.021563000
6	-2.962562000	2.747324000	-0.334193000
6	1.326708000	2.484520000	-0.248248000
6	2.139217000	3.598590000	0.007015000
6	3.495653000	3.462750000	0.208734000
6	4.071695000	2.196065000	0.183512000
6	3.332621000	1.052813000	-0.100321000
6	1.941447000	1.203269000	-0.363362000
6	3.971703000	-0.293040000	-0.063619000
6	3.185872000	-1.455024000	-0.133155000
6	3.800409000	-2.705413000	-0.002293000
6	5.169460000	-2.830115000	0.179584000
6	5.952887000	-1.678375000	0.203910000
6	5.362808000	-0.430614000	0.081384000
5	1.648187000	-1.383740000	-0.501765000
8	1.273240000	-2.232741000	-1.636715000
7	1.184193000	0.091547000	-0.714109000
5	-0.189439000	0.231357000	-0.898939000
7	-0.983400000	-1.018391000	-1.080676000
8	0.721951000	-1.815838000	0.652274000
1	5.125625000	2.113578000	0.408561000
1	4.108266000	4.332415000	0.411426000
1	1.699600000	4.585798000	0.053116000
1	-4.040703000	2.830556000	-0.297360000
1	-0.270518000	4.728584000	0.265941000
1	-2.696733000	4.795545000	0.239667000
1	3.179907000	-3.595591000	-0.050123000
1	5.626948000	-3.806813000	0.287139000
1	7.028413000	-1.751998000	0.317146000
1	6.009316000	0.436542000	0.091625000
1	-5.017696000	1.212052000	-0.999065000
1	-6.225792000	-0.792332000	-1.683829000
1	-4.984174000	-2.889181000	-2.194152000
1	-2.518590000	-2.932550000	-1.929772000
1	-0.523274000	-1.643195000	-1.751609000
6	-0.547022000	-2.024561000	0.423161000
1	-0.820708000	-2.976965000	-0.042279000
1	2.014893000	-2.371605000	-2.226710000
6	-1.489026000	-1.523027000	1.458875000
6	-2.740499000	-2.113618000	1.625544000
6	-1.141114000	-0.396206000	2.205302000
6	-3.649245000	-1.573165000	2.528176000
6	-2.053210000	0.145829000	3.100832000
6	-3.307441000	-0.439616000	3.259306000
1	-3.004782000	-2.991208000	1.045486000
1	-0.158344000	0.042717000	2.070949000

```
1       -4.621486000     -2.032959000      2.657732000
1       -1.787761000      1.025541000      3.674546000
1       -4.017469000     -0.014110000      3.958817000
```

Transition state with p-hydroxy benzaldehyde (C_1), S_0

```
60
scf done: -1579.46671915

6       -2.168000000     -0.811866000     -1.595287000
6       -2.846604000      0.392265000     -1.325309000
6       -4.232531000      0.398980000     -1.536034000
6       -4.911550000     -0.716922000     -2.001504000
6       -4.213653000     -1.885556000     -2.295079000
6       -2.843803000     -1.926554000     -2.089344000
6       -2.120548000      1.615003000     -0.892983000
6       -0.714255000      1.566114000     -0.803825000
6        0.058312000      2.667166000     -0.399623000
6       -0.617635000      3.865982000     -0.107763000
6       -1.998448000      3.920610000     -0.201737000
6       -2.758750000      2.810846000     -0.581645000
6        1.512958000      2.493670000     -0.230045000
6        2.318579000      3.596039000      0.090265000
6        3.661170000      3.445216000      0.368308000
6        4.224663000      2.172562000      0.364178000
6        3.489837000      1.039105000      0.027688000
6        2.120214000      1.206547000     -0.328346000
6        4.109436000     -0.315206000      0.101274000
6        3.321892000     -1.466245000     -0.069114000
6        3.911405000     -2.726906000      0.086313000
6        5.255878000     -2.872999000      0.395636000
6        6.043312000     -1.730201000      0.529656000
6        5.479012000     -0.472405000      0.382238000
5        1.817561000     -1.373011000     -0.563716000
8        1.536615000     -2.184265000     -1.749533000
7        1.378400000      0.111619000     -0.757133000
5        0.016327000      0.268669000     -1.027822000
7       -0.774509000     -0.957723000     -1.316573000
8        0.814015000     -1.847752000      0.502389000
1        5.264079000      2.079796000      0.645802000
1        4.269283000      4.306640000      0.614965000
1        1.885880000      4.586706000      0.126781000
1       -3.835458000      2.909956000     -0.617703000
1       -0.088255000      4.750406000      0.219927000
1       -2.506907000      4.846904000      0.040043000
1        3.293036000     -3.609394000     -0.049797000
1        5.692441000     -3.857545000      0.518365000
1        7.101313000     -1.818356000      0.748649000
1        6.129843000      0.385166000      0.486269000
1       -4.797262000      1.301723000     -1.344963000
1       -5.983220000     -0.669164000     -2.150354000
1       -4.730949000     -2.756664000     -2.677475000
1       -2.283195000     -2.830714000     -2.304194000
1       -0.289569000     -1.565783000     -1.982706000
6       -0.442652000     -2.045978000      0.183549000
1       -0.681226000     -2.968293000     -0.352691000
1        2.285901000     -2.198689000     -2.347985000
6       -1.450069000     -1.598118000      1.168356000
6       -2.708370000     -2.201723000      1.224467000
6       -1.181329000     -0.494646000      1.980684000
6       -3.689698000     -1.710578000      2.070464000
6       -2.157265000      0.008539000      2.826390000
6       -3.415098000     -0.597292000      2.865136000
1       -2.922405000     -3.061503000      0.599093000
1       -0.202350000     -0.029262000      1.939203000
1       -4.668557000     -2.170173000      2.126313000
1       -1.950844000      0.868238000      3.454876000
8       -4.410955000     -0.146645000      3.668492000
1       -4.114113000      0.621073000      4.168638000
```

Transition state with p-nitro benzaldehyde (C_1), S_0

```
61
scf done: -1708.72869223

6       -1.635047000     -2.173729000     -1.102781000
6       -2.527007000     -1.140579000     -1.448493000
6       -3.852043000     -1.504704000     -1.723264000
6       -4.280315000     -2.820865000     -1.641416000
6       -3.382099000     -3.827537000     -1.290945000
6       -2.062218000     -3.500142000     -1.025609000
6       -2.071681000      0.268245000     -1.526687000
6       -0.687042000      0.534025000     -1.480586000
6       -0.175183000      1.840080000     -1.501709000
6       -1.090198000      2.904184000     -1.591589000
6       -2.451027000      2.646059000     -1.634109000
6       -2.953284000      1.342635000     -1.597363000
6        1.272607000      2.041511000     -1.310180000
6        1.833772000      3.311624000     -1.503595000
6        3.156036000      3.563021000     -1.200035000
6        3.940279000      2.547913000     -0.661440000
6        3.454891000      1.254993000     -0.481034000
6        2.111546000      0.979263000     -0.863401000
6        4.304236000      0.212313000      0.158812000
6        3.741057000     -1.014258000      0.547502000
6        4.533579000     -1.944638000      1.230828000
6        5.865578000     -1.691489000      1.525903000
6        6.433445000     -0.490858000      1.101782000
6        5.665264000      0.444704000      0.425637000
5        2.278814000     -1.420519000      0.096174000
8        2.193331000     -2.743982000     -0.507001000
7        1.616315000     -0.321770000     -0.775981000
5        0.280709000     -0.569671000     -1.123810000
7       -0.286404000     -1.887221000     -0.763646000
8        1.281019000     -1.480742000      1.314068000
1        4.951849000      2.790224000     -0.367203000
1        3.574950000      4.549903000     -1.352316000
1        1.222673000      4.113240000     -1.897101000
1       -4.026085000      1.196627000     -1.593652000
1       -0.759376000      3.934204000     -1.578185000
1       -3.145707000      3.477276000     -1.671377000
1        4.089152000     -2.890713000      1.525934000
1        6.461690000     -2.420660000      2.062339000
1        7.479455000     -0.283184000      1.295993000
1        6.148985000      1.356769000      0.102595000
1       -4.562461000     -0.744584000     -2.021562000
1       -5.312384000     -3.064248000     -1.861581000
1       -3.706362000     -4.859000000     -1.231928000
1       -1.346477000     -4.270112000     -0.756486000
1        0.357770000     -2.665970000     -0.929685000
6        0.047196000     -1.851045000      1.176912000
1       -0.193114000     -2.913697000      1.264674000
1        2.990763000     -2.962489000     -0.993286000
6       -0.999073000     -0.889796000      1.609515000
6       -2.321742000     -1.309410000      1.761125000
6       -0.667087000      0.464313000      1.721275000
6       -3.327646000     -0.374440000      1.964988000
6       -1.659260000      1.408414000      1.925553000
6       -2.972218000      0.964864000      2.019404000
1       -2.572288000     -2.361840000      1.688789000
1        0.367075000      0.769418000      1.610458000
1       -4.363538000     -0.668932000      2.058171000
1       -1.433768000      2.464089000      1.984895000
7       -4.043711000      1.970316000      2.165839000
8       -5.191677000      1.577118000      2.181748000
8       -3.719636000      3.136022000      2.249336000
```

Transition state with p-fluoro benzaldehyde (C_1), S_0

```
59
scf done: -1603.47981099

6       -2.174031000     -0.771321000     -1.593640000
6       -2.845350000      0.432252000     -1.302907000
6       -4.232933000      0.447751000     -1.502885000
6       -4.920229000     -0.658543000     -1.978919000
6       -4.229553000     -1.826003000     -2.294208000
```

6	-2.858620000	-1.876179000	-2.098609000
6	-2.109367000	1.645441000	-0.861549000
6	-0.702898000	1.586428000	-0.777675000
6	0.077252000	2.678625000	-0.364015000
6	-0.590205000	3.878156000	-0.056899000
6	-1.970903000	3.942774000	-0.146396000
6	-2.739056000	2.842117000	-0.535924000
6	1.531451000	2.495065000	-0.201128000
6	2.343687000	3.589910000	0.127902000
6	3.686170000	3.429562000	0.400929000
6	4.242763000	2.154237000	0.382709000
6	3.501024000	1.028127000	0.036694000
6	2.131406000	1.205912000	-0.314275000
6	4.114553000	-0.329372000	0.095625000
6	3.320685000	-1.474382000	-0.083866000
6	3.903176000	-2.739956000	0.057197000
6	5.247626000	-2.896320000	0.361477000
6	6.041472000	-1.759138000	0.504791000
6	5.483902000	-0.496783000	0.371404000
5	1.816926000	-1.366036000	-0.572460000
8	1.518219000	-2.175661000	-1.752185000
7	1.382455000	0.118991000	-0.753874000
5	0.019657000	0.287507000	-1.021398000
7	-0.781222000	-0.926692000	-1.324885000
8	0.807643000	-1.832967000	0.505015000
1	5.282297000	2.052964000	0.660844000
1	4.299271000	4.285343000	0.654701000
1	1.916246000	4.582338000	0.175629000
1	-3.815175000	2.948540000	-0.567975000
1	-0.054399000	4.755328000	0.279518000
1	-2.472784000	4.869431000	0.107253000
1	3.279793000	-3.617858000	-0.085800000
1	5.679147000	-3.884347000	0.473276000
1	7.099494000	-1.855264000	0.720208000
1	6.139766000	0.356043000	0.482291000
1	-4.792163000	1.350187000	-1.294988000
1	-5.992681000	-0.603958000	-2.119524000
1	-4.753449000	-2.689131000	-2.685627000
1	-2.303509000	-2.779672000	-2.330246000
1	-0.303721000	-1.537496000	-1.993087000
6	-0.437042000	-2.047648000	0.177052000
1	-0.662219000	-2.958639000	-0.383085000
1	2.271454000	-2.222856000	-2.343847000
6	-1.462827000	-1.613718000	1.153285000
6	-2.710984000	-2.235778000	1.188251000
6	-1.207562000	-0.509466000	1.970303000
6	-3.710172000	-1.757869000	2.026830000
6	-2.197120000	-0.016984000	2.808379000
6	-3.428757000	-0.652513000	2.810703000
1	-2.906720000	-3.094775000	0.556770000
1	-0.232154000	-0.036799000	1.937019000
1	-4.687089000	-2.221001000	2.076129000
1	-2.031889000	0.840705000	3.447722000
9	-4.393702000	-0.176647000	3.618551000

p-hydroxy benzaldehyde (C_s), S_0

15
scf done: -420.751938717

6	0.936215000	-1.227679000	0.000018000
6	-0.435100000	-1.070101000	0.000009000
6	1.760841000	-0.095832000	0.000029000
1	-1.089521000	-1.933862000	0.000002000
6	-1.001178000	0.211327000	0.000012000
6	1.210117000	1.185995000	0.000031000
1	1.859138000	2.054527000	0.000040000
6	-0.169718000	1.331156000	0.000021000
1	-0.605202000	2.325131000	0.000023000
1	1.395418000	-2.208393000	0.000017000
6	-2.461714000	0.392630000	0.000009000
8	-3.267466000	-0.510963000	-0.000136000
1	-2.801523000	1.445133000	-0.000123000
8	3.096467000	-0.310816000	0.000038000
1	3.572892000	0.526725000	0.000047000

p-nitro benzaldehyde (C_s), S_0

```
16
scf done: -550.011721900

6       -0.284324000     -1.159377000     -0.000006000
6        1.096061000     -1.048504000      0.000023000
6       -1.034345000      0.010918000     -0.000024000
1        1.722864000     -1.931637000      0.000038000
6        1.692740000      0.213971000      0.000031000
6       -0.470781000      1.276969000     -0.000016000
1       -1.101154000      2.154934000     -0.000031000
6        0.915077000      1.370185000      0.000012000
1        1.391133000      2.344296000      0.000019000
1       -0.778285000     -2.120892000     -0.000013000
6        3.175917000      0.338340000      0.000062000
8        3.923666000     -0.606505000      0.000063000
1        3.563653000      1.372302000      0.000046000
7       -2.509634000     -0.100130000     -0.000054000
8       -2.991855000     -1.212262000     -0.000039000
8       -3.153418000      0.927130000     -0.000046000
```

p-fluoro benzaldehyde (C_s), S_0

```
14
scf done: -444.764217366

6       -0.954252000     -1.224726000     -0.000019000
6        0.421519000     -1.068743000     -0.000044000
6       -1.743101000     -0.082113000     -0.000015000
1        1.075614000     -1.932364000     -0.000050000
6        0.982764000      0.211905000     -0.000067000
6       -1.221529000      1.199755000     -0.000034000
1       -1.886730000      2.053330000     -0.000029000
6        0.160581000      1.338896000     -0.000058000
1        0.602624000      2.329510000     -0.000073000
1       -1.423559000     -2.200087000     -0.000003000
6        2.450441000      0.387408000     -0.000112000
8        3.244445000     -0.523628000      0.000241000
1        2.797712000      1.436687000      0.000243000
9       -3.077750000     -0.230261000      0.000009000
```

Compound **B** with p-hydroxy benzaldehyde (C_1), S_0

```
60
scf done: -1579.46965305

6       -2.385638000     -1.476226000     -1.137721000
6       -3.131201000     -0.284226000     -1.184083000
6       -4.515508000     -0.421285000     -1.355563000
6       -5.125496000     -1.661145000     -1.472501000
6       -4.360268000     -2.822713000     -1.442627000
6       -2.987113000     -2.722309000     -1.277037000
6       -2.499654000      1.061248000     -1.096906000
6       -1.094479000      1.137517000     -1.084173000
6       -0.392613000      2.351802000     -1.005857000
6       -1.154230000      3.534691000     -0.964685000
6       -2.537021000      3.466388000     -0.977743000
6       -3.221246000      2.246520000     -1.035514000
6        1.078895000      2.325183000     -0.909130000
6        1.815247000      3.518430000     -0.942262000
6        3.186277000      3.513548000     -0.786874000
6        3.852590000      2.314623000     -0.543969000
6        3.184264000      1.094333000     -0.494218000
6        1.784666000      1.097120000     -0.750664000
6        3.900271000     -0.165264000     -0.128260000
6        3.220655000     -1.396755000     -0.098445000
```

6	3.908752000	-2.543487000	0.314904000
6	5.246482000	-2.505015000	0.682032000
6	5.920650000	-1.285929000	0.641837000
6	5.255015000	-0.134583000	0.248723000
5	1.709282000	-1.508543000	-0.579172000
8	1.504789000	-2.258410000	-1.833084000
7	1.099530000	-0.106476000	-0.827444000
5	-0.268306000	-0.108471000	-1.016815000
7	-0.944163000	-1.470039000	-0.912690000
8	0.866514000	-2.169395000	0.506633000
1	4.921886000	2.353986000	-0.390945000
1	3.743787000	4.440735000	-0.834338000
1	1.309273000	4.461093000	-1.102750000
1	-4.302917000	2.259204000	-1.018961000
1	-0.685601000	4.507073000	-0.893448000
1	-3.109994000	4.384972000	-0.927035000
1	3.374699000	-3.489238000	0.354230000
1	5.759678000	-3.405725000	0.999000000
1	6.965026000	-1.228622000	0.926389000
1	5.812751000	0.792147000	0.253196000
1	-5.133858000	0.464330000	-1.411542000
1	-6.199142000	-1.718887000	-1.602241000
1	-4.823801000	-3.794999000	-1.550428000
1	-2.373433000	-3.616685000	-1.254638000
1	-0.462569000	-2.104853000	-1.570203000
6	-0.485781000	-2.040319000	0.518760000
1	-0.991190000	-3.009559000	0.566362000
1	1.947129000	-3.110327000	-1.794336000
6	-1.019025000	-1.102998000	1.578549000
6	-2.356462000	-1.167624000	1.975783000
6	-0.191292000	-0.135334000	2.145003000
6	-2.871002000	-0.260024000	2.889760000
6	-0.694308000	0.777593000	3.062296000
6	-2.039330000	0.722127000	3.425452000
1	-3.008041000	-1.933999000	1.567845000
1	0.855792000	-0.101518000	1.866869000
1	-3.907296000	-0.302059000	3.201545000
1	-0.044785000	1.529750000	3.497453000
8	-2.591597000	1.591070000	4.313285000
1	-1.930073000	2.222398000	4.615004000

Compound **B** with p-nitro benzaldehyde (C_1), S_0

```
61
scf done: -1708.73436038
```

6	1.864971000	2.335452000	-0.659772000
6	2.698037000	1.406820000	-1.308888000
6	4.022945000	1.807250000	-1.529497000
6	4.494207000	3.048006000	-1.127176000
6	3.641791000	3.952133000	-0.500943000
6	2.322743000	3.589759000	-0.272443000
6	2.209358000	0.079474000	-1.772233000
6	0.829520000	-0.188738000	-1.690750000
6	0.262023000	-1.411036000	-2.087723000
6	1.131169000	-2.381657000	-2.620970000
6	2.488204000	-2.122085000	-2.706669000
6	3.041854000	-0.908986000	-2.280127000
6	-1.177010000	-1.641281000	-1.861708000
6	-1.787594000	-2.816826000	-2.322955000
6	-3.111377000	-3.087444000	-2.044998000
6	-3.851294000	-2.203203000	-1.263820000
6	-3.312800000	-1.013369000	-0.781353000
6	-1.969368000	-0.705120000	-1.134263000
6	-4.102757000	-0.116618000	0.115223000
6	-3.534037000	1.055939000	0.644688000
6	-4.288170000	1.844309000	1.522283000
6	-5.582584000	1.503161000	1.885734000
6	-6.150194000	0.348296000	1.348984000
6	-5.421672000	-0.447036000	0.478146000
5	-2.088694000	1.554896000	0.213083000
8	-2.066313000	2.885273000	-0.425886000
7	-1.420406000	0.509241000	-0.743247000
5	-0.094505000	0.777960000	-1.019656000
7	0.476493000	2.018905000	-0.335327000
8	-1.159124000	1.693403000	1.395721000

1	-4.872255000	-2.470674000	-1.031398000
1	-3.571443000	-3.995510000	-2.414357000
1	-1.219910000	-3.527354000	-2.908605000
1	4.113738000	-0.777456000	-2.345424000
1	0.770161000	-3.349410000	-2.941866000
1	3.146585000	-2.887634000	-3.100302000
1	-3.838942000	2.749004000	1.920915000
1	-6.148046000	2.125021000	2.570302000
1	-7.163345000	0.064801000	1.610122000
1	-5.903376000	-1.333812000	0.089464000
1	4.702056000	1.138088000	-2.040486000
1	5.526472000	3.314744000	-1.317127000
1	3.995633000	4.929465000	-0.198811000
1	1.640066000	4.283140000	0.207593000
1	-0.149493000	2.810278000	-0.567076000
6	0.182843000	1.799115000	1.214530000
1	0.593172000	2.697801000	1.684485000
1	-2.712922000	2.944547000	-1.133336000
6	0.961163000	0.568507000	1.649607000
6	2.329003000	0.661960000	1.910706000
6	0.312209000	-0.662188000	1.746862000
6	3.063322000	-0.475302000	2.217012000
6	1.030780000	-1.808918000	2.053008000
6	2.396156000	-1.689962000	2.267791000
1	2.829498000	1.623100000	1.870575000
1	-0.756334000	-0.717168000	1.578665000
1	4.125175000	-0.427184000	2.413715000
1	0.550018000	-2.774844000	2.122021000
7	3.170959000	-2.906371000	2.579853000
8	4.368921000	-2.791285000	2.736426000
8	2.570208000	-3.957156000	2.659378000

Compound **B** with p-fluoro benzaldehyde (C_1), S_0

```
59
scf done: -1603.48397291
```

6	-2.331926000	-1.557601000	-1.085930000
6	-3.088068000	-0.378259000	-1.208579000
6	-4.465075000	-0.539216000	-1.414419000
6	-5.057926000	-1.790816000	-1.487949000
6	-4.282033000	-2.940523000	-1.377491000
6	-2.915027000	-2.816304000	-1.179373000
6	-2.472206000	0.975825000	-1.160542000
6	-1.067586000	1.068820000	-1.138735000
6	-0.382090000	2.293513000	-1.082677000
6	-1.158792000	3.467608000	-1.083240000
6	-2.540271000	3.382303000	-1.108268000
6	-3.208894000	2.152723000	-1.137055000
6	1.087049000	2.287849000	-0.953562000
6	1.805649000	3.491911000	-0.984375000
6	3.169583000	3.512512000	-0.778519000
6	3.846532000	2.328141000	-0.497917000
6	3.198877000	1.096090000	-0.462363000
6	1.805670000	1.072720000	-0.751263000
6	3.932231000	-0.150495000	-0.087240000
6	3.261123000	-1.384032000	-0.003505000
6	3.972434000	-2.521357000	0.398621000
6	5.320978000	-2.467729000	0.718744000
6	5.987482000	-1.246719000	0.623617000
6	5.303496000	-0.108224000	0.226468000
5	1.736844000	-1.540453000	-0.428017000
8	1.510106000	-2.489795000	-1.537023000
7	1.139392000	-0.143640000	-0.812190000
5	-0.226907000	-0.163454000	-1.015260000
7	-0.896496000	-1.520874000	-0.826654000
8	0.884138000	-2.063975000	0.699080000
1	4.907091000	2.390143000	-0.299608000
1	3.712366000	4.448925000	-0.813815000
1	1.290728000	4.423895000	-1.175307000
1	-4.290794000	2.151002000	-1.125842000
1	-0.703449000	4.447441000	-1.032284000
1	-3.124615000	4.294832000	-1.087553000
1	3.444774000	-3.468872000	0.453868000
1	5.851896000	-3.359327000	1.032354000

```
1        7.043155000     -1.179876000      0.860656000
1        5.861985000      0.816124000      0.169843000
1       -5.089752000      0.335723000     -1.534024000
1       -6.126410000     -1.867892000     -1.646954000
1       -4.732282000     -3.922275000     -1.449753000
1       -2.292071000     -3.700545000     -1.096250000
1       -0.392192000     -2.198550000     -1.423868000
6       -0.472793000     -1.982169000      0.646357000
1       -0.947878000     -2.962863000      0.744241000
1        2.091626000     -2.304392000     -2.278286000
6       -1.071332000     -0.993360000      1.624847000
6       -2.411840000     -1.097404000      1.997267000
6       -0.296920000      0.055761000      2.120379000
6       -2.992215000     -0.142913000      2.824773000
6       -0.861126000      1.018149000      2.948248000
6       -2.201651000      0.900624000      3.271600000
1       -3.014362000     -1.925705000      1.639164000
1        0.752359000      0.115317000      1.856049000
1       -4.030692000     -0.201630000      3.124321000
1       -0.281229000      1.843744000      3.340742000
9       -2.757129000      1.833502000      4.069625000
```

pTSA (C_1), S_0

```
19
scf done: -895.303141303

6        0.122167000      0.000533000     -0.095948000
6       -0.551414000      1.215451000     -0.090677000
6       -0.553556000     -1.215152000     -0.057674000
1       -0.000941000      2.146998000     -0.138980000
1       -0.003261000     -2.147872000     -0.078107000
6       -1.939877000      1.205203000     -0.042537000
6       -1.939332000     -1.201633000     -0.008908000
1       -2.478955000      2.145589000     -0.047431000
1       -2.480400000     -2.140907000      0.013375000
6       -2.649983000      0.003557000      0.004697000
16       1.888128000     -0.003882000     -0.117491000
8        2.361612000     -1.233672000     -0.703405000
8        2.362181000      1.277984000     -0.593829000
8        2.289900000     -0.130735000      1.440253000
6       -4.152029000     -0.001538000      0.084687000
1       -4.472791000     -0.156382000      1.118371000
1       -4.568787000      0.945190000     -0.258654000
1       -4.572446000     -0.809217000     -0.515861000
1        2.242129000      0.731573000      1.881132000
```

pTSA anion (C_1), S_0

```
18
scf done: -894.861777275

6       -0.159317000      0.007497000     -0.045554000
6        0.528777000     -1.200881000     -0.028402000
6        0.534130000      1.210921000     -0.028321000
1       -0.024509000     -2.132708000     -0.046471000
1       -0.016298000      2.143949000     -0.046287000
6        1.918414000     -1.198890000      0.001071000
6        1.925377000      1.200826000      0.000934000
1        2.455038000     -2.141999000      0.012797000
1        2.466849000      2.141156000      0.012917000
6        2.636697000     -0.000239000      0.015004000
16      -1.954616000      0.000289000      0.003389000
8       -2.371527000      1.303736000     -0.550983000
8       -2.365666000     -1.153025000     -0.822626000
8       -2.309288000     -0.160557000      1.430134000
6        4.143367000     -0.005219000      0.010892000
1        4.535227000     -0.884702000      0.523910000
1        4.523686000     -0.022230000     -1.014329000
1        4.541051000      0.886591000      0.497291000
```

Compound **D** with benzaldehyde (C_1), S_0

```
57
scf done: -1428.22462532

6       -2.591424000     -0.807840000     -1.312642000
6       -3.221799000      0.384781000     -0.928199000
6       -4.617251000      0.412114000     -1.058017000
6       -5.333019000     -0.667536000     -1.551554000
6       -4.670694000     -1.818689000     -1.965242000
6       -3.290919000     -1.881841000     -1.847702000
6       -2.470941000      1.582374000     -0.465461000
6       -1.062878000      1.540887000     -0.470371000
6       -0.263395000      2.623281000     -0.058347000
6       -0.920178000      3.791284000      0.356383000
6       -2.305011000      3.837087000      0.361946000
6       -3.088066000      2.750373000     -0.037774000
6        1.207157000      2.478039000     -0.054025000
6        2.032141000      3.582866000      0.185138000
6        3.407576000      3.449557000      0.239723000
6        3.994412000      2.204519000      0.061305000
6        3.229491000      1.066295000     -0.199265000
6        1.825529000      1.221766000     -0.266177000
6        3.868028000     -0.262643000     -0.375208000
6        3.075730000     -1.427214000     -0.453008000
6        3.675197000     -2.690616000     -0.553906000
6        5.052108000     -2.816287000     -0.601088000
6        5.839456000     -1.663779000     -0.551745000
6        5.262394000     -0.408391000     -0.439201000
5        1.564124000     -1.247216000     -0.480648000
7        1.023792000      0.094798000     -0.544106000
5       -0.353372000      0.264450000     -0.755675000
7       -1.129999000     -0.986731000     -1.184216000
8        0.677195000     -2.306409000     -0.444308000
1        5.069977000      2.128856000      0.136112000
1        4.028429000      4.315744000      0.429447000
1        1.596285000      4.562051000      0.327500000
1       -4.163928000      2.846892000      0.007340000
1       -0.372041000      4.657407000      0.700372000
1       -2.799490000      4.740719000      0.697941000
1        3.043623000     -3.570852000     -0.603407000
1        5.516009000     -3.791390000     -0.682805000
1        6.918798000     -1.746525000     -0.601843000
1        5.916151000      0.452224000     -0.411392000
1       -5.160096000      1.305012000     -0.781285000
1       -6.410595000     -0.600786000     -1.632391000
1       -5.217359000     -2.656385000     -2.378019000
1       -2.759696000     -2.769425000     -2.174009000
1       -0.784820000     -1.277738000     -2.108058000
6       -0.686115000     -2.134506000     -0.231988000
1       -1.199379000     -3.025067000     -0.588098000
6       -1.079037000     -1.817882000      1.194915000
6       -2.412020000     -1.997630000      1.574744000
6       -0.151643000     -1.365563000      2.133457000
6       -2.818280000     -1.687945000      2.866895000
6       -0.561314000     -1.062062000      3.427385000
6       -1.894741000     -1.212078000      3.792591000
1       -3.133952000     -2.391095000      0.868039000
1        0.898059000     -1.266538000      1.884390000
1       -3.853270000     -1.830245000      3.151731000
1        0.166817000     -0.715595000      4.150103000
1       -2.210375000     -0.974962000      4.801275000
```

Compound **D** with 4-hydroxy benzaldehyde (C_1), S_0

```
58
scf done: -1503.45378808

6       -2.440338000     -0.626374000     -1.671675000
6       -3.078437000      0.540342000     -1.223890000
6       -4.465975000      0.595512000     -1.415086000
```

```
6       -5.167273000     -0.431318000     -2.027536000
6       -4.496144000     -1.553419000     -2.501972000
6       -3.124365000     -1.644775000     -2.323833000
6       -2.340516000      1.688670000     -0.632545000
6       -0.935192000      1.624643000     -0.562487000
6       -0.146459000      2.660616000     -0.028719000
6       -0.810825000      3.804987000      0.436242000
6       -2.193040000      3.873862000      0.367347000
6       -2.965893000      2.833310000     -0.155921000
6        1.320034000      2.492072000      0.042464000
6        2.144166000      3.563167000      0.405494000
6        3.513215000      3.404646000      0.521150000
6        4.093816000      2.166936000      0.281883000
6        3.330306000      1.062782000     -0.101035000
6        1.933838000      1.245110000     -0.230030000
6        3.961408000     -0.259680000     -0.342196000
6        3.160662000     -1.401152000     -0.556279000
6        3.749336000     -2.662468000     -0.724563000
6        5.125023000     -2.807360000     -0.704471000
6        5.922337000     -1.676087000     -0.517170000
6        5.355273000     -0.424009000     -0.337050000
5        1.654718000     -1.195692000     -0.650200000
7        1.134831000      0.155401000     -0.634747000
5       -0.226926000      0.362079000     -0.906488000
7       -0.990802000     -0.837122000     -1.478525000
8        0.755993000     -2.241047000     -0.744326000
1        5.163256000      2.070012000      0.404434000
1        4.133424000      4.244980000      0.805643000
1        1.713421000      4.536490000      0.596147000
1       -4.040943000      2.946979000     -0.167501000
1       -0.272146000      4.633622000      0.874471000
1       -2.694197000      4.758740000      0.741197000
1        3.110682000     -3.525091000     -0.880008000
1        5.580645000     -3.780550000     -0.838823000
1        7.001654000     -1.773020000     -0.511493000
1        6.017298000      0.419746000     -0.200717000
1       -5.013884000      1.468664000     -1.089784000
1       -6.239325000     -0.345065000     -2.151866000
1       -5.029945000     -2.348201000     -3.006325000
1       -2.589160000     -2.512616000     -2.693392000
1       -0.593076000     -1.059045000     -2.400219000
6       -0.615699000     -2.066087000     -0.592588000
1       -1.119140000     -2.915113000     -1.050221000
6       -1.079058000     -1.852937000      0.827323000
6       -2.436353000     -2.014650000      1.129582000
6       -0.199970000     -1.502155000      1.850927000
6       -2.910850000     -1.782923000      2.408566000
6       -0.664596000     -1.275594000      3.139051000
6       -2.025119000     -1.398472000      3.415952000
1       -3.133331000     -2.333581000      0.362879000
1        0.865956000     -1.422608000      1.673884000
1       -3.959887000     -1.905174000      2.646431000
1        0.031162000     -1.011020000      3.927400000
8       -2.544202000     -1.178344000      4.645411000
1       -1.853836000     -0.916070000      5.263916000
```

Compound **D** with 4-nitro benzaldehyde (C_1), S_0

```
59
scf done: -1632.71284199

6        2.034779000     -0.814190000     -2.145537000
6        2.677943000     -1.622023000     -1.195721000
6        4.020632000     -1.927909000     -1.457773000
6        4.672064000     -1.474333000     -2.594051000
6        3.990436000     -0.711722000     -3.536733000
6        2.662249000     -0.386472000     -3.308941000
6        1.983091000     -2.182958000     -0.006254000
6        0.602403000     -1.946287000      0.143930000
6       -0.146439000     -2.440474000      1.228578000
6        0.531613000     -3.212893000      2.183038000
6        1.889475000     -3.448010000      2.039561000
6        2.624400000     -2.941681000      0.963419000
6       -1.582671000     -2.108882000      1.329305000
6       -2.390226000     -2.722467000      2.293458000
```

```
6       -3.724736000     -2.385371000      2.427312000
6       -4.285801000     -1.419740000      1.603289000
6       -3.539746000     -0.782823000      0.610108000
6       -2.180982000     -1.150248000      0.475870000
6       -4.147494000      0.258777000     -0.256275000
6       -3.341498000      1.012231000     -1.135546000
6       -3.898854000      2.040483000     -1.909247000
6       -5.251700000      2.320268000     -1.840188000
6       -6.057890000      1.559758000     -0.990230000
6       -5.519853000      0.548191000     -0.209905000
5       -1.873192000      0.630179000     -1.239763000
7       -1.402050000     -0.539946000     -0.530596000
5       -0.098709000     -1.003792000     -0.767262000
7        0.631171000     -0.380624000     -1.966949000
8       -0.952820000      1.363268000     -1.969523000
1       -5.324890000     -1.161327000      1.750406000
1       -4.332275000     -2.869542000      3.181044000
1       -1.974386000     -3.477605000      2.945985000
1        3.684563000     -3.148892000      0.921010000
1        0.025879000     -3.612888000      3.050864000
1        2.403271000     -4.034337000      2.791927000
1       -3.255561000      2.610278000     -2.570752000
1       -5.684010000      3.111760000     -2.439578000
1       -7.121490000      1.759859000     -0.935575000
1       -6.188309000     -0.013642000      0.427356000
1        4.569271000     -2.550322000     -0.764941000
1        5.710754000     -1.734875000     -2.753196000
1        4.481580000     -0.376204000     -4.440661000
1        2.117750000      0.200492000     -4.040729000
1        0.124442000     -0.652741000     -2.819438000
6        0.415492000      1.151961000     -1.879109000
1        0.883548000      1.573086000     -2.766849000
6        1.064048000      1.697174000     -0.619508000
6        2.453947000      1.843351000     -0.594998000
6        0.307220000      2.054354000      0.496045000
6        3.091836000      2.293949000      0.551191000
6        0.932028000      2.510873000      1.648897000
6        2.313058000      2.605582000      1.653677000
1        3.047997000      1.618165000     -1.472201000
1       -0.773973000      2.005874000      0.484509000
1        4.165820000      2.409873000      0.589399000
1        0.361437000      2.789427000      2.523728000
7        2.985528000      3.078573000      2.883444000
8        4.194002000      3.166758000      2.864483000
8        2.289144000      3.345571000      3.838233000
```

Compound **D** with 4-fluoro benzaldehyde (C_1), S_0

```
57
scf done: -1527.46578150

6       -2.443305000     -0.587012000     -1.672565000
6       -3.075662000      0.576637000     -1.208917000
6       -4.462544000      0.641912000     -1.402021000
6       -5.168173000     -0.372448000     -2.030037000
6       -4.502271000     -1.491200000     -2.519530000
6       -3.131229000     -1.592158000     -2.340880000
6       -2.332836000      1.712827000     -0.600678000
6       -0.927413000      1.643435000     -0.536039000
6       -0.134056000      2.668256000      0.012512000
6       -0.793724000      3.806468000      0.498724000
6       -2.175921000      3.880055000      0.436054000
6       -2.953449000      2.850567000     -0.102230000
6        1.331917000      2.494547000      0.076929000
6        2.160528000      3.558800000      0.449648000
6        3.529342000      3.394295000      0.559064000
6        4.105013000      2.157303000      0.304588000
6        3.336705000      1.059823000     -0.087839000
6        1.940849000      1.249017000     -0.211684000
6        3.962118000     -0.262546000     -0.343784000
6        3.156546000     -1.398096000     -0.571605000
6        3.739626000     -2.660070000     -0.754603000
6        5.114579000     -2.811151000     -0.735559000
6        5.916664000     -1.685716000     -0.533794000
6        5.355150000     -0.433308000     -0.339124000
```

```
5        1.652209000     -1.184932000     -0.662460000
7        1.136515000      0.167034000     -0.627845000
5       -0.223825000      0.383725000     -0.897664000
7       -0.993721000     -0.807070000     -1.482460000
8        0.748292000     -2.226039000     -0.767952000
1        5.174495000      2.055736000      0.422603000
1        4.153349000      4.229304000      0.850784000
1        1.733469000      4.531322000      0.652229000
1       -4.028276000      2.966720000     -0.106919000
1       -0.251167000      4.625678000      0.949696000
1       -2.673412000      4.759412000      0.827377000
1        3.097321000     -3.517999000     -0.920677000
1        5.566038000     -3.784621000     -0.881311000
1        6.995511000     -1.787587000     -0.528013000
1        6.020959000      0.405484000     -0.191294000
1       -5.006091000      1.513986000     -1.066629000
1       -6.239457000     -0.278486000     -2.155339000
1       -5.039254000     -2.275592000     -3.036588000
1       -2.599898000     -2.456755000     -2.723366000
1       -0.597606000     -1.017370000     -2.407941000
6       -0.622279000     -2.048338000     -0.620125000
1       -1.126451000     -2.890972000     -1.088827000
6       -1.090833000     -1.860529000      0.805696000
6       -2.447142000     -2.037943000      1.095025000
6       -0.208664000     -1.526314000      1.833471000
6       -2.927330000     -1.840540000      2.381731000
6       -0.674204000     -1.331475000      3.127321000
6       -2.027526000     -1.480738000      3.369768000
1       -3.138668000     -2.343906000      0.318691000
1        0.855683000     -1.436375000      1.655222000
1       -3.973531000     -1.973412000      2.624226000
1       -0.003905000     -1.076301000      3.937615000
9       -2.483308000     -1.288870000      4.616413000
```

protonated compound **A** (C_1), S_0

```
46
scf done: -1159.10105732

6        5.019979000     -0.491674000      0.053586000
6        3.621628000     -0.373309000     -0.011577000
6        2.886807000     -1.541735000     -0.292792000
6        3.539562000     -2.755332000     -0.530181000
6        4.918527000     -2.834578000     -0.473862000
6        5.664451000     -1.694807000     -0.169566000
6        2.938565000      0.925606000      0.151965000
6        1.533577000      0.974897000      0.055339000
6        0.822337000      2.186004000      0.120960000
6        1.536788000      3.361252000      0.358673000
6        2.921818000      3.314190000      0.487980000
6        3.626543000      2.123571000      0.373588000
6       -0.646523000      2.167970000     -0.079645000
6       -1.339694000      3.366789000     -0.249716000
6       -2.719032000      3.396771000     -0.381990000
6       -3.436807000      2.217424000     -0.332556000
6       -2.798750000      0.979034000     -0.190158000
6       -1.386441000      0.959860000     -0.094826000
6       -3.599257000     -0.259431000     -0.099740000
6       -4.984597000     -0.276163000     -0.334087000
6       -5.713608000     -1.442840000     -0.186854000
6       -5.095100000     -2.638780000      0.191709000
6       -3.731579000     -2.649162000      0.404635000
6       -2.975975000     -1.472162000      0.262367000
5       -1.473757000     -1.412891000      0.347014000
7       -0.705762000     -0.285790000      0.020207000
5        0.753850000     -0.307393000     -0.114757000
7        1.475493000     -1.520069000     -0.326988000
1       -4.514394000      2.266167000     -0.392825000
1       -3.232625000      4.341315000     -0.506985000
1       -0.795310000      4.300239000     -0.281667000
1        4.704223000      2.149309000      0.458727000
1        1.041342000      4.316974000      0.459298000
1        3.464623000      4.233148000      0.675446000
1       -3.252523000     -3.587845000      0.665007000
1       -5.677006000     -3.545010000      0.300360000
```

1	-6.780521000	-1.427154000	-0.374701000
1	-5.508392000	0.616584000	-0.644647000
1	5.619928000	0.380425000	0.275845000
1	6.744364000	-1.747007000	-0.113972000
1	5.411731000	-3.780730000	-0.659466000
1	2.948999000	-3.638245000	-0.751352000
1	1.084860000	-2.288387000	-0.862287000
8	-0.721434000	-2.604313000	0.781944000
1	0.248099000	-2.503346000	0.934215000
1	-1.143827000	-3.269852000	1.350134000

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