Supporting Information

Tuning of electronic properties via labile N→B-coordination in conjugated organoboranes

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Contents

1. Experimental Section

1.1. Materials and Instrumentation

All reactions and manipulations of sensitive compounds were carried out under an atmosphere of pre-purified argon using either Schlenk techniques or an inert-atmosphere glovebox (MBraun Labmaster). Toluene, Et_2O, THF, DMF and dichloromethane were purified using a solvent purification system (MBraun; alumina / copper columns for hydrocarbon solvents). *N*-hexane, and benzene were dried by distillation from CaH_2 under argon atmosphere prior to use. Mes_2BF[1], different phenylazides[2] and 1,12-diazidododecane[3] were prepared according to literature.

Other reagents were commercially available (Aldrich, Acros, Alfa Aesar) and were either used as obtained or purified by standard procedures.[4] ^1H-, ^{13}C-, ^{19}F- and ^{11}B-NMR spectra were recorded at 293 K on a Bruker Avance DRX 400 (400 MHz) spectrometer or a Bruker Avance 500 AMX (500 MHz). Solution ^1H and ^{13}C NMR spectra were referenced internally to the solvent residual signals.[5] Solution ^{11}B-NMR spectra were recorded either on the Bruker Avance DRX 400 (400 MHz) spectrometer at the University of Ulm, or on a Bruker Avance III DPX 600 spectrometer at the Department of Inorganic Chemistry at the University of Heidelberg. ^{11}B-NMR spectra were referenced externally to $BF_3 \cdot Et_2O$ (10% in $CHCl_3$). Individual signals are referred to as singlet (s), doublet (d), triplet (t), multiplet (m), and broadened (br). Temperature calibration of the NMR spectrometer was performed using CH_3OH/CD_3OD (<298 K) and $HOCH_2CH_2OH/DMSO\text{-}d_6$ (>298 K).[6] High resolution mass spectrometry measurements were performed on a Bruker SolariX FTMS using MALDI (Matrix Assisted Laser Desorption Ionization). *Trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) was used as matrix in MALDI measurements. UV-visible absorption spectra and photoluminescence spectra were acquired on a Perkin Elmer Lambda 19 UV-vis/NIR spectrometer and a Perkin Elmer LS 55 fluorescence spectrometer, respectively. Fluorescence Lifetimes were measured on a **HORIBA** JOBIN YVON FluoroCube spectrometer equipped with a NanoLED light source and a TBX Picosecond Photon Detection Module. Elemental analyses were performed on an Elemental Vario EL analyzer. Melting points were measured on a Büchi M-565 melting point apparatus with a heating rate of 2 K/min. Cyclic voltammetry measurements were performed with an Autolab Potentiostat Galvanostat with a three electrode system, consisting of a Pt working electrode (0.785 mm^2), a Pt-counter electrode, and an Ag/AgCl-reference electrode. The measurements were carried out in THF or NCMe with $[N(n\text{-}Bu)_4][PF_6]$ (0.1 M) as supporting electrolyte, and were internally referenced against the ferrocene/ferrocenium redox-

couple.Thermalgravimetry measurements were recorded on a Mettler Toledo TGA/SDTA 851e, with an Alox70µL sample holder. Binding constants were determined by numerical fit of the UV-vis absorption titration spectra using the program HypSpec2014™ by Protonic Software (http://www.hyperquad.co.uk.). Deconvolution of UV-vis spectra was performed with Spekwin32-free optical spectroscopy software, Version 1.71.5, 2010, http://www.effemm2.de/spekwin/.
X-ray diffraction intensities were collected on an Agilent Technologies SuperNova single-crystal X-ray diffractometer at 150 K with Mo-Kα radiation. Crystal data and refinement parameters are collected in the Supporting Information. The structures were solved using direct methods (SIR92[ix] or Shlexs-2014[x]), completed by subsequent difference Fourier syntheses, and refined by full-matrix least-squares procedures. The crystallographic data for **Trz-Me** and **B_2-H** has been deposited with the Cambridge Crystallographic Data Centre under CCDC 1521412 and CCDC 1521490. These data can be obtained free of charge from www.ccdc.cam.ac.uk/data_request/cif.

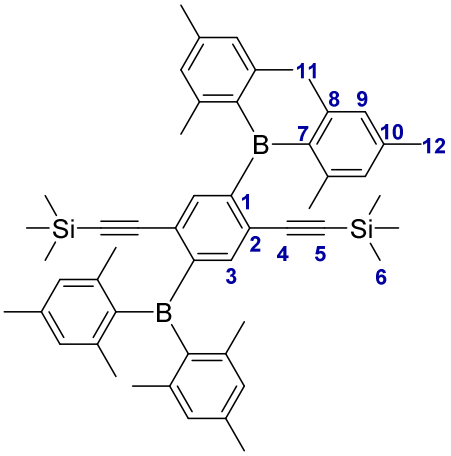
1.2. Synthetic Procedures

1.2.1. Preparation of 1,4-dibromo-2,5-bis(trimethylsilylethynyl)benzene (S1)[7,8]

Under an argon atmosphere 200 mL THF were added to 10.0 g (20.5 mmol) 1,4-dibromo-2,5-diiodobenzene, CuI (602 mg, 3.16 mmol) und $(Ph_3P)_2PdCl_2$ (1.02 g, 1.46 mmol). After the addition of DIPA (13.0 mL, 92.5 mmol), the solution was stirred for 10 min and was then cooled to 0 °C. According to trimethylsilylacetylene (6.40 mL, 45.1 mmol) was added dropwise, the mixture was stirred at room temperature for 48 h. Then water and diluted HCl (5%) were added followed by the extraction with diethyl ether. The combined organic layer was washed twice with saturated ammonium chloride-solution, 5% HCl, 1 M $NaHCO_3$-solution and saturated NaCl-solution and subsequent dried over Na_2SO_4. After the solvents were removed under reduced pressure and the residue was purified by a column chromatography over silica gel (SiO_2, petroleum ether/ethylacetat 100/1). Further purification by recrystallization from isopropanol gave **S1** in 58% yield (5.10 g, 11.9 mmol) as a pale yellow solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.68 (s, 2 H, 3), 0.28 (s, 18 H, 6) ppm.
^{13}C-NMR (100 MHz, $CDCl_3$): δ = 136.1 (3), 126.1 (2), 123.4 (1), 102.8 (4), 101.1 (5), -0.6 (6) ppm.

1.2.2. Preparation of 1,4-Bis(dimesitylboryl)-2,5-bis(trimethylsilylethynyl)-benzene (B_2-TMS)[9]



To a solution of 1,4-dibromo-2,5-bis(trimethylsilyl-ethynyl)benzene (429 mg, 1.00 mmol) in 8.0 mL dry THF was added a *n*-hexane solution of *n*-BuLi (1.31 mL, 2.10 mmol) dropwise at -78 °C. The mixture was stirred at the same temperature for 20 min. A solution of dimesitylboron fluoride (600 mg, 2.24 mmol) in THF (3 mL) was added to the mixture via syringe. The reaction mixture was warmed to room temperature gradually and stirred for 14 h. After the solvents were removed under reduced pressure, the resulting residue was suspended in *n*-hexane. The residue was separated through centrifugation (4000 U/5 min) and washed with diethyl ether to get 56% yield (431 mg, 562 µmol) of a white-yellow solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.33 (s, 2 H, 3), 6.75 (s, 8 H, 9), 2.27 (s, 12 H, 12), 1.98 (s, 24 H, 11), -0.06 (s, 18 H, 6) ppm.

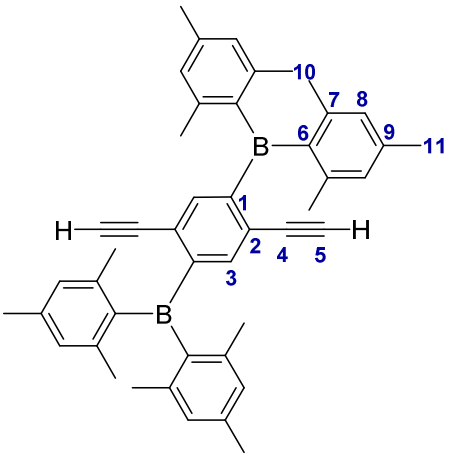
^{13}C-NMR (100 MHz, $CDCl_3$): δ = 152.7 (1), 142.5 (8), 141.1 (7), 139.4 (10), 137.5 (3), 128.5 (9), 125.8 (2), 104.6 (4), 99.2 (5), 23.5 (11), 21.4 (12), -0.17 (6) ppm.

mp 312.9-314.9 °C [Lit.: >300 °C]

MS (HR-MALDI, matrix: DCTB) for $C_{52}H_{64}B_2Si_2$: calc. m/z = 766.4733, found m/z = 766.4719([M^+]).

1.2.3. Preparation of 1,4-Diethynyl-2,5-bis(dimesitylboryl)benzene (B_2-H)[9]

To a solution of 300 mg (391 µmol) **B_2-TMS** in 8.0 mL dry THF was added a suspension of TBAF·SiO_2 (7.82 g, ca. 11.7 mmol F^-) in 11 mL THF. The mixture was stirred at room temperature for 17 h. The reaction mixture was filtered off and washed with THF. The resulting mixture was subjected to a silica gel column chromatography (petroleum ether/chloroform 2/1, R_f = 0.75) to afford 86% yield (208 mg, 335 mmol) of a white-yellow solid.

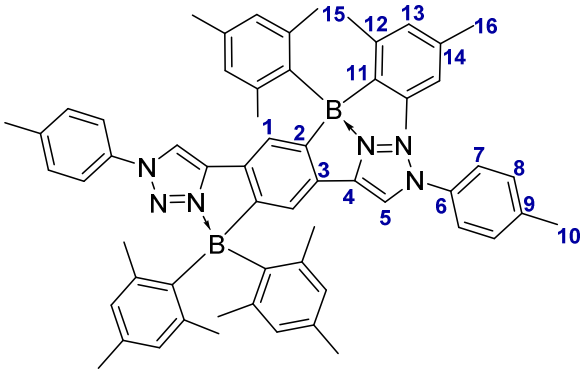


^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.40 (s, 2 H, 3), 6.75 (s, 8 H, 8), 2.74 (s, 2 H, 5), 2.28 (s, 12 H, 11), 2.00 (s, 24 H, 10) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 153.2 (1), 142.5 (7), 141.1 (6), 139.6 (9), 137.9 (3), 128.3 (8), 125.2 (2), 83.2(4), 81.7(5), 23.3 (10), 21.4 (11) ppm.

1.2.4. Preparation of 1,4-Bis(dimesitylboryl)-2,5-(Bis(1-(p-tolyl)-1*H*-1,2,3-triazol-4-yl))benzene (Trz-Me)

To a solution of 100 mg (87.1 µmol) **B_2-H** in 13 mL dry THF were added 3.24 mg (5.59 µmol, 15 mol%) CuI, 0.06 mL (345 µmol) diisopropylethylamine (DIPEA) and 64.4 mg (211 µmol) 4-azidotoluene. The mixture was stirred at 60-70 °C for 33 h, until repeated TLC control indicated that the reaction had come to completion. Subsequently, the solvent was removed under reduced pressure, and the residue was purified by repeated washing with dry *n*-hexane and diethyl ether to afford **Trz-Me** in 29% (41.2 mg, 46.1 µmol) yield as colorless solid.



^{1}H-NMR (400 MHz, C_6D_6): δ = 8.23 (s, 2 H, 5), 6.99 (s, 8 H, 13), 6.82 (d, 4 H, $^{3}J_{HH}$ = 8.5 Hz, 7/8), 6.87 (d, 4 H, $^{3}J_{HH}$ = 8.5 Hz, 7/8), 6.36 (s, 2 H, 1), 2.48 (br, 24 H, 15), 2.25 (s, 12 H, 16), 1.94 (s, 6 H, 10) ppm.

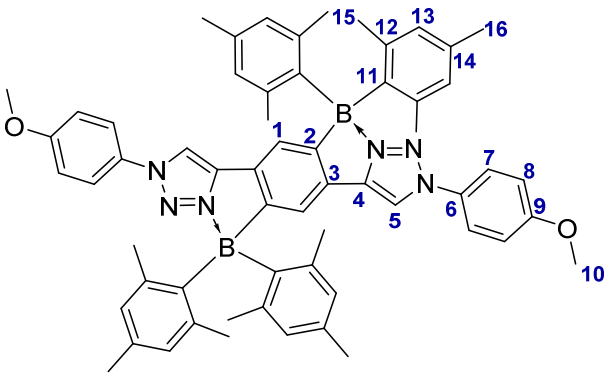
^{1}H-NMR (400 MHz, THF-d_8): δ = 8.89 (s, 2 H, 5), 7.90 (s, 2 H, 1), 7.75 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz, 7), 7.37 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz, 8), 6.52 (s, 8 H, 13), 2.39 (s, 6 H, 10), 2.10 (s, 12 H, 16), 1.90 (br, 24 H, 15) ppm.

^{13}C-NMR (100 MHz, THF-d_8): δ = 151.6 (4), 140.9 (9), 140.8 (12), 135.4 (9), 133.5 (14), 130.9 (8), 130.6 (3), 129.8 (13), 125.9 (1), 120.9 (7), 116.2 (5), 25.6 (15), 20.9 (10), 20.8 (16) ppm.

^{13}C-resonances of carbon atoms directly bonded to boron could not be observed.

MS (HR-MALDI, matrix: DCTB) for $C_{60}H_{62}B_2N_6$: calc. m/z = 888.5222, found m/z = 888.5203 ([M$^+$]). Also observed: ([M-Mes]$^+$): calc. m/z = 769.4361, found m/z = 769.4350, ([M-CH_3]$^+$): calc. m/z = 874.5066, found m/z = 874.5013.

1.2.5. Preparation of 1,4-Bis(dimesitylboryl)-2,5-(Bis(1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl))benzene (Trz-OMe)



To a solution of 50.2 mg (80.6 µmol) **B_2-H** in 6.0 mL dry THF were added 1.98 mg (10.4 µmol) CuI, 27.1 mg (204 µmol) 1-azido-4-methoxybenzene and 0.04 mL (230 µmol) DIPEA. The mixture was stirred at ambient temperature for several days, additional azide was then added and the mixture was heated to 70°C overnight, until TLC control indicated that the reaction had come to completion. Subsequently, the solvent was removed under reduced pressure, and the residue was washed with dry *n*-hexane to afford **Trz-OMe** in 68% yield (50.0 mg, 54.2 µmol) as a tanned solid.

^{1}H-NMR (400 MHz, C_6D_6): δ = 8.24 (s, 2 H, 5), 7.00 (s, 8 H, 13), 6.81 (d, 4 H, $^{3}J_{HH}$ = 9.1 Hz, 7/8), 6.45 (d, 4 H, $^{3}J_{HH}$ = 9.1 Hz, 7/8), 6.31 (s, 2 H, 1), 3.17 (s, 6 H, 10), 2.49 (br, 24 H, 15), 2.26 (s, 12 H, 16) ppm.

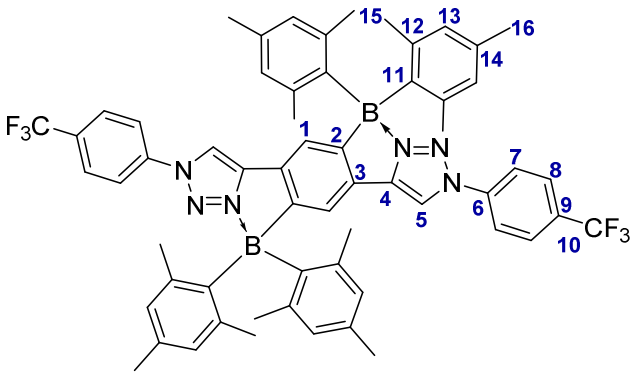
^{1}H-NMR (400 MHz, THF-d_8): δ = 8.80 (s, 2 H, 5), 7.90 (s, 2 H, 1), 7.75 (d, 4 H, $^{3}J_{HH}$ = 9.1 Hz, 7/8), 7.07 (d, 4 H, $^{3}J_{HH}$ = 9.1 Hz, 7/8), 6.52 (s, 8 H, 13), 3.83 (s, 6 H, 10), 2.10 (s, 12 H, 16), 1.90 (br, 24 H, 15) ppm.

^{13}C-NMR (100 MHz, THF-d_8): δ = 161.6 (9), 151.5 (4), 140.8 (12), 133.4 (14), 130.8 (6), 130.6 (3), 129.8 (13), 125.8 (1), 122.6 (7/8), 116.2 (5), 115.5 (7/8), 55.8 (10), 25.6 (15), 20.8 (16) ppm.

^{13}C-resonances of carbon atoms directly bonded to boron could not be observed.

MS (HR-MALDI, matrix: DCTB) for $C_{60}H_{62}B_2N_6O_2$: calc. m/z = 920.5120, found m/z = 920.5120 ([M$^+$]). Also observed: ([M-Mes]$^+$): calc. m/z = 801.4260, found m/z = 801.4248, ([M-CH_3]$^+$): calc. m/z = 906.4964, found m/z = 906.4905.

1.2.6. Preparation of 1,4-Bis(dimesitylboryl)-2,5-(Bis(1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl))benzene (Trz-CF_3)



To a solution of 30.1 mg (48.4 µmol) **B_2-H** in 3.9 mL dry THF, were added 1.23 mg (6.46 µmol) CuI, 0.02 mL (115 µmol) DIPEA and an initial amount of 43.4 mg (232 µmol) 1-azido-4-(trifluormethyl)-benzene. The mixture was stirred at ambient temperature for several days, additional azide was then added and the mixture was heated to 70°C for 21 h, until TLC control indicated that the reaction had come to completion. Subsequently, the solvent was removed under reduced pressure, and the resulting residue was washed with dry *n*-hexane to afford **Trz-CF_3** in 81% yield (39.0 mg, 39.1 µmol) as a pale yellow solid.

^{1}H-NMR (400 MHz, C_6D_6): δ = 8.23 (s, 2 H, 5), 7.06 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz 7/8), 7.00 (s, 8 H, 13), 6.70 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz, 7/8), 6.28 (s, 2 H, 1), 2.45 (b, 24 H, 15), 2.25 (s, 12 H, 16) ppm.

^{1}H-NMR (400 MHz, THF-d_8): δ = 9.06 (s, 2 H, 5), 8.09 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz, 7/8), 7.94 (s, 2 H, 1), 7.93 (d, 4 H, $^{3}J_{HH}$ = 8.4 Hz, 7/8), 6.54 (s, 8 H, 13), 2.10 (s, 12 H, 16), 1.91 (br, 24 H, 15) ppm.

^{13}C-NMR (100 MHz, THF-d_8): δ = 151.8 (4), 140.9 (12), 140.2 (9), 133.7 (14), 130.5 (3), 129.9 (13), 127.9 (7/8), 126.1 (1), 121.7 (7/8), 116.8 (5), 25.6 (15), 20.8 (16) ppm.

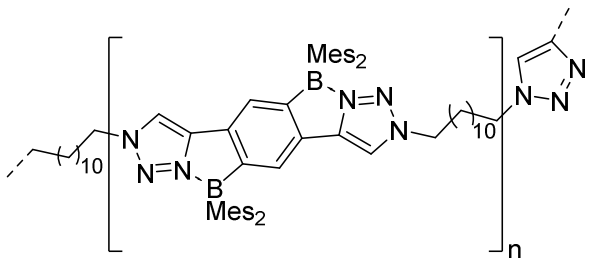
^{13}C-resonances of carbon atoms directly bonded to boron could not be observed.

^{19}F-NMR (125 MHz, C_6D_6): δ = -62.4 ppm.

MS (HR-MALDI, matrix: DCTB) for $C_{60}H_{56}B_2F_6N_6$: calc. m/z = 996.4657, found m/z = 996.4651 ([M$^+$]). Also observed: ([M-Mes]$^+$): calc. m/z = 877.3796, found m/z = 877.3787, ([M-CH_3]$^+$): calc. m/z = 982.4500, found m/z = 982.4445.

1.2.7. Preparation of Polymer PTrz

To a solution of 20.0 mg (33.7 µmol) **B_2-H** and 8.50 mg (33.7 µmol) of 1,12-diazidododecane in 2.0 mL of dry toluene were added 100 µL of a 25 mM 1:1 solution of CuI and PMDETA in dry THF. The reaction mixture was stirred at 60 °C for 3 d and for another 20 h at 100 °C, and was subsequently poured into petroleum ether to precipitate the product. The colorless participate were filtered off and washed with petroleum ether, diethyl ether, and acetonitrile. The residue was then taken up in DCM, filtered, and evaporated to dryness to give 18.0 mg (61%) of a colorless solid.



GPC ($CHCl_3$ vs. PS): M_n = 7.2 kDa; PDI = 2.1

^{1}H-NMR (400 MHz, THF-d_8): δ = 8.17, 7.78, 6.49, 4.34, 2.08, 1.83, 1.24 ppm.

^{13}C-NMR (100 MHz, THF-d_8): δ = 161.7, 151.0, 147.1, 140.7, 133.2, 130.6, 129.7, 125.6, 118.0, 52.8 (CH_2-), 51.9 (CH_2-), 30.5 (CH_2-), 30.4 (CH_2-), 30.3 (CH_2-), 30.2 (CH_2-), 30.1 (CH_2-), 29.7 (CH_2-), 29.6 (CH_2-), 29.5 (CH_2-), 26.9 (CH_2-), 20.8 ppm.
Uv-vis (THF) λ_{max} = 276 nm; λ_{em} = 374 nm.
Anal. calc. for $C_{464}H_{577}B_{16}N_{48}$ C 79.62; H 8.31; N 9.60. Found: C 77.68; H 8.39; N 9.93.

2. Supplementary Analytical Data

2.1. Electrochemical and Uv-vis-spectroscopic Data

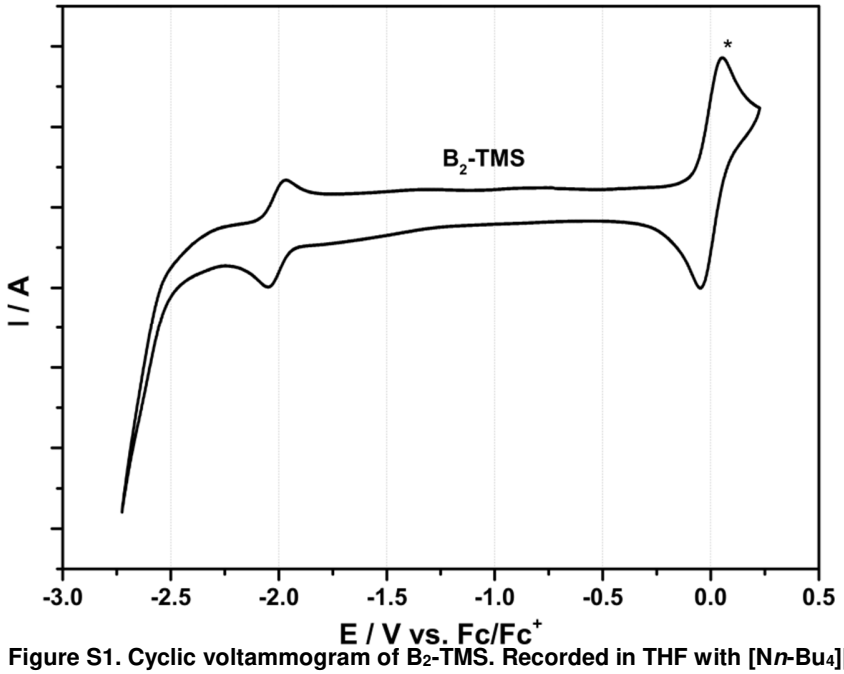


Figure S1. Cyclic voltammogram of B_2-TMS. Recorded in THF with [N*n*-Bu_4][PF_6] (0.1 M) as electrolyte at 300 mV/s. * = internal standard ferrocene.

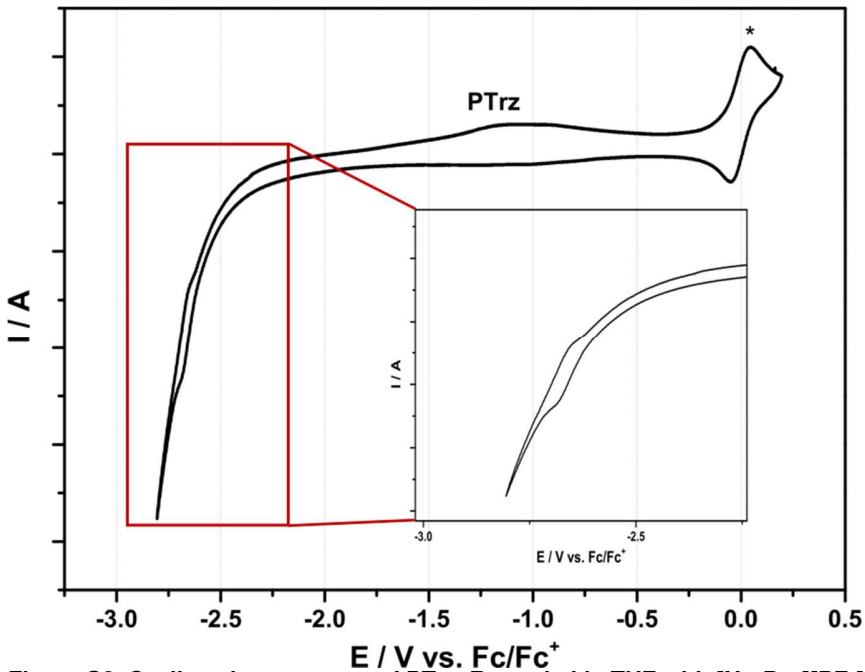


Figure S2. Cyclic voltammogram of PTrz. Recorded in THF with [N*n*-Bu_4][PF_6] (0.1 M) as electrolyte at 300 mV/s. * = internal standard ferrocene.

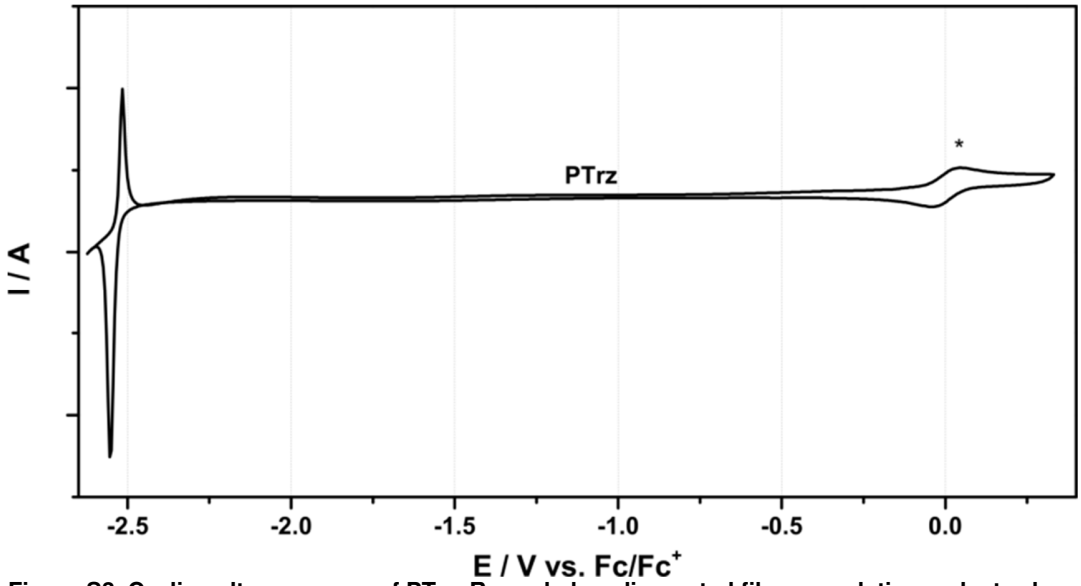


Figure S3. Cyclic voltammogram of PTrz. Recorded as dip-coated film on a platinum electrode vs. 0.1 M [N*n*Bu$_4$][PF$_6$] in NCMe-solution. * = internal standard ferrocene.

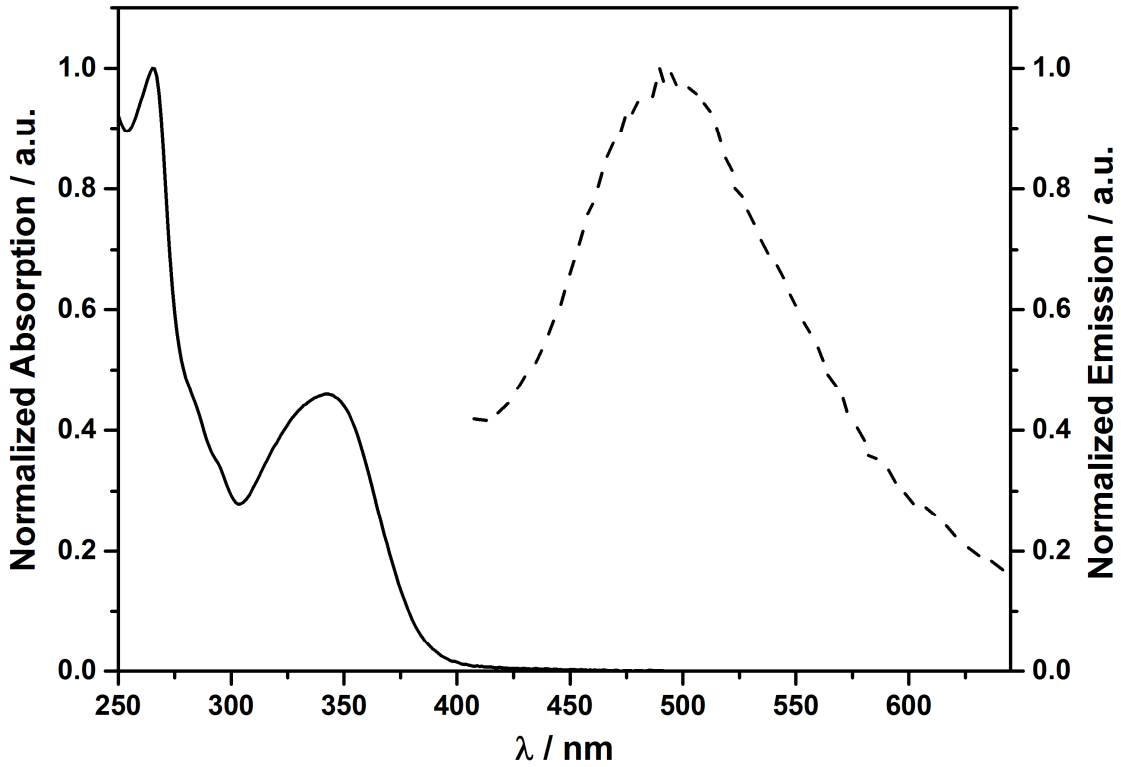


Figure S4. UV-vis absorption (solid) and emission (dashed) spectra of B$_2$-H in THF solution.

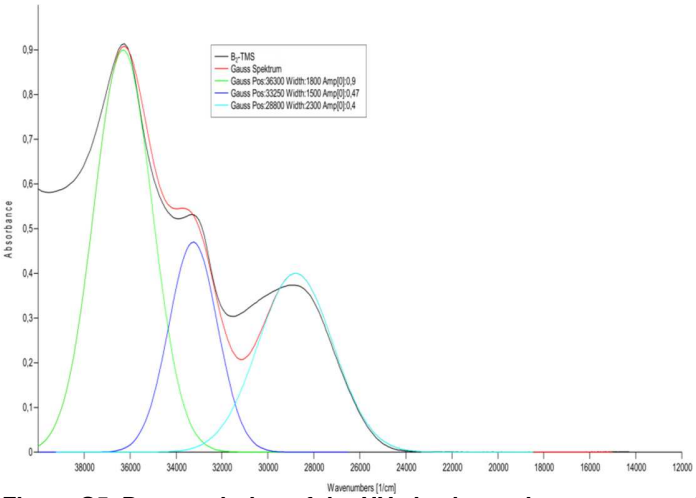


Figure S5. Deconvolution of the UV-vis absorption spectrum of B_2-TMS in THF solution at ambient temperature.

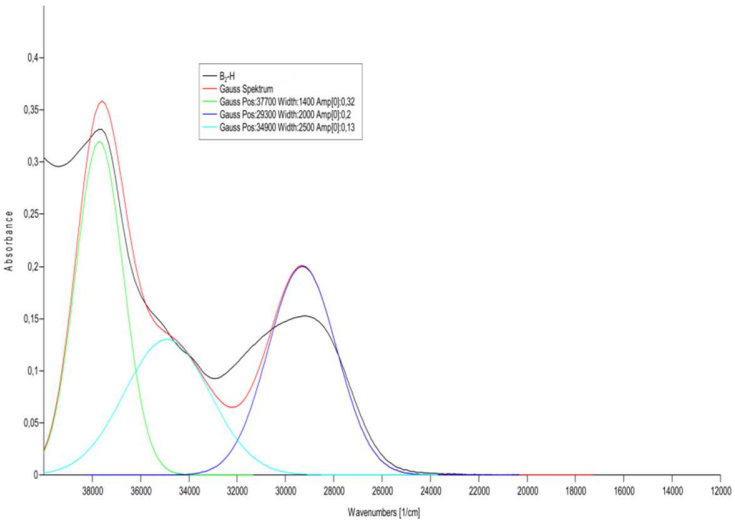


Figure S6. Deconvolution of the UV-vis absorption spectrum of B_2-H in THF solution at ambient temperature.

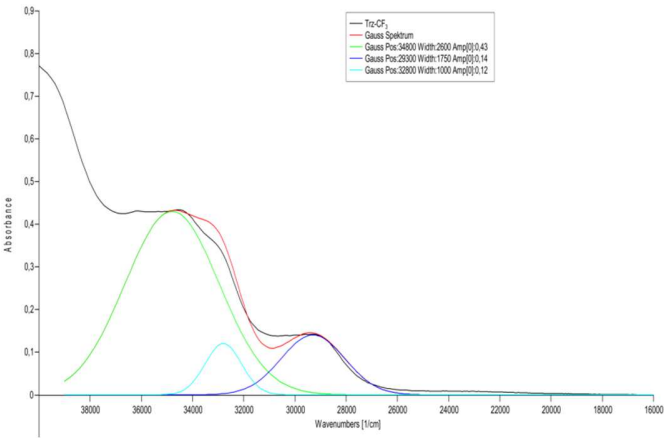


Figure S7. Deconvolution of the UV-vis absorption spectrum of Trz-CF_3 in THF solution at ambient temperature.

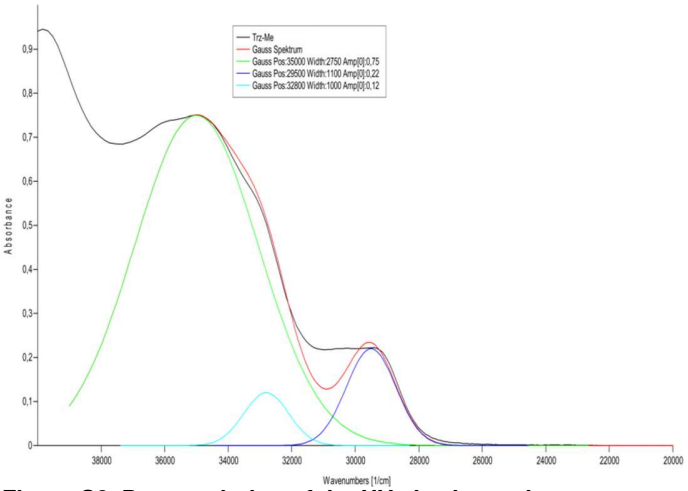


Figure S8. Deconvolution of the UV-vis absorption spectrum of Trz-Me in THF solution at ambient temperature.

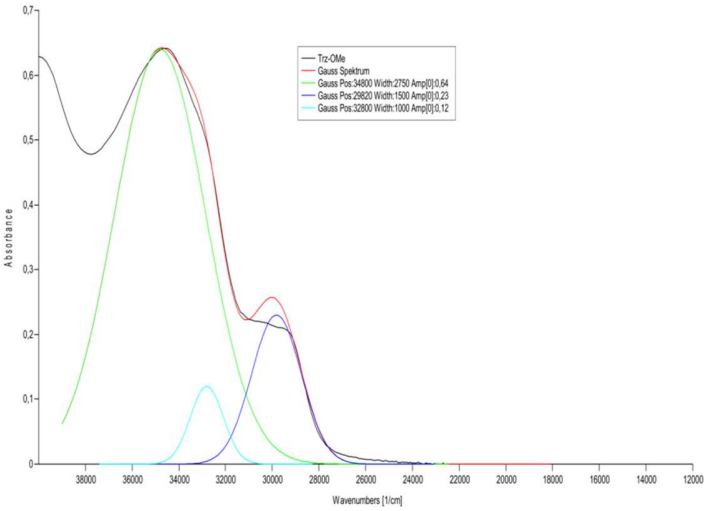


Figure S9. Deconvolution of the UV-vis absorption spectrum of Trz-OMe in THF solution at ambient temperature.

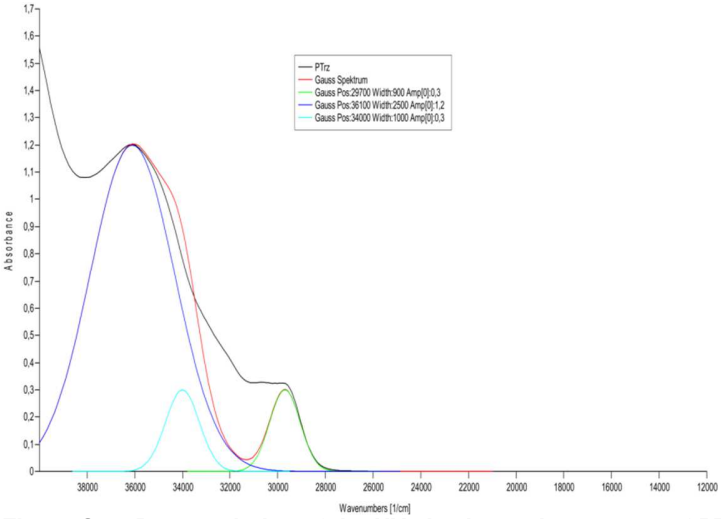


Figure S10. Deconvolution of the UV-vis absorption spectra of PTrz in THF solution at ambient temperature.

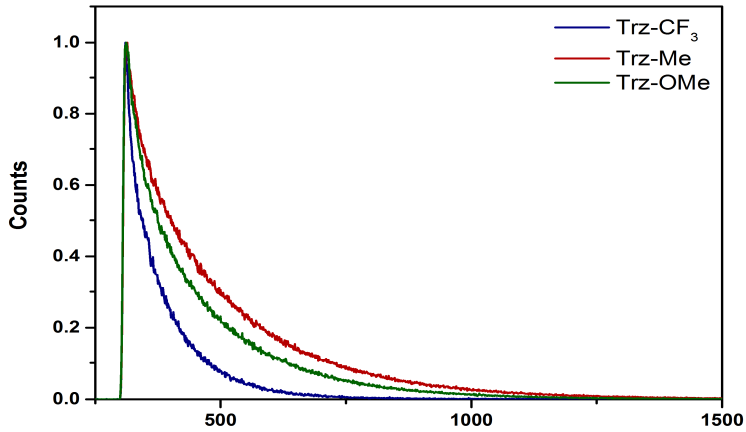


Figure S11. Fluorescence lifetimes of Trz-CF_3 (c = $4.0 \cdot 10^{-7}$ M), Trz-OMe (c = $1.3 \cdot 10^{-6}$ M), and Trz-Me (c = $1.1 \cdot 10^{-6}$ M) in THF solution at ambient temperature.

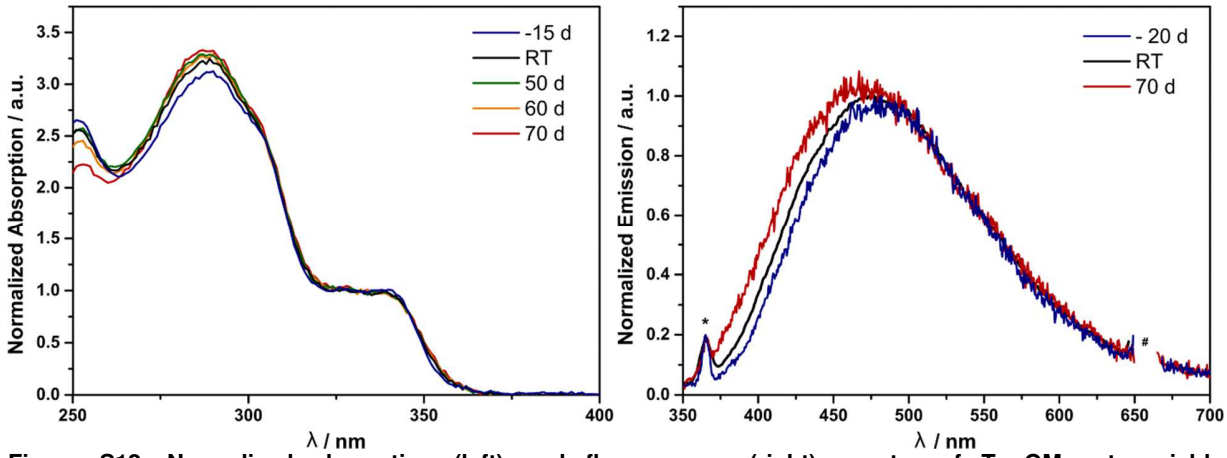


Figure S12. Normalized absorption (left) and fluorescence (right) spectra of Trz-OMe at variable temperatures. Recorded in THF; excitation wavelength 330 nm.

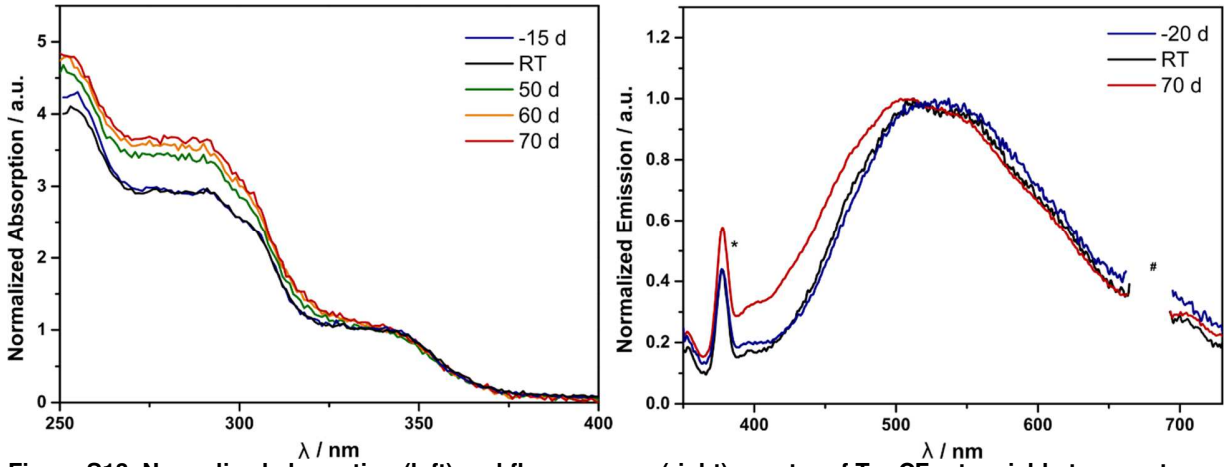


Figure S13. Normalized absorption (left) and fluorescence (right) spectra of Trz-CF_3 at variable temperatures. Recorded in THF; excitation wavelength 340 nm.

2.2. ^{11}B NMR Spectra

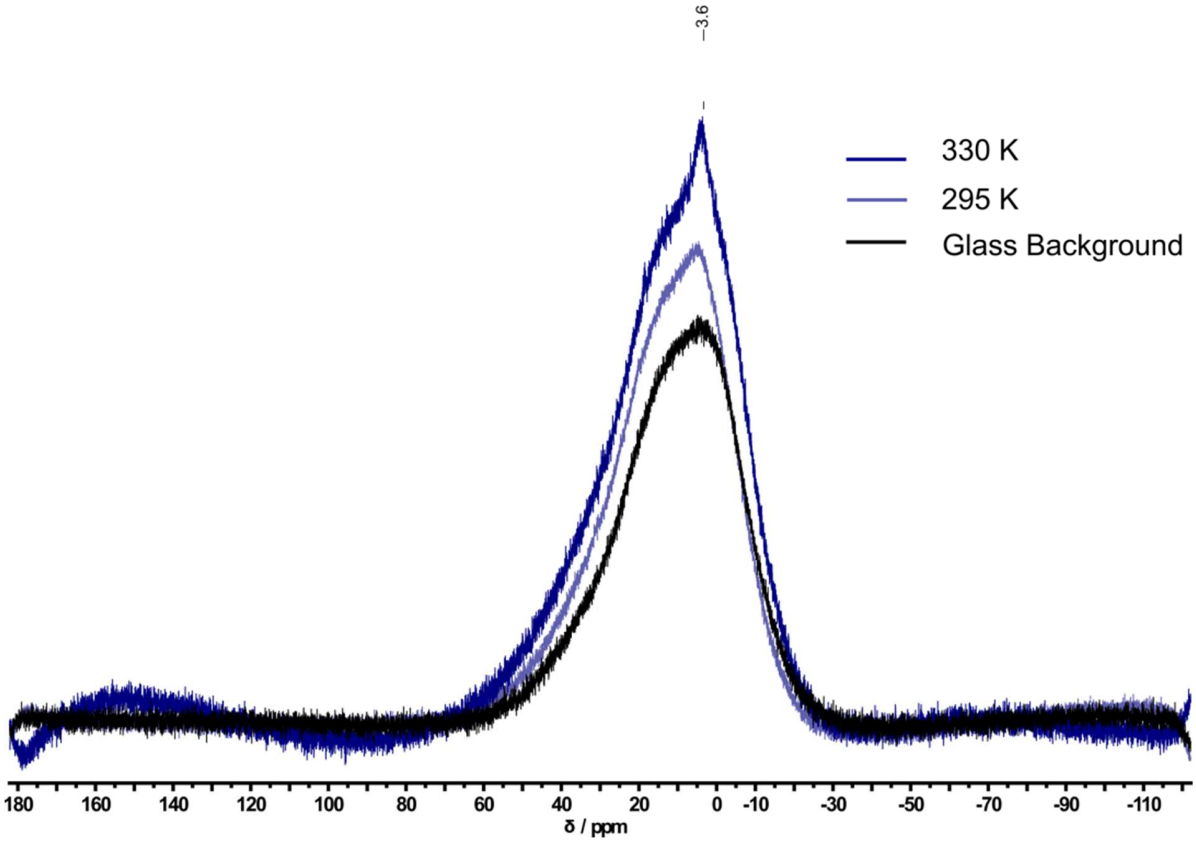


Figure S14. ^{11}B NMR-spectrum of Trz-CF_3 in THF-d_8. Glass background of the NMR-probe-head (black).

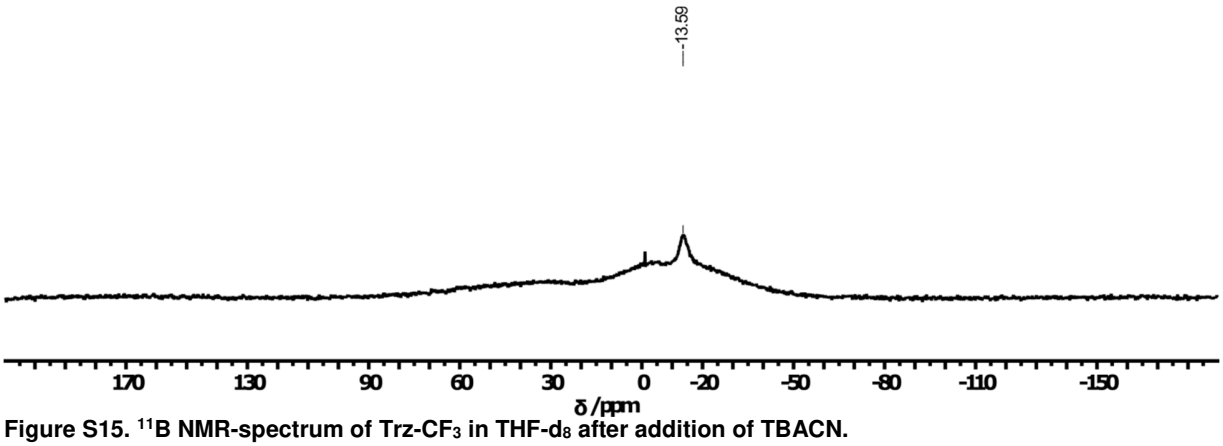


Figure S15. ^{11}B NMR-spectrum of Trz-CF_3 in THF-d_8 after addition of TBACN.

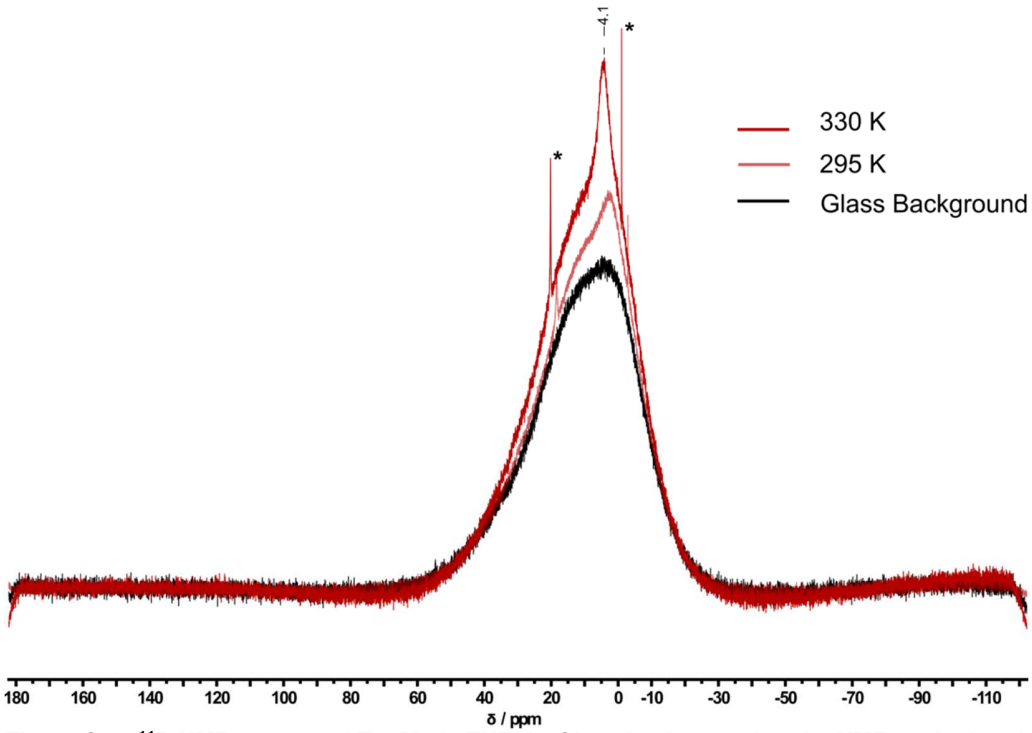


Figure S16. ^{11}B NMR-spectra of Trz-Me in THF-d$_8$. Glass background of the NMR-probe-head (black). * Trace amounts of hydrolyzed borane.

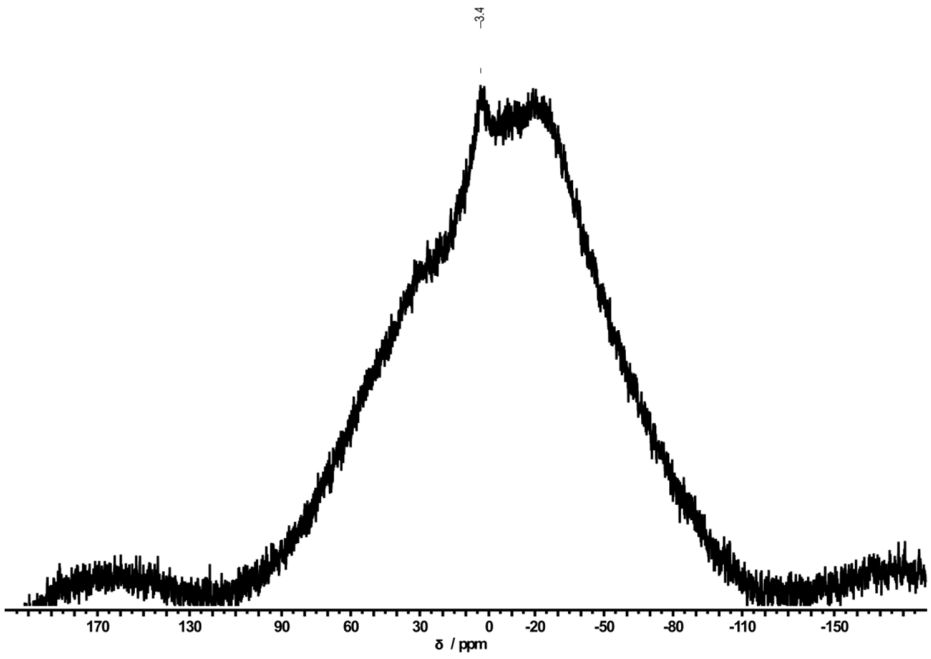


Figure S17. ^{11}B NMR-spectrum of Trz-OMe in THF-d$_8$.

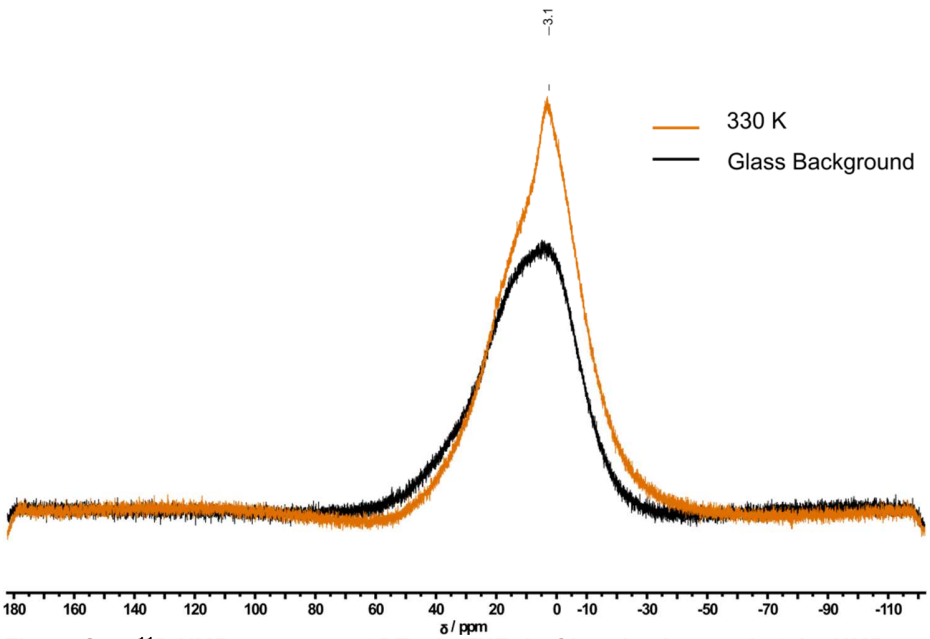


Figure S18. ^{11}B NMR-spectrum of PTrz in THF-d_8. Glass background of the NMR-probe-head (black).

2.3. Dynamic ^{1}H NMR Experiments

Hindered rotation of the mesityl-groups strongly affects chemical shifts of the *ortho*-methyl-groups and aromatic *meta*-protons in ^{1}H NMR spectra of **Trz-OMe**, **Trz-Me**, and **Trz-CF$_3$**. The system, presumably, eventually becomes locked in ***closed***, twofold N→B-coordinated conformation, wherein the four *ortho*-methyl-groups and aromatic *meta*-protons on each $BMes_2$-group become magnetically inequivalent.

2.3.1. $\Delta G^{\ddagger}$ estimate from T_C

The signals of the aromatic mesityl protons appear sharp at elevated temperature (340 K), but split into two broadened signals below a coalescence temperature of 235 K (T_C1) and appear further resolved into four individual signals below 220 K (T_C2) (see Figure S22, Figure S23, and Figure S24). The Gibbs activation energy dynamic exchange processes in **Trz-OMe**, **Trz-Me**, and **Trz-CF$_3$** has been estimated from the signal separations at 208 K ($\Delta\nu1$, $\Delta\nu2$ in Hz) in ^{1}H NMR experiments at 500 MHz in THF-d_8, and from the coalescence temperatures (T_C in K) in the same solvent, according to:

$$\Delta G^{\ddagger} = R*T_C[9.972+\log(T_C/\Delta\nu)]\ [J*mol^{-1}]$$

Table S1. $\Delta G^{\ddagger}$ according to dynamic NMR experiments.

Trz-CF_3	$\Delta v1$[a] (208 K) [Hz]	T_C1 [K]	$\Delta G^{\ddagger}_1$ [kJ/mol]	$\Delta v2$[b] (208 K) [Hz]	T_C2 [K]	$\Delta G^{\ddagger}_2$ [kJ/mol]
	28	220±3K	45.9 ±0.6	128	235±3K	46.0 ±0.6
Trz-OMe	$\Delta v1$ (208 K) [Hz]	T_C1 [K]	$\Delta G^{\ddagger}_1$ [kJ/mol]	$\Delta v2$ (208 K) [Hz]	T_C2 [K]	$\Delta G^{\ddagger}_2$ [kJ/mol]
	21	220±3	46.3 ±0.6	125	235±3	46.1 ±0.6
Trz-Me	$\Delta v1$ (208 K) [Hz]	T_C1 [K]	$\Delta G^{\ddagger}_1$ [kJ/mol]	$\Delta v2$ (208 K) [Hz]	T_C2 [K]	$\Delta G^{\ddagger}_2$ [kJ/mol]
	23	220±3	46.1±0.7	126	235±3	46.1 ±0.6

[a] Signal separation within each pseudo-doublet at 208 K. Averaged over both signal pairs. [b] Averaged separation of pseudo-doublets at 208 K.

2.3.2. Line shape analyses

General method: The signals of the aromatic mesityl protons of **Trz-OMe**, **Trz-Me** and **Trz-CF_3** in variable temperature ^{1}H NMR spectra (see Figure S22, Figure S23, and Figure S24) were fitted as a four-spin systems without scalar coupling, based on the line-width and chemical shifts of 500 MHz ^{1}H NMR spectra at 208 K in THF-d_8. The spectra were simulated and compared to the experimental spectra using the WINDNMR program package (version 7.1.14).[10] The rate constants (k_r) for theThermalexchange could then be determined from these simulations as a function of temperature. According to the Eyring equation, linear fit (y = a + b*x) of the plot of ln(kr/T) versus 1/T then allowed to derive the activation parameters as followes:

$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - \Delta S^{\ddagger} * T$$

$$k_r = k_B * T * R^{-1} * \exp(-\Delta G^{\ddagger} * R^{-1} * T^{-1}) \text{ (Eyring equation)}$$

⇨ **$\Delta H^{\ddagger} = -(m)*R$; $\Delta S^{\ddagger} = ([b]+\ln(h/k_B))/R$**

With: R: gas constant, 8.3144 $J*K^{-1}mol^{-1}$; k_B: Boltzman's constant, $1.3805*10^{-23}$ $J*K^{-1}$
h: Planck's constant, $6.6256*10^{-34}$ J*s; a, b = intercept and slope of linear fit (y = a + b*x)

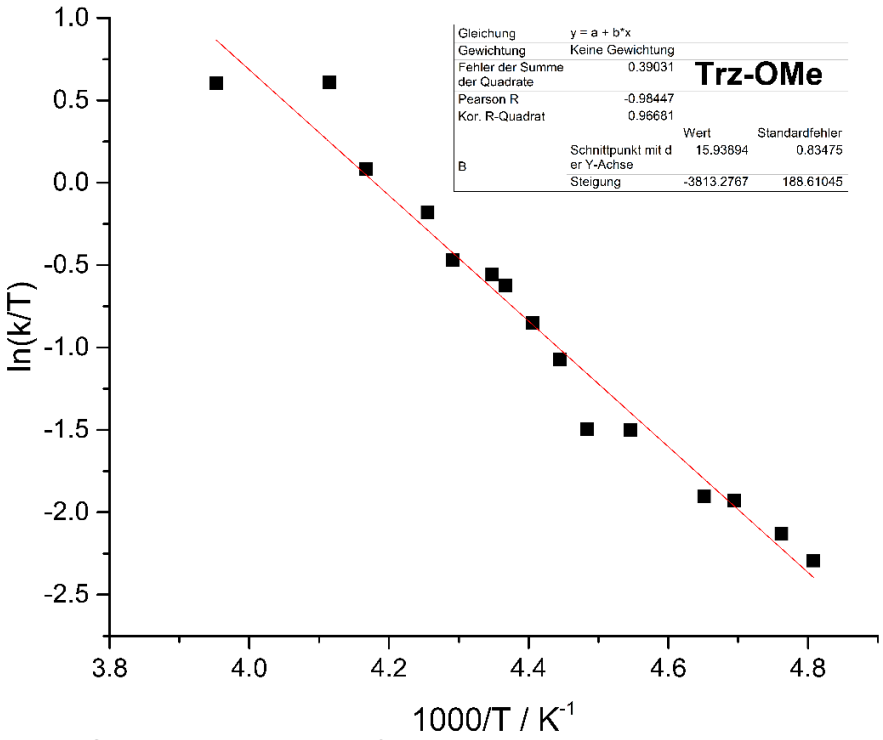


Figure S19. Eyring plot of Trz-OMe.

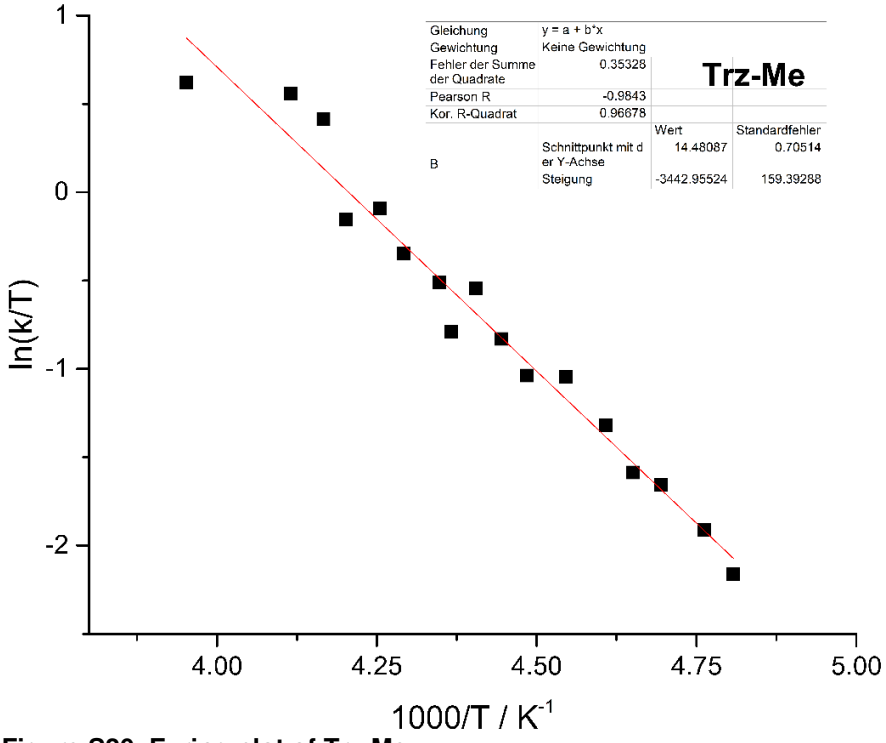


Figure S20. Eyring plot of Trz-Me.

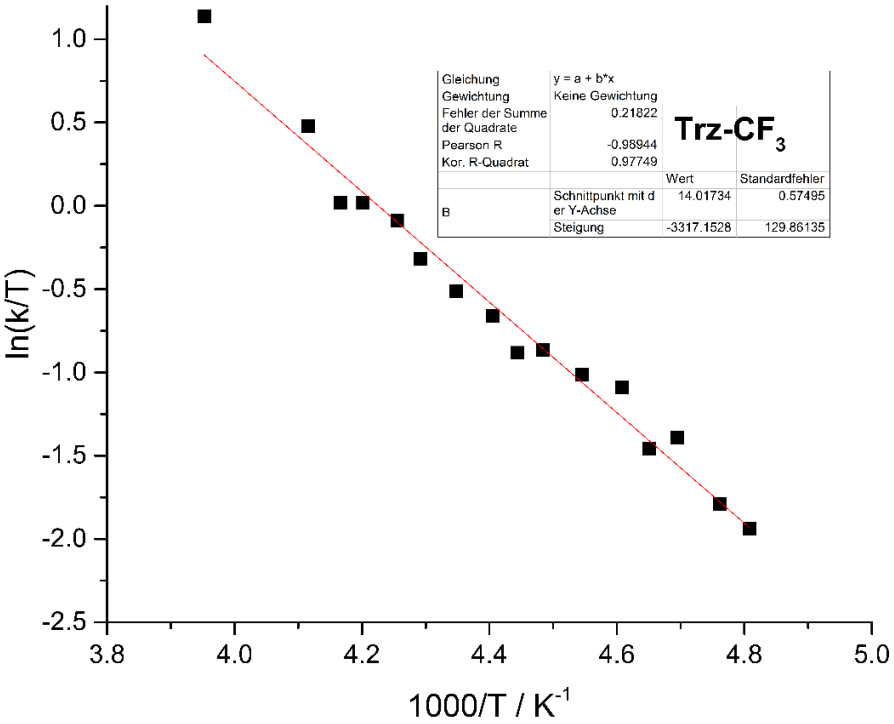


Figure S21. Eyring plot of Trz-CF_3.

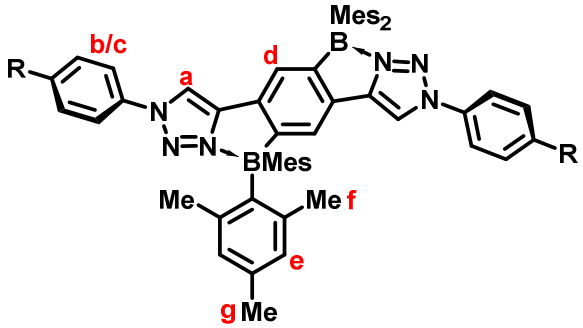


Chart S1. Signal assignment in dynamic NMR experiments.

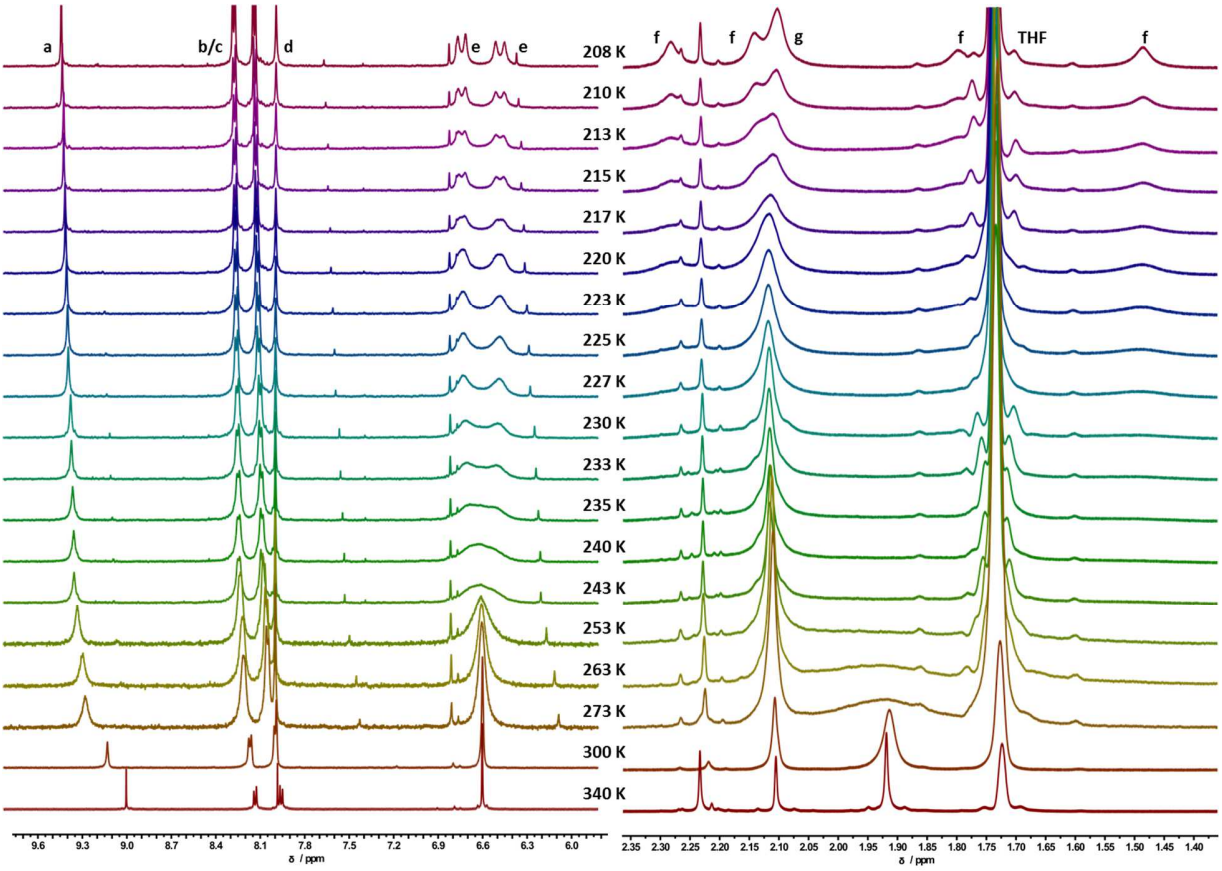


Figure S22. Dynamic ^{1}H NMR of Trz-CF_3 in THF-d_8 at 500 MHz. Signal assignment according to Chart S1.

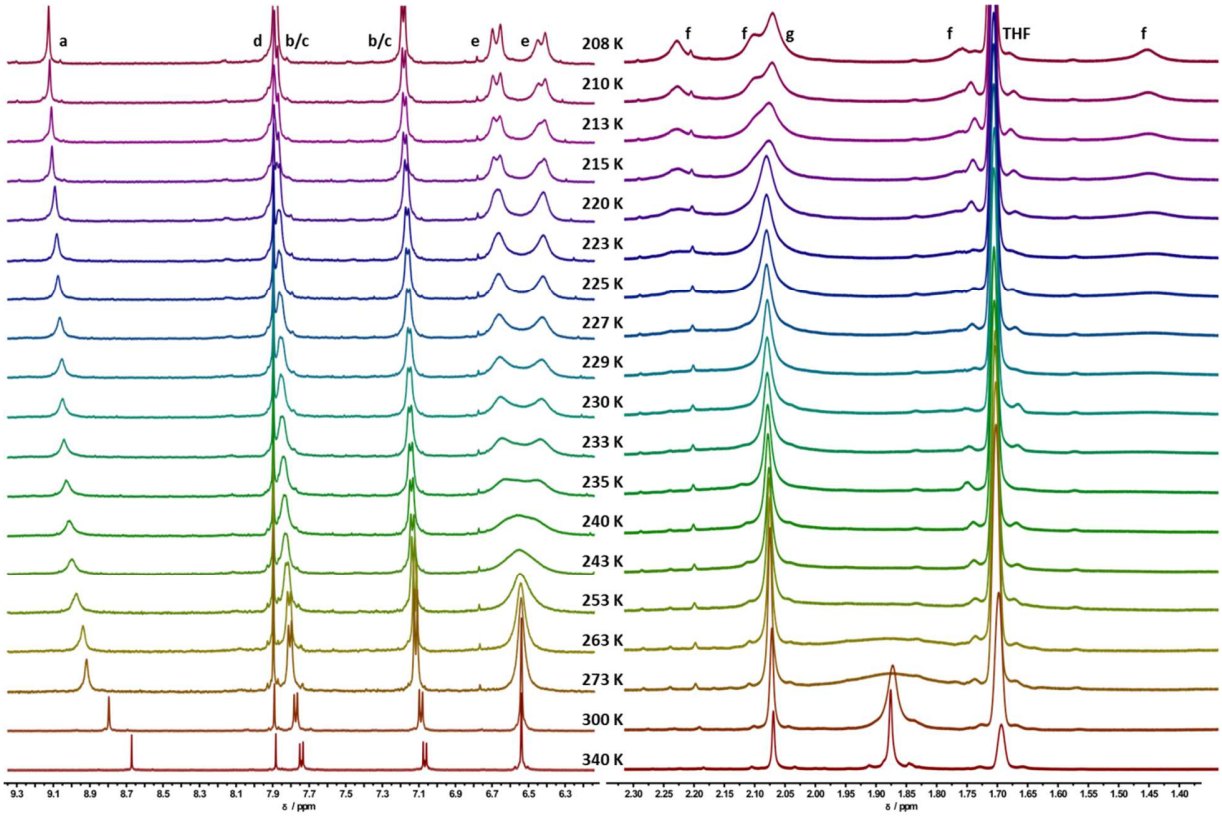


Figure S23. Dynamic ^{1}H NMR of Trz-OMe in THF-d_8 at 500 MHz. Signal assignment according to Chart S1.

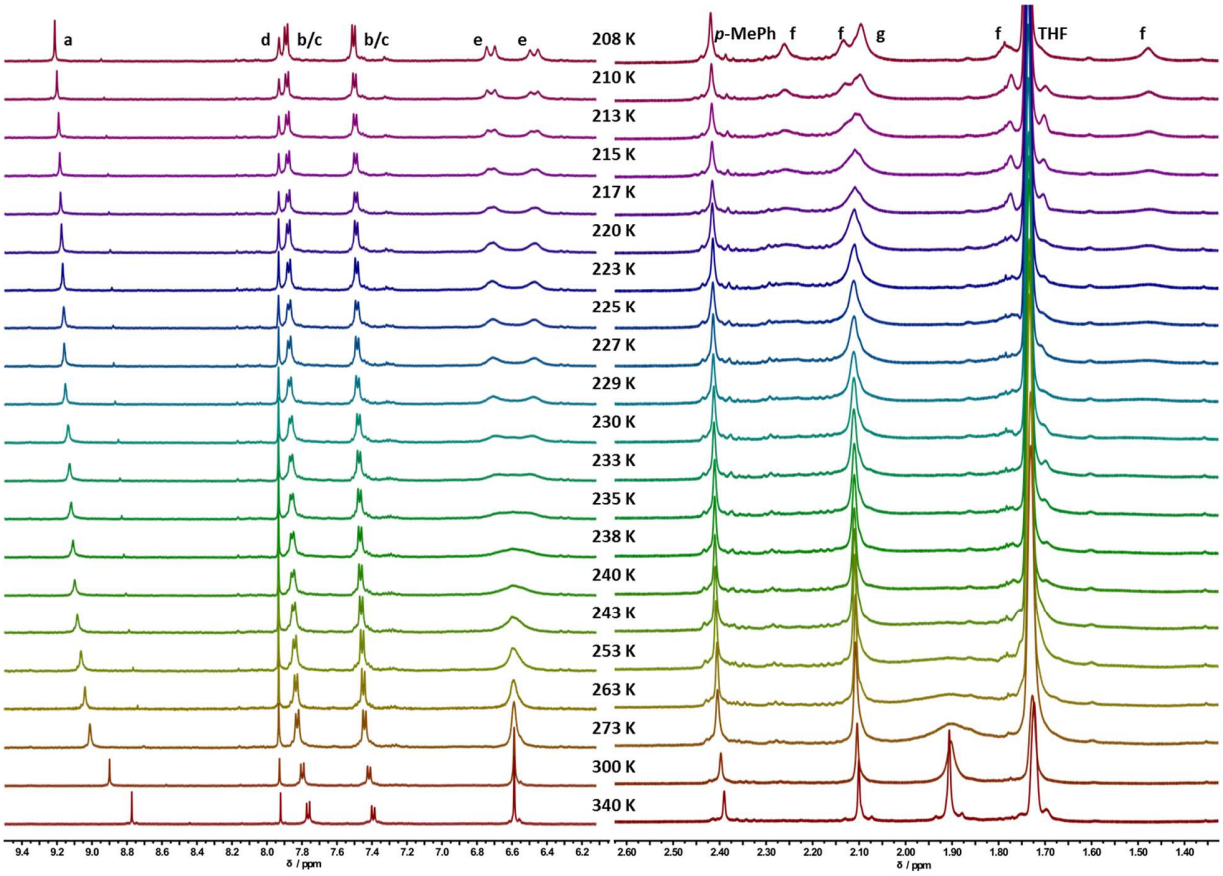


Figure S24. Dynamic ^{1}H NMR of Trz-Me in THF-d_8 at 500 MHz. Signal assignment according to Chart S1.

2.4. NMR and MS Spectra

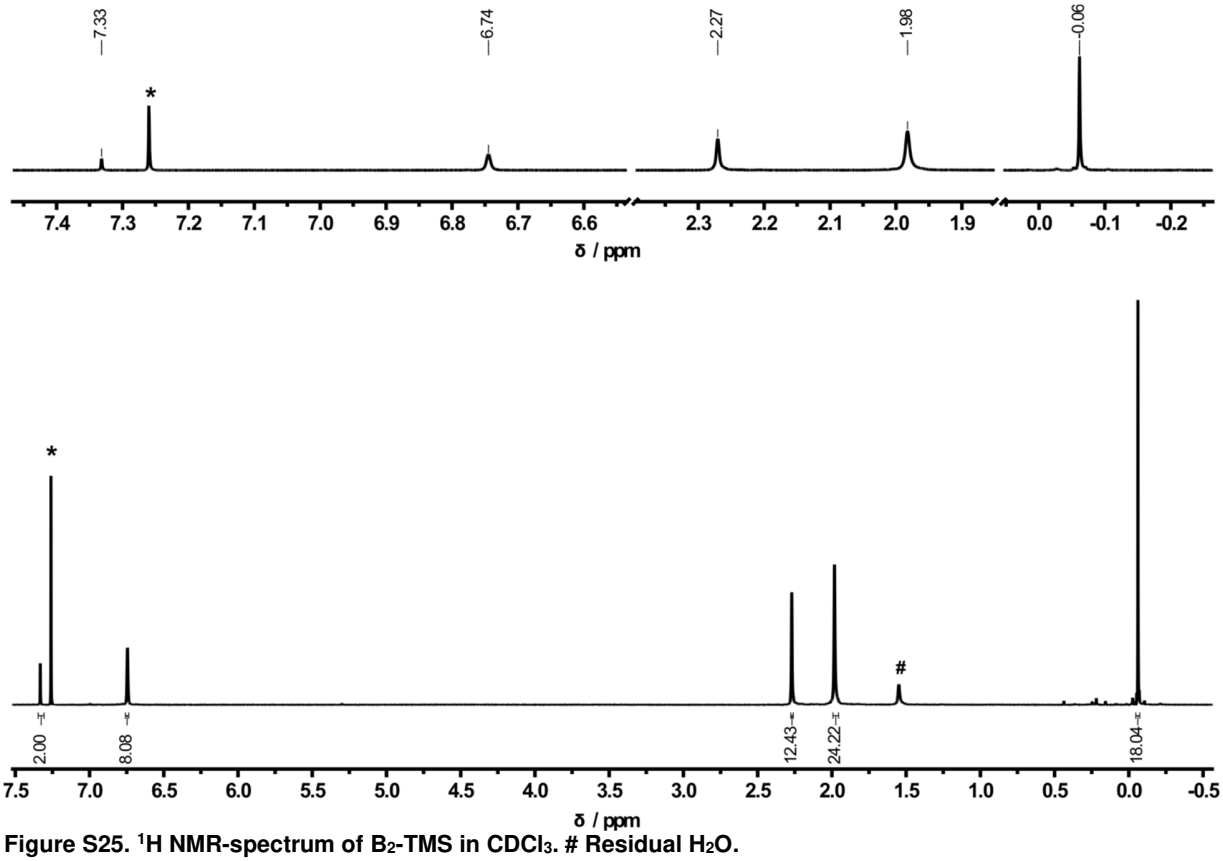


Figure S25. ^{1}H NMR-spectrum of B_2-TMS in $CDCl_3$. # Residual H_2O.

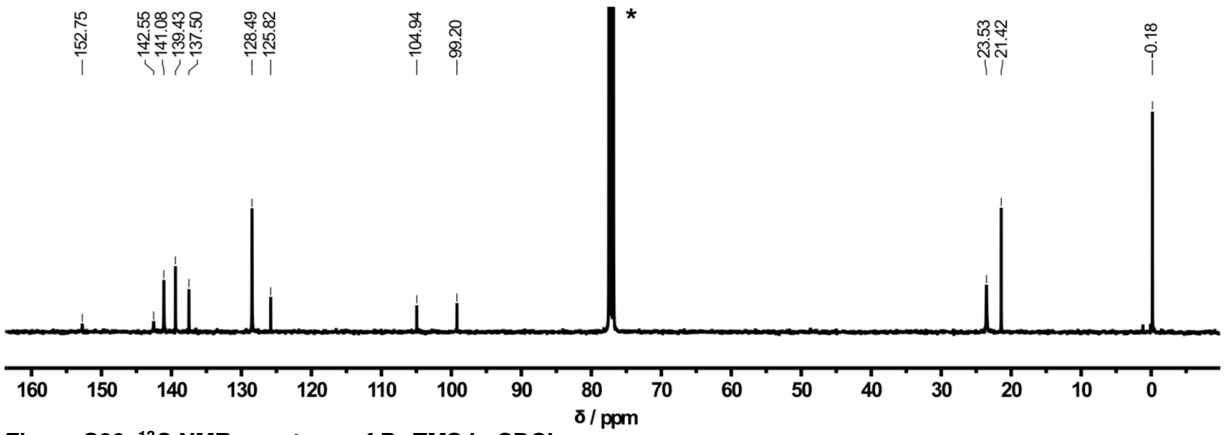


Figure S26. ^{13}C NMR-spectrum of B_2-TMS in $CDCl_3$.

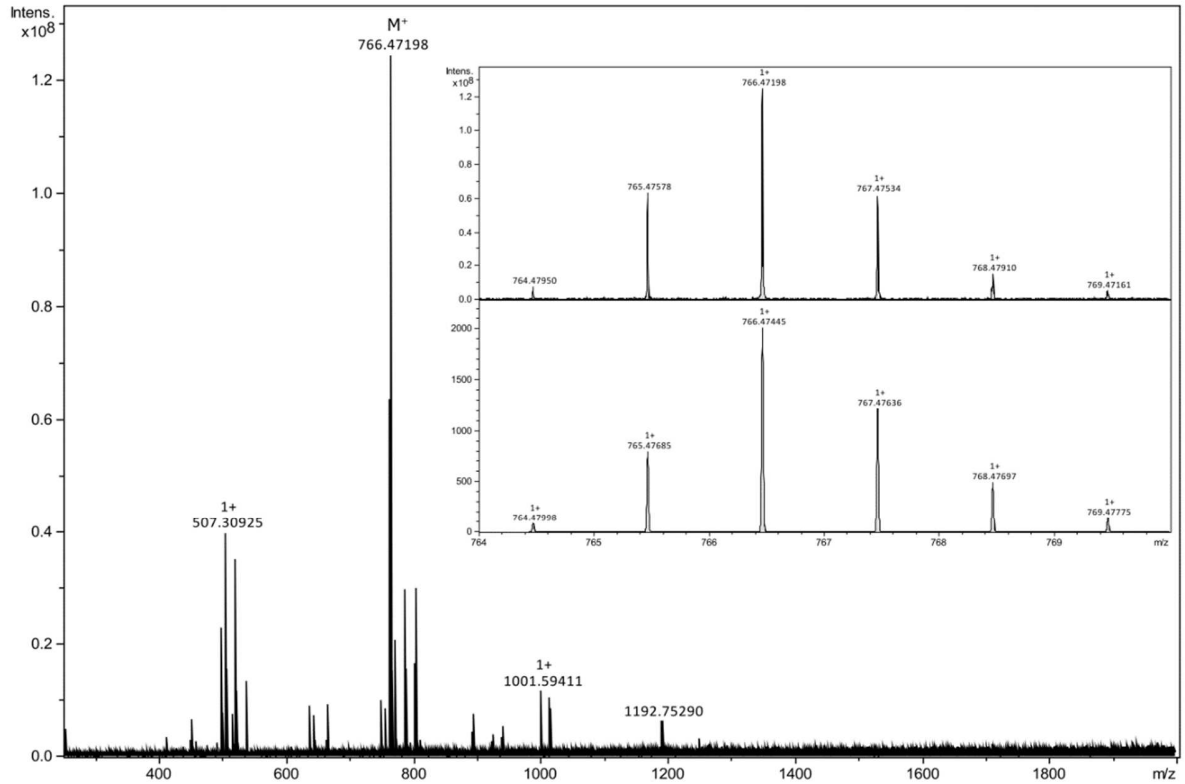


Figure S27. HR-FTMS-spectrum of B_2-TMS. The insert shows enlarged the experimental (top) and calculated (bottom) isotope-pattern of the molecular ion.

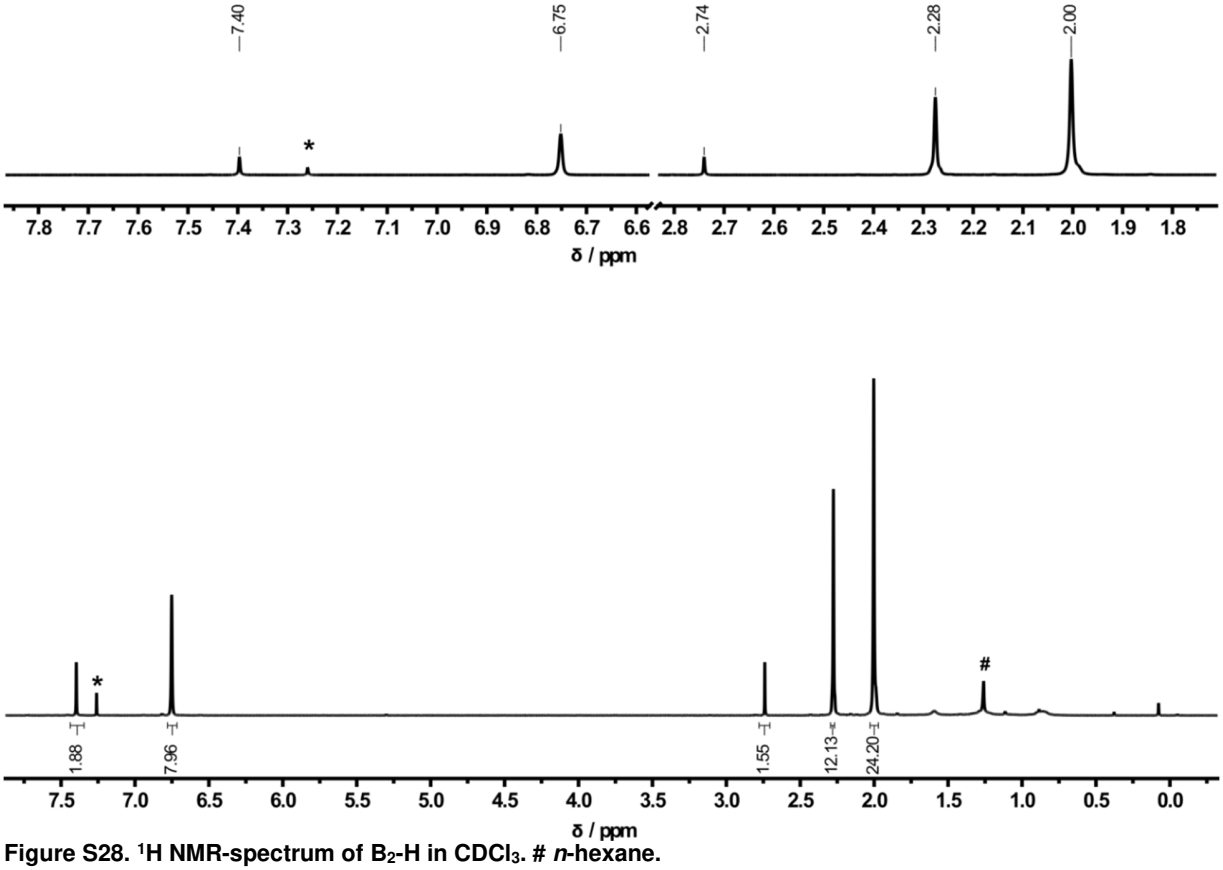


Figure S28. ^{1}H NMR-spectrum of B_2-H in $CDCl_3$. # *n*-hexane.

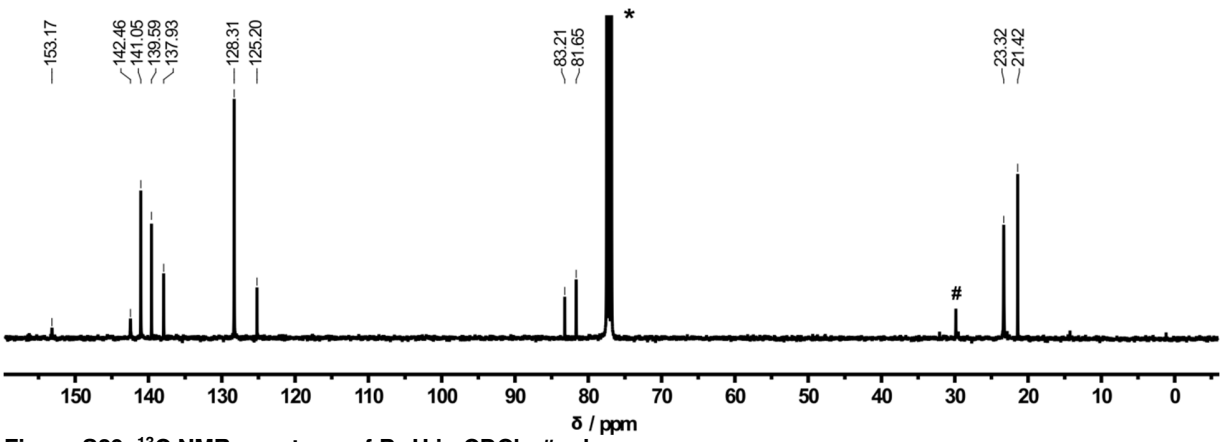


Figure S29. ^{13}C NMR-spectrum of B_2-H in $CDCl_3$. # *n*-hexane.

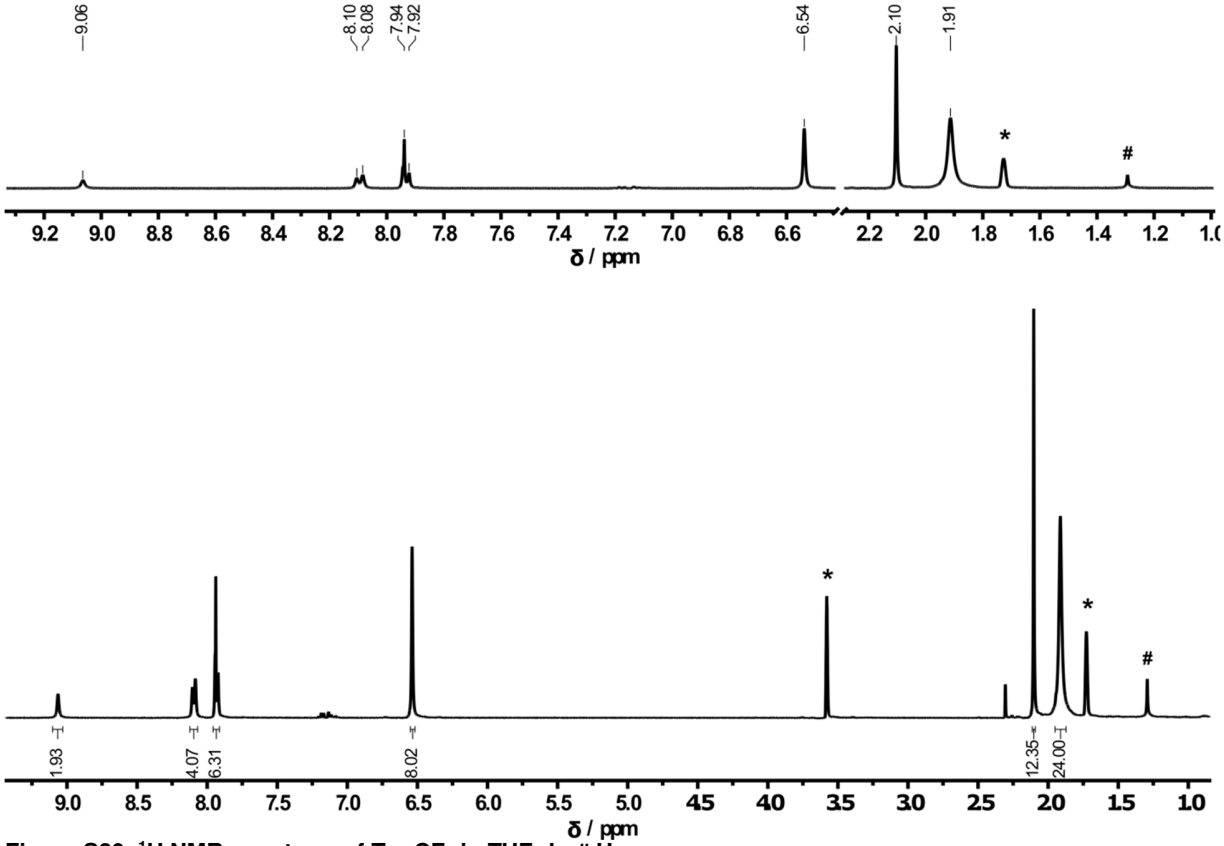


Figure S30. ^{1}H NMR-spectrum of Trz-CF_3 in THF-d_8. # H grease.

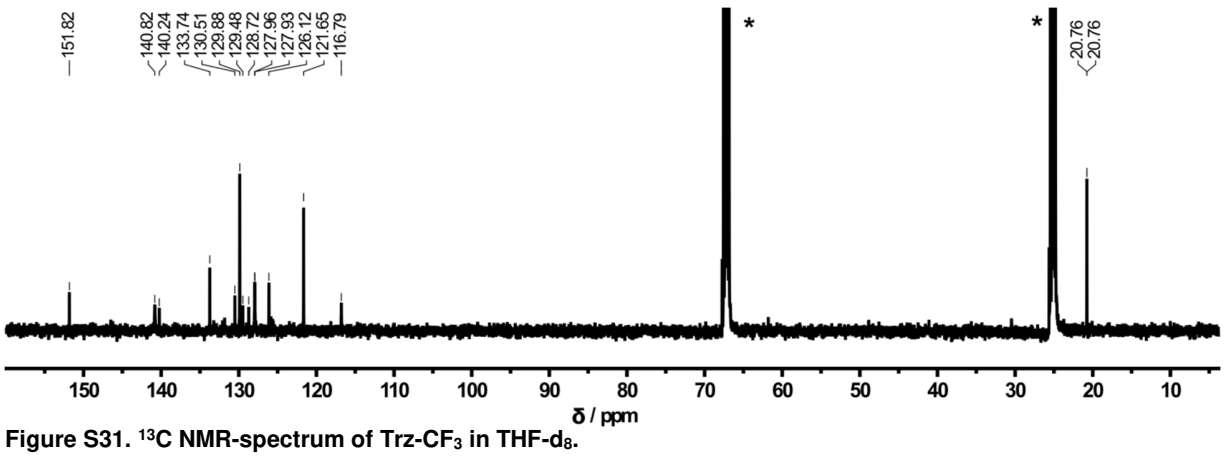


Figure S31. ^{13}C NMR-spectrum of Trz-CF_3 in THF-d_8.

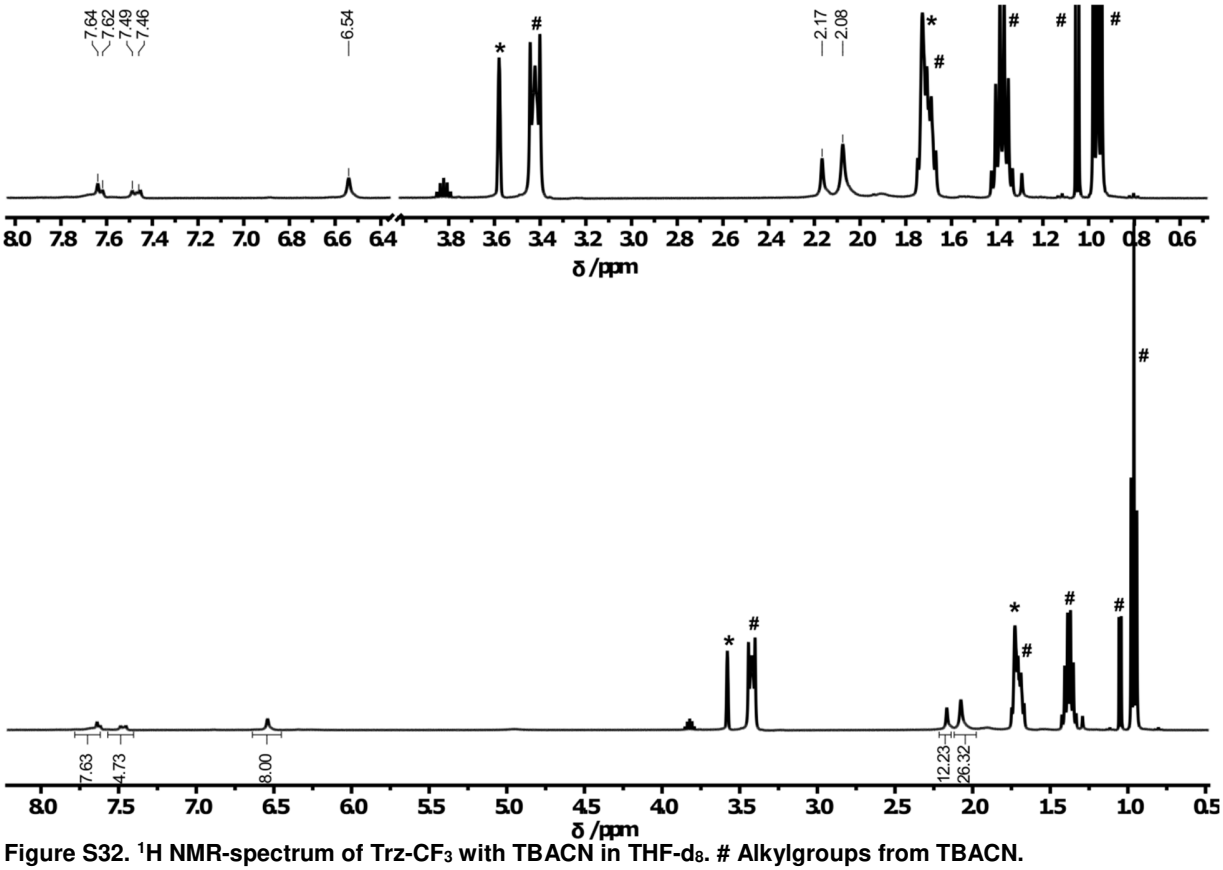


Figure S32. ^{1}H NMR-spectrum of Trz-CF_3 with TBACN in THF-d_8. # Alkylgroups from TBACN.

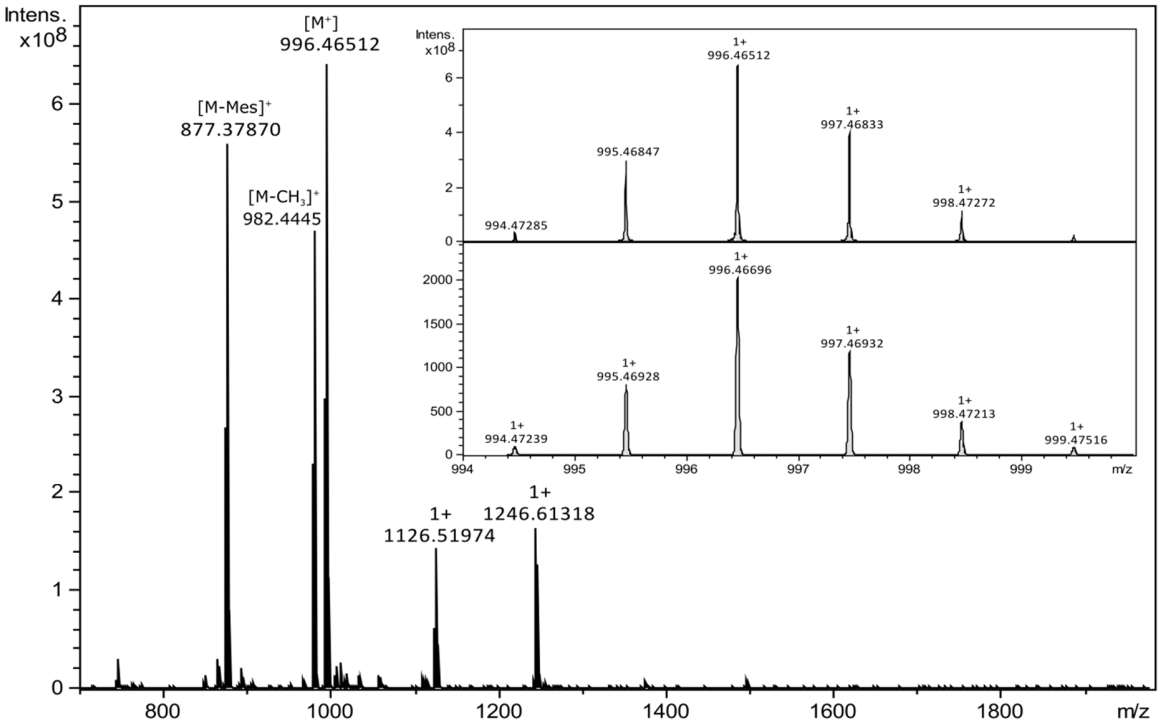


Figure S33. HR-FTMS-spectrum of Trz-CF_3. The insert shows enlarged the experimental (top) and calculated (bottom) isotope-pattern of the molecular ion.

Mass spectra of all three model boranes, as well as **PTrz**, showed signals corresponding to the molecular monocations after loss of one equivalent of either mesityl- ($[M\text{-}Mes]^+$), or methyl-groups ($[M\text{-}CH_3]^+$), that are more prominent than those of the molecular ions ($[M]^+$). See also Figure S36, Figure S39, and Figure S42.

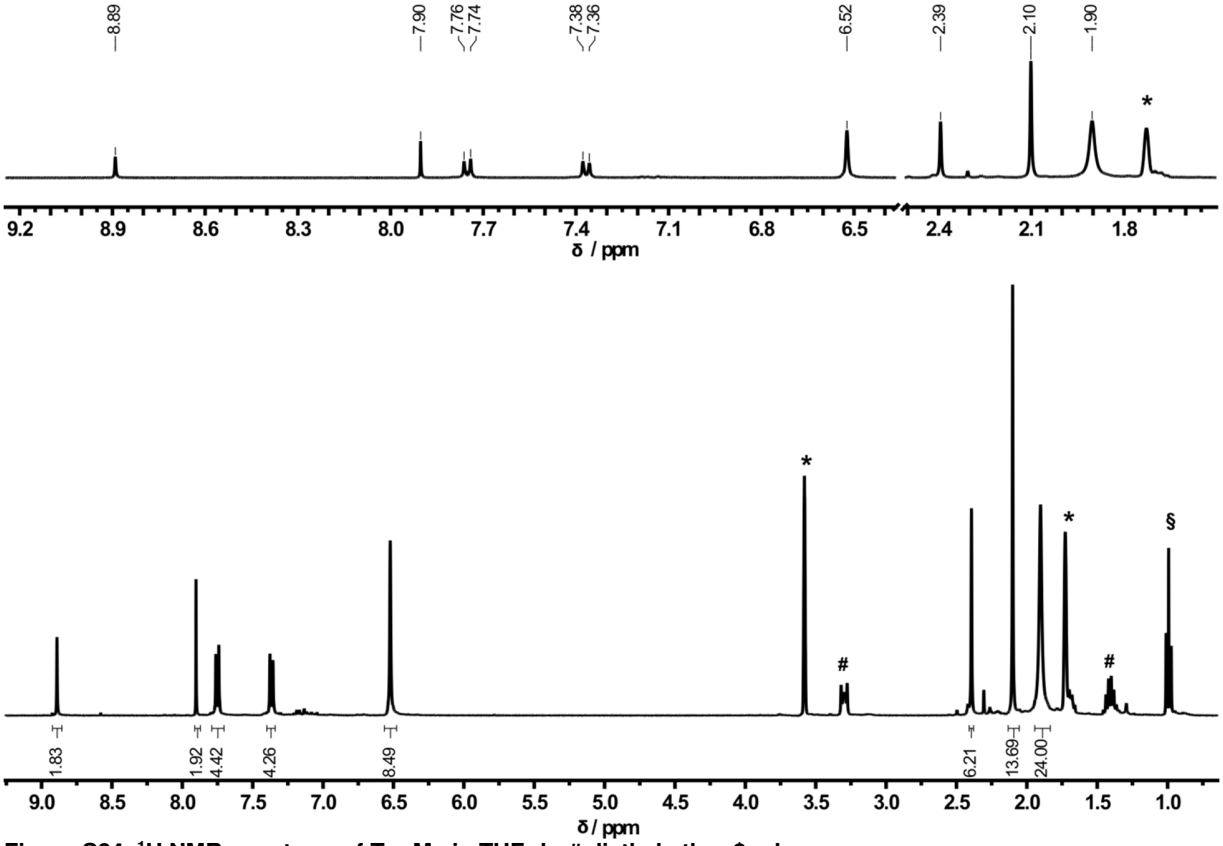


Figure S34. ^{1}H NMR-spectrum of Trz-Me in THF-d_8. # diethyl ether $ *n*-hexane.

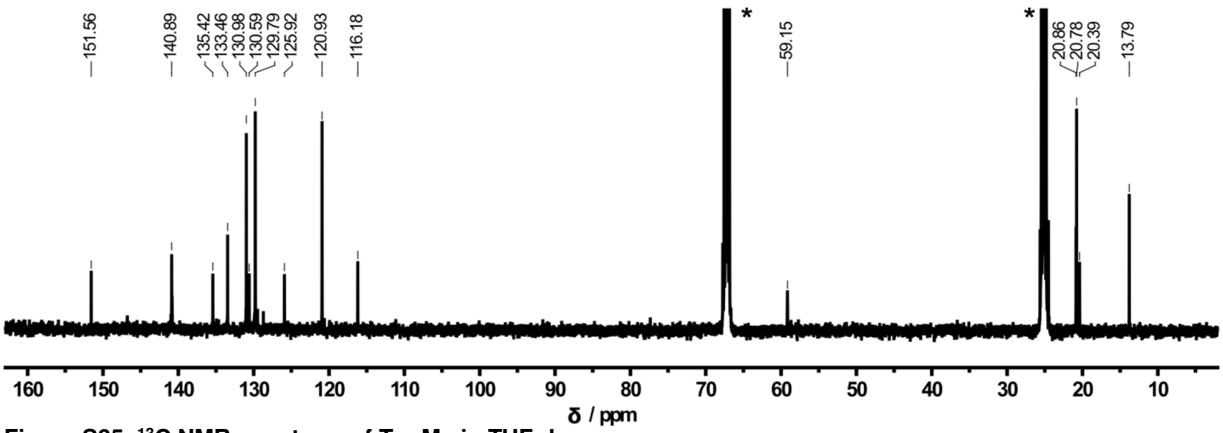


Figure S35. ^{13}C NMR-spectrum of Trz-Me in THF-d_8.

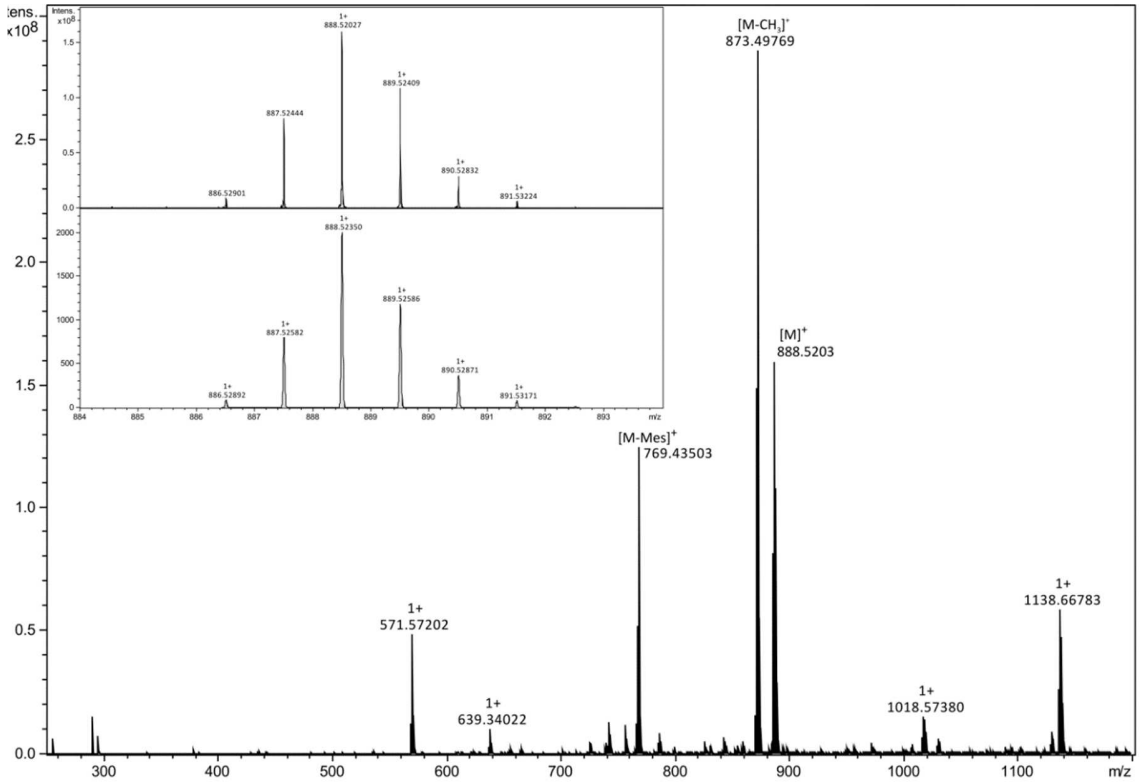


Figure S36. HR-FTMS-spectrum of Trz-Me. The insert shows enlarged the experimental (top) and calculated (bottom) isotope-pattern of the molecular ion.

Mass spectra of all three model boranes, as well as **PTrz**, showed signals corresponding to the molecular monocations after loss of one equivalent of either mesityl- ($[M\text{-}Mes]^+$), or methyl-groups ($[M\text{-}CH_3]^+$), that are more prominent than those of the molecular ions ($[M]^+$). See also Figure S33, Figure S39, and Figure S42.

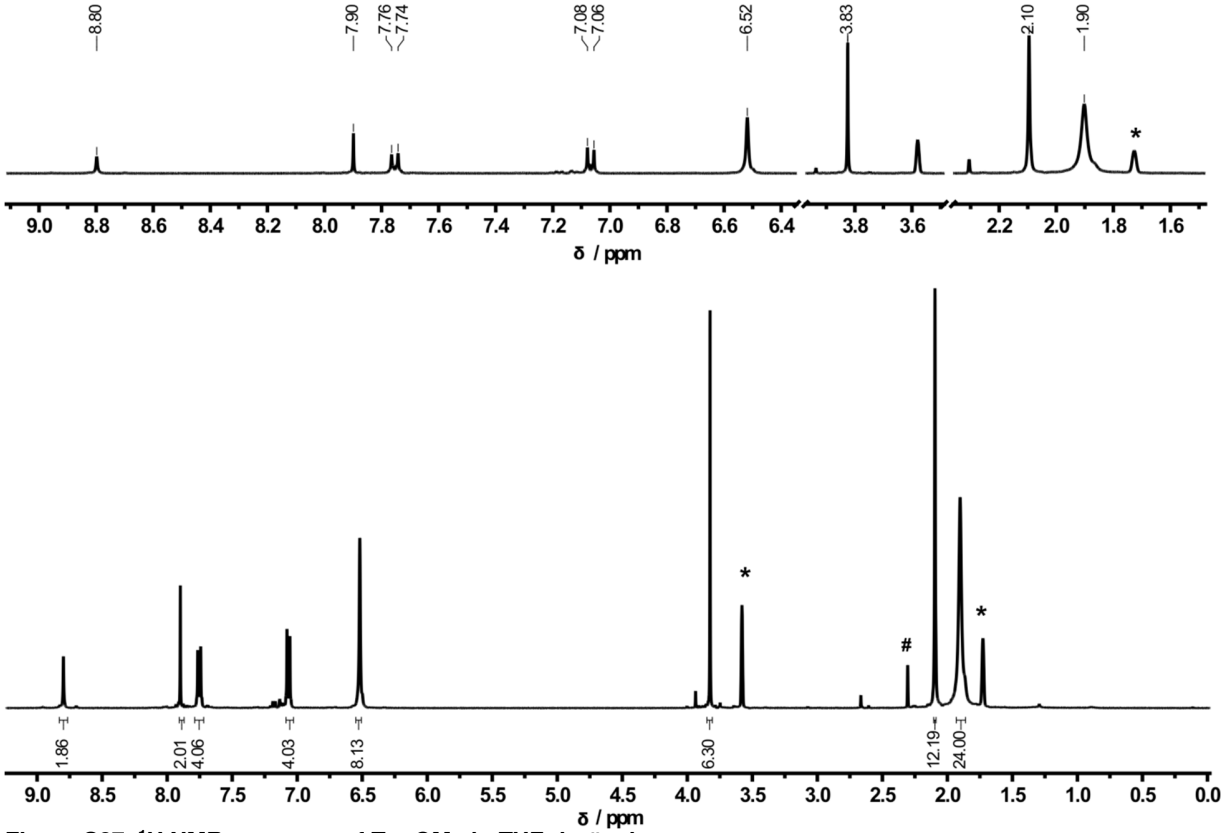


Figure S37. ^{1}H NMR-spectrum of Trz-OMe in THF-d_8. # toluene.

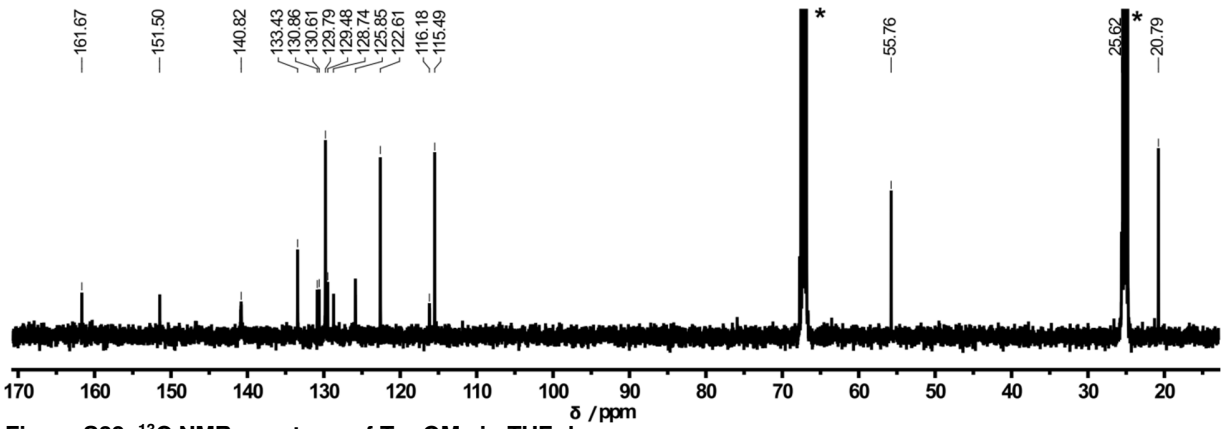


Figure S38. ^{13}C NMR-spectrum of Trz-OMe in THF-d_8.

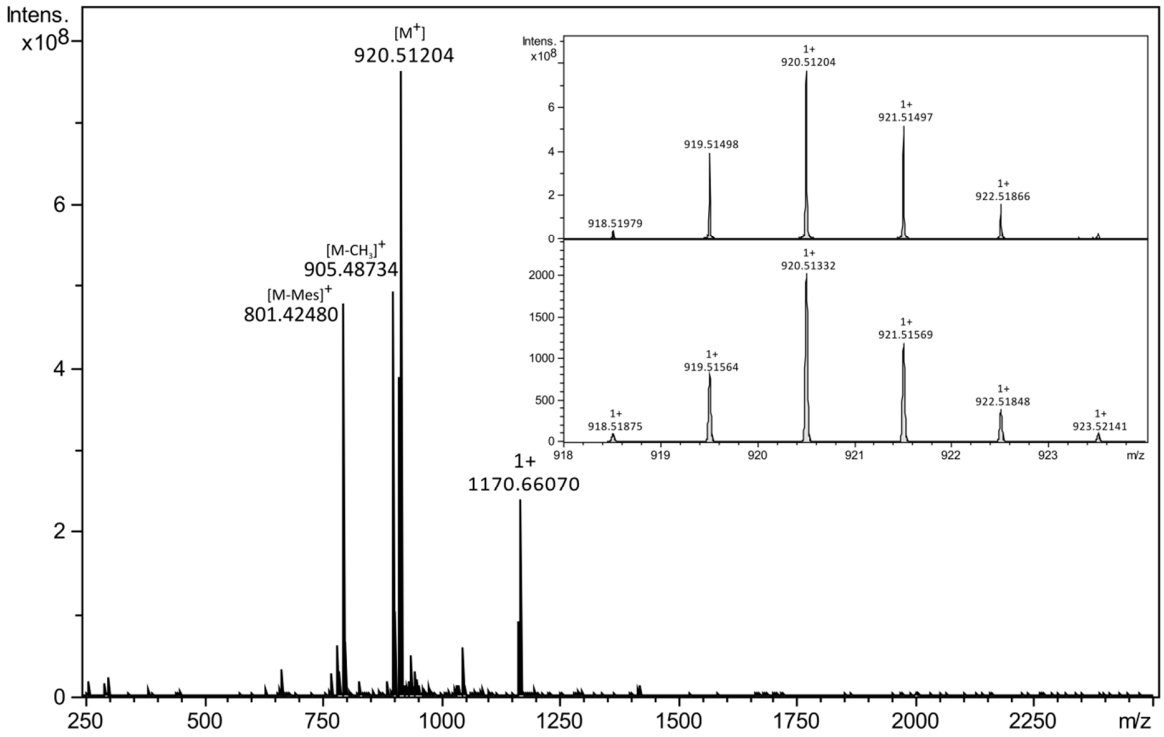


Figure S39. HR-FTMS-spectrum of Trz-OMe. The insert shows enlarged the experimental (top) and calculated (bottom) isotope-pattern of the molecular ion.

Mass spectra of all three model boranes, as well as **PTrz**, showed signals corresponding to the molecular monocations after loss of one equivalent of either mesityl- ($[M\text{-}Mes]^+$), or methyl-groups ($[M\text{-}CH_3]^+$), that are more prominent than those of the molecular ions ($[M]^+$). See also Figure S33, Figure S36, and Figure S42.

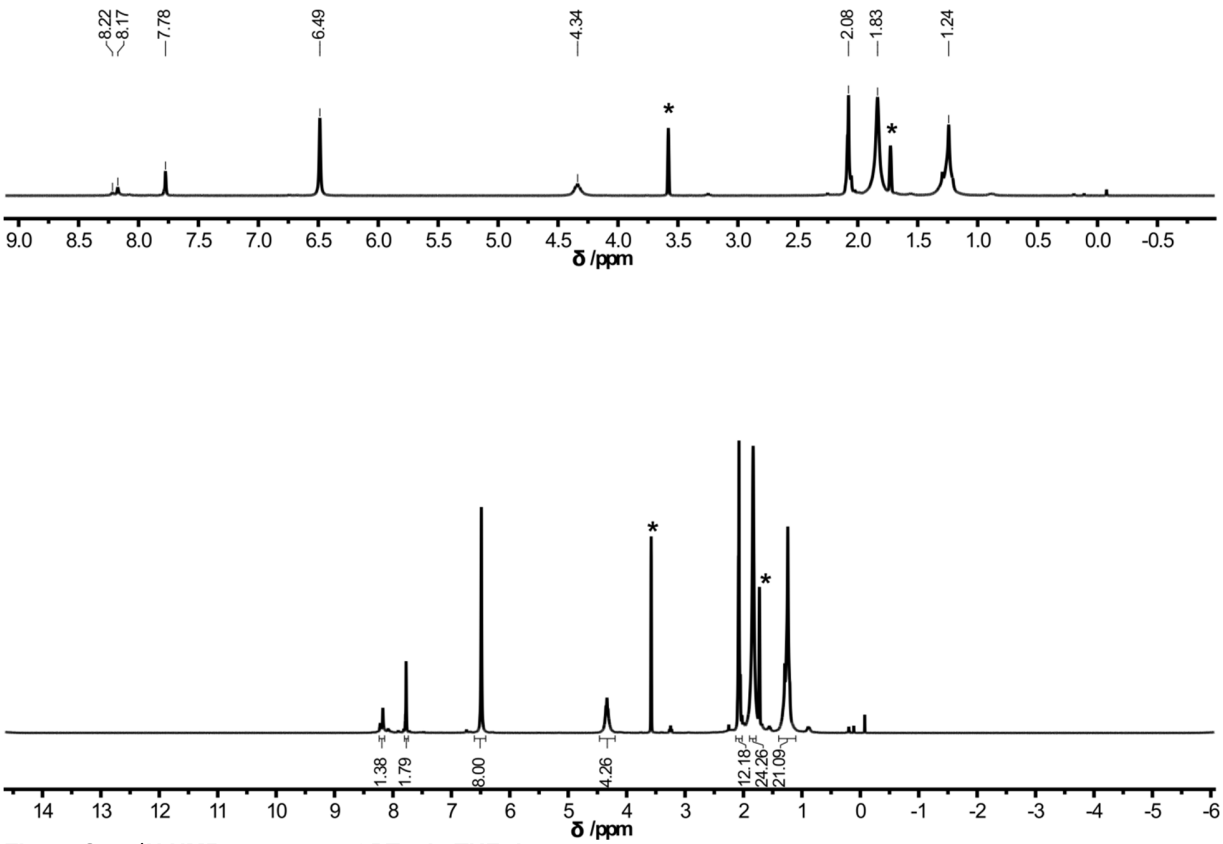


Figure S40. ^{1}H NMR-spectrum of PTrz in THF-d_8.

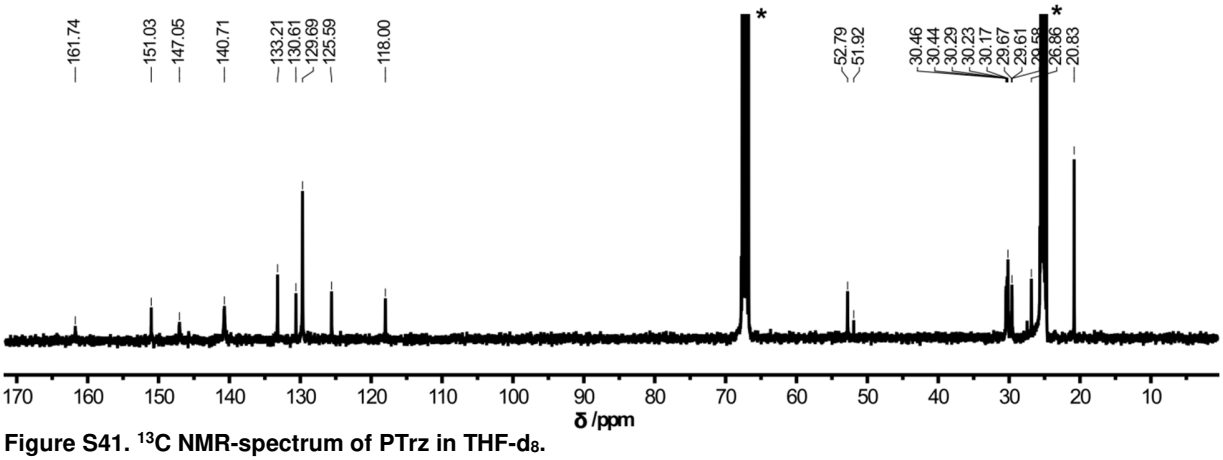


Figure S41. ^{13}C NMR-spectrum of PTrz in THF-d_8.

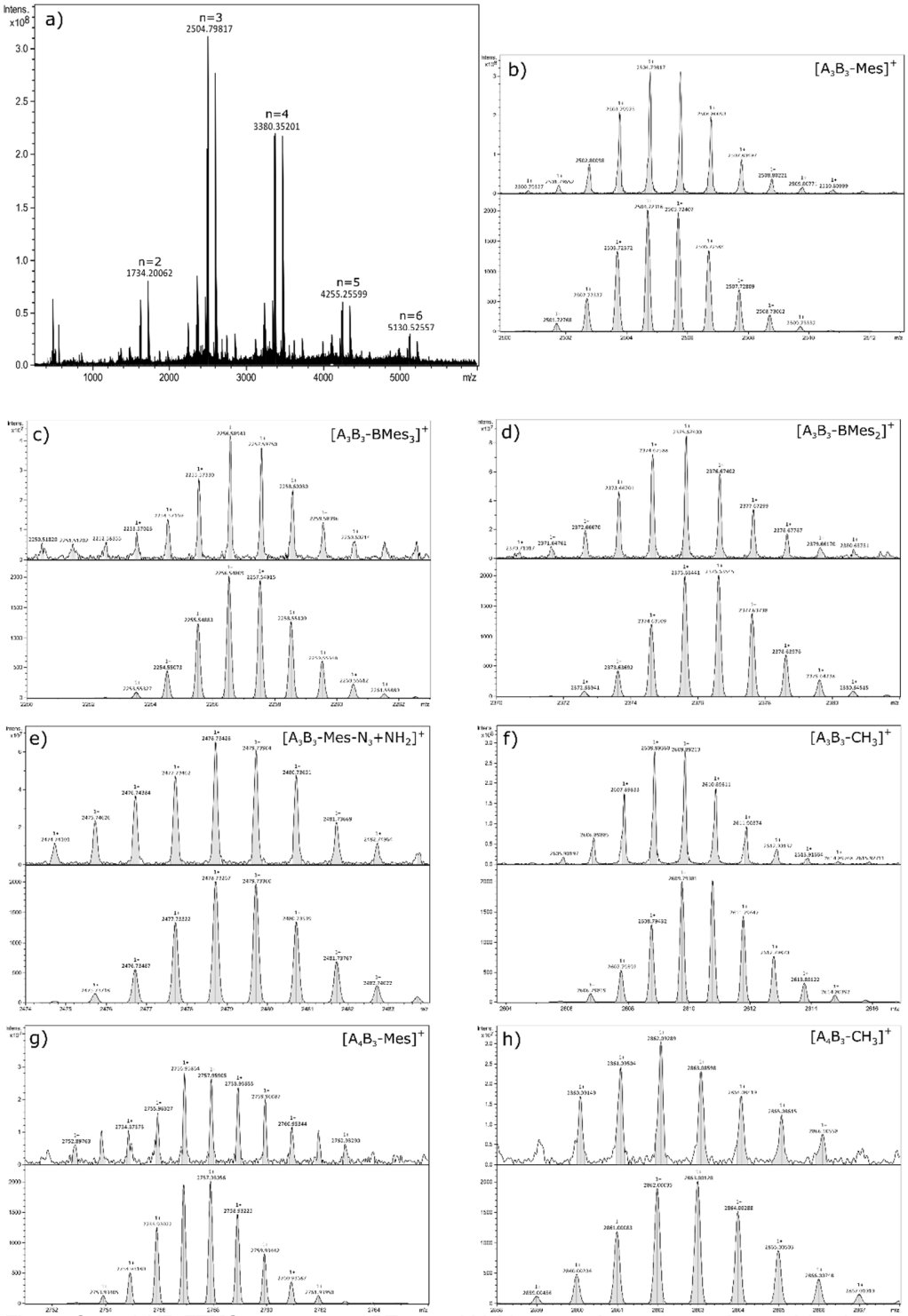


Figure S42. a) HR-FTMS-spectrum of PTrz, and b)-h) comparison of experimental (top) and calculated (bottom) isotope-patterns. A_xB_y corresponds to the diazide / stoichiometry. e) Species wherein an azide-end-group has been reduced to NH_2. Originates either from impurity in the reactant, or decomposed during the polymerization or ionization.

The molecular compounds **Trz-Me**, **Trz-OMe**, and **Trz-CF**3 showed similar fragmentation patternsn (See Figure S33,Figure S36, and Figure S39).

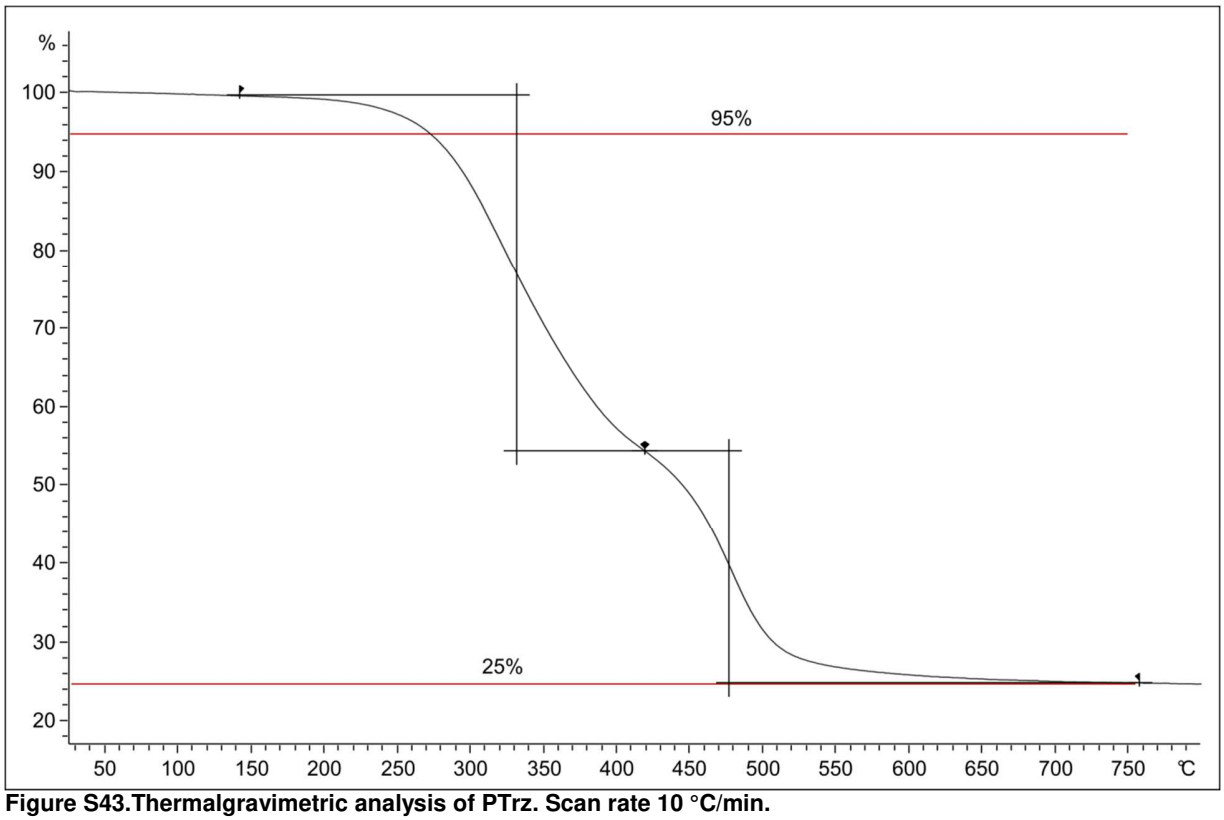
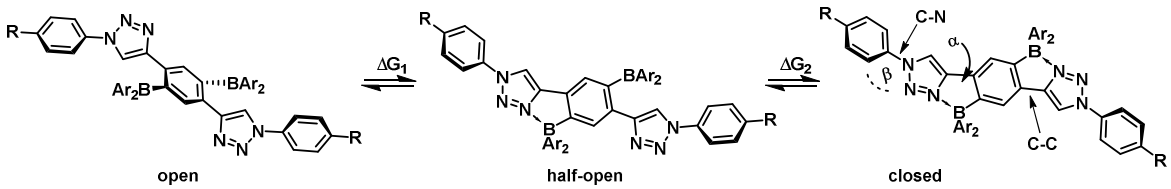


Figure S43.Thermalgravimetric analysis of PTrz. Scan rate 10 °C/min.

3. DFT Study



Scheme S1. Simulated conformers of Trz-boranes.

Trz-OMe': R = OMe, **Trz-Me'**: R = Me, **Trz-CF_3'**: R = CF_3, **PTrz':** Me instead of *p*-R-Ph.

Table S2. Calculated structural parameters for Trz-boranes.

Optimizations of **Trz-OMe'**, **Trz-Me**, **Trz-CF_3'** and **PTrz'**, performed at the B3LYP-D2/tzvp level. **TS'**-structures optimized at the B3LYP-D2/def2-TZVP-level including PCM-emulation of solvent THF.

Trz-R'	Trz-OMe'		Trz-Me'		Trz-Me^{XRD}		Trz-CF_3'		PTrz'		TS'		
	Closed	*Open*	*Closed*	*Open*			*Closed*	*Open*	*Closed*	*Open*	*Closed*	*TS*	*open*
d(N→B) / Å	1.661 1.660		1.659		1.655(0)	1.664(0)	1.667		1.661		1.664		
Angle α / °[a]	+5.4 -5.3	±52.6	±5.0	-132.7 -132.6	±6.5(1)	±6.1(1)	±5.7	±55.8	5.4	51.6 -31.7	4.6	-52.9	-56.2
d(C-N) / Å	1.424	1.417	1.425	1.418	1.442(1)	1.440(1)	1.421	1.412	1.455	1.450	1.457	1.452	1.451
d(C-B) / Å	1.628	1.569	1.627	1.574	1.642(1)	1.645(1)	1.627	1.571	1.628	1.569 1.570	1.633	1.574	1.568
d(C-C) / Å	1.445	1.465	1.445	1.465	1.459(1)	1.457(1)	1.444	1.466	1.445	1.466 1.465	1.447	1.472	1.468
Angle β/ °[b]	30.8	±34.7	±27.3	-9.5 9.3	±31.0(1)	±40.9(1)	±24.7	±17.9					
Angle γ/°[c]		17.3		17.3 17.4				11.0		15.9 16.0		47.3	15.4
C_{Trz}-C_{Mes}[d]		3.008		3.107				2.996		3.006 3.012		3.573	3.007

[a] Dihedral angle (N-C-C-C) within the N→B-ring. [b] Dihedral angle (N=N-C-C) between triazole and terminal phenyl ring. [c] Angle between the triazole ring and the closest mesityl-ring. [d] Distance C-4 of the triazole ring and C-1 of the closest mesityl ring.

Table S3. Calculated electronic properties of Trz-boranes.

Optimizations of Trz-OMe', Trz-Me, Trz-CF_3' and PTrz', performed at the B3LYP-D2/tzvp level.

	Energy	HOMO-2 eV	HOMO-1 eV	HOMO eV	LUMO eV	LUMO+1 eV	HOMO/LUMO-gap eV
PTrz'							
open	**0.0**	**-6.20**	**-6.14**	**-6.01**	**-2.06**	**-1.44**	**3.95**
half-open	**-0.4**	**-5.86**	**-5.72**	**-5.63**	**-1.73**	**-1.55**	**3.90**
closed	**:=0**	**-5.67**	**-5.63**	**-5.47**	**-1.56**	**-1.53**	**3.91**
Trz-Me'							
open	**-2.1**	**-6.24**	**-6.08**	**-5.80**	**-2.36**	**-1.49**	**3.44**
half-open	**-2.1**	**-5.83**	**-5.69**	**-5.62**	**-2.06**	**-1.76**	**3.55**
closed	**:=0**	**-5.63**	**-5.60**	**-5.44**	**-2.01**	**1.95**	**3.42**
Trz-OMe'							
open	**-14.8**	**-6.16**	**-6.02**	**-5.85**	**-2.22**	**-1.51**	**3.64**
half-open	**-4.0**	**-5.80**	**-5.66**	**-5.58**	**-1.94**	**-1.65**	**3.64**
closed	**:=0**	**-5.60**	**-5.58**	**-5.41**	**-1.87**	**-1.81**	**3.54**
Trz-CF_3'							
open	**-17.8**	**-6.41**	**-6.32**	**-6.25**	**-2.45**	**-2.11**	**3.80**
half-open	**-2.8**	**-6.07**	**-5.92**	**-5.85**	**-2.69**	**-2.16**	**3.16**
closed	**:=0**	**-5.85**	**-5.82**	**-5.68**	**-2.63**	**-2.57**	**3.05**
B_2-H		**-6.23**	**-6.20**	**-6.11**	**-2.40**	**-1.59**	**3.71**
B_2-TMS		**-6.23**	**-6.18**	**-5.98**	**-2.41**	**-1.55**	**3.56**

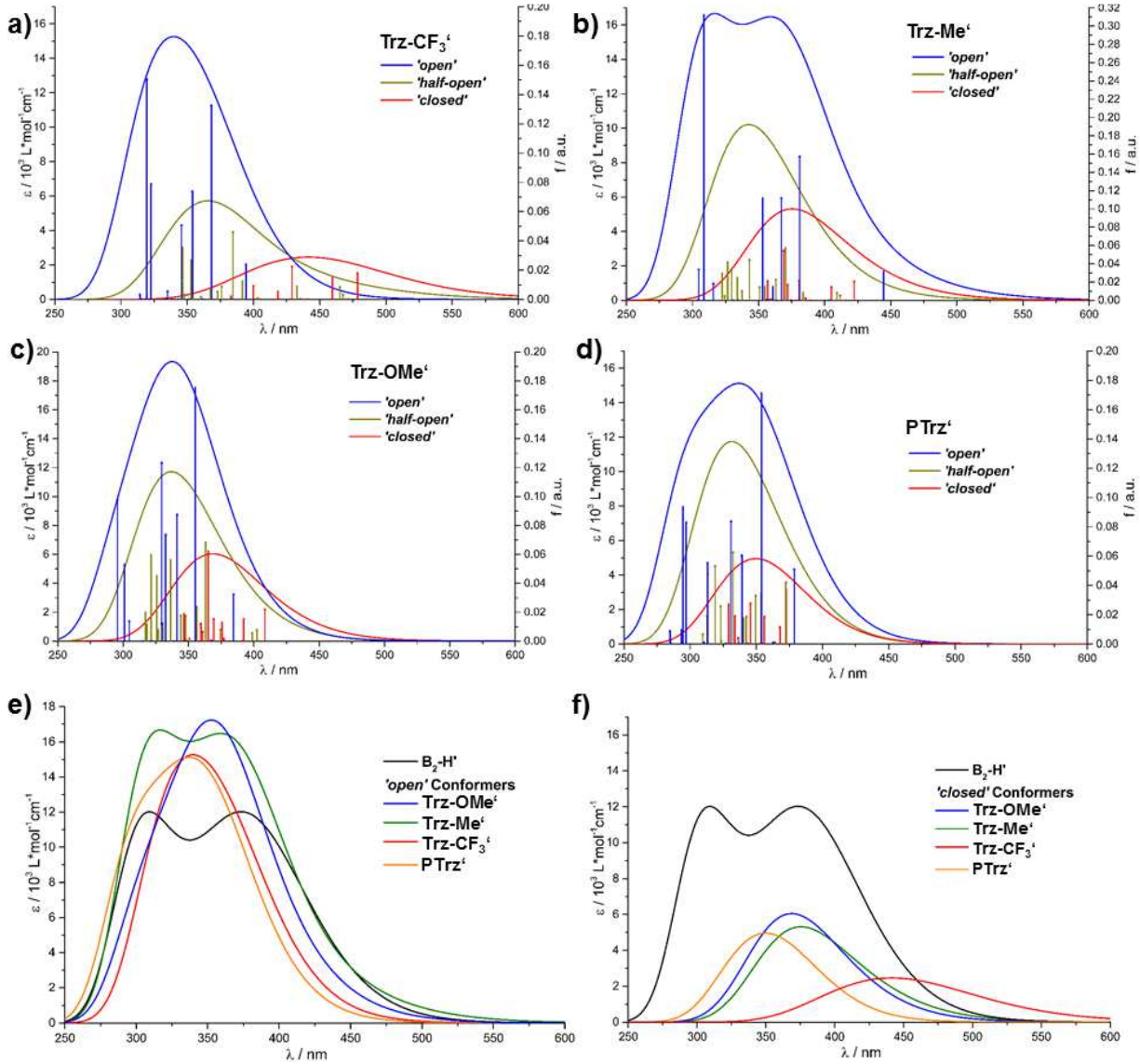


Figure S44. Calculated electronic transitions and corresponding simulated UV-vis spectra of triazolyl boranes. Simulated spectra based on first 15 excited states superimposed with a half-width at half-height of 0.333 eV. Geometry and TDDFT: B3LYP-D2/TZVP.

Table S4. Energies, oscillator strengths and orbital contributions of calculated electronic transitions. Optimizations of **Trz-OMe'**, **Trz-Me**, **Trz-CF_3'** and **PTrz'**, performed at the B3LYP-D2/tzvp level. Data extracted with GaussSum 3.0.[11]

PTrz' *,open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	26405.79	378.70	0.0510	Singlet-A	HOMO->LUMO (96%)	
2	27564.80	362.78	0.0010	Singlet-A	H-1->LUMO (91%)	HOMO->L+1 (4%)
3	28255.21	353.92	0.1713	Singlet-A	H-2->LUMO (92%)	H-1->L+1 (2%)
4	29137.59	343.20	0.0005	Singlet-A	H-3->LUMO (88%)	H-2->L+1 (3%), HOMO->L+1 (4%)
5	29479.56	339.22	0.0606	Singlet-A	H-5->LUMO (25%), H-4->LUMO (64%)	H-6->LUMO (3%)
6	29694.11	336.77	0.0003	Singlet-A	H-5->LUMO (68%), H-4->LUMO (26%)	H-4->L+1 (2%)
7	30225.63	330.85	0.0837	Singlet-A	H-6->LUMO (86%)	H-7->LUMO (5%), H-7->L+1 (4%), H-4->LUMO (2%)
8	30575.67	327.06	0.0001	Singlet-A	H-7->LUMO (88%)	H-6->LUMO (5%), H-6->L+1 (4%)
9	31929.07	313.19	0.0554	Singlet-A	H-8->LUMO (77%)	H-9->LUMO (9%), H-3->L+1 (3%), HOMO->L+1 (3%)
10	32219.43	310.37	0.0010	Singlet-A	HOMO->L+1 (86%)	H-8->LUMO (3%), H-3->LUMO (4%), H-1->LUMO (3%)
11	33668.81	297.01	0.0830	Singlet-A	H-1->L+1 (84%)	H-9->LUMO (3%), H-8->LUMO (5%), H-2->LUMO (2%)
12	33943.84	294.60	0.0936	Singlet-A	H-9->LUMO (67%), H-8->LUMO (10%)	H-2->L+1 (9%), H-1->L+1 (4%), HOMO->L+2 (2%)
13	34071.28	293.50	0.0095	Singlet-A	H-2->L+1 (80%)	H-9->LUMO (7%), H-1->LUMO (2%), H-1->L+1 (4%)
14	35064.95	285.19	0.0028	Singlet-A	H-4->L+1 (82%)	H-5->L+1 (4%), H-4->LUMO (4%)
15	35108.51	284.83	0.0088	Singlet-A	H-3->L+1 (82%)	H-9->LUMO (3%)

PTrz' *,half-open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	26856.65	372.35	0.0423	Singlet-A	HOMO->LUMO (86%)	HOMO->L+1 (8%), HOMO->L+2 (2%)
2	27452.69	364.26	0.0013	Singlet-A	H-1->LUMO (69%), H-1->L+1 (26%)	H-1->L+2 (3%)
3	28273.77	353.68	0.0347	Singlet-A	H-3->LUMO (35%), H-2->LUMO (17%), HOMO->L+1 (35%)	H-3->L+1 (3%), H-1->L+1 (6%)
4	28617.36	349.44	0.0330	Singlet-A	H-3->LUMO (17%), H-2->LUMO (12%), HOMO->L+1 (55%)	H-1->L+1 (2%), HOMO->LUMO (8%)
5	29202.92	342.43	0.0187	Singlet-A	H-3->LUMO (23%), H-2->LUMO (49%), H-2->L+1 (21%)	H-5->LUMO (2%), H-2->L+2 (2%)
6	29382.78	340.34	0.0178	Singlet-A	H-1->LUMO (24%), H-1->L+1 (62%)	H-5->LUMO (3%), H-3->LUMO (5%)
7	30076.41	332.49	0.0625	Singlet-A	H-5->LUMO (69%)	H-5->L+1 (4%), H-2->L+1 (8%), H-1->L+1 (2%), HOMO->L+2 (9%)
8	30531.31	327.53	0.0005	Singlet-A	H-4->LUMO (67%), H-2->L+1 (13%)	H-4->L+1 (9%), H-2->LUMO (4%)
9	30909.59	323.52	0.0021	Singlet-A	H-4->LUMO (16%), H-2->LUMO (12%), H-2->L+1 (55%)	H-5->LUMO (6%), H-4->L+1 (3%), H-3->LUMO (5%)
10	30949.11	323.11	0.0258	Singlet-A	HOMO->L+2 (76%)	H-6->LUMO (6%), H-5->LUMO (6%), HOMO->LUMO (3%)
11	31359.64	318.88	0.0530	Singlet-A	H-6->LUMO (83%)	H-6->L+1 (6%), HOMO->L+2 (5%)
12	31903.26	313.45	0.0477	Singlet-A	H-7->LUMO (20%), H-1->L+2 (65%)	H-3->L+1 (4%), H-1->LUMO (3%)
13	31989.56	312.60	0.0192	Singlet-A	H-7->LUMO (65%), H-1->L+2 (22%)	H-7->L+1 (5%)
14	32170.23	310.85	0.0006	Singlet-A	H-4->LUMO (11%), H-4->L+1 (85%)	
15	32312.18	309.48	0.0068	Singlet-A	H-3->L+1 (72%)	H-8->LUMO (4%), H-5->L+1 (6%), H-3->LUMO (5%), H-1->L+2 (3%)

PTrz' ,*closed'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	26832.45	372.68	0.0369	Singlet-A	HOMO->LUMO (24%), HOMO->L+1 (70%)	H-1->L+2 (4%)
2	27182.50	367.88	0.0115	Singlet-A	HOMO->LUMO (73%), HOMO->L+1 (20%)	H-1->L+2 (4%)
3	27447.85	364.33	0.0000	Singlet-A	H-1->L+1 (27%), HOMO->L+2 (71%)	
4	28086.64	356.04	0.0187	Singlet-A	H-3->L+2 (25%), H-2->L+1 (64%)	H-1->L+2 (8%)
5	28142.30	355.34	0.0000	Singlet-A	H-3->L+1 (41%), H-2->L+2 (39%), H-1->L+1 (15%)	H-3->LUMO (2%)
6	28390.72	352.23	0.0000	Singlet-A	H-1->LUMO (82%)	H-3->L+1 (3%), H-1->L+1 (9%), HOMO->L+2 (4%)
7	28937.56	345.57	0.0278	Singlet-A	H-2->LUMO (91%)	H-2->L+1 (6%)
8	29204.53	342.41	0.0000	Singlet-A	H-3->LUMO (71%), H-3->L+1 (17%)	H-1->LUMO (4%), H-1->L+1 (3%)
9	29422.30	339.88	0.0000	Singlet-A	H-3->LUMO (16%), H-1->LUMO (12%), H-1->L+1 (41%), HOMO->L+2 (20%)	H-4->L+2 (2%), H-3->L+1 (6%)
10	29725.56	336.41	0.0043	Singlet-A	H-5->L+2 (10%), H-4->L+1 (45%), H-3->L+2 (12%), H-1->L+2 (27%)	HOMO->L+1 (2%)
11	29950.59	333.88	0.0190	Singlet-A	H-5->L+2 (12%), H-4->L+1 (25%), H-1->L+2 (50%)	H-2->L+1 (2%), HOMO->L+1 (6%)
12	29994.15	333.40	0.0000	Singlet-A	H-5->L+1 (49%), H-4->L+2 (38%)	H-2->L+2 (4%)
13	30381.29	329.15	0.0273	Singlet-A	H-4->LUMO (91%)	H-4->L+1 (4%)
14	30589.38	326.91	0.0000	Singlet-A	H-5->LUMO (83%), H-5->L+1 (11%)	
15	30924.91	323.36	0.0000	Singlet-A	H-3->L+1 (25%), H-2->L+2 (51%)	H-5->LUMO (5%), H-5->L+1 (4%), H-3->LUMO (7%), H-1->L+1 (4%)

Trz-Me' ,*open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	22490.77	444.63	0.0313	Singlet-A	HOMO->LUMO (98%)	
2	24782.19	403.52	0.0000	Singlet-A	H-1->LUMO (95%)	HOMO->L+1 (3%)
3	26240.44	381.09	0.1572	Singlet-A	H-2->LUMO (86%)	H-4->LUMO (9%), H-3->L+1 (2%)
4	26697.76	374.56	0.0000	Singlet-A	H-3->LUMO (95%)	
5	27237.34	367.14	0.1118	Singlet-A	H-4->LUMO (82%), H-2->LUMO (10%)	H-10->LUMO (2%), H-6->LUMO (3%)
6	27520.44	363.37	0.0001	Singlet-A	H-5->LUMO (95%)	H-6->L+1 (2%)
7	27706.76	360.92	0.0145	Singlet-A	H-6->LUMO (92%)	H-5->L+1 (2%), H-4->LUMO (3%)
8	28081.00	356.11	0.0005	Singlet-A	H-7->LUMO (94%)	
9	28313.29	353.19	0.1116	Singlet-A	H-8->LUMO (94%)	
10	29902.20	334.42	0.0000	Singlet-A	H-9->LUMO (40%), HOMO->L+1 (54%)	H-1->LUMO (2%)
11	30239.34	330.70	0.0000	Singlet-A	H-9->LUMO (55%), HOMO->L+1 (40%)	
12	31672.59	315.73	0.0182	Singlet-A	H-10->LUMO (51%), HOMO->L+2 (32%)	H-11->LUMO (3%), H-4->LUMO (2%), H-1->L+1 (3%)
13	32401.71	308.63	0.3118	Singlet-A	H-10->LUMO (21%), H-1->L+1 (15%), HOMO->L+2 (54%)	H-1->L+3 (6%)
14	32825.15	304.64	0.0337	Singlet-A	H-10->LUMO (18%), H-1->L+1 (69%)	H-11->LUMO (4%), HOMO->L+2 (4%)
15	32854.99	304.37	0.0003	Singlet-A	H-1->L+2 (19%), HOMO->L+3 (76%)	

Trz-Me‘ ,*half-open‘*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	24286.16	411.76	0.0051	Singlet-A	HOMO->LUMO (94%)	H-1->LUMO (4%)
2	24428.92	409.35	0.0084	Singlet-A	H-1->LUMO (94%)	HOMO->LUMO (4%)
3	26057.35	383.77	0.0083	Singlet-A	H-2->LUMO (94%)	H-3->LUMO (4%)
4	27003.44	370.32	0.0572	Singlet-A	H-3->L+1 (19%), HOMO->L+1 (64%)	H-3->LUMO (4%), H-2->L+1 (7%), H-1->L+1 (4%)
5	27539.80	363.11	0.0226	Singlet-A	H-3->LUMO (17%), H-3->L+1 (32%), HOMO->L+1 (30%)	H-2->L+1 (8%), H-1->L+1 (7%)
6	27784.19	359.92	0.0008	Singlet-A	H-4->LUMO (98%)	
7	28182.62	354.83	0.0146	Singlet-A	H-3->LUMO (22%), H-1->L+1 (70%)	
8	28499.60	350.88	0.0144	Singlet-A	H-3->LUMO (44%), H-3->L+1 (24%), H-1->L+1 (13%)	H-5->LUMO (4%), H-5->L+1 (2%), H-2->LUMO (3%), H-2->L+1 (5%)
9	29148.07	343.08	0.0441	Singlet-A	H-5->LUMO (29%), H-5->L+1 (37%), H-2->L+1 (21%)	H-3->LUMO (3%)
10	29630.39	337.49	0.0100	Singlet-A	H-5->LUMO (23%), H-3->L+1 (18%), H-2->L+1 (50%)	H-3->LUMO (2%)
11	29947.37	333.92	0.0246	Singlet-A	H-6->LUMO (16%), H-5->LUMO (19%), H-5->L+1 (41%)	H-6->L+1 (8%), H-2->L+1 (5%)
12	30341.77	329.58	0.0339	Singlet-A	H-6->LUMO (14%), H-6->L+1 (21%), H-5->LUMO (13%), HOMO->L+2 (32%)	H-5->L+1 (3%), HOMO->L+3 (9%), HOMO->L+4 (3%)
13	30625.68	326.52	0.0419	Singlet-A	H-6->LUMO (25%), HOMO->L+2 (35%)	H-6->L+1 (8%), H-5->LUMO (5%), H-5->L+1 (7%), HOMO->L+3 (8%)
14	30841.03	324.24	0.0044	Singlet-A	H-4->L+1 (92%)	
15	31015.24	322.42	0.0297	Singlet-A	H-6->LUMO (24%), H-6->L+1 (50%)	H-9->LUMO (9%), H-5->LUMO (3%), H-1->L+2 (4%)

Trz-Me‘ ,*closed‘*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	23683.66	422.23	0.0205	Singlet-A	HOMO->LUMO (92%)	H-1->L+1 (5%)
2	24039.35	415.98	0.0000	Singlet-A	H-1->LUMO (13%), HOMO->L+1 (83%)	H-3->LUMO (2%)
3	24687.02	405.07	0.0147	Singlet-A	H-3->L+1 (23%), H-2->LUMO (61%), H-1->L+1 (13%)	
4	24716.05	404.60	0.0000	Singlet-A	H-3->LUMO (34%), H-2->L+1 (43%), H-1->LUMO (20%)	
5	25704.89	389.03	0.0000	Singlet-A	H-3->LUMO (22%), H-1->LUMO (59%), HOMO->L+1 (14%)	
6	25926.69	385.70	0.0025	Singlet-A	H-3->L+1 (16%), H-1->L+1 (60%), HOMO->L+2 (11%)	H-4->LUMO (3%), HOMO->LUMO (7%)
7	26265.44	380.73	0.0213	Singlet-A	H-5->L+1 (21%), H-4->LUMO (60%)	H-3->L+1 (4%), H-2->LUMO (6%), H-1->L+1 (4%), HOMO->L+2 (2%)
8	26371.91	379.19	0.0000	Singlet-A	H-5->LUMO (42%), H-4->L+1 (40%)	H-3->LUMO (4%), H-2->L+1 (9%), H-1->LUMO (3%)
9	26883.27	371.98	0.0169	Singlet-A	H-3->L+1 (35%), H-2->LUMO (29%), H-1->L+1 (11%), HOMO->L+2 (11%)	H-5->L+1 (5%), H-4->LUMO (5%), H-2->L+2 (3%)
10	26888.91	371.90	0.0000	Singlet-A	H-5->LUMO (10%), H-3->LUMO (35%), H-2->L+1 (43%)	H-4->L+1 (5%), H-1->LUMO (5%)
11	27117.97	368.76	0.0541	Singlet-A	H-3->L+1 (13%), HOMO->L+2 (72%)	H-4->LUMO (3%), H-1->L+1 (6%)
12	27820.48	359.45	0.0000	Singlet-A	H-7->LUMO (43%), H-6->L+1 (18%), H-5->LUMO (21%), H-4->L+1 (13%)	
13	27891.46	358.53	0.0013	Singlet-A	H-7->L+1 (32%), H-6->LUMO (64%)	
14	28005.99	357.07	0.0000	Singlet-A	H-7->LUMO (20%), H-6->L+1 (15%), H-5->LUMO (24%), H-4->L+1 (37%)	
15	28021.31	356.87	0.0214	Singlet-A	H-5->L+1 (64%), H-4->LUMO (26%)	H-8->LUMO (4%), H-3->L+1 (2%)

Trz-CF_3' *,open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25358.88	394.34	0.0240	Singlet-A	HOMO->LUMO (93%)	H-1->L+1 (3%)
2	26070.26	383.58	0.0000	Singlet-A	H-1->LUMO (88%)	HOMO->L+1 (7%)
3	27151.04	368.31	0.1325	Singlet-A	H-2->LUMO (92%)	H-3->L+1 (2%)
4	27655.14	361.60	0.0000	Singlet-A	H-3->LUMO (83%)	H-2->L+1 (4%), H-1->LUMO (2%), HOMO->L+1 (5%)
5	28253.60	353.94	0.0738	Singlet-A	H-6->LUMO (10%), H-5->LUMO (76%)	H-4->LUMO (4%), H-4->L+1 (3%)
6	28445.56	351.55	0.0000	Singlet-A	H-4->LUMO (84%)	H-5->LUMO (5%), H-5->L+1 (3%)
7	28925.46	345.72	0.0506	Singlet-A	H-6->LUMO (81%), H-5->LUMO (11%)	H-7->L+1 (3%)
8	29138.39	343.19	0.0000	Singlet-A	H-7->LUMO (81%)	H-6->L+1 (5%), H-4->LUMO (3%), HOMO->L+1 (5%)
9	29507.79	338.89	0.0000	Singlet-A	HOMO->L+1 (73%)	H-7->LUMO (5%), H-3->LUMO (8%), H-3->L+2 (2%), H-1->LUMO (3%), H-1->L+2 (6%)
10	29830.42	335.23	0.0055	Singlet-A	H-1->L+1 (62%), HOMO->L+2 (25%)	H-8->LUMO (3%), H-3->L+1 (6%)
11	30993.47	322.65	0.0789	Singlet-A	H-8->LUMO (52%), H-3->L+1 (19%), H-1->L+1 (10%)	H-9->LUMO (4%), H-7->L+1 (2%), H-4->L+1 (2%)
12	31059.60	321.96	0.0000	Singlet-A	H-2->L+1 (81%)	H-7->LUMO (2%), H-7->L+2 (2%), H-3->LUMO (3%), H-1->L+2 (4%)
13	31295.92	319.53	0.1505	Singlet-A	H-8->LUMO (16%), H-1->L+1 (17%), HOMO->L+2 (46%)	H-3->L+1 (9%), H-1->L+3 (5%), HOMO->LUMO (2%)
14	31685.49	315.60	0.0000	Singlet-A	H-1->L+2 (58%), HOMO->L+3 (18%)	H-8->L+1 (2%), H-3->L+2 (2%), H-2->L+1 (6%), H-1->LUMO (4%), HOMO->L+1 (5%)
15	31813.73	314.33	0.0034	Singlet-A	H-8->LUMO (18%), H-3->L+1 (27%), HOMO->L+2 (11%)	H-7->L+1 (8%), H-6->L+2 (4%), H-5->L+2 (3%), H-4->L+1 (8%), H-2->L+2 (7%), H-1->L+1 (3%), H-1->L+3 (3%)

Trz-CF_3' *,half-open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	21383.37	467.65	0.0034	Singlet-A	HOMO->LUMO (91%)	H-1->LUMO (8%)
2	21490.64	465.32	0.0084	Singlet-A	H-1->LUMO (90%)	HOMO->LUMO (8%)
3	23106.98	432.77	0.0089	Singlet-A	H-2->LUMO (97%)	
4	24808.81	403.08	0.0004	Singlet-A	H-4->LUMO (97%)	
5	25526.64	391.75	0.0123	Singlet-A	H-3->LUMO (92%)	H-5->LUMO (2%)
6	26010.57	384.46	0.0461	Singlet-A	HOMO->L+1 (87%)	H-3->L+1 (5%), HOMO->L+3 (2%)
7	26599.36	375.95	0.0089	Singlet-A	H-5->LUMO (88%)	H-8->LUMO (2%), H-6->LUMO (4%), H-3->LUMO (3%)
8	26813.10	372.95	0.0054	Singlet-A	H-3->L+1 (49%), H-1->L+1 (30%)	H-2->L+1 (8%), HOMO->L+1 (7%)
9	27204.27	367.59	0.0083	Singlet-A	H-3->L+1 (29%), H-1->L+1 (60%)	H-2->L+1 (3%), H-1->L+2 (3%)
10	27743.05	360.45	0.0018	Singlet-A	H-6->LUMO (91%)	H-9->LUMO (2%), H-5->LUMO (5%)
11	28220.53	354.35	0.0020	Singlet-A	H-7->LUMO (86%)	H-9->LUMO (3%), H-8->LUMO (7%), H-5->LUMO (3%)
12	28344.74	352.80	0.0267	Singlet-A	H-5->L+1 (14%), H-3->L+1 (10%), H-2->L+1 (66%)	
13	28743.99	347.90	0.0033	Singlet-A	H-5->L+1 (29%), H-2->L+1 (11%), HOMO->L+2 (32%)	H-8->LUMO (8%), H-6->L+1 (2%), HOMO->L+4 (4%)
14	28844.81	346.68	0.0354	Singlet-A	H-5->L+1 (34%), HOMO->L+2 (39%)	H-7->L+1 (2%), H-6->L+1 (7%), H-2->L+1 (3%), HOMO->L+3 (3%), HOMO->L+4 (3%)
15	28853.68	346.58	0.0127	Singlet-A	H-8->LUMO (73%), HOMO->L+2 (11%)	H-7->LUMO (8%)

Trz-CF_3' *,closed'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	20895.41	478.57	0.0181	Singlet-A	HOMO->LUMO (92%)	H-1->L+1 (6%)
2	21222.87	471.19	0.0000	Singlet-A	H-1->LUMO (17%), HOMO->L+1 (81%)	
3	21755.19	459.66	0.0149	Singlet-A	H-3->L+1 (22%), H-2->LUMO (62%), H-1->L+1 (14%)	
4	21784.23	459.05	0.0000	Singlet-A	H-3->LUMO (33%), H-2->L+1 (42%), H-1->LUMO (21%)	HOMO->L+1 (2%)
5	22694.02	440.64	0.0000	Singlet-A	H-3->LUMO (23%), H-1->LUMO (56%), HOMO->L+1 (15%)	H-2->L+1 (3%)
6	22977.93	435.20	0.0005	Singlet-A	H-3->L+1 (15%), H-1->L+1 (70%)	H-4->LUMO (3%), H-2->LUMO (3%), HOMO->LUMO (7%)
7	23302.16	429.14	0.0225	Singlet-A	H-5->L+1 (23%), H-4->LUMO (60%)	H-3->L+1 (4%), H-2->LUMO (6%), H-1->L+1 (4%)
8	23376.37	427.78	0.0000	Singlet-A	H-5->LUMO (44%), H-4->L+1 (39%)	H-3->LUMO (4%), H-2->L+1 (8%), H-1->LUMO (2%)
9	23843.36	419.40	0.0000	Singlet-A	H-5->LUMO (10%), H-3->LUMO (36%), H-2->L+1 (44%)	H-4->L+1 (5%), H-1->LUMO (4%)
10	23897.40	418.46	0.0055	Singlet-A	H-3->L+1 (53%), H-2->LUMO (28%)	H-5->L+1 (6%), H-4->LUMO (7%), H-1->L+1 (4%)
11	24774.13	403.65	0.0000	Singlet-A	H-7->L+1 (23%), H-6->LUMO (56%), H-5->LUMO (14%)	H-4->L+1 (5%)
12	24801.55	403.20	0.0009	Singlet-A	H-7->LUMO (65%), H-6->L+1 (30%)	H-4->LUMO (3%)
13	24953.18	400.75	0.0000	Singlet-A	H-7->L+1 (10%), H-5->LUMO (31%), H-4->L+1 (48%)	H-6->LUMO (9%)
14	25003.99	399.94	0.0093	Singlet-A	H-5->L+1 (68%), H-4->LUMO (26%)	H-6->L+1 (3%)
15	26106.55	383.05	0.0020	Singlet-A	H-7->LUMO (31%), H-6->L+1 (61%)	HOMO->L+2 (5%)

Trz-OMe' *,open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	26011.38	384.45	0.0325	Singlet-A	HOMO->LUMO (95%)	H-1->L+1 (2%)
2	27165.56	368.11	0.0000	Singlet-A	H-1->LUMO (92%)	HOMO->L+1 (5%)
3	28150.36	355.24	0.1753	Singlet-A	H-2->LUMO (91%)	H-3->L+1 (2%)
4	28819.80	346.98	0.0000	Singlet-A	H-3->LUMO (91%)	H-2->L+1 (3%), HOMO->L+1 (3%)
5	29307.77	341.21	0.0874	Singlet-A	H-5->LUMO (84%)	H-8->LUMO (3%), H-6->LUMO (6%), H-4->L+1 (2%)
6	29510.21	338.87	0.0000	Singlet-A	H-7->LUMO (15%), H-4->LUMO (79%)	H-5->L+1 (3%)
7	30074.80	332.50	0.0737	Singlet-A	H-8->LUMO (90%)	H-9->L+1 (3%), H-5->LUMO (4%)
8	30347.42	329.52	0.1233	Singlet-A	H-6->LUMO (75%)	H-11->LUMO (2%), H-10->LUMO (3%), H-9->LUMO (7%), H-5->LUMO (3%)
9	30347.42	329.52	0.0119	Singlet-A	H-9->LUMO (70%), H-7->LUMO (13%)	H-8->L+1 (4%), H-6->LUMO (7%)
10	31080.57	321.74	0.0000	Singlet-A	H-9->LUMO (16%), H-7->LUMO (66%), H-4->LUMO (14%)	
11	31760.50	314.86	0.0000	Singlet-A	HOMO->L+1 (88%)	H-3->LUMO (3%), H-1->LUMO (4%)
12	32814.67	304.74	0.0139	Singlet-A	H-10->LUMO (56%), H-1->L+1 (19%)	H-11->LUMO (9%), H-6->LUMO (6%), H-3->L+1 (3%)
13	33216.33	301.06	0.0531	Singlet-A	H-10->LUMO (22%), H-1->L+1 (71%)	
14	33798.66	295.87	0.0000	Singlet-A	H-2->L+1 (91%)	H-3->LUMO (3%)
15	33823.67	295.65	0.0977	Singlet-A	H-11->LUMO (69%), H-10->LUMO (12%)	H-3->L+1 (5%), H-1->L+1 (3%), HOMO->L+6 (4%)

Trz-OMe' *,half-open'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	24854.78	402.34	0.0077	Singlet-A	HOMO->LUMO (98%)	
2	25074.16	398.82	0.0056	Singlet-A	H-1->LUMO (98%)	
3	26722.76	374.21	0.0079	Singlet-A	H-2->LUMO (91%)	H-3->LUMO (7%)
4	27536.57	363.15	0.0684	Singlet-A	H-3->L+1 (12%), HOMO->L+1 (70%)	H-3->LUMO (4%), H-2->L+1 (8%), H-1->L+1 (2%)
5	28064.06	356.33	0.0237	Singlet-A	H-3->LUMO (24%), H-3->L+1 (27%), H-2->L+1 (11%), HOMO->L+1 (23%)	H-1->L+1 (7%), HOMO->L+3 (2%)
6	28495.57	350.93	0.0007	Singlet-A	H-4->LUMO (97%)	
7	28746.41	347.87	0.0175	Singlet-A	H-3->LUMO (26%), H-1->L+1 (64%)	H-2->LUMO (3%), H-1->L+3 (2%)
8	29060.16	344.11	0.0178	Singlet-A	H-3->LUMO (29%), H-3->L+1 (23%), H-1->L+1 (21%)	H-5->LUMO (5%), H-5->L+1 (4%), H-2->LUMO (4%), H-2->L+1 (9%)
9	29728.79	336.37	0.0563	Singlet-A	H-5->LUMO (31%), H-5->L+1 (34%), H-2->L+1 (18%)	H-3->LUMO (4%), HOMO->L+2 (2%), HOMO->L+3 (2%)
10	30265.95	330.40	0.0124	Singlet-A	H-5->LUMO (18%), H-3->L+1 (27%), H-2->L+1 (45%)	H-3->LUMO (2%)
11	30591.00	326.89	0.0077	Singlet-A	H-5->LUMO (25%), H-5->L+1 (32%)	H-9->LUMO (2%), H-7->LUMO (3%), H-6->LUMO (8%), H-6->L+1 (5%), H-2->L+1 (4%), HOMO->L+2 (8%), HOMO->L+3 (3%)
12	30692.62	325.81	0.0450	Singlet-A	H-6->L+1 (14%), HOMO->L+2 (46%), HOMO->L+3 (17%)	H-6->LUMO (7%), H-5->L+1 (4%)
13	31111.22	321.43	0.0598	Singlet-A	H-7->LUMO (13%), H-7->L+1 (10%), H-6->LUMO (18%), H-6->L+1 (14%), H-5->LUMO (10%), H-5->L+1 (14%), HOMO->L+2 (12%)	
14	31428.20	318.19	0.0116	Singlet-A	H-4->L+1 (10%), H-1->L+2 (68%)	H-7->LUMO (4%), H-1->L+3 (7%)
15	31535.47	317.10	0.0198	Singlet-A	H-4->L+1 (76%)	H-6->LUMO (2%), H-1->L+2 (9%)

Trz-OMe' *,closed'*

No.	Energy (cm^{-1})	λ (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	24483.77	408.43	0.0219	Singlet-A	HOMO->LUMO (91%)	H-1->L+1 (5%)
2	24830.58	402.73	0.0000	Singlet-A	H-1->LUMO (12%), HOMO->L+1 (83%)	H-3->LUMO (2%)
3	25495.19	392.23	0.0151	Singlet-A	H-3->L+1 (23%), H-2->LUMO (55%), H-1->L+1 (14%)	H-1->LUMO (3%)
4	25528.25	391.72	0.0003	Singlet-A	H-3->LUMO (36%), H-2->L+1 (40%), H-1->LUMO (15%)	H-2->LUMO (3%)
5	26514.67	377.15	0.0017	Singlet-A	H-3->LUMO (15%), H-1->LUMO (49%), HOMO->L+1 (10%)	H-1->L+1 (9%), HOMO->LUMO (3%), HOMO->L+2 (7%)
6	26621.94	375.63	0.0129	Singlet-A	H-1->LUMO (10%), H-1->L+1 (30%), HOMO->L+2 (30%)	H-3->LUMO (4%), H-3->L+1 (8%), H-2->LUMO (2%), H-2->L+1 (4%), HOMO->LUMO (4%), HOMO->L+1 (3%)
7	27083.29	369.23	0.0154	Singlet-A	H-5->L+1 (18%), H-4->LUMO (55%)	H-3->L+1 (9%), H-2->LUMO (4%), HOMO->L+2 (8%)
8	27227.66	367.27	0.0005	Singlet-A	H-5->LUMO (39%), H-4->L+1 (39%)	H-3->LUMO (4%), H-2->L+1 (9%), H-1->LUMO (4%)
9	27394.62	365.04	0.0621	Singlet-A	H-1->L+1 (36%), HOMO->L+2 (47%)	H-4->LUMO (3%), H-2->LUMO (7%)
10	27712.40	360.85	0.0063	Singlet-A	H-3->LUMO (20%), H-3->L+1 (10%), H-2->LUMO (13%), H-2->L+1 (23%)	H-5->LUMO (9%), H-5->L+1 (3%), H-4->LUMO (3%), H-4->L+1 (2%), H-1->LUMO (5%), H-1->L+2 (3%)
11	27821.29	359.44	0.0119	Singlet-A	H-3->LUMO (14%), H-3->L+1 (34%), H-2->LUMO (13%), H-2->L+1 (13%)	H-5->LUMO (2%), H-5->L+1 (4%), H-4->LUMO (6%), H-4->L+1 (3%), H-2->L+2 (5%)
12	28518.96	350.64	0.0017	Singlet-A	H-1->L+2 (81%)	H-3->L+2 (4%), H-1->L+4 (2%)
13	28693.17	348.51	0.0003	Singlet-A	H-6->LUMO (36%), H-6->L+1 (20%), H-5->LUMO (17%)	H-7->LUMO (3%), H-4->LUMO (4%), H-4->L+1 (9%), H-1->L+2 (6%)
14	28793.99	347.29	0.0015	Singlet-A	H-7->LUMO (34%), H-7->L+1 (12%), H-6->LUMO (16%), H-6->L+1 (14%)	H-5->LUMO (9%), H-4->L+1 (8%)
15	28848.84	346.63	0.0188	Singlet-A	H-7->LUMO (26%), H-7->L+1 (10%), H-5->L+1 (19%), H-4->LUMO (16%), H-4->L+1 (11%)	H-6->LUMO (2%), H-6->L+1 (4%), H-5->LUMO (3%), H-2->L+2 (3%)

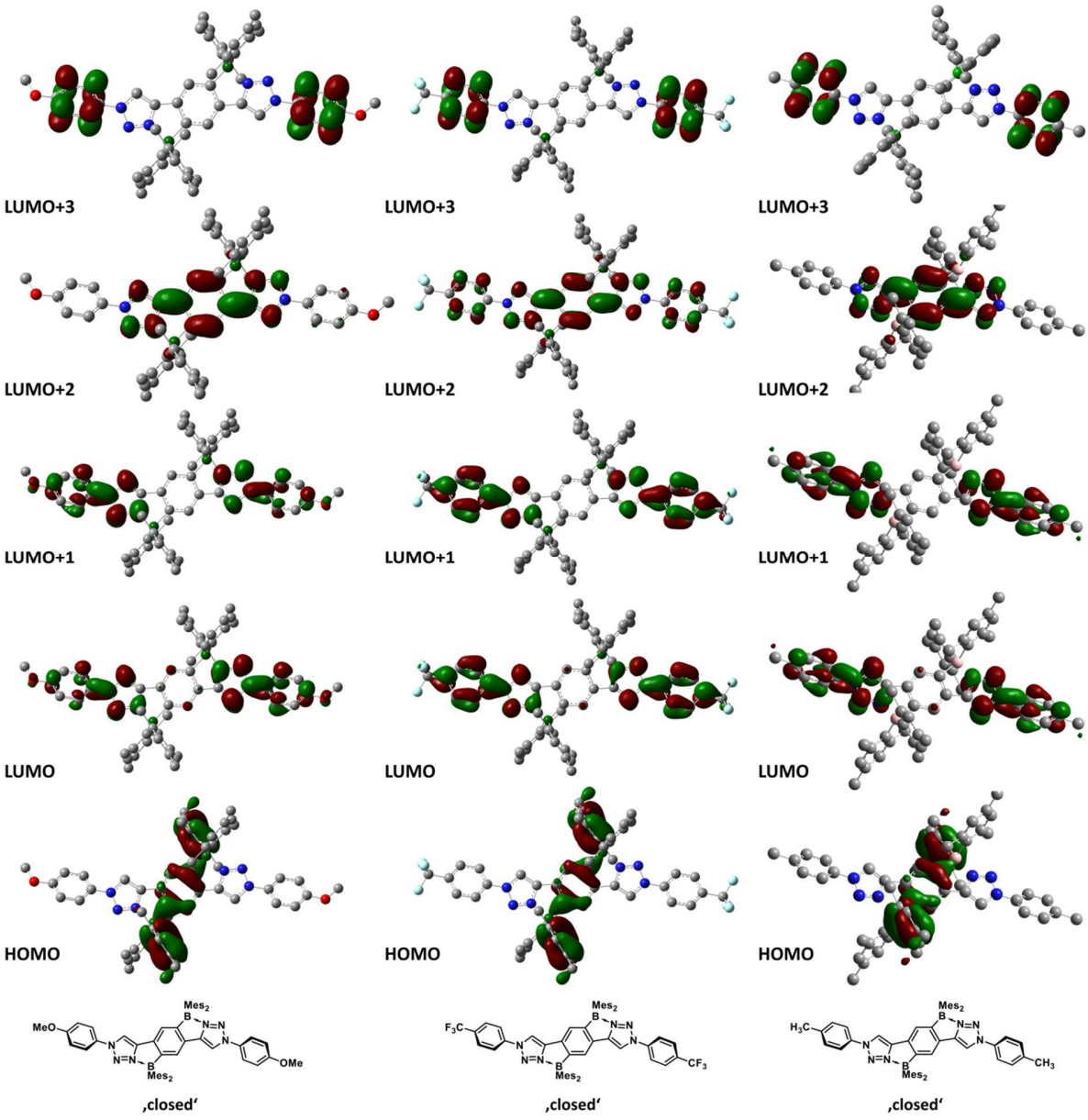


Figure S45. Frontier orbital plots of closed conformers. Iso-value 0.03.

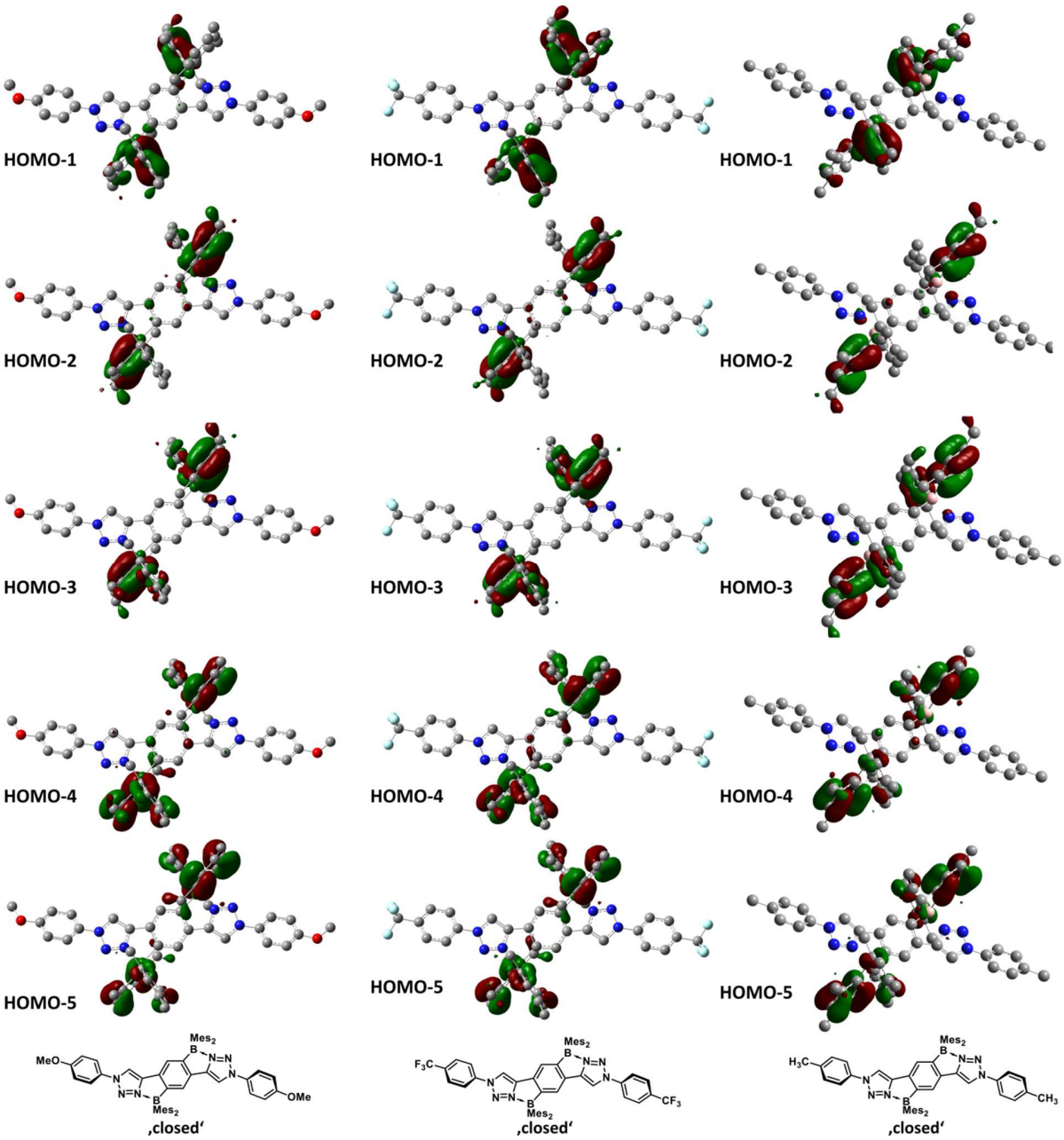


Figure S46. Frontier orbital plots of *closed* conformers. Iso-value 0.03.

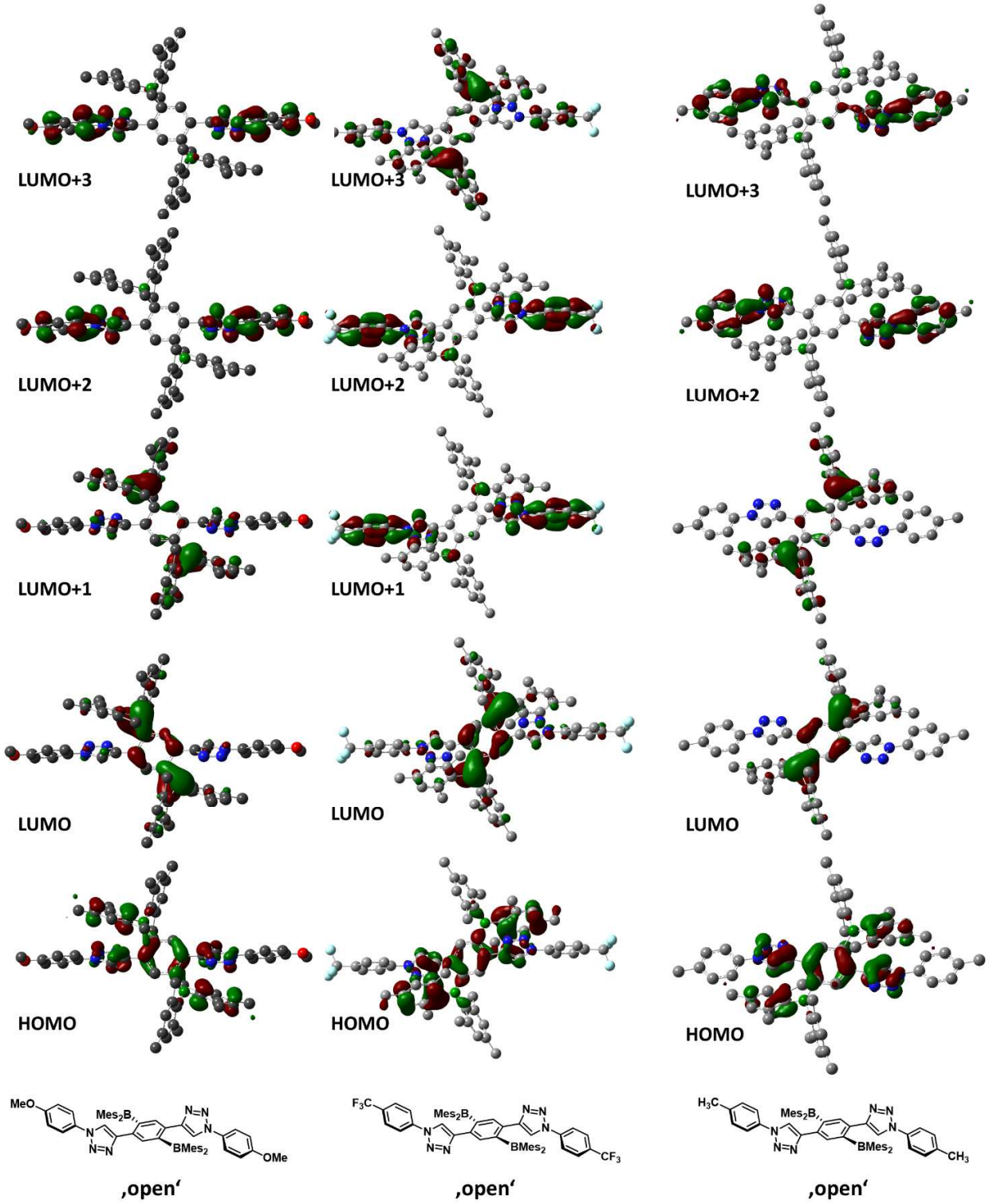


Figure S47. Frontier orbital plots of *open* conformers.

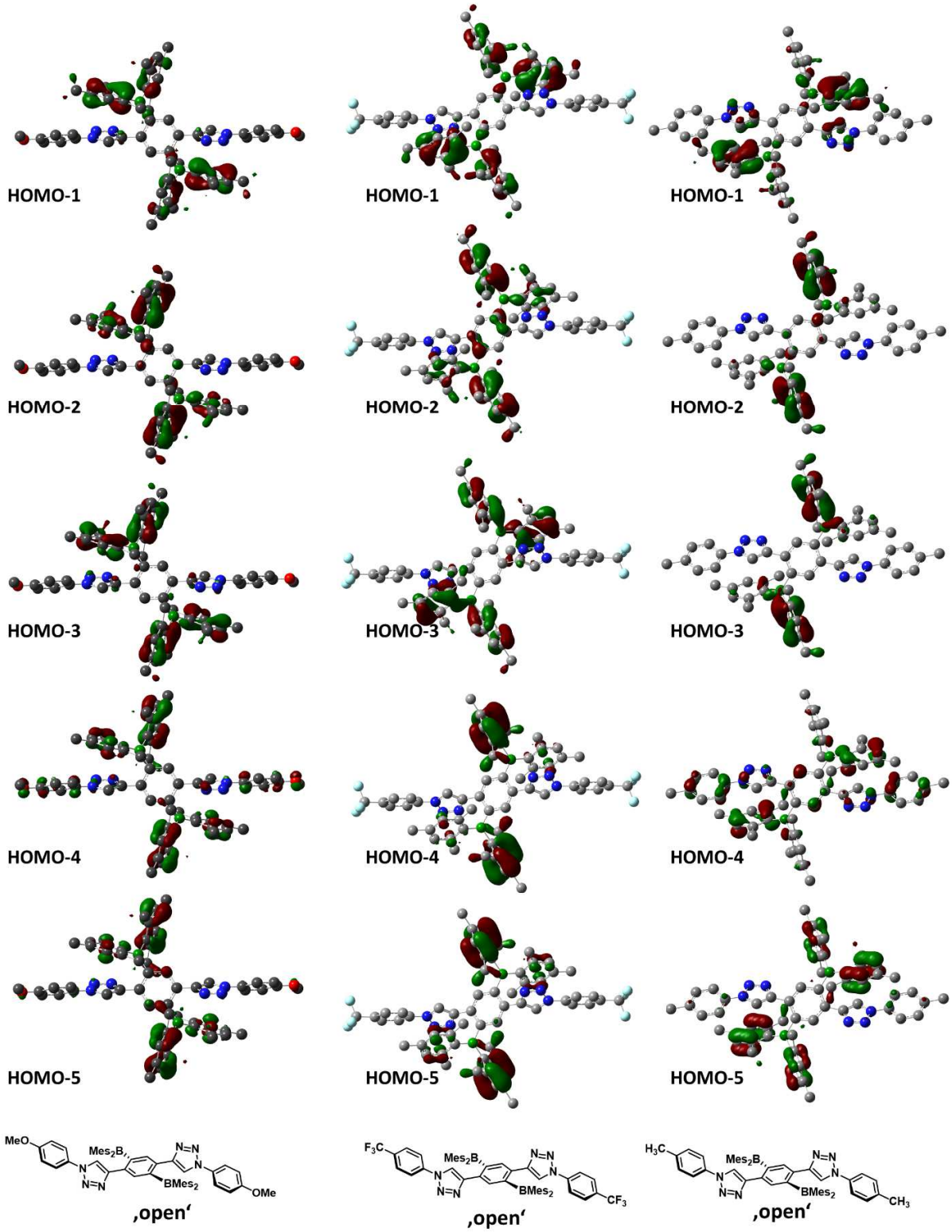


Figure S48. Frontier orbital plots of *open* conformers.

3.1. Optimized Structures

3.1.1. PTrz'

***closed*-PTrz'**

HF zero-point energy = -2240.7802001
Zero-point correction= 0.917806 (Hartree/Particle)
Thermal correction to Energy= 0.972759
Thermal correction to Enthalpy= 0.973703
Thermal correction to Gibbs Free Energy= 0.824271
Sum of electronic and zero-point Energies=-2239.862394
Sum of electronic and Thermal Energies=-2239.807441
Sum of electronic and Thermal Enthalpies= -2239.806497
Sum of electronic and Thermal Free Energies=-2239.955929

C	-1.42656900	-0.07531400	0.02597100
C	-0.70195300	0.52516500	-1.02893300
C	0.68683800	0.62681900	-1.06228000
C	1.42645900	0.07554900	-0.02572600
C	0.70184100	-0.52491200	1.02919300
C	-0.68694400	-0.62656900	1.06253700
C	1.63695600	-0.96051500	2.04128600
C	-1.63705700	0.96066600	-2.04108200
N	-2.91173700	0.56785600	-1.75108300
N	-3.76472300	0.97407900	-2.64438800
N	-3.04310600	1.62996000	-3.54430600
C	-1.71871700	1.65357800	-3.22515800
N	2.91166000	-0.56783200	1.75121500
N	3.76465900	-0.97417900	2.64445000
N	3.04303300	-1.63003000	3.54438700
C	1.71861700	-1.65346600	3.22534000
B	-3.03301500	-0.09916700	-0.23449500
B	3.03292100	0.09921900	0.23465100
C	3.68969800	-2.19656100	4.71866800
C	-3.68975500	2.19639000	-4.71864500
C	4.03808100	-0.96924800	-0.49523100
C	5.42990700	-0.85211200	-0.26668600
C	6.32609100	-1.74751800	-0.85326700
C	5.90139400	-2.78368900	-1.67547900
C	4.53393800	-2.91796700	-1.87816200
C	3.60641300	-2.04472100	-1.30267200
C	3.46692700	1.66795300	0.15394300
C	3.87386600	2.18420900	-1.09778500
C	4.19963500	3.53480300	-1.23881700
C	4.13230300	4.42604400	-0.17528500
C	3.67971600	3.93131200	1.04196100
C	3.33535200	2.58957700	1.21511300
C	-3.46676000	-1.66797300	-0.15376900
C	-3.33488800	-2.58964200	-1.21486800
C	-3.67886400	-3.93146100	-1.04162100
C	-4.13135000	-4.42623300	0.17565100
C	-4.19900600	-3.53492500	1.23910200
C	-3.87362800	-2.18424300	1.09797100
C	-4.03838900	0.96920400	0.49522500
C	-3.60694200	2.04477500	1.30262700
C	-4.53462200	2.91818300	1.87765000
C	-5.90200800	2.78392200	1.67456100
C	-6.32649800	1.74753200	0.85249600
C	-5.43017000	0.85198300	0.26638000
H	1.18473200	1.11676200	-1.89103300
H	-1.18484000	-1.11654000	1.89127300
H	-0.98686900	2.15286400	-3.83426900
H	0.98675500	-2.15269200	3.83448300
H	7.38762900	-1.62976800	-0.65633700
H	4.17095900	-3.73370400	-2.49628500
H	4.51109700	3.89824200	-2.21392600
H	3.57159000	4.61231400	1.88105000
H	-3.57051000	-4.61250000	-1.88065000
H	-4.51042000	-3.89836900	2.21422500
H	-4.17181500	3.73401200	2.49575000
H	-7.38798500	1.62972800	0.65531600
C	-6.03609100	-0.24529300	-0.58238900
H	-6.08397300	-1.18717400	-0.02994900
H	-7.05198600	0.02938600	-0.87785000
H	-5.45955800	-0.44087000	-1.48413800
C	-2.15122700	2.32139600	1.60854300
H	-1.70128800	1.51754400	2.19516300
H	-1.54682700	2.41550600	0.70549300
H	-2.05650500	3.24871300	2.17825900
C	-3.99298400	-1.32912900	2.34276700
H	-3.19546200	-0.59070000	2.42061400
H	-4.92805900	-0.76358800	2.34934800
H	-3.97041900	-1.96186300	3.23412800
C	-2.78956300	-2.19817900	-2.57053400
H	-3.47406500	-1.54086600	-3.11261900
H	-1.83316800	-1.67910100	-2.47656400
H	-2.62771000	-3.08789900	-3.18276600
C	2.15060600	-2.32142600	-1.60808600
H	1.54650100	-2.41537000	-0.70482700
H	1.70044700	-1.51770600	-2.19472100
H	2.05573200	-3.24885900	-2.17758700
C	6.03608800	0.24490200	0.58224000
H	7.05186500	-0.03014100	0.87777200
H	6.08434700	1.18681500	0.02987900
H	5.45954300	0.44059400	1.48394800
C	3.99289100	1.32918300	-2.34267600
H	4.92788700	0.76351000	-2.34947200
H	3.19525500	0.59087600	-2.42046000
H	3.97026500	1.96200500	-3.23397300
C	2.78997000	2.19816500	2.57077100
H	1.83348300	1.67926100	2.47679700
H	3.47436000	1.54071100	3.11283300
H	2.62828200	3.08789400	3.18303400
C	-6.88619100	3.71660600	2.33209000
H	-7.18275200	3.34277900	3.31852300
H	-6.45355900	4.71026800	2.47478500
H	-7.79475500	3.81754400	1.73292100
C	-4.53260200	-5.87013400	0.33359800
H	-5.59107300	-6.01357000	0.08901500
H	-3.95265900	-6.51600300	-0.33095000
H	-4.38457000	-6.21058000	1.36169200
C	4.53399400	5.86983300	-0.33313900
H	3.95438400	6.51581500	0.33159000

H	5.59255700	6.01289600	-0.08873600
H	4.38588400	6.21044600	-1.36116600
C	6.88536700	-3.71618900	-2.33358400
H	6.45367200	-4.71060800	-2.47387700
H	7.17941600	-3.34354000	-3.32121300
H	7.79526900	-3.81509400	-1.73612000
H	3.38264400	-3.23627300	4.83288800
H	4.76441100	-2.14211700	4.56075000
H	3.41430900	-1.62641800	5.60731600
H	-4.76447500	2.14167500	-4.56086800
H	-3.38294200	3.23618300	-4.83277800
H	-3.41411000	1.62635500	-5.60728300

half-open-PTrz'

HF zero-point energy = -2240.7773578
Zero-point correction= 0.915675 (Hartree/Particle)
Thermal correction to Energy= 0.971752
Thermal correction to Enthalpy= 0.972696
Thermal correction to Gibbs Free Energy= 0.821270
Sum of electronic and zero-point Energies= -2239.861683
Sum of electronic and thermal Energies= -2239.805606
Sum of electronic and thermal Enthalpies= -2239.804662
Sum of electronic and thermal Free Energies= -2239.956088

C	1.42530200	-0.55530000	0.19333900
C	0.79475200	0.50544000	0.88911700
C	-0.58452200	0.68776600	0.84363000
C	-1.40132800	-0.18954000	0.13627300
C	-0.76459600	-1.25409400	-0.53288000
C	0.61025800	-1.45662900	-0.49318000
C	-1.75538900	-2.00452000	-1.27012600
C	1.64065200	1.42217800	1.65538000
N	2.56873300	0.97247900	2.54994400
N	3.27698900	1.97379600	2.97682300
N	2.81554500	3.08165200	2.36899300
C	1.78812500	2.78398900	1.54508200
N	-2.97708300	-1.39870200	-1.21625400
N	-3.88529400	-2.06810800	-1.86307600
N	-3.25175500	-3.11812600	-2.36813300
C	-1.93045100	-3.13356100	-2.03340000
B	2.96868900	-0.62836000	-0.05231300
B	-2.99878000	-0.10881200	-0.17318900
C	-3.98777900	-4.10402000	-3.14592800
C	3.51848600	4.34196300	2.50941100
C	-4.12573200	-0.58777400	0.91006200
C	-5.49223700	-0.41413300	0.58664200
C	-6.48947100	-0.81633000	1.47605600
C	-6.19244600	-1.39881300	2.70270200
C	-4.85234300	-1.59763300	3.00807300
C	-3.82694500	-1.21479200	2.13850500
C	-3.21398300	1.36590600	-0.83819400
C	-3.52472200	2.44212800	0.02463600
C	-3.65864700	3.73879700	-0.47655000
C	-3.48713000	4.03309400	-1.82310100
C	-3.13118900	2.98474600	-2.66320300
C	-2.97865200	1.67852900	-2.19488800
C	3.65858700	-2.03239200	-0.12378700
C	3.47946500	-2.96949200	0.91950800
C	4.11704600	-4.20698100	0.85634600
C	4.91344700	-4.56798600	-0.22769400
C	5.07258600	-3.64822200	-1.26145800
C	4.47816600	-2.38842500	-1.21717000
C	3.75599300	0.70550800	-0.34156000
C	3.27936700	1.65430400	-1.27290000
C	3.95737700	2.85704100	-1.45307400
C	5.09763900	3.17270700	-0.71611300
C	5.56971600	2.23045900	0.19177400
C	4.93595900	1.00119100	0.37302300
H	-1.01992400	1.52405100	1.37683100
H	1.06836300	-2.27984800	-1.03178700
H	1.30503600	3.51602500	0.92269900
H	-1.26539300	-3.91866900	-2.34526200
H	-7.52895700	-0.66941900	1.19769800
H	-4.59093200	-2.07342300	3.94838900
H	-3.90047400	4.54245000	0.21291000
H	-2.94819200	3.18878500	-3.71410500
H	3.98713000	-4.90731700	1.67564100
H	5.68173400	-3.91463500	-2.11961600
H	3.58329300	3.56860400	-2.18319000
H	6.45645400	2.45323300	0.77679200
C	5.51589700	0.02874200	1.37047300
H	5.85197000	-0.88512400	0.87522000
H	6.36336100	0.47603300	1.89360000
H	4.76897800	-0.25530400	2.11351100
C	2.03897800	1.40873900	-2.10171700
H	1.99019800	0.37933400	-2.46211800
H	1.12879800	1.57766800	-1.52037900
H	2.01857000	2.07615000	-2.96614600
C	4.72921600	-1.43506800	-2.36363700
H	3.80244600	-0.99357100	-2.73711100
H	5.36321000	-0.60341200	-2.04777200
H	5.22089400	-1.95132500	-3.19113400
C	2.63995300	-2.65165900	2.13602100
H	2.81957300	-1.64048800	2.50681200
H	1.57434000	-2.70977500	1.89941600
H	2.85005400	-3.36220100	2.93871100
C	-2.41441700	-1.50134500	2.59486400
H	-1.84977800	-2.06800100	1.85291300
H	-1.85135900	-0.58302300	2.77433600
H	-2.42639400	-2.07515000	3.52423800
C	-5.95808800	0.23343300	-0.69988500
H	-7.00246300	-0.02612900	-0.89158000
H	-5.88303600	1.32227800	-0.64045300
H	-5.36630600	-0.07444800	-1.55955200
C	-3.74343500	2.27275000	1.51390900
H	-4.75200400	1.91004400	1.72841100
H	-3.06261300	1.54874700	1.95913600
H	-3.61049900	3.23135400	2.02193100
C	-2.52309700	0.64730700	-3.20374600
H	-1.63264200	0.11930500	-2.85554100
H	-3.29582700	-0.09869400	-3.40580400
H	-2.27407700	1.13165500	-4.15041500

C	-7.28279200	-1.78493800	3.66839900
H	-6.95040800	-2.57847300	4.34233200
H	-7.57971000	-0.93023100	4.28632700
H	-8.17469200	-2.13105800	3.13930800
C	-3.68129300	5.43030200	-2.35296300
H	-3.00182100	5.63601200	-3.18443200
H	-4.70315200	5.57266900	-2.72199700
H	-3.50748900	6.17531300	-1.57235500
C	5.81915100	4.47871700	-0.92808600
H	5.11629200	5.29426600	-1.11917500
H	6.42714800	4.73921100	-0.05819900
H	6.49010900	4.41924300	-1.79183900
C	5.60989500	-5.90310400	-0.26449100
H	5.78586100	-6.22871600	-1.29250900
H	6.58331300	-5.84696600	0.23504100
H	5.02254800	-6.66900100	0.24798400
H	2.79909400	5.15737700	2.58922000
H	4.12060600	4.28760400	3.41441700
H	4.16651200	4.49477500	1.64316100
H	-4.98806700	-3.71086400	-3.31229900
H	-3.48526300	-4.26296800	-4.10035400
H	-4.04586200	-5.04293200	-2.59338200

open-PTrz'

HF zero-point energy = -2240.7732901
Zero-point correction= 0.913416 (Hartree/Particle)
Thermal correction to Energy= 0.970632
Thermal correction to Enthalpy= 0.971577
Thermal correction to Gibbs Free Energy= 0.817356
Sum of electronic and zero-point Energies=-2239.859874
Sum of electronic and Thermal Energies=-2239.802658
Sum of electronic and Thermal Enthalpies= -2239.801713
Sum of electronic and Thermal Free Energies=-2239.955934

C	1.37461000	0.27786500	0.05218700
C	0.90563200	-0.91819800	-0.52591500
C	-0.44476800	-1.24765500	-0.46182800
C	-1.38334700	-0.39503800	0.12863400
C	-0.91298800	0.79520900	0.71807200
C	0.43814300	1.12006500	0.66105300
C	-1.88033600	1.68390800	1.36571900
C	1.86841900	-1.78252500	-1.21593300
N	2.66219900	-1.30910100	-2.22076500
N	3.52869100	-2.21876000	-2.55134800
N	3.30463500	-3.29044400	-1.77139700
C	2.27133500	-3.06442400	-0.93120800
N	-2.76515100	1.23031400	2.30085900
N	-3.60792100	2.17506000	2.59170900
N	-3.27784100	3.25006500	1.85460400
C	-2.20022500	2.99030200	1.08364300
B	2.89667000	0.64219000	0.17206900
B	-2.90469800	-0.69650000	-0.10899100
C	-4.14292500	4.41351200	1.82689300
C	4.22644900	-4.40984600	-1.78077000
C	-3.83545100	0.48439900	-0.57739100
C	-5.05812800	0.72612700	0.08532100
C	-5.82102000	1.84399900	-0.25054800
C	-5.43635800	2.71841000	-1.26227800
C	-4.25233500	2.44843700	-1.94563600
C	-3.44812700	1.36078400	-1.61434400
C	-3.41917800	-2.16685800	0.01970900
C	-4.19072600	-2.75923700	-1.00539900
C	-4.63747800	-4.07128400	-0.87055100
C	-4.37889600	-4.81719500	0.27759500
C	-3.63048000	-4.22522100	1.29118600
C	-3.13443800	-2.92760900	1.17636300
C	3.31477600	2.14030000	-0.00067200
C	2.89013800	2.88043500	-1.12785800
C	3.28625400	4.20844400	-1.27337900
C	4.07143400	4.84938400	-0.31827700
C	4.47074800	4.12164300	0.80003000
C	4.12419600	2.78200300	0.96272900
C	3.93552000	-0.47979400	0.54624100
C	3.70008000	-1.37929500	1.60860900
C	4.60653400	-2.40269500	1.87249700
C	5.74891500	-2.58660600	1.09546900
C	5.98141900	-1.69339600	0.05494000
C	5.11202000	-0.63724400	-0.21734800
H	-0.79014200	-2.16377300	-0.92868600
H	0.78184500	2.04135200	1.11868900
H	1.95906700	-3.77424500	-0.18619500
H	-1.80258200	3.69746400	0.37777400
H	-6.74149100	2.03153500	0.29337200
H	-3.94493900	3.10437600	-2.75455000
H	-5.20789900	-4.51989600	-1.67788000
H	-3.42504100	-4.78911500	2.19572900
H	2.97165800	4.75723600	-2.15564400
H	5.07238100	4.60727700	1.56189900
H	4.41590800	-3.07513200	2.70359800
H	6.86390900	-1.81822800	-0.56446900
C	5.44401000	0.29330900	-1.35789000
H	5.65551000	1.30029400	-0.99079000
H	6.31547300	-0.06988900	-1.90587400
H	4.60889800	0.36636800	-2.05597300
C	2.47919900	-1.26628600	2.49215400
H	2.26261800	-0.22939200	2.75727700
H	1.58778000	-1.64894000	1.98839100
H	2.62074000	-1.83278800	3.41500500
C	4.62551700	2.05489000	2.19008300
H	3.82758200	1.50318900	2.69209300
H	5.39137800	1.32246500	1.92430100
H	5.05472500	2.76082500	2.90432800
C	2.04457100	2.25957100	-2.21701300
H	2.38855300	1.25878700	-2.48657700
H	1.00623300	2.15367500	-1.89177300
H	2.05839900	2.88647100	-3.11148900
C	-2.17251300	1.15766500	-2.39998600
H	-1.29966800	1.50940700	-1.84352700
H	-1.99254600	0.10404200	-2.62076400
H	-2.21466200	1.70257500	-3.34566600
C	-5.55143000	-0.18178800	1.18483100
H	-6.44765400	0.23281100	1.65046700
H	-5.78646100	-1.17457200	0.79409200

H	-4.79210100	-0.30517500	1.95861400
C	-4.54569300	-2.00678600	-2.26791500
H	-5.29418800	-1.23690600	-2.06548200
H	-3.68083500	-1.49510100	-2.69539700
H	-4.94643900	-2.68943200	-3.02034600
C	-2.33531900	-2.35796000	2.32622400
H	-1.27225600	-2.31151200	2.07482000
H	-2.64072300	-1.33962000	2.57570000
H	-2.44778000	-2.98432900	3.21408200
C	-6.29727200	3.89656800	-1.63899300
H	-6.88598700	4.24536300	-0.78655500
H	-5.69157400	4.72817200	-2.00840700
H	-7.00150400	3.62716000	-2.43347500
C	6.72293400	-3.69526900	1.40064900
H	6.20635200	-4.59252000	1.75218100
H	7.31356100	-3.95582700	0.51881900
H	7.42311100	-3.39428700	2.18731900
C	4.50367300	6.28008200	-0.50495900
H	4.64091400	6.77952000	0.45710900
H	5.45763700	6.33010000	-1.04135100
H	3.76957400	6.84180300	-1.08761300
C	-4.92081300	-6.21446600	0.42699400
H	-5.95963100	-6.19231900	0.77405500
H	-4.90606100	-6.74730700	-0.52714400
H	-4.34098500	-6.78701500	1.15450600
H	-3.53855900	5.32065400	1.80361700
H	-4.78549400	4.36558700	0.94461800
H	-4.75267400	4.39615100	2.72824200
H	4.93624200	-4.30111500	-0.95734400
H	3.67157100	-5.34277600	-1.67898000
H	4.75839500	-4.39565400	-2.73018500

3.1.2. Trz-Me'

closed-Trz-Me'

HF zero-point energy = -2703.0629056
Zero-point correction= 1.076947 (Hartree/Particle)
Thermal correction to Energy= 1.141445
Thermal correction to Enthalpy= 1.142389
Thermal correction to Gibbs Free Energy= 0.968649
Sum of electronic and zero-point Energies=-2701.985958
Sum of electronic and Thermal Energies=-2701.921461
Sum of electronic and Thermal Enthalpies= -2701.920516
Sum of electronic and Thermal Free Energies=-2702.094257

C	1.14630900	0.85016500	0.06026600
C	1.23087400	-0.55613100	-0.05779700
C	0.12564500	-1.40306700	-0.09638500
C	-1.14622200	-0.85015100	-0.06043500
C	-1.23078400	0.55614000	0.05765500
C	-0.12555700	1.40308000	0.09625300
C	-2.62325400	0.92630000	0.16746200
C	2.62335000	-0.92630600	-0.16755100
N	3.43080400	0.17320000	-0.23733900
N	4.68579100	-0.14286500	-0.32976600
N	4.71355700	-1.47507600	-0.34703700
C	3.45856200	-2.01141800	-0.25070200
N	-3.43069400	-0.17321400	0.23723600
N	-4.68567500	0.14284000	0.32974000
N	-4.71345100	1.47505300	0.34703900
C	-3.45846700	2.01140800	0.25065400
B	2.59873300	1.58369100	0.02714500
B	-2.59863700	-1.58369400	-0.02728100
C	-5.95284200	2.16692700	0.46856200
C	-7.02299200	1.55578000	1.11658700
C	-8.22366800	2.24102900	1.22807500
C	-8.37574500	3.53378700	0.71743100
C	-7.28685100	4.12051700	0.07169300
C	-6.07951800	3.44521300	-0.06314400
C	5.95294700	-2.16696200	-0.46848800
C	6.07958300	-3.44524500	0.06323500
C	7.28691700	-4.12056200	-0.07152900
C	8.37585200	-3.53384600	-0.71721400
C	8.22381600	-2.24109200	-1.22787500
C	7.02313800	-1.55582900	-1.11645900
C	-3.32224000	-2.12125500	-1.39619500
C	-4.56068100	-2.79686900	-1.28452300
C	-5.21966400	-3.26865200	-2.42103700
C	-4.70139300	-3.09714100	-3.69853800
C	-3.50169100	-2.40695500	-3.81298600
C	-2.81625100	-1.91485700	-2.69859500
C	-2.53780800	-2.63930400	1.21386300
C	-2.13034100	-3.96629000	0.94654000
C	-2.01964400	-4.89848100	1.98054300
C	-2.29065000	-4.57095400	3.30305800
C	-2.63270800	-3.25163100	3.57468100
C	-2.73965400	-2.29104700	2.56742300
C	2.53792800	2.63931400	-1.21399100
C	2.73983300	2.29108900	-2.56754900
C	2.63289800	3.25169000	-3.57479300
C	2.29079100	4.57099700	-3.30315800
C	2.01972100	4.89848900	-1.98064600
C	2.13040200	3.96627900	-0.94665800
C	3.32217900	2.12127300	1.39613600
C	2.81601100	1.91477100	2.69844100
C	3.50123800	2.40685300	3.81296700
C	4.70090200	3.09714100	3.69873500
C	5.21934900	3.26877100	2.42132000
C	4.56057800	2.79700200	1.28467400
H	0.25487600	-2.47705800	-0.16512500
H	-0.25478900	2.47706900	0.16502200
H	3.28317200	-3.07049800	-0.26581400
H	-3.28308400	3.07048800	0.26577800
H	-6.90710900	0.55795200	1.51558500
H	-9.05895500	1.76412000	1.72731500
H	-7.38749600	5.11465400	-0.34702200
H	-5.25559100	3.90048600	-0.59670900
H	5.25562300	-3.90050500	0.59676100
H	7.38752900	-5.11469500	0.34720200
H	9.05913400	-1.76419400	-1.72706800
H	6.90728900	-0.55800300	-1.51546900
H	-6.16863200	-3.78274200	-2.30004600
H	-3.08563200	-2.23436800	-4.80105700

H	-1.70647300	-5.91050800	1.74037900
H	-2.80031100	-2.95136400	4.60484700
H	2.80054700	2.95144700	-4.60495800
H	1.70650600	5.91050100	-1.74047500
H	3.08503900	2.23418100	4.80096500
H	6.16828800	3.78295400	2.30050300
C	5.22931000	3.08469900	-0.04280000
H	4.78671900	3.96206500	-0.52154800
H	6.29347500	3.28146800	0.11143100
H	5.13249500	2.26227800	-0.74767400
C	1.52584800	1.17656600	2.98023400
H	0.65969600	1.71015800	2.58289800
H	1.50787300	0.18418800	2.52831900
H	1.38634900	1.06154400	4.05758200
C	1.80012500	4.46286000	0.44596100
H	1.26370700	3.72091100	1.03715000
H	2.70509800	4.70071600	1.01042500
H	1.18855300	5.36701700	0.38380600
C	3.03831500	0.87549500	-3.00883700
H	4.03899000	0.55234300	-2.71045900
H	2.32023200	0.17086400	-2.58405300
H	2.97636500	0.79909000	-4.09643100
C	-1.52609500	-1.17675900	-2.98068600
H	-1.50796500	-0.18434600	-2.52885900
H	-0.65990300	-1.71038100	-2.58348600
H	-1.38680200	-1.06183300	-4.05807200
C	-5.22923400	-3.08439000	0.04307600
H	-6.29344100	-3.28108500	-0.11097000
H	-4.78663800	-3.96174400	0.52183800
H	-5.13223900	-2.26190700	0.74785700
C	-1.80013900	-4.46292100	-0.44608000
H	-2.70514000	-4.70077200	-1.01050100
H	-1.26372600	-3.72100500	-1.03731400
H	-1.18858900	-5.36709200	-0.38392400
C	-3.03808500	-0.87543800	3.00869500
H	-2.32000100	-0.17083400	2.58387000
H	-4.03876200	-0.55226700	2.71034600
H	-2.97609300	-0.79901500	4.09628600
C	2.21505100	5.60196900	-4.39947300
H	3.18969300	6.07572800	-4.56208500
H	1.90870400	5.14958000	-5.34639800
H	1.50359400	6.39300700	-4.14866900
C	5.40507900	3.64974700	4.91092200
H	5.07435700	4.67233600	5.12471700
H	5.19723900	3.04534900	5.79762100
H	6.48706900	3.68027400	4.75877800
C	-5.40579800	-3.64975500	-4.91058800
H	-5.19798600	-3.04546300	-5.79736400
H	-5.07524500	-4.67241000	-5.12433500
H	-6.48777400	-3.68012000	-4.75830600
C	-2.21489900	-5.60190400	4.39939300
H	-1.90829800	-5.14954200	5.34625000
H	-3.18960000	-6.07547600	4.56219900
H	-1.50363400	-6.39308100	4.14848600
C	-9.67552400	4.27560000	0.87941900
H	-10.52917000	3.61197100	0.72284900
H	-9.76179400	4.68927700	1.88955200
H	-9.74749400	5.10437900	0.17249200
C	9.67562200	-4.27568800	-0.87913700
H	9.74770200	-5.10423600	-0.17195100
H	9.76175600	-4.68969900	-1.88914600
H	10.52927600	-3.61199400	-0.72290400

half-open-Trz-Me'

HF zero-point energy = -2703.0625689
Zero-point correction= 1.075141 (Hartree/Particle)
Thermal correction to Energy= 1.140691
Thermal correction to Enthalpy= 1.141636
Thermal correction to Gibbs Free Energy= 0.967513
Sum of electronic and zero-point Energies=-2701.987427
Sum of electronic and Thermal Energies=-2701.921877
Sum of electronic and Thermal Enthalpies= -2701.920933
Sum of electronic and Thermal Free Energies=-2702.095056

C	-0.95986600	1.23849100	0.37121300
C	-1.18551000	-0.11245700	0.73289500
C	-0.14992500	-1.04159300	0.76229300
C	1.15700200	-0.66676200	0.46500100
C	1.37089700	0.67956800	0.11066300
C	0.35137400	1.62448800	0.08768500
C	2.75887400	0.85341000	-0.25314700
C	-2.55463100	-0.51565000	1.06544800
N	-3.29566900	0.13547200	2.01267400
N	-4.51246300	-0.30438800	1.98869400
N	-4.58602000	-1.24684600	1.01845900
C	-3.37311000	-1.41476500	0.43447400
N	3.41960200	-0.34193100	-0.27195400
N	4.67123600	-0.20707200	-0.58758000
N	4.84127600	1.09588300	-0.80619300
C	3.68375400	1.79996500	-0.61328700
B	-2.10870200	2.25377300	0.05203000
B	2.49427900	-1.58410500	0.32652600
C	6.11591400	1.60006500	-1.19507100
C	6.99592800	0.78243900	-1.89900400
C	8.23426600	1.28613600	-2.26846400
C	8.60926400	2.59779100	-1.96138300
C	7.70765100	3.39341500	-1.25358600
C	6.46739800	2.90321300	-0.86216400
C	-5.82550200	-1.82410400	0.64750300
C	-5.85094000	-2.99788000	-0.09862200
C	-7.07005500	-3.52237700	-0.51285100
C	-8.27455000	-2.90219400	-0.18214300
C	-8.22262600	-1.73073800	0.57881800
C	-7.01583500	-1.18506900	0.98895700
C	3.37446100	-2.03468600	1.62979400
C	4.49664600	-2.87252700	1.42892500
C	5.29271800	-3.26446500	2.50610900
C	5.02409500	-2.85877700	3.80777500
C	3.93653200	-2.01760800	4.00346200
C	3.12236600	-1.59728300	2.94802400
C	2.09145700	-2.76741600	-0.72039800
C	1.57641100	-3.97499100	-0.19478400
C	1.16052100	-5.00002500	-1.04726500
C	1.22188900	-4.88299200	-2.43019200
C	1.67668000	-3.67592800	-2.94745800
C	2.09001100	-2.62624900	-2.12504800
C	-1.89315800	3.76347200	0.41020500

C	-1.50858600	4.13981400	1.71717300
C	-1.32878000	5.48667700	2.02574500
C	-1.49143200	6.48647200	1.06986900
C	-1.85715000	6.10968300	-0.22022700
C	-2.07824500	4.77543300	-0.55713700
C	-3.38647900	1.73973100	-0.71008800
C	-3.28106000	0.92373000	-1.85628300
C	-4.42734500	0.39543900	-2.44551900
C	-5.69575100	0.62727400	-1.91872300
C	-5.79770600	1.46358300	-0.81150400
C	-4.67539500	2.03244600	-0.21319400
H	-0.37112300	-2.06714100	1.03189600
H	0.55054200	2.65360500	-0.19280000
H	-3.21358700	-2.05624900	-0.41153300
H	3.62641600	2.86223100	-0.75830500
H	6.70782300	-0.23110200	-2.13999800
H	8.92235500	0.64898200	-2.81150100
H	7.98436500	4.40687000	-0.98896900
H	5.79352000	3.52138700	-0.28370600
H	-4.92873800	-3.50212700	-0.35475100
H	-7.08257800	-4.43182300	-1.10202700
H	-9.14552100	-1.22511800	0.83902000
H	-6.97737700	-0.26632500	1.55469600
H	6.14924700	-3.90532300	2.31832300
H	3.71543900	-1.66635100	5.00673600
H	0.77161800	-5.91568400	-0.61143900
H	1.69501000	-3.53583700	-4.02432300
H	-1.05388100	5.76186500	3.03933400
H	-1.98211100	6.87415400	-0.98077200
H	-4.32710400	-0.22180400	-3.33328400
H	-6.77722500	1.67087500	-0.39373700
C	-4.86796500	2.91556600	0.99515800
H	-4.51957000	3.93188300	0.79894400
H	-5.92212700	2.95529500	1.27724900
H	-4.30185200	2.53392800	1.84718300
C	-1.94550700	0.58986900	-2.48164300
H	-1.27760300	1.45350700	-2.50032300
H	-1.42585000	-0.19229700	-1.92162200
H	-2.08186200	0.23977800	-3.50724600
C	-2.50667900	4.44984400	-1.96984500
H	-1.88502900	3.66879000	-2.41434100
H	-3.53303600	4.07693200	-1.98920800
H	-2.44613400	5.33721100	-2.60371000
C	-1.32506700	3.11692500	2.81549800
H	-2.10737400	2.35539800	2.80348500
H	-0.37567100	2.58750600	2.70077100
H	-1.32703900	3.60459500	3.79296500
C	1.97750000	-0.67726800	3.30781300
H	1.99538300	0.24815600	2.73005100
H	1.00847600	-1.14183700	3.11505700
H	2.02079900	-0.41719500	4.36778800
C	4.88485100	-3.41993400	0.07207500
H	5.92526900	-3.75455000	0.08805600
H	4.25675900	-4.27213300	-0.20000200
H	4.77482500	-2.68492100	-0.72221100
C	1.44903500	-4.24210700	1.29067200
H	2.40551100	-4.54484800	1.72417400
H	1.13000600	-3.36258700	1.84869200
H	0.72626300	-5.04320100	1.46501800
C	2.49494100	-1.34304700	-2.81679100
H	1.95066900	-0.48613200	-2.41355900
H	3.56309600	-1.13829800	-2.70998400
H	2.27440100	-1.40515400	-3.88455400
C	-6.91373200	-0.03583700	-2.50343900
H	-7.79612600	0.60138800	-2.40529700
H	-6.76745200	-0.26804000	-3.56110000
H	-7.12733400	-0.97295600	-1.97916300
C	-1.31172700	7.93767300	1.43169300
H	-1.01661900	8.52829300	0.56109700
H	-2.24643300	8.36061300	1.81599500
H	-0.55326500	8.05969200	2.20896700
C	0.81280700	-6.01786900	-3.33311100
H	0.38870100	-5.64514300	-4.26929000
H	1.67306700	-6.64607600	-3.59008900
H	0.07169900	-6.65890500	-2.84891200
C	5.87039400	-3.32685500	4.96332500
H	5.85372700	-2.60399600	5.78288900
H	5.50239600	-4.28053200	5.35792900
H	6.90857400	-3.47817900	4.65633500
C	-9.59463000	-3.48526100	-0.61156900
H	-9.46788300	-4.17046800	-1.45226600
H	-10.05857400	-4.04454100	0.20771100
H	-10.29382200	-2.69978600	-0.90894900
C	9.94380700	3.13790200	-2.40071100
H	9.92094100	3.41043500	-3.46093600
H	10.21462500	4.03001200	-1.83281400
H	10.73176600	2.39232600	-2.27078000

open-Trz-Me'

HF zero-point energy = -2703.0548771
Zero-point correction= 1.072582 (Hartree/Particle)
Thermal correction to Energy= 1.139727
Thermal correction to Enthalpy= 1.140672
Thermal correction to Gibbs Free Energy= 0.959823
Sum of electronic and zero-point Energies=-2701.982295
Sum of electronic and Thermal Energies=-2701.915150
Sum of electronic and Thermal Enthalpies= -2701.914206
Sum of electronic and Thermal Free Energies=-2702.095054

C	1.12011000	0.88603100	0.12123200
C	1.31109800	-0.49664400	-0.10254500
C	0.20620200	-1.33940800	-0.20328200
C	-1.11845000	-0.88688300	-0.12311400
C	-1.30951800	0.49575700	0.10012100
C	-0.20465100	1.33841600	0.20162600
C	-2.63720000	1.10969500	0.18414600
C	2.63865200	-1.11058800	-0.18837500
N	2.93529900	-2.25573300	0.50034100
N	4.18373400	-2.54905500	0.34037500
N	4.72622800	-1.60368000	-0.47257400
C	3.77952900	-0.70176200	-0.82944900
N	-2.93333400	2.25344200	-0.50708900
N	-4.18196500	2.54687600	-0.34893400
N	-4.72510600	1.60299500	0.46527800
C	-3.77865900	0.70184500	0.82481000
B	2.23668700	1.95459300	0.41757000
B	-2.23528100	-1.95564800	-0.41782900
C	-6.10868500	1.61782700	0.77584300
C	-6.88981300	2.71302600	0.41018700
C	-8.24914700	2.70738600	0.69166600
C	-8.85776400	1.62862600	1.33677100
C	-8.05380500	0.54797900	1.70081800
C	-6.69329200	0.53194000	1.42207700
C	6.10954400	-1.61798500	-0.78437300

C	6.69300500	-0.53233500	-1.43202800
C	8.05329700	-0.54783600	-1.71191600
C	8.85817800	-1.62773500	-1.34773600
C	8.25071000	-2.70630000	-0.70121600
C	6.89165300	-2.71241900	-0.41846400
C	-3.58724400	-1.55381300	-1.10335700
C	-4.81315800	-1.98240100	-0.53856500
C	-6.01323200	-1.46114700	-1.00796100
C	-6.05576600	-0.52791800	-2.04128400
C	-4.85655500	-0.16838700	-2.64375000
C	-3.63285100	-0.66339700	-2.19579800
C	-1.94299800	-3.44450300	-0.02010200
C	-2.08969200	-4.47852700	-0.96987100
C	-1.82200600	-5.79738700	-0.60943000
C	-1.43771900	-6.13879700	0.68500600
C	-1.31676300	-5.11798600	1.62463100
C	-1.54292200	-3.78585700	1.28947600
C	1.94255800	3.44533500	0.02774400
C	1.53529800	3.79380900	-1.27772500
C	1.29676800	5.12657200	-1.60143800
C	1.41794600	6.14152900	-0.65560300
C	1.80332500	5.79230200	0.63636100
C	2.08272600	4.47276200	0.98560500
C	3.59004700	1.55164000	1.09994500
C	3.63774000	0.66058000	2.19166800
C	4.86242700	0.16597000	2.63743100
C	6.06052300	0.52639900	2.03326100
C	6.01587000	1.45988200	1.00024600
C	4.81473600	1.98080300	0.53321800
H	0.38610500	-2.39560400	-0.35877300
H	-0.38471000	2.39450200	0.35764700
H	3.98102500	0.13968200	-1.46281000
H	-3.98076900	-0.13835500	1.45966100
H	-6.42668800	3.54985400	-0.09173000
H	-8.84942600	3.56312900	0.40471100
H	-8.49914600	-0.30220600	2.20457500
H	-6.10287700	-0.33324800	1.68526700
H	6.10191100	0.33227100	-1.69561600
H	8.49771800	0.30217400	-2.21677800
H	8.85171100	-3.56146400	-0.41404000
H	6.42948500	-3.54904700	0.08465200
H	-6.94117300	-1.76358000	-0.53491000
H	-4.86870100	0.53456900	-3.47026600
H	-1.92293000	-6.57905000	-1.35573200
H	0.99909800	5.37852300	-2.61445300
H	1.88993100	6.56738400	1.39125500
H	4.87621500	-0.53736700	3.46360400
H	6.94285700	1.76280000	0.52563000
C	-2.38629400	-0.19226200	-2.90737500
H	-2.06477400	0.77669100	-2.51460700
H	-1.55560000	-0.88853600	-2.79391400
H	-2.58818000	-0.06710700	-3.97414500
C	-4.87261500	-2.93533100	0.63480400
H	-4.52552700	-3.93361200	0.36177100
H	-4.23293700	-2.60974300	1.46054500
H	-5.89677000	-3.01532300	1.00667400
C	-2.52884100	-4.19231800	-2.38808800
H	-3.57885500	-3.89207500	-2.41879200
H	-1.95714800	-3.37415200	-2.83285800
H	-2.40178900	-5.07754500	-3.01477800
C	-1.38349300	-2.74071600	2.37089000
H	-0.42067400	-2.23181000	2.28303900
H	-2.15497900	-1.96914200	2.31135400
H	-1.43711300	-3.20150600	3.35961600
C	1.37237900	2.75506100	-2.36468700
H	2.14150800	1.98095500	-2.30893600
H	0.40785900	2.24882500	-2.27968300
H	1.42759000	3.22094900	-3.35095200
C	2.39239000	0.18822900	2.90451800
H	1.56111900	0.88404600	2.79245400
H	2.07100900	-0.78067800	2.51150300
H	2.59557700	0.06255700	3.97098000
C	4.87111700	2.93374800	-0.64027000
H	4.23013900	2.60738700	-1.46477500
H	4.52338900	3.93156300	-0.36645700
H	5.89444300	3.01477700	-1.01421700
C	2.51828200	4.17726900	2.40306500
H	1.94627500	3.35558400	2.84099000
H	3.56846800	3.87779900	2.43423600
H	2.38895200	5.05810700	3.03544400
C	-7.35917900	0.10664500	-2.44174200
H	-7.28044600	0.59502600	-3.41518400
H	-8.16445000	-0.63166000	-2.48420400
H	-7.64603000	0.86543500	-1.70521800
C	1.16377200	7.57858800	-1.02752700
H	0.84491500	8.15949000	-0.15906000
H	2.07298200	8.04546300	-1.42217300
H	0.39341900	7.65495600	-1.79858700
C	7.36492500	-0.10751300	2.43159800
H	7.28782500	-0.59644900	3.40489400
H	7.65135100	-0.86571600	1.69431200
H	8.16973600	0.63133300	2.47342300
C	-10.33971200	1.61912600	1.60378200
H	-10.71486200	2.62992700	1.77943700
H	-10.88729100	1.20827400	0.74867700
H	-10.57953400	1.00556500	2.47503000
C	10.33988000	-1.61769300	-1.61607900
H	10.57884000	-1.00276200	-2.48659000
H	10.88821000	-1.20815600	-0.76082600
H	10.71496400	-2.62819000	-1.79365200
H	-1.03446000	-5.36538100	2.64311200
C	-1.13285400	-7.56688400	1.05218300
H	-1.68387000	-8.26456400	0.41715300
H	-0.06509800	-7.77764600	0.92774700
H	-1.38770500	-7.76885100	2.09534300

3.1.3. Trz-OMe'

closed-Trz-OMe'

HF zero-point energy = -2853.5332029
Zero-point correction= 1.087225 (Hartree/Particle)
Thermal correction to Energy= 1.153159
Thermal correction to Enthalpy= 1.154103
Thermal correction to Gibbs Free Energy= 0.979775
Sum of electronic and zero-point Energies=-2852.445978
Sum of electronic and Thermal Energies=-2852.380044
Sum of electronic and Thermal Enthalpies= -2852.379100
Sum of electronic and Thermal Free Energies=-2852.553428

C	-1.02888100	-0.98878400	0.03128200
C	-1.28809100	0.39676700	-0.07649100
C	-0.29729800	1.37573300	-0.09103200
C	1.03325000	0.98604600	-0.04000000

C	1.29235700	-0.39940800	0.06766500
C	0.30157900	-1.37849500	0.08218700
C	2.71849800	-0.59310300	0.19397100
C	-2.71431700	0.59030100	-0.20355500
N	-3.37594600	-0.59941700	-0.30796400
N	-4.66215100	-0.44062500	-0.39477800
N	-4.85774900	0.87635400	-0.35664600
C	-3.68135500	1.56349500	-0.23866400
N	3.38136100	0.59639100	0.29341200
N	4.66669000	0.43617900	0.39186800
N	4.85863600	-0.88212900	0.38435100
C	3.68143700	-1.56794600	0.26536900
B	-2.37781600	-1.89802700	-0.02958100
B	2.38260800	1.89486000	0.01935700
C	6.17289700	-1.41912600	0.48887300
C	7.14835300	-0.73130600	1.21239800
C	8.42207100	-1.25727400	1.30724000
C	8.73434200	-2.47762700	0.69366500
C	7.75187500	-3.16141500	-0.02651600
C	6.47339100	-2.62198100	-0.13327600
C	-6.17679300	1.40856800	-0.41193600
C	-6.39577100	2.64409500	-1.00283900
C	-7.67930100	3.18143900	-1.03754300
C	-8.74552400	2.46324200	-0.49041200
C	-8.51292200	1.21034800	0.09245800
C	-7.23611900	0.68591200	0.13991500
O	10.00999100	-2.91059300	0.85119700
O	-10.03213700	2.89235400	-0.47753100
C	3.05766800	2.52031800	-1.33683200
C	4.20401000	3.33963500	-1.20281800
C	4.82979700	3.87837300	-2.32777700
C	4.36381300	3.64125400	-3.61533100
C	3.25320200	2.81910500	-3.75078200
C	2.60551500	2.25466500	-2.64767100
C	2.15994500	2.93041000	1.25749300
C	1.57773000	4.18820600	0.97905500
C	1.30495000	5.08951900	2.01053700
C	1.57991300	4.79605200	3.34025600
C	2.10289000	3.53908900	3.62017400
C	2.37771000	2.61034300	2.61503400
C	-2.15015200	-2.94072400	-1.25924400
C	-2.36449000	-2.62905200	-2.61907600
C	-2.08150700	-3.56224600	-3.61766900
C	-1.55481400	-4.81563900	-3.32822400
C	-1.28550500	-5.10140300	-1.99561200
C	-1.56614000	-4.19508300	-0.97058500
C	-3.06415300	-2.51207300	1.32690700
C	-2.62092200	-2.23738600	2.63900400
C	-3.28366300	-2.78396800	3.74207900
C	-4.40044500	-3.59769100	3.60516800
C	-4.85579200	-3.84583300	2.31581900
C	-4.21505600	-3.32463700	1.19054100
H	-0.55895800	2.42567900	-0.15528300
H	0.56310500	-2.42861000	0.14479000
H	-3.64815600	2.63307100	-0.14939100
H	3.63947900	-2.64082000	0.25888500
H	6.89871100	0.20814600	1.68515400
H	9.19509900	-0.74203800	1.86171600
H	7.97181800	-4.09691900	-0.51910700
H	5.72286800	-3.13464600	-0.72047200
H	-5.57420900	3.18632400	-1.45265000
H	-7.83555200	4.14383000	-1.50201000
H	-9.35025800	0.67038300	0.51412900
H	-7.04497500	-0.27491000	0.59737700
H	5.70980800	4.49987400	-2.18984900
H	2.87981500	2.59804200	-4.74618800
H	0.85947100	6.04876800	1.76284600
H	2.28637600	3.26164100	4.65404400
H	-2.26279200	-3.29174400	-4.65375700
H	-0.83914600	-6.05827800	-1.74036500
H	-2.91665800	-2.55618800	4.73832300
H	-5.73769000	-4.46443300	2.17642500
C	-4.79819900	-3.70792700	-0.15283200
H	-4.20991700	-4.50057500	-0.62213500
H	-5.82123600	-4.07155600	-0.02634100
H	-4.81640600	-2.87570300	-0.85341000
C	-1.42050400	-1.36854000	2.94280800
H	-0.49888100	-1.80426900	2.55105600
H	-1.50254000	-0.37622700	2.49764800
H	-1.30615300	-1.24828200	4.02251700
C	-1.22540100	-4.63906800	0.43702800
H	-0.80996500	-3.83221300	1.04088300
H	-2.11447200	-4.98603100	0.96939600
H	-0.50284600	-5.45895100	0.40650300
C	-2.87518900	-1.27925600	-3.07081800
H	-3.91453700	-1.11645100	-2.77506900
H	-2.27817500	-0.46894600	-2.64624500
H	-2.82140400	-1.19977700	-4.15868300
C	1.41149000	1.37672300	-2.95113400
H	1.50153500	0.38461700	-2.50716500
H	0.48637600	1.80446800	-2.55863800
H	1.29736200	1.25678900	-4.03095000
C	4.79901500	3.71095400	0.13870000
H	5.82321000	4.06906400	0.00652500
H	4.21872800	4.50354300	0.61821100
H	4.81746000	2.87352400	0.83293400
C	1.22839900	4.64192300	-0.42345400
H	2.11337600	4.99545900	-0.95825200
H	0.81174600	3.83882500	-1.03123800
H	0.50387600	5.45963400	-0.38216400
C	2.88090800	1.25511500	3.05961100
H	2.28126200	0.44996300	2.62945000
H	3.92013800	1.08820300	2.76528700
H	2.82482100	1.16938700	4.14682900
C	-1.28980100	-5.82338200	-4.41683000
H	-2.18612500	-6.41614900	-4.63137200
H	-0.99275200	-5.33141600	-5.34688900
H	-0.49819300	-6.51872100	-4.12594300
C	-5.08078900	-4.20355500	4.80560000
H	-4.66205900	-5.18907600	5.03824300
H	-4.95301600	-3.57525400	5.69079700
H	-6.15102000	-4.33660900	4.62712100
C	5.02936100	4.26478500	-4.81500200
H	4.86307900	3.66585300	-5.71397900

H	4.63146000	5.26732600	-5.00824500
H	6.10695900	4.36503300	-4.66058300
C	1.32285900	5.79875200	4.43535600
H	1.03523700	5.30239200	5.36599600
H	2.21985200	6.39263300	4.64400100
H	0.52712900	6.49348500	4.15454600
C	10.38097900	-4.14120900	0.23740100
H	9.78245600	-4.97094100	0.62848600
H	10.26225900	-4.08842500	-0.85004800
H	11.42897900	-4.29460200	0.48599900
C	-10.32171500	4.16132900	-1.05555800
H	-9.77845700	4.96052500	-0.53998300
H	-10.06456700	4.17539300	-2.12006500
H	-11.39297900	4.30718900	-0.93401300

half-open-Trz-OMe'

HF zero-point energy = -2853.5317849
Zero-point correction= 1.085255 (Hartree/Particle)
Thermal correction to Energy= 1.152293
Thermal correction to Enthalpy= 1.153237
Thermal correction to Gibbs Free Energy= 0.976841
Sum of electronic and zero-point Energies=-2852.446530
Sum of electronic and Thermal Energies=-2852.379492
Sum of electronic and Thermal Enthalpies= -2852.378548
Sum of electronic and Thermal Free Energies=-2852.554944

C	-0.86866800	1.36478600	0.52957400
C	-1.22399100	0.02213800	0.80791600
C	-0.27242100	-0.99334600	0.82438400
C	1.07267800	-0.71866300	0.59627400
C	1.41893400	0.62646800	0.35695000
C	0.48360400	1.65528300	0.34483400
C	2.83049600	0.70141100	0.05547600
C	-2.63525700	-0.27551100	1.05454800
N	-3.38588100	0.45329200	1.93377800
N	-4.62444400	0.08055900	1.86336300
N	-4.69808500	-0.90097900	0.93362500
C	-3.47132200	-1.15911000	0.41980500
N	3.38010700	-0.54373900	-0.04165000
N	4.64965300	-0.50273700	-0.31385300
N	4.94278600	0.79112300	-0.42710600
C	3.84826800	1.58285600	-0.20851800
B	-1.90779700	2.46602700	0.13903000
B	2.32328400	-1.74113600	0.39113500
C	6.26605700	1.20342600	-0.75384500
C	7.08299800	0.37187900	-1.50779900
C	8.37438300	0.77476100	-1.82759700
C	8.84266800	2.02157800	-1.40223600
C	8.00879200	2.85287700	-0.64485100
C	6.73026900	2.44326600	-0.31448200
C	-5.94646300	-1.44509700	0.54126900
C	-6.14946300	-1.81204500	-0.78916900
C	-7.36994700	-2.33102000	-1.18125800
C	-8.40733800	-2.47072500	-0.25334700
C	-8.20467600	-2.08491900	1.07425500
C	-6.96987900	-1.57916800	1.46908400
C	3.10835800	-2.43701500	1.64436900
C	4.13939400	-3.36581200	1.36854100
C	4.84728500	-3.97114000	2.40769400
C	4.57752800	-3.69442000	3.74276400
C	3.58424700	-2.76255000	4.01428600
C	2.86063000	-2.13027300	2.99917200
C	1.83615100	-2.73775700	-0.80911200
C	1.19279100	-3.94597700	-0.45210800
C	0.70837000	-4.81113100	-1.43523600
C	0.82142400	-4.52819400	-2.79064100
C	1.40001800	-3.31438100	-3.14068400
C	1.88511000	-2.41986600	-2.18440300
C	-1.63121400	3.95254700	0.54581100
C	-1.34606400	4.28558900	1.88969000
C	-1.11995900	5.61486500	2.24149800
C	-1.13545200	6.63702900	1.29565200
C	-1.39651400	6.30136800	-0.03050400
C	-1.66185000	4.98781900	-0.41384600
C	-3.12705900	2.05567100	-0.77001000
C	-2.95082400	1.26663600	-1.92582900
C	-4.05946300	0.86326100	-2.67002000
C	-5.35712600	1.19592500	-2.29318300
C	-5.52555600	1.97964600	-1.15441400
C	-4.44051100	2.43192600	-0.40824600
H	-0.59226100	-2.01010300	1.01772600
H	0.78018300	2.67712100	0.13141500
H	-3.30333000	-1.88644100	-0.35288600
H	3.89164800	2.65360300	-0.27485500
H	6.71061500	-0.58828300	-1.83617600
H	8.99934000	0.11636600	-2.41273000
H	8.38987100	3.80882900	-0.31130800
H	6.10214500	3.07649400	0.29809700
H	-5.36563100	-1.65052500	-1.51646900
H	-7.54885300	-2.61451700	-2.20993700
H	-8.99215200	-2.18085900	1.80736100
H	-6.79958900	-1.27650600	2.49285000
H	5.63423400	-4.67824700	2.16217900
H	3.36843500	-2.50790000	5.04751600
H	0.22240900	-5.73195700	-1.12618500
H	1.46054800	-3.04212800	-4.19030200
H	-0.92377600	5.85762100	3.28129200
H	-1.40134300	7.08264800	-0.78421400
H	-3.90446600	0.27350300	-3.56866100
H	-6.52820500	2.24768700	-0.83708300
C	-4.70234100	3.29379700	0.80263700
H	-4.28210900	4.29320000	0.66733600
H	-5.77520400	3.38567500	0.98270300
H	-4.24357500	2.86314800	1.69411600
C	-1.58382700	0.83776700	-2.41131300
H	-0.84342100	1.63107400	-2.29459000
H	-1.20923300	-0.02217300	-1.84965900
H	-1.62542100	0.55949600	-3.46676400
C	-1.96881600	4.71348600	-1.86896600
H	-1.39804700	3.86567900	-2.25412000
H	-3.02385300	4.46434400	-2.00616700
H	-1.73825700	5.58898700	-2.48017900
C	-1.31310500	3.23645800	2.97738300
H	-2.13652300	2.52494300	2.88926900
H	-0.39120600	2.65120100	2.92425100
H	-1.36050600	3.70799100	3.96165800
C	1.81642100	-1.12892100	3.43846400
H	1.94995600	-0.15839200	2.95801800
H	0.80617300	-1.45996900	3.18841300
H	1.86453500	-0.98287600	4.51995900
C	4.51422900	-3.78627700	-0.03626300
H	5.50885800	-4.23967100	-0.03745600

H	3.80421300	-4.51928800	-0.42771400
H	4.51774500	-2.95138600	-0.73399300
C	0.99650400	-4.38444300	0.98421000
H	1.90946700	-4.82388000	1.39369300
H	0.73930700	-3.55606000	1.64323800
H	0.20134600	-5.13219200	1.04052600
C	2.41512400	-1.10115300	-2.70320700
H	1.92744100	-0.25831700	-2.20906800
H	3.49242400	-0.99952600	-2.55078700
H	2.22322100	-1.01409300	-3.77469400
O	10.08029700	2.50754900	-1.66847100
O	-9.57285400	-2.98101700	-0.73695600
C	-6.54641100	0.74507600	-3.09982300
H	-7.01500100	1.59115300	-3.61291000
H	-6.25299300	0.01471200	-3.85780000
H	-7.30304100	0.28687900	-2.45805000
C	-0.90792100	8.06965500	1.70180500
H	-0.49597500	8.65385900	0.87543000
H	-1.84948500	8.54213900	2.00261600
H	-0.22272300	8.13539000	2.55059400
C	0.33631800	-5.49671700	-3.83802200
H	0.00874600	-4.97217400	-4.73948100
H	1.13279300	-6.18950000	-4.13196300
H	-0.49792400	-6.09630700	-3.46477500
C	5.32406200	-4.38990500	4.85168900
H	5.33342700	-3.78383800	5.76106500
H	4.85503900	-5.34876200	5.09909100
H	6.35801100	-4.59644200	4.56280800
C	-10.66111600	-3.12771900	0.16713400
H	-10.95580100	-2.16073600	0.58950900
H	-11.48234800	-3.53909300	-0.41665300
H	-10.40695000	-3.81438800	0.98204800
C	10.97380700	1.69111800	-2.42041200
H	11.16759800	0.74464800	-1.90490000
H	10.57212400	1.48610800	-3.41834600
H	11.89724000	2.26001900	-2.50534500

open-Trz-OMe'

HF zero-point energy = -2853.5292113
Zero-point correction= 1.082495 (Hartree/Particle)
Thermal correction to Energy= 1.150998
Thermal correction to Enthalpy= 1.151942
Thermal correction to Gibbs Free Energy= 0.970138
Sum of electronic and zero-point Energies=-2852.446716
Sum of electronic and Thermal Energies=-2852.378214
Sum of electronic and Thermal Enthalpies= -2852.377270
Sum of electronic and Thermal Free Energies=-2852.559073

C	-0.85034200	1.13652600	0.01494800
C	-1.31526200	-0.12054800	0.44933800
C	-0.47859500	-1.23119400	0.41033800
C	0.85016300	-1.13716900	-0.01612300
C	1.31502900	0.11987100	-0.45067200
C	0.47836700	1.23052000	-0.41165100
C	2.68987900	0.22301800	-0.94642100
C	-2.69007800	-0.22363600	0.94523900
N	-3.16381900	0.60153500	1.92599000
N	-4.43492400	0.40582400	2.08448600
N	-4.80777400	-0.55339100	1.20626200
C	-3.73981800	-0.97885700	0.48847100
N	3.16400500	-0.60255200	-1.92665300
N	4.43509400	-0.40662700	-2.08500600
N	4.80755900	0.55309100	-1.20716300
C	3.73935600	0.97871900	-0.48983900
B	-1.79035500	2.37259800	-0.20711800
B	1.79034800	-2.37293900	0.20682400
C	6.16791600	0.92316900	-1.05970800
C	7.01620800	0.91587300	-2.16807900
C	8.34645700	1.25853100	-2.01336300
C	8.84268000	1.62463500	-0.75612700
C	7.99042400	1.62736500	0.34945900
C	6.65532300	1.26519100	0.19317900
C	-6.16824000	-0.92312000	1.05894500
C	-6.65601100	-1.26442000	-0.19399500
C	-7.99123200	-1.62620100	-0.35015200
C	-8.84323700	-1.62381100	0.75562700
C	-8.34663800	-1.25846400	2.01293500
C	-7.01627400	-0.91618900	2.16751600
C	3.20926000	-2.13743000	0.84484000
C	4.35806100	-2.69938900	0.24226900
C	5.62196000	-2.40735900	0.74835400
C	5.79500500	-1.60725900	1.87457100
C	4.65836300	-1.09007200	2.48905500
C	3.37937900	-1.32924100	1.98727900
C	1.24483300	-3.80295800	-0.11456800
C	1.33833100	-4.84513500	0.83514600
C	0.83573700	-6.10859700	0.53366500
C	0.27243100	-6.39420300	-0.70818200
C	0.19465200	-5.36832300	-1.64602200
C	0.65131000	-4.08148500	-1.36652600
C	-1.24435300	3.80227500	0.11498800
C	-0.65023100	4.07985000	1.36689500
C	-0.19304000	5.36636400	1.64697800
C	-0.27085700	6.39284700	0.70979300
C	-0.83475300	6.10818600	-0.53199200
C	-1.33787500	4.84506100	-0.83404300
C	-3.20950500	2.13774900	-0.84482200
C	-3.38012900	1.33007400	-1.98755100
C	-4.65929700	1.09140500	-2.48907100
C	-5.79565100	1.60860100	-1.87405300
C	-5.62211700	2.40816400	-0.74753600
C	-4.35800500	2.69967000	-0.24165300
H	-0.85084500	-2.18910700	0.75725000
H	0.85064800	2.18844900	-0.75848700
H	-3.81629000	-1.72352100	-0.28201100
H	3.81550700	1.72378100	0.28028900
H	6.62232200	0.63288000	-3.13419100
H	9.02202200	1.25981800	-2.85867200
H	8.35380000	1.88516900	1.33325300
H	6.00700500	1.20851500	1.05675100
H	-6.00786900	-1.20746700	-1.05768000
H	-8.35489500	-1.88342700	-1.33399200
H	-9.02200900	-1.26001300	2.85839800
H	-6.62210300	-0.63376800	3.13367900
H	6.49365300	-2.81781300	0.24901500
H	4.76906200	-0.48434800	3.38366900
H	0.89196100	-6.89152800	1.28353100

H	-0.23554900	-5.57392800	-2.62125600
H	0.23762200	5.57123600	2.62216400
H	-0.89100500	6.89158700	-1.28136300
H	-4.77038500	0.48606900	-3.38390100
H	-6.49358100	2.81856600	-0.24775700
C	-4.25302400	3.59249700	0.97062200
H	-3.75468500	4.53207000	0.72027600
H	-5.24520100	3.81638900	1.36711100
H	-3.67176700	3.11319200	1.75960400
C	-2.20877700	0.70862900	-2.71434000
H	-1.36143700	1.39307700	-2.78506900
H	-1.84349100	-0.18185500	-2.19535500
H	-2.49835100	0.41778300	-3.72655200
C	-1.96560400	4.62905400	-2.19275200
H	-1.59772500	3.71923200	-2.67183500
H	-3.04974000	4.52077300	-2.10966700
H	-1.75165100	5.47364100	-2.85131300
C	-0.52693500	3.02403800	2.44238200
H	-1.42882100	2.41518000	2.52864400
H	0.29422100	2.33686400	2.21992500
H	-0.32598200	3.49001000	3.40982000
C	2.20771600	-0.70772800	2.71351900
H	1.84263200	0.18268800	2.19427300
H	1.36035000	-1.39215900	2.78400500
H	2.49688800	-0.41672800	3.72580100
C	4.25360300	-3.59288100	-0.96956100
H	5.24592500	-3.81664400	-1.36575900
H	3.75554300	-4.53249000	-0.71879600
H	3.67232300	-3.11419700	-1.75889900
C	1.96550400	-4.62808000	2.19393900
H	3.04964000	-4.51956200	2.11116300
H	1.59721100	-3.71804400	2.67229400
H	1.75153800	-5.47229300	2.85297500
C	0.52815600	-3.02631500	-2.44265200
H	-0.29302500	-2.33900700	-2.22071000
H	1.43005200	-2.41748800	-2.52910700
H	0.32737200	-3.49283800	-3.40985800
C	7.17279600	-1.33076600	2.41610800
H	7.83942500	-0.98244700	1.62307600
H	7.14153000	-0.56801600	3.19816800
H	7.61331100	-2.23555000	2.84718200
C	-7.17364600	1.33265900	-2.41535400
H	-7.14281400	0.56988300	-3.19740600
H	-7.84028300	0.98461900	-1.62221000
H	-7.61386000	2.23761100	-2.84638600
C	0.21177100	7.78125500	1.03789900
H	0.63199300	8.27161500	0.15628500
H	-0.61496600	8.40389600	1.39711600
H	0.97336800	7.75985600	1.82086000
C	-0.20962700	-7.78297900	-1.03557300
H	0.61780000	-8.40613100	-1.39230100
H	-0.63168700	-8.27222700	-0.15421200
H	-0.96963200	-7.76248500	-1.82009800
O	10.16234000	1.95295800	-0.71001600
O	-10.16299000	-1.95178100	0.70965200
C	10.71018700	2.33045700	0.54693700
C	-10.71125800	-2.32833300	-0.54740000
H	10.62989700	1.51435200	1.27356300
H	11.75890500	2.55467800	0.36176900
H	10.20692800	3.21840900	0.94524100
H	-11.76001400	-2.55229200	-0.36212700
H	-10.63084000	-1.51182000	-1.27355400
H	-10.20841000	-3.21622600	-0.94635500

3.1.4. Trz-CF_3'

***closed*-Trz-CF_3'**

HF zero-point energy = -3298.7576642
Zero-point correction= 1.031737 (Hartree/Particle)
Thermal correction to Energy= 1.099968
Thermal correction to Enthalpy= 1.100912
Thermal correction to Gibbs Free Energy= 0.915797
Sum of electronic and zero-point Energies=-3297.725928
Sum of electronic and Thermal Energies=-3297.657697
Sum of electronic and Thermal Enthalpies= -3297.656752
Sum of electronic and Thermal Free Energies=-3297.841867

C	-0.94126900	-1.07321100	0.05499100
C	-1.32042900	0.28665400	-0.02034500
C	-0.41854100	1.34766500	-0.05253400
C	0.94126500	1.07321900	-0.05486200
C	1.32043300	-0.28664200	0.02046700
C	0.41854300	-1.34764900	0.05264700
C	2.76083000	-0.35998800	0.09638500
C	-2.76081300	0.35999500	-0.09631600
N	-3.32422900	-0.88254900	-0.19920000
N	-4.61651900	-0.83293100	-0.25507200
N	-4.92349800	0.46558200	-0.20931600
C	-3.80402100	1.24898600	-0.11208500
N	3.32430000	0.88253300	0.19932700
N	4.61659300	0.83287400	0.25513800
N	4.92352900	-0.46564200	0.20925800
C	3.80401900	-1.24900500	0.11206400
B	-2.20466600	-2.09810600	0.02198300
B	2.20467900	2.09806800	-0.02185100
C	6.28244400	-0.87929200	0.25955900
C	7.23123100	-0.05230100	0.85597000
C	8.55479600	-0.46394700	0.89741500
C	8.92370800	-1.69197700	0.35274600
C	7.96779700	-2.51319200	-0.23827800
C	6.64329100	-2.10386200	-0.29574600
C	-6.28242300	0.87918400	-0.25972300
C	-6.64333400	2.10380300	0.29543300
C	-7.96785100	2.51308200	0.23786800
C	-8.92371200	1.69177000	-0.35310300
C	-8.55473700	0.46369300	-0.89762200
C	-7.23116000	0.05209600	-0.85608000
C	2.78564800	2.79523100	-1.38465000
C	3.87252100	3.69497800	-1.26945600
C	4.42689200	4.28938000	-2.40340500
C	3.94262900	4.03504600	-3.68127000
C	2.88611500	3.14187600	-3.79740900
C	2.31190200	2.51871400	-2.68520700

C	1.93854900	3.09381900	1.23787600
C	1.24298900	4.29968800	0.99538500
C	0.93478900	5.16540600	2.04744600
C	1.28367600	4.88459400	3.36224500
C	1.91979600	3.67308500	3.60803600
C	2.23288000	2.78013400	2.58239200
C	-1.93849100	-3.09385000	-1.23773200
C	-2.23277000	-2.78012100	-2.58224700
C	-1.91961100	-3.67302500	-3.60791100
C	-1.28346600	-4.88452400	-3.36213600
C	-0.93463600	-5.16538100	-2.04733100
C	-1.24291800	-4.29971500	-0.99525200
C	-2.78564700	-2.79519700	1.38482000
C	-2.31193900	-2.51858500	2.68535700
C	-2.88631100	-3.14152900	3.79761600
C	-3.94292400	-4.03456800	3.68153800
C	-4.42710600	-4.28906300	2.40366100
C	-3.87259500	-3.69489100	1.26967600
H	-0.77087800	2.37195800	-0.08865100
H	0.77087700	-2.37194400	0.08874000
H	-3.84903900	2.32112400	-0.07868800
H	3.84900700	-2.32114100	0.07860700
H	6.92884200	0.89745300	1.27263600
H	9.30202400	0.17207700	1.35211000
H	8.26025100	-3.45908600	-0.67337400
H	5.90560100	-2.72252100	-0.78780400
H	-5.90568500	2.72254200	0.78745200
H	-8.26035300	3.45901400	0.67284800
H	-9.30192500	-0.17240700	-1.35227600
H	-6.92872500	-0.89769600	-1.27262900
H	5.26443200	4.96991700	-2.28074000
H	2.49824900	2.91102900	-4.78484300
H	0.40099000	6.08553300	1.82800000
H	2.16495800	3.40290500	4.63093700
H	-2.16473500	-3.40281500	-4.63081300
H	-0.40083000	-6.08550500	-1.82789300
H	-2.49846300	-2.91062000	4.78504100
H	-5.26468200	-4.96956300	2.28102400
C	-4.47468100	-4.09662700	-0.06011500
H	-3.85542100	-4.84714100	-0.55835300
H	-5.46904100	-4.52329500	0.09417800
H	-4.56474300	-3.26005800	-0.74946200
C	-1.16754900	-1.57040000	2.96663600
H	-0.23329200	-1.92794600	2.52826700
H	-1.33897000	-0.57585700	2.55287900
H	-1.01857000	-1.46907900	4.04392300
C	-0.80065500	-4.73478500	0.38711500
H	-0.44964700	-3.90216500	0.99635800
H	-1.62332800	-5.18992300	0.94467200
H	0.00372800	-5.47084300	0.30678700
C	-2.86234400	-1.46695900	-2.99023500
H	-3.90325300	-1.39321500	-2.66456600
H	-2.32007900	-0.61919500	-2.56526100
H	-2.84642200	-1.36168200	-4.07688800
C	1.16764300	1.57038300	-2.96652100
H	1.33916400	0.57587500	-2.55272900
H	0.23331800	1.92782600	-2.52820200
H	1.01872600	1.46902000	-4.04381200
C	4.47471200	4.09654200	0.06034200
H	5.46910400	4.52313100	-0.09396600
H	3.85554500	4.84707600	0.55866800
H	4.56473300	3.25990700	0.74961300
C	0.80062800	4.73471700	-0.38696600
H	1.62325200	5.18989200	-0.94456700
H	0.44962900	3.90207800	-0.99618300
H	-0.00378500	5.47073900	-0.30659500
C	2.86244600	1.46697900	2.99040900
H	2.32013200	0.61920000	2.56552800
H	3.90333000	1.39319600	2.66466700
H	2.84660400	1.36176600	4.07707000
C	10.35136100	-2.16233400	0.45684600
C	-10.35137800	2.16206400	-0.45730800
F	11.22357400	-1.13322800	0.47971100
F	10.55335900	-2.87504600	1.59116800
F	10.69656600	-2.96257600	-0.57439500
F	-11.22355200	1.13292300	-0.48008100
F	-10.55336400	2.87463400	-1.59172100
F	-10.69664800	2.96241500	0.57382700
C	-4.53299000	-4.71455800	4.88979000
H	-4.11201900	-5.71759900	5.02043100
H	-4.32605400	-4.14810100	5.80098500
H	-5.61604900	-4.82594700	4.79047900
C	-0.98578500	-5.85221200	-4.47806400
H	-1.85475000	-6.48428000	-4.69226600
H	-0.72958100	-5.32538400	-5.40114000
H	-0.15553000	-6.51262900	-4.21566000
C	0.98607700	5.85233600	4.47814700
H	0.73003100	5.32555200	5.40129100
H	1.85502800	6.48447700	4.69219200
H	0.15574400	6.51268300	4.21580900
C	4.53242600	4.71534300	-4.88947900
H	4.32777300	4.14763900	-5.80041900
H	4.10924400	5.71728100	-5.02146600
H	5.61510700	4.82932600	-4.78908700

***half-open*-Trz-CF_3'**

HF zero-point energy = -3298.7596871
Zero-point correction= 1.030145 (Hartree/Particle)
Thermal correction to Energy= 1.099227
Thermal correction to Enthalpy= 1.100171
Thermal correction to Gibbs Free Energy= 0.916752
Sum of electronic and zero-point Energies=-3297.729542
Sum of electronic and Thermal Energies=-3297.660460
Sum of electronic and Thermal Enthalpies= -3297.659516
Sum of electronic and Thermal Free Energies=-3297.842935

C	-0.76533900	1.40190300	0.59234300
C	-1.21582600	0.09798700	0.91580900
C	-0.34653900	-0.98742800	0.94923400
C	1.01154300	-0.82611100	0.68775700
C	1.45186600	0.47802200	0.38855400
C	0.59960800	1.57689600	0.36351700
C	2.85766000	0.43455900	0.05894700

C	-2.64342800	-0.08874000	1.18699900
N	-3.31700100	0.66421900	2.11234400
N	-4.58211700	0.42223600	2.03152600
N	-4.75951600	-0.49493400	1.04556300
C	-3.56102600	-0.84616800	0.51151900
N	3.31060600	-0.85417900	-0.01032500
N	4.57261000	-0.91788300	-0.29278100
N	4.96694800	0.34879400	-0.43599100
C	3.93675800	1.22854700	-0.22927600
B	-1.72293200	2.58574800	0.22315300
B	2.17233400	-1.95222800	0.50552700
C	6.31953200	0.64295600	-0.76076500
C	7.09479400	-0.31559400	-1.40948000
C	8.41270400	-0.01882600	-1.72097600
C	8.94802600	1.22493900	-1.39189100
C	8.16515200	2.17698200	-0.74629900
C	6.84858700	1.88410000	-0.41878400
C	-6.05321700	-0.86057000	0.61448000
C	-6.22651900	-1.99347400	-0.17687800
C	-7.49119400	-2.31593900	-0.64918200
C	-8.57919400	-1.51175500	-0.32632700
C	-8.40274400	-0.39000200	0.48275600
C	-7.14215100	-0.05449500	0.94683900
C	2.94711600	-2.63586000	1.77021000
C	3.90206000	-3.64654600	1.51143600
C	4.60383400	-4.24436000	2.55910900
C	4.40019100	-3.88080000	3.88501100
C	3.47969400	-2.87157400	4.13770800
C	2.76432800	-2.24513800	3.11364700
C	1.57341200	-2.96865700	-0.62093800
C	0.83122100	-4.08591400	-0.17214900
C	0.22917500	-4.95120800	-1.08773400
C	0.32234900	-4.75767200	-2.46060900
C	1.01110700	-3.63383800	-2.90016900
C	1.61498100	-2.74047600	-2.01301200
C	-1.30502400	4.04382200	0.60447000
C	-0.92976800	4.35711700	1.93101700
C	-0.58347300	5.66561000	2.26215600
C	-0.56657600	6.68332300	1.31155000
C	-0.91969600	6.36590600	0.00199000
C	-1.30508300	5.07655300	-0.35911100
C	-3.01898800	2.26678600	-0.61070700
C	-2.97568300	1.44209300	-1.75453600
C	-4.15613500	1.08363400	-2.40288900
C	-5.40162300	1.50415400	-1.94340700
C	-5.43601700	2.34865000	-0.83725000
C	-4.27501500	2.74776900	-0.17891800
H	-0.74047000	-1.96915100	1.18197200
H	0.97083400	2.56516200	0.11268800
H	-3.46249200	-1.49791200	-0.33565800
H	4.05871100	2.29165500	-0.31540800
H	6.66554200	-1.27572400	-1.65643100
H	9.02714600	-0.75659900	-2.21901300
H	8.58729700	3.13613400	-0.47964600
H	6.25002900	2.60876800	0.11568700
H	-5.38314600	-2.62397300	-0.42159900
H	-7.62772200	-3.18867900	-1.27283500
H	-9.25055000	0.23619200	0.72670400
H	-6.98284800	0.82618700	1.55001500
H	5.33195700	-5.01631400	2.32838600
H	3.31530300	-2.55218400	5.16227500
H	-0.33258800	-5.80100200	-0.71113300
H	1.06765300	-3.43276500	-3.96583800
H	-0.32019000	5.89621500	3.28973900
H	-0.90333600	7.14364500	-0.75505000
H	-4.10220200	0.45672300	-3.28763500
H	-6.39413800	2.70433300	-0.47265600
C	-4.39833000	3.65589900	1.02016500
H	-3.89446800	4.60878600	0.84481200
H	-5.44842400	3.85296800	1.24562500
H	-3.94056500	3.20177600	1.90134200
C	-1.67271500	0.91966300	-2.31690800
H	-0.88718200	1.67762400	-2.29114300
H	-1.30075400	0.06624400	-1.74362300
H	-1.80627800	0.59968100	-3.35251700
C	-1.71035300	4.82386900	-1.79385300
H	-1.22739000	3.93462900	-2.20478500
H	-2.78720000	4.65569300	-1.87214700
H	-1.44814300	5.67804200	-2.42197900
C	-0.93248800	3.31465300	3.02631200
H	-1.81065300	2.66772800	2.97777200
H	-0.06014100	2.66077000	2.94528000
H	-0.90697100	3.79468400	4.00714100
C	1.79653400	-1.16082900	3.53032100
H	1.98094900	-0.22041300	3.00826700
H	0.76212400	-1.43636100	3.31337500
H	1.87651300	-0.97476200	4.60357500
C	4.19537700	-4.16447900	0.11992300
H	5.15116400	-4.69442700	0.11164000
H	3.41735700	-4.85726500	-0.21094000
H	4.23860400	-3.36866100	-0.62118400
C	0.65322100	-4.42425800	1.29319200
H	1.54266700	-4.91434000	1.69681400
H	0.49062400	-3.54212500	1.91190200
H	-0.19708900	-5.09865400	1.42104800
C	2.27386200	-1.52251800	-2.62142600
H	1.89158200	-0.60079300	-2.17688900
H	3.35839900	-1.53233700	-2.48678300
H	2.07403700	-1.48158700	-3.69404600
C	10.36169000	1.55716900	-1.79419700
C	-9.96092900	-1.87079900	-0.79817000
F	11.16389400	0.47258200	-1.75974000
F	10.41160000	2.04263200	-3.05794100
F	10.91135900	2.49321900	-0.99224200
F	-10.68864700	-0.77318800	-1.10707300
F	-10.65662100	-2.54050000	0.15339800
F	-9.94043200	-2.65936500	-1.89457100
C	5.13676800	-4.56731300	5.00594700
H	5.27032900	-3.89750200	5.85910700
H	4.58256700	-5.44391700	5.35925200
H	6.12095500	-4.91176300	4.67845000
C	-0.29247800	-5.73037700	-3.43324100
H	-0.58540000	-5.23070800	-4.36022300
H	0.41695700	-6.52257800	-3.69687700
H	-1.17572600	-6.21151400	-3.00530900
C	-6.67504500	1.04214400	-2.59984400
H	-6.48942100	0.68371400	-3.61471400
H	-7.12625000	0.22270700	-2.03163200
H	-7.41122500	1.84860900	-2.64560400
C	-0.21131500	8.09547600	1.69643400
H	0.22986000	8.63521700	0.85511200
H	-1.10413700	8.64736400	2.01010400
H	0.49438800	8.11221100	2.53043500

***open*-Trz-CF_3'**

HF zero-point energy = -3298.7602936
Zero-point correction= 1.027628 (Hartree/Particle)
Thermal correction to Energy= 1.098013
Thermal correction to Enthalpy= 1.098957
Thermal correction to Gibbs Free Energy= 0.911633
Sum of electronic and zero-point Energies=-3297.732666
Sum of electronic and Thermal Energies=-3297.662281
Sum of electronic and Thermal Enthalpies= -3297.661337
Sum of electronic and Thermal Free Energies=-3297.848660

C	0.82019100	-1.16077700	-0.01609400
C	1.31593000	0.07135600	0.45361500
C	0.50984100	1.20464100	0.44693500
C	-0.82017700	1.16104100	0.01572800
C	-1.31590100	-0.07107700	-0.45401000
C	-0.50979900	-1.20435900	-0.44735000
C	-2.69669900	-0.13008300	-0.94431300
C	2.69671200	0.13034500	0.94398100
N	3.14768900	-0.69055200	1.94346300
N	4.42632500	-0.56253300	2.06800400
N	4.83571300	0.34629200	1.14707300
C	3.77222900	0.80861200	0.43942700
N	-3.14780900	0.69089800	-1.94367200
N	-4.42642700	0.56280900	-2.06816200
N	-4.83570000	-0.34619900	-1.14732000
C	-3.77213200	-0.80850400	-0.43979300
B	1.71985600	-2.42578000	-0.25707700
B	-1.71987600	2.42595700	0.25702700
C	-6.20715900	-0.61037600	-0.93975600
C	-7.16023600	0.30133100	-1.39327400
C	-8.50116100	0.06120900	-1.14574300
C	-8.89326800	-1.07118200	-0.43283900
C	-7.93938900	-1.98138500	0.01006100
C	-6.59416500	-1.75400900	-0.24575900
C	6.20721100	0.61029800	0.93951000
C	6.59435800	1.75386700	0.24548900
C	7.93960400	1.98106200	-0.01036900
C	8.89336900	1.07073400	0.43252200
C	8.50112400	-0.06159200	1.14545000
C	7.16016800	-0.30153100	1.39301700
C	-3.15862800	2.21960800	0.85665000
C	-4.27591100	2.81763000	0.23293900
C	-5.56249200	2.51431500	0.67486600
C	-5.79029700	1.65602300	1.74579400
C	-4.68183200	1.12010400	2.39828900
C	-3.38298300	1.37782800	1.96687400
C	-1.11850500	3.83830400	-0.03492700
C	-1.18687100	4.86816400	0.93042100
C	-0.63405400	6.11645900	0.65589300
C	-0.04371300	6.40036000	-0.57394800
C	0.00771500	5.38753900	-1.52792000
C	-0.50035600	4.11465900	-1.27553100
C	1.11844600	-3.83802700	0.03523000
C	0.50021600	-4.11404200	1.27590600
C	-0.00791400	-5.38681200	1.52859300
C	0.04352400	-6.39990000	0.57486700
C	0.63394700	-6.11635700	-0.65498400
C	1.18684800	-4.86813200	-0.92980600
C	3.15862700	-2.21961600	-0.85672300
C	3.38298600	-1.37801800	-1.96709400
C	4.68185300	-1.12035200	-2.39849900
C	5.79031000	-1.65615100	-1.74587900
C	5.56248000	-2.51430100	-0.67484500
C	4.27588700	-2.81754200	-0.23291400
H	0.90878400	2.14211200	0.81868300
H	-0.90874900	-2.14182100	-0.81911400
H	3.86988200	1.47588100	-0.39579900
H	-3.86966200	-1.47589600	0.39535100
H	-6.83634800	1.18621500	-1.91939500
H	-9.24628800	0.76909500	-1.48373200
H	-8.24354600	-2.86282800	0.55751100
H	-5.85331600	-2.46674400	0.08885600
H	5.85359300	2.46670000	-0.08910800
H	8.24386900	2.86244900	-0.55785000
H	9.24615100	-0.76958200	1.48344000
H	6.83618400	-1.18637000	1.91915500
H	-6.41050200	2.96015500	0.16583100
H	-4.83332300	0.48326600	3.26463600
H	-0.67206600	6.88937200	1.41705800
H	0.45587800	5.59364300	-2.49489200
H	-0.45615900	-5.59263200	2.49559000
H	0.67197000	-6.88947300	-1.41593700
H	4.83338500	-0.48364200	-3.26493300
H	6.41046900	-2.96003600	-0.16568100
C	4.11842300	-3.75114600	0.94249800
H	3.56307700	-4.64807700	0.66081900
H	5.09571100	-4.05167800	1.32575500
H	3.56908500	-3.26833400	1.75325100
C	2.24349600	-0.73220700	-2.72244800
H	1.39660500	-1.41043000	-2.84332000
H	1.86250200	0.14754000	-2.19607400
H	2.57305000	-0.41779000	-3.71500100
C	1.84145400	-4.65176600	-2.27549200
H	1.50328800	-3.72740900	-2.74898700
H	2.92646300	-4.57162600	-2.17411200
H	1.61755000	-5.48222100	-2.94829200
C	0.40745700	-3.07402600	2.37009800
H	1.32906000	-2.49807500	2.47252900
H	-0.38873400	-2.35480300	2.15840400
H	0.18709300	-3.55017500	3.32811800
C	-2.24346700	0.73189200	2.72208900
H	-1.86266600	-0.14790400	2.19565500
H	-1.39647100	1.41000000	2.84283900
H	-2.57292400	0.41750200	3.71468200
C	-4.11854800	3.75142200	-0.94233200
H	-5.09587100	4.05206600	-1.32541000
H	-3.56311800	4.64828800	-0.66061000
H	-3.56934600	3.26870600	-1.75323700
C	-1.84136900	4.65141200	2.27609200
H	-2.92641100	4.57158000	2.17479200
H	-1.50338700	3.72678700	2.74918400
H	-1.61719800	5.48155300	2.94919300
C	-0.40759300	3.07493700	-2.36999600
H	0.38872800	2.35576700	-2.15858700
H	-1.32913200	2.49889200	-2.47247700
H	-0.18740300	3.55135300	-3.32792400
C	-10.35708600	-1.32240000	-0.19702500
C	10.35722100	1.32174900	0.19670700
F	-11.02611300	-0.17896900	0.07562400
F	-10.95238200	-1.86867700	-1.28540600
F	-10.57321200	-2.16860300	0.83306700
F	11.02609900	0.17825100	-0.07596200
F	10.95258600	1.86795300	1.28508100
F	10.57344500	2.16794100	-0.83339100

C	-7.19017900	1.29391400	2.16374800
H	-7.53648400	0.40875000	1.62055900
H	-7.23892300	1.06850400	3.23159400
H	-7.88995300	2.10399500	1.94637900
C	7.19019500	-1.29403800	-2.16380100
H	7.23900100	-1.06879300	-3.23168100
H	7.53642200	-0.40876200	-1.62073700
H	7.89000500	-2.10404100	-1.94625800
C	-0.49353700	-7.77457600	0.87420900
H	-0.91688300	-8.23667500	-0.02095100
H	0.30492500	-8.43142100	1.23626900
H	-1.26569000	-7.73770500	1.64610300
C	0.49334500	7.77515200	-0.87276100
H	-0.30622400	8.43380300	-1.22903100
H	0.92180400	8.23462100	0.02134200
H	1.26151200	7.73927500	-1.64864800

3.1.5. Transitional State Optimization

Open*/*closed conformers and transitional state of *ortho*-dimesitylboryl-(1-methyl-1,2,3-triazol-4-yl)-phenylene optimized at B3LYP-D2/def2-TZVP, solvent: PCM; THF

Open-Conformer (TS^{o})

HF zero-point energy = -1236.6136061
Zero-point correction= 0.506507 (Hartree/Particle)
Thermal correction to Energy= 0.537162
Thermal correction to Enthalpy= 0.538106
Thermal correction to Gibbs Free Energy= 0.443885
Sum of electronic and zero-point Energies= -1236.107099
Sum of electronic and thermal Energies= -1236.076444
Sum of electronic and thermal Enthalpies= -1236.075500
Sum of electronic and thermal Free Energies=-1236.169721

C	0.35935300	1.78937000	0.43182200
C	-0.83702300	2.39831700	-0.00193600
C	-1.10603200	3.73030200	0.30508900
C	-0.19377300	4.48216600	1.03983900
C	1.00785400	3.90931800	1.44570900
C	1.27993400	2.58316400	1.12841800
C	-1.78338600	1.61081500	-0.80071800
N	-1.41734100	1.00479300	-1.96410200
N	-2.40118600	0.26883900	-2.39338400
N	-3.40819000	0.39118700	-1.52049700
C	-3.07284100	1.22665200	-0.51874800
B	0.64155800	0.25167200	0.31128200
C	-4.59800800	-0.43066600	-1.63956300
C	2.10961300	-0.23030100	0.05538700
C	2.85464500	0.27792300	-1.03082700
C	4.14602600	-0.18761400	-1.26744400
C	4.74975700	-1.12939800	-0.43827000
C	4.01928000	-1.61209700	0.64434000
C	2.71270400	-1.19541400	0.89026600
C	-0.52929300	-0.77566400	0.53136400
C	-1.39066000	-0.68569900	1.64506700
C	-2.45446800	-1.57197100	1.78056900
C	-2.72210700	-2.54723800	0.82185800
C	-1.86742500	-2.63640000	-0.27123400
C	-0.77061200	-1.78843600	-0.41938500
H	-2.02597400	4.18233200	-0.04538500
H	2.21598900	2.13823900	1.44483300
H	-3.72643600	1.43099500	0.31012000
H	4.69623200	0.19730700	-2.11990400
H	4.47624100	-2.33651100	1.31045300
H	-3.09849100	-1.49218300	2.65065200
H	-2.05888200	-3.38441500	-1.03340200
C	0.11069000	-1.95908700	-1.63131000
H	1.11498000	-2.27656100	-1.34247000
H	-0.30955800	-2.70473400	-2.30861100
H	0.21019200	-1.01876200	-2.17619200
C	-1.19842000	0.36181700	2.71486800
H	-0.14536400	0.49727400	2.96805600
H	-1.56661500	1.33574600	2.38176400
H	-1.73868300	0.08542700	3.62237800
C	1.98008500	-1.79527600	2.06757500
H	1.50205900	-1.03000000	2.68256100
H	1.18675400	-2.46639500	1.73068200
H	2.66784400	-2.36149800	2.69844500
C	2.27483100	1.29701300	-1.98335800
H	1.24052800	1.06783100	-2.24642000
H	2.26880200	2.29247900	-1.53196800
H	2.86837800	1.34221900	-2.89870900
C	-3.88520300	-3.48920300	0.98122100
H	-4.75948100	-2.97170600	1.38404100
H	-4.15703800	-3.94334000	0.02622200
H	-3.63960100	-4.29915600	1.67591300
C	6.13931700	-1.63243600	-0.72223400
H	6.63563200	-1.95834100	0.19426900
H	6.10836600	-2.48973100	-1.40306600
H	6.74878300	-0.86008300	-1.19654200
H	-4.49052100	-1.31494300	-1.00885700
H	-5.46786800	0.14557200	-1.32843700
H	-4.70232200	-0.72985000	-2.68009400
H	1.72913100	4.49509500	2.00209700
H	-0.41286900	5.51586200	1.27686500

Transitional State (TS‡)

HF zero-point energy = -1236.6016961
Zero-point correction= 0.505659 (Hartree/Particle)
Thermal correction to Energy= 0.535879
Thermal correction to Enthalpy= 0.536823
Thermal correction to Gibbs Free Energy= 0.441976
Sum of electronic and zero-point Energies= -1236.096037
Sum of electronic and thermal Energies= -1236.065817
Sum of electronic and thermal Enthalpies= -1236.064873
Sum of electronic and thermal Free Energies= -1236.159721

C	-1.08443800	-3.26100100	2.97424000
C	0.13018100	-2.63819900	3.24094100
C	0.57023300	-1.61540000	2.41024800
C	-0.19193400	-1.14920500	1.32974300
C	-1.41581300	-1.79531200	1.06485600
C	-1.83834400	-2.84897500	1.88262500
C	-2.22677500	-1.49612200	-0.12606100
N	-2.63855700	-0.25741800	-0.51270700
N	-3.33362600	-0.35735600	-1.60906400
N	-3.38181300	-1.65466600	-1.94647300
C	-2.70926100	-2.40013500	-1.04957100
B	0.44543900	0.03521300	0.51170100
C	-4.08017500	-2.09222700	-3.14245100
C	-0.23332200	1.43139700	0.34819000

C	-0.23620000	2.07661100	-0.90748400
C	-0.79925800	3.34177900	-1.04046300
C	-1.34329300	4.02035400	0.04702800
C	-1.32842100	3.38565400	1.28536400
C	-0.80575800	2.10481100	1.44769100
C	1.89350900	-0.20595300	-0.04891400
C	2.94237800	0.68593000	0.25564500
C	4.22355200	0.44934100	-0.24187500
C	4.49970300	-0.63118500	-1.07385000
C	3.45676600	-1.50255400	-1.38175800
C	2.17537800	-1.31762700	-0.87200100
H	1.53624900	-1.16271600	2.60222300
H	-2.77595600	-3.34292200	1.65854900
H	-2.60869600	-3.46738300	-1.13806200
H	-0.81282000	3.81254200	-2.01805500
H	-1.74052300	3.89898200	2.14796400
H	5.02453200	1.13174000	0.02312100
H	3.64831400	-2.35013700	-2.03178600
C	-0.84543400	1.49209100	2.82636700
H	-1.49188000	0.61207500	2.84613400
H	0.14297600	1.16019900	3.15343300
H	-1.22117000	2.21337700	3.55426500
C	0.31634400	1.41111200	-2.14508700
H	0.03007900	1.96996800	-3.03794500
H	1.40591500	1.34819500	-2.11016200
H	-0.05954800	0.39076500	-2.24838200
C	2.72897400	1.90725600	1.11984400
H	2.19391800	2.68421600	0.56873400
H	2.13034600	1.68484400	2.00510100
H	3.68771500	2.31433400	1.44667200
C	1.09724900	-2.30238800	-1.25578000
H	0.80939900	-2.92208600	-0.40335900
H	0.19003200	-1.79694800	-1.59489700
H	1.44195600	-2.95785500	-2.05769100
C	-1.95923900	5.38300700	-0.11890800
H	-3.02363900	5.29883200	-0.36267400
H	-1.87820700	5.96659300	0.80064900
H	-1.48001700	5.93617400	-0.92966500
C	5.87545200	-0.83927800	-1.64683500
H	6.10582400	-1.90276100	-1.74282000
H	5.94909300	-0.39752300	-2.64624900
H	6.63769500	-0.37006400	-1.02161500
H	-1.43830200	-4.06838000	3.60299200
H	0.73850500	-2.95907700	4.07754100
H	-4.86553000	-2.79942500	-2.87525800
H	-4.51858300	-1.21317500	-3.60918200
H	-3.37923200	-2.56505200	-3.83083900

Closed Conformer (TS^{c})

HF zero-point energy = -1236.6206856
Zero-point correction= 0.509217 (Hartree/Particle)
Thermal correction to Energy= 0.538429
Thermal correction to Enthalpy= 0.539373
Thermal correction to Gibbs Free Energy= 0.449204
Sum of electronic and zero-point Energies= -1236.111468
Sum of electronic and thermal Energies= -1236.082257
Sum of electronic and thermal Enthalpies= -1236.081313
Sum of electronic and thermal Free Energies=-1236.171481

C	0.40541900	1.26618800	-1.30178700
C	0.15015400	2.58603600	-0.87790800
C	-0.39928300	2.55164400	0.46019900
N	-0.41575900	1.28514800	0.95452300
N	-0.92142000	1.23694900	2.15338300
C	1.00992300	3.50851300	-2.90717400
C	1.30902500	2.21402400	-3.33925200
C	1.02261500	1.10950400	-2.54071000
C	0.43605500	3.70419300	-1.65709500
N	-1.22015200	2.48801000	2.45739500
C	-0.92313900	3.34787600	1.45012700
B	0.03961000	0.16136300	-0.15583800
C	-1.84618700	2.80045100	3.73500900
C	-1.30296800	-0.77855200	-0.24970800
C	-1.51095700	-1.76943900	0.73848300
C	-2.64488700	-2.58329700	0.70691500
C	-3.61293700	-2.46359000	-0.28229700
C	-3.42664500	-1.47144600	-1.23621400
C	-2.30813300	-0.63305700	-1.23009500
C	1.43374800	-0.63878200	0.13819700
C	1.71085100	-1.79831500	-0.62131200
C	2.90405500	-2.50147600	-0.44181400
C	3.86804400	-2.10083400	0.47407500
C	3.62013900	-0.93240000	1.18451200
C	2.44389200	-0.19800500	1.02101500
H	1.28246800	0.12012500	-2.89520400
H	0.22618900	4.70350100	-1.29478600
H	-1.10955200	4.40396600	1.52133800
H	-2.77343000	-3.33140600	1.48328600
H	-4.17897400	-1.33436000	-2.00669400
H	3.08399300	-3.38702000	-1.04384400
H	4.37314300	-0.56627100	1.87566900
C	-2.24668800	0.40850900	-2.32278400
H	-2.10244200	1.41299800	-1.92279900
H	-1.41417500	0.22739900	-3.00527700
H	-3.17106500	0.39984800	-2.90424000
C	-0.53196400	-2.03592000	1.86075600
H	-1.03044200	-2.57451000	2.67030100
H	0.30474900	-2.64605800	1.51116200
H	-0.10616300	-1.12145500	2.26716300
C	0.75357100	-2.36213300	-1.64948000
H	-0.01900300	-2.97310200	-1.17522400
H	0.22969200	-1.58592200	-2.20438300
H	1.29648700	-2.99081700	-2.35918200
C	2.33648000	1.08592300	1.81200700
H	2.08340700	1.92988700	1.16777900
H	1.57175100	1.02623200	2.58959400
H	3.28818000	1.30877700	2.29796800
H	1.24121300	4.35781700	-3.53740300
H	1.77538200	2.07023300	-4.30664100
C	5.12831200	-2.89666300	0.68818000
C	-4.80832400	-3.37835200	-0.32416700
H	-5.65690500	-2.89598100	-0.81475600
H	-4.58243100	-4.29309300	-0.88278900
H	-5.11141900	-3.67761500	0.68204900
H	5.96383200	-2.24715800	0.96027000
H	5.00159300	-3.62289900	1.49847900
H	5.39963800	-3.45400500	-0.21141600
H	-1.66820200	1.96675700	4.40910600
H	-1.39805200	3.70866900	4.13355100
H	-2.91721300	2.94429400	3.59294200

4. Crystal Data

4.1. Trz-Me

Table S5. Crystal data and structure refinement for Trz-Me.

Empirical formula	$C_{60.50}H_{63}B_2ClN_6$	
Formula weight	931.24	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.9954(7) Å	α= 69.831(4)°.
	b = 14.3264(6) Å	β= 78.920(4)°.
	c = 14.4940(7) Å	γ = 85.791(4)°.
Volume	2677.0(2) $Å^3$	
Z	2	
Density (calculated)	1.155 Mg/m^3	
Absorption coefficient	0.959 mm^{-1}	
F(000)	990	
Crystal colour and habit	Colorless prism	
Crystal size	0.274 x 0.173 x 0.105 mm^3	
Theta range for data collection	3.218 to 74.112°.	
Index ranges	-17<=h<=17, -17<=k<=9, -17<=l<=17	
Reflections collected	19208	
Independent reflections	10567 [R(int) = 0.0368]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.88923	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10567 / 0 / 654	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0637, wR2 = 0.1873	
R indices (all data)	R1 = 0.0837, wR2 = 0.1969	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.608 and -0.352 $e.Å^{-3}$	

Definitions:

$$R_1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \qquad wR_2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right]}{\sum \left[w\left(F_o^2\right)^2 \right]}}$$

$$GooF = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right) \right]}{(n-p)}}$$

n = number of reflections; p = number of parameters

Notes on the refinement of Trz-Me.

All hydrogen atoms were placed in calculated positions and refined by using a riding model.

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Trz-Me. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9998(2)	189(2)	3962(2)	31(1)
C(2)	9690(2)	893(2)	4439(2)	32(1)
C(3)	9673(2)	723(2)	5448(2)	33(1)
C(4)	9425(2)	1813(2)	3704(2)	34(1)
C(5)	9034(2)	2736(2)	3614(2)	38(1)
C(6)	8718(2)	4181(2)	2132(2)	38(1)
C(7)	9241(2)	4773(2)	1244(2)	54(1)
C(8)	8923(3)	5745(2)	820(2)	61(1)
C(9)	8101(2)	6118(2)	1260(2)	52(1)
C(10)	7591(2)	5503(2)	2153(2)	51(1)
C(11)	7896(2)	4541(2)	2594(2)	45(1)
C(12)	7761(3)	7177(2)	807(3)	72(1)
C(13)	11122(2)	505(2)	2241(2)	34(1)
C(14)	11404(2)	-413(2)	2103(2)	38(1)
C(15)	12386(2)	-623(2)	1822(2)	50(1)
C(16)	13121(2)	42(3)	1669(2)	55(1)
C(17)	12846(2)	939(3)	1775(2)	51(1)
C(18)	11876(2)	1185(2)	2055(2)	43(1)
C(19)	10687(2)	-1213(2)	2242(2)	43(1)
C(20)	14180(3)	-224(4)	1411(3)	79(1)
C(21)	11692(3)	2208(3)	2138(3)	59(1)
C(22)	9149(2)	332(2)	2270(2)	29(1)
C(23)	8328(2)	-254(2)	2831(2)	34(1)
C(24)	7659(2)	-497(2)	2354(2)	37(1)
C(25)	7737(2)	-160(2)	1328(2)	37(1)
C(26)	8530(2)	432(2)	772(2)	36(1)
C(27)	9222(2)	681(2)	1214(2)	33(1)
C(28)	8112(2)	-647(2)	3962(2)	42(1)
C(29)	6967(2)	-382(2)	833(2)	50(1)
C(30)	10047(2)	1335(2)	514(2)	37(1)
C(40)	5111(2)	1014(2)	4930(2)	35(1)
C(41)	5459(2)	650(2)	4137(2)	35(1)
C(42)	5364(2)	-331(2)	4191(2)	35(1)
C(43)	5897(2)	1470(2)	3269(2)	36(1)
C(44)	6412(2)	1688(2)	2319(2)	40(1)
C(45)	7021(2)	3309(2)	1017(2)	41(1)
C(46)	6693(3)	4278(2)	621(2)	60(1)
C(47)	7152(3)	4850(2)	-318(3)	65(1)
C(48)	7918(3)	4469(2)	-867(2)	52(1)
C(49)	8205(3)	3504(2)	-439(2)	55(1)
C(50)	7761(2)	2914(2)	512(2)	51(1)
C(51)	8399(3)	5097(3)	-1908(2)	68(1)
C(52)	6118(2)	2658(2)	4980(2)	33(1)
C(53)	6821(2)	2066(2)	5516(2)	36(1)
C(54)	7460(2)	2494(2)	5881(2)	41(1)
C(55)	7460(2)	3502(2)	5727(2)	42(1)
C(56)	6814(2)	4097(2)	5152(2)	39(1)
C(57)	6159(2)	3700(2)	4776(2)	35(1)
C(58)	6937(2)	957(2)	5718(2)	46(1)
C(59)	8137(3)	3934(3)	6164(3)	63(1)
C(60)	5510(2)	4433(2)	4137(2)	38(1)

C(61)	4177(2)	2678(2)	4828(2)	37(1)
C(62)	3817(2)	2727(2)	5796(2)	41(1)
C(63)	2852(2)	3003(2)	6051(3)	53(1)
C(64)	2206(2)	3239(2)	5397(3)	60(1)
C(65)	2551(2)	3197(2)	4456(3)	58(1)
C(66)	3512(2)	2920(2)	4163(2)	48(1)
C(67)	4426(2)	2492(2)	6605(2)	45(1)
C(68)	1157(3)	3500(3)	5713(4)	91(2)
C(69)	3781(3)	2886(3)	3119(3)	72(1)
B(1)	9994(2)	634(2)	2753(2)	31(1)
B(2)	5268(2)	2215(2)	4618(2)	35(1)
N(1)	9640(2)	1764(1)	2768(2)	32(1)
N(2)	9402(2)	2593(2)	2094(2)	34(1)
N(3)	9040(2)	3185(2)	2619(2)	35(1)
N(4)	5749(2)	2349(2)	3444(2)	35(1)
N(5)	6146(2)	3100(2)	2672(2)	38(1)
N(6)	6543(2)	2687(2)	1986(2)	39(1)
C(31)	4112(9)	6877(8)	1345(11)	121(5)
Cl(1)	4488(3)	5762(3)	1998(3)	137(1)
Cl(2)	4891(4)	7484(4)	287(5)	207(3)

Table S7. Bond lengths [Å] and angles [°] for Trz-Me.

C(1)-C(3)#1	1.394(3)
C(1)-C(2)	1.408(3)
C(1)-B(1)	1.646(3)
C(2)-C(3)	1.394(3)
C(2)-C(4)	1.457(3)
C(3)-C(1)#1	1.394(3)
C(3)-H(3)	0.9500
C(4)-N(1)	1.357(3)
C(4)-C(5)	1.366(4)
C(5)-N(3)	1.360(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.374(4)
C(6)-C(11)	1.375(4)
C(6)-N(3)	1.439(3)
C(7)-C(8)	1.392(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.382(4)
C(9)-C(12)	1.512(4)
C(10)-C(11)	1.379(4)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.412(4)
C(13)-C(14)	1.415(4)
C(13)-B(1)	1.637(4)
C(14)-C(15)	1.397(4)
C(14)-C(19)	1.515(4)
C(15)-C(16)	1.389(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.365(5)
C(16)-C(20)	1.511(4)
C(17)-C(18)	1.396(4)
C(17)-H(17)	0.9500
C(18)-C(21)	1.511(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.413(3)
C(22)-C(27)	1.422(3)
C(22)-B(1)	1.636(4)
C(23)-C(24)	1.393(4)
C(23)-C(28)	1.514(4)
C(24)-C(25)	1.382(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.387(4)
C(25)-C(29)	1.510(4)
C(26)-C(27)	1.386(4)
C(26)-H(26)	0.9500
C(27)-C(30)	1.514(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(40)-C(42)#2	1.391(4)
C(40)-C(41)	1.410(4)
C(40)-B(2)	1.642(4)
C(41)-C(42)	1.396(3)
C(41)-C(43)	1.459(4)
C(42)-C(40)#2	1.390(4)
C(42)-H(42)	0.9500
C(43)-N(4)	1.361(3)
C(43)-C(44)	1.367(4)
C(44)-N(6)	1.358(3)
C(44)-H(44)	0.9500
C(45)-C(50)	1.355(4)
C(45)-C(46)	1.388(4)
C(45)-N(6)	1.441(3)
C(46)-C(47)	1.381(5)
C(46)-H(46)	0.9500
C(47)-C(48)	1.403(5)
C(47)-H(47)	0.9500
C(48)-C(49)	1.371(4)
C(48)-C(51)	1.517(4)
C(49)-C(50)	1.394(4)
C(49)-H(49)	0.9500
C(50)-H(50)	0.9500
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.417(4)
C(52)-C(57)	1.420(3)
C(52)-B(2)	1.636(4)
C(53)-C(54)	1.394(4)
C(53)-C(58)	1.514(4)
C(54)-C(55)	1.383(4)
C(54)-H(54)	0.9500
C(55)-C(56)	1.388(4)
C(55)-C(59)	1.507(4)
C(56)-C(57)	1.395(4)
C(56)-H(56)	0.9500
C(57)-C(60)	1.516(4)
C(58)-H(58A)	0.9800

C(58)-H(58B)	0.9800	C(6)-C(7)-C(8)	118.8(3)
C(58)-H(58C)	0.9800	C(6)-C(7)-H(7)	120.6
C(59)-H(59A)	0.9800	C(8)-C(7)-H(7)	120.6
C(59)-H(59B)	0.9800	C(9)-C(8)-C(7)	121.7(3)
C(59)-H(59C)	0.9800	C(9)-C(8)-H(8)	119.2
C(60)-H(60A)	0.9800	C(7)-C(8)-H(8)	119.2
C(60)-H(60B)	0.9800	C(8)-C(9)-C(10)	118.2(3)
C(60)-H(60C)	0.9800	C(8)-C(9)-C(12)	121.7(3)
C(61)-C(66)	1.409(4)	C(10)-C(9)-C(12)	120.1(3)
C(61)-C(62)	1.420(4)	C(11)-C(10)-C(9)	121.3(3)
C(61)-B(2)	1.635(4)	C(11)-C(10)-H(10)	119.3
C(62)-C(63)	1.396(4)	C(9)-C(10)-H(10)	119.3
C(62)-C(67)	1.511(4)	C(6)-C(11)-C(10)	119.5(3)
C(63)-C(64)	1.375(5)	C(6)-C(11)-H(11)	120.3
C(63)-H(63)	0.9500	C(10)-C(11)-H(11)	120.3
C(64)-C(65)	1.377(6)	C(9)-C(12)-H(12A)	109.5
C(64)-C(68)	1.512(5)	C(9)-C(12)-H(12B)	109.5
C(65)-C(66)	1.402(4)	H(12A)-C(12)-H(12B)	109.5
C(65)-H(65)	0.9500	C(9)-C(12)-H(12C)	109.5
C(66)-C(69)	1.504(5)	H(12A)-C(12)-H(12C)	109.5
C(67)-H(67A)	0.9800	H(12B)-C(12)-H(12C)	109.5
C(67)-H(67B)	0.9800	C(18)-C(13)-C(14)	116.4(2)
C(67)-H(67C)	0.9800	C(18)-C(13)-B(1)	124.9(2)
C(68)-H(68A)	0.9800	C(14)-C(13)-B(1)	118.0(2)
C(68)-H(68B)	0.9800	C(15)-C(14)-C(13)	120.4(3)
C(68)-H(68C)	0.9800	C(15)-C(14)-C(19)	116.3(3)
C(69)-H(69A)	0.9800	C(13)-C(14)-C(19)	123.3(2)
C(69)-H(69B)	0.9800	C(16)-C(15)-C(14)	122.4(3)
C(69)-H(69C)	0.9800	C(16)-C(15)-H(15)	118.8
B(1)-N(1)	1.664(3)	C(14)-C(15)-H(15)	118.8
B(2)-N(4)	1.655(4)	C(17)-C(16)-C(15)	117.1(3)
N(1)-N(2)	1.320(3)	C(17)-C(16)-C(20)	121.6(4)
N(2)-N(3)	1.338(3)	C(15)-C(16)-C(20)	121.3(4)
N(4)-N(5)	1.318(3)	C(16)-C(17)-C(18)	122.6(3)
N(5)-N(6)	1.339(3)	C(16)-C(17)-H(17)	118.7
C(31)-Cl(1)	1.658(11)	C(18)-C(17)-H(17)	118.7
C(31)-Cl(2)	1.694(15)	C(17)-C(18)-C(13)	120.9(3)
C(31)-H(31A)	0.9900	C(17)-C(18)-C(21)	116.2(3)
C(31)-H(31B)	0.9900	C(13)-C(18)-C(21)	122.9(3)
C(3)#1-C(1)-C(2)	116.4(2)	C(14)-C(19)-H(19A)	109.5
C(3)#1-C(1)-B(1)	130.5(2)	C(14)-C(19)-H(19B)	109.5
C(2)-C(1)-B(1)	112.9(2)	H(19A)-C(19)-H(19B)	109.5
C(3)-C(2)-C(1)	124.4(2)	C(14)-C(19)-H(19C)	109.5
C(3)-C(2)-C(4)	126.6(2)	H(19A)-C(19)-H(19C)	109.5
C(1)-C(2)-C(4)	109.0(2)	H(19B)-C(19)-H(19C)	109.5
C(1)#1-C(3)-C(2)	119.2(2)	C(16)-C(20)-H(20A)	109.5
C(1)#1-C(3)-H(3)	120.4	C(16)-C(20)-H(20B)	109.5
C(2)-C(3)-H(3)	120.4	H(20A)-C(20)-H(20B)	109.5
N(1)-C(4)-C(5)	106.6(2)	C(16)-C(20)-H(20C)	109.5
N(1)-C(4)-C(2)	111.2(2)	H(20A)-C(20)-H(20C)	109.5
C(5)-C(4)-C(2)	142.2(2)	H(20B)-C(20)-H(20C)	109.5
N(3)-C(5)-C(4)	104.8(2)	C(18)-C(21)-H(21A)	109.5
N(3)-C(5)-H(5)	127.6	C(18)-C(21)-H(21B)	109.5
C(4)-C(5)-H(5)	127.6	H(21A)-C(21)-H(21B)	109.5
C(7)-C(6)-C(11)	120.6(2)	C(18)-C(21)-H(21C)	109.5
C(7)-C(6)-N(3)	120.8(2)	H(21A)-C(21)-H(21C)	109.5
C(11)-C(6)-N(3)	118.6(2)	H(21B)-C(21)-H(21C)	109.5

C(23)-C(22)-C(27)	116.4(2)	C(46)-C(47)-C(48)	121.6(3)
C(23)-C(22)-B(1)	124.5(2)	C(46)-C(47)-H(47)	119.2
C(27)-C(22)-B(1)	119.1(2)	C(48)-C(47)-H(47)	119.2
C(24)-C(23)-C(22)	120.5(2)	C(49)-C(48)-C(47)	117.8(3)
C(24)-C(23)-C(28)	116.0(2)	C(49)-C(48)-C(51)	121.1(3)
C(22)-C(23)-C(28)	123.5(2)	C(47)-C(48)-C(51)	121.1(3)
C(25)-C(24)-C(23)	122.7(2)	C(48)-C(49)-C(50)	121.7(3)
C(25)-C(24)-H(24)	118.6	C(48)-C(49)-H(49)	119.1
C(23)-C(24)-H(24)	118.6	C(50)-C(49)-H(49)	119.1
C(24)-C(25)-C(26)	117.0(2)	C(45)-C(50)-C(49)	118.7(3)
C(24)-C(25)-C(29)	121.6(3)	C(45)-C(50)-H(50)	120.6
C(26)-C(25)-C(29)	121.3(3)	C(49)-C(50)-H(50)	120.6
C(27)-C(26)-C(25)	122.3(2)	C(48)-C(51)-H(51A)	109.5
C(27)-C(26)-H(26)	118.9	C(48)-C(51)-H(51B)	109.5
C(25)-C(26)-H(26)	118.9	H(51A)-C(51)-H(51B)	109.5
C(26)-C(27)-C(22)	121.0(2)	C(48)-C(51)-H(51C)	109.5
C(26)-C(27)-C(30)	116.5(2)	H(51A)-C(51)-H(51C)	109.5
C(22)-C(27)-C(30)	122.5(2)	H(51B)-C(51)-H(51C)	109.5
C(23)-C(28)-H(28A)	109.5	C(53)-C(52)-C(57)	116.5(2)
C(23)-C(28)-H(28B)	109.5	C(53)-C(52)-B(2)	124.2(2)
H(28A)-C(28)-H(28B)	109.5	C(57)-C(52)-B(2)	119.3(2)
C(23)-C(28)-H(28C)	109.5	C(54)-C(53)-C(52)	120.5(2)
H(28A)-C(28)-H(28C)	109.5	C(54)-C(53)-C(58)	116.2(2)
H(28B)-C(28)-H(28C)	109.5	C(52)-C(53)-C(58)	123.3(2)
C(25)-C(29)-H(29A)	109.5	C(55)-C(54)-C(53)	122.7(3)
C(25)-C(29)-H(29B)	109.5	C(55)-C(54)-H(54)	118.7
H(29A)-C(29)-H(29B)	109.5	C(53)-C(54)-H(54)	118.7
C(25)-C(29)-H(29C)	109.5	C(54)-C(55)-C(56)	117.3(3)
H(29A)-C(29)-H(29C)	109.5	C(54)-C(55)-C(59)	121.3(3)
H(29B)-C(29)-H(29C)	109.5	C(56)-C(55)-C(59)	121.5(3)
C(27)-C(30)-H(30A)	109.5	C(55)-C(56)-C(57)	121.9(2)
C(27)-C(30)-H(30B)	109.5	C(55)-C(56)-H(56)	119.0
H(30A)-C(30)-H(30B)	109.5	C(57)-C(56)-H(56)	119.0
C(27)-C(30)-H(30C)	109.5	C(56)-C(57)-C(52)	121.0(2)
H(30A)-C(30)-H(30C)	109.5	C(56)-C(57)-C(60)	116.7(2)
H(30B)-C(30)-H(30C)	109.5	C(52)-C(57)-C(60)	122.4(2)
C(42)#2-C(40)-C(41)	116.2(2)	C(53)-C(58)-H(58A)	109.5
C(42)#2-C(40)-B(2)	130.5(2)	C(53)-C(58)-H(58B)	109.5
C(41)-C(40)-B(2)	113.1(2)	H(58A)-C(58)-H(58B)	109.5
C(42)-C(41)-C(40)	124.4(2)	C(53)-C(58)-H(58C)	109.5
C(42)-C(41)-C(43)	126.9(2)	H(58A)-C(58)-H(58C)	109.5
C(40)-C(41)-C(43)	108.6(2)	H(58B)-C(58)-H(58C)	109.5
C(40)#2-C(42)-C(41)	119.4(2)	C(55)-C(59)-H(59A)	109.5
C(40)#2-C(42)-H(42)	120.3	C(55)-C(59)-H(59B)	109.5
C(41)-C(42)-H(42)	120.3	H(59A)-C(59)-H(59B)	109.5
N(4)-C(43)-C(44)	106.4(2)	C(55)-C(59)-H(59C)	109.5
N(4)-C(43)-C(41)	110.9(2)	H(59A)-C(59)-H(59C)	109.5
C(44)-C(43)-C(41)	142.7(2)	H(59B)-C(59)-H(59C)	109.5
N(6)-C(44)-C(43)	104.9(2)	C(57)-C(60)-H(60A)	109.5
N(6)-C(44)-H(44)	127.6	C(57)-C(60)-H(60B)	109.5
C(43)-C(44)-H(44)	127.6	H(60A)-C(60)-H(60B)	109.5
C(50)-C(45)-C(46)	122.2(3)	C(57)-C(60)-H(60C)	109.5
C(50)-C(45)-N(6)	118.5(2)	H(60A)-C(60)-H(60C)	109.5
C(46)-C(45)-N(6)	119.2(3)	H(60B)-C(60)-H(60C)	109.5
C(47)-C(46)-C(45)	117.9(3)	C(66)-C(61)-C(62)	116.4(3)
C(47)-C(46)-H(46)	121.0	C(66)-C(61)-B(2)	124.9(3)
C(45)-C(46)-H(46)	121.0	C(62)-C(61)-B(2)	118.2(2)

C(63)-C(62)-C(61)	120.4(3)
C(63)-C(62)-C(67)	115.9(3)
C(61)-C(62)-C(67)	123.7(2)
C(64)-C(63)-C(62)	122.8(3)
C(64)-C(63)-H(63)	118.6
C(62)-C(63)-H(63)	118.6
C(63)-C(64)-C(65)	117.1(3)
C(63)-C(64)-C(68)	121.2(4)
C(65)-C(64)-C(68)	121.7(4)
C(64)-C(65)-C(66)	122.4(3)
C(64)-C(65)-H(65)	118.8
C(66)-C(65)-H(65)	118.8
C(65)-C(66)-C(61)	120.8(3)
C(65)-C(66)-C(69)	116.6(3)
C(61)-C(66)-C(69)	122.6(3)
C(62)-C(67)-H(67A)	109.5
C(62)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
0C(62)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(64)-C(68)-H(68A)	109.5
C(64)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(64)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(66)-C(69)-H(69A)	109.5
C(66)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(66)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5

C(22)-B(1)-C(13)	116.4(2)
C(22)-B(1)-C(1)	121.6(2)
C(13)-B(1)-C(1)	104.25(19)
C(22)-B(1)-N(1)	102.47(18)
C(13)-B(1)-N(1)	117.1(2)
C(1)-B(1)-N(1)	93.44(18)
C(61)-B(2)-C(52)	115.4(2)
C(61)-B(2)-C(40)	105.3(2)
C(52)-B(2)-C(40)	121.7(2)
C(61)-B(2)-N(4)	117.2(2)
C(52)-B(2)-N(4)	102.4(2)
C(40)-B(2)-N(4)	93.48(19)
N(2)-N(1)-C(4)	111.9(2)
N(2)-N(1)-B(1)	134.43(19)
C(4)-N(1)-B(1)	113.04(19)
N(1)-N(2)-N(3)	104.42(19)
N(2)-N(3)-C(5)	112.3(2)
N(2)-N(3)-C(6)	121.0(2)
C(5)-N(3)-C(6)	126.7(2)
N(5)-N(4)-C(43)	112.0(2)
N(5)-N(4)-B(2)	133.9(2)
C(43)-N(4)-B(2)	113.3(2)
N(4)-N(5)-N(6)	104.35(19)
N(5)-N(6)-C(44)	112.4(2)
N(5)-N(6)-C(45)	119.5(2)
C(44)-N(6)-C(45)	128.0(2)
Cl(1)-C(31)-Cl(2)	115.0(8)
Cl(1)-C(31)-H(31A)	108.5
Cl(2)-C(31)-H(31A)	108.5
Cl(1)-C(31)-H(31B)	108.5
Cl(2)-C(31)-H(31B)	108.5
H(31A)-C(31)-H(31B)	107.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+1; #2 -x+1,-y,-z+1

Table S8. Anisotropic displacement parameters ($Å^2$x 10^3) for Trz-Me. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	30(1)	29(1)	-9(1)	-6(1)	-2(1)
C(2)	36(1)	28(1)	30(1)	-8(1)	-8(1)	-1(1)
C(3)	38(1)	30(1)	30(1)	-10(1)	-7(1)	1(1)
C(4)	42(1)	30(1)	28(1)	-8(1)	-7(1)	0(1)
C(5)	52(2)	29(1)	29(1)	-8(1)	-5(1)	2(1)
C(6)	47(2)	27(1)	35(1)	-7(1)	-6(1)	3(1)
C(7)	61(2)	40(2)	41(2)	-3(1)	9(1)	13(1)
C(8)	72(2)	39(2)	45(2)	5(1)	13(2)	8(1)
C(9)	59(2)	33(1)	51(2)	-5(1)	-1(1)	8(1)
C(10)	52(2)	36(1)	55(2)	-10(1)	5(1)	6(1)
C(11)	51(2)	32(1)	41(1)	-8(1)	5(1)	0(1)
C(12)	77(2)	39(2)	70(2)	2(2)	10(2)	15(2)
C(13)	37(1)	36(1)	28(1)	-7(1)	-7(1)	0(1)
C(14)	40(1)	42(1)	30(1)	-9(1)	-8(1)	7(1)
C(15)	48(2)	57(2)	41(2)	-15(1)	-8(1)	16(1)
C(16)	37(2)	77(2)	44(2)	-14(2)	-8(1)	7(1)
C(17)	38(2)	67(2)	43(2)	-10(1)	-9(1)	-8(1)
C(18)	40(1)	50(2)	36(1)	-9(1)	-9(1)	-4(1)
C(19)	51(2)	34(1)	44(2)	-15(1)	-9(1)	9(1)
C(20)	41(2)	120(4)	71(2)	-30(2)	-7(2)	14(2)
C(21)	50(2)	56(2)	76(2)	-25(2)	-8(2)	-17(2)
C(22)	33(1)	26(1)	29(1)	-10(1)	-5(1)	3(1)
C(23)	36(1)	31(1)	33(1)	-10(1)	-3(1)	2(1)
C(24)	34(1)	34(1)	40(1)	-12(1)	-2(1)	-1(1)
C(25)	40(1)	33(1)	43(1)	-17(1)	-11(1)	3(1)
C(26)	42(1)	33(1)	33(1)	-13(1)	-9(1)	5(1)
C(27)	37(1)	28(1)	31(1)	-9(1)	-5(1)	6(1)
C(28)	43(2)	47(2)	33(1)	-11(1)	1(1)	-13(1)
C(29)	50(2)	51(2)	53(2)	-18(1)	-18(1)	-4(1)
C(30)	41(1)	37(1)	29(1)	-7(1)	-5(1)	1(1)
C(40)	36(1)	31(1)	38(1)	-12(1)	-8(1)	1(1)
C(41)	38(1)	29(1)	37(1)	-10(1)	-7(1)	-2(1)
C(42)	40(1)	30(1)	36(1)	-13(1)	-6(1)	1(1)
C(43)	44(1)	27(1)	37(1)	-11(1)	-9(1)	1(1)
C(44)	55(2)	29(1)	37(1)	-11(1)	-7(1)	1(1)
C(45)	57(2)	31(1)	33(1)	-7(1)	-9(1)	-1(1)
C(46)	88(3)	38(2)	46(2)	-11(1)	-1(2)	8(2)
C(47)	103(3)	34(2)	48(2)	-6(1)	-5(2)	8(2)
C(48)	76(2)	42(2)	36(1)	-7(1)	-10(1)	-10(1)
C(49)	60(2)	48(2)	46(2)	-9(1)	1(1)	2(1)
C(50)	59(2)	37(1)	45(2)	-5(1)	-4(1)	7(1)
C(51)	103(3)	51(2)	42(2)	-6(1)	-5(2)	-15(2)
C(52)	35(1)	30(1)	33(1)	-11(1)	-1(1)	-1(1)
C(53)	38(1)	34(1)	37(1)	-15(1)	-4(1)	1(1)
C(54)	39(1)	42(1)	42(1)	-15(1)	-11(1)	5(1)
C(55)	41(1)	43(2)	47(2)	-19(1)	-8(1)	-3(1)
C(56)	42(1)	32(1)	44(1)	-15(1)	-4(1)	-6(1)
C(57)	36(1)	32(1)	34(1)	-11(1)	-1(1)	-1(1)
C(58)	50(2)	37(1)	58(2)	-19(1)	-22(1)	9(1)
C(59)	65(2)	53(2)	82(2)	-26(2)	-32(2)	-2(2)
C(60)	44(1)	28(1)	41(1)	-11(1)	-6(1)	-1(1)

C(61)	38(1)	26(1)	49(2)	-12(1)	-10(1)	-3(1)
C(62)	40(1)	27(1)	53(2)	-12(1)	1(1)	-6(1)
C(63)	45(2)	37(2)	67(2)	-14(1)	8(1)	-4(1)
C(64)	39(2)	38(2)	87(3)	-7(2)	2(2)	-2(1)
C(65)	40(2)	40(2)	84(2)	-5(2)	-19(2)	-2(1)
C(66)	44(2)	35(1)	64(2)	-13(1)	-17(1)	-3(1)
C(67)	49(2)	41(2)	44(2)	-17(1)	5(1)	-8(1)
C(68)	43(2)	72(3)	128(4)	-7(3)	5(2)	5(2)
C(69)	61(2)	96(3)	75(2)	-39(2)	-39(2)	16(2)
B(1)	37(1)	26(1)	28(1)	-7(1)	-7(1)	0(1)
B(2)	39(2)	29(1)	35(1)	-10(1)	-7(1)	1(1)
N(1)	39(1)	28(1)	28(1)	-7(1)	-7(1)	0(1)
N(2)	44(1)	26(1)	31(1)	-7(1)	-6(1)	3(1)
N(3)	46(1)	26(1)	30(1)	-7(1)	-4(1)	2(1)
N(4)	43(1)	27(1)	36(1)	-10(1)	-8(1)	0(1)
N(5)	50(1)	29(1)	35(1)	-9(1)	-7(1)	-1(1)
N(6)	52(1)	30(1)	33(1)	-9(1)	-6(1)	1(1)
C(31)	107(8)	73(6)	192(13)	-27(7)	-76(9)	-5(6)
Cl(1)	185(4)	114(2)	130(3)	-45(2)	-90(3)	60(2)
Cl(2)	179(5)	191(5)	212(5)	7(4)	-50(4)	-80(4)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Trz-Me.

	x	y	z	U(eq)
H(3)	9441	1222	5731	39
H(5)	8807	3005	4132	45
H(7)	9808	4524	925	64
H(8)	9286	6161	210	73
H(10)	7019	5748	2469	62
H(11)	7542	4131	3211	53
H(12A)	8050	7610	1075	108
H(12B)	7050	7211	973	108
H(12C)	7965	7398	80	108
H(15)	12556	-1245	1732	60
H(17)	13335	1415	1653	61
H(19A)	10336	-1010	1680	64
H(19B)	10221	-1310	2866	64
H(19C)	11039	-1837	2272	64
H(20A)	14448	197	730	118
H(20B)	14235	-924	1457	118
H(20C)	14544	-118	1880	118
H(21A)	12305	2574	1925	89
H(21B)	11424	2145	2833	89
H(21C)	11227	2569	1710	89
H(24)	7128	-912	2751	44
H(26)	8601	676	65	43
H(28A)	7458	-933	4191	63
H(28B)	8146	-102	4217	63
H(28C)	8592	-1161	4211	63
H(29A)	6518	-879	1330	75
H(29B)	7278	-639	302	75
H(29C)	6606	230	545	75
H(30A)	10636	928	460	55
H(30B)	10170	1851	778	55
H(30C)	9870	1648	-147	55
H(42)	5622	-531	3631	42
H(44)	6630	1239	1969	48
H(46)	6170	4541	984	72
H(47)	6943	5518	-599	78
H(49)	8720	3230	-800	66
H(50)	7974	2249	800	61
H(51A)	8967	4741	-2138	103
H(51B)	8606	5729	-1893	103
H(51C)	7934	5226	-2365	103
H(54)	7914	2076	6251	49
H(56)	6818	4796	5010	47
H(58A)	7537	723	5983	69
H(58B)	6969	821	5095	69
H(58C)	6378	611	6207	69
H(59A)	8079	3561	6880	95
H(59B)	7964	4633	6066	95
H(59C)	8809	3889	5830	95
H(60A)	4845	4391	4515	57
H(60B)	5511	4274	3532	57
H(60C)	5755	5108	3952	57

H(63)	2631	3029	6703	64
H(65)	2121	3361	3988	69
H(67A)	4841	3061	6477	68
H(67B)	4834	1906	6606	68
H(67C)	3997	2358	7255	68
H(68A)	884	3000	6349	136
H(68B)	782	3516	5202	136
H(68C)	1125	4155	5792	136
H(69A)	3211	3065	2789	108
H(69B)	4000	2214	3145	108
H(69C)	4306	3359	2741	108
H(31A)	3995	7294	1777	146
H(31B)	3482	6803	1163	146

4.2. B_2-H

Table S10. Crystal data and structure refinement for B_2-H.

Empirical formula	$C_{46}H_{48}B_2$
Formula weight	622.46
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal System	Triclinic
Space group	P-1
Unit cell dimensions	a = 6.9356(5) Å α= 69.417(8)°
	b = 11.2669(9) Å β= 88.074(7)°
	c = 12.5929(13) Å γ = 78.462(6)°
Volume	901.89(14) Å^3
Z	1
Density (calculated)	1.146 Mg/m^3
Absorption coefficient	0.063 mm^{-1}
F(000)	334
Crystal colour and habit	Colorless prism
Crystal size	0.173 x 0.090 x 0.089 mm^3
Theta range for data collection	3.000 to 29.237°
Index ranges	-8 ≤ h ≤ 8, -15 ≤ k ≤ 13, -16 ≤ l ≤ 15
Reflections collected	8238
Independent reflections	4241 [R(int) = 0.0246]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.91812
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4241 / 0 / 223
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0509, wR2 = 0.1188
R indices (all data)	R1 = 0.0667, wR2 = 0.1307
Extinction coefficient	n/a
Largest diff. peak and hole	0.247 and -0.223 e.Å^{-3}

Definitions:

$$R_1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \qquad wR_2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right]}{\sum \left[w\left(F_o^2\right)^2 \right]}} \qquad GooF = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right) \right]}{(n-p)}}$$

n = number of reflections; p = number of parameters

Notes on the refinement of B_2-H.

All hydrogen atoms were placed in calculated positions and refined by using a riding model.

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B_2-H. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(Eq)
C(1)	1433(2)	2998(1)	5546(1)	29(1)
C(2)	2478(2)	2157(1)	5317(1)	22(1)
C(3)	3760(2)	1087(1)	5118(1)	20(1)
C(4)	4376(2)	1147(1)	4022(1)	21(1)
C(5)	5603(2)	38(1)	3943(1)	21(1)
C(6)	3564(2)	3785(1)	2874(1)	20(1)
C(7)	4973(2)	4149(1)	3417(1)	23(1)
C(8)	4726(2)	5420(1)	3392(1)	26(1)
C(9)	3103(2)	6355(1)	2854(1)	26(1)
C(10)	1724(2)	6002(1)	2316(1)	26(1)
C(11)	1923(2)	4755(1)	2297(1)	22(1)
C(12)	6818(2)	3216(2)	4010(1)	33(1)
C(13)	2847(3)	7723(2)	2834(2)	36(1)
C(14)	346(2)	4502(2)	1661(1)	33(1)
C(15)	3509(2)	2062(1)	1786(1)	20(1)
C(16)	4649(2)	2510(1)	829(1)	23(1)
C(17)	4361(2)	2233(1)	-141(1)	26(1)
C(18)	2968(2)	1534(1)	-212(1)	27(1)
C(19)	1828(2)	1115(1)	724(1)	26(1)
C(20)	2092(2)	1350(1)	1718(1)	23(1)
C(21)	6240(2)	3249(2)	842(1)	32(1)
C(22)	2744(3)	1203(2)	-1259(1)	36(1)
C(23)	791(2)	858(2)	2699(1)	30(1)
B(1)	3793(2)	2362(2)	2894(1)	20(1)

Table S12. Bond lengths [Å] and angles [°] for B_2-H.

C(1)-C(2)	1.186(2)	C(9)-C(8)-C(7)	121.80(14)
C(1)-H(1)	0.9500	C(9)-C(8)-H(8)	119.1
C(2)-C(3)	1.4409(19)	C(7)-C(8)-H(8)	119.1
C(3)-C(5)#1	1.4000(18)	C(8)-C(9)-C(10)	117.84(13)
C(3)-C(4)	1.4136(19)	C(8)-C(9)-C(13)	121.44(15)
C(4)-C(5)	1.3964(18)	C(10)-C(9)-C(13)	120.71(14)
C(4)-B(1)	1.5819(19)	C(9)-C(10)-C(11)	122.55(13)
C(5)-C(3)#1	1.3999(18)	C(9)-C(10)-H(10)	118.7
C(5)-H(5)	0.9500	C(11)-C(10)-H(10)	118.7
C(6)-C(7)	1.411(2)	C(10)-C(11)-C(6)	119.60(14)
C(6)-C(11)	1.4205(19)	C(10)-C(11)-C(14)	117.40(13)
C(6)-B(1)	1.571(2)	C(6)-C(11)-C(14)	123.00(12)
C(7)-C(8)	1.397(2)	C(7)-C(12)-H(12A)	109.5
C(7)-C(12)	1.508(2)	C(7)-C(12)-H(12B)	109.5
C(8)-C(9)	1.382(2)	H(12A)-C(12)-H(12B)	109.5
C(8)-H(8)	0.9500	C(7)-C(12)-H(12C)	109.5
C(9)-C(10)	1.385(2)	H(12A)-C(12)-H(12C)	109.5
C(9)-C(13)	1.507(2)	H(12B)-C(12)-H(12C)	109.5
C(10)-C(11)	1.3921(19)	C(9)-C(13)-H(13A)	109.5
C(10)-H(10)	0.9500	C(9)-C(13)-H(13B)	109.5
C(11)-C(14)	1.504(2)	H(13A)-C(13)-H(13B)	109.5
C(12)-H(12A)	0.9800	C(9)-C(13)-H(13C)	109.5
C(12)-H(12B)	0.9800	H(13A)-C(13)-H(13C)	109.5
C(12)-H(12C)	0.9800	H(13B)-C(13)-H(13C)	109.5
C(13)-H(13A)	0.9800	C(11)-C(14)-H(14A)	109.5
C(13)-H(13B)	0.9800	C(11)-C(14)-H(14B)	109.5
C(13)-H(13C)	0.9800	H(14A)-C(14)-H(14B)	109.5
C(14)-H(14A)	0.9800	C(11)-C(14)-H(14C)	109.5
C(14)-H(14B)	0.9800	H(14A)-C(14)-H(14C)	109.5
C(14)-H(14C)	0.9800	H(14B)-C(14)-H(14C)	109.5
C(15)-C(20)	1.409(2)	C(20)-C(15)-C(16)	118.21(13)
C(15)-C(16)	1.4139(19)	C(20)-C(15)-B(1)	120.69(12)
C(15)-B(1)	1.574(2)	C(16)-C(15)-B(1)	121.10(13)
C(16)-C(17)	1.393(2)	C(17)-C(16)-C(15)	119.81(14)

C(16)-C(21)	1.513(2)	C(17)-C(16)-C(21)	118.56(13)
C(17)-C(18)	1.386(2)	C(15)-C(16)-C(21)	121.59(13)
C(17)-H(17)	0.9500	C(18)-C(17)-C(16)	122.18(14)
C(18)-C(19)	1.390(2)	C(18)-C(17)-H(17)	118.9
C(18)-C(22)	1.511(2)	C(16)-C(17)-H(17)	118.9
C(19)-C(20)	1.392(2)	C(17)-C(18)-C(19)	117.78(13)
C(19)-H(19)	0.9500	C(17)-C(18)-C(22)	121.00(14
C(20)-C(23)	1.514(2)	C(19)-C(18)-C(22)	121.20(15)
C(21)-H(21A)	0.9800	C(18)-C(19)-C(20)	121.90(14)
C(21)-H(21B)	0.9800	C(18)-C(19)-H(19)	119.1
C(21)-H(21C)	0.9800	C(20)-C(19)-H(19)	119.1
C(22)-H(22A)	0.9800	C(19)-C(20)-C(15)	120.10(13)
C(22)-H(22B)	0.9800	C(19)-C(20)-C(23)	118.55(14)
C(22)-H(22C)	0.9800	C(15)-C(20)-C(23)	121.32(13)
C(23)-H(23A)	0.9800	C(16)-C(21)-H(21A)	109.5
C(23)-H(23B)	0.9800	C(16)-C(21)-H(21B)	109.5
C(23)-H(23C)	0.9800	H(21A)-C(21)-H(21B)	109.5
		C(16)-C(21)-H(21C)	109.5
C(2)-C(1)-H(1)	180.0	H(21A)-C(21)-H(21C)	109.5
C(1)-C(2)-C(3)	176.28(15)	H(21B)-C(21)-H(21C)	109.5
C(5)#1-C(3)-C(4)	120.10(12)	C(18)-C(22)-H(22A)	109.5
C(5)#1-C(3)-C(2)	117.58(12)	C(18)-C(22)-H(22B)	109.5
C(4)-C(3)-C(2)	122.31(12)	H(22A)-C(22)-H(22B)	109.5
C(5)-C(4)-C(3)	116.60(12)	C(18)-C(22)-H(22C)	109.5
C(5)-C(4)-B(1)	118.15(12)	H(22A)-C(22)-H(22C)	109.5
C(3)-C(4)-B(1)	125.24(12)	H(22B)-C(22)-H(22C)	109.5
C(4)-C(5)-C(3)#1	123.29(12)	C(20)-C(23)-H(23A)	109.5
C(4)-C(5)-H(5)	118.4	C(20)-C(23)-H(23B)	109.5
C(3)#1-C(5)-H(5)	118.4	H(23A)-C(23)-H(23B)	109.5
C(7)-C(6)-C(11)	117.74(12)	C(20)-C(23)-H(23C)	109.5
C(7)-C(6)-B(1)	121.61(12)	H(23A)-C(23)-H(23C)	109.5
C(11)-C(6)-B(1)	120.64(13)	H(23B)-C(23)-H(23C)	109.5
C(8)-C(7)-C(6)	120.43(13)	C(6)-B(1)-C(15)	121.79(11)
C(8)-C(7)-C(12)	117.17(14)	C(6)-B(1)-C(4)	122.04(12)
C(6)-C(7)-C(12)	122.38(13)	C(15)-B(1)-C(4)	116.15(12)

Table S13. Anisotropic displacement parameters ($Å^2$x 10^3) for B_2-H. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	31(1)	27(1)	27(1)	-11(1)	3(1)	0(1)
C(2)	26(1)	20(1)	18(1)	-5(1)	0(1)	-3(1)
C(3)	22(1)	19(1)	20(1)	-8(1)	-1(1)	-2(1)
C(4)	24(1)	19(1)	19(1)	-7(1)	-1(1)	-3(1)
C(5)	26(1)	21(1)	16(1)	-7(1)	1(1)	-3(1)
C(6)	26(1)	18(1)	14(1)	-4(1)	1(1)	-4(1)
C(7)	25(1)	25(1)	18(1)	-7(1)	2(1)	-5(1)
C(8)	31(1)	30(1)	24(1)	-13(1)	2(1)	-12(1)
C(9)	36(1)	21(1)	23(1)	-10(1)	9(1)	-8(1)
C(10)	29(1)	20(1)	24(1)	-6(1)	2(1)	0(1)
C(11)	27(1)	19(1)	17(1)	-5(1)	0(1)	-2(1)
C(12)	29(1)	34(1)	34(1)	-11(1)	-7(1)	-5(1)
C(13)	50(1)	24(1)	40(1)	-16(1)	10(1)	-10(1)
C(14)	34(1)	25(1)	37(1)	-10(1)	-13(1)	2(1)
C(15)	25(1)	16(1)	18(1)	-5(1)	-2(1)	0(1)
C(16)	26(1)	20(1)	19(1)	-4(1)	-2(1)	-1(1)
C(17)	30(1)	28(1)	17(1)	-6(1)	2(1)	-2(1)
C(18)	30(1)	26(1)	22(1)	-10(1)	-6(1)	3(1)
C(19)	27(1)	23(1)	29(1)	-11(1)	-5(1)	-3(1)
C(20)	27(1)	18(1)	23(1)	-7(1)	-1(1)	-1(1)
C(21)	34(1)	37(1)	26(1)	-9(1)	4(1)	-14(1)
C(22)	40(1)	41(1)	28(1)	-18(1)	-7(1)	0(1)
C(23)	33(1)	28(1)	32(1)	-12(1)	5(1)	-9(1)
B(1)	18(1)	22(1)	20(1)	-7(1)	2(1)	-2(1)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for B^2-H.

	x	y	z	U(eq)
H(1)	597	3671	5728	35
H(5)	6026	48	3215	25
H(8)	5700	5647	3754	32
H(10)	599	6634	1946	31
H(12A)	7830	3701	4038	49
H(12B)	7297	2633	3594	49
H(12C)	6525	2709	4785	49
H(13A)	2694	8324	2046	55
H(13B)	4007	7814	3199	55
H(13C)	1672	7922	3244	55
H(14A)	-729	5264	1417	49
H(14B)	-163	3753	2158	49
H(14C)	901	4323	994	49
H(17)	5146	2532	-775	32
H(19)	841	655	684	31
H(21A)	6818	3510	95	48
H(21B)	7266	2695	1418	48
H(21C)	5667	4021	1023	48
H(22A)	2859	1949	-1938	53
H(22B)	1450	985	-1277	53
H(22C)	3777	461	-1240	53
H(23A)	-310	594	2434	45
H(23B)	279	1548	3000	45
H(23C)	1562	115	3298	45

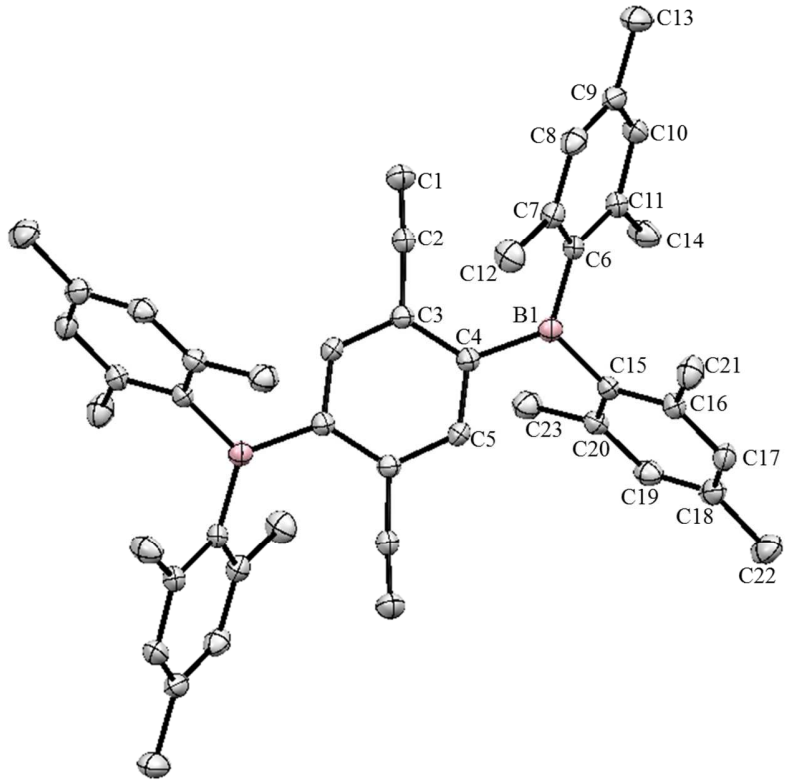


Figure S49. Crystal structure of 1,4-Diethynyl-2,5-bis(dimesitylboryl)benzene (B_2-H). Hydrogen atoms have been omitted for clarity

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