Supporting Information

Carboboration of isocyanates with tris(pentafluorophenyl)borane and evidence for dissociative FLP chemistry of an acid–base pair

Meera Mehta,* and Jose M. Goicoechea*

Department of Chemistry, University of Oxford, Chemistry Research Laboratory, 12 Mansfield Road, Oxford, OX1 3TA, U.K.

E-mail: meera.mehta@chem.ox.ac.uk; jose.goicoechea@chem.ox.ac.uk

Table of Contents

1. Methods and Materials

1.1. General Remarks

All reactions and product manipulations were carried out under an inert atmosphere of argon or dinitrogen using standard Schlenk-line or glovebox techniques (MBraun UNIlab glovebox maintained at < 0.1 ppm H_2O and < 0.1 ppm O_2). Hexane (hex; Sigma-Aldrich, HPLC grade) and toluene (Sigma-Aldrich; HPLC grade) were purified using an MBraun SPS-800 solvent system. All dry solvents were stored under argon in gas-tight ampoules. d_8-Toluene (Sigma-Aldrich, 99.5%) and C_6D_6 (Sigma-Aldrich, 99.5%) were degassed and stored over 3 Å molecular sieves. $B(C_6F_5)_3$, phenyl isocyanate, cyclohexyl isocyanate, allyl isocyanate, 4-bromophenyl isocyanate, 4-chlorophenyl isocyanate, 4-nitrophenyl isocyanate, 4-methoxyphenyl isocyanate, benzyl isocyanate, 2-(trifluoromethyl)phenyl isocyanate were purchased from either Sigma-Aldrich or Alfa Aesar and used without further purification Whereas, $Al(C_6F_5)_3$ and $Ga(C_6F_5)_3$ were prepared according to known procedures.[1,2]

Additional characterization techniques: ^{1}H, ^{13}C, ^{11}B, ^{19}F NMR spectra were acquired at 298 K with a Bruker Ascend 400 NMR spectrometer and with a Bruker AV III 500 MHz NMR spectrometer. ^{1}H and ^{13}C NMR spectra were referenced to the most downfield solvent resonance. ^{11}B and ^{19}F spectra were externally referenced to $BF_3{\cdot}Et_2O$ in C_6D_6 and $CFCl_3$ (δ = 0 ppm), respectively. Multiplicity is indicated using the following abbreviations: b = broad, s = singlet, d = doublet, t = triplet, and q = quartet. ^{13}C NMR resonances for C_6F_5 could not always be observed. Elemental analyses were carried out by Elemental Microanalyses Ltd. (Devon, U.K.). Samples (approx. 5 mg) were submitted in sealed Pyrex ampoules. In cases where elemental analysis data deviate significantly from expected values, the best obtainable analysis is presented.

1.2. X-ray Diffraction Studies

Single crystal X-ray structure determination: Single-crystal X-ray diffraction data were collected using an Oxford Diffraction Supernova dual-source diffractometer equipped with a 135 mm Atlas CCD area detector. Crystals were selected under Paratone-N oil, mounted on micromount loops and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device.[3] Data were collected at 150 K using mirror monochromated Cu Kα radiation (λ = 1.5418 Å; Oxford Diffraction Supernova). Data collected on the Oxford Diffraction

Supernova diffractometer were processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[4] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Structures were subsequently solved using direct methods and refined on F^2 using the ShelXL 2013 package and ShelXle.[5,6]

1.3. Kinetic Studies

A stock solution of **1a** was prepared by dissolving 0.2 g of **1a** (25 mg/ sample, 0.03 mmol) in 4 mL of d_8-toluene. The NMR instrument was pre-warmed to 353 K, pre-locked, pre-tuned, and pre-shimmed to a dummy sample. To an air tight J. Young NMR tube 0.5 mL of stock solution was added along with the appropriate equivalents of CyNCO using a micro-syringe. The sample was cooled to 4 °C before being quickly inserted into the NMR instrument. The sample was shimmed and monitored by $^{19}F\{^1H\}$ NMR spectroscopy.

1.4. Thermodynamic Studies

A stock solution of **1a** was prepared by dissolving 0.2 g of **1a** (25 mg/ sample, 0.03 mmol) in 4 mL of d_8-toluene. The NMR instrument was pre-warmed to the appropriate temperature. To an air tight J. Young NMR tube 0.5 mL of stock solution was added along with 4.3 μL of CyNCO (0.03 mmol, 1 eq) using a microsyringe. The sample was inserted into the NMR instrument and monitored by $^{19}F\{^1H\}$ NMR spectroscopy until equilibrium was reached.

1.5. Computational Studies

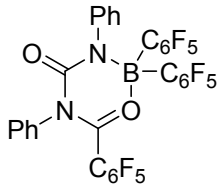
All calculations were performed with the Gaussian09 program package3 (version g09, rev.d01). The theoretical approach is based on the framework of density functional theory (DFT).[7,8] All calculations were performed with the PBE1PBE functional and employing 6-31G(d,p) basis set. Transition states and ground states were fully optimized without constraints at the corresponding level of theory and uniquely characterized by occurrence of one or none imaginary frequency respectively and verified by the corresponding frequency calculation. The imaginary frequencies for the transition state calculations can be found together with the *x*,*y*,*z* coordinates. Gibbs free reaction energies and enthalpies were calculated for standard conditions (p = 1 atm, T = 298 K) and are unscaled. Geometry optimizations were performed using the Gaussian 09, Revision D.01.[9,10]

1.6. General Procedure for Scrambled Products

A solution of **1b** (50 mg, 0.07 mmol) and isocyanate (0.7 mmol, 10 eq) in toluene (0.5 mL) was sealed in an air tight J. Young NMR tube and heated to 110 °C overnight. The solution was cooled to room temperature and solvent removed under reduced pressure. Crystals suitable for X-ray diffraction studies could be obtained by extracting the product in hexane.

2. Synthesis and Characterization Data

2.1. Compound 1a



In a Schlenk flask charged with a stir bar $B(C_6F_5)_3$ (1.0 g, 2.0 mmol) was dissolved in 30 mL of toluene. To this mixture PhNCO (1.0 g, 8.4 mmol, 4.2 eq) was added dropwise and stirred overnight. The solvent was removed under reduced pressure to give a pale yellow oil, which was further washed with hexane (3 × 20 mL) to yield a white precipitate. Crystals suitable for X-ray diffraction studies could be obtained from the hexane filtrate.

^{1}H NMR (500 MHz, C_6D_6): δ = 7.36 (d, $^3J_{H–H}$ = 7.5 Hz, 2H, *Ph*), 6.96 (m, 2H, *Ph*), 6.92 (m, 2H, *Ph*), 6.77 (m, 1H, *Ph*), 6.62 (m, 3H, *Ph*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.0 (d, $^3J_{F–F}$ = 22 Hz, 4F, *o*-C_6F_5), –139.1(d, $^3J_{F–F}$ = 20 Hz, 2F, *o*-C_6F_5), –142.8 (t, $^3J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –153.2 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –157.4 (m, 2F, *m*-C_6F_5), –162.5 (td, $^3J_{F–F}$ = 23, 9.4 Hz, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 4.0 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 166.7 (s, N*C*N), 148.5 (b*d*, $^1J_{C–F}$ = 245 Hz, *C*$_6$F$_5$), 147.7 (s, *Ph*), 142.3 (bd, $^1J_{C–F}$ = 258 Hz, *C*$_6$F$_5$), 141.2 (bd, $^1J_{C–F}$ = 247 Hz, *C*$_6$F$_5$), 139.7 (s, *Ph*), 137.5 (bd, $^1J_{C–F}$ = 250 Hz, *C*$_6$F$_5$), 133.6 (s, *Ph*), 130.9 (s, *Ph*), 129.4 (s, *Ph*), 128.9 (s, *Ph*), 127.1 (s, *Ph*), 126.4 (s, *Ph*), 105.6 (s, N*C*O) ppm.

Isolated Yield = 68%.

Elemental analysis for $C_{32}H_{10}BF_{15}N_2O_2$: calcd.: C 51.23, H 1.34, N 3.73; found: C 51.07, H 1.31, N 3.82.

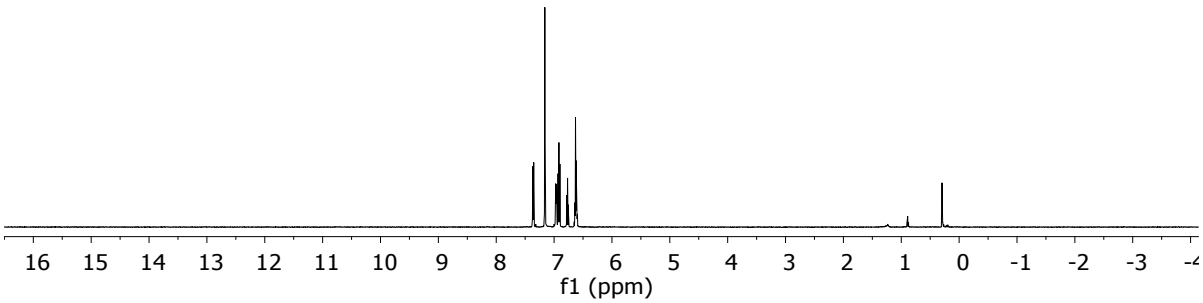


Figure S1. ^{1}H NMR spectrum (C_6D_6) of **1a**.

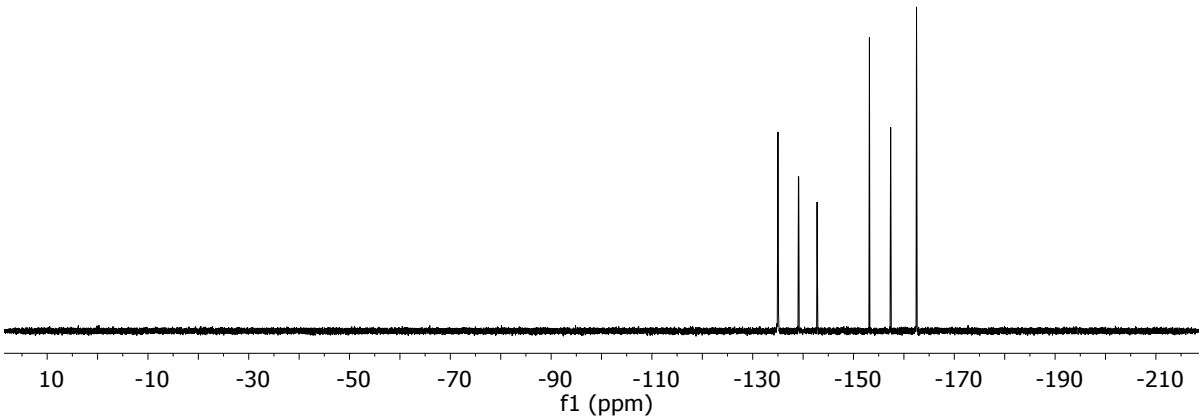


Figure S2. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **1a**.

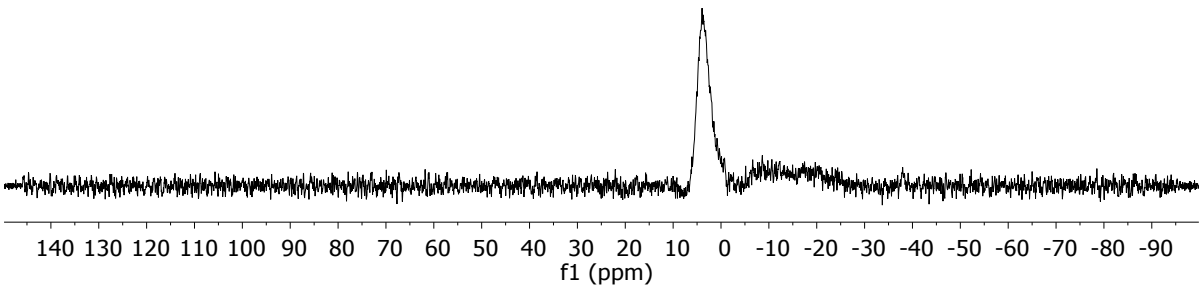


Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **1a**.

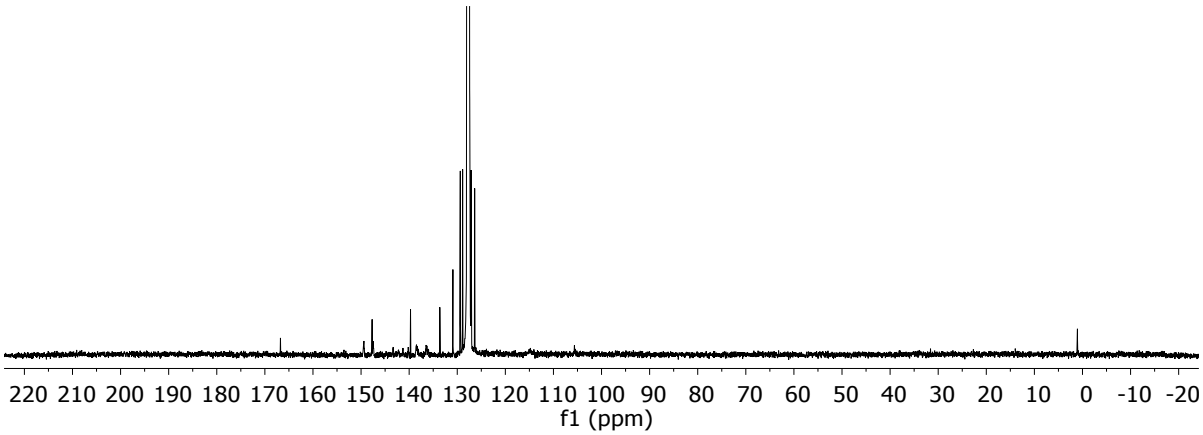


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **1a**.

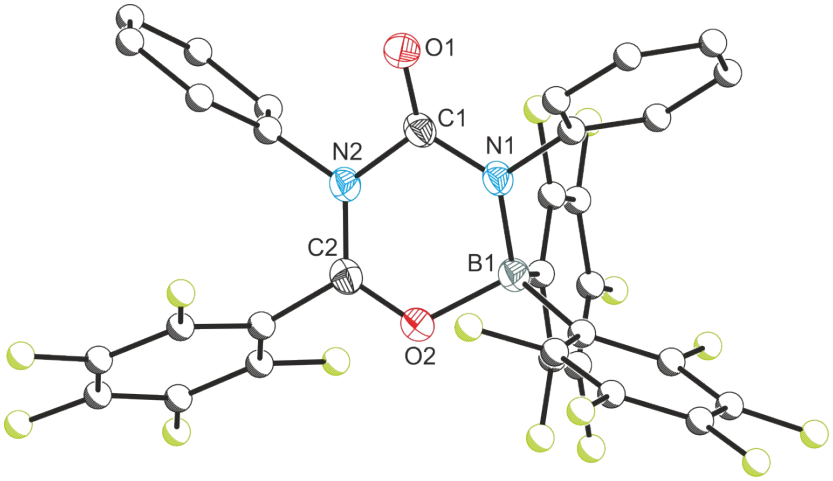
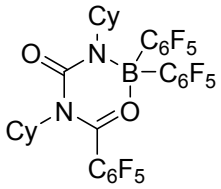


Figure S5. Single crystal X-ray structure of **1a**. Atoms of the Ph and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.2. Compound 1b



In a Schlenk flask charged with a stir bar $B(C_6F_5)_3$ (1.0 g, 2.0 mmol) was dissolved in 30 mL of toluene. To this mixture CyNCO (1.0 g, 8.0 mmol, 4 eq) was added dropwise and stirred overnight. Crystals suitable for X-ray diffraction studies grew from the solution overnight. The solvent was decanted and the product dried under reduced pressure to yield a white precipitate.

^{1}H NMR (500 MHz, C_6D_6): δ = 3.28 (m, 2H, *Cy*), 2.47 (qd, $^3J_{H–H}$ = 12.8, 3.8 Hz, 2H, *Cy*), 2.36 (bq, $^3J_{H–H}$ = 12.7 Hz, 2H, *Cy*), 1.84 (bd, $^3J_{H–H}$ = 12.0 Hz, 2H, *Cy*), 1.58 (m, 4H, *Cy*), 1.38 (m, 3H, *Cy*), 1.15 (d, $^3J_{H–H}$ = 10.0 Hz, 1H, *Cy*), 0.95 (m, 4H, *Cy*), 0.81 (qt, $^3J_{H–H}$ = 13.2, 3.5 Hz, 1H, *Cy*), 0.60 (dddd, $^3J_{H–H}$ = 17.2, 13.5, 8.4, 3.6 Hz, 2H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –134.0 (d, $^3J_{F–F}$ = 23 Hz, 4F, *o*-C_6F_5), –40.3 (m, 2F, *o*-C_6F_5), –143.6 (t, $^3J_{F–F}$ = 21 Hz, 1F, *p*-C_6F_5), –154.1 (t, $^3J_{F–F}$ = 20 Hz, 2F, *p*-C_6F_5), –156.7 (m, 2F, *m*-C_6F_5), –162.9 (m, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.7 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 164.5 (s, N*C*N), 148.6 (bd, $^1J_{C–F}$ = 239 Hz, C_6F_5), 146.2 (s, N*C*O), 137.4 (bd, $^3J_{C–F}$ = 251 Hz, C_6F_5), 66.0 (s, *Cy*), 59.7 (s, *Cy*), 30.6 (s, *Cy*), 29.2 (s, *Cy*), 26.4 (s, *Cy*), 25.7 (s, *Cy*), 25.4 (s, *Cy*), 24.3 (s, *Cy*) ppm.

Isolated Yield = 70%.

Elemental analysis for $C_{32}H_{22}BF_{15}N_2O_2$: calcd.: C 50.42, H 2.91, N 3.67; found: C 50.93, H 2.87, N 3.77.

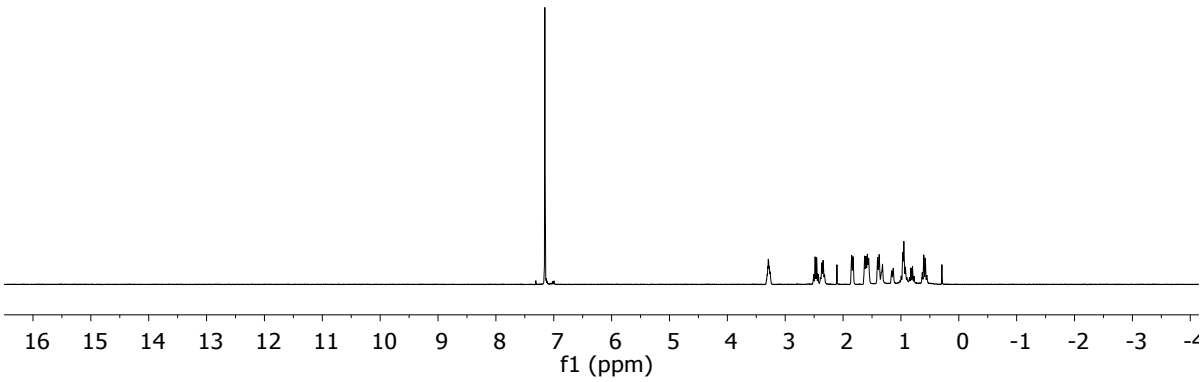


Figure S6. ^{1}H NMR spectrum (C_6D_6) of **1b**.

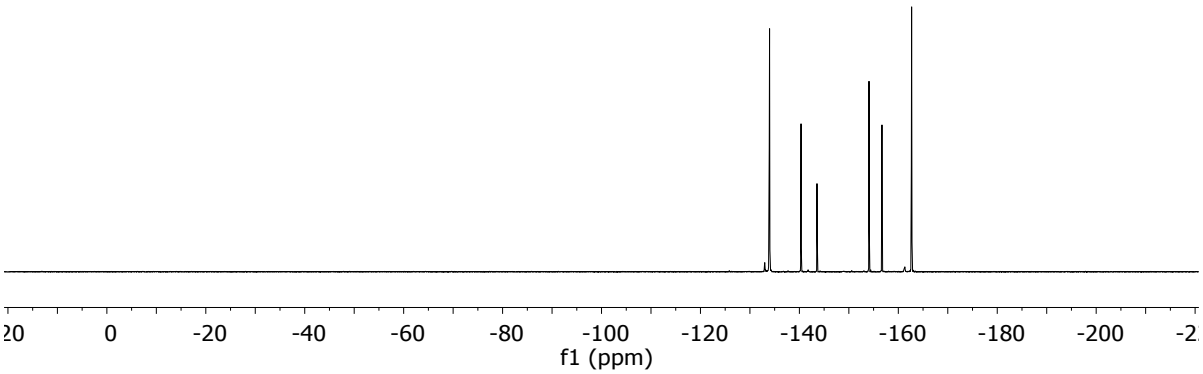


Figure S7. ^{19}F{^{1}H} NMR spectrum (C_6D_6) of **1b**.

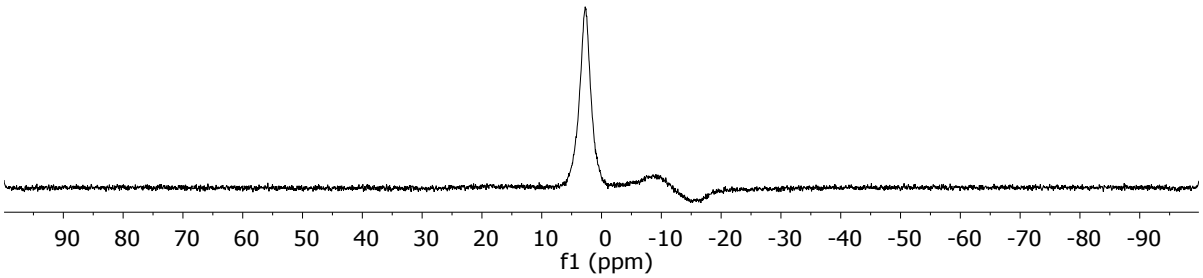


Figure S8. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **1b**.

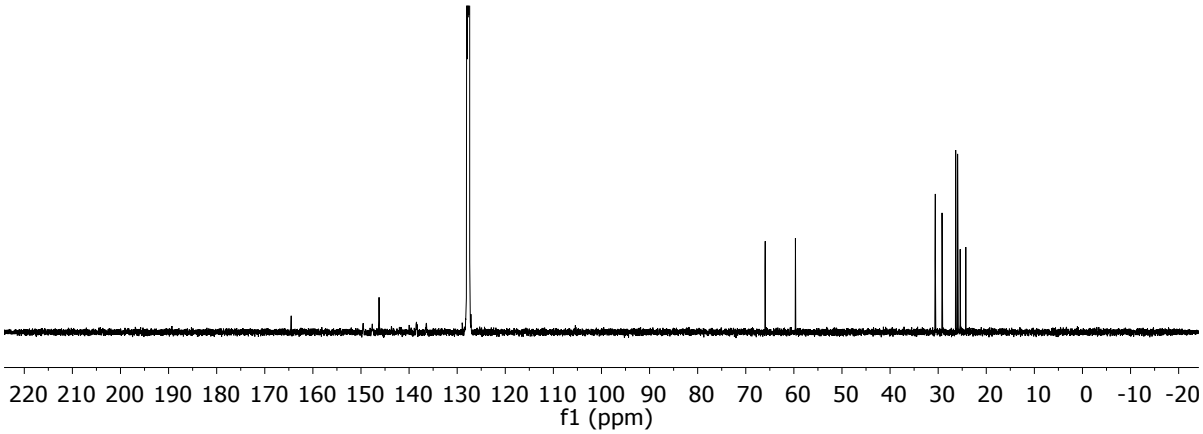


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **1b**.

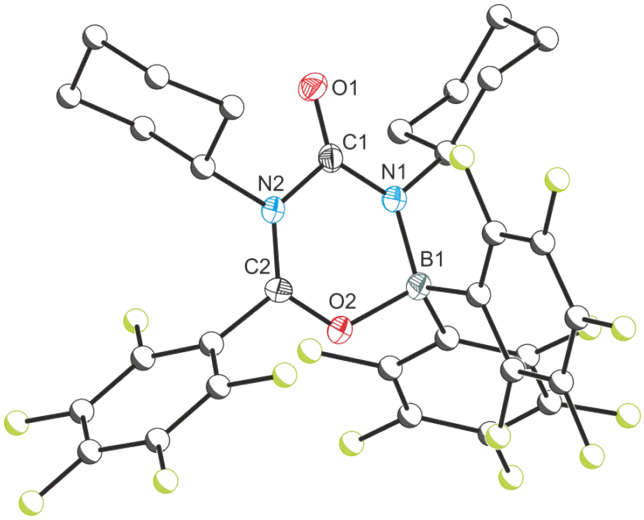
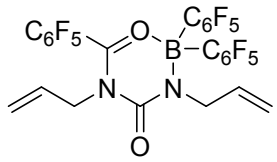


Figure S10. Single crystal X-ray structure of **1b**. Atoms of the Cy and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.3. Compound 1c



In a Schlenk flask charged with a stir bar $B(C_6F_5)_3$ (1.0 g, 2.0 mmol) was dissolved in 30 mL of toluene. To this mixture allyl isocyanate (1.0 g, 10 mmol, 5 eq) was added dropwise and stirred overnight. The solvent was removed under reduced pressure to give a pale-yellow oil, which was further washed with hexane (3 × 20 mL) to yield a white precipitate. Crystals suitable for X-ray diffraction studies could be obtained from the hexane filtrate.

^{1}H NMR (500 MHz, C_6D_6): δ = 5.59 (ddt, $^3J_{H–H}$ = 16.5, 10.4, 5.9 Hz, 1H, CH_2CHCH_2), 5.21 (ddt, $^3J_{H–H}$ = 17.2, 10.7, 5.5 Hz, 1H, CH_2CHCH_2), 4.64 (m, 3H, NCH_2CHCH_2), 4.45 (m, 1H, NCH_2CHCH_2), 3.34 (m, 4H, NCH_2CHCH_2); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –136.1 (dd, $^3J_{F–F}$ = 24, 9 Hz, 4F, *o*-C_6F_5), –139.3 (d, $^3J_{F–F}$ = 18 Hz, 2F, *o*-C_6F_5), –143.1 (m, 1F, *p*-C_6F_5), –154.0 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.5 (dd, $^3J_{F–F}$ = 22, 18 Hz, 2F, *m*-C_6F_5), –162.9 (m, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.9 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 165.3 (s, N*C*N), 148.51 (bd, $^1J_{C–F}$ = 246 Hz, C_6F_5), 143.8 (bd, $^1J_{C–F}$ = 275 Hz, C_6F_5), 142.7 (bd, $^1J_{C–F}$ = 256 Hz, C_6F_5), 141.1 (bd, $^1J_{C–F}$ = 253 Hz, C_6F_5), 137.4 (bd, $^1J_{C–F}$ = 249 Hz, C_6F_5), 132.0 (s, NCH_2CHCH_2), 129.5 (s, NCH_2CHCH_2), 118.8 (s, NCH_2CHCH_2), 116.3 (s, NCH_2CHCH_2), 48.8 (s, NCH_2CHCH_2), 48.5 (s, NCH_2CHCH_2) ppm.

Isolated Yield = 63%.

Elemental analysis for $C_{26}H_{10}BF_{15}N_2O_2$: calcd.: C 46.05, H 1.49, N 4.13; found: C 45.96, H 1.48, N 4.21.

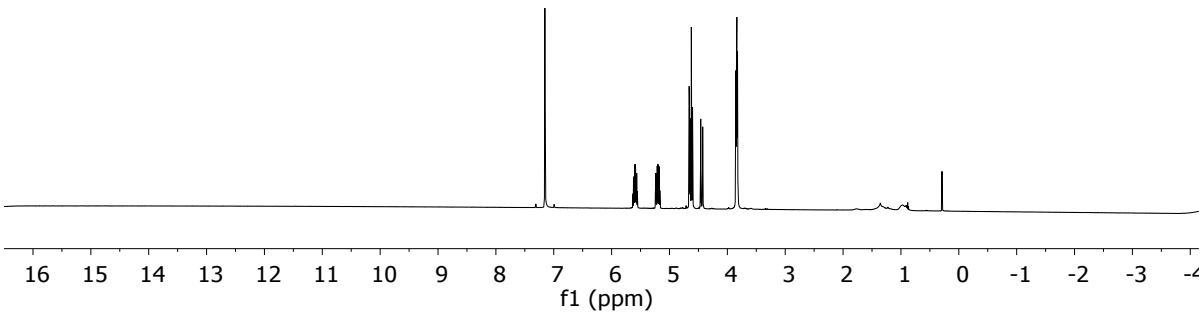


Figure S11. ^{1}H NMR spectrum (C_6D_6) of **1c**.

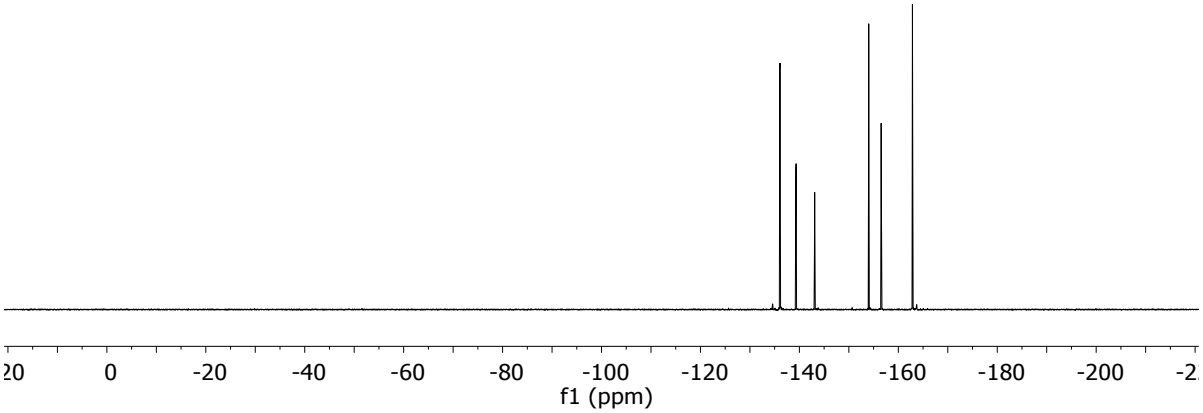


Figure S12. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **1c**.

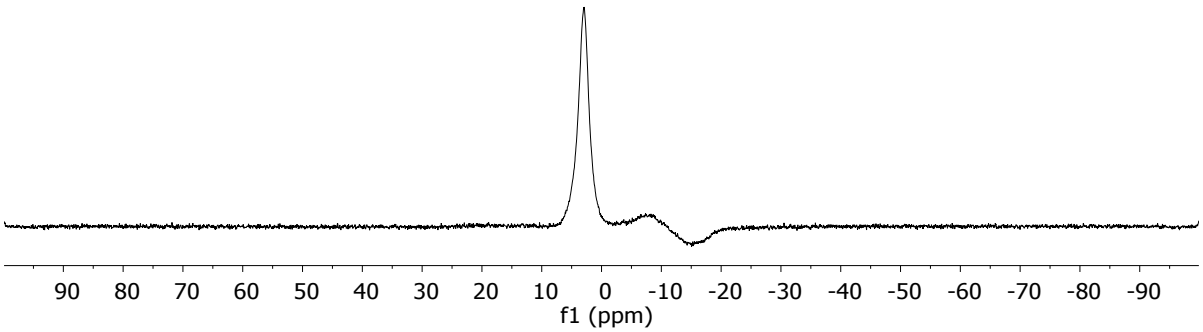


Figure S13. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **1c**.

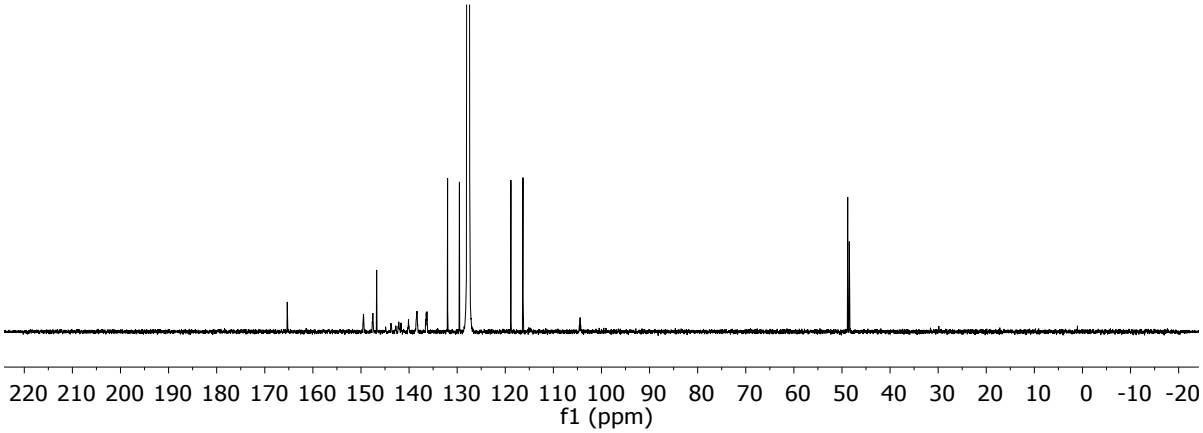


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **1c**.

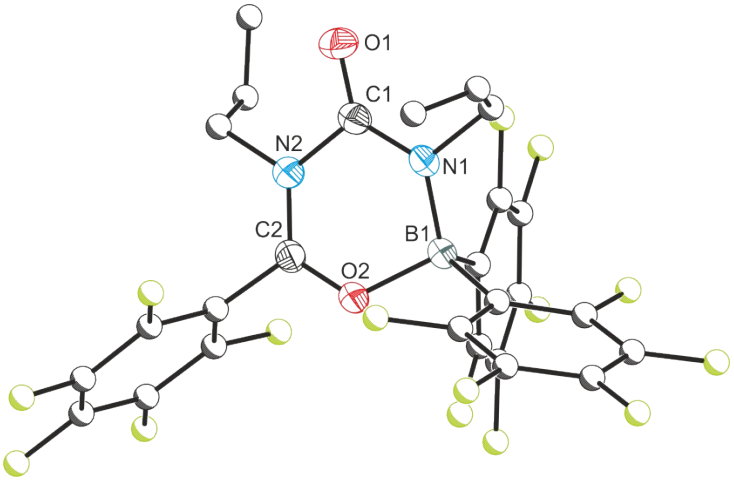
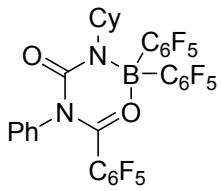


Figure S15. Single crystal X-ray structure of **1c**. Atoms of the allyl and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.4. Compound 2



^{1}H NMR (500 MHz, C_6D_6): δ = 7.30 (d, $^3J_{H–H}$ = 8.5 Hz, 2H, *Ph*), 6.91 (dd, $^3J_{H–H}$ = 8.5, 7.4 Hz, 2H, *Ph*), 6.76 (t, $^3J_{H–H}$ = 7.4 Hz, 1H, *Ph*), 3.33 (tt, $^3J_{H–H}$ = 12.1, 3.5 Hz, 1H, *Cy*), 2.45 (qd, $^3J_{H–H}$ = 12.7, 3.8 Hz, 1H, *Cy*), 1.63 (m, 1H, *Cy*), 1.34 (d, $^3J_{H–H}$ = 12.8 Hz, 1H, *Cy*), 1.23 (m, 2H, *Cy*), 1.09 (d, $^3J_{H–H}$ = 13.5 Hz, 1H, *Cy*), 0.88 (t, $^3J_{H–H}$ = 7.0 Hz, 2H, *Cy*), 0.71 (qt, $^3J_{H–H}$ = 13.1, 3.1 Hz, 1H, *Cy*), 0.56 (qt, $^3J_{H–H}$ = 13.3, 3.6 Hz, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.0 (d, $^3J_{F–F}$ = 23 Hz, 4F, *o*-C_6F_5), –140.3 (d, $^3J_{F–F}$ = 20 Hz, 2F, *o*-C_6F_5), –142.7 (m, 1F, *p*-C_6F_5), –153.5 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.2 (m, 2F, *m*-C_6F_5), –162.8 (m, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 3.4 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 165.9 (s, NCN), 148.3 (bd, $^1J_{C–F}$ = 244 Hz, C_6F_5), 147.8 (s, *Ph*), 142.9 (bd, $^1J_{C–F}$ = 222 Hz, C_6F_5), 140.9 (bd, $^1J_{C–F}$ = 213 Hz, C_6F_5), 139.9 (s, *Ph*), 137.5 (bd, $^1J_{C–F}$ = 256 Hz, C_6F_5), 128.7 (s, *Ph*), 127.2 (s, *Ph*), 126.4 (s, *Ph*), 66.4 (s, NCO), 31.6 (s, *Cy*), 30.5 (s, *Cy*), 25.9 (s, *Cy*), 24.1 (s, *Cy*), 22.7 (s, *Cy*), 14.0 (s, *Cy*) ppm.

Isolated Yield = 16%.

Elemental analysis for $C_{32}H_{16}BF_{15}N_2O_2$: calcd.: C 50.82, H 2.13, N 3.70; found: C 51.63, H 2.35, N 3.95.

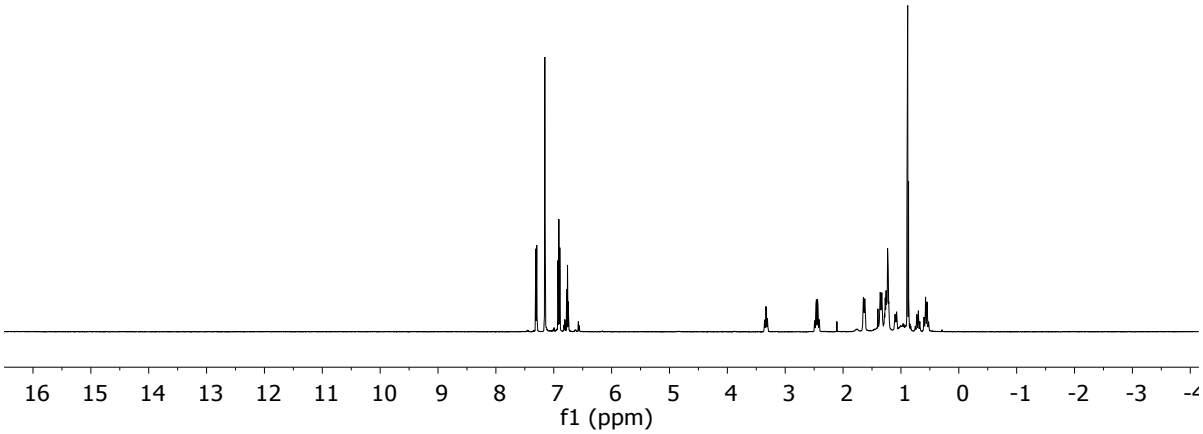


Figure S16. ^{1}H NMR spectrum (C_6D_6) of **2**.

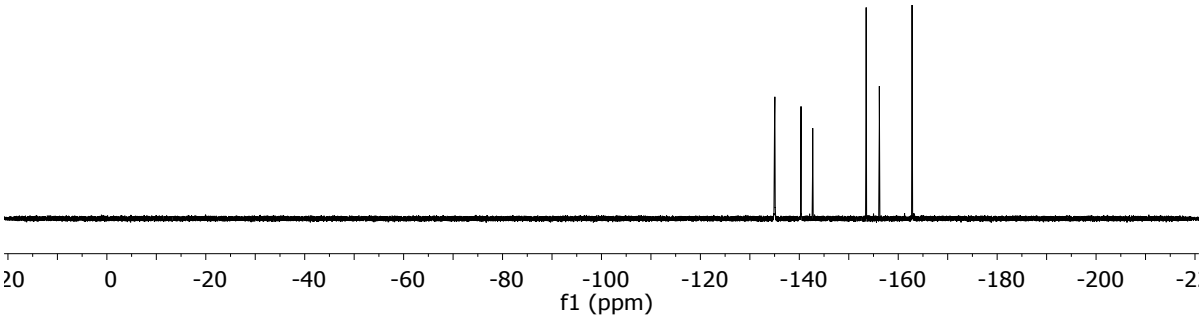


Figure S17. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **2**.

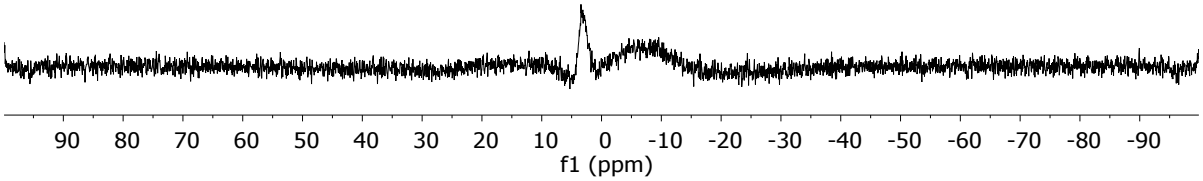


Figure S18. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **2**.

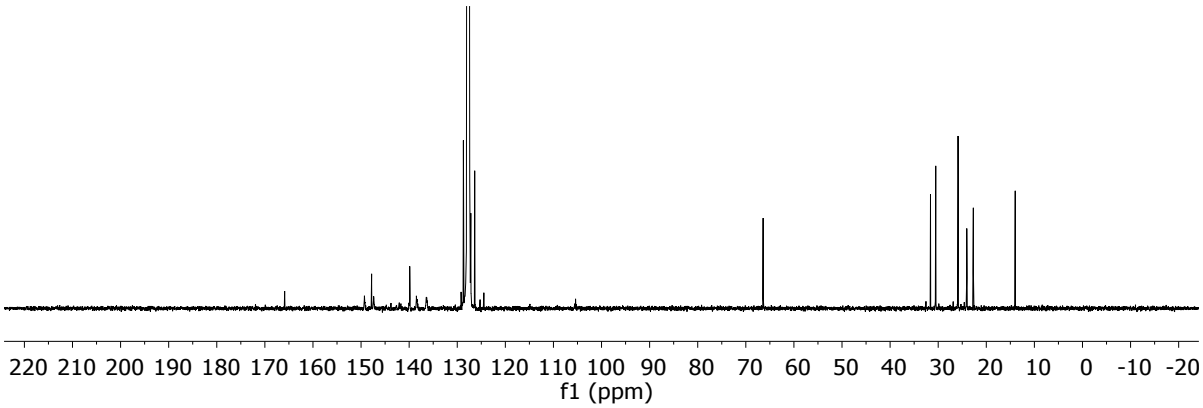


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **2**.

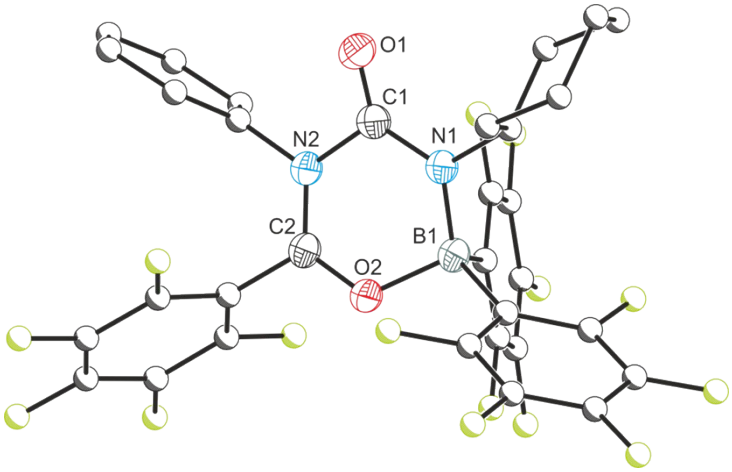
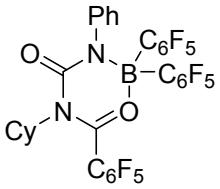


Figure S20. Single crystal X-ray structure of **2**. . Atoms of the Cy, Ph and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.5. Compound 3a



^{1}H NMR (500 MHz, C_6D_6): δ = 7.30 (d, $^{3}J_{H–H}$ = 7.9 Hz, 2H, *Ph*), 6.91 (t, $^{3}J_{H–H}$ = 7.9 Hz, 2H, *Ph*), 6.76 (t, $^{3}J_{H–H}$ = 7.4 Hz, 1H, *Ph*), 3.33 (tt, $^{3}J_{H–H}$ = 12.0, 3.7 Hz, 1H, *Cy*), 2.45 (qd, $^{3}J_{H–H}$ = 12.6, 3.8 Hz, 1H, *Cy*), 1.65 (m, 1H, *Cy*), 1.34 (d, $^{3}J_{H–H}$ = 13.3 Hz, 1H, *Cy*), 1.25 (m, 2H, *Cy*), 1.09 (d, $^{3}J_{H–H}$ = 13.3 Hz, 1H, *Cy*), 0.88 (t, $^{3}J_{H–H}$ = 7.0 Hz, 2H, *Cy*), 0.72 (m, 1H, *Cy*), 0.56 (qt, $^{3}J_{H–H}$ = 13.0, 3.3 Hz, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.0 (d, $^{3}J_{F–F}$ = 9 Hz,

4F, *o*-C_6F_5), –140.3 (d, $^3J_{F–F}$ = 19 Hz, 2F, *o*-C_6F_5), –142.7 (t, $^3J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –153.5 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.2 (m, 2F, *m*-C_6F_5), –162.8 (td, $^3J_{F–F}$ = 21, 9 Hz, 4F, *m*-C_6F_5); **$^{11}B\{^1H\}$ NMR (128 MHz, C_6D_6):** δ = 3.5 (s); **$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6):** δ = 165.9 (s, N*C*N), 148.3 (bd, $^1J_{C–F}$ = 254 Hz, C_6F_5), 147.8 (s, *Ph*), 142.79 (bd, $^1J_{C–F}$ = 258 Hz, C_6F_5), 139.9 (s, *Ph*), 137.4 (bd, $^1J_{CF}$ = 243 Hz, C_6F_5), 128.7 (s, *Ph*), 127.2 (s, *Ph*), 126.4 (s, *Ph*), 66.4 (s, N*C*O), 31.6 (s, *Cy*), 30.5 (s, *Cy*), 25.9 (s, *Cy*), 24.1 (s, *Cy*), 22.7 (s, *Cy*), 13.9 (s, *Cy*) ppm.

Isolated Yield = 76%.

Elemental analysis for $C_{32}H_{16}BF_{15}N_2O_2$: calcd.: C 50.82, H 2.13, N 3.70; found: C 51.30, H 2.15, N 3.84.

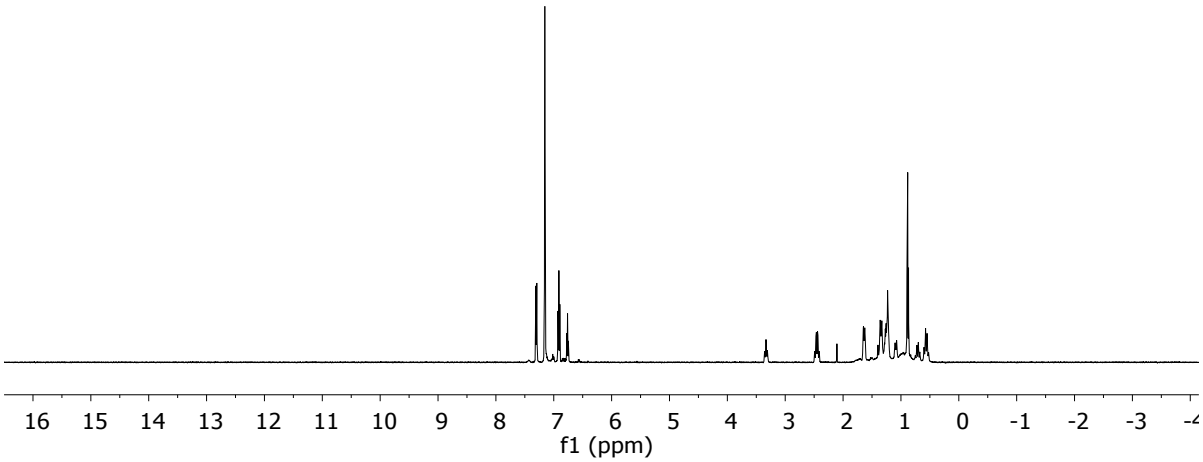


Figure S21. ^1H NMR spectrum (C_6D_6) of **3a**.

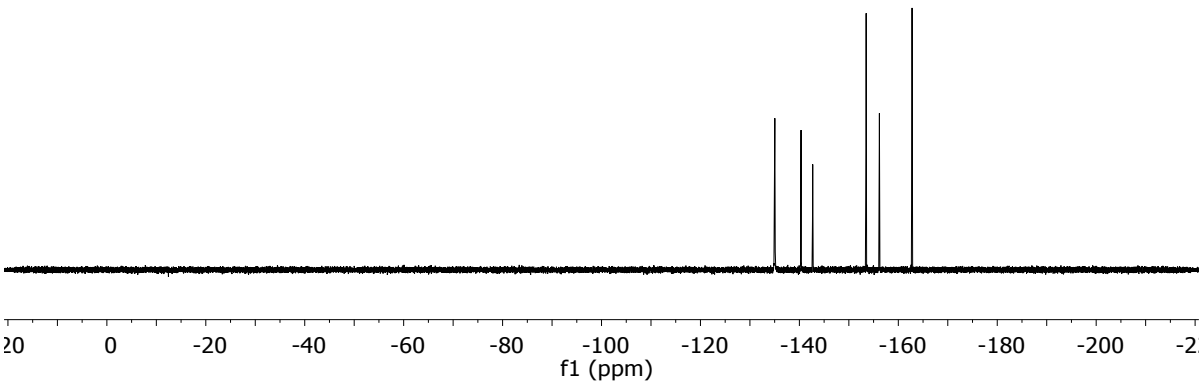


Figure S22. $^{19}F\{^1H\}$ NMR spectrum (C_6D_6) of **3a**.

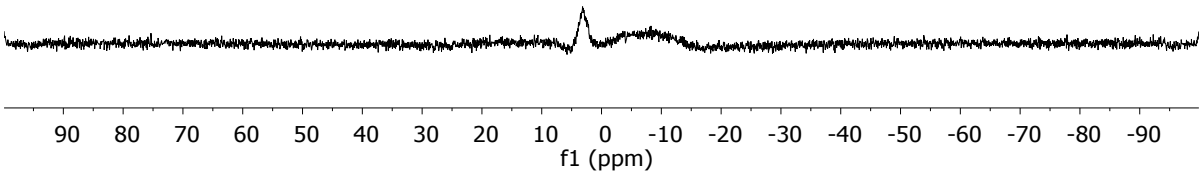


Figure S23. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3a**.

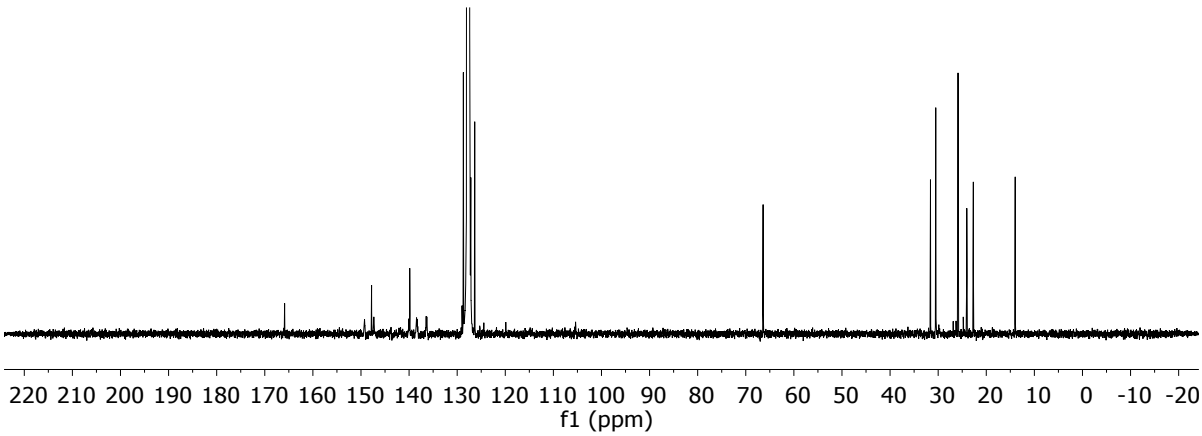


Figure S24. $^{11}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3a**.

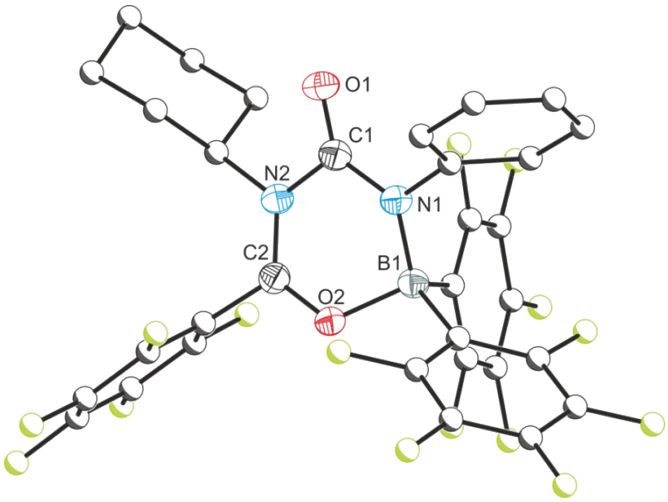
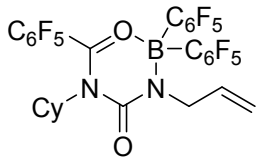


Figure S25. Single crystal X-ray structure of **3a**. . Atoms of the Cy, Ph and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.6. Compound 3b



^{1}H NMR (500 MHz, C_6D_6): δ = 5.63 (m, 1H, NCH_2CHCH_2), 4.69 (b, 1H, NCH_2CHCH_2), 4.66 (dd, $^3J_{H–H}$ = 8.6, 1.5 Hz, 1H, NCH_2CHCH_2), 3.85 (bd, $^3J_{H–H}$ = 5.9 Hz, 2H, NCH_2CHCH_2), 3.26 (tt, $^3J_{H–H}$ = 12.0, 3.7 Hz, 1H, *Cy*), 2.45 (qd, $^3J_{H–H}$ = 12.7, 3.8 Hz, 2H, *Cy*), 1.50 (m, 1H, *Cy*), 1.35 (dt, $^3J_{H–H}$ = 14.1, 3.3 Hz, 2H, *Cy*), 1.12 (dt, $^3J_{H–H}$ = 13.4, 3.4 Hz, 1H, *Cy*), 0.96 (m, 1H, *Cy*), 0.78 (qt, $^3J_{H–H}$ = 13.2, 3.6 Hz, 1H, *Cy*), 0.56 (qt, $^3J_{H–H}$ = 13.3, 3.6 Hz, 2H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –136.0 (dd, $^3J_{F–F}$ = 23.9, 9.4 Hz, 4F, *o*-C_6F_5), –140.2 (d, $^3J_{F–F}$ = 20 Hz, 2F, *o*-C_6F_5), –142.9 (t, $^3J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –154.0 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.4 (m, 2F, *m*-C_6F_5), –136.0 (m, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.4 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 165.0 (s, N*C*N), 148.5 (bd, $^1J_{C–F}$ = 239 Hz, C_6F_5), 143.7 (bd, $^1J_{C–F}$ = 270 Hz, C_6F_5), 142.7 (bd, $^1J_{C–F}$ = 260 Hz, C_6F_5), 141.1 (bd, $^1J_{C–F}$ = 247 Hz, C_6F_5), 137.5 (bd, $^1J_{C–F}$ = 256 Hz, C_6F_5), 132.2 (s, NCH_2CHCH_2), 116.6 (s, NCH_2CHCH_2), 66.3 (s, N*C*O), 48.2 (s, NCH_2CHCH_2), 30.4 (s, *Cy*), 25.9 (s, *Cy*), 24.1 (s, *Cy*) ppm.

Isolated Yield = 79%.

Elemental analysis for $C_{29}H_{16}BF_{15}N_2O_2$: calcd.: C 48.36, H 2.24, N 3.89; found: C 48.12, H 2.26, N 4.17.

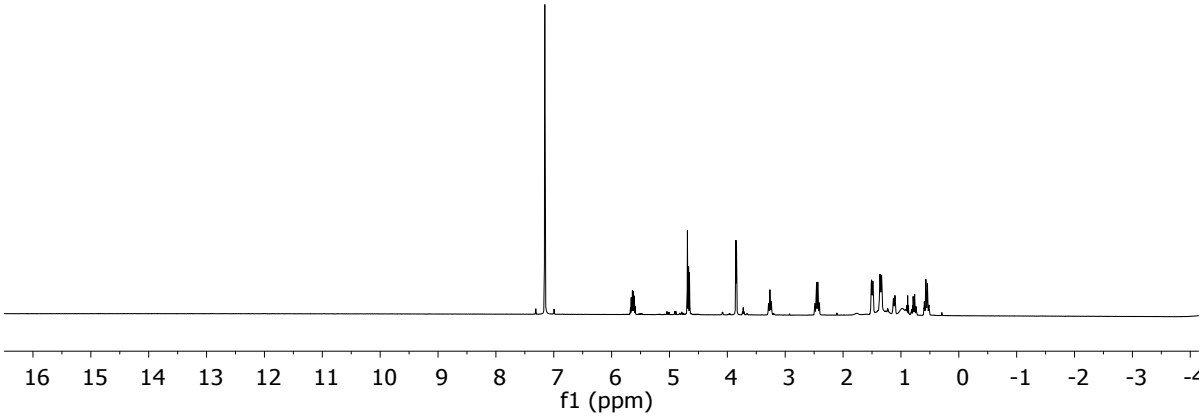


Figure S26. ^{1}H NMR spectrum (C_6D_6) of **3b**.

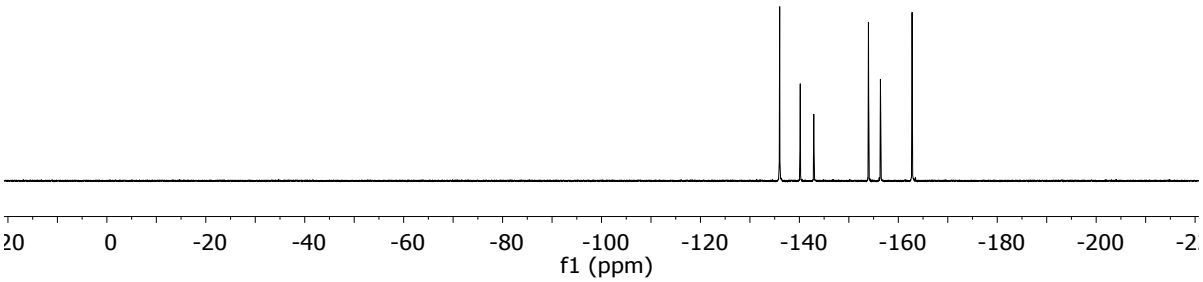


Figure S27. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **3b**.

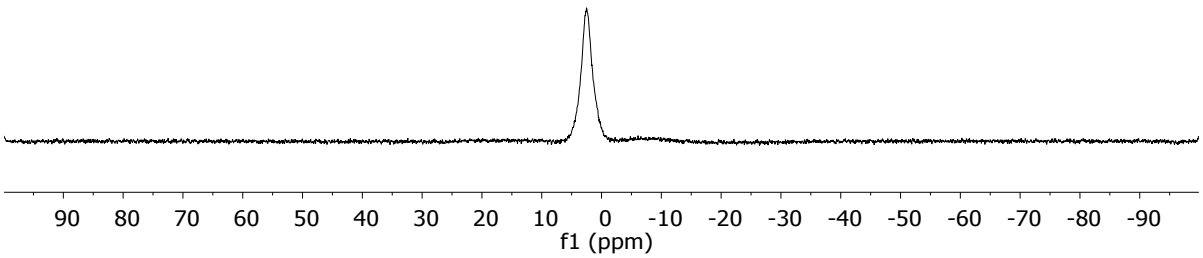


Figure S28. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3b**.

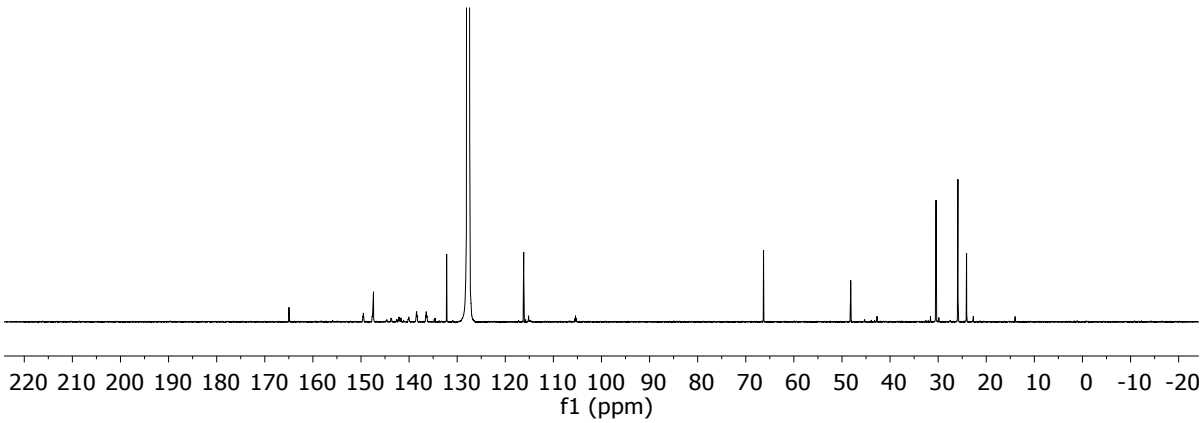


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3b**.

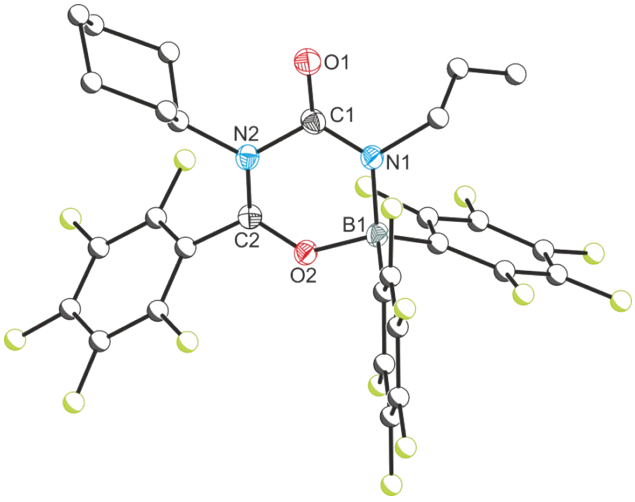
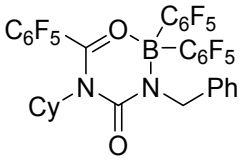


Figure S30. Single crystal X-ray structure of **3b**. Atoms of the Cy, allyl and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.7. Compound 3c



^{1}H NMR (500 MHz, C_6D_6): δ = 6.98 (d, $^3J_{H–H}$ = 7.2 Hz, 2H, *Ph*), 6.94 (t, $^3J_{H–H}$ = 7.6 Hz, 2H, *Ph*), 6.88 (m, 1H, *Ph*), 4.58 (s, 2H, C*H*$_2$Ph), 3.31 (tt, $^3J_{H–H}$ = 12.0, 3.7 Hz, 1H, *Cy*), 2.51 (qd, $^3J_{H–H}$ = 12.7, 3.8 Hz, 2H, *Cy*), 1.56 (m, 1H, *Cy*), 1.38 (dt, $^3J_{H–H}$ = 14.1, 3.3 Hz, 2H, *Cy*), 1.13 (dd, $^3J_{H–H}$ = 9.7, 6.3 Hz, 1H, *Cy*), 0.96 (m, 2H, *Cy*), 0.80 (qt, $^3J_{H–H}$ = 13.3, 3.6 Hz, 1H, *Cy*), 0.58 (qt, $^3J_{H–H}$ = 13.3, 3.6 Hz, 2H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –136.0 (m, 4F, *o*-C_6F_5), –140.2 (d, $^3J_{F–F}$ = 19 Hz, 2F, *o*-C_6F_5), –142.9 (t, $^3J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –154.4 (t, $^3J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.4 (m, 2F, *m*-C_6F_5), –163.1 (m, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.8 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 165.1 (s, N*C*N), 148.9 (s, *Ph*), 148.4 (bd, $^1J_{C–F}$ = 239 Hz, C_6F_5), 143.6 (bd, $^1J_{C–F}$ = 257 Hz, C_6F_5), 142.7 (bd, $^1J_{C–F}$ = 265 Hz, C_6F_5), 141.0 (bd, $^1J_{CF}$ = 248 Hz, C_6F_5), 137.4 (bd, $^1J_{C–F}$ = 248 Hz, C_6F_5), 137.3 (s, *Ph*), 127.1 (s, *Ph*), 126.7 (s, *Ph*), 66.5 (s, N*C*O), 48.8 (s, *C*H$_2$Ph), 30.5 (s, *Cy*), 25.9 (s, *Cy*), 24.1 (s, *Cy*) ppm.

Isolated Yield = 70%.

Elemental analysis for $C_{33}H_{18}BF_{15}N_2O_2$: calcd.: C 51.46, H 2.36, N 3.64; found: C 51.66, H 2.38, N 3.79.

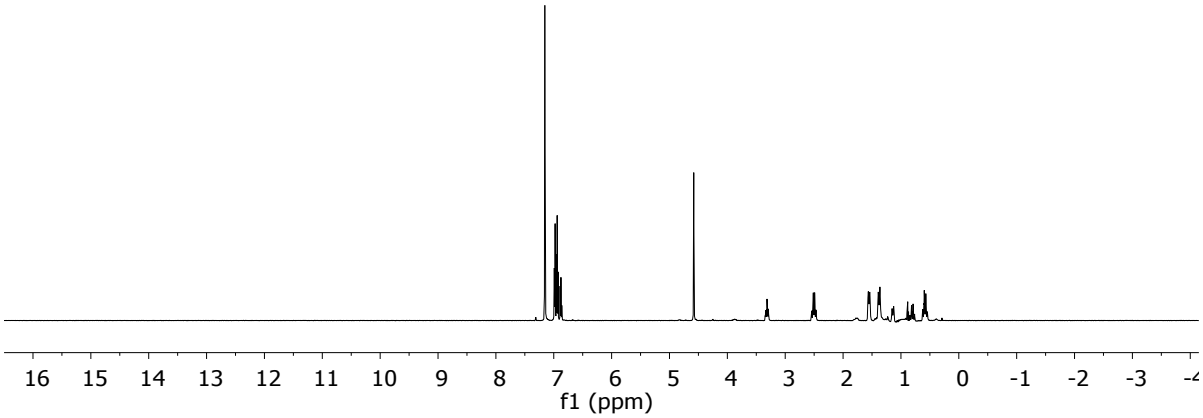


Figure S31. ^{1}H NMR spectrum (C_6D_6) of **3c**.

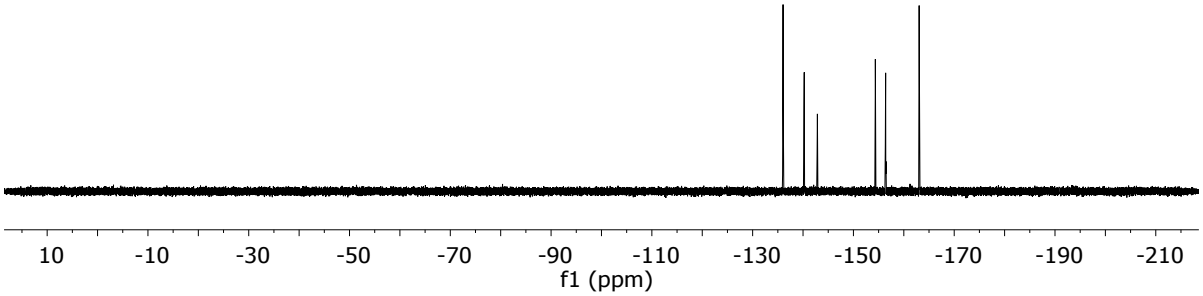


Figure S32. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **3c**.

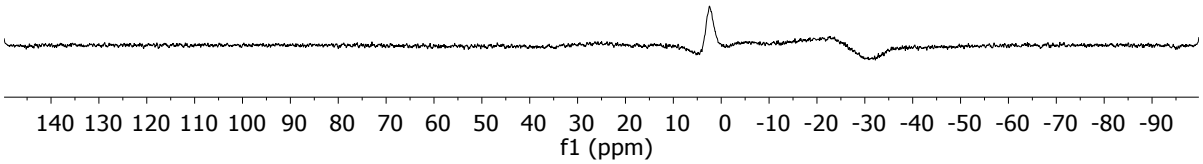


Figure S33. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3c**.

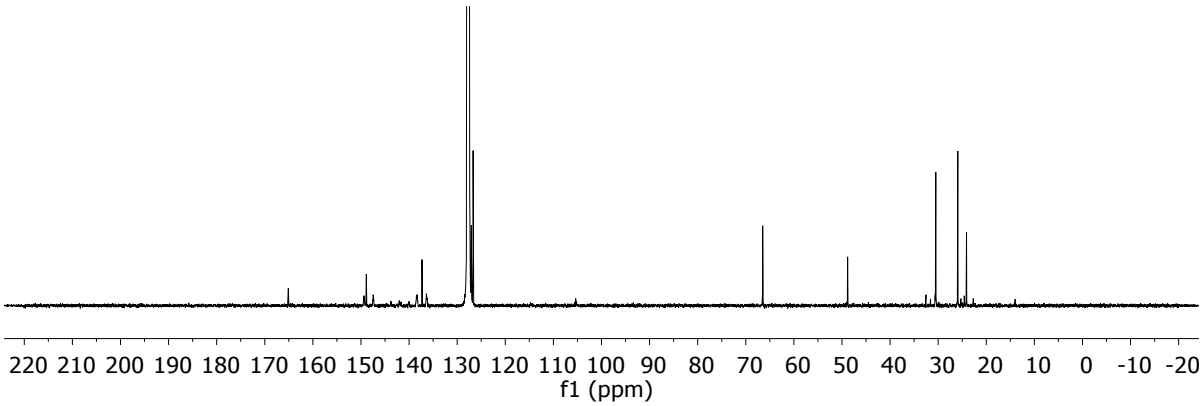


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3c**.

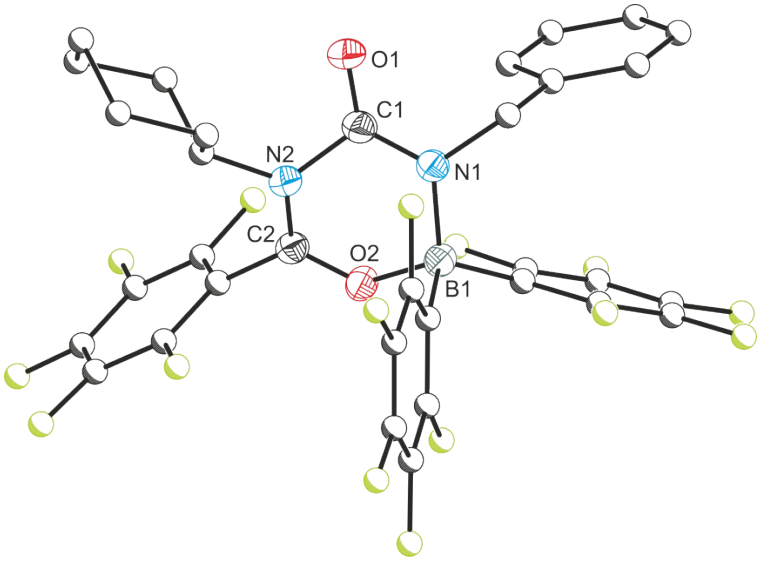
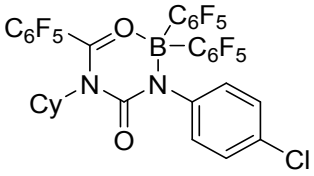


Figure S35. Single crystal X-ray structure of **3c**. Atoms of the Cy, benzyl and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.8. Compound 3d



^{1}H NMR (500 MHz, C_6D_6): δ = 7.07 (d, $^{3}J_{H–H}$ = 8.8 Hz, 2H, C_6H_4Cl), 6.90 (d, $^{3}J_{H–H}$ = 8.8 Hz, 2H, C_6H_4Cl), 3.32 (tt, $^{3}J_{H–H}$ = 12.1, 3.7 Hz, 1H, *Cy*), 2.43 (qd, $^{3}J_{H–H}$ = 12.7, 3.8 Hz, 2H, *Cy*), 1.62 (d, $^{3}J_{H–H}$ = 11.4 Hz, 2H, *Cy*), 1.35 (dd, $^{3}J_{H–H}$ = 10.6, 3.2 Hz, 2H, *Cy*), 1.09 (d, $^{3}J_{H–H}$ = 13.4 Hz, 1H, *Cy*), 0.93 (m, 1H, *Cy*), 1.09 (d, $^{3}J_{H–H}$ = 13.4 Hz, 1H, *Cy*), 0.56 (dddd, $^{3}J_{H–H}$ =

16.8, 13.2, 8.4, 3.5 Hz, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.2 (d, $^{3}J_{F–F}$ = 17 Hz, 4F, *o*-C_6F_5), –140.3 (d, $^{3}J_{F–F}$ = 19 Hz, 2F, *o*-C_6F_5), –142.3 (t, $^{3}J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –152.8 (t, $^{3}J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.0 (m, 2F, *m*-C_6F_5), –162.4 (dt, $^{3}J_{F–F}$ = 21, 17 Hz, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 3.2 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 166.0 (s, N*C*N), 148.27 (bd, $^{1}J_{C–F}$ = 240 Hz, C_6F_5), 147.8 (s, C_6H_4Cl), 142.7 (bd, $^{1}J_{C–F}$ = 253 Hz, C_6F_5), 141.2 (bd, $^{1}J_{C–F}$ = 248 Hz, C_6F_5), 138.3 (s, C_6H_4Cl), 137.4 (bd, $^{1}J_{C–F}$ = 269 Hz, C_6F_5), 133.0 (s, C_6H_4Cl), 129.0 (s, C_6H_4Cl), 66.5 (s, N*C*O), 30.5 (s, *Cy*), 25.9 (s, *Cy*), 24.0 (s, *Cy*) ppm.

Isolated Yield = 60%.

Elemental analysis for $C_{32}H_{15}BF_{15}N_2O_2Cl$: calcd.: C 48.61, H 1.91, N 3.54; found: C 48.34, H 1.85, N 3.67.

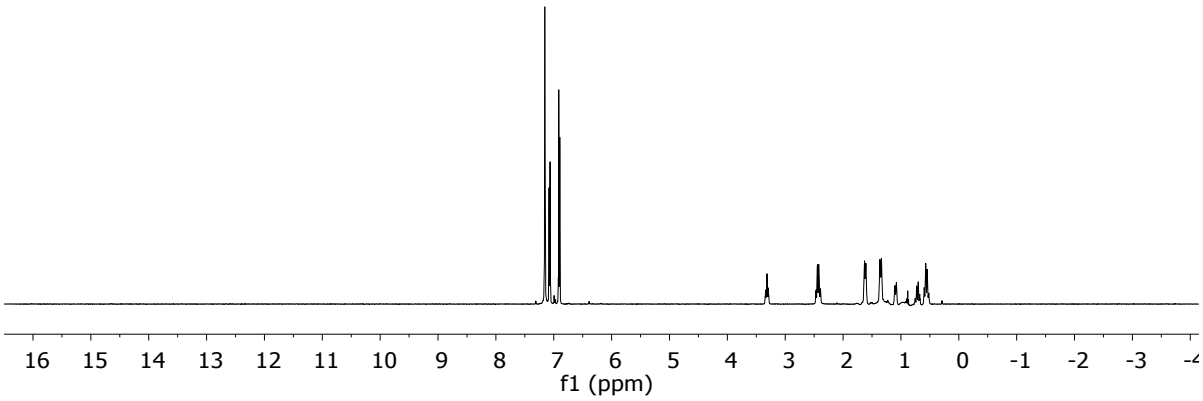


Figure S36. ^{1}H NMR spectrum (C_6D_6) of **3d**.

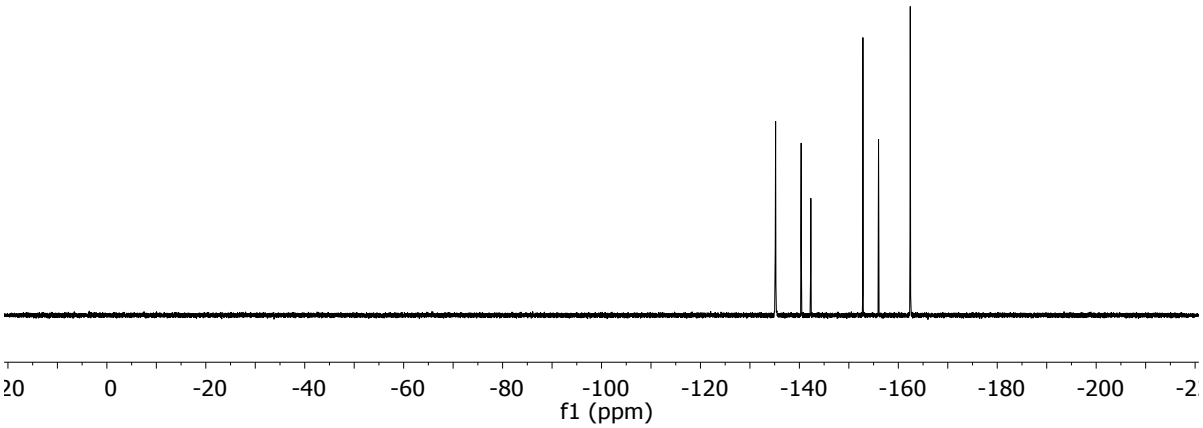


Figure S37. ^{19}F{^{1}H} NMR spectrum (C_6D_6) of **3d**.

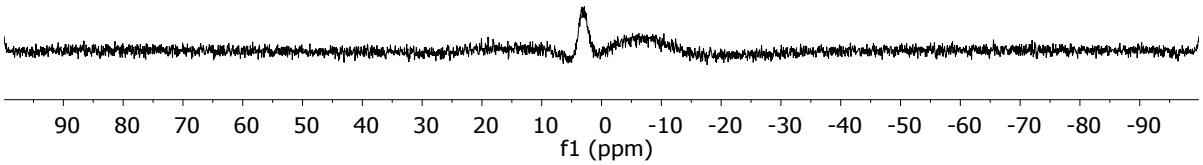


Figure S38. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3d**.

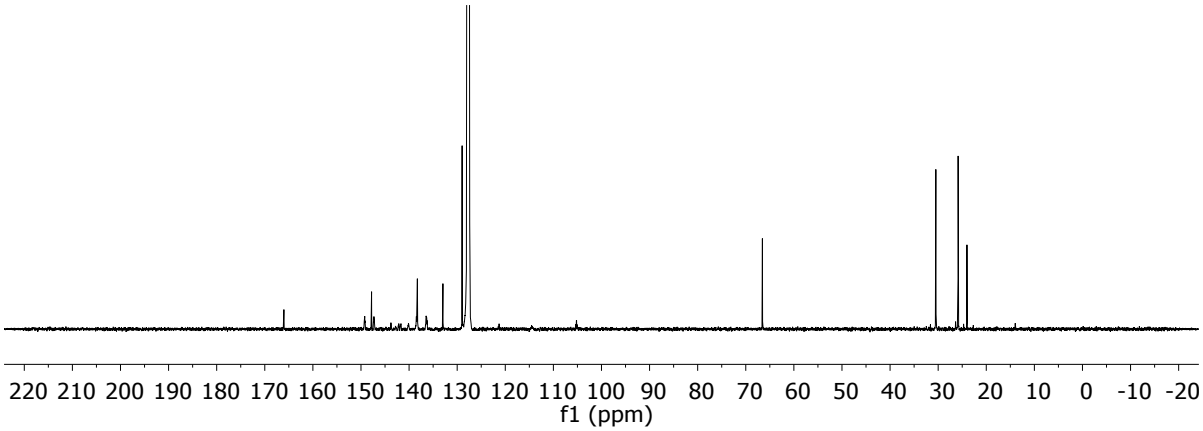


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3d**.

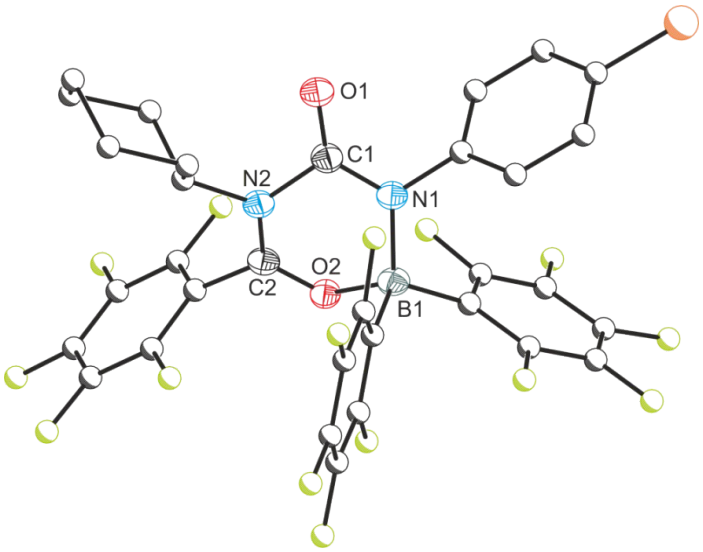
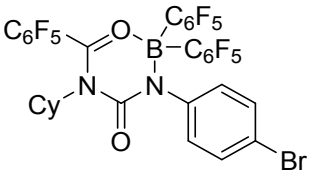


Figure S40. Single crystal X-ray structure of **3d**. Atoms of the Cy and aromatic moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.9. Compound 3e



^{1}H NMR (500 MHz, C_6D_6): δ = 7.07 (d, $^{3}J_{H–H}$ = 8.8 Hz, 2H, C_6H_4Br), 7.01 (d, $^{3}J_{H–H}$ = 8.8 Hz, 2H, C_6H_4Br), 3.31 (tt, $^{3}J_{H–H}$ = 12.3, 6.1 Hz, 1H, *Cy*), 2.43 (qd, $^{3}J_{H–H}$ = 12.8, 3.7 Hz, 1H, *Cy*), 1.63 (t, $^{3}J_{H–H}$ = 16.0 Hz, 1H, *Cy*), 1.51 (d, $^{3}J_{H–H}$ = 13.4 Hz, 1H, *Cy*), 1.35 (d, $^{3}J_{H–H}$ = 13.5 Hz, 1H, *Cy*), 1.26 (m, 1H, *Cy*), 1.09 (d, $^{3}J_{H–H}$ = 13.5 Hz, 1H, *Cy*), 0.93 (m, 2H, *Cy*), 0.73 (m, 1H, *Cy*), 0.55 (q, $^{3}J_{H–H}$ = 13.4 Hz, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.2 (d, $^{3}J_{F–F}$ = 9 Hz, 4F, *o*-C_6F_5), –140.3 (d, $^{3}J_{F–F}$ = 21 Hz, 2F, *o*-C_6F_5), –142.3 (t, $^{3}J_{F–F}$ = 22 Hz, 1F, *p*-C_6F_5), –152.8 (t, $^{3}J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.0 (m, 2F, *m*-C_6F_5), –162.4 (td, $^{3}J_{F–F}$ = 21, 9 Hz, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.8 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 166.0 (s, N*C*N), 148.2 (bd, $^{1}J_{C–F}$ = 255 Hz, C_6F_5), 147.7 (s, C_6H_5Br), 138.8 (s, C_6H_5Br), 137.3 (bd, $^{1}J_{C–F}$ = 252 Hz, C_6F_5), 132.0 (s, C_6H_5Br), 131.9 (s, C_6H_5Br), 121.6 (s, C_6H_5Br), 121.0 (s, C_6H_5Br), 66.5 (s, N*C*O), 31.6 (s, *Cy*), 30.5 (s, *Cy*), 26.4 (s, *Cy*), 25.9 (s, *Cy*), 24.7 (s, *Cy*), 24.0 (s, *Cy*) ppm.

Isolated Yield = 58%.

Elemental analysis for $C_{32}H_{15}BF_{15}N_2O_2Br$: calcd.: C 46.02, H 1.81, N 3.35; found: C 46.32, H 1.87, N 3.46.

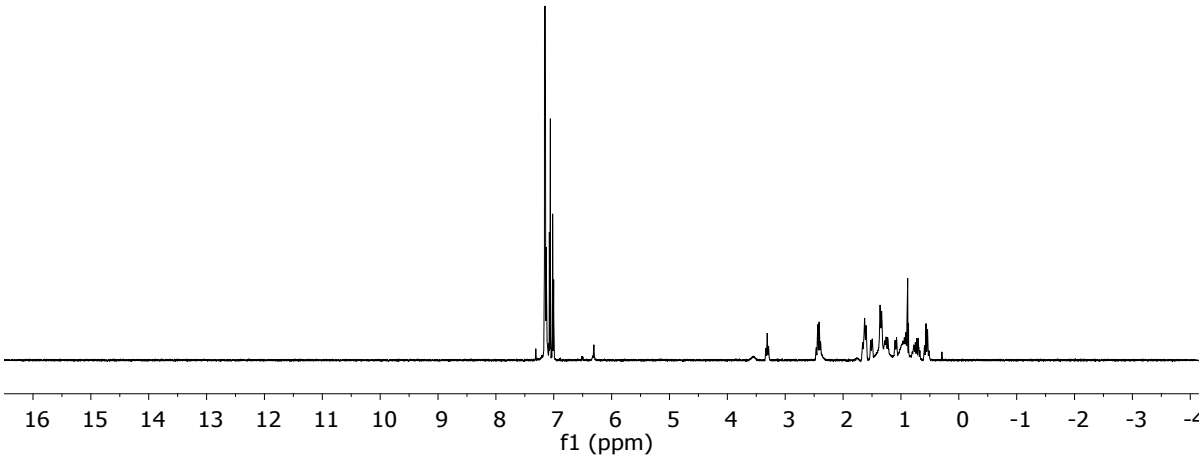


Figure S41. ^{1}H NMR spectrum (C_6D_6) of **3e**.

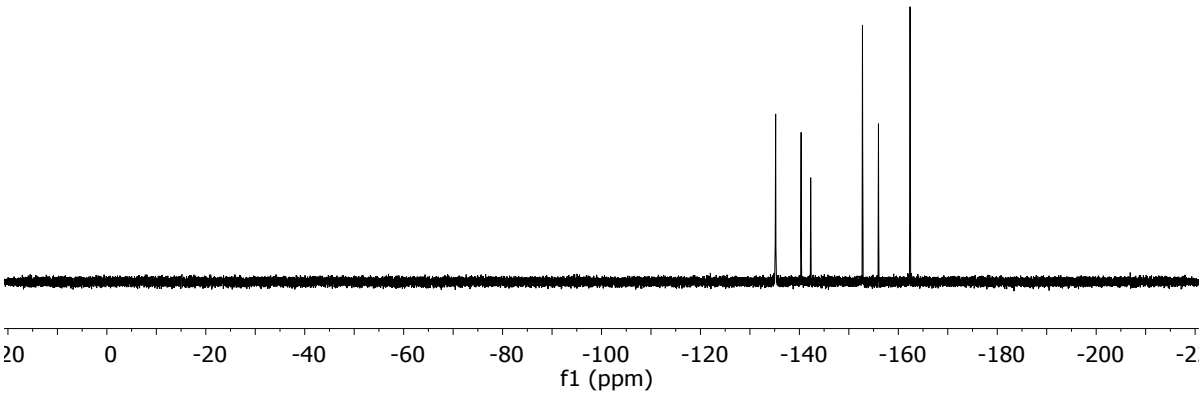


Figure S42. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **3e**.

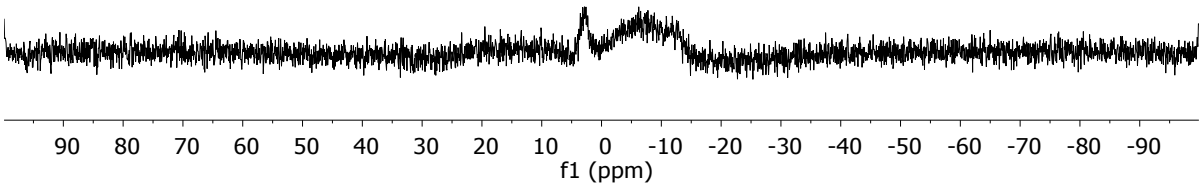


Figure S43. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3e**.

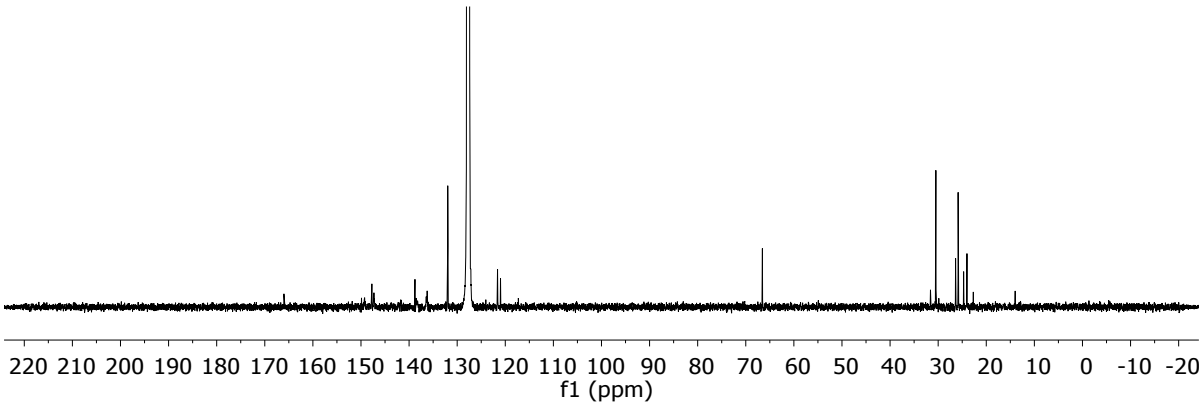


Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3e**.

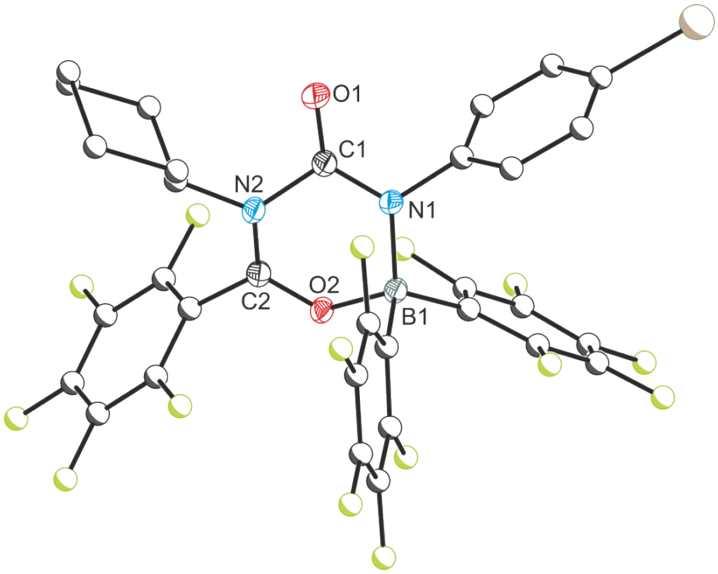
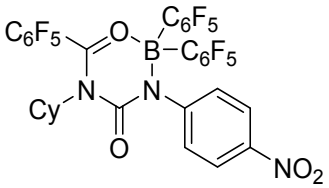
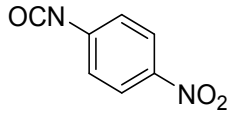


Figure S45. Single crystal X-ray structure of **3e**. Atoms of the Cy and aromatic moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.10. Compound 3f



^{1}H NMR (500 MHz, C_6D_6): δ = 7.67 (d, $^{3}J_{H–H}$ = 8.9 Hz, 2H, $C_6H_4NO_2$), 7.07 (d, $^{3}J_{H–H}$ = 8.9 Hz, 2H, $C_6H_4NO_2$), 3.32 (tt, $^{3}J_{H–H}$ = 12.0, 3.7 Hz, 1H, *Cy*), 2.40 (qd, $^{3}J_{H–H}$ = 12.6, 3.8 Hz, 2H, *Cy*), 2.11 (s, 1H, *Cy*), 1.61 (d, $^{3}J_{H–H}$ = 11.3 Hz, 1H, *Cy*), 1.36 (m, 2H, *Cy*), 1.09 (d, $^{3}J_{H–H}$ = 12.5 Hz, 1H, *Cy*), 0.93 (bm, 2H, *Cy*), 0.70 (m, 1H, *Cy*), 0.57 (m, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.3 (d, $^{3}J_{F–F}$ = 24 Hz, 4F, *o*-C_6F_5), –140.3 (d, $^{3}J_{F–F}$ = 20 Hz, 2F, *o*-C_6F_5), –141.7 (m, 1F, *p*- C_6F_5), –152.1 (m, 1F, *p*- C_6F_5), –155.7 (m, 2F, *m*- C_6F_5), –162.0 (m, 4F, *m*- C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 2.5 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** *δ* = 166.4 (s, N*C*N), 148.3 (bd, $^{1}J_{C–F}$ = 241 Hz, C_6F_5), 147.7 (s, $C_6H_4NO_2$), 146.2 (s, $C_6H_4NO_2$), 142.8 (bd, $^{1}J_{C–F}$ = 257 Hz, C_6F_5), 141.3 (bd, $^{1}J_{C–F}$ = 256, Hz, C_6F_5), 137.4 (bd, $^{1}J_{C–F}$ = 247.9 Hz, C_6F_5), 129.0 (s, $C_6H_4NO_2$), 128.2 (s, $C_6H_4NO_2$), 126.9 (s, $C_6H_4NO_2$), 125.3 (s, $C_6H_4NO_2$), 124.0 (s, $C_6H_4NO_2$), 66.8 (s, N*C*O), 30.5 (s, *Cy*), 25.8 (s, *Cy*), 24.0 (s, *Cy*), 21.1 (s, *Cy*) ppm.



^{1}H NMR (500 MHz, C_6D_6): δ = 7.53 (d, $^{3}J_{H–H}$ = 9.0 Hz, 2H, $C_6H_4NO_2$), 6.06 (d, $^{3}J_{H–H}$ = 9.0 Hz, 2H, $C_6H_4NO_2$); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 144.9 (s, $C_6H_4NO_2$), 138.8 (s, $C_6H_4NO_2$), 124.7 (s, $C_6H_4NO_2$), 124.5 (s, $C_6H_4NO_2$) ppm.

Isolated Yield = 68%.

Elemental analysis for $C_{32}H_{15}BF_{15}N_3O_4$+1/2$C_7H_4N_2O_3$+1/2tol: calcd.: C 50.40, H 2.28, N 6.03; found: C 50.29, H 2.41, N 6.92.

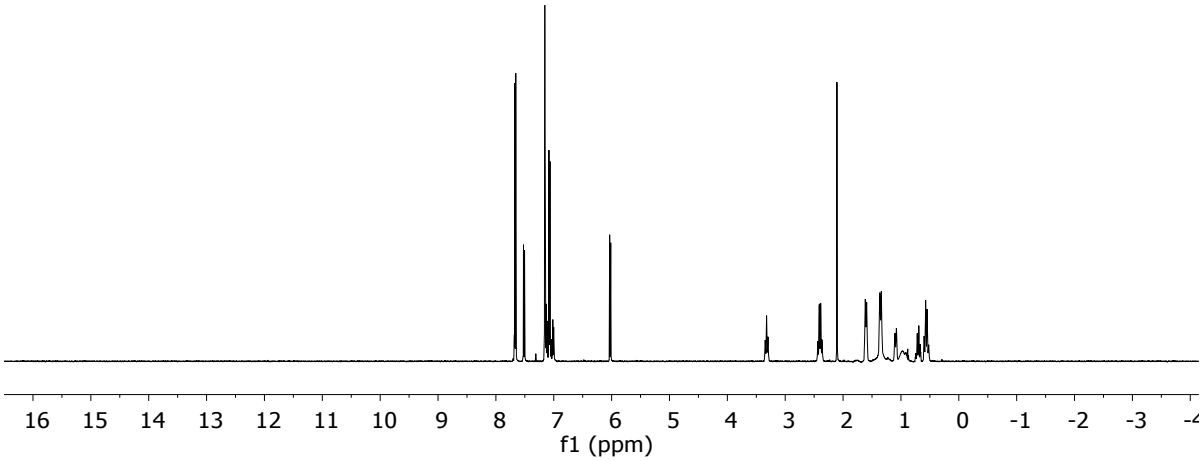


Figure S46. ^{1}H NMR spectrum (C_6D_6) of **3f**.

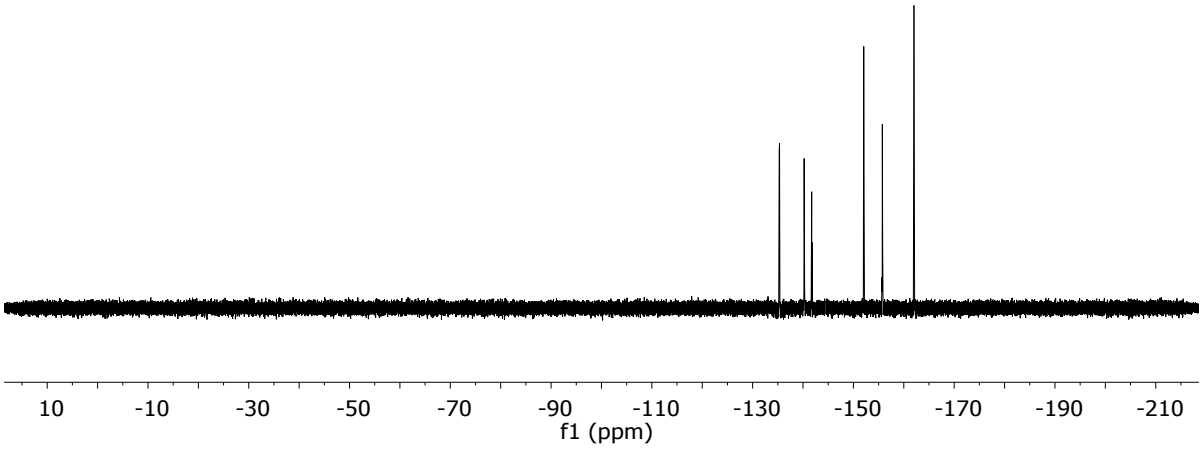


Figure S47. ^{19}F{^{1}H} NMR spectrum (C_6D_6) of **3f**.

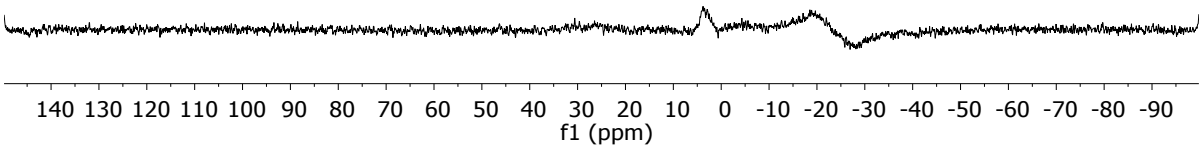


Figure S48. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3f**.

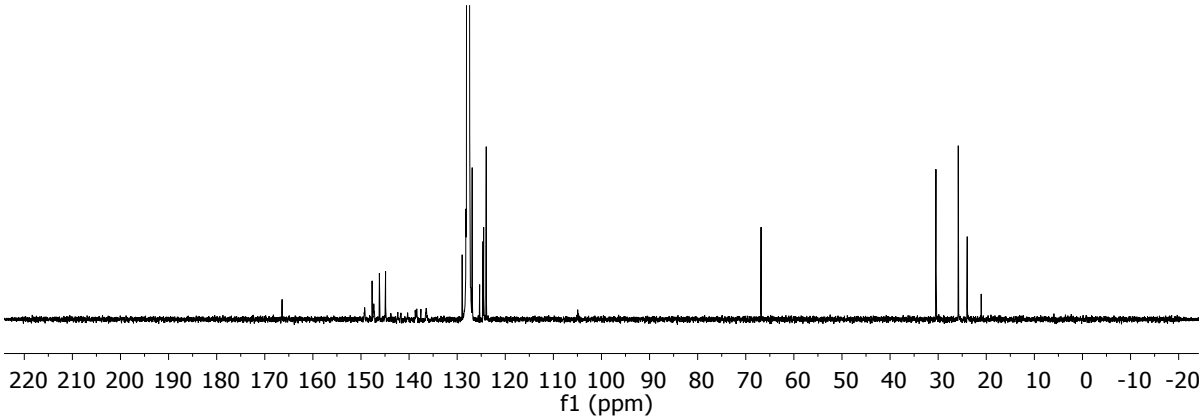


Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3f**.

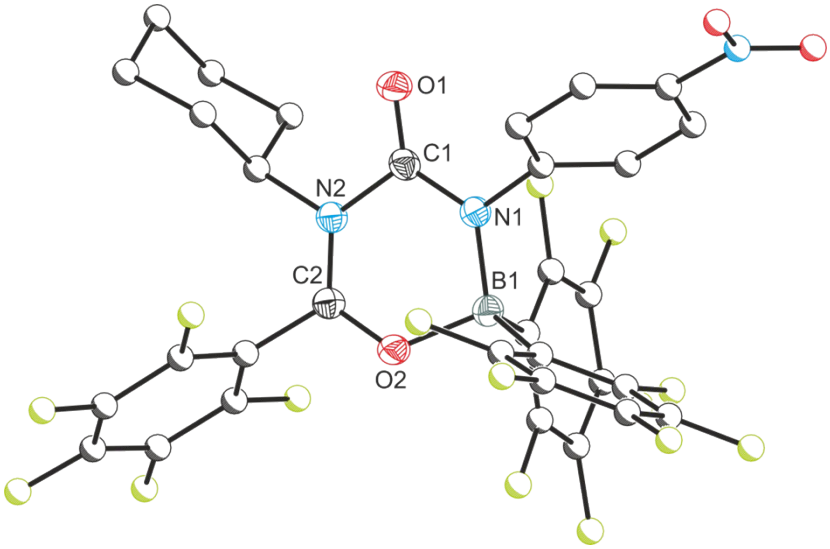
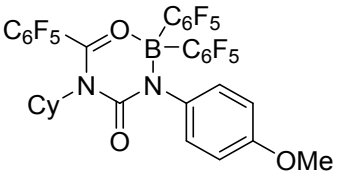


Figure S50. Single crystal X-ray structure of **3f**. Atoms of the Cy and aromatic moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.11. Compound 3g



^{1}H NMR (500 MHz, C_6D_6): δ = 7.25 (d, $^{3}J_{H–H}$ = 9.0 Hz, 2H, C_6H_4OMe), 6.55 (d, $^{3}J_{H–H}$ = 9.0 Hz, 2H, C_6H_4OMe), 3.36 (tt, $^{3}J_{H–H}$ = 12.0, 3.6 Hz, 1H, *Cy*), 3.04 (s, 3H, C_6H_4O*Me*), 2.48 (qd, $^{3}J_{H–H}$ = 12.6, 3.8 Hz, 2H, *Cy*), 1.65 (m, 2H, *Cy*), 1.37 (m, 2H, *Cy*), 1.10 (m, 1H, *Cy*), 0.73 (qt, $^{3}J_{H–H}$ = 13.1, 3.5 Hz, 1H, *Cy*), 0.59 (qt, $^{3}J_{H–H}$ = 13.2, 3.5 Hz, 2H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –135.0 (d, $^{3}J_{F–F}$ = 26 Hz, 4F, *o*-C_6F_5), –140.3 (d, $^{3}J_{F–F}$ = 21 Hz, 2F, *o*-C_6F_5), –142.9 (m, 1F, *p*-C_6F_5), –153.7 (t, $^{3}J_{F–F}$ = 21 Hz, 2F, *p*-C_6F_5), –156.3 (m, 2F, *m*-C_6F_5), –162.9 (td, $^{3}J_{F–F}$ = 26, 23, 4F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 3.3 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 165.8 (s, N*C*N), 158.6 (s, C_6H_4OMe), 148.4 (bd, $^{1}J_{C–F}$ = 246 Hz, C_6F_5), 148.1 (s, C_6H_4OMe), 143.7 (bd, $^{1}J_{C–F}$ = 263 Hz, C_6F_5), 142.8 (bd, $^{1}J_{C–F}$ = 261 Hz, C_6F_5), 141.0 (bd, $^{1}J_{C–F}$ = 253 Hz, C_6F_5), 137.5 (bd, $^{1}J_{C–F}$ = 255 Hz, C_6F_5), 132.5 (s, C_6H_4OMe), 125.4 (s, C_6H_4OMe), 114.5 (s, C_6H_4OMe), 114.0 (s, C_6H_4OMe), 66.4 (s, N*C*O), 54.3 (s, C_6H_4O*Me*), 30.5 (s, *Cy*), 25.9 (s, *Cy*), 24.1 (s, *Cy*) ppm.

Isolated Yield = 66%.

Elemental analysis for $C_{33}H_{18}BF_{15}N_2O_3$: calcd.: C 50.41, H 2.31, N 3.56; found: C 51.22, H 2.33, N 3.98.

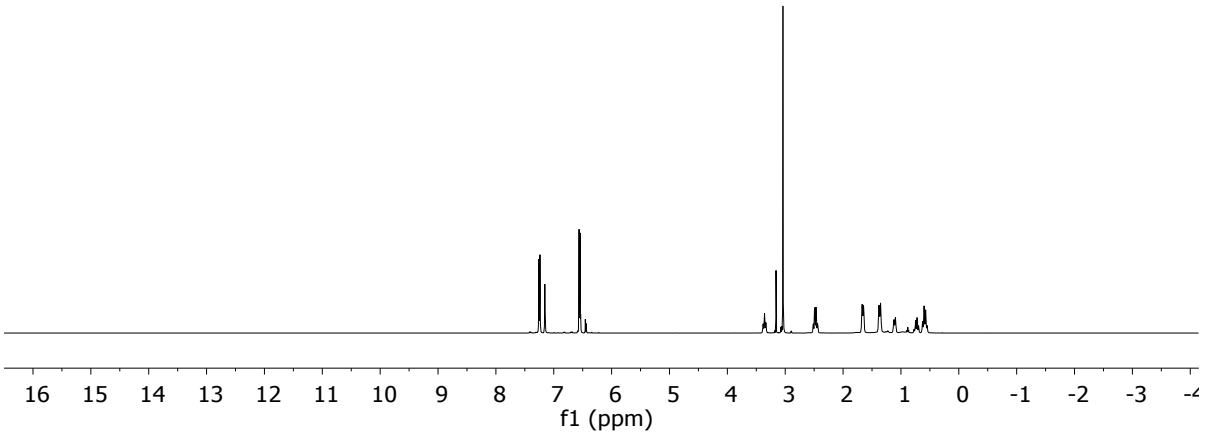


Figure S51. ^{13}C{^{1}H} NMR spectrum (C_6D_6) of **3g**.

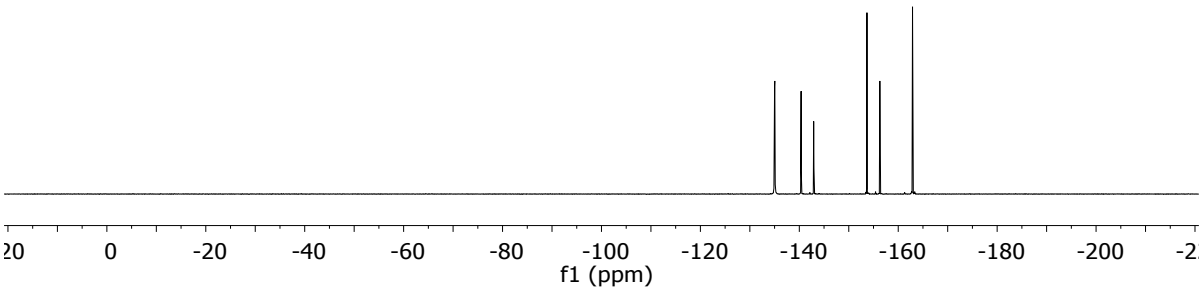


Figure S52. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **3g**.

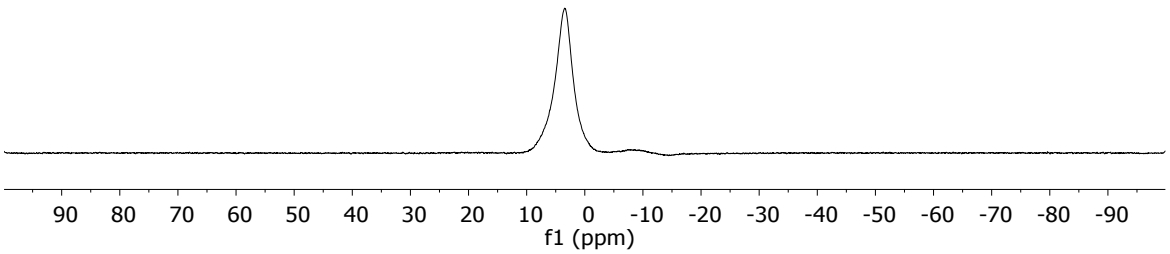


Figure S53. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3g**.

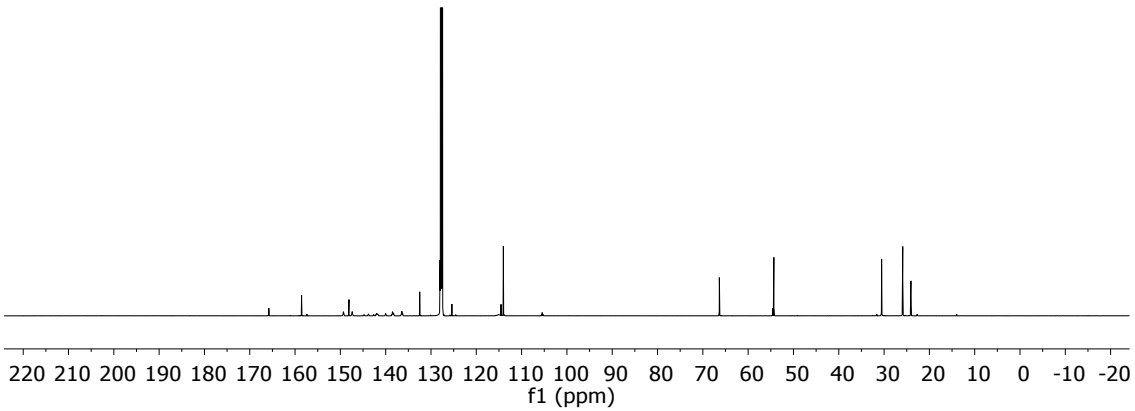


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3g**.

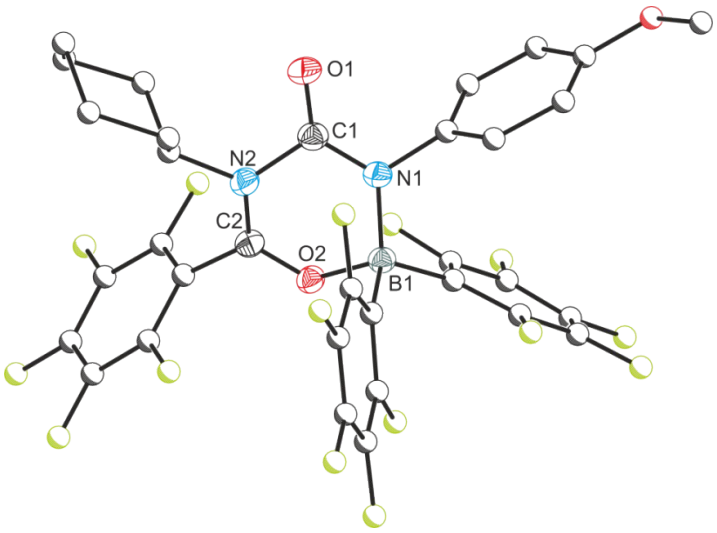
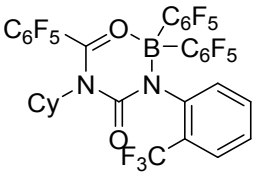


Figure S55. Single crystal X-ray structure of **3g**. Atoms of the Cy and aromatic moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.12. Compound 3h



^{1}H NMR (500 MHz, C_6D_6): δ = 7.64 (d, $^{3}J_{H–H}$ = 8.1 Hz, 1H, $C_6H_4CF_3$), 7.20 (d, $^{3}J_{H–H}$ = 7.9 Hz, 1H, $C_6H_4CF_3$), 6.93 (t, $^{3}J_{H–H}$ = 7.8 Hz, 1H, $C_6H_4CF_3$), 6.62 (t, $^{3}J_{H–H}$ = 7.7 Hz, 1H, $C_6H_4CF_3$), 3.32 (tt, $^{3}J_{H–H}$ = 12.1, 3.7 Hz, 1H, *Cy*), 2.51 (qd, $^{3}J_{H–H}$ = 12.9, 3.9 Hz, 1H, *Cy*), 2.33 (qd, $^{3}J_{H–H}$ = 12.3, 3.9 Hz, 1H, *Cy*), 1.65 (d, $^{3}J_{H–H}$ = 13.1 Hz, 1H, *Cy*), 1.51 (d, $^{3}J_{H–H}$ = 12.3 Hz, 1H, *Cy*), 1.31 (m, 2H, *Cy*), 0.96 (m, 2H, *Cy*), 0.64 (m, 1H, *Cy*), 0.46 (m, 1H, *Cy*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –59.8 (m, 3F, CF_3), –137.8 (d, $^{3}J_{F–F}$ = 23 Hz, 2F, *o*-C_6F_5), –142.6 (m, 3F, *o*-C_6F_5), –153.0 (t, $^{3}J_{F–F}$ = 21 Hz, 1F, *o*-C_6F_5), –153.3 (t, $^{3}J_{F–F}$ = 21 Hz, 1F, *p*-C_6F_5), –155.9 (m, 1F, *p*-C_6F_5), –156.4 (m, 1F, *p*-C_6F_5), –162.1 (m, 4F, *m*-C_6F_5), –163.3 (b, 2F, *m*-C_6F_5); **^{11}B{^{1}H} NMR (128 MHz, C_6D_6):** δ = 3.4 (s); **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 166.8 (s, N*C*N), 148.9 (s, $C_6H_4CF_3$), 137.1 (s, $C_6H_4CF_3$), 132.3 (s, $C_6H_4CF_3$), 129.3 (s, $C_6H_4CF_3$), 127.2 (s, $C_6H_4CF_3$), 66.4 (s, N*C*O), 30.4 (s, *Cy*), 29.9 (s, *Cy*), 25.9 (s, *Cy*), 25.7 (s, *Cy*), 24.0 (s, *Cy*) ppm. $C_6H_4CF_3$ could not be observed by ^{13}C NMR spectroscopy.

Isolated Yield = 29%

Elemental analysis for $C_{33}H_{15}BF_{18}N_2O_2$: calcd.: C 48.02, H 1.83, N 3.40; found: C 48.98, H 1.97, N 3.93.

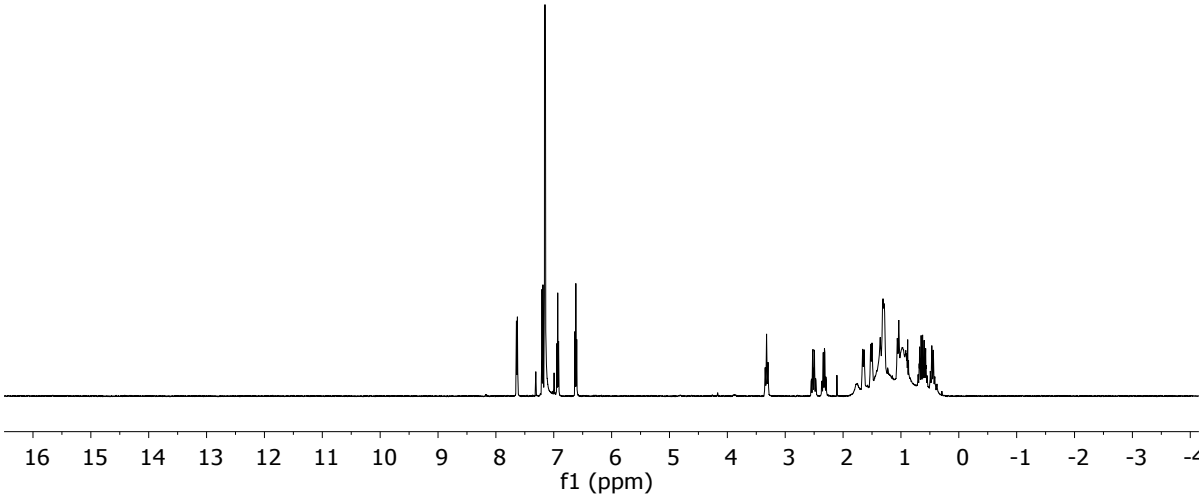


Figure S56. ^{1}H NMR spectrum (C_6D_6) of **3h**.

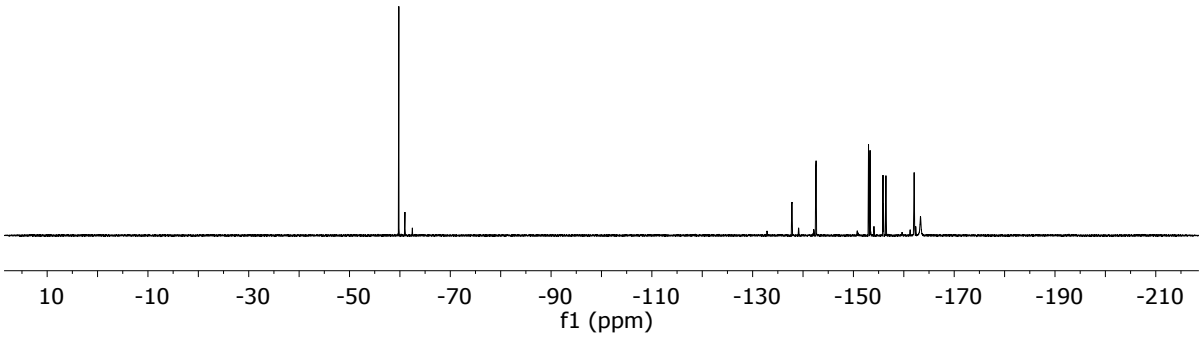


Figure S57. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **3h**.

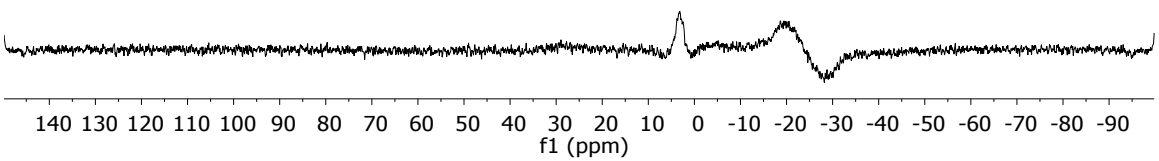


Figure S58. $^{11}B\{^{1}H\}$ NMR spectrum (C_6D_6) of **3h**.

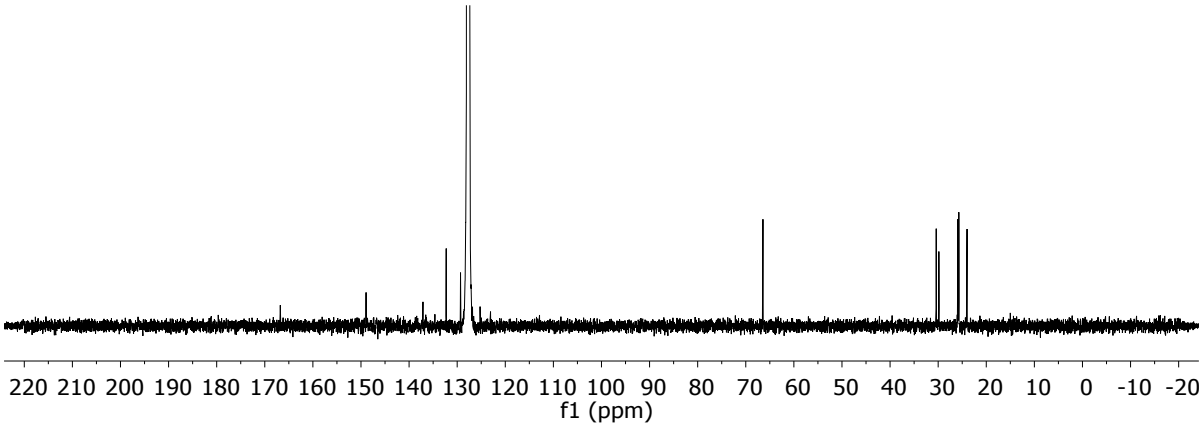


Figure S59. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **3h**.

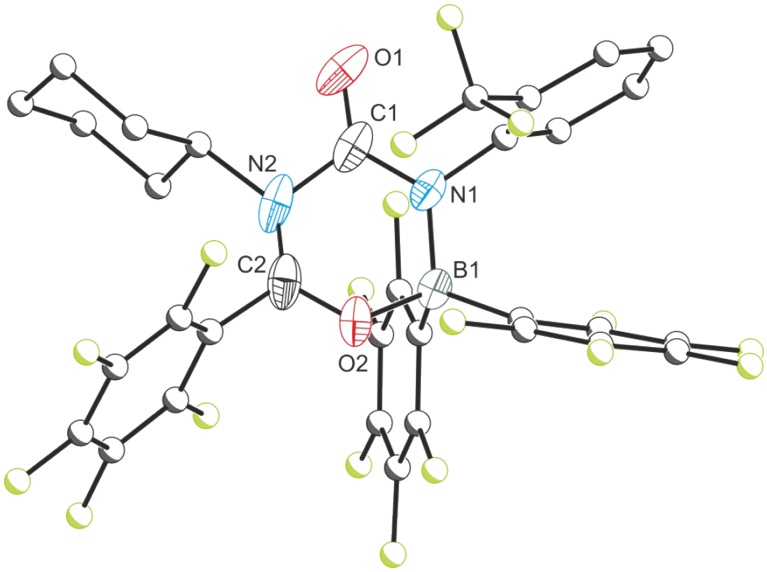
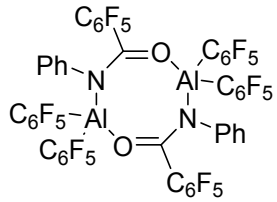


Figure S60. Single crystal X-ray structure of **3h**. Atoms of the Cy and aromatic moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.13. Compound 4



In a Schlenk flask charged with a stir bar $Al(C_6F_5)_3$ (0.10 g, 0.5 mmol) was dissolved in 5 mL of toluene. To this mixture PhNCO (0.25 g, 2.1 mmol, 4.2 eq) was added dropwise and

stirred overnight. The solvent was removed under reduced pressure to give a pale-yellow oil, which was further washed with hexane (3 × 7 mL) to yield a white precipitate. Crystals suitable for X-ray diffraction studies could be obtained from the hexane filtrate.

$^{19}F\{^1H\}$ NMR (377 MHz, C_6D_6): δ = –132.6 (bm, 2F, *o*-C_6F_5), –133.1 (bm, 4F, *o*-C_6F_5), -135.2 (b, 1F, *p*-C_6F_5), –163.7 (t, *J* = 21 Hz, 2F, *p*-C_6F_5), –167.7 (bm, 4F, *m*-C_6F_5), –167.8 (bm, 2F, *m*-C_6F_5) ppm.

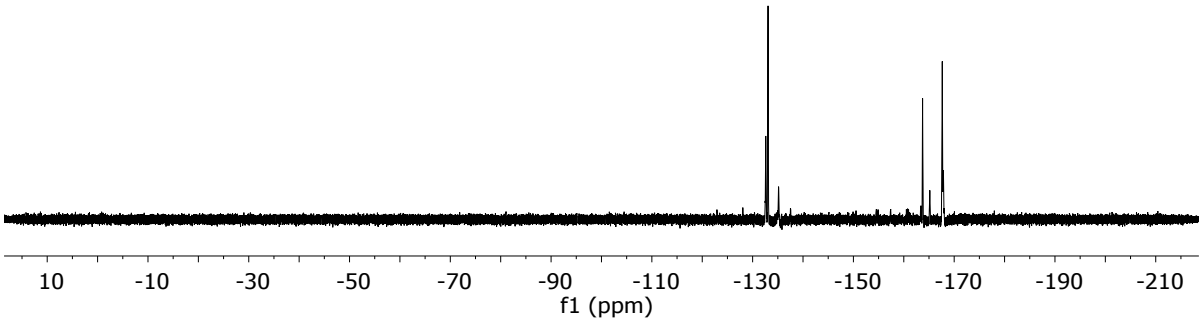


Figure S61. $^{19}F\{^1H\}$ NMR spectrum (C_6D_6) of **4**.

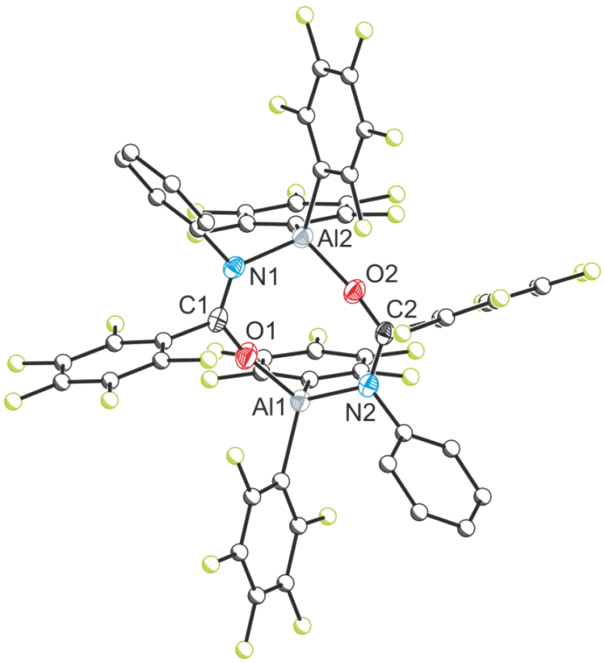
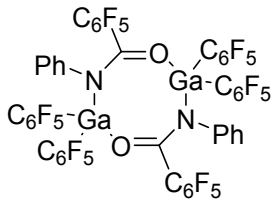


Figure S62. Single crystal X-ray structure of **4**. Atoms of the Ph and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

2.14. Compound 5



In a Schlenk flask charged with a stir bar $Ga(C_6F_5)_3$ (0.10 g, 0.4 mmol) was dissolved in 5 mL of toluene. To this mixture PhNCO (0.25 g, 5.2 mmol, 4.2 eq) was added dropwise and stirred overnight. The solvent was removed under reduced pressure to give a pale-yellow oil, which was further washed with hexane (3 × 7 mL) to yield a white precipitate. Crystals suitable for X-ray diffraction studies could be obtained from the hexane filtrate.

Note: NMR spectroscopy could only be performed on a sample contaminated with solvent. Solvent-free samples displayed poor solubility in d_8-toluene, C_6D_6, CD_2Cl_2, and d_8-THF.

^{1}H NMR (500 MHz, C_6D_6): δ = 6.91 (d, $^3J_{H–H}$ = 7.4 Hz, 4H, *Ph*), 6.57 (m, 6H, *Ph*); **^{19}F{^{1}H} NMR (377 MHz, C_6D_6):** δ = –124.6 (d, $^3J_{F–F}$ = 25 Hz, 4F, *o*-C_6F_5), –137.2 (m, 2F, *o*-C_6F_5), -146.6 (t, $^3J_{F–F}$ = 21 Hz, 1F, *p*-C_6F_5), –149.4 (t, $^3J_{F–F}$ = 20 Hz, 2F, *p*-C_6F_5), –159.3 (m, 2F, *m*-C_6F_5), –159.9 (m, 4F, *p*-C_6F_5), **^{13}C{^{1}H} NMR (126 MHz, C_6D_6):** δ = 167.7 (s, N*C*O), 148.8 (bd, $^1J_{C–F}$ = 231 Hz, C_6F_5), 142.4 (bd, $^1J_{C–F}$ = 288 Hz, C_6F_5), 138.7 (s, *Ph*), 137.1 (bd, $^1J_{C–F}$ = 270 Hz, C_6F_5), 129.3 (s, *Ph*), 128.9 (s, *Ph*), 125.3 (s, *Ph*), 124.5 (s, *Ph*) ppm.

Isolated Yield = 33%.

Elemental analysis for $C_{32}H_{22}BF_{15}N_2O_2$: calcd.: C 43.5, H 0.7, N 2.0; found: C 40.92, H 0.71, N 2.61.

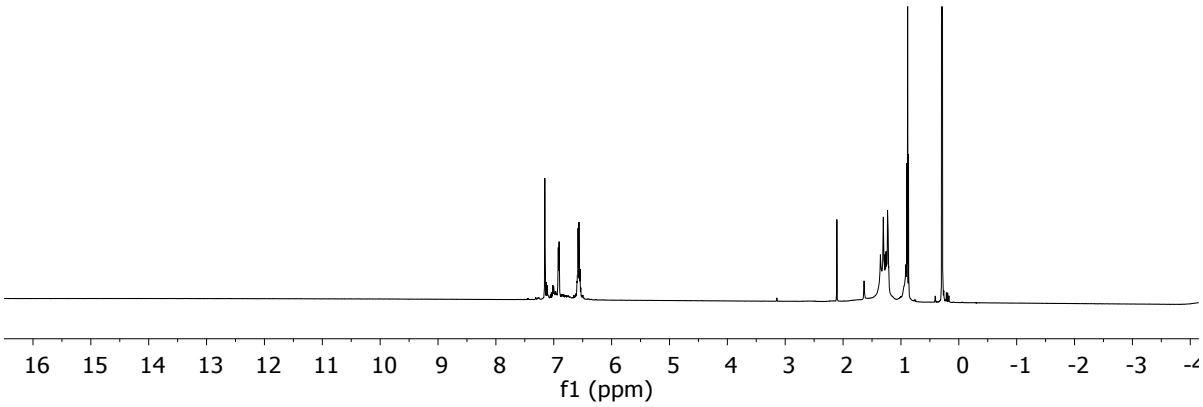


Figure S63. ^{1}H NMR spectrum (C_6D_6) of **5**.

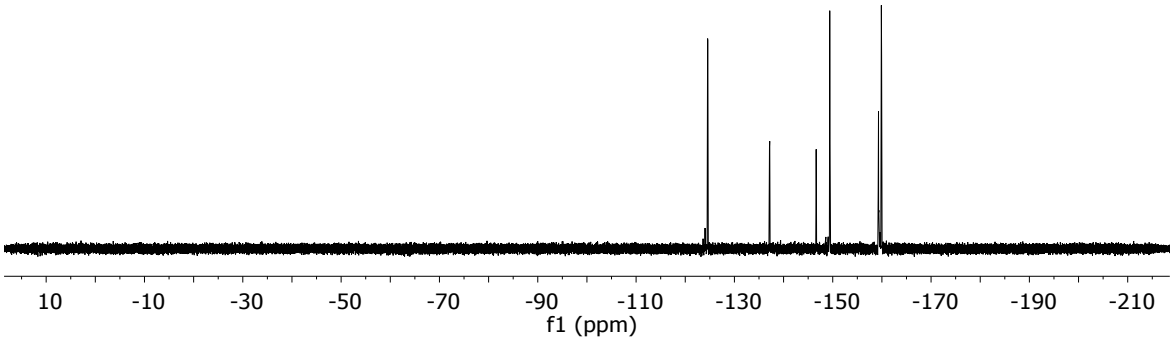


Figure S64. $^{19}F\{^{1}H\}$ NMR spectrum (C_6D_6) of **5**.

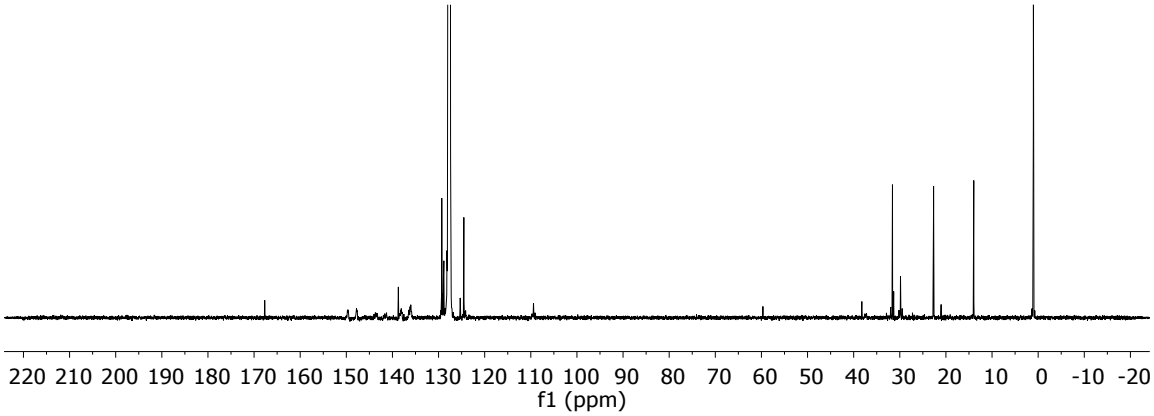


Figure S65. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6) of **5**.

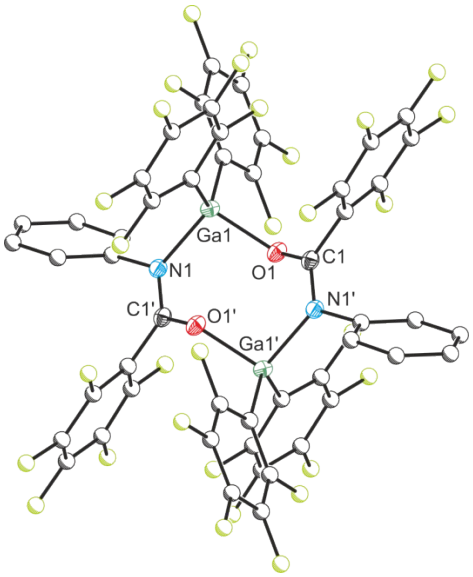


Figure S66. Single crystal X-ray structure of **5**. Atoms of the Ph and C_6F_5 moieties are pictured as spheres of arbitrary radius. Anisotropic displacement ellipsoids pictured at 50% probability. Hydrogen atoms omitted for clarity.

3. Kinetic Studies

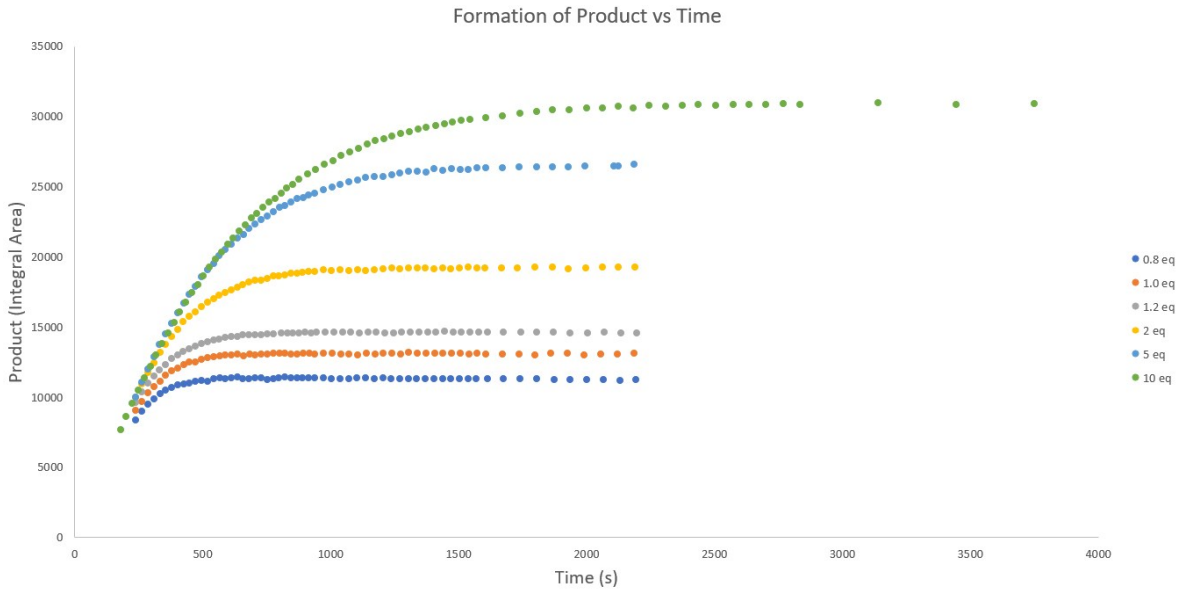


Figure S68. Formation of **2** vs. time (s). Experimental conditions as described in section 1.3.

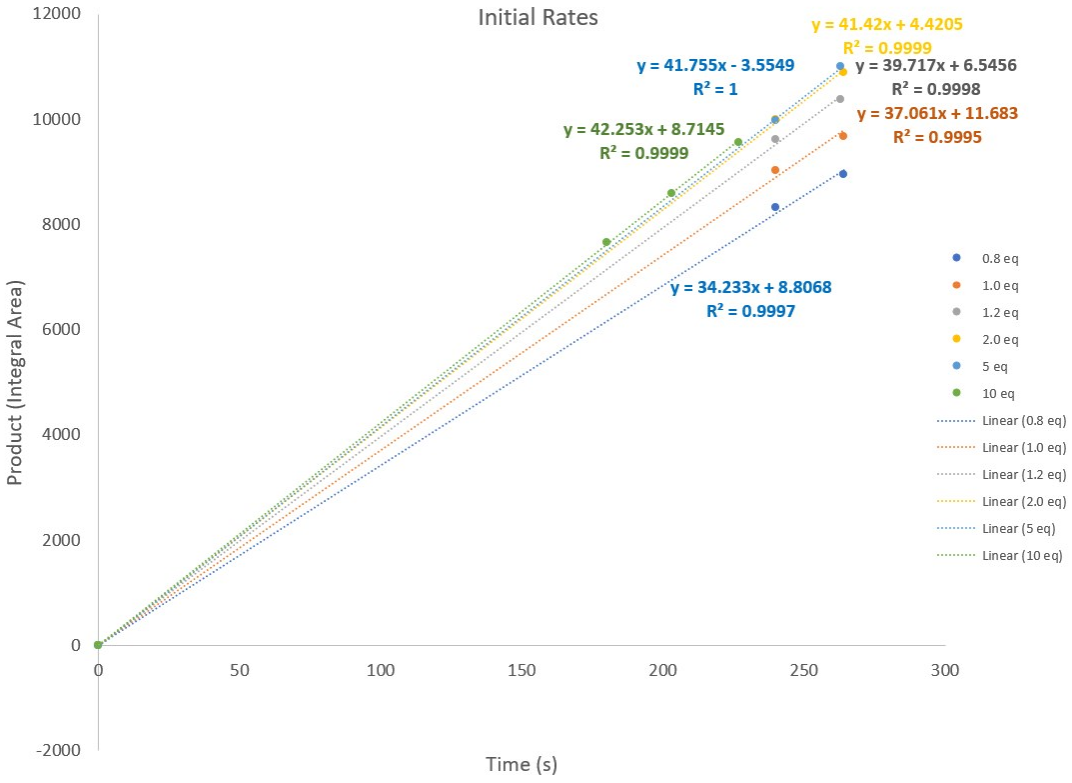


Figure S69. Initial Formation of **2** vs. time (s). Experimental conditions as described in section 1.3.

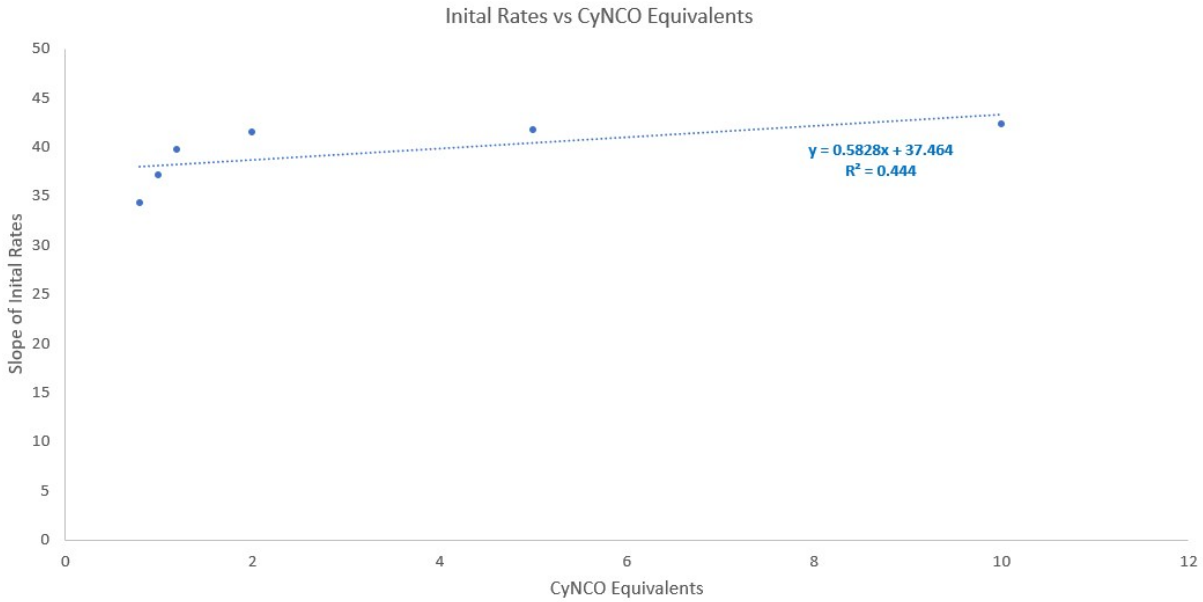


Figure S70. Slope of initial formation of **2** vs. CyNCO equivalents. Experimental conditions as described in section 1.3.

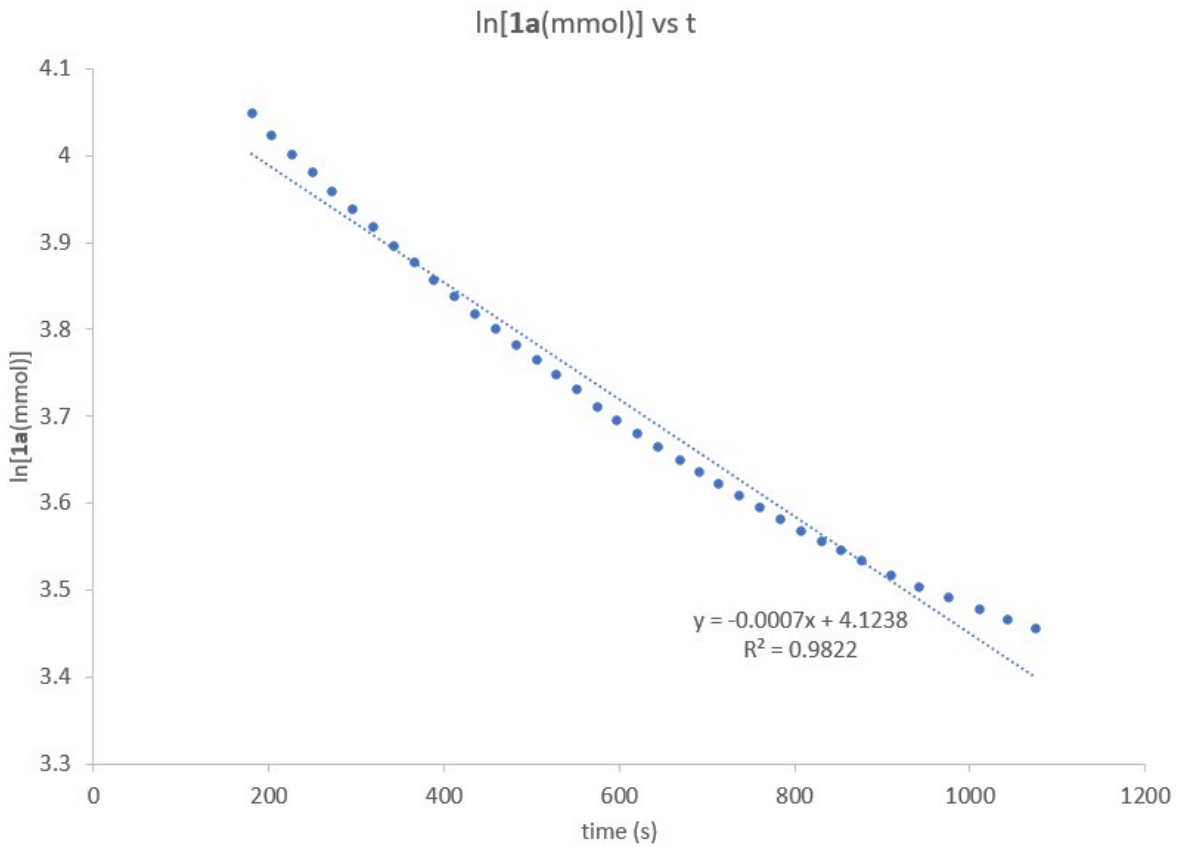


Figure S71. ln[**1a**(mmol)] vs t (s) for consumption of **1a** with 10 eq of CyNCO. Experimental conditions as described in section 1.3.

4. Thermodynamic Studies

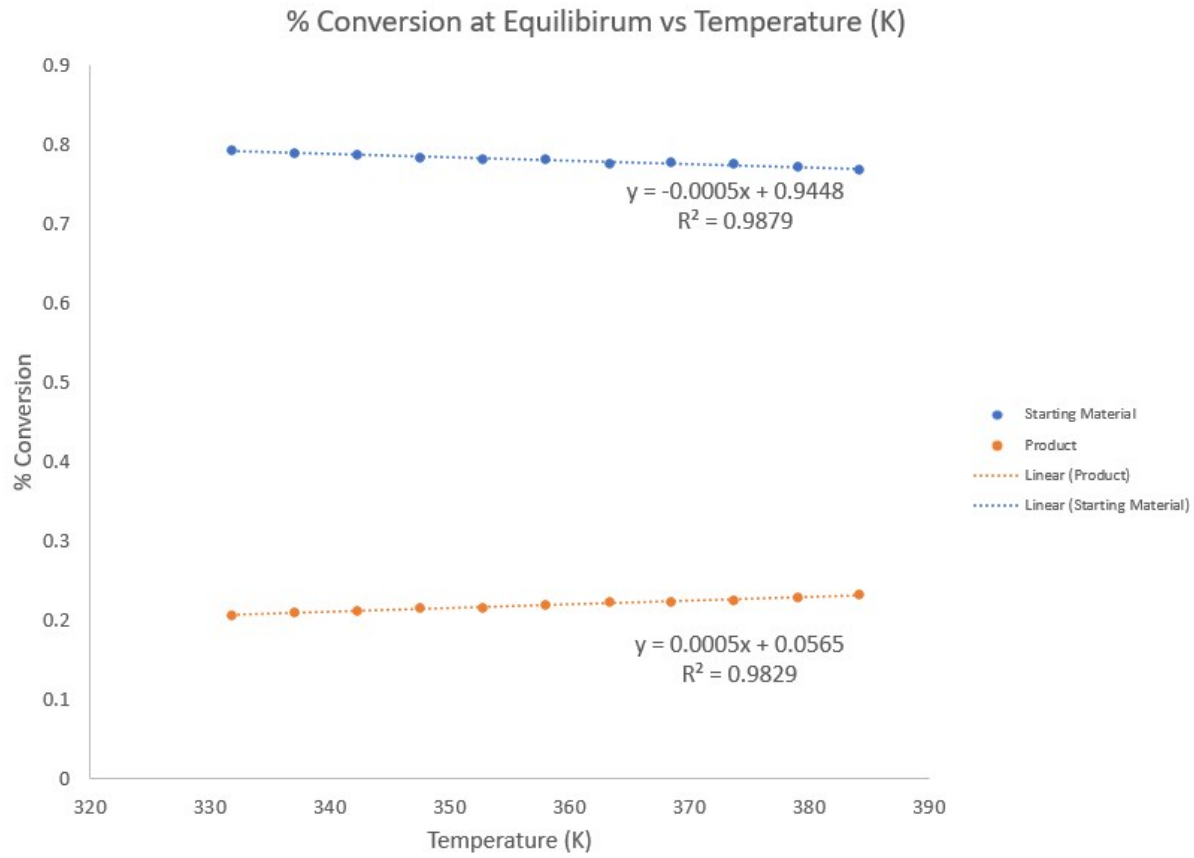


Figure S72. Conversion of **1a** to **2** at Equilibrium vs Temperature (K). Experimental conditions as described in section 1.4.

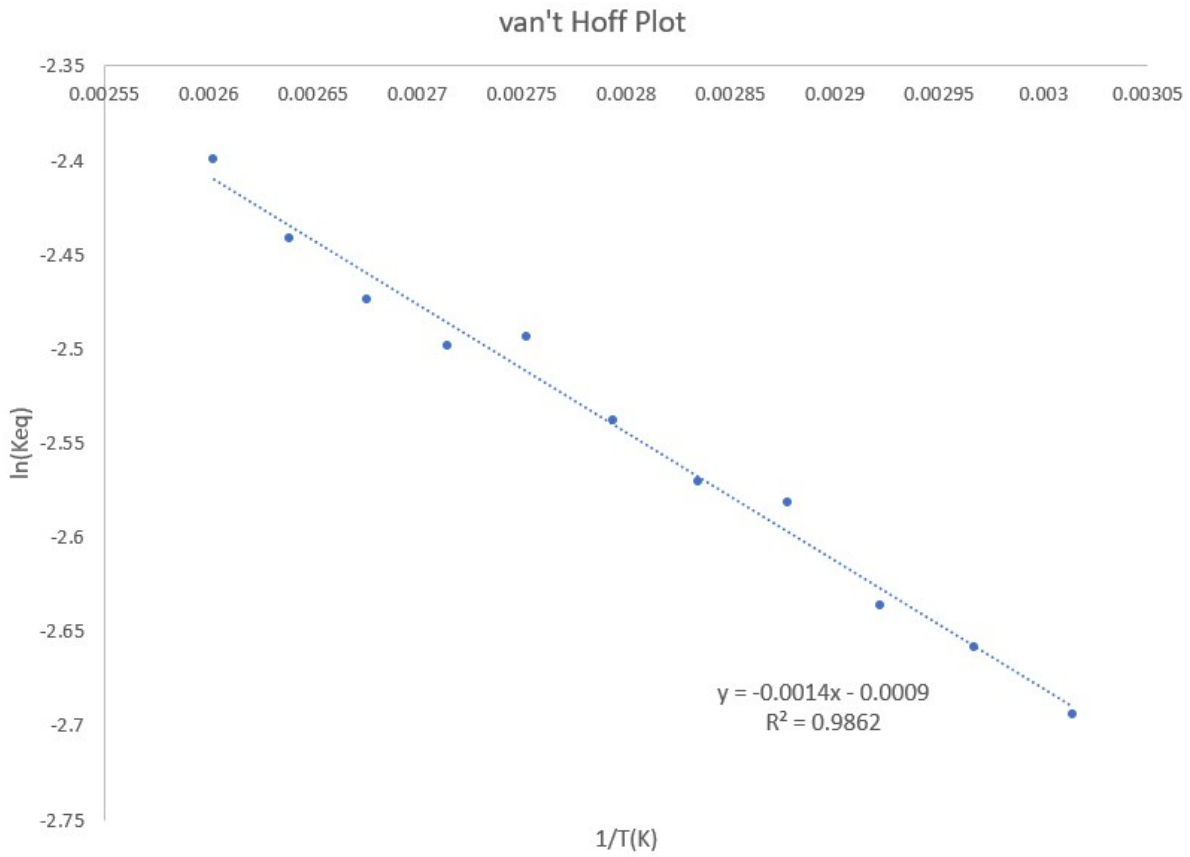


Figure S73. Van't Hoff Plot for Conversion of **1a** to **2**. Experimental conditions as described in section 1.4.

5. Crystallographic Tables

Table S1. Selected X-ray data collection and refinement parameters for **1a 1b**, **1c** and **2**.

	1a	**1b**	**1c**	**2**
Formula	$C_{32}H_{10}BF_{15}N_2O_2$	$C_{32}H_{22}BF_{15}N_2O_2$	$C_{26}H_{10}BF_{15}N_2O_2$	$C_{32}H_{16}BF_{15}N_2O_2$
CCDC	1907920	1907921	1907922	1907923
Fw [g mol^{-1}]	750.23	762.32	678.17	756.28
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	*P*–1	*C*2/*c*	$P2_1/c$	$P2_1/c$
a (Å)	9.1684(3)	16.6110(5)	8.63710(10)	13.9196(2)
b (Å)	12.0068(3)	10.3630(2)	20.2199(2)	9.8620(2)
c (Å)	14.3299(4)	36.6152(9)	15.13590(10)	22.3185(5)
α (°)	100.589(2)	90	90	90
β (°)	91.900(2)	103.060(2)	93.8880(10)	96.685(2)
γ (°)	105.332(2)	90	90	90
V (Å^3)	1489.86(8)	6139.9(3)	2637.27(4)	3042.94(10)
Z	2	8	4	4
Radiation, λ (Å)	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184
Temp (K)	150(2)	150(2)	150(2)	150(2)
ρ_{calc} (g cm^{-3})	1.672	1.649	1.708	1.651
μ (mm^{-1})	1.523	1.480	1.639	1.492
Reflections collected	30308	31445	32653	25771
Independent reflections	6085	6370	5481	6309
Parameters	469	469	431	469
R(int)	0.0241	0.0381	0.0231	0.0335
R1/wR2,[a] $I \geq 2\sigma I$ (%)	3.33/8.92	6.78/20.33	3.50/9.13	4.09/10.81
R1/wR2,[a] all data (%)	3.83/9.52	7.32/21.17	3.72/9.35	5.45/12.00
GOF	1.068	1.119	1.027	1.032

[a] $R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0459 and 0.56 for **1a**, 0.0810 and 39.59 for **1b**, 0.0475 and 0.98 for **1c**, and 0.0618 and 0.85 for **2**.

Table S2. Selected X-ray data collection and refinement parameters for **3a**·0.75hex, **3b**, **3c** and **3d**.

	3a·0.75hex	**3b**	**3c**	**3d**
Formula	$C_{36.5}H_{26.5}BF_{15}N_2O_2$	$C_{29}H_{16}BF_{15}N_2O_2$	$C_{33}H_{18}BF_{15}N_2O_2$	$C_{32}H_{15}BClF_{15}N_2O_2$
CCDC	1907924	1907925	1907926	1907927
Fw [g mol^{-1}]	820.91	720.25	770.30	790.72
Crystal system	triclinic	triclinic	monoclinic	monoclinic
Space group	*P*–1	*P*–1	$P2_1/n$	$P2_1$
a (Å)	12.7339(4)	9.1546(3)	14.4113(2)	15.00220(10)
b (Å)	14.6283(5)	10.4650(3)	12.5047(2)	12.8083(2)
c (Å)	21.2277(7)	32.5941(9)	35.4165(4)	17.2649(2)
α (°)	77.984(3)	89.932(2)	90	90
β (°)	76.287(3)	87.734(2)	91.0590(10)	104.1050(10)
γ (°)	69.659(3)	64.836(3)	90	90
V (Å^3)	3567.4(2)	2823.63(16)	6381.28(15)	3217.48(7)
Z	4	4	8	4
Radiation, λ (Å)	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184
Temp (K)	150(2)	150(2)	150(2)	150(2)
ρ_{calc} (g cm^{-3})	1.528	1.694	1.604	1.632
μ (mm^{-1})	1.319	1.570	1.435	2.187
Reflections collected	39525	25899	36270	41515
Independent reflections	14767	9955	13144	12803
Parameters	1073	883	955	955
R(int)	0.0350	0.0237	0.0288	0.0429
R1/wR2,[a] $I \geq 2\sigma I$ (%)	4.50/11.20	6.97/19.98	4.77/11.34	3.35/8.41
R1/wR2,[a] all data (%)	6.13/12.38	7.28/20.10	5.54/11.73	3.65/8.73
GOF	1.016	1.174	1.137	1.033

[a] $R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0539 and 1.09 for **3a**·0.75hex, 0.0546 and 13.21 for **3b**, 0.0279 and 5.45 for **3c**, and 0.0445 and 0.39 for **3d**.

Table S3. Selected X-ray data collection and refinement parameters for **3e**, **3f**, **3g** and **3h**.

	3e	**3f**	**3g**	**3h**
Formula	$C_{32}H_{15}BBrF_{15}N_2O_2$	$C_{32}H_{15}BF_{15}N_3O_4$	$C_{33}H_{18}BF_{15}N_2O_3$	$C_{33}H_{15}BF_{18}N_2O_2$
CCDC	1907928	1907929	1907930	1907931
Fw [g mol^{-1}]	835.18	801.28	786.30	824.28
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_12_12_1$
a (Å)	15.5607(5)	12.78170(10)	15.4749(2)	9.5724(2)
b (Å)	12.1150(3)	16.79680(10)	12.27710(10)	15.9011(3)
c (Å)	33.7225(10)	18.1486(2)	33.3387(3)	41.7343(6)
α (°)	90	90	90	90
β (°)	93.091(3)	100.3400(10)	93.7040(10)	90
γ (°)	90	90	90	90
V (Å^3)	6348.0(3)	3833.08(6)	6320.68(11)	6352.4(2)
Z	8	4	8	8
Radiation, λ (Å)	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184
Temp (K)	150(2)	150(2)	150(2)	150(2)
ρ_{calc} (g cm^{-3})	1.748	1.388	1.653	1.724
μ (mm^{-1})	2.918	1.266	1.487	1.629
Reflections collected	29127	31854	66784	44949
Independent reflections	12289	7947	13136	12989
Parameters	955	497	975	1028
R(int)	0.0249	0.0238	0.0256	0.0383
R1/wR2,[a] $I \geq 2\sigma I$ (%)	3.92/9.14	3.88/10.49	3.20/8.55	4.19/10.08
R1/wR2,[a] all data (%)	4.82/9.59	4.33/10.94	3.86/9.00	5.47/11.10
GOF	1.071	1.028	1.023	0.999

[a] $R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0358 and 5.88 for **3e**, 0.0581 and 1.38 for **3f**, 0.0440 and 2.24 for **3g**, and 0.0533 and 1.23 for **3d**.

Table S4. Selected X-ray data collection and refinement parameters for **4**·tol and **5**·hex.

	4·tol	**5**·hex
Formula	$C_{57}H_{18}Al_2F_{30}N_2O_2$	$C_{56}H_{24}F_{30}Ga_2N_2O_2$
CCDC	1907932	1907933
Fw [g mol^{-1}]	1386.69	1466.21
Crystal system	triclinic	triclinic
Space group	*P*–1	*P*–1
a (Å)	11.8016(3)	9.8455(5)
b (Å)	14.1317(3)	11.6923(5)
c (Å)	17.4036(5)	13.4043(7)
α (°)	78.018(2)	67.685(4)
β (°)	75.621(2)	79.756(4)
γ (°)	80.479(2)	71.222(4)
V (Å^3)	2730.41(12)	1348.79(12)
Z	2	1
Radiation, λ (Å)	Cu Kα, 1.54184	Cu Kα, 1.54184
Temp (K)	150(2)	150(2)
ρ_{calc} (g cm^{-3})	1.687	1.805
μ (mm^{-1})	1.866	2.619
Reflections collected	44233	12718
Independent reflections	11307	5570
Parameters	881	415
R(int)	0.0349	0.0355
R1/wR2,[a] I ≥ 2σI (%)	10.82/41.24	3.19/8.09
R1/wR2,[a] all data (%)	11.56/42.19	3.75/8.56
GOF	1.999	1.037

[a] $R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.2000 and 0 for **4**·tol, and 0.0438 and 0.29 for **5**·hex.

6. DFT Studies

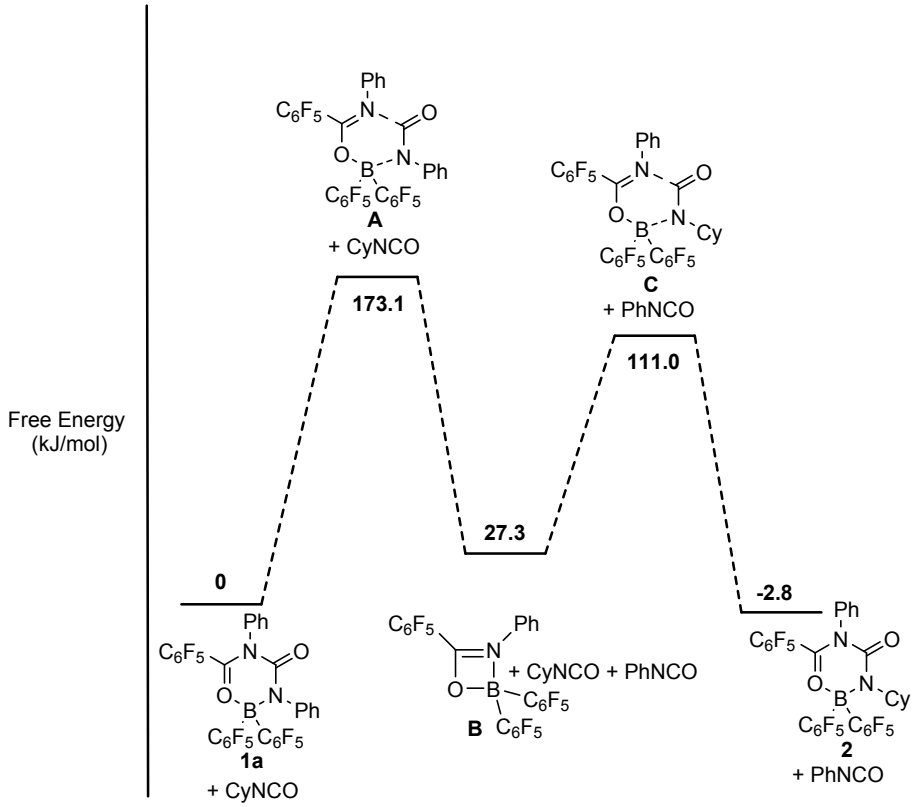


Figure S74. Computed isocyanate exchange using CyNCO via disassociative mechanism.

Table S5. Computed isocyanate exchange via dissociative mechanism.

Description	E [a.u.]	ΔE [kJ/mol]	G [a.u]	ΔG (kJ/mol}
1a + CyNCO	–3407.61	0	–3407.18	0
A + CyNCO	–3407.54	183.3278	–3407.11	173.1333
B + CyNCO + PhNCO	–3407.57	104.3116	–3407.17	27.26844
C + PhNCO	–3407.57	119.0768	–3407.14	111.0481
2 + PhNCO	–3407.62	-8.81611	–3407.18	-2.79878

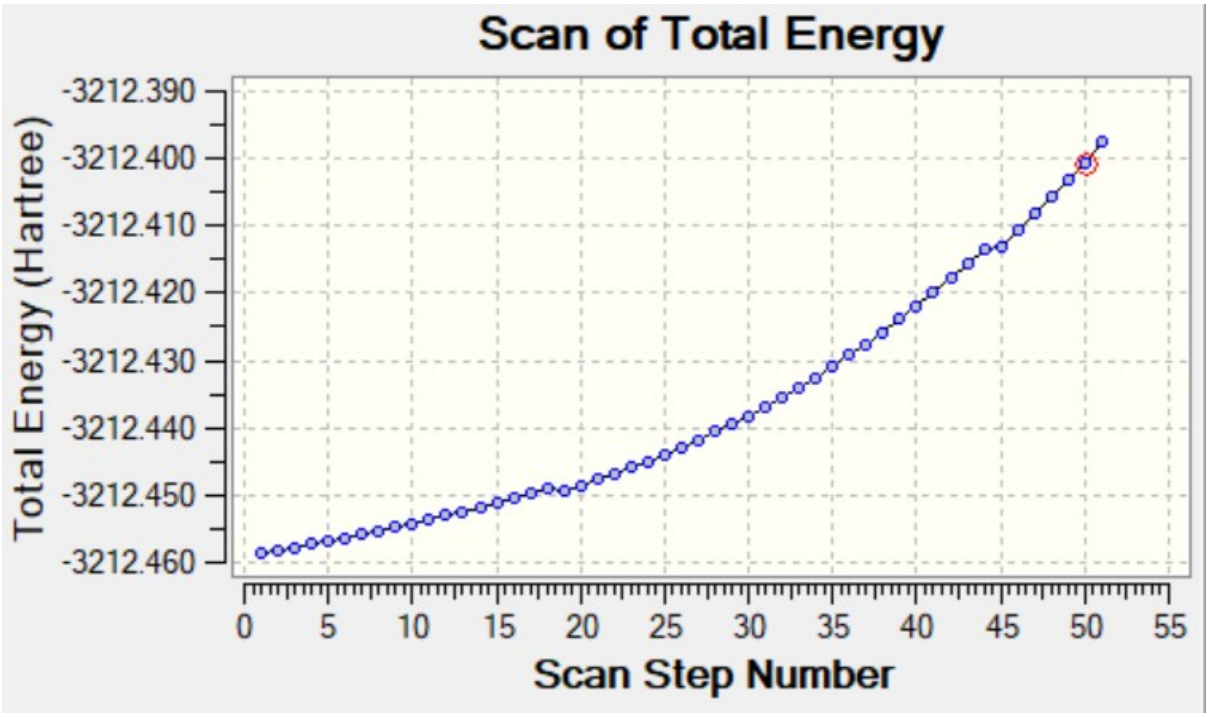


Figure S75. Exponential increase in energy for computed isocyanate exchange using MeNCO via associative mechanism.

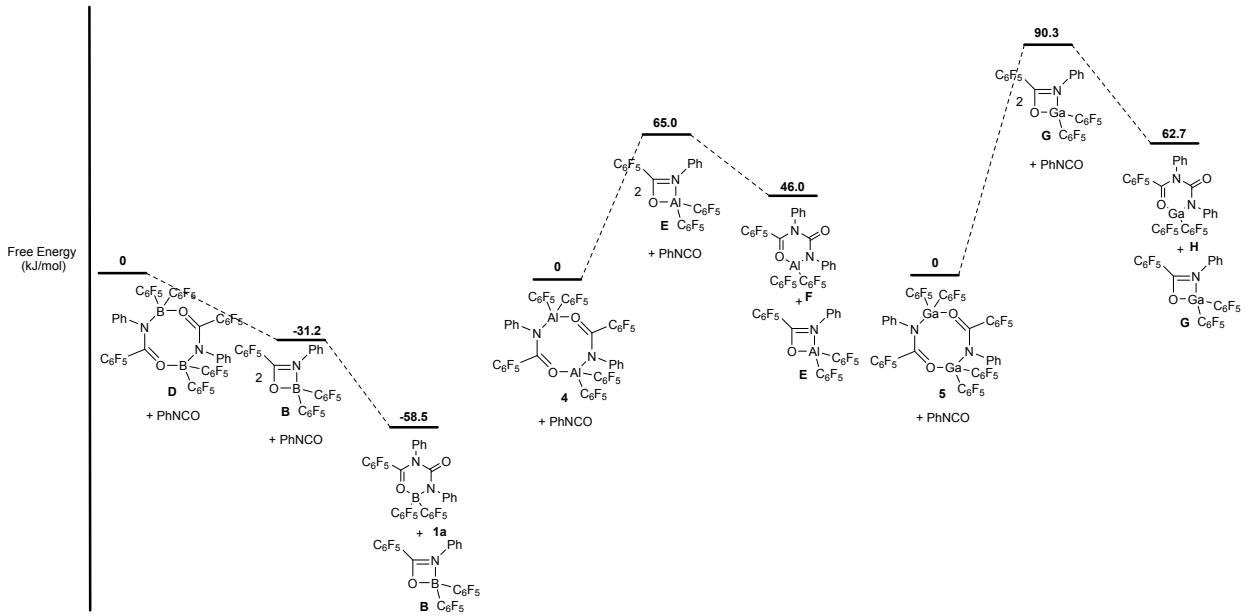


Figure S76. Computed energies for head-to-tail dimerization vs PhNCO capture.

Table S6. Computed energies for head-to-tail dimerization vs PhNCO capture

Description	E [a.u.]	ΔE [kJ/mol]	G [a.u]	ΔG (kJ/mol}
D + PhNCO	-5610.07	0	-5609.58	0
2**B** + PhNCO	-5610.05	62.08404	-5609.59	-31.2461
1a + **B**	-5610.09	-42.2275	-5609.6	-58.5145
4 + PhNCO	-6045.17	0	-6044.7	0
2**E** + PhNCO	-6045.12	143.4915	-6044.68	65.04414
F+ **E**	-6045.15	53.41148	-6044.68	45.96463
5 + PhNCO	-9405.81	0	-9405.34	0
2**G** + PhNCO	-9405.74	176.4574	-9405.3	90.3067
H + **G**	-9405.78	78.17722	-9405.31	62.7337

6.1 Geometry Optimized Structures

6.1.1. PhNCO

Charge = 0 Multiplicity = 1

O	-2.0722	-0.46787	0.
C	-0.6422	-0.46789	0.
N	0.6514	-0.4679	0.00001
C	2.1214	-0.46791	0.00002
C	2.81892	-0.94869	-1.10848
C	2.8189	0.0128	1.10815
C	4.21364	-0.94934	-1.1085
H	2.26874	-1.32832	-1.98164
C	4.21404	0.01314	1.1079
H	2.2693	0.39193	1.98184
C	4.91146	-0.46794	-0.00011
H	4.7635	-1.32885	-1.98194
H	4.76372	0.39261	1.98159
H	6.01114	-0.4685	-0.00038

6.1.2. CyNCO

Charge = 0 Multiplicity = 1

O	-2.0722	-0.46787	0.
C	-0.6422	-0.46789	0.
N	0.6514	-0.4679	0.00001
C	2.1214	-0.46791	0.00002
C	2.62941	-1.89081	-0.11423
C	2.62942	0.38976	-1.1414
H	2.45877	-0.02855	0.97537
C	4.14144	-1.93166	-0.20157
H	2.19035	-2.37077	-1.02814
H	2.28865	-2.48352	0.77414
C	4.14152	0.34954	-1.22821
H	2.19049	0.02384	-2.10669
H	2.2896	1.44803	-0.99635
C	4.65049	-1.073	-1.3412
H	4.48075	-2.98991	-0.3481
H	4.58052	-1.5676	0.76438
H	4.48228	0.94184	-2.11681
H	4.57991	0.8305	-0.31444
H	5.77146	-1.07208	-1.33891
H	4.31568	-1.51248	-2.31747

6.1.3. Compound 1a

Charge = 0 Multiplicity = 1

F	-2.9232	6.49211	9.10782
F	-1.87491	10.3524	7.27272
F	2.05138	7.30538	13.32688
F	0.7327	8.99796	7.45296
F	4.25924	5.78904	13.5981
F	1.77703	6.08986	8.78543

F	-3.01237	5.14959	6.81364
F	5.26393	4.45317	11.44788
F	4.06716	4.65928	9.03005
F	-0.235	10.72488	11.70136
F	-1.96669	12.98113	7.08543
F	0.61111	7.6371	5.15378
O	0.41058	8.4176	10.26051
F	-1.34277	14.54872	9.22374
O	-2.59879	6.92106	12.44527
F	-1.25336	5.68893	4.82357
F	-0.42718	13.3904	11.51684
N	-0.50957	6.74842	11.5086
N	-1.99896	8.44756	10.83098
C	0.52325	7.34867	10.93943
C	-1.83987	7.39506	11.63867
C	-1.11969	7.86338	8.37309
C	-2.03509	6.84045	8.15163
C	-1.47022	11.04828	8.35427
C	1.86839	6.71775	11.05073
C	-3.24778	9.16744	10.9692
C	-1.02178	10.39763	9.49161
C	2.41703	6.06641	9.9567
C	2.5351	6.64788	12.26143
C	3.57314	5.31543	10.07629
C	-0.22411	8.06003	7.32447
C	3.67726	5.8929	12.40396
C	-0.39434	5.42719	12.1101
C	-2.09762	6.12041	6.97664
C	4.18513	5.22052	11.30916
C	-0.25537	7.36841	6.14159
C	-1.56454	12.42471	8.24049
C	-4.10015	9.28936	9.88464
H	-3.8806	8.89656	9.07076

C	-0.68056	11.24519	10.53614
C	-1.20961	6.39175	5.96585
C	-0.22448	5.29917	13.47856
H	-0.12973	6.05012	14.01892
C	-1.23815	13.21482	9.31536
C	-0.78576	12.62026	10.47334
C	-0.53352	4.3366	11.28436
H	-0.64221	4.44556	10.36719
C	-3.56084	9.75744	12.17904
H	-2.98568	9.66972	12.90457
B	-1.00311	8.7909	9.70959
C	-5.60151	10.59831	11.23004
H	-6.39376	11.07701	11.31992
C	-5.28728	10.00313	10.01973
H	-5.8688	10.08029	9.29809
C	-4.73911	10.48221	12.30579
H	-4.94861	10.89	13.11494
C	-0.19905	4.02403	14.02396
H	-0.07754	3.91364	14.93935
C	-0.50811	3.06549	11.85197
H	-0.59574	2.31401	11.31113
C	-0.35354	2.91859	13.21214
H	-0.35322	2.06747	13.58699

6.1.4. Compound A

Charge = 0 Multiplicity = 1

F	1.57204	1.73299	2.28988
F	3.16526	2.27492	-0.75515
F	-2.45793	-2.95679	-1.18524
F	-0.55167	2.35037	-1.88768
F	-4.79826	-2.89296	-2.54094
F	-2.83408	1.6544	-0.3215

F	0.87974	4.19575	2.99674
F	-6.14555	-0.55301	-2.79726
F	-5.16425	1.72114	-1.6912
F	1.52018	-2.10523	-1.51355
F	5.51437	1.55032	-1.77888
F	-1.22954	4.84604	-1.16074
O	-0.26473	-0.2737	-0.80283
F	5.89531	-0.98427	-2.6705
O	-0.00553	-3.05019	2.00299
F	-0.51657	5.78338	1.2959
F	3.8828	-2.79775	-2.53337
N	-1.11145	-1.22399	1.10478
N	1.24369	-1.12652	1.49499
C	-1.25312	-0.69425	-0.07466
C	0.22748	-1.92481	1.60863
C	0.5208	1.92534	0.16959
C	0.87861	2.44854	1.40973
C	3.29097	1.01967	-1.18673
C	-2.58143	-0.64721	-0.74503
C	2.5431	-1.63357	1.6767
C	2.21791	0.12528	-1.10384
C	-3.28692	0.54203	-0.89288
C	-3.10963	-1.80636	-1.30807
C	-4.49249	0.58458	-1.57802
C	-0.19113	2.78058	-0.67102
C	-4.31036	-1.78421	-2.00403
C	-2.29165	-1.47552	1.88714
C	0.53078	3.738	1.79906
C	-4.9987	-0.58321	-2.13978
C	-0.54877	4.07378	-0.32052
C	4.52511	0.66569	-1.71219
C	3.56861	-0.70985	1.92755
H	3.31154	0.3375	2.03063

C	2.46603	-1.17143	-1.57518
C	-0.18389	4.55312	0.93099
C	-2.80153	-2.76278	2.03389
H	-2.30335	-3.59227	1.54976
C	4.72305	-0.63143	-2.16821
C	3.68935	-1.55818	-2.09979
C	-2.89066	-0.38312	2.51198
H	-2.46037	0.60661	2.39189
C	2.88302	-2.99089	1.54948
H	2.10427	-3.72073	1.3643
B	0.8746	0.50028	-0.42417
C	5.21872	-2.47309	1.92078
H	6.25032	-2.79886	2.0156
C	4.88813	-1.12649	2.05083
H	5.66323	-0.39137	2.25039
C	4.20731	-3.39675	1.67156
H	4.44863	-4.45133	1.56867
C	-3.93744	-2.94604	2.81556
H	-4.34367	-3.94542	2.93674
C	-4.02733	-0.58166	3.28767
H	-4.49805	0.26518	3.77718
C	-4.55058	-1.86276	3.44011
H	-5.43575	-2.01771	4.04948

6.1.5. Compound B

Charge = 0 Multiplicity = 1

F	0.95004	2.25489	2.17371
F	3.55836	1.33294	-1.01499
F	-2.99465	-2.74255	0.68235
F	0.7644	1.30823	-2.46237
F	-5.17474	-3.344	-0.79023
F	-2.19606	1.01619	-2.04898

F	0.55531	4.82399	1.65107
F	-5.85633	-1.77896	-2.89597
F	-4.36784	0.39491	-3.52962
F	1.27493	-2.7742	-0.43859
F	5.48847	0.06136	-2.32771
F	0.37039	3.90641	-2.96211
O	-0.23139	-0.55025	-0.56471
F	5.35458	-2.62724	-2.71988
F	0.26122	5.6911	-0.91042
F	3.22757	-4.02932	-1.75882
N	-1.32861	-0.30073	1.41105
C	-1.30179	-0.54619	0.10267
C	0.88007	1.64723	-0.12739
C	0.81329	2.60014	0.88602
C	3.4108	0.01508	-1.20027
C	-2.54549	-0.84364	-0.6429
C	2.29429	-0.6525	-0.70672
C	-2.90141	-0.06482	-1.74423
C	-3.32753	-1.95591	-0.33349
C	-4.02256	-0.36773	-2.50341
C	0.7197	2.14645	-1.42079
C	-4.44603	-2.27839	-1.08791
C	-2.56505	0.01644	2.07145
C	0.61062	3.95655	0.64301
C	-4.79037	-1.48073	-2.17451
C	0.51632	3.48814	-1.70731
C	4.44209	-0.62651	-1.87647
C	2.28515	-2.0312	-0.91294
C	0.4596	4.40196	-0.66154
C	-3.10687	-0.83815	3.02717
H	-2.59021	-1.7526	3.28795
C	4.37846	-1.99842	-2.07525
C	3.29178	-2.71078	-1.58532

C	-3.19153	1.21509	1.7364
H	-2.73089	1.87769	1.00895
B	1.06888	0.04085	0.08267
C	-4.30399	-0.48594	3.63978
H	-4.7337	-1.14469	4.38778
C	-4.39274	1.55201	2.35012
H	-4.88516	2.48423	2.09221
C	-4.94871	0.70158	3.30169
H	-5.88289	0.968	3.78657

6.1.6. Compound C

Charge = 0 Multiplicity = 1

F	-3.12905	-0.57865	2.01355
F	-1.17363	-3.09873	-0.73291
F	-4.76682	1.25349	2.99304
F	-0.19647	0.04974	2.67531
F	-0.61704	-5.05835	0.93936
F	-1.32042	2.66297	-0.93901
O	0.27858	0.70769	-0.14817
F	2.45166	0.68098	2.13371
F	-4.72115	3.80478	2.04692
F	2.84729	1.61671	-2.46468
F	5.67888	3.7281	0.61976
F	4.46765	2.40661	2.65708
F	-2.97768	4.47538	0.06693
F	0.17593	-4.5392	3.49353
F	0.38305	-1.9567	4.33665
F	4.87175	3.32921	-1.94129
O	-0.27101	-1.49783	-3.38072
N	-1.48841	-0.51655	-1.56207
N	1.56166	-0.94225	-1.03228
C	2.58598	1.12356	-0.17518

C	-2.07859	0.95702	0.53171
C	1.45086	0.19672	-0.47523
C	-0.7069	-1.40642	0.88545
C	-3.01531	0.65968	1.52207
C	-3.89925	1.59799	2.04549
C	-2.11578	2.27415	0.06615
C	-0.79758	-2.74214	0.51005
C	-0.51111	-3.8012	1.36448
C	-0.29726	-1.19868	2.20348
C	-2.9473	-0.39389	-1.9754
H	-3.43234	-0.06677	-1.05296
C	2.813	-1.51947	-1.30216
C	3.23051	1.80161	-1.20348
C	-2.98605	3.23873	0.55789
C	-3.87978	2.89902	1.56492
C	4.05831	2.21807	1.408
C	-0.78062	-1.03472	-2.45339
C	3.01432	1.34688	1.12801
C	-0.10434	-3.54071	2.66415
C	0.00324	-2.22322	3.08985
C	4.68281	2.89157	0.3639
C	3.17621	-1.79492	-2.62386
H	2.50345	-1.51209	-3.42691
C	3.6679	-1.89455	-0.25956
H	3.36499	-1.70409	0.76637
B	-0.95288	-0.08158	-0.02375
C	-3.11232	0.68186	-3.04185
H	-2.56044	0.38049	-3.94431
H	-2.67304	1.62063	-2.69277
C	4.27259	2.68304	-0.94765
C	-3.54238	-1.72898	-2.40691
H	-3.40643	-2.4721	-1.61661
H	-3.01415	-2.1016	-3.2962

C	-5.0228	-1.5441	-2.74674
H	-5.44107	-2.50039	-3.07767
H	-5.56996	-1.26479	-1.83581
C	-4.592	0.85477	-3.38863
H	-5.1231	1.25155	-2.51242
H	-4.69608	1.60514	-4.17927
C	-5.22514	-0.46873	-3.81191
H	-4.77102	-0.80314	-4.75504
H	-6.29323	-0.33073	-4.01156
C	5.24677	-2.77799	-1.8585
H	6.19151	-3.26687	-2.07568
C	4.87796	-2.51901	-0.54131
H	5.53356	-2.80722	0.27545
C	4.39125	-2.41281	-2.89546
H	4.66973	-2.61341	-3.92607

6.1.7. Compound 2

Charge = 0 Multiplicity = 1

F	5.39753	4.26692	17.0257
F	9.37736	3.54783	15.54727
F	2.76281	4.61804	17.23602
F	6.85788	7.00777	17.58443
F	10.78619	3.28716	17.75778
F	5.47737	7.34957	13.42884
O	7.75072	7.02069	14.71963
F	10.11075	8.11993	16.32055
F	1.46055	6.31245	15.59681
F	8.91926	8.84649	11.82379
F	11.46066	12.03507	14.11075
F	11.36297	10.52263	16.35274
F	2.84747	7.69054	13.69406
F	10.2854	4.85453	19.9302

F	8.31588	6.7204	19.80226
F	10.2285	11.18764	11.84514
O	8.92242	4.1858	12.16166
N	7.47755	4.70165	13.88009
N	9.32828	6.08676	13.38364
C	9.5112	8.41778	14.06181
C	5.57999	5.82927	15.24882
C	8.82456	7.09692	14.05279
C	8.00775	5.27742	16.45429
C	4.81818	5.14891	16.18778
C	3.44866	5.30459	16.31242
C	4.85885	6.66968	14.41814
C	9.037	4.3545	16.57385
C	9.79951	4.19778	17.72047
C	7.81076	6.04866	17.59057
C	6.56151	3.57049	13.58199
H	5.92499	3.57298	14.32715
C	10.65995	6.1804	12.79975
C	9.54238	9.22558	12.94241
C	3.49041	6.8547	14.51514
C	2.79248	6.16403	15.47576
C	10.75811	10.10457	15.2376
C	8.53363	4.85293	13.08275
C	10.11452	8.88239	15.21667
C	9.55372	4.98139	18.80999
C	8.54835	5.92555	18.74936
C	10.80666	10.87269	14.1016
C	10.82646	6.55339	11.49025
H	10.09207	6.70989	10.94156
C	11.72311	5.90851	13.62732
H	11.58633	5.63906	14.50685
B	7.18452	5.61629	15.07492
C	5.72303	3.84234	12.38359

H	6.29359	3.88896	11.60053
H	5.28988	4.704	12.48769
C	10.19447	10.44601	12.94445
C	7.14785	2.20025	13.60524
H	7.58103	2.04986	14.46001
H	7.82106	2.12629	12.91083
C	6.08846	1.14928	13.38925
H	6.51786	0.2847	13.29429
H	5.51831	1.11164	14.17309
C	4.67287	2.78543	12.16647
H	4.00004	2.85967	12.86122
H	4.23768	2.94146	11.31374
C	5.23725	1.40526	12.18021
H	5.77122	1.27211	11.38143
H	4.50967	0.76401	12.16203
C	13.20177	6.44288	11.81493
H	14.06428	6.54322	11.48189
C	13.01224	6.04717	13.11378
H	13.74731	5.87026	13.65534
C	12.1221	6.69135	11.00475
H	12.25832	6.95435	10.12318

6.1.8. Compound D

Charge = 0 Multiplicity = 1

F	1.44404	8.45374	4.20154
F	7.56381	12.52469	1.87866
F	3.35802	14.61265	1.73805
F	1.58032	12.2969	1.46581
O	4.24318	9.37695	3.89776
F	2.43962	10.15881	7.07838
O	4.4801	12.30309	3.61074
F	2.49606	14.22616	4.68793

F	5.79561	7.72578	2.0103
F	-0.11694	10.56066	7.71085
F	7.57443	8.47776	4.0538
F	-0.08985	14.60651	5.28554
F	6.18413	5.75628	0.24569
F	3.627	7.34619	6.36124
F	-0.9566	12.84693	2.11654
F	7.2143	13.23965	4.46881
N	4.49977	11.27052	1.62766
F	-1.0955	9.04082	4.88049
F	8.73642	14.82564	1.09894
F	-2.30337	11.23152	3.84795
F	4.35825	5.27684	-1.68327
F	1.70938	8.79873	-0.06142
N	5.25911	10.32178	5.66071
F	-1.4209	12.76768	6.81775
F	2.10718	6.78603	-1.82604
F	7.2116	16.98586	0.48473
F	4.5254	16.88714	0.81674
F	8.89352	15.01759	5.61589
F	4.63103	4.89225	6.89079
F	4.43469	13.41915	8.23044
F	6.16333	15.11766	9.40906
F	8.58217	6.01215	4.55679
C	4.78802	12.29121	2.37053
F	7.08768	4.21312	5.99106
F	8.37305	15.94399	8.10926
C	3.71868	8.32019	1.07736
C	2.58358	12.18646	5.86489
C	5.73276	13.30961	6.27326
C	1.62235	10.34146	2.80379
C	5.00852	9.30146	4.91203
C	5.43337	13.52441	1.82604

C	4.80348	11.27695	0.2075
C	4.84008	7.51969	1.08234
C	1.86425	11.29411	6.61855
C	6.11266	10.14451	6.82439
C	5.59105	7.9539	5.2042
C	6.80445	13.59838	1.65339
C	0.87417	9.5558	3.67199
C	5.85898	10.50926	-0.25565
H	6.4057	10.05031	0.34031
C	4.00141	11.9875	-0.67563
H	3.29933	12.50913	-0.35857
C	7.41108	14.76722	1.2334
C	0.94821	11.45416	2.31076
C	1.86556	13.28605	5.43162
C	0.52594	11.46387	6.95553
C	4.68437	14.65639	1.55213
C	-1.03917	10.93882	3.50931
C	-0.42421	9.83779	4.0289
C	6.63231	15.86383	0.93294
C	6.91182	13.7269	5.69391
C	5.50608	13.77186	7.53821
C	-0.35007	11.77327	2.64111
C	2.82964	8.06875	0.0664
C	5.29829	11.1273	-2.51163
H	5.46124	11.06991	-3.42631
C	7.47139	10.33028	6.71649
H	7.85106	10.55782	5.89975
C	6.08944	10.43377	-1.62683
H	6.78641	9.90738	-1.94722
C	-0.1311	12.58135	6.49737
C	5.53441	9.81747	8.03953
H	4.61629	9.69125	8.10594
C	0.53561	13.50861	5.72047

C	4.84247	7.02376	5.90971
C	5.07754	6.49962	0.17762
C	5.26648	15.81121	1.0923
C	8.27305	10.1778	7.84697
H	9.19397	10.29735	7.78223
C	4.26239	11.90901	-2.04018
H	3.73438	12.38549	-2.63945
C	6.35087	9.68024	9.16172
H	5.97149	9.47339	9.98509
C	6.6085	5.42271	5.73043
C	4.1548	6.26404	-0.80678
C	6.85044	7.59552	4.75433
C	7.79555	14.61008	6.25832
C	7.70947	9.84907	9.06045
H	8.24935	9.74218	9.81079
C	3.00392	7.02535	-0.8599
C	7.35521	6.33473	5.02492
C	5.34059	5.76363	6.19192
C	6.393	14.67837	8.15574
C	7.54185	15.07284	7.51828
B	3.47813	9.80533	2.36621
B	4.49349	12.071	5.36224

6.1.9. Compound 4

Charge = 0 Multiplicity = 1

Al	1.62228	0.53318	1.01907
Al	-1.65411	0.1548	-1.1871
F	3.45843	2.79141	0.10669
F	-0.87543	-3.27291	2.5078
F	-3.23308	0.80415	2.45903
F	-0.77388	2.4253	2.18225
O	1.14826	0.28457	-0.71144

F	0.48006	2.25431	-2.61063
O	-1.21684	-0.21361	0.51586
F	-3.60162	2.20272	-0.23021
F	2.27692	-2.39899	0.65535
F	0.46446	4.92578	-2.56271
F	1.30595	-3.30401	-2.17417
F	-3.6317	4.90132	-0.24013
F	4.53142	-3.84383	0.91785
F	3.33671	0.96049	-2.28314
F	-1.07354	5.07059	2.00826
F	-2.68238	-2.68117	-0.38645
N	0.28274	-0.38319	2.11895
F	3.18118	5.46102	0.02927
F	-2.92465	-4.44147	3.8215
F	0.90213	6.61476	0.96755
F	6.8211	-2.64038	1.77117
F	4.59361	1.45437	2.10306
N	-0.1891	-0.75298	-2.12331
F	-1.57668	6.26777	-1.3844
F	6.82899	0.00975	2.35207
F	-5.12955	-2.9914	4.45119
F	-5.28687	-0.37143	3.7726
F	-5.09641	-3.84386	-0.63753
F	5.6153	-0.15929	-3.15694
F	-4.24301	1.05394	-2.81899
F	-6.64769	-0.1148	-3.06076
F	3.58291	-4.40085	-3.0746
C	-0.9192	-0.56316	1.67159
F	5.74444	-2.83776	-3.56087
F	-7.08583	-2.56609	-1.98048
C	3.34247	-0.40517	1.34418
C	-1.57231	2.11561	-1.42271
C	-3.37423	-0.75057	-1.56499

C	1.39044	2.49273	1.20269
C	1.00616	-0.51192	-1.67899
C	-1.99438	-1.19834	2.48186
C	0.5772	-0.62841	3.50093
C	3.39809	-1.76556	1.0712
C	-0.55732	2.86094	-2.00817
C	-0.39303	-1.3146	-3.41952
C	2.23205	-1.13015	-2.24092
C	-1.9373	-2.54332	2.83282
C	2.35691	3.32816	0.65153
C	1.34303	-1.73615	3.86096
H	1.66824	-2.42864	3.0935
C	0.12658	0.26886	4.47049
H	-0.44746	1.13777	4.16506
C	-2.98946	-3.15718	3.49833
C	0.2461	3.13465	1.65876
C	-2.59747	2.85334	-0.84244
C	-0.53768	4.25034	-2.0038
C	-3.14599	-0.47849	2.79083
C	1.06251	5.30059	1.04387
C	2.2242	4.70842	0.56215
C	-4.12245	-2.4157	3.81519
C	-3.65314	-2.00343	-1.03561
C	-4.42089	-0.14429	-2.24892
C	0.05695	4.5086	1.58517
C	4.5374	0.16214	1.7725
C	1.18786	-1.06911	6.17612
H	1.4268	-1.24222	7.22095
C	-1.18717	-2.45179	-3.56357
H	-1.59034	-2.93469	-2.68011
C	1.6415	-1.95441	5.20162
H	2.22843	-2.82299	5.48425
C	-1.58475	4.94077	-1.40395

C	0.13649	-0.67553	-4.5429
H	0.69576	0.24674	-4.41786
C	-2.6311	4.24128	-0.81474
C	3.37209	-0.35186	-2.46348
C	4.54015	-2.54228	1.19941
C	-4.20505	-1.07201	3.46306
C	-1.42403	-2.96485	-4.83352
H	-2.03361	-3.85636	-4.9442
C	0.43062	0.03975	5.80863
H	0.07802	0.73531	6.56409
C	-0.10662	-1.19772	-5.80887
H	0.30034	-0.69633	-6.68169
C	4.61986	-2.29036	-3.1334
C	5.71006	-1.92834	1.63251
C	2.33036	-2.50791	-2.44665
C	-4.88199	-2.63681	-1.15799
C	-0.88259	-2.34393	-5.95674
H	-1.07255	-2.74829	-6.94617
C	5.71148	-0.56983	1.92517
C	3.50742	-3.08986	-2.89472
C	4.55399	-0.91723	-2.92132
C	-5.67294	-0.73021	-2.3978
C	-5.9006	-1.98459	-1.84436

6.1.10. Compound E

Charge = 0 Multiplicity = 1

F	0.95004	2.25489	2.17371
F	3.55836	1.33294	-1.01499
F	-2.99465	-2.74255	0.68235
F	0.7644	1.30823	-2.46237
F	-5.17474	-3.344	-0.79023
F	-2.19606	1.01619	-2.04898
F	0.55531	4.82399	1.65107
F	-5.85633	-1.77896	-2.89597

F	-4.36784	0.39491	-3.52962
F	1.27493	-2.7742	-0.43859
F	5.48847	0.06136	-2.32771
F	0.37039	3.90641	-2.96211
O	-0.23139	-0.55025	-0.56471
F	5.35458	-2.62724	-2.71988
F	0.26122	5.6911	-0.91042
F	3.22757	-4.02932	-1.75882
N	-1.32861	-0.30073	1.41105
C	-1.30179	-0.54619	0.10267
C	0.88007	1.64723	-0.12739
C	0.81329	2.60014	0.88602
C	3.4108	0.01508	-1.20027
C	-2.54549	-0.84364	-0.6429
C	2.29429	-0.6525	-0.70672
C	-2.90141	-0.06482	-1.74423
C	-3.32753	-1.95591	-0.33349
C	-4.02256	-0.36773	-2.50341
C	0.7197	2.14645	-1.42079
C	-4.44603	-2.27839	-1.08791
C	-2.56505	0.01644	2.07145
C	0.61062	3.95655	0.64301
C	-4.79037	-1.48073	-2.17451
C	0.51632	3.48814	-1.70731
C	4.44209	-0.62651	-1.87647
C	2.28515	-2.0312	-0.91294
C	0.4596	4.40196	-0.66154
C	-3.10687	-0.83815	3.02717
H	-2.59021	-1.7526	3.28795
C	4.37846	-1.99842	-2.07525
C	3.29178	-2.71078	-1.58532
C	-3.19153	1.21509	1.7364
H	-2.73089	1.87769	1.00895
C	-4.30399	-0.48594	3.63978
H	-4.7337	-1.14469	4.38778
C	-4.39274	1.55201	2.35012
H	-4.88516	2.48423	2.09221
C	-4.94871	0.70158	3.30169
H	-5.88289	0.968	3.78657

Al	1.06888	0.04085	0.08267

6.1.11. Compound F

Charge = 0 Multiplicity = 1

F	-2.9232	6.49211	9.10782
F	-1.87491	10.3524	7.27272
F	2.05138	7.30538	13.32688
F	0.7327	8.99796	7.45296
F	4.25924	5.78904	13.5981
F	1.77703	6.08986	8.78543
F	-3.01237	5.14959	6.81364
F	5.26393	4.45317	11.44788
F	4.06716	4.65928	9.03005
F	-0.235	10.72488	11.70136
F	-1.96669	12.98113	7.08543
F	0.61111	7.6371	5.15378
O	0.41058	8.4176	10.26051
F	-1.34277	14.54872	9.22374
O	-2.59879	6.92106	12.44527
F	-1.25336	5.68893	4.82357
F	-0.42718	13.3904	11.51684
N	-0.50957	6.74842	11.5086
N	-1.99896	8.44756	10.83098
C	0.52325	7.34867	10.93943
C	-1.83987	7.39506	11.63867
C	-1.11969	7.86338	8.37309
C	-2.03509	6.84045	8.15163
C	-1.47022	11.04828	8.35427
C	1.86839	6.71775	11.05073
C	-3.24778	9.16744	10.9692
C	-1.02178	10.39763	9.49161
C	2.41703	6.06641	9.9567

C	2.5351	6.64788	12.26143
C	3.57314	5.31543	10.07629
C	-0.22411	8.06003	7.32447
C	3.67726	5.8929	12.40396
C	-0.39434	5.42719	12.1101
C	-2.09762	6.12041	6.97664
C	4.18513	5.22052	11.30916
C	-0.25537	7.36841	6.14159
C	-1.56454	12.42471	8.24049
C	-4.10015	9.28936	9.88464
H	-3.8806	8.89656	9.07076
C	-0.68056	11.24519	10.53614
C	-1.20961	6.39175	5.96585
C	-0.22448	5.29917	13.47856
H	-0.12973	6.05012	14.01892
C	-1.23815	13.21482	9.31536
C	-0.78576	12.62026	10.47334
C	-0.53352	4.3366	11.28436
H	-0.64221	4.44556	10.36719
C	-3.56084	9.75744	12.17904
H	-2.98568	9.66972	12.90457
C	-5.60151	10.59831	11.23004
H	-6.39376	11.07701	11.31992
C	-5.28728	10.00313	10.01973
H	-5.8688	10.08029	9.29809
C	-4.73911	10.48221	12.30579
H	-4.94861	10.89	13.11494
C	-0.19905	4.02403	14.02396
H	-0.07754	3.91364	14.93935
C	-0.50811	3.06549	11.85197
H	-0.59574	2.31401	11.31113
C	-0.35354	2.91859	13.21214
H	-0.35322	2.06747	13.58699

Al	-1.00311	8.7909	9.70959

6.1.12. Compound 5

Charge = 0 Multiplicity = 1

Ga	1.82332	0.81301	-0.65233
F	-1.74301	3.55948	0.26774
F	4.2862	-0.92175	-0.68738
F	-2.82538	0.37521	-3.04191
O	-0.99631	-0.00772	-0.88001
F	-4.13661	4.7288	-0.07824
F	-5.22056	1.56767	-3.39136
F	1.87353	2.60819	1.90133
F	0.41482	-0.36327	-3.33787
F	3.80576	4.21707	2.88407
F	1.25165	-2.32574	-4.95363
F	4.57575	1.6668	-1.8467
F	3.57693	-3.62083	-4.45131
F	5.09432	-2.9228	-2.29961
F	6.49382	3.28895	-0.86559
F	6.11364	4.55954	1.49925
F	-5.87707	3.74305	-1.91492
N	0.24279	1.81742	-1.23915
C	3.18229	2.04419	0.01997
C	3.02005	2.72831	1.21425
C	2.31565	-0.58146	-1.93521
C	0.41891	3.09637	-1.84209
C	5.17275	3.7532	1.02479
C	-0.92439	1.23461	-1.16199
C	-2.19721	1.96297	-1.41373
C	3.99061	3.57339	1.73477
C	0.79969	4.19051	-1.06696
H	0.8616	4.07477	0.00955

C	-2.55913	3.08305	-0.66817
C	4.36599	2.26347	-0.66569
C	0.91033	5.54339	-3.06403
H	1.09536	6.50203	-3.53889
C	3.51303	-1.25125	-1.73938
C	-3.79831	3.68649	-0.8245
C	-3.1235	1.44964	-2.32158
C	0.55862	4.43943	-3.83603
H	0.47777	4.53003	-4.91496
C	0.32637	3.20948	-3.22968
H	0.0776	2.32852	-3.81423
C	3.95729	-2.28105	-2.55414
C	1.57097	-0.97074	-3.03816
C	3.17873	-2.64452	-3.64723
C	5.36599	3.09937	-0.18687
C	-4.69534	3.17205	-1.75333
C	-4.35932	2.05226	-2.50701
C	1.9841	-1.98051	-3.89929
C	1.02887	5.41629	-1.68195
H	1.30703	6.2745	-1.07789
Ga	-1.82333	-0.81302	0.65233
F	1.74299	-3.55947	-0.26778
F	-4.28623	0.92174	0.68747
F	2.82539	-0.37521	3.04187
O	0.99628	0.00771	0.88
F	4.13661	-4.72877	0.07815
F	5.22058	-1.56766	3.39128
F	-1.8736	-2.60819	-1.90134
F	-0.41474	0.36325	3.33781
F	-3.80587	-4.21704	-2.88405
F	-1.25152	2.3257	4.95362
F	-4.57576	-1.66678	1.84674
F	-3.57682	3.6208	4.45139

F	-5.09428	2.92278	2.29974
F	-6.49385	-3.28891	0.86565
F	-6.11373	-4.55949	-1.4992
F	5.87709	-3.74301	1.91481
N	-0.24281	-1.81743	1.23913
C	-3.18233	-2.04419	-0.01995
C	-3.02012	-2.72829	-1.21424
C	-2.31563	0.58144	1.93523
C	-0.41892	-3.09639	1.84208
C	-5.17282	-3.75316	-1.02475
C	0.92437	-1.23462	1.16197
C	2.19721	-1.96298	1.4137
C	-3.99069	-3.57336	-1.73475
C	-0.79964	-4.19054	1.06695
H	-0.86151	-4.07481	-0.00957
C	2.55912	-3.08304	0.66812
C	-4.36602	-2.26345	0.66572
C	-0.91031	-5.54341	3.06401
H	-1.09533	-6.50206	3.53888
C	-3.51302	1.25123	1.73944
C	3.79831	-3.68647	0.82443
C	3.12351	-1.44964	2.32153
C	-0.55864	-4.43944	3.83602
H	-0.47782	-4.53003	4.91495
C	-0.3264	-3.20949	3.22967
H	-0.07767	-2.32852	3.81423
C	-3.95725	2.28103	2.55423
C	-1.57091	0.97071	3.03816
C	-3.17865	2.6445	3.6473
C	-5.36604	-3.09934	0.18691
C	4.69536	-3.17203	1.75324
C	4.35933	-2.05225	2.50694
C	-1.98401	1.98047	3.89931

C	-1.02881	-5.41632	1.68193
H	-1.30693	-6.27455	1.07787

6.1.13. Compound G

Charge = 0 Multiplicity = 1

F	0.95004	2.25489	2.17371
F	3.55836	1.33294	-1.01499
F	-2.99465	-2.74255	0.68235
F	0.7644	1.30823	-2.46237
F	-5.17474	-3.344	-0.79023
F	-2.19606	1.01619	-2.04898
F	0.55531	4.82399	1.65107
F	-5.85633	-1.77896	-2.89597
F	-4.36784	0.39491	-3.52962
F	1.27493	-2.7742	-0.43859
F	5.48847	0.06136	-2.32771
F	0.37039	3.90641	-2.96211
O	-0.23139	-0.55025	-0.56471
F	5.35458	-2.62724	-2.71988
F	0.26122	5.6911	-0.91042
F	3.22757	-4.02932	-1.75882
N	-1.32861	-0.30073	1.41105
C	-1.30179	-0.54619	0.10267
C	0.88007	1.64723	-0.12739
C	0.81329	2.60014	0.88602
C	3.4108	0.01508	-1.20027
C	-2.54549	-0.84364	-0.6429
C	2.29429	-0.6525	-0.70672
C	-2.90141	-0.06482	-1.74423
C	-3.32753	-1.95591	-0.33349
C	-4.02256	-0.36773	-2.50341
C	0.7197	2.14645	-1.42079

C	-4.44603	-2.27839	-1.08791
C	-2.56505	0.01644	2.07145
C	0.61062	3.95655	0.64301
C	-4.79037	-1.48073	-2.17451
C	0.51632	3.48814	-1.70731
C	4.44209	-0.62651	-1.87647
C	2.28515	-2.0312	-0.91294
C	0.4596	4.40196	-0.66154
C	-3.10687	-0.83815	3.02717
H	-2.59021	-1.7526	3.28795
C	4.37846	-1.99842	-2.07525
C	3.29178	-2.71078	-1.58532
C	-3.19153	1.21509	1.7364
H	-2.73089	1.87769	1.00895
C	-4.30399	-0.48594	3.63978
H	-4.7337	-1.14469	4.38778
C	-4.39274	1.55201	2.35012
H	-4.88516	2.48423	2.09221
C	-4.94871	0.70158	3.30169
H	-5.88289	0.968	3.78657
Ga	1.06888	0.04085	0.08267

6.1.14. Compound H

Charge = 0 Multiplicity = 1

F	-2.9232	6.49211	9.10782
F	-1.87491	10.3524	7.27272
F	2.05138	7.30538	13.32688
F	0.7327	8.99796	7.45296
F	4.25924	5.78904	13.5981
F	1.77703	6.08986	8.78543
F	-3.01237	5.14959	6.81364
F	5.26393	4.45317	11.44788

F	4.06716	4.65928	9.03005
F	-0.235	10.72488	11.70136
F	-1.96669	12.98113	7.08543
F	0.61111	7.6371	5.15378
O	0.41058	8.4176	10.26051
F	-1.34277	14.54872	9.22374
O	-2.59879	6.92106	12.44527
F	-1.25336	5.68893	4.82357
F	-0.42718	13.3904	11.51684
N	-0.50957	6.74842	11.5086
N	-1.99896	8.44756	10.83098
C	0.52325	7.34867	10.93943
C	-1.83987	7.39506	11.63867
C	-1.11969	7.86338	8.37309
C	-2.03509	6.84045	8.15163
C	-1.47022	11.04828	8.35427
C	1.86839	6.71775	11.05073
C	-3.24778	9.16744	10.9692
C	-1.02178	10.39763	9.49161
C	2.41703	6.06641	9.9567
C	2.5351	6.64788	12.26143
C	3.57314	5.31543	10.07629
C	-0.22411	8.06003	7.32447
C	3.67726	5.8929	12.40396
C	-0.39434	5.42719	12.1101
C	-2.09762	6.12041	6.97664
C	4.18513	5.22052	11.30916
C	-0.25537	7.36841	6.14159
C	-1.56454	12.42471	8.24049
C	-4.10015	9.28936	9.88464
H	-3.8806	8.89656	9.07076
C	-0.68056	11.24519	10.53614
C	-1.20961	6.39175	5.96585

C	-0.22448	5.29917	13.47856
H	-0.12973	6.05012	14.01892
C	-1.23815	13.21482	9.31536
C	-0.78576	12.62026	10.47334
C	-0.53352	4.3366	11.28436
H	-0.64221	4.44556	10.36719
C	-3.56084	9.75744	12.17904
H	-2.98568	9.66972	12.90457
C	-5.60151	10.59831	11.23004
H	-6.39376	11.07701	11.31992
C	-5.28728	10.00313	10.01973
H	-5.8688	10.08029	9.29809
C	-4.73911	10.48221	12.30579
H	-4.94861	10.89	13.11494
C	-0.19905	4.02403	14.02396
H	-0.07754	3.91364	14.93935
C	-0.50811	3.06549	11.85197
H	-0.59574	2.31401	11.31113
C	-0.35354	2.91859	13.21214
H	-0.35322	2.06747	13.58699
Ga	-1.00311	8.7909	9.70959

7. References

1. C. H. Lee, S. J. Lee, J. W. Park, K. H. Kim, B. Y. Lee, J. S. Oh, *J. Mol. Catal. A: Chem* **1998**, *132*, 231.
2. K. Ludovici, W. Tyrra, D. Naumann, *J. Organomet. Chem.* **1992**, *441*, 363.
3. J. Cosier, A. M. Glazer, *J. Appl. Cryst.* **1986**, *19*, 105.
4. CrysAlisPro, Agilent Technologies, Version 1.171.35.8.
5. G. M. Sheldrick, **2013**, SHELXS-2013.
6. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281.
7. P. Hohenberg, W. Kohn, *Phys. Rev. B* **1964**, *136*, B864.
8. W. Kohn, L. Sham, *J. Phys. Rev.* **1965**, *140*, A1133.
9. C. Peng, H. B. Schlegel, *Israel J. of Chem.* **1993**, *33*, 449.
10. C. Peng, P. Y. Ayala, H. B. Schlegel, M. J. J. Frisch, *Comp. Chem.* **1996**, *17*, 49.