BN-Doped Diphenylacetylene: A Basic Model for Conjugated Pi-Systems Containing the BN Bond Pair

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Electronic Supplementary Information

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General

All oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box.

THF, Et_2O, CH_2Cl_2, and pentane were purified by passing through a neutral alumina column under argon. Cyclohexene was dried over CaH_2 and distilled under N_2 prior to use.

Trisacetonitrile(tricarbonyl)chromium(0) was purchased from Acros or Aldrich and used as received. 1,2-Azaborine precursor **3** was prepared according to literature procedures.[1] All other chemicals and solvents were purchased (Aldrich or Strem) and used as received.

Silica gel (230-400 mesh) was heated under vacuum in a 200 °C sand bath for 12 hours. Flash chromatography was performed with this silica gel under an inert atmosphere.

^{11}B NMR spectra were recorded on a Varian Unity/Inova 600 spectrometer at ambient temperature. ^{1}H NMR spectra were recorded on a Varian Unity/Inova 300 or Varian Unity/Inova 600 spectrometer. ^{13}C NMR spectra were recorded on a Varian Unity/Inova 300 or Varian Unity/Inova 500 spectrometer. ^{11}B NMR spectra were externally referenced to $BF_3 \bullet Et_2O$ (δ 0).

IR spectra were recorded on a Nicolet Magna 550 FT-IR instrument with OMNIC software. UV-Vis spectra were recorded on an Agilent 8453 spectrometer with ChemStation software. Fluorescence spectra were recorded on a Hitachi F-4500 Fluorometer. Fluorescence quantum yields were determined using the comparative method[2] and were referenced to naphthalene (Φ_F = 0.21).[3] All quantum yields are reported as the average of three runs at three different concentrations (1.0×10^{-5} M, 5.0×10^{-6} M, and 2.5×10^{-6} M in THF). Emission spectra for the determination of quantum yields were collected using excitation and emission slit widths of 10 nm. Fine structure in the emission spectrum of tolan was observed when using a 2 nm emission slit width; an emission maximum at 303 nm was observed under these conditions and is consistent with reported values for tolan.[4]

High-resolution mass spectroscopy data were obtained at the Mass Spectroscopy Facilities and Services Core of the Environmental Health Sciences Center at Oregon State University. Financial support for this facility has been furnished in part by the National Institute of Environmental Health Sciences, NIH (P30 ES00210).

Synthesis of 1 and 2

Compound 4. 1,2-Azaborine **3** (0.500 g, 2.20 mmol) and Et_2O (20 mL) were combined in a flask and cooled to –10 °C. A solution of phenylethylnylmagnesium bromide (0.7 M in THF; 3.45 mL, 2.42 mmol) was added dropwise with stirring. The mixture was allowed to warm to rt, whereupon approximately one-half of the solvent was removed under reduced pressure. Solids were removed by filtration, and the filtrate was concentrated under reduced pressure. The crude material was purified by column chromatography (Et_2O/pentane) to yield **4** as a white, crystalline solid (0.490 g, 76%).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 7.60 (dd, $^3J_{HH}$ = 11.2, 5.6 Hz, 1H), 7.51 (m, 2H), 7.35 (m, 4H), 6.90 (d, $^3J_{HH}$ = 11.1 Hz, 1H), 6.40 (app t, $^3J_{HH}$ = 6.4 Hz, 1H), 0.95 (s, 9H), 0.63 (s, 6H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 144.0, 139.3, 134 (br), 132.6, 131.9, 128.9, 128.8, 124.7, 112.8, 27.0, 19.6, –1.9. The signal for the boron-bound alkyne carbon was not detected. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 29.3. FTIR (thin film) 3065, 3031, 2956, 2929, 2884, 2858, 2175, 1602, 1504, 1490, 1470, 1452, 1391, 1363, 1274, 1253, 1194, 1126, 1070, 1017, 987, 938, 913, 843, 822, 786, 710, 690, 626 cm^{-1}. HRMS (EI) calcd for $C_{18}H_{24}BNSi$ (M^+) 293.17711, found 293.17778.

Compound 5. A vial was charged with a solution of **4** (0.500 g, 1.70 mmol in 30 mL THF) and $(MeCN)_3Cr(CO)_3$ (0.663 g, 2.56 mmol) and stirred at rt for 1 h. Solvents were removed under reduced pressure. The crude material was purified by column chromatography (CH_2Cl_2/pentane) to provide **5** as a red, crystalline solid (0.667 g, 91%).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 7.52 (m, 2H), 7.37 (m, 3H), 6.03 (dd, $^3J_{HH}$ = 7.9, 5.2 Hz, 2H), 5.23 (app t, $^3J_{HH}$ = 5.8 Hz, 1H), 4.74 (d, $^3J_{HH}$ = 9.7 Hz, 1H), 1.00 (s, 9H), 0.73 (s, 3H), 0.46 (s, 3H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 230.6, 132.1, 129.5, 129.0, 123.6, 108.4, 103.8, 88 (br), 83.4, 27.1, 20.2, –1.1, –3.8. The signal for the boron-bound alkyne carbon was not detected. ^{11}B NMR (96.3 MHz, CD_2Cl_2): δ 14.3. FTIR (CH_2Cl_2) 1971, 1902, 1879 cm^{-1}. HRMS (EI) calcd for $C_{21}H_{24}BNSiCrO_3$ (M^+) 429.10237, found 429.10066.

Compound 6. A vial was charged with a solution of **5** (0.667 g, 1.55 mmol in 10 mL THF) and cooled to –20 °C. A solution of HF-pyridine (0.5 M in THF; 3.1 mL, 1.55 mmol) was added dropwise. The reaction was allowed to warm to rt and stirred for 10 min. Solvents were removed under reduced pressure. The resulting crude material was purified by column chromatography (CH_2Cl_2/pentane) to provide **6** as an orange-red solid (0.416 g, 85%).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 7.52 (m, 2H), 7.34 (m, 3H), 6.15 (app t, $^3J_{HH}$ = 5.3 Hz, 1H), 5.91 (dd, $^3J_{HH}$ = 8.6, 6.2 Hz, 1H), 5.34 (br, 1H), 5.26 (dd, $^3J_{HH}$ = 7.2, 5.0 Hz, 1H), 4.76 (d, $^3J_{HH}$ = 5.5 Hz, 1H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 230.0, 132.6, 129.7, 129.0, 122.9, 107.9, 98.6, 86 (br), 82.1. The alkyne carbon signals were not observed. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 11.7. FTIR (CH_2Cl_2) 3361, 2185, 1976, 1906, 1880 cm^{-1}. HRMS (EI) calcd for $C_{15}H_{10}BNCrO_3$ (M^+) 315.01589, found 315.01578.

Compound 1. Complex **6** (0.383 g, 1.22 mmol) and MeCN (10 mL) were combined in a vial and stirred at rt for 12 h. Approximately two-thirds of the solvent was removed under reduced pressure. Column chromatography (CH_2Cl_2/pentane) provided BN tolan **1** as a white, crystalline solid (0.198 g, 91%).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 8.44 (br, 1H), 7.76 (dd, $^3J_{HH}$ = 10.8, 6.7 Hz, 1H), 7.59 (m, 2H), 7.40 (m, 4H), 7.00 (d, $^3J_{HH}$ = 11.1 Hz, 1H), 6.44 (app t, $^3J_{HH}$ = 6.5 Hz, 1H). ^{13}C NMR (125.8 MHz, CD_2Cl_2): δ 145.1, 134.9, 134.8, 132.4, 132 (br), 129.0, 124.1, 111.9, 104.8, 84 (br). ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 25.8. FTIR (thin film) 3380, 3140, 3075, 3049, 3027, 2178, 1606, 1538, 1487, 1460, 1440, 1421, 1349, 1265, 1235, 1213, 1191, 1126, 1108, 1080, 995, 842, 793, 760, 733, 692, 681 cm^{-1}. HRMS (EI) calcd for $C_{12}H_{10}BN$ (M^+) 179.09063, found 179.09122.

Compound 8. Ethylmagnesium bromide (1.0 M in THF; 1.96 mL, 1.96 mmol) and ethynylmagnesium bromide (0.5 M in THF; 3.91 mL, 1.96 mmol) were combined in a vial and stirred at rt for 30 minutes during which time significant gas evolution was observed. The reaction was stirred for an additional 12 h. This Grignard mixture was then added to a solution of **3** (0.890 g, 3.91 mmol in 10 mL THF) at rt. The reaction was stirred an additional 48 h at rt. At the conclusion of the reaction, the solvent was removed under reduced pressure. The resulting crude material was subjected to column chromatography (CH_2Cl_2/pentane) to yield **8** as a light-yellow solid (0.732 g, 91%).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 7.58 (dd, $^3J_{HH}$ = 11.0, 6.1 Hz, 2H), 7.28 (d, $^3J_{HH}$ = 6.3 Hz, 2H), 6.82 (d, $^3J_{HH}$ = 11.2 Hz, 2H), 6.38 (app t, $^3J_{HH}$ = 6.3, 6.1 Hz, 2H), 0.98 (s, 18H), 0.61 (s, 12H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 143.7, 139.3, 122 (br), 112.5, 27.0, 19.6, –1.8. The signal for the boron-bound alkyne carbon was not detected. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 28.7. FTIR (thin film) 3007, 2927, 2882, 2857, 1875, 1600, 1503, 1467, 1450, 1389, 1364, 1270, 1257, 1216, 1173, 1153, 1097, 989, 938, 842, 822, 810, 739, 705, 694, 634 cm^{-1}. HRMS (EI) calcd for $C_{22}H_{38}B_2N_2Si_2$ (M^+) 408.27597, found 408.27775.

Compound 10. To a stirred solution of **8** (0.732 g, 1.79 mmol in 18 mL THF) was added $(MeCN)_3Cr(CO)_3$ (0.976 g, 3.76 mmol). The reaction was stirred at rt for 1 h. Solvents were removed under reduced pressure. The crude material was subjected to column chromatography (CH_2Cl_2/pentane) to give a mixture of **9** and **10**. The mixture was taken up in THF (15 mL) and additional $(MeCN)_3Cr(CO)_3$ (0.300 g, 1.16 mmol) was added. The reaction was stirred at rt for 1 h. Solvents were removed and the crude material was subjected to column chromatography (CH_2Cl_2/pentane) to ultimately provide **10** as an orange-red, crystalline solid (0.365 g, 30%, single diastereomer).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 5.9-6.0 (m, 4H), 5.19 (app t, $^3J_{HH}$ = 6.1 Hz, 2H), 4.61 (d, $^3J_{HH}$ = 6.2 Hz, 2H), 1.00 (s, 18H), 0.81 (s, 6H), 0.44 (s, 6H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 230.3, 108.0, 103.5, 83.3, 27.2, –0.8, –3.9. The signals for the boron-bound carbons were not detected. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 13.6. FTIR (CH_2Cl_2) 1971, 1899 (br) cm^{-1}.

Compound 11. A solution of complex **10** (0.228 g, 0.335 mmol in 15 mL) was cooled to –20 °C, whereupon HF-pyridine (0.5 M in THF; 1.34 mL, 0.67 mmol) was added dropwise. The reaction was kept at –20 °C for 30 min., then allowed to warm to rt. Solvents were removed under reduced pressure to provide a crude mixture which was used directly in the preparation of **2**.

Compound 2. The crude material containing complex **11** was combined in a vial with MeCN (5 mL) and stirred at rt for 10 min. Solvents were removed under reduced pressure. The resulting crude material was purified by column chromatograpy (Et_2O/pentane) to give **2** as a white, crystalline solid (0.028 g, 47% from **10**).

^{1}H NMR (300 MHz, CH_2Cl_2): δ 8.43 (br, 2H), 7.71 (dd, $^3J_{HH}$ = 10.8, 6.6 Hz, 2H), 7.36 (app t, $^3J_{HH}$ = 7.2 Hz, 2H), 6.89 (d, $^3J_{HH}$ = 11.1 Hz, 2H), 6.40 (app t, $^3J_{HH}$ = 6.5 Hz, 2H?). ^{13}C NMR (125.8 MHz, CD_2Cl_2): δ 145.1, 134.8, 131 (br), 111.8. The signal for the boron-bound alkyne carbon was not detected. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 25.4. FTIR (CH_2Cl_2) 3370, 3091, 3053, 3031, 2978, 1611, 1532, 1464, 1420, 1352, 1223, 1202, 1151, 1082, 998, 852, 740, 677 cm^{-1}. HRMS (EI) calcd for $C_{10}H_{10}B_2N_2$ (M^+) 180.10301, found 180.10330.

Absorption and Emission Spectra for 1 and 2

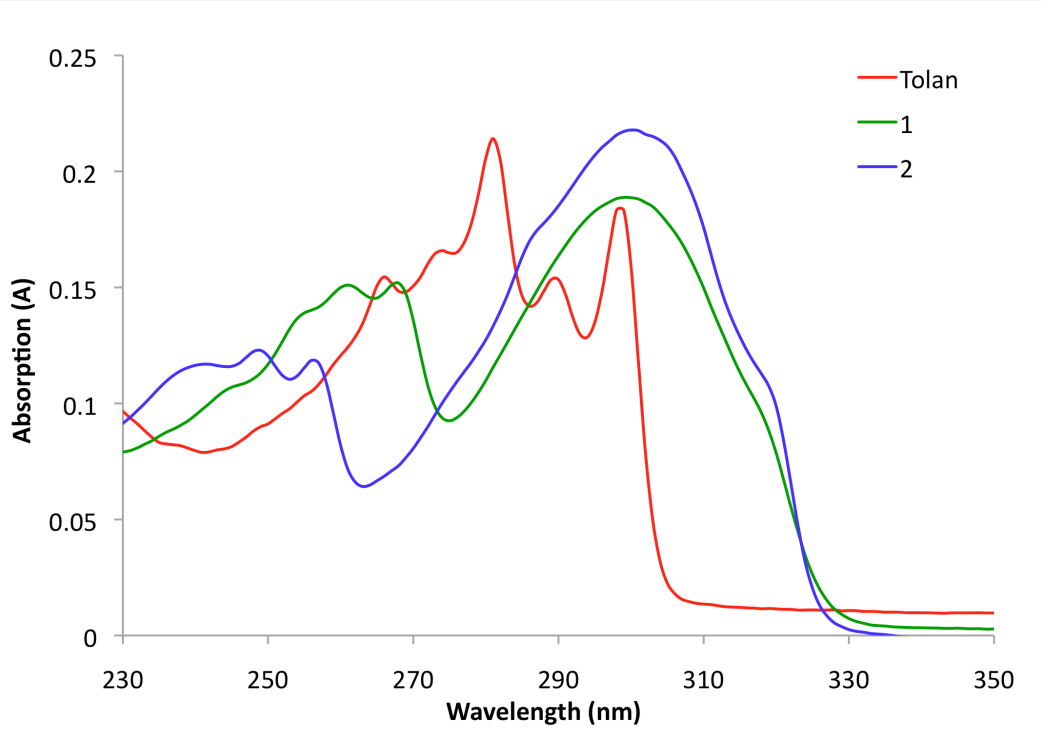


Figure S1. Absorption spectra of **1**, **2**, and tolan (10^{-5} M in THF).

λ_{abs}, Tolan:
281 nm, 21409 $M^{-1}cm^{-1}$
298 nm, 18327 $M^{-1}cm^{-1}$

λ_{abs}, **1**:
261 nm, 15101 $M^{-1}cm^{-1}$
268 nm, 15187 $M^{-1}cm^{-1}$
299 nm, 18880 $M^{-1}cm^{-1}$

λ_{abs}, **2**:
249 nm, 12286 $M^{-1}cm^{-1}$
256 nm, 11857 $M^{-1}cm^{-1}$
300 nm, 21785 $M^{-1}cm^{-1}$

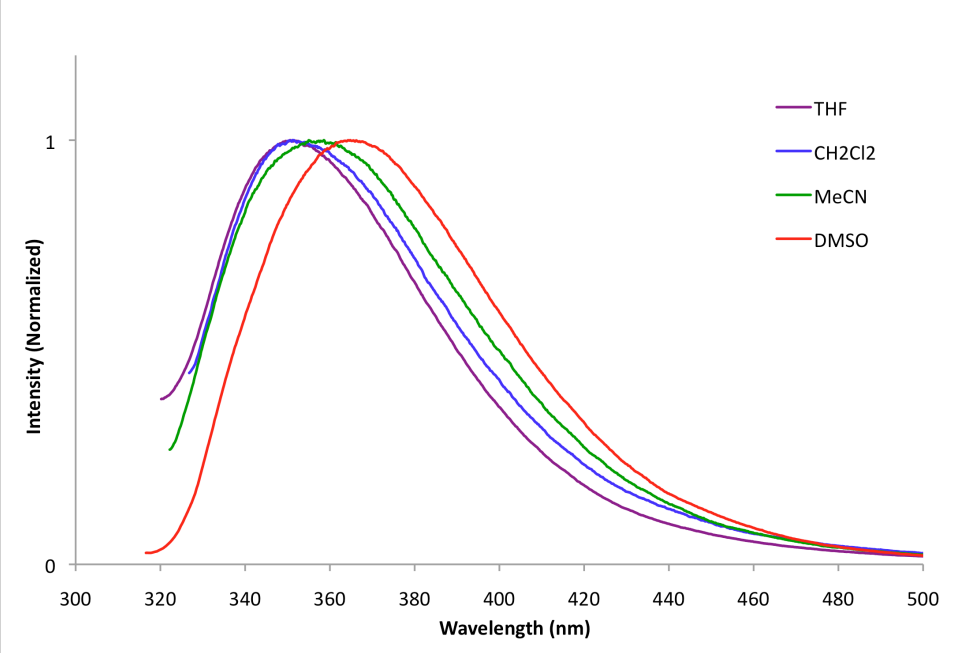


Figure S2. Normalized emission spectra of **1** in various solvents.

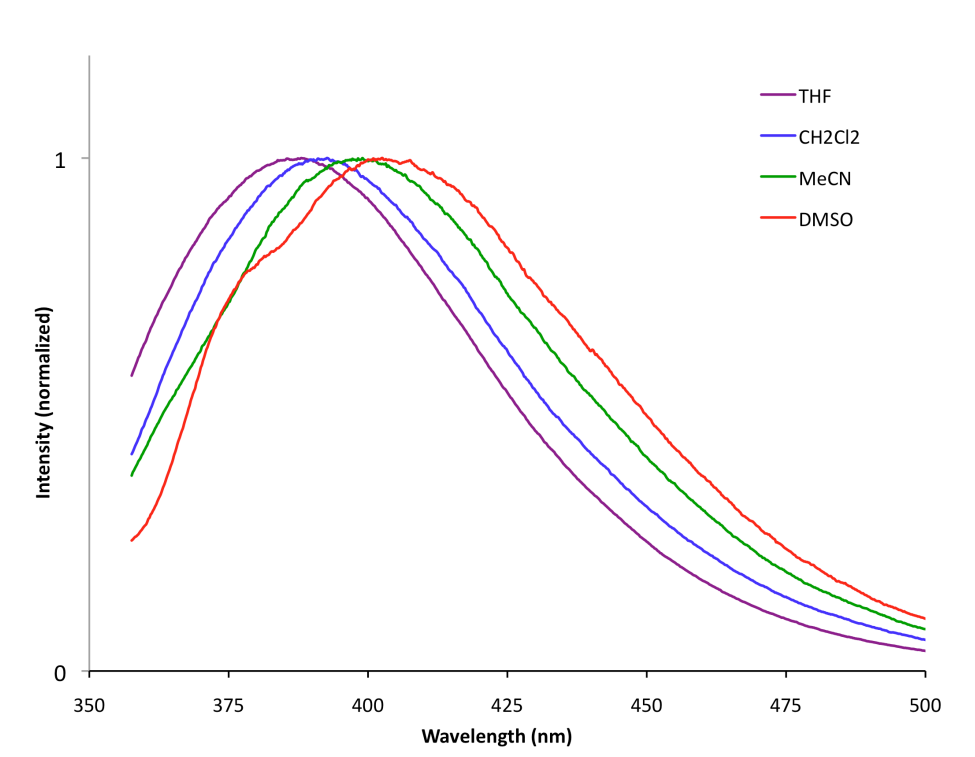
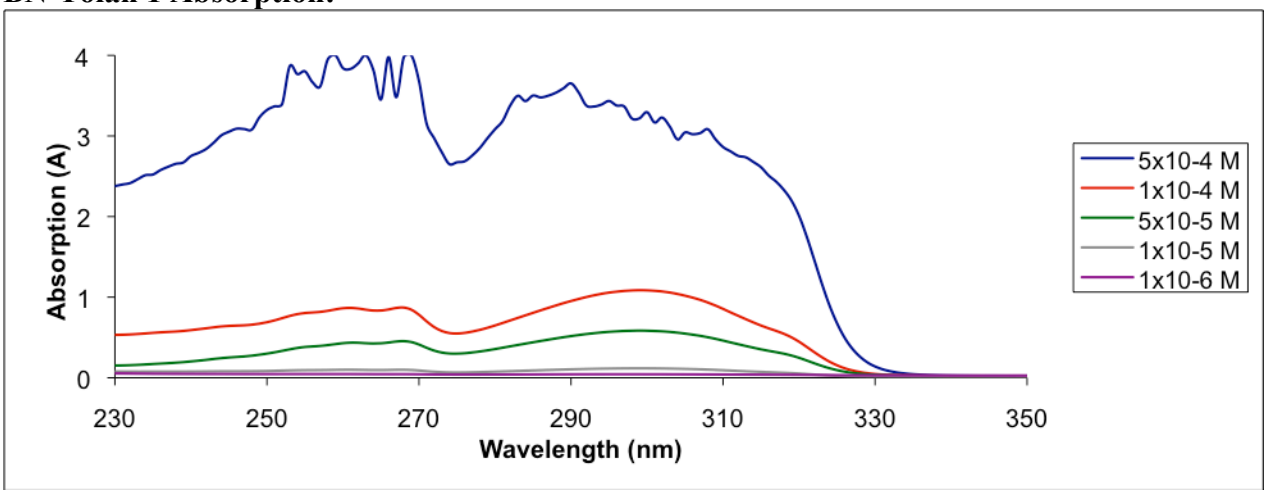


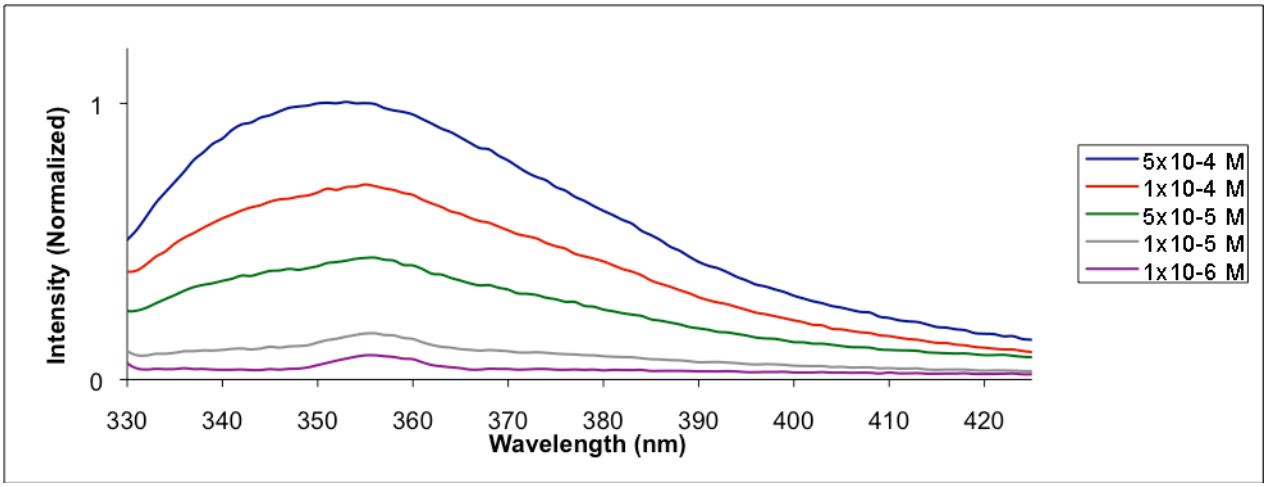
Figure S3. Normalized emission spectra of **2** in various solvents.

Concentration-Dependent Absorption and Emission Spectra

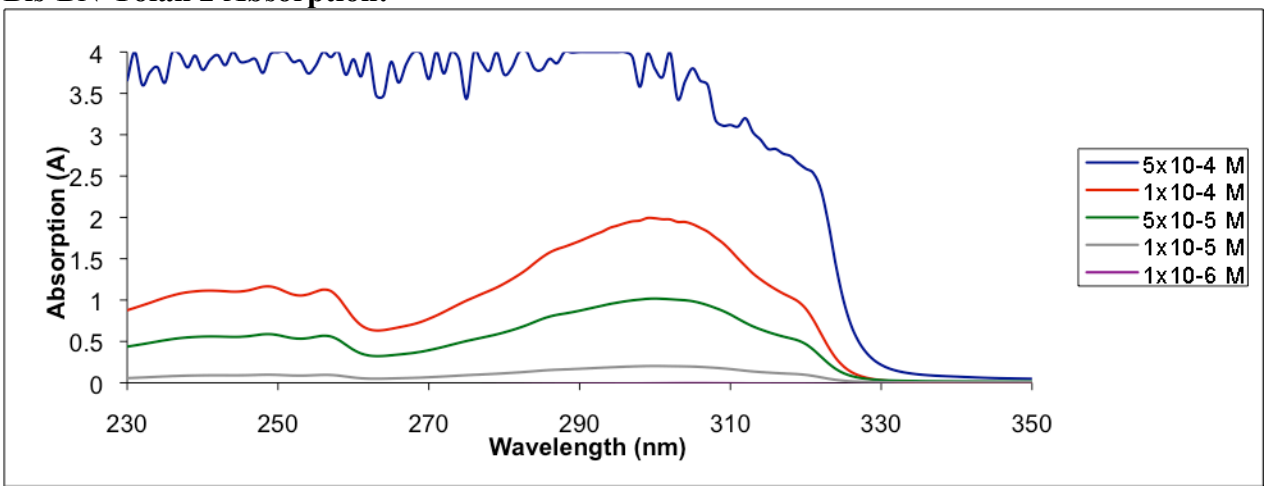
BN-Tolan 1 Absorption:



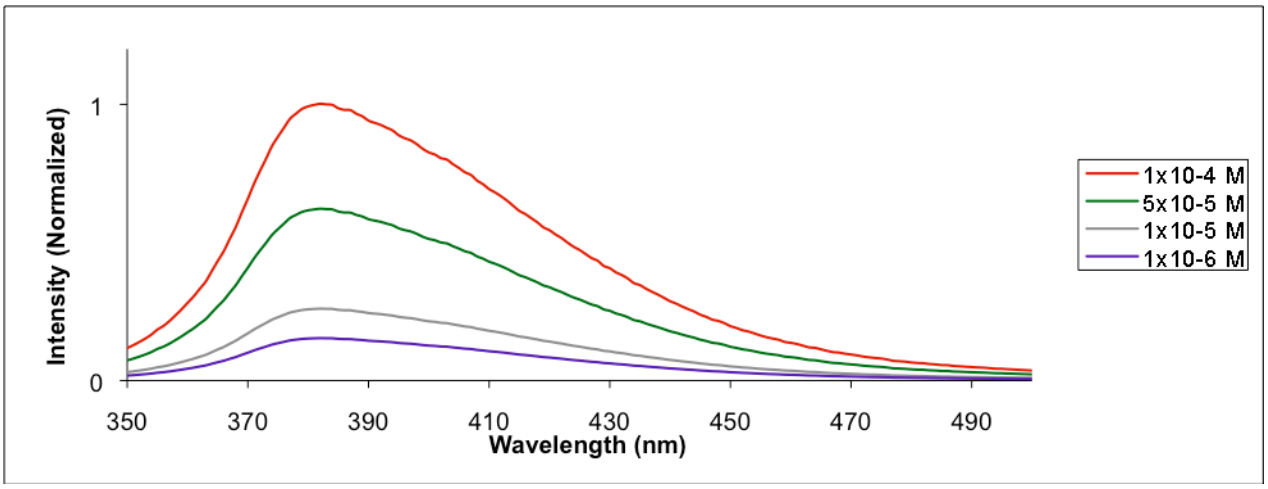
BN-Tolan 1 Emission:



Bis-BN-Tolan 2 Absorption:



Bis-BN-Tolan 2 Emission:



Infrared Spectra for 1,2-Dihydro-1,2-azaborine, 1, and 2 (Thin Film)

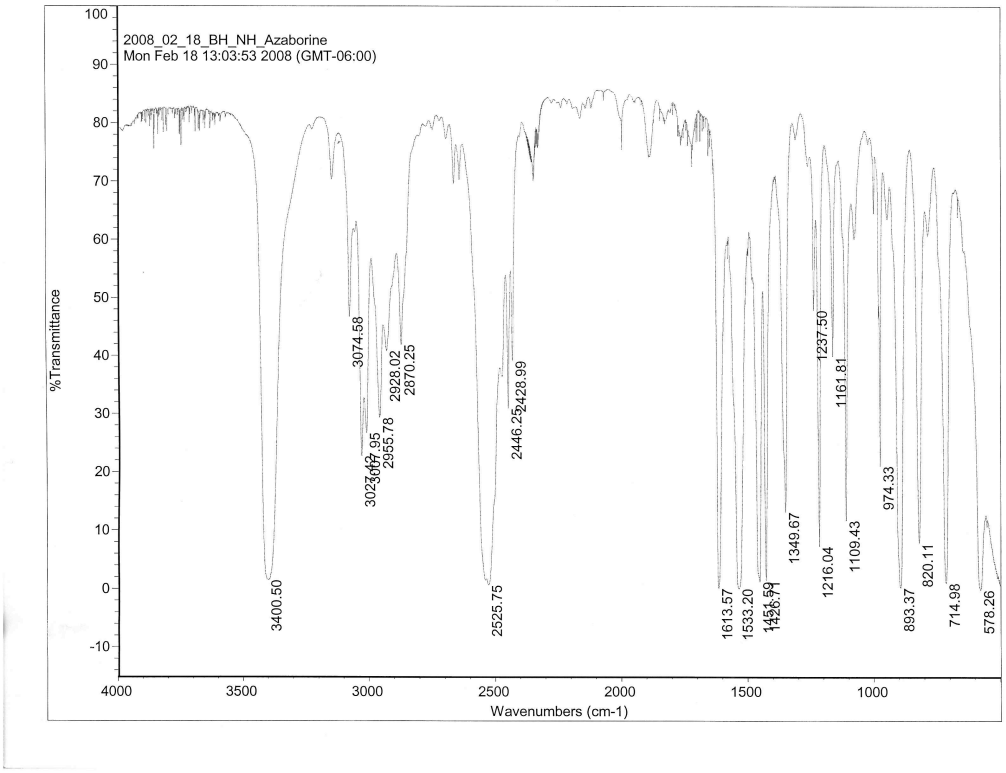


Figure S4. Infrared spectrum of 1,2-dihydro-1,2-azaborine.

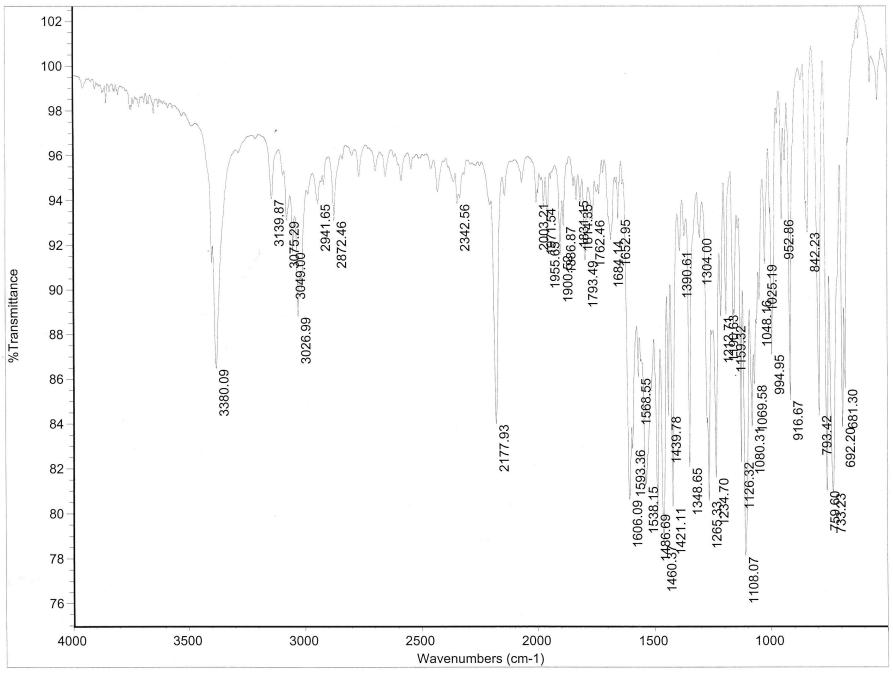


Figure S5. Infrared spectrum of **1**.

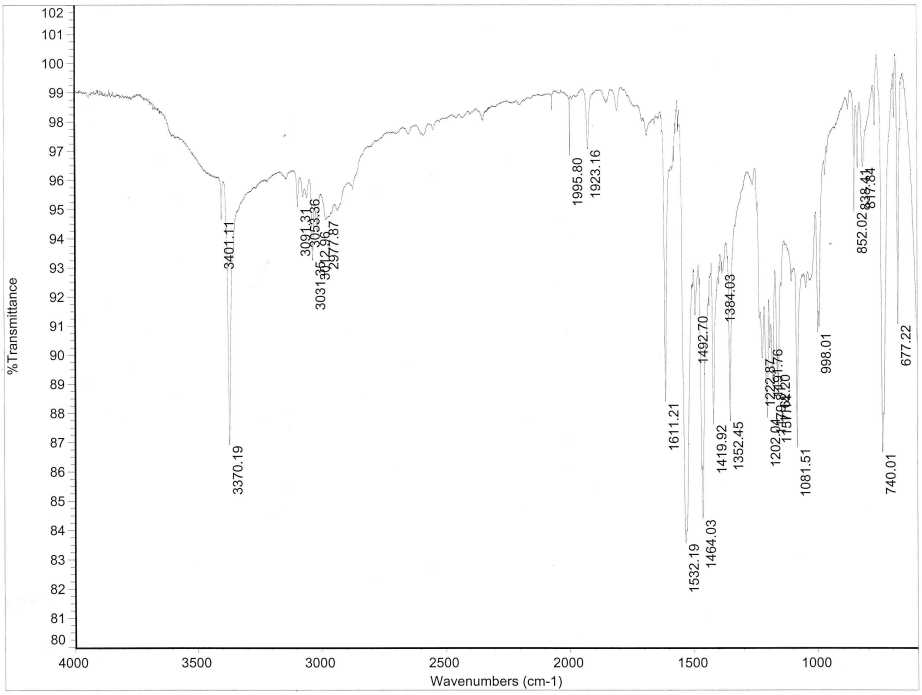
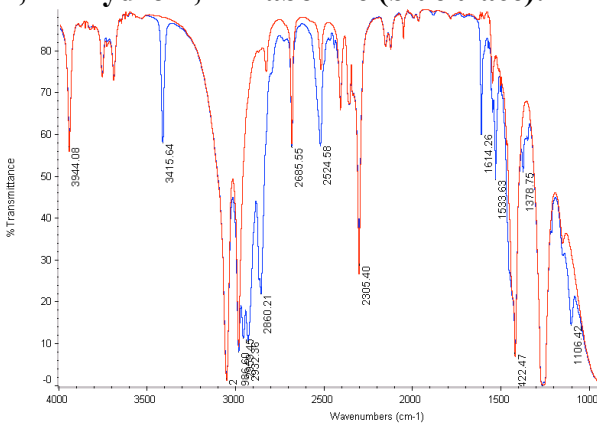


Figure S6. Infrared spectrum of **2**.

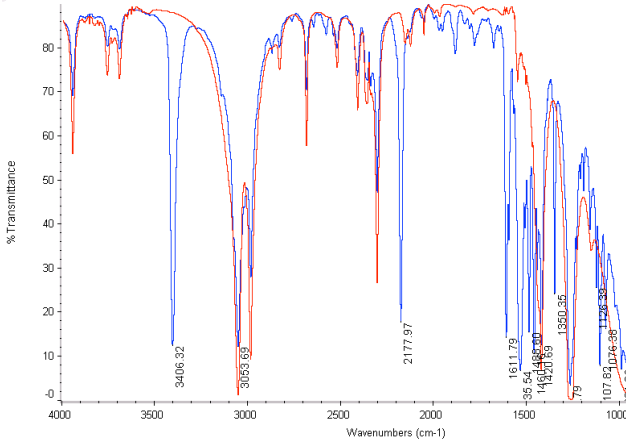
Infrared Spectra for 1,2-Dihydro-1,2-azaborine, 1, and 2 (Solution in CH_2Cl_2)

1,2-Dihydro-1,2-Azaborine (blue trace):



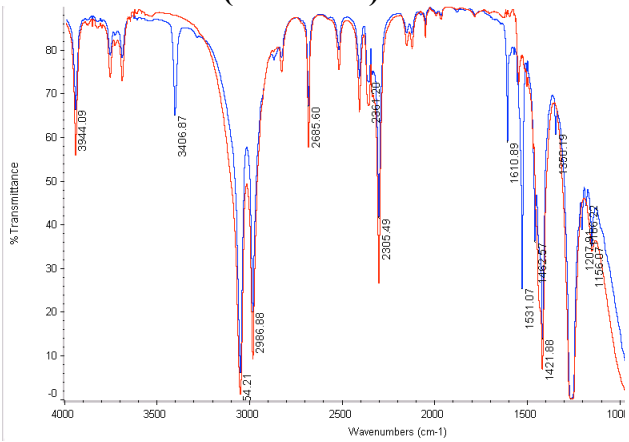
The red trace is the IR spectrum of CH_2Cl_2.

BN-Tolan 1 (blue trace):



The red trace is the IR spectrum of CH_2Cl_2.

Bis-BN-Tolan 2 (blue trace):



The red trace is the IR spectrum of CH_2Cl_2.

Computational Results

The geometries of tolan, **1**, **2**(cis) and **2**(trans) were calculated initially at the density functional theory (DFT) level with the B3LYP hybrid exchange-correlation functional and the DZVP2 basis set. Vibrational frequencies were calculated to show that the structures were minima. The molecules all exhibited the two rings in the same plane. Time-dependent density functional theory at the B3LYP/DZVP2 level was used to calculate the excited states. The calculated excitations were dominated by the HOMO-LUMO transition. The B3LYP/DZVP2 geometries were used as starting points for G3MP2 and G3MP2B3 calculations.

Table ST1. Total Energies of the ground states in a.u.

Compound	B3LYP/DZVP2		G3MP2		G3MP2B3	
	0 K	298 K	0 K	298 K	0 K	298 K
Tolan	-539.361055	-539.348942	-538.525809	-538.513549	-538.550584	-538.538157
1	-542.820098	-542.807613	-541.975253	-541.962486	-541.999869	-541.987070
2 (cis)	-546.277108	-546.265138	-545.422887	-545.410533	-545.447423	-545.435117
2 (trans)	-546.277860	-546.265906	-545.423371	-545.411027	-545.448013	-545.435723

Figure ST1. Perpendicular structure and two views of the parallel dimer structure.

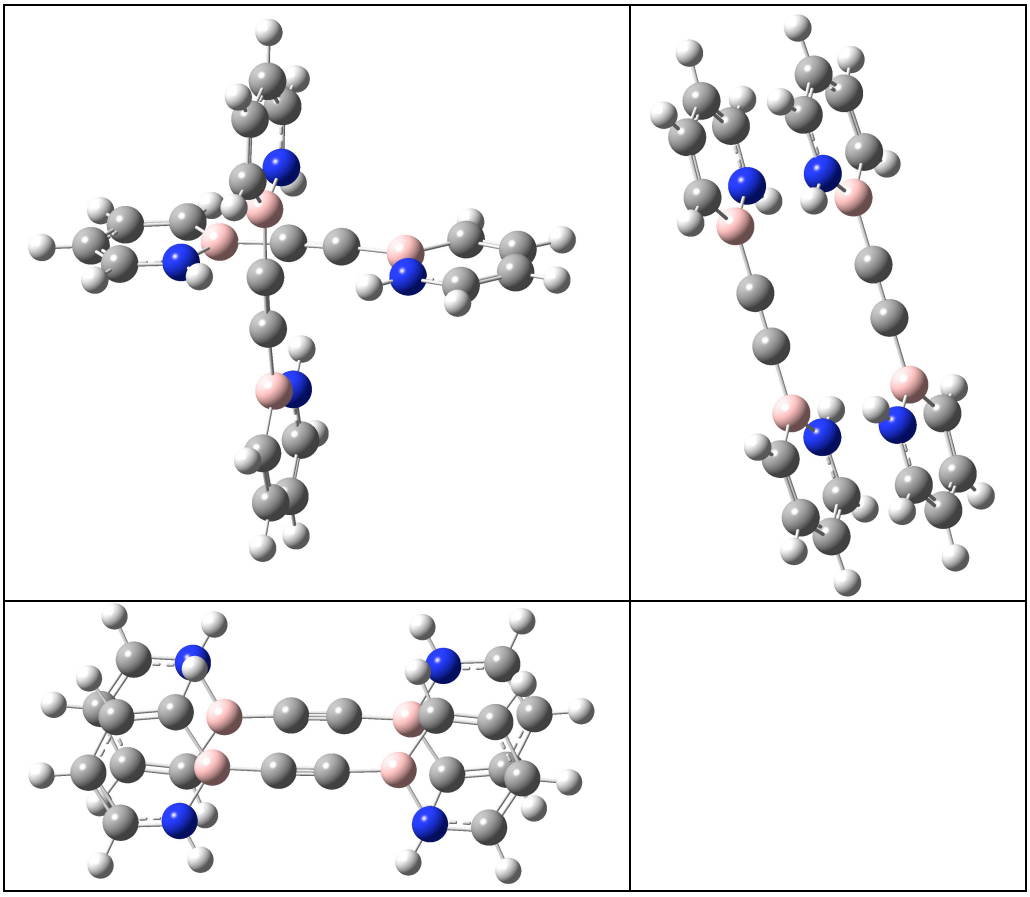


Table ST2. Selected geometry parameters (angstroms and degrees) of the dimer structures at wB97xD/DZVP2 level.

Dimer	r(C≡C)	r(C-B)	r(N-H···π(C≡C)	r(B….B)	∠N-H - π(C≡C)
Perpendicular	1.224	1.547	2.36		164.3
Parallel	1.222	1.539		3.54	

Table ST3. Total Energies of the dimer and monomer structures in a.u.

Dimer	wB97xD/DZVP2			MP2/aug-cc-pvTZ
	ΔH (0 K)	ΔH (298 K)	ΔG (298 K)	E_{elec}
Perpendicular	-1092.165574	-1092.139798	-1092.223133	-1090.452809
Parallel	-1092.149941	-1092.125065	-1092.205481	-1090.439349
Monomer				
2 (cis)	-546.066801	-546.054887	-546.104350	-545.206976

Table ST4. Dimerization energies in kcal/mol.

Dimer	Functional	ΔE_{elec}	ΔH (0 K)	ΔH (298 K)	ΔG (298 K)
Perpendicular	wB97xD	-22.3	-20.1	-18.8	-9.1
	MP2	-24.4	-22.2	-20.9	-11.2
Parallel	wB97xD	-10.6	-10.3	-9.6	2.0
	MP2	-15.9	-15.6	-14.9	-3.3

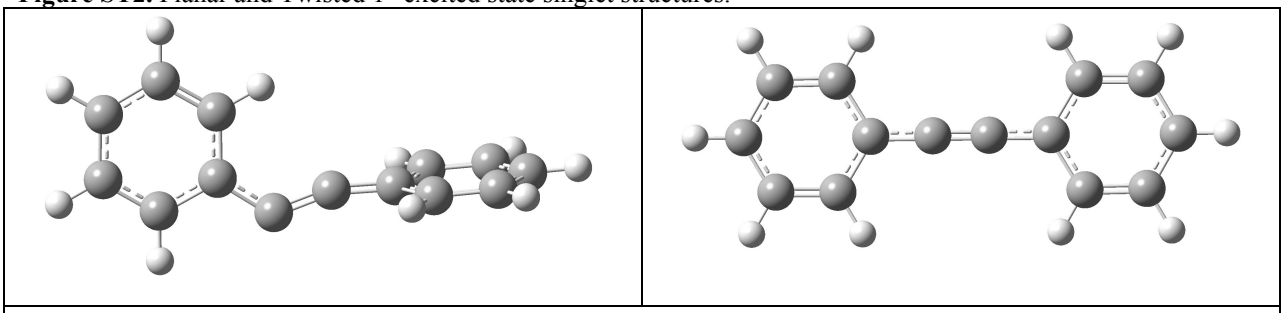
Table ST5. Total Energies of the optimized excited state singlet structures in a.u at the TD-DFT/B3LYP/DZVP2 level.

Compound	Planar singlet		Twisted singlet	
	0 K	298 K	0 K	298 K
Tolan	-539.223489	-539.210844	-539.227302	-539.214922
1	-542.685804	-542.672717	-542.682575	-542.669644
2 (cis)	-546.141155	-546.127638	-546.134824	-546.121477
2 (trans)	-546.141867	-546.128373		

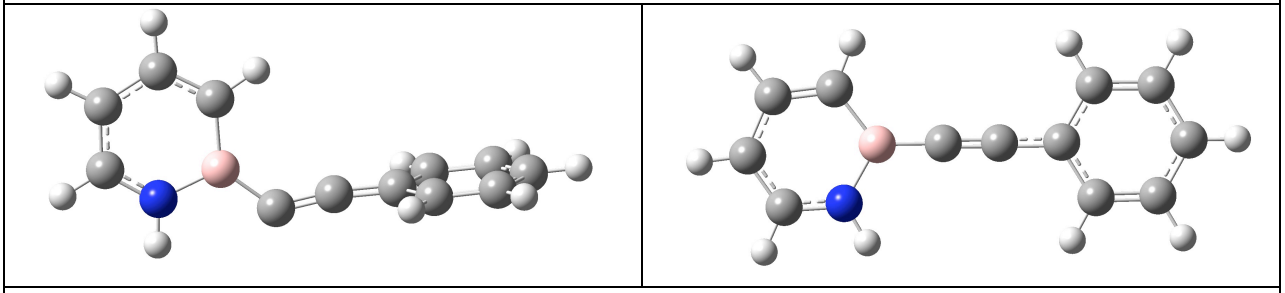
Table ST6. Comparison of selected bond distances for the ground states, 1st excited state singlet and twisted 1st excited state singlet structures in Å at the B3LYP/DZVP2 level.

Compound	C≡C	C-C(ring)	C-B
Ground states			
Tolan	1.221	1.431	
1	1.225	1.432	1.533
2 (cis)	1.230		1.536
2 (trans)	1.229		1.536
1st excited states singlet			
Tolan	1.259	1.387	
1	1.257	1.391	1.477
2 (cis)	1.261		1.493
2 (trans)	1.261		1.494
twisted 1st excited state singlet			
Tolan	1.323	1.373, 1.427	
1	1.291	1.377	1.493
2 (cis)	1.298		1.496, 1.493

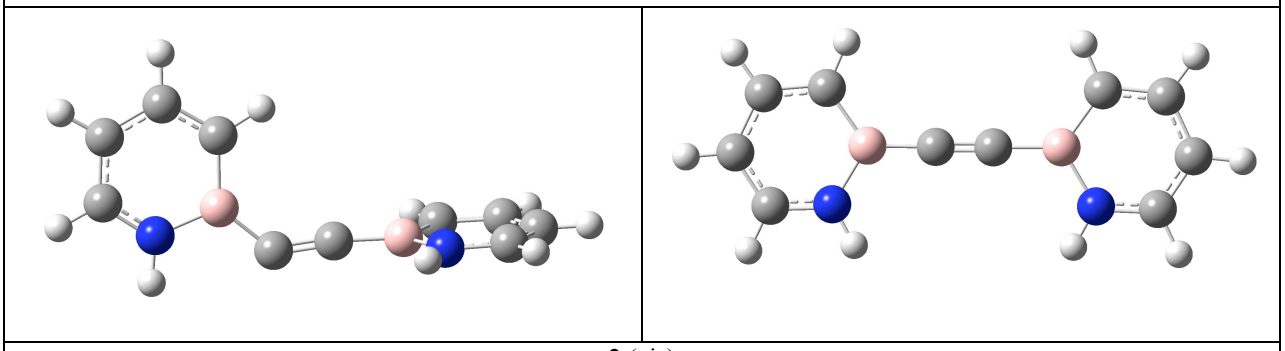
Figure ST2. Planar and Twisted 1st excited state singlet structures.



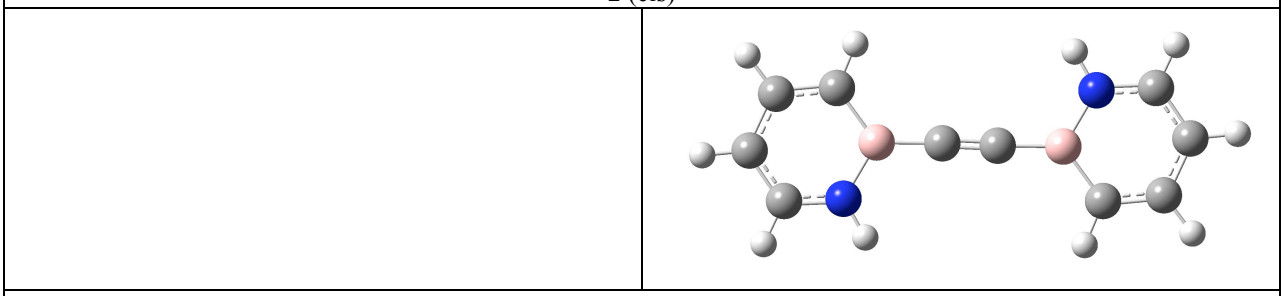
Tolan



1



2 (cis)



2 (trans)

Table ST7. Calculated vertical 1st singlet excitation energies from the ground state structures.

Molecules	State	Transition (eV)	Transition (nm)	Oscillator strength
Tolan	$^1B_{1u}$	4.08	304.1	0.937
1	$^1A'$	3.99	310.4	0.716
2 (cis)	$^1B_2$	4.01	309.2	0.633
2 (trans)	^1B_u	4.01	309.3	0.640

Table ST8. Emission from the Optimized TD-DFT singlets.

Molecule	State	Transition (eV)	Transition (nm)	Oscillator strength
Tolan	$^1B_{1u}$	3.61	343	0.99
1	$^1A'$	3.52	352	0.74
2 (cis)	$^1B_2$	3.65	339	0.72
2 (trans)	^1B_u	3.66	339	0.72

Table ST9. Emission from optimized twisted TD-DFT singlets

Molecule	State	Transition (eV)	Transition (nm)	Oscillator strength
Tolan	^1A	2.53	489	0.005
Tolan	^1A	3.93	316	0.14
1	^1A	2.87	432	0.0003
1	^1A	4.11	302	0.20
2	^1A	3.08	403	0.002
2	^1A	4.07	305	0.22

Table ST10. ΔE ground state energy differences of the twisted structures.

Molecule	ΔE(kcal/mol)	ΔE(eV)
Tolan	27.5	1.19
1	22.3	0.96
2	20.5[a]	0.89[a]
	21.0[b]	0.91[b]

[a] Compared to **2** (cis). [b] Compared to **2** (trans)

Table ST11. Solvation effects (THF) for the optimized 1st exited state singlet.

Molecule	State	Transition (eV)	Transition (nm)	Oscillator strength
Tolan	$^1B_{2u}$	3.47	357	1.20
1	$^1A'$	3.40	365	0.93
2 (cis)	$^1B_2$	3.51	353	0.91
2 (trans)	^1B_u	3.51	353	0.91

Table ST12. Solvation (THF) for the optimized twisted 1st excited state singlet structures.

Molecule	State	Transition (eV)	Transition (nm)	Oscillator strength
Tolan	^1A	2.64	470	0.0009
Tolan	^1A	3.85	322	0.27
1	^1A	2.95	421	0.0005
1	^1A	4.04	307	0.38
2	^1A	3.12	398	0.003
2	^1A	3.93	316	0.48

Table ST13. Dipole moments in Debye.

Molecule	Ground state	1st exited state singlet	twisted 1st excited state singlet
Tolan	0.00	0.00	2.42
1	1.72	1.79	0.90
2 (cis)	3.42	3.46	1.95

Figure ST3. Excitation and emission energy diagrams from the singlet excited state. Dashed lines are the adiabatic transition.

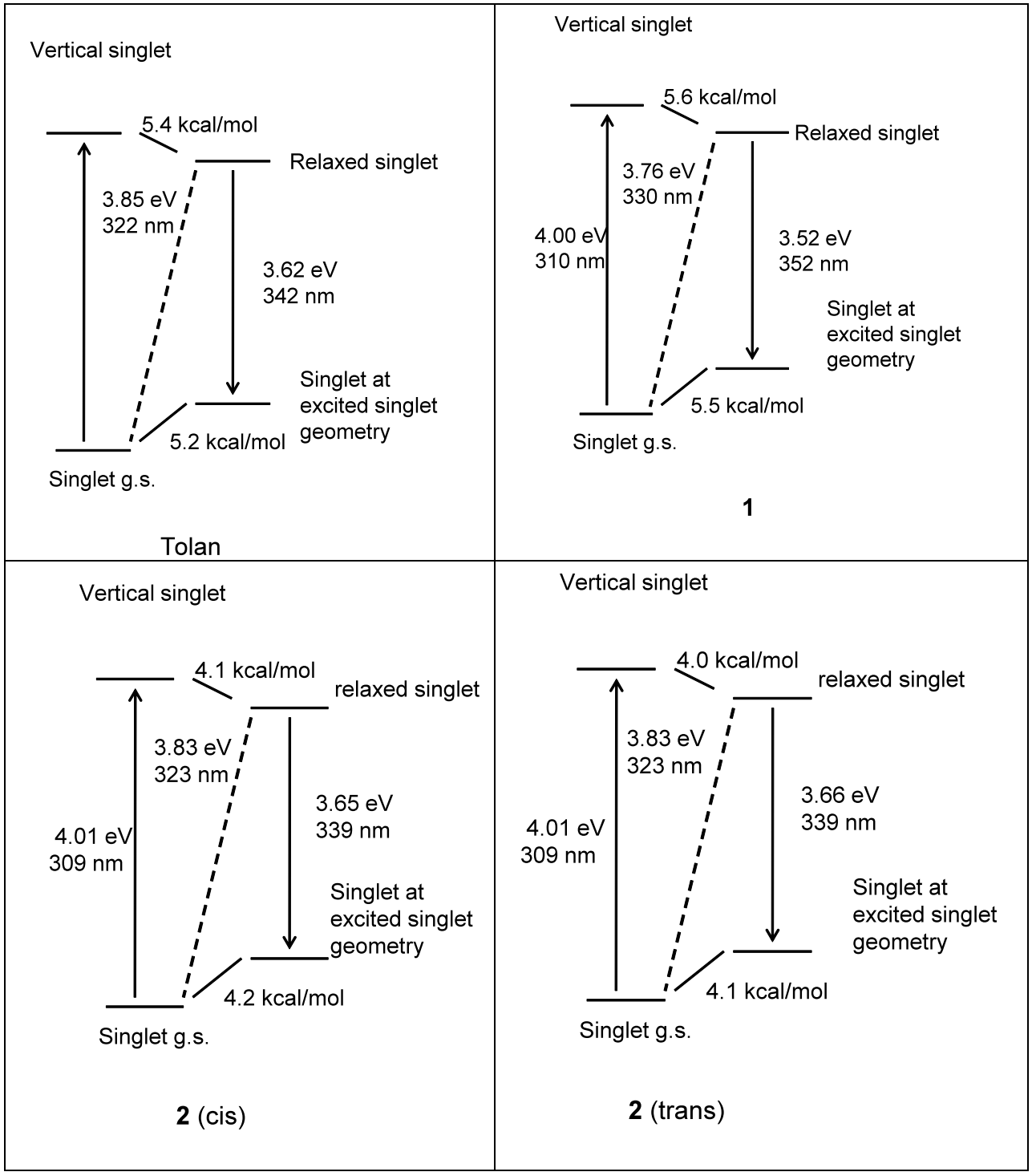


Figure ST4. Excitation and emission energy diagrams from the triplet excited state. Dashed lines are the adiabatic transition.

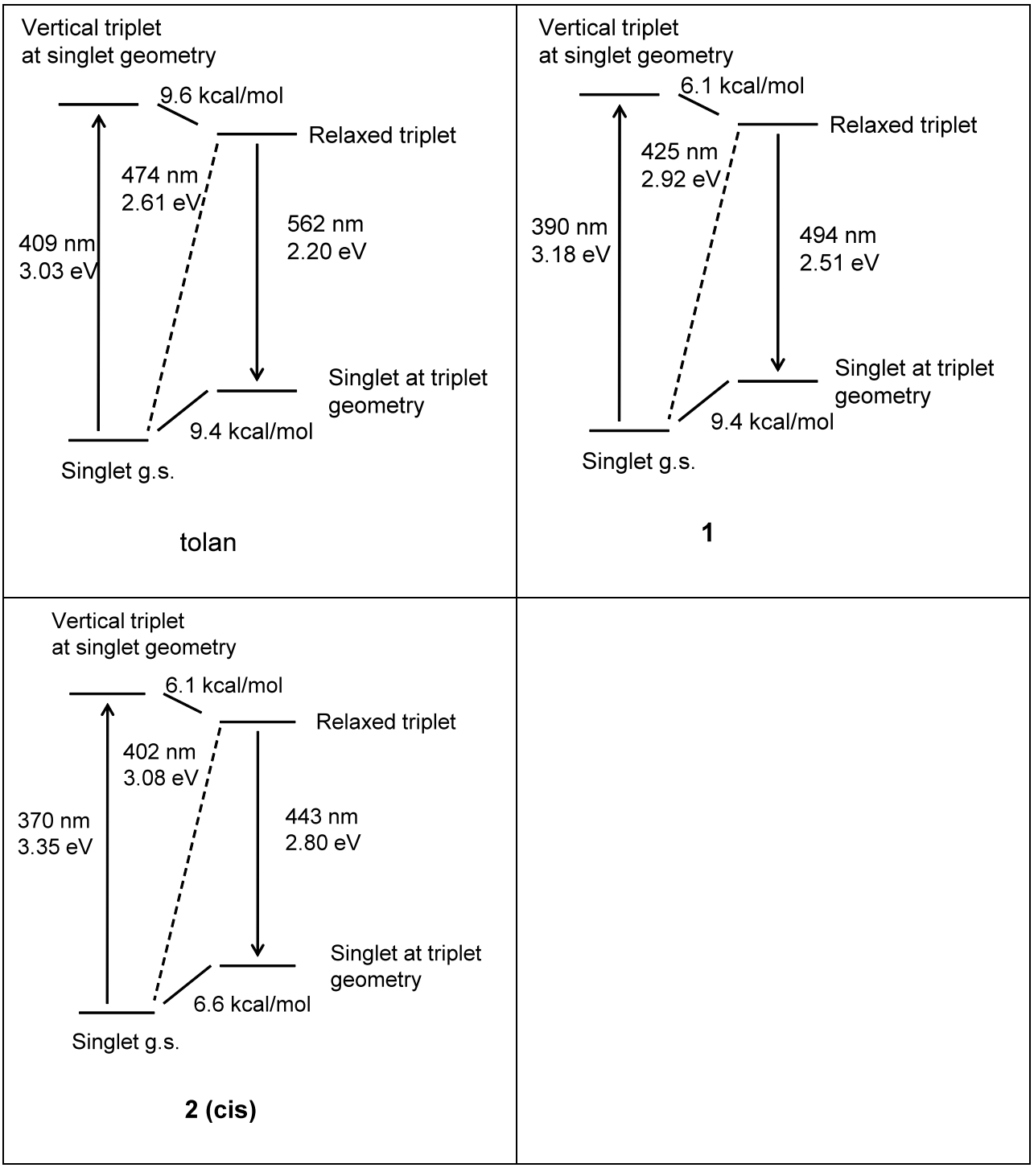


Table S14. Optimized B3LYP/DZVP2 x,y,z coordinates in angstroms.

A. Optimized Ground States:

Tolan (D_{2h})

C	0.000000	0.000000	0.610250
C	0.000000	0.000000	-0.610250
C	0.000000	0.000000	-2.041057
C	0.000000	1.216553	-2.759234
C	0.000000	-1.216553	-2.759234
C	0.000000	1.211916	-4.155966
H	0.000000	2.153701	-2.212760
C	0.000000	-1.211916	-4.155966
H	0.000000	-2.153701	-2.212760
C	0.000000	0.000000	-4.860187
H	0.000000	2.153141	-4.698148
H	0.000000	-2.153141	-4.698148
H	0.000000	0.000000	-5.946021
C	0.000000	0.000000	2.041057
C	0.000000	1.216553	2.759234
C	0.000000	-1.216553	2.759234
C	0.000000	1.211916	4.155966
H	0.000000	2.153701	2.212760
C	0.000000	-1.211916	4.155966
H	0.000000	-2.153701	2.212760
C	0.000000	0.000000	4.860187
H	0.000000	2.153141	4.698148
H	0.000000	-2.153141	4.698148
H	0.000000	0.000000	5.946021

BN-Tolan, **1** (C_s)

C	-1.572564	4.048318	0.000000
C	1.088532	3.039241	0.000000
C	0.831801	4.396371	0.000000
C	-0.502882	4.910167	0.000000
H	-2.596909	4.406938	0.000000
H	-2.219768	2.124117	0.000000
H	2.124340	2.708630	0.000000
H	1.649798	5.115705	0.000000
H	-0.682960	5.979270	0.000000
C	0.000000	0.535617	0.000000
C	0.072213	-0.687430	0.000000
C	0.182308	-2.114832	0.000000
C	-0.972406	-2.927909	0.000000
C	1.452234	-2.733375	0.000000
C	-0.857152	-4.319877	0.000000
H	-1.950093	-2.457431	0.000000
C	1.559350	-4.125914	0.000000
H	2.341428	-2.111835	0.000000
C	0.407404	-4.924702	0.000000
H	-1.751996	-4.935864	0.000000
H	2.540965	-4.591119	0.000000
H	0.494338	-6.007130	0.000000
B	-0.079926	2.066541	0.000000

N	-1.383219	2.694568	0.000000

Bis-Cis-BN-Tolan, **2**(cis) (C_{2v})

C	0.000000	4.238318	-1.236504
C	0.000000	3.034180	1.342056
C	0.000000	4.406688	1.187149
C	0.000000	5.018250	-0.105687
H	0.000000	4.671867	-2.231464
H	0.000000	2.367694	-2.024077
H	0.000000	2.626632	2.349909
H	0.000000	5.063193	2.056413
H	0.000000	6.097850	-0.205743
C	0.000000	0.614776	0.073274
C	0.000000	-0.614776	0.073274
C	0.000000	-3.034180	1.342056
C	0.000000	-4.238318	-1.236504
H	0.000000	-2.367694	-2.024077
C	0.000000	-4.406688	1.187149
H	0.000000	-2.626632	2.349909
C	0.000000	-5.018250	-0.105687
H	0.000000	-4.671867	-2.231464
H	0.000000	-5.063193	2.056413
H	0.000000	-6.097850	-0.205743
B	0.000000	2.150295	0.104998
N	0.000000	2.874118	-1.147395
N	0.000000	-2.874118	-1.147395
B	0.000000	-2.150295	0.104998

Bis-Trans-BN-Tolan, **2**(trans) (C_{2h})

C	-1.212821	4.253976	0.000000
C	1.348506	3.013699	0.000000
C	1.212821	4.388545	0.000000
C	-0.070875	5.018244	0.000000
H	-2.201585	4.701469	0.000000
H	-2.025677	2.393230	0.000000
H	2.351462	2.593819	0.000000
H	2.091229	5.032828	0.000000
H	-0.155600	6.099120	0.000000
C	0.033357	0.613778	0.000000
C	-0.033357	-0.613778	0.000000
C	-1.348506	-3.013699	0.000000
C	1.212821	-4.253976	0.000000
H	2.025677	-2.393230	0.000000
C	-1.212821	-4.388545	0.000000
H	-2.351462	-2.593819	0.000000
C	0.070875	-5.018244	0.000000
H	2.201585	-4.701469	0.000000
H	-2.091229	-5.032828	0.000000
H	0.155600	-6.099120	0.000000
B	0.098986	2.147984	0.000000
N	-1.142867	2.889406	0.000000
N	1.142867	-2.889406	0.000000
B	-0.098986	-2.147984	0.000000

B. Optimized 1st Excited Singlet State:

Tolan (D_{2h})

C	0.000000	0.000000	0.629342
C	0.000000	0.000000	-0.629342
C	0.000000	0.000000	-2.015858
C	0.000000	1.239328	-2.760384
C	0.000000	-1.239328	-2.760384
C	0.000000	1.222865	-4.145110
H	0.000000	2.176783	-2.214043
C	0.000000	-1.222865	-4.145110
H	0.000000	-2.176783	-2.214043
C	0.000000	0.000000	-4.855513
H	0.000000	2.160756	-4.693778
H	0.000000	-2.160756	-4.693778
H	0.000000	0.000000	-5.941030
C	0.000000	0.000000	2.015858
C	0.000000	1.239328	2.760384
C	0.000000	-1.239328	2.760384
C	0.000000	1.222865	4.145110
H	0.000000	2.176783	2.214043
C	0.000000	-1.222865	4.145110
H	0.000000	-2.176783	2.214043
C	0.000000	0.000000	4.855513
H	0.000000	2.160756	4.693778
H	0.000000	-2.160756	4.693778
H	0.000000	0.000000	5.941030

BN-Tolan (C_s)

C	-1.714850	3.973078	0.000000
C	0.989431	3.082662	0.000000
C	0.698067	4.437468	0.000000
C	-0.654764	4.886418	0.000000
H	-2.741963	4.327522	0.000000
H	-2.333575	2.049910	0.000000
H	2.033546	2.778800	0.000000
H	1.489217	5.184083	0.000000
H	-0.887922	5.945390	0.000000
C	0.000000	0.553410	0.000000
C	0.117528	-0.698500	0.000000
C	0.261727	-2.082165	0.000000
C	-0.889151	-2.953383	0.000000
C	1.569451	-2.693464	0.000000
C	-0.728817	-4.329666	0.000000
H	-1.880879	-2.512299	0.000000
C	1.699762	-4.072876	0.000000
H	2.445966	-2.053582	0.000000
C	0.560626	-4.912577	0.000000
H	-1.606328	-4.971331	0.000000
H	2.692072	-4.516538	0.000000
H	0.674709	-5.991762	0.000000
B	-0.150367	2.023003	0.000000
N	-1.512438	2.643194	0.000000

Bis-Cis-BN-Tolan (C_{2v})

C	0.000000	4.241181	-1.233869
C	0.000000	3.020707	1.338592
C	0.000000	4.404206	1.213642
C	0.000000	5.014571	-0.079471
H	0.000000	4.710953	-2.213563
H	0.000000	2.399647	-2.075153
H	0.000000	2.594498	2.339448
H	0.000000	5.050144	2.089157
H	0.000000	6.094548	-0.181036
C	0.000000	0.630641	0.077832
C	0.000000	-0.630641	0.077832
C	0.000000	-3.020707	1.338592
C	0.000000	-4.241181	-1.233869
H	0.000000	-2.399647	-2.075153
C	0.000000	-4.404206	1.213642
H	0.000000	-2.594498	2.339448
C	0.000000	-5.014571	-0.079471
H	0.000000	-4.710953	-2.213563
H	0.000000	-5.050144	2.089157
H	0.000000	-6.094548	-0.181036
B	0.000000	2.124031	0.092006
N	0.000000	2.887110	-1.188462
N	0.000000	-2.887110	-1.188462
B	0.000000	-2.124031	0.092006

Bis-Trans-BN-Tolan (C_{2h})

C	-1.224709	4.252594	0.000000
C	1.334895	3.004618	0.000000
C	1.224709	4.389563	0.000000
C	-0.061754	5.013760	0.000000
H	-2.199386	4.732660	0.000000
H	-2.084206	2.418337	0.000000
H	2.332002	2.569285	0.000000
H	2.106997	5.026276	0.000000
H	-0.151610	6.094735	0.000000
C	0.036528	0.629445	0.000000
C	-0.036528	-0.629445	0.000000
C	-1.334895	-3.004618	0.000000
C	1.224709	-4.252594	0.000000
H	2.084206	-2.418337	0.000000
C	-1.224709	-4.389563	0.000000
H	-2.332002	-2.569285	0.000000
C	0.061754	-5.013760	0.000000
H	2.199386	-4.732660	0.000000
H	-2.106997	-5.026276	0.000000
H	0.151610	-6.094735	0.000000
B	0.078657	2.122366	0.000000
N	-1.193416	2.898738	0.000000
N	1.193416	-2.898738	0.000000
B	-0.078657	-2.122366	0.000000

C. Optimized Twisted 1st Excited State Singlet Structures:

Tolan (C_1)

C	4.392534	-0.699508	-0.000862
C	2.134416	0.989967	0.001456
C	3.404662	1.543259	0.002643
C	4.538040	0.703229	0.001516
H	5.275160	-1.331742	-0.001703
H	2.980807	-2.336251	-0.003964
H	1.248609	1.616296	0.002284
H	3.535234	2.621290	0.004448
H	5.531977	1.141378	0.002476
C	0.667999	-1.057867	-0.002333
C	-0.511587	-0.459332	-0.001282
C	-1.866253	-0.230709	-0.000645
C	-2.599953	-0.088073	1.236503
C	-2.600356	-0.082854	-1.236938
C	-3.960070	0.177084	1.213897
H	-2.076478	-0.199925	2.179566
C	-3.960470	0.182196	-1.212768
H	-2.077189	-0.190724	-2.180638
C	-4.666769	0.319753	0.000976
H	-4.490165	0.271573	2.158385
H	-4.490876	0.280664	-2.156675
H	-5.730511	0.529550	0.001593
C	3.124280	-1.261069	-0.002126
C	1.952433	-0.436429	-0.000998

BN-Tolan (C_1)

C	-4.386830	-0.727514	-0.035454
C	-2.244563	1.139500	0.074418
C	-3.561226	1.583039	0.127587
C	-4.628611	0.661026	0.073775
H	-5.218612	-1.425127	-0.074398
H	-3.026418	-2.216624	-0.172541
H	-1.448180	1.877109	0.120031
H	-3.799821	2.640938	0.213008
H	-5.657945	0.998852	0.115730
C	-0.594169	-1.081509	-0.128383
C	0.607684	-0.611615	-0.077725
C	1.947096	-0.296554	-0.036549
C	2.685994	0.019237	-1.243795
C	2.671825	-0.252023	1.218883
C	4.027314	0.353001	-1.176040
H	2.175917	-0.017083	-2.200549
C	4.013008	0.087919	1.241248
H	2.150665	-0.495189	2.138726
C	4.722518	0.400903	0.056550
H	4.557511	0.580768	-2.098000
H	4.531983	0.109360	2.196838
H	5.772954	0.666239	0.091773
B	-1.909507	-0.379838	-0.049259
N	-3.150110	-1.210359	-0.093059

Bis-BN-Tolan (C_1)

C	4.482717	-0.699110	0.165112
C	2.327007	1.099008	-0.291511
C	3.641038	1.529761	-0.436363
C	4.715269	0.640494	-0.211598
H	5.317413	-1.373282	0.334715
H	3.128796	-2.138290	0.600081
H	1.523764	1.808540	-0.470234
H	3.873701	2.552586	-0.725754
H	5.742052	0.970434	-0.323594
C	0.686591	-1.026531	0.354665
C	-0.538430	-0.617493	0.219502
C	-2.792060	0.351474	1.274167
C	-4.125730	0.651082	1.092140
H	-2.341226	0.582280	2.237453
C	-4.109275	-0.209973	-1.195070
H	-2.370654	-0.985534	-1.901321
C	-4.792911	0.370727	-0.160687
H	-4.709815	1.106617	1.890290
H	-4.598277	-0.431260	-2.139681
H	-5.841392	0.614406	-0.292594
B	2.006055	-0.365540	0.126405
N	3.246754	-1.166892	0.322725
B	-1.996104	-0.290967	0.137691
N	-2.780956	-0.541763	-1.093005

D. Optimized Dimers at wB97xD/DZVP2 level:

Perpendicular Dimer

C	-2.831389	-2.745759	0.049369
C	-3.256493	-3.156304	-2.298594
C	-3.523109	-3.416007	-0.922532
H	-3.008889	-2.918935	1.104463
H	-1.409775	-1.367562	0.498284
H	-2.152541	-2.084350	-3.759808
H	-3.830589	-3.712786	-3.036292
H	-4.271815	-4.143051	-0.634238
C	-0.440194	-0.426127	-1.812293
C	0.438827	0.425085	-1.812499
C	2.831244	2.745114	0.047169
H	1.410962	1.365960	0.497358
C	3.253383	3.156592	-2.301165
H	2.148274	2.084496	-3.761396
C	3.521414	3.416084	-0.925342
H	3.009851	2.918096	1.102109
H	3.826306	3.713592	-3.039385
H	4.270007	4.143502	-0.637704
B	-1.543185	-1.495268	-1.627591
B	1.541685	1.494520	-1.628630
C	2.745542	-2.831125	-0.048928
C	2.242174	-2.306573	2.697207
C	3.160370	-3.252002	2.299048
C	3.418213	-3.520464	0.922996
H	2.917278	-3.010045	-1.104019
H	1.364755	-1.412009	-0.497864
H	2.089346	-2.147106	3.760230

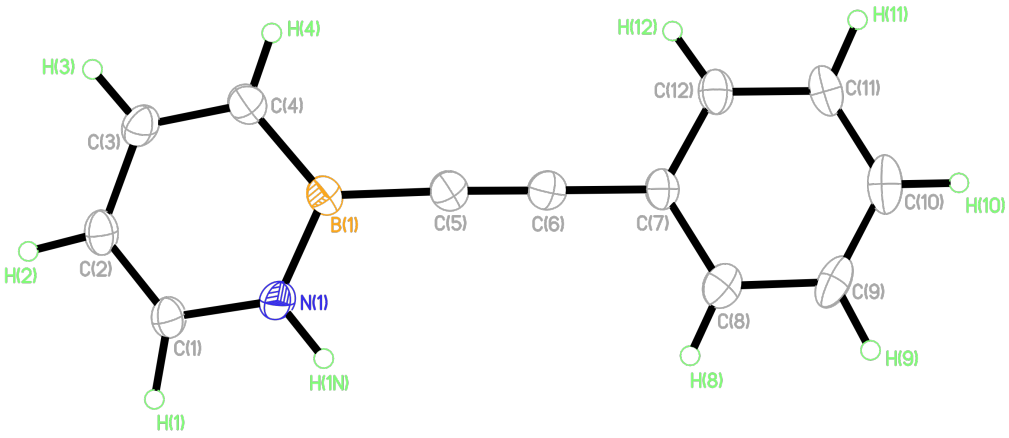
H	3.718619	-3.824363	3.036760
H	4.145707	-4.268742	0.634727
C	0.426483	-0.439309	1.812668
C	-0.425059	0.439396	1.812707
C	-2.238280	2.308595	2.698089
C	-2.746099	2.830205	-0.047767
H	-1.367261	1.409471	-0.497466
C	-3.156531	3.254180	2.300418
H	-2.083816	2.150172	3.761032
C	-3.416584	3.521189	0.924500
H	-2.919517	3.008024	-1.102769
H	-3.713201	3.827680	3.038438
H	-4.144063	4.269622	0.636599
B	1.496294	-1.541670	1.627993
N	1.825673	-1.884260	0.274785
N	-1.826311	1.883091	0.275454
B	-1.494742	1.541956	1.628487
C	2.307506	2.238502	-2.698507
C	-2.310614	-2.238582	-2.696781
N	1.883890	1.825461	-0.275719
N	-1.883926	-1.826506	-0.274367

Parallel Dimer

C	4.277037	2.339069	0.781296
C	4.395260	1.170030	-1.336040
C	5.030270	1.782847	-0.212250
H	4.730778	2.808605	1.646771
H	2.426536	2.756169	1.492708
H	2.598909	0.633285	-2.324265
H	5.035611	0.736439	-2.101152
H	6.110029	1.807496	-0.133916
C	0.637926	1.778277	-0.319063
C	-0.584203	1.781480	-0.320077
C	-4.221062	2.373882	0.771367
H	-2.368626	2.776185	1.486342
C	-4.344667	1.199595	-1.342595
H	-2.550630	0.641704	-2.323489
C	-4.976843	1.822311	-0.222798
H	-4.672695	2.849536	1.634594
H	-4.987001	0.769898	-2.108230
H	-6.056513	1.857502	-0.147509
B	2.175806	1.726175	-0.353685
B	-2.122435	1.739195	-0.356670
C	4.344992	-1.202310	1.340372
C	4.220559	-2.368714	-0.777932
C	4.976694	-1.819432	0.217228
H	4.987707	-0.774822	2.106921
H	2.551411	-0.651970	2.326294
H	2.367810	-2.771686	-1.491813
H	4.671847	-2.840379	-1.643527
H	6.056319	-1.852246	0.140218
C	0.584208	-1.785862	0.320346
C	-0.637913	-1.782208	0.320436
C	-4.393477	-1.166974	1.339381
H	-2.595553	-0.632800	2.326083

C	-4.278647	-2.337530	-0.777338
H	-2.429316	-2.758709	-1.489540
C	-5.030235	-1.779214	0.216271
H	-5.032531	-0.731758	2.104649
H	-4.733828	-2.806510	-1.642361
H	-6.110079	-1.802094	0.138580
B	2.122412	-1.742084	0.355423
B	-2.175661	-1.728032	0.356061
N	-2.859061	2.347419	0.716512
N	-2.916605	-2.326872	-0.719438
C	-2.978775	1.131400	-1.454054
C	-3.027233	-1.115146	1.454302
C	2.979131	-1.136898	1.453982
C	3.029189	1.115769	-1.451869
N	2.858602	-2.345145	-0.720965
N	2.915056	2.325690	0.722634

X-ray Crystal Structure Determination of 1. Crystals of **1** suitable for X-ray diffraction were obtained by slow evaporation of a solution of **1** in Et_2O.



Diffraction intensity data were collected with a Bruker Smart Apex CCD diffractometer at 173(2) K using MoKα - radiation (0.71073 Å). The structure was solved using direct methods, completed by subsequent difference Fourier syntheses, and refined by full matrix least-squares procedures on F^2. All non-H atoms were refined with anisotropic thermal parameters. H atoms were found on the residual density map and refined with isotropic thermal parameters. The Flack parameter is 0.00(8). All software and sources scattering factors are contained in the SHELXTL (6.10) program package (G.Sheldrick, Bruker XRD, Madison, WI). Crystallographic data and some details of data collection and crystal structure refinement for $C_{12}H_{10}BN$ are given in the following tables.

Table S1. Crystal data and structure refinement for **1** (liu72).

Identification code	liu72	
Empirical formula	C_{12} H_{10} B N	
Formula weight	179.02	
Temperature	173(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	Fdd2	
Unit cell dimensions	a = 23.388(11) Å	α= 90°.
	b = 31.934(15) Å	β= 90°.
	c = 5.423(3) Å	γ = 90°.
Volume	4051(3) $Å^3$	
Z	16	
Density (calculated)	1.174 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	1504	
Crystal size	0.21 x 0.12 x 0.02 mm^3	
Theta range for data collection	2.16 to 25.00°.	
Index ranges	-27<=h<=27, -37<=k<=37, -6<=l<=6	
Reflections collected	8757	
Independent reflections	1791 [R(int) = 0.0942]	
Completeness to theta = 25.00∞	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9987 and 0.9860	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1791 / 1 / 167	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1043	
R indices (all data)	R1 = 0.0946, wR2 = 0.1198	
Absolute structure parameter	0(6)	
Largest diff. peak and hole	0.143 and -0.161 e.$≈^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	601(1)	1001(1)	4888(6)	41(1)
B(1)	122(2)	917(1)	3334(8)	33(1)
C(1)	1013(2)	1296(1)	4348(8)	42(1)
C(2)	974(2)	1525(1)	2256(7)	40(1)
C(3)	514(2)	1462(1)	595(8)	42(1)
C(4)	95(2)	1173(1)	1045(7)	41(1)
C(5)	-319(1)	596(1)	4301(7)	37(1)
C(6)	-665(1)	352(1)	5158(7)	36(1)
C(7)	-1077(1)	65(1)	6161(6)	33(1)
C(8)	-965(2)	-154(1)	8367(7)	40(1)
C(9)	-1367(2)	-438(1)	9266(8)	49(1)
C(10)	-1877(2)	-502(1)	8034(9)	55(1)
C(11)	-1999(2)	-280(1)	5913(9)	49(1)
C(12)	-1601(2)	0(1)	4952(7)	41(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

N(1)-C(1)	1.380(4)
N(1)-B(1)	1.427(5)
N(1)-H(1N)	0.92(5)
B(1)-C(4)	1.488(5)
B(1)-C(5)	1.545(5)
C(1)-C(2)	1.352(5)
C(1)-H(1)	1.04(4)
C(2)-C(3)	1.417(5)
C(2)-H(2)	0.95(3)
C(3)-C(4)	1.368(5)
C(3)-H(3)	0.91(3)
C(4)-H(4)	0.93(3)
C(5)-C(6)	1.216(4)
C(6)-C(7)	1.436(5)
C(7)-C(12)	1.406(5)
C(7)-C(8)	1.410(5)
C(8)-C(9)	1.395(5)
C(8)-H(8)	0.95(5)
C(9)-C(10)	1.383(6)
C(9)-H(9)	0.96(4)
C(10)-C(11)	1.381(6)

C(10)-H(10)	0.96(4)
C(11)-C(12)	1.391(5)
C(11)-H(11)	0.99(4)
C(12)-H(12)	0.94(3)

C(1)-N(1)-B(1)	123.5(3)
C(1)-N(1)-H(1N)	120(3)
B(1)-N(1)-H(1N)	116(3)
N(1)-B(1)-C(4)	114.9(3)
N(1)-B(1)-C(5)	116.6(3)
C(4)-B(1)-C(5)	128.3(3)
C(2)-C(1)-N(1)	120.0(4)
C(2)-C(1)-H(1)	130(2)
N(1)-C(1)-H(1)	110(2)
C(1)-C(2)-C(3)	120.5(3)
C(1)-C(2)-H(2)	115(2)
C(3)-C(2)-H(2)	125(2)
C(4)-C(3)-C(2)	121.7(4)
C(4)-C(3)-H(3)	118.8(19)
C(2)-C(3)-H(3)	119.4(19)
C(3)-C(4)-B(1)	119.4(4)
C(3)-C(4)-H(4)	121(2)
B(1)-C(4)-H(4)	120(2)
C(6)-C(5)-B(1)	177.2(4)
C(5)-C(6)-C(7)	179.7(4)
C(12)-C(7)-C(8)	119.0(3)
C(12)-C(7)-C(6)	120.1(3)
C(8)-C(7)-C(6)	120.9(3)
C(9)-C(8)-C(7)	119.6(4)
C(9)-C(8)-H(8)	117(3)
C(7)-C(8)-H(8)	123(3)
C(10)-C(9)-C(8)	120.6(4)
C(10)-C(9)-H(9)	123(2)
C(8)-C(9)-H(9)	116(2)
C(11)-C(10)-C(9)	120.2(4)
C(11)-C(10)-H(10)	119(3)
C(9)-C(10)-H(10)	120(3)
C(10)-C(11)-C(12)	120.3(4)
C(10)-C(11)-H(11)	124(2)
C(12)-C(11)-H(11)	115(2)

C(11)-C(12)-C(7)	120.2(4)
C(11)-C(12)-H(12)	124(2)
C(7)-C(12)-H(12)	116(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for **1**. 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}
N(1)	49(2)	30(2)	43(2)	8(2)	-6(2)	-7(2)
B(1)	32(2)	19(2)	47(2)	-2(2)	-1(2)	4(2)
C(1)	47(3)	34(2)	46(3)	4(2)	-2(2)	-13(2)
C(2)	42(2)	26(2)	52(2)	2(2)	6(2)	-5(2)
C(3)	46(2)	35(2)	45(3)	11(2)	3(2)	4(2)
C(4)	37(2)	36(2)	48(3)	1(2)	-3(2)	0(2)
C(5)	36(2)	27(2)	48(2)	0(2)	-1(2)	6(2)
C(6)	41(2)	25(2)	43(2)	-2(2)	-2(2)	6(2)
C(7)	39(2)	19(2)	41(2)	-6(2)	4(2)	1(1)
C(8)	55(3)	21(2)	44(2)	-6(2)	5(2)	7(2)
C(9)	77(3)	28(2)	42(3)	4(2)	19(2)	3(2)
C(10)	57(3)	35(2)	73(3)	-6(2)	27(3)	-7(2)
C(11)	43(2)	36(2)	66(3)	-7(2)	8(2)	-11(2)
C(12)	46(2)	28(2)	49(3)	-5(2)	7(2)	-3(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(1N)	625(18)	847(13)	6320(90)	95(17)
H(1)	1305(18)	1315(12)	5800(80)	86(14)
H(2)	1276(13)	1720(9)	2020(60)	38(9)
H(3)	510(12)	1603(9)	-870(60)	27(9)
H(4)	-198(13)	1130(9)	-80(70)	37(10)
H(8)	-627(19)	-114(13)	9310(90)	86(16)
H(9)	-1282(15)	-564(11)	10830(80)	53(11)
H(10)	-2172(17)	-674(12)	8760(80)	74(14)
H(11)	-2353(14)	-314(10)	4930(80)	51(11)
H(12)	-1658(13)	156(9)	3510(70)	39(10)

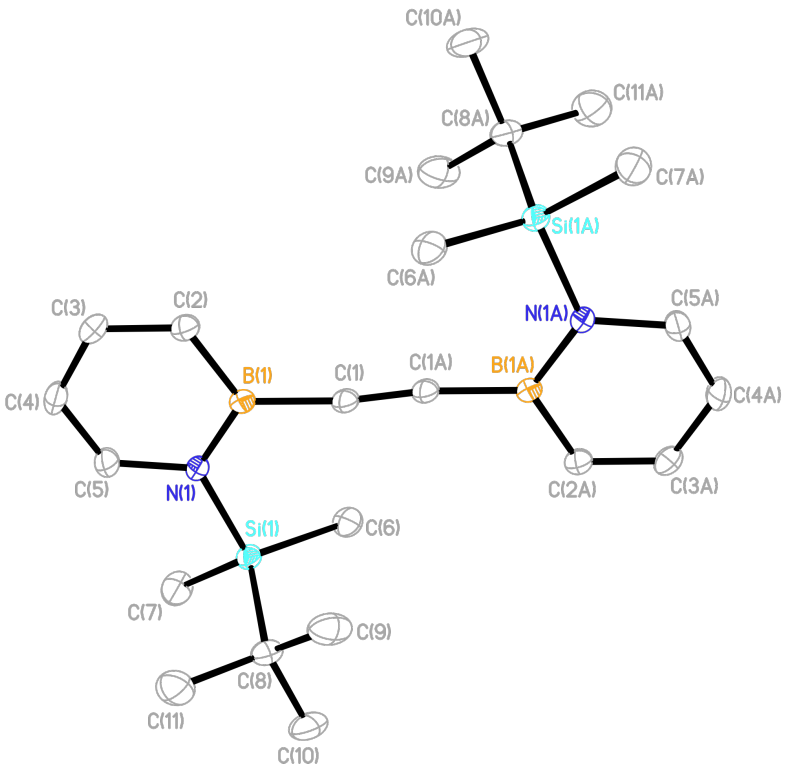
Table S6. Torsion angles [°] for **1**.

C(1)-N(1)-B(1)-C(4)	0.2(5)
C(1)-N(1)-B(1)-C(5)	-176.1(3)

B(1)-N(1)-C(1)-C(2)	0.1(5)
N(1)-C(1)-C(2)-C(3)	-0.4(5)
C(1)-C(2)-C(3)-C(4)	0.3(6)
C(2)-C(3)-C(4)-B(1)	0.0(5)
N(1)-B(1)-C(4)-C(3)	-0.2(5)
C(5)-B(1)-C(4)-C(3)	175.6(4)
N(1)-B(1)-C(5)-C(6)	47(7)
C(4)-B(1)-C(5)-C(6)	-129(7)
B(1)-C(5)-C(6)-C(7)	120(100)
C(5)-C(6)-C(7)-C(12)	6(92)
C(5)-C(6)-C(7)-C(8)	-173(100)
C(12)-C(7)-C(8)-C(9)	1.9(4)
C(6)-C(7)-C(8)-C(9)	-178.5(3)
C(7)-C(8)-C(9)-C(10)	-1.0(5)
C(8)-C(9)-C(10)-C(11)	-1.0(6)
C(9)-C(10)-C(11)-C(12)	2.1(6)
C(10)-C(11)-C(12)-C(7)	-1.2(5)
C(8)-C(7)-C(12)-C(11)	-0.8(5)
C(6)-C(7)-C(12)-C(11)	179.6(3)

Symmetry transformations used to generate equivalent atoms:

X-ray Crystal Structure Determination of 8. Crystals of **8** suitable for X-ray diffraction were obtained by slow evaporation of a solution of **8** in Et_2O.



Diffraction intensity data were collected with a Bruker Smart Apex CCD diffractometer at 173(2) K using MoKα - radiation (0.71073 Å). The structure was solved using direct methods, completed by subsequent difference Fourier syntheses, and refined by full matrix least-squares procedures on F^2. All non-H atoms were refined with anisotropic thermal parameters. H atoms were found on the residual density map and refined with isotropic thermal parameters. The Flack parameter is 0.00(8). All software and sources scattering factors are contained in the SHELXTL (6.10) program package (G.Sheldrick, Bruker XRD, Madison, WI). Crystallographic data and some details of data collection and crystal structure refinement for $C_{22}H_{38}B_2N_2Si_2$ are given in the following tables.

Table S7. Crystal data and structure refinement for **8** (liu49).

Identification code	liu49	
Empirical formula	C_{22} H_{38} B_2 N_2 Si_2	
Formula weight	408.34	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.3135(12) Å	α= 90°.
	b = 8.3715(9) Å	β= 101.892(2)°.
	c = 13.7353(14) Å	γ = 90°.
Volume	1273.0(2) $Å^3$	
Z	2	
Density (calculated)	1.065 Mg/m^3	
Absorption coefficient	0.149 mm^{-1}	
F(000)	444	
Crystal size	0.19 x 0.12 x 0.05 mm^3	
Theta range for data collection	2.13 to 27.00°.	
Index ranges	-14<=h<=14, -10<=k<=10, -17<=l<=17	
Reflections collected	13631	
Independent reflections	2780 [R(int) = 0.0429]	
Completeness to theta = 27.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9926 and 0.9722	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2780 / 0 / 203	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1194	
R indices (all data)	R1 = 0.0712, wR2 = 0.1301	
Largest diff. peak and hole	0.340 and -0.165 e.$Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	7763(1)	2417(1)	5157(1)	27(1)
N(1)	6997(1)	2347(2)	6184(1)	26(1)
B(1)	5893(2)	1485(3)	6194(2)	26(1)
C(1)	5284(2)	437(2)	5312(1)	28(1)
C(2)	5356(2)	1622(3)	7109(1)	32(1)
C(3)	5916(2)	2529(3)	7882(2)	39(1)
C(4)	6994(2)	3330(3)	7833(2)	47(1)
C(5)	7489(2)	3234(3)	7019(2)	40(1)
C(6)	7796(3)	419(3)	4574(2)	39(1)
C(7)	9363(2)	2986(4)	5673(2)	47(1)
C(8)	7014(2)	3968(3)	4241(2)	35(1)
C(9)	5686(3)	3583(4)	3828(2)	56(1)
C(10)	7683(3)	4052(4)	3377(2)	54(1)
C(11)	7109(3)	5618(3)	4743(2)	55(1)

Table S9. Bond lengths [Å] and angles [°] for **8**.

Si(1)-N(1)	1.8010(16)
Si(1)-C(6)	1.858(2)
Si(1)-C(7)	1.865(3)
Si(1)-C(8)	1.884(2)
N(1)-C(5)	1.384(3)
N(1)-B(1)	1.445(3)
B(1)-C(2)	1.508(3)
B(1)-C(1)	1.539(3)
C(1)-C(1)#1	1.206(4)
C(2)-C(3)	1.352(3)
C(2)-H(2)	0.97(2)
C(3)-C(4)	1.405(3)
C(3)-H(3)	0.93(2)
C(4)-C(5)	1.352(3)
C(4)-H(4)	0.93(3)
C(5)-H(5)	0.98(2)
C(6)-H(6A)	0.92(4)
C(6)-H(6B)	0.92(3)
C(6)-H(6C)	0.95(3)
C(7)-H(7A)	0.99(3)
C(7)-H(7B)	0.90(3)

C(7)-H(7C)	0.94(4)
C(8)-C(9)	1.527(3)
C(8)-C(10)	1.536(3)
C(8)-C(11)	1.537(3)
C(9)-H(9A)	0.98(3)
C(9)-H(9B)	0.99(3)
C(9)-H(9C)	0.92(3)
C(10)-H(10A)	1.04(3)
C(10)-H(10B)	0.98(3)
C(10)-H(10C)	0.98(3)
C(11)-H(11A)	0.96(3)
C(11)-H(11B)	0.98(3)
C(11)-H(11C)	0.95(3)

N(1)-Si(1)-C(6)	111.34(10)
N(1)-Si(1)-C(7)	107.24(10)
C(6)-Si(1)-C(7)	106.84(14)
N(1)-Si(1)-C(8)	108.84(9)
C(6)-Si(1)-C(8)	112.24(11)
C(7)-Si(1)-C(8)	110.21(12)
C(5)-N(1)-B(1)	117.42(16)
C(5)-N(1)-Si(1)	117.09(13)
B(1)-N(1)-Si(1)	125.46(13)
N(1)-B(1)-C(2)	117.90(18)
N(1)-B(1)-C(1)	121.65(16)
C(2)-B(1)-C(1)	120.45(17)
C(1)#1-C(1)-B(1)	172.5(2)
C(3)-C(2)-B(1)	119.53(19)
C(3)-C(2)-H(2)	120.1(13)
B(1)-C(2)-H(2)	120.3(13)
C(2)-C(3)-C(4)	120.1(2)
C(2)-C(3)-H(3)	122.2(15)
C(4)-C(3)-H(3)	117.6(15)
C(5)-C(4)-C(3)	121.5(2)
C(5)-C(4)-H(4)	117.8(17)
C(3)-C(4)-H(4)	120.7(17)
C(4)-C(5)-N(1)	123.6(2)
C(4)-C(5)-H(5)	120.4(13)
N(1)-C(5)-H(5)	116.0(13)
Si(1)-C(6)-H(6A)	112(2)

Si(1)-C(6)-H(6B)	113(2)
H(6A)-C(6)-H(6B)	112(3)
Si(1)-C(6)-H(6C)	107.5(16)
H(6A)-C(6)-H(6C)	100(3)
H(6B)-C(6)-H(6C)	112(2)
Si(1)-C(7)-H(7A)	109.5(16)
Si(1)-C(7)-H(7B)	115.7(19)
H(7A)-C(7)-H(7B)	106(2)
Si(1)-C(7)-H(7C)	109(2)
H(7A)-C(7)-H(7C)	106(3)
H(7B)-C(7)-H(7C)	109(3)
C(9)-C(8)-C(10)	109.1(2)
C(9)-C(8)-C(11)	109.2(2)
C(10)-C(8)-C(11)	107.8(2)
C(9)-C(8)-Si(1)	112.04(16)
C(10)-C(8)-Si(1)	108.81(17)
C(11)-C(8)-Si(1)	109.85(17)
C(8)-C(9)-H(9A)	112.7(17)
C(8)-C(9)-H(9B)	110.9(17)
H(9A)-C(9)-H(9B)	109(2)
C(8)-C(9)-H(9C)	111.4(18)
H(9A)-C(9)-H(9C)	107(2)
H(9B)-C(9)-H(9C)	105(2)
C(8)-C(10)-H(10A)	108.7(17)
C(8)-C(10)-H(10B)	110.7(17)
H(10A)-C(10)-H(10B)	106(2)
C(8)-C(10)-H(10C)	115.0(17)
H(10A)-C(10)-H(10C)	104(2)
H(10B)-C(10)-H(10C)	112(2)
C(8)-C(11)-H(11A)	111.4(19)
C(8)-C(11)-H(11B)	110(2)
H(11A)-C(11)-H(11B)	107(3)
C(8)-C(11)-H(11C)	108.1(19)
H(11A)-C(11)-H(11C)	106(3)
H(11B)-C(11)-H(11C)	114(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **8**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	27(1)	33(1)	24(1)	-1(1)	9(1)	-4(1)
N(1)	30(1)	29(1)	20(1)	-2(1)	6(1)	-5(1)
B(1)	29(1)	26(1)	21(1)	3(1)	4(1)	-2(1)
C(1)	28(1)	34(1)	24(1)	1(1)	9(1)	-5(1)
C(2)	34(1)	37(1)	27(1)	1(1)	10(1)	-5(1)
C(3)	52(1)	45(1)	24(1)	-5(1)	16(1)	-6(1)
C(4)	61(2)	54(2)	28(1)	-17(1)	14(1)	-22(1)
C(5)	45(1)	44(1)	31(1)	-10(1)	11(1)	-19(1)
C(6)	45(1)	40(1)	38(1)	-5(1)	20(1)	2(1)
C(7)	32(1)	67(2)	43(1)	-6(1)	10(1)	-8(1)
C(8)	37(1)	39(1)	30(1)	6(1)	12(1)	-1(1)
C(9)	44(2)	65(2)	54(2)	27(2)	-2(1)	-3(1)
C(10)	69(2)	60(2)	39(1)	12(1)	25(1)	-4(2)
C(11)	71(2)	40(2)	57(2)	5(1)	17(2)	7(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(2)	4600(20)	1080(30)	7138(16)	40(6)
H(3)	5590(20)	2700(30)	8440(18)	41(6)
H(4)	7400(20)	3930(30)	8370(20)	68(8)
H(5)	8260(20)	3770(30)	7007(16)	35(6)
H(6A)	8170(30)	-330(50)	5020(30)	110(13)
H(6B)	7050(30)	90(40)	4240(20)	82(10)
H(6C)	8350(20)	470(30)	4140(20)	58(8)
H(7A)	9710(20)	2250(30)	6220(20)	62(8)
H(7B)	9480(30)	3990(40)	5920(20)	66(9)
H(7C)	9820(30)	2850(40)	5180(30)	89(11)
H(9A)	5200(30)	3560(40)	4350(20)	69(9)
H(9B)	5330(30)	4360(30)	3310(20)	66(8)
H(9C)	5600(30)	2600(30)	3510(20)	55(8)
H(10A)	7290(30)	4940(40)	2890(20)	77(9)
H(10B)	7590(30)	3050(40)	3000(20)	68(9)
H(10C)	8530(30)	4380(30)	3560(20)	67(9)
H(11A)	6710(30)	6420(40)	4300(20)	80(10)
H(11B)	7960(30)	5930(40)	4940(20)	85(11)
H(11C)	6690(30)	5570(40)	5270(20)	77(10)

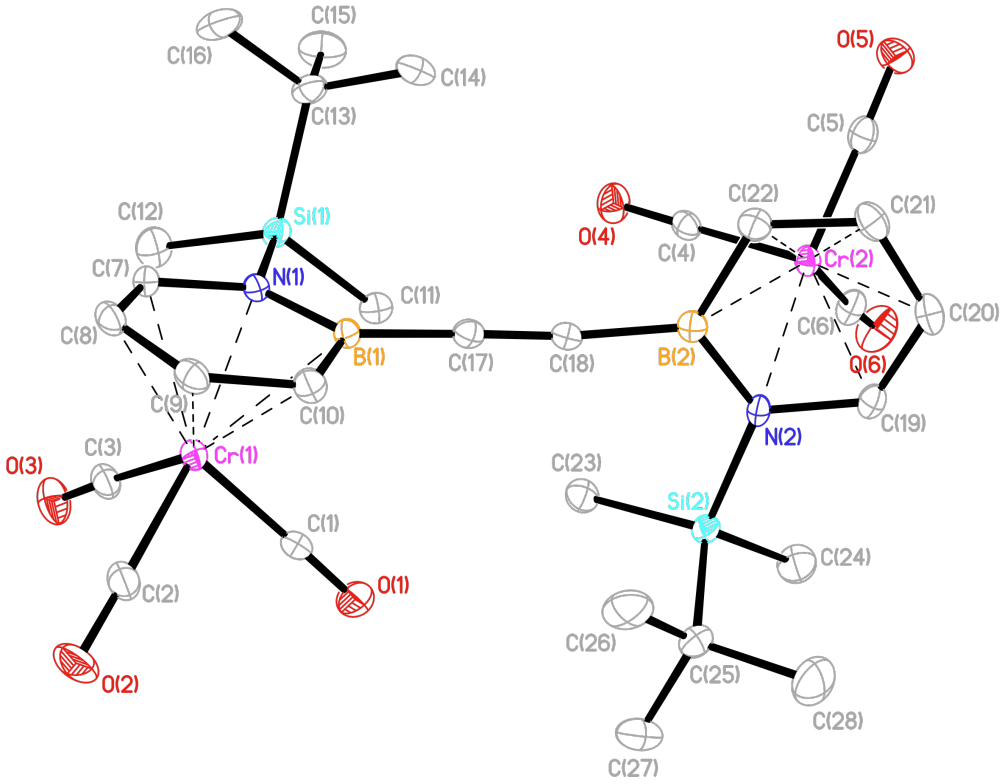
Table S12. Torsion angles [°] for **8**.

C(6)-Si(1)-N(1)-C(5)	139.95(18)
C(7)-Si(1)-N(1)-C(5)	23.4(2)
C(8)-Si(1)-N(1)-C(5)	-95.81(18)
C(6)-Si(1)-N(1)-B(1)	-42.3(2)
C(7)-Si(1)-N(1)-B(1)	-158.80(18)
C(8)-Si(1)-N(1)-B(1)	81.98(17)
C(5)-N(1)-B(1)-C(2)	0.3(3)
Si(1)-N(1)-B(1)-C(2)	-177.52(14)
C(5)-N(1)-B(1)-C(1)	-178.83(19)
Si(1)-N(1)-B(1)-C(1)	3.4(3)
N(1)-B(1)-C(1)-C(1)#1	174(2)
C(2)-B(1)-C(1)-C(1)#1	-5(2)
N(1)-B(1)-C(2)-C(3)	-0.1(3)
C(1)-B(1)-C(2)-C(3)	179.0(2)
B(1)-C(2)-C(3)-C(4)	-0.3(3)
C(2)-C(3)-C(4)-C(5)	0.7(4)
C(3)-C(4)-C(5)-N(1)	-0.6(4)
B(1)-N(1)-C(5)-C(4)	0.1(3)
Si(1)-N(1)-C(5)-C(4)	178.1(2)
N(1)-Si(1)-C(8)-C(9)	-60.5(2)
C(6)-Si(1)-C(8)-C(9)	63.2(2)
C(7)-Si(1)-C(8)-C(9)	-177.8(2)
N(1)-Si(1)-C(8)-C(10)	178.84(17)
C(6)-Si(1)-C(8)-C(10)	-57.5(2)
C(7)-Si(1)-C(8)-C(10)	61.5(2)
N(1)-Si(1)-C(8)-C(11)	61.1(2)
C(6)-Si(1)-C(8)-C(11)	-175.23(18)
C(7)-Si(1)-C(8)-C(11)	-56.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

X-ray Crystal Structure Determination of 10. Crystals of **10** suitable for X-ray diffraction were obtained by slow evaporation of a solution of **10** in Et_2O.



Diffraction intensity data were collected with a Bruker Smart Apex CCD diffractometer at 173(2) K using MoKα - radiation (0.71073 Å). The structure was solved using direct methods, completed by subsequent difference Fourier syntheses, and refined by full matrix least-squares procedures on F^2. All non-H atoms were refined with anisotropic thermal parameters. H atoms were found on the residual density map and refined with isotropic thermal parameters. The Flack parameter is 0.00(8). All software and sources scattering factors are contained in the SHELXTL (6.10) program package (G.Sheldrick, Bruker XRD, Madison, WI). Crystallographic data and some details of data collection and crystal structure refinement for $C_{28}H_{38}B_2N_2O_6Si_2$ are given in the following tables.

Table S13. Crystal data and structure refinement for **10** (liu50).

Identification code	liu50	
Empirical formula	$C_{28}H_{38}B_2Cr_2N_2O_6Si_2$	
Formula weight	680.40	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 12.8679(12) Å	α= 90°.
	b = 20.821(2) Å	β= 90°.
	c = 25.082(2) Å	γ = 90°.
Volume	6719.9(11) $Å^3$	
Z	8	
Density (calculated)	1.345 Mg/m^3	
Absorption coefficient	0.759 mm^{-1}	
F(000)	2832	
Crystal size	0.12 x 0.04 x 0.02 mm^3	
Theta range for data collection	1.62 to 25.00°.	
Index ranges	-15<=h<=15, -24<=k<=24, -29<=l<=29	
Reflections collected	52442	
Independent reflections	5928 [R(int) = 0.1524]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9850 and 0.9145	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5928 / 0 / 379	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0610, wR2 = 0.1073	
R indices (all data)	R1 = 0.1086, wR2 = 0.1262	
Largest diff. peak and hole	0.412 and -0.367 $e.Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	6961(1)	1763(1)	6635(1)	23(1)
Cr(2)	7037(1)	419(1)	3540(1)	23(1)
Si(1)	8380(1)	331(1)	6166(1)	24(1)
Si(2)	7451(1)	2074(1)	3982(1)	26(1)
O(1)	7840(3)	2564(2)	5746(1)	49(1)
O(2)	6167(3)	2944(2)	7181(1)	48(1)
O(3)	8953(3)	2022(2)	7214(1)	45(1)
O(4)	8613(3)	-12(2)	4340(1)	40(1)
O(5)	7081(3)	-902(2)	3071(1)	44(1)
O(6)	8790(3)	692(2)	2788(1)	52(1)
N(1)	7186(3)	765(2)	6348(1)	20(1)
N(2)	6620(3)	1372(2)	3864(1)	21(1)
B(1)	6447(4)	1050(2)	5962(2)	21(1)
B(2)	6272(4)	914(3)	4277(2)	22(1)
C(1)	7495(4)	2256(2)	6080(2)	30(1)
C(2)	6474(4)	2492(3)	6967(2)	32(1)
C(3)	8195(4)	1906(2)	6991(2)	30(1)
C(4)	7995(4)	159(2)	4033(2)	25(1)
C(5)	7051(4)	-388(3)	3249(2)	31(1)
C(6)	8108(4)	610(2)	3081(2)	32(1)
C(7)	6951(4)	781(2)	6894(2)	24(1)
C(8)	6058(4)	1060(2)	7095(2)	26(1)
C(9)	5366(4)	1390(2)	6755(2)	26(1)
C(10)	5538(4)	1402(2)	6209(2)	26(1)
C(11)	8959(4)	726(2)	5578(2)	28(1)
C(12)	9298(4)	396(3)	6740(2)	40(1)
C(13)	8010(4)	-529(2)	6053(2)	30(1)
C(14)	7231(4)	-597(2)	5589(2)	38(1)
C(15)	8994(4)	-911(3)	5909(2)	47(2)
C(16)	7518(4)	-818(2)	6555(2)	43(1)
C(17)	6568(3)	1008(2)	5357(2)	23(1)
C(18)	6510(3)	995(2)	4875(2)	21(1)
C(19)	6253(4)	1303(2)	3343(2)	27(1)
C(20)	5583(4)	814(2)	3194(2)	30(1)
C(21)	5316(4)	320(2)	3554(2)	31(1)
C(22)	5645(3)	351(2)	4082(2)	26(1)
C(23)	8432(4)	1878(2)	4498(2)	33(1)

C(24)	8145(4)	2265(3)	3354(2)	45(2)
C(25)	6561(4)	2748(2)	4174(2)	36(1)
C(26)	5838(4)	2571(3)	4637(2)	50(2)
C(27)	7243(5)	3321(3)	4344(2)	60(2)
C(28)	5895(5)	2951(3)	3693(2)	65(2)

Table S15. Bond lengths [Å] and angles [°] for **10**.

Cr(1)-C(2)	1.841(5)
Cr(1)-C(3)	1.846(5)
Cr(1)-C(1)	1.859(5)
Cr(1)-C(7)	2.145(4)
Cr(1)-C(8)	2.196(5)
Cr(1)-C(9)	2.215(5)
Cr(1)-N(1)	2.217(4)
Cr(1)-C(10)	2.249(5)
Cr(1)-B(1)	2.341(5)
Cr(2)-C(4)	1.828(5)
Cr(2)-C(5)	1.831(5)
Cr(2)-C(6)	1.840(5)
Cr(2)-C(19)	2.156(5)
Cr(2)-N(2)	2.211(4)
Cr(2)-C(20)	2.221(5)
Cr(2)-C(21)	2.225(5)
Cr(2)-C(22)	2.253(4)
Cr(2)-B(2)	2.334(5)
Si(1)-N(1)	1.840(4)
Si(1)-C(11)	1.846(5)
Si(1)-C(12)	1.866(5)
Si(1)-C(13)	1.875(5)
Si(2)-N(2)	1.834(4)
Si(2)-C(23)	1.853(5)
Si(2)-C(24)	1.854(5)
Si(2)-C(25)	1.875(5)
O(1)-C(1)	1.146(5)
O(2)-C(2)	1.153(5)
O(3)-C(3)	1.151(5)
O(4)-C(4)	1.163(5)
O(5)-C(5)	1.161(5)
O(6)-C(6)	1.156(6)
N(1)-C(7)	1.402(5)

N(1)-B(1)	1.481(6)
N(2)-C(19)	1.397(5)
N(2)-B(2)	1.477(6)
B(1)-C(10)	1.513(7)
B(1)-C(17)	1.529(7)
B(2)-C(22)	1.506(7)
B(2)-C(18)	1.540(7)
C(7)-C(8)	1.382(6)
C(7)-H(7A)	1.0000
C(8)-C(9)	1.411(6)
C(8)-H(8A)	1.0000
C(9)-C(10)	1.387(6)
C(9)-H(9A)	1.0000
C(10)-H(10A)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(16)	1.533(6)
C(13)-C(15)	1.537(7)
C(13)-C(14)	1.542(7)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.211(6)
C(19)-C(20)	1.387(6)
C(19)-H(19A)	1.0000
C(20)-C(21)	1.411(7)
C(20)-H(20A)	1.0000
C(21)-C(22)	1.392(6)
C(21)-H(21A)	1.0000
C(22)-H(22A)	1.0000

C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.533(7)
C(25)-C(28)	1.539(7)
C(25)-C(27)	1.539(7)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800

C(2)-Cr(1)-C(3)	86.6(2)
C(2)-Cr(1)-C(1)	90.5(2)
C(3)-Cr(1)-C(1)	87.4(2)
C(2)-Cr(1)-C(7)	130.25(19)
C(3)-Cr(1)-C(7)	90.7(2)
C(1)-Cr(1)-C(7)	139.02(19)
C(2)-Cr(1)-C(8)	97.5(2)
C(3)-Cr(1)-C(8)	107.95(19)
C(1)-Cr(1)-C(8)	162.96(19)
C(7)-Cr(1)-C(8)	37.12(17)
C(2)-Cr(1)-C(9)	84.9(2)
C(3)-Cr(1)-C(9)	141.96(19)
C(1)-Cr(1)-C(9)	129.6(2)
C(7)-Cr(1)-C(9)	67.61(18)
C(8)-Cr(1)-C(9)	37.31(16)
C(2)-Cr(1)-N(1)	164.44(18)
C(3)-Cr(1)-N(1)	101.27(18)
C(1)-Cr(1)-N(1)	103.12(17)
C(7)-Cr(1)-N(1)	37.44(14)
C(8)-Cr(1)-N(1)	67.36(15)
C(9)-Cr(1)-N(1)	80.61(15)

C(2)-Cr(1)-C(10)	102.3(2)
C(3)-Cr(1)-C(10)	169.7(2)
C(1)-Cr(1)-C(10)	97.51(19)
C(7)-Cr(1)-C(10)	79.66(18)
C(8)-Cr(1)-C(10)	66.16(17)
C(9)-Cr(1)-C(10)	36.19(16)
N(1)-Cr(1)-C(10)	68.88(15)
C(2)-Cr(1)-B(1)	138.8(2)
C(3)-Cr(1)-B(1)	133.9(2)
C(1)-Cr(1)-B(1)	85.19(19)
C(7)-Cr(1)-B(1)	67.20(17)
C(8)-Cr(1)-B(1)	78.85(17)
C(9)-Cr(1)-B(1)	67.31(18)
N(1)-Cr(1)-B(1)	37.79(15)
C(10)-Cr(1)-B(1)	38.42(17)
C(4)-Cr(2)-C(5)	89.5(2)
C(4)-Cr(2)-C(6)	88.9(2)
C(5)-Cr(2)-C(6)	86.7(2)
C(4)-Cr(2)-C(19)	136.30(19)
C(5)-Cr(2)-C(19)	134.1(2)
C(6)-Cr(2)-C(19)	91.3(2)
C(4)-Cr(2)-N(2)	100.40(17)
C(5)-Cr(2)-N(2)	166.47(19)
C(6)-Cr(2)-N(2)	102.57(18)
C(19)-Cr(2)-N(2)	37.29(14)
C(4)-Cr(2)-C(20)	160.51(19)
C(5)-Cr(2)-C(20)	101.1(2)
C(6)-Cr(2)-C(20)	107.8(2)
C(19)-Cr(2)-C(20)	36.90(17)
N(2)-Cr(2)-C(20)	66.88(15)
C(4)-Cr(2)-C(21)	129.37(19)
C(5)-Cr(2)-C(21)	86.0(2)
C(6)-Cr(2)-C(21)	140.9(2)
C(19)-Cr(2)-C(21)	67.46(18)
N(2)-Cr(2)-C(21)	80.55(16)
C(20)-Cr(2)-C(21)	37.00(17)
C(4)-Cr(2)-C(22)	96.32(18)
C(5)-Cr(2)-C(22)	100.94(19)
C(6)-Cr(2)-C(22)	170.7(2)
C(19)-Cr(2)-C(22)	79.66(18)

N(2)-Cr(2)-C(22)	69.03(15)
C(20)-Cr(2)-C(22)	65.78(17)
C(21)-Cr(2)-C(22)	36.23(16)
C(4)-Cr(2)-B(2)	83.09(19)
C(5)-Cr(2)-B(2)	136.4(2)
C(6)-Cr(2)-B(2)	135.7(2)
C(19)-Cr(2)-B(2)	66.87(18)
N(2)-Cr(2)-B(2)	37.81(15)
C(20)-Cr(2)-B(2)	77.96(18)
C(21)-Cr(2)-B(2)	66.98(18)
C(22)-Cr(2)-B(2)	38.29(17)
N(1)-Si(1)-C(11)	108.45(19)
N(1)-Si(1)-C(12)	107.5(2)
C(11)-Si(1)-C(12)	109.2(2)
N(1)-Si(1)-C(13)	107.2(2)
C(11)-Si(1)-C(13)	114.0(2)
C(12)-Si(1)-C(13)	110.3(2)
N(2)-Si(2)-C(23)	109.5(2)
N(2)-Si(2)-C(24)	108.4(2)
C(23)-Si(2)-C(24)	108.2(2)
N(2)-Si(2)-C(25)	106.4(2)
C(23)-Si(2)-C(25)	113.7(2)
C(24)-Si(2)-C(25)	110.6(2)
C(7)-N(1)-B(1)	119.3(4)
C(7)-N(1)-Si(1)	115.7(3)
B(1)-N(1)-Si(1)	124.8(3)
C(7)-N(1)-Cr(1)	68.5(2)
B(1)-N(1)-Cr(1)	75.7(2)
Si(1)-N(1)-Cr(1)	130.55(19)
C(19)-N(2)-B(2)	119.1(4)
C(19)-N(2)-Si(2)	115.4(3)
B(2)-N(2)-Si(2)	125.3(3)
C(19)-N(2)-Cr(2)	69.2(2)
B(2)-N(2)-Cr(2)	75.6(2)
Si(2)-N(2)-Cr(2)	129.25(19)
N(1)-B(1)-C(10)	115.0(4)
N(1)-B(1)-C(17)	124.1(4)
C(10)-B(1)-C(17)	120.8(4)
N(1)-B(1)-Cr(1)	66.5(2)
C(10)-B(1)-Cr(1)	67.5(3)

C(17)-B(1)-Cr(1)	136.3(3)
N(2)-B(2)-C(22)	115.9(4)
N(2)-B(2)-C(18)	123.5(4)
C(22)-B(2)-C(18)	120.6(4)
N(2)-B(2)-Cr(2)	66.6(2)
C(22)-B(2)-Cr(2)	67.9(3)
C(18)-B(2)-Cr(2)	137.4(3)
O(1)-C(1)-Cr(1)	178.6(5)
O(2)-C(2)-Cr(1)	179.1(5)
O(3)-C(3)-Cr(1)	177.1(4)
O(4)-C(4)-Cr(2)	178.9(4)
O(5)-C(5)-Cr(2)	178.4(5)
O(6)-C(6)-Cr(2)	176.0(5)
C(8)-C(7)-N(1)	123.0(4)
C(8)-C(7)-Cr(1)	73.5(3)
N(1)-C(7)-Cr(1)	74.1(2)
C(8)-C(7)-H(7A)	118.2
N(1)-C(7)-H(7A)	118.2
Cr(1)-C(7)-H(7A)	118.2
C(7)-C(8)-C(9)	120.6(4)
C(7)-C(8)-Cr(1)	69.4(3)
C(9)-C(8)-Cr(1)	72.1(3)
C(7)-C(8)-H(8A)	118.9
C(9)-C(8)-H(8A)	118.9
Cr(1)-C(8)-H(8A)	118.9
C(10)-C(9)-C(8)	120.3(4)
C(10)-C(9)-Cr(1)	73.2(3)
C(8)-C(9)-Cr(1)	70.6(3)
C(10)-C(9)-H(9A)	119.4
C(8)-C(9)-H(9A)	119.4
Cr(1)-C(9)-H(9A)	119.4
C(9)-C(10)-B(1)	121.2(4)
C(9)-C(10)-Cr(1)	70.6(3)
B(1)-C(10)-Cr(1)	74.1(3)
C(9)-C(10)-H(10A)	119.0
B(1)-C(10)-H(10A)	119.0
Cr(1)-C(10)-H(10A)	119.0
Si(1)-C(11)-H(11A)	109.5
Si(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5

Si(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(1)-C(12)-H(12A)	109.5
Si(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(16)-C(13)-C(15)	109.2(4)
C(16)-C(13)-C(14)	108.4(4)
C(15)-C(13)-C(14)	108.1(4)
C(16)-C(13)-Si(1)	110.8(3)
C(15)-C(13)-Si(1)	108.7(3)
C(14)-C(13)-Si(1)	111.5(3)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-B(1)	170.5(5)
C(17)-C(18)-B(2)	170.5(5)
C(20)-C(19)-N(2)	122.6(4)
C(20)-C(19)-Cr(2)	74.1(3)
N(2)-C(19)-Cr(2)	73.5(2)
C(20)-C(19)-H(19A)	118.4
N(2)-C(19)-H(19A)	118.4

Cr(2)-C(19)-H(19A)	118.4
C(19)-C(20)-C(21)	120.9(4)
C(19)-C(20)-Cr(2)	69.0(3)
C(21)-C(20)-Cr(2)	71.6(3)
C(19)-C(20)-H(20A)	118.5
C(21)-C(20)-H(20A)	118.5
Cr(2)-C(20)-H(20A)	118.5
C(22)-C(21)-C(20)	120.2(4)
C(22)-C(21)-Cr(2)	73.0(3)
C(20)-C(21)-Cr(2)	71.4(3)
C(22)-C(21)-H(21A)	119.6
C(20)-C(21)-H(21A)	119.6
Cr(2)-C(21)-H(21A)	119.6
C(21)-C(22)-B(2)	120.5(4)
C(21)-C(22)-Cr(2)	70.8(3)
B(2)-C(22)-Cr(2)	73.8(3)
C(21)-C(22)-H(22A)	119.4
B(2)-C(22)-H(22A)	119.4
Cr(2)-C(22)-H(22A)	119.4
Si(2)-C(23)-H(23A)	109.5
Si(2)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
Si(2)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
Si(2)-C(24)-H(24A)	109.5
Si(2)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
Si(2)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(28)	108.7(5)
C(26)-C(25)-C(27)	108.9(4)
C(28)-C(25)-C(27)	108.8(5)
C(26)-C(25)-Si(2)	112.6(3)
C(28)-C(25)-Si(2)	110.1(4)
C(27)-C(25)-Si(2)	107.6(4)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5

C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	28(1)	23(1)	18(1)	-2(1)	1(1)	1(1)
Cr(2)	25(1)	26(1)	17(1)	-2(1)	1(1)	1(1)
Si(1)	27(1)	23(1)	23(1)	2(1)	1(1)	6(1)
Si(2)	30(1)	23(1)	23(1)	4(1)	-2(1)	-4(1)
O(1)	80(3)	34(2)	34(2)	7(2)	9(2)	-10(2)
O(2)	67(3)	33(2)	45(2)	-17(2)	14(2)	3(2)
O(3)	40(3)	62(3)	33(2)	-10(2)	-5(2)	-9(2)
O(4)	37(2)	47(2)	37(2)	-2(2)	-7(2)	11(2)
O(5)	66(3)	32(2)	33(2)	-12(2)	5(2)	3(2)
O(6)	41(3)	72(3)	43(2)	12(2)	21(2)	7(2)
N(1)	23(2)	20(2)	17(2)	-1(2)	1(2)	-1(2)
N(2)	21(2)	26(2)	16(2)	1(2)	-3(2)	3(2)
B(1)	24(3)	21(3)	18(3)	0(2)	-4(2)	-3(2)
B(2)	20(3)	25(3)	22(3)	-2(2)	2(2)	3(2)
C(1)	44(3)	20(3)	27(3)	-5(2)	-1(3)	1(2)
C(2)	36(3)	34(3)	25(3)	-5(2)	1(2)	-5(3)
C(3)	34(3)	33(3)	23(3)	-6(2)	3(2)	-5(2)
C(4)	27(3)	26(3)	23(3)	-5(2)	5(2)	-2(2)
C(5)	34(3)	40(3)	20(3)	2(2)	4(2)	3(3)
C(6)	34(3)	38(3)	26(3)	4(2)	2(3)	9(3)

C(7)	31(3)	23(3)	17(2)	0(2)	-3(2)	-2(2)
C(8)	29(3)	27(3)	21(2)	-6(2)	5(2)	-4(2)
C(9)	26(3)	26(3)	27(3)	-6(2)	5(2)	0(2)
C(10)	25(3)	27(3)	26(3)	-2(2)	-2(2)	3(2)
C(11)	22(3)	29(3)	34(3)	1(2)	0(2)	2(2)
C(12)	33(3)	46(4)	41(3)	0(3)	-7(3)	15(3)
C(13)	35(3)	23(3)	33(3)	4(2)	6(3)	5(2)
C(14)	47(4)	24(3)	42(3)	-7(2)	-1(3)	-5(2)
C(15)	40(4)	34(3)	68(4)	-5(3)	8(3)	15(3)
C(16)	52(4)	25(3)	53(4)	12(3)	9(3)	3(3)
C(17)	20(3)	20(3)	27(3)	0(2)	-2(2)	2(2)
C(18)	20(3)	19(3)	25(3)	-2(2)	1(2)	-1(2)
C(19)	30(3)	31(3)	20(2)	4(2)	0(2)	2(2)
C(20)	24(3)	43(3)	24(3)	-6(2)	-3(2)	-1(2)
C(21)	22(3)	38(3)	34(3)	-7(2)	-4(2)	-4(2)
C(22)	20(3)	28(3)	28(3)	2(2)	1(2)	-5(2)
C(23)	28(3)	35(3)	36(3)	0(2)	-3(2)	-9(2)
C(24)	49(4)	46(4)	41(3)	9(3)	6(3)	-16(3)
C(25)	46(4)	29(3)	33(3)	3(2)	-7(3)	8(3)
C(26)	56(4)	37(4)	57(4)	0(3)	12(3)	20(3)
C(27)	95(6)	27(3)	59(4)	-3(3)	-3(4)	-2(3)
C(28)	77(5)	62(5)	55(4)	0(3)	-18(4)	32(4)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**.

	x	y	z	U(eq)
H(7A)	7498	640	7151	29
H(8A)	5992	1119	7489	31
H(9A)	4824	1676	6913	32
H(10A)	5128	1707	5984	31
H(11A)	9132	1172	5666	42
H(11B)	8461	719	5282	42
H(11C)	9592	496	5473	42
H(12A)	9485	847	6795	60
H(12B)	9926	146	6664	60
H(12C)	8964	228	7062	60
H(14A)	7055	-1051	5540	57
H(14B)	7545	-430	5261	57
H(14C)	6600	-354	5671	57
H(15A)	8810	-1362	5849	71
H(15B)	9494	-882	6203	71

H(15C)	9303	-733	5585	71
H(16A)	7331	-1267	6488	65
H(16B)	6893	-575	6649	65
H(16C)	8017	-798	6850	65
H(19A)	6557	1582	3058	33
H(20A)	5445	746	2805	36
H(21A)	4987	-82	3417	38
H(22A)	5562	-34	4316	31
H(23A)	8869	1523	4373	49
H(23B)	8079	1751	4828	49
H(23C)	8866	2255	4566	49
H(24A)	8606	1908	3260	68
H(24B)	8558	2656	3403	68
H(24C)	7639	2332	3067	68
H(26A)	5390	2938	4722	75
H(26B)	6254	2458	4950	75
H(26C)	5406	2203	4534	75
H(27A)	6797	3682	4447	91
H(27B)	7688	3449	4045	91
H(27C)	7677	3195	4647	91
H(28A)	5433	3303	3797	97
H(28B)	5478	2585	3572	97
H(28C)	6349	3094	3403	97

Table S18. Torsion angles [°] for **10**.

C(11)-Si(1)-N(1)-C(7)	-147.3(3)
C(12)-Si(1)-N(1)-C(7)	-29.4(4)
C(13)-Si(1)-N(1)-C(7)	89.2(3)
C(11)-Si(1)-N(1)-B(1)	37.0(4)
C(12)-Si(1)-N(1)-B(1)	154.9(4)
C(13)-Si(1)-N(1)-B(1)	-86.5(4)
C(11)-Si(1)-N(1)-Cr(1)	-64.5(3)
C(12)-Si(1)-N(1)-Cr(1)	53.5(3)
C(13)-Si(1)-N(1)-Cr(1)	172.1(2)
C(2)-Cr(1)-N(1)-C(7)	-43.3(7)
C(3)-Cr(1)-N(1)-C(7)	76.1(3)
C(1)-Cr(1)-N(1)-C(7)	166.1(3)
C(8)-Cr(1)-N(1)-C(7)	-28.8(3)
C(9)-Cr(1)-N(1)-C(7)	-65.2(3)
C(10)-Cr(1)-N(1)-C(7)	-100.8(3)

B(1)-Cr(1)-N(1)-C(7)	-130.1(4)
C(2)-Cr(1)-N(1)-B(1)	86.8(7)
C(3)-Cr(1)-N(1)-B(1)	-153.8(3)
C(1)-Cr(1)-N(1)-B(1)	-63.8(3)
C(7)-Cr(1)-N(1)-B(1)	130.1(4)
C(8)-Cr(1)-N(1)-B(1)	101.3(3)
C(9)-Cr(1)-N(1)-B(1)	64.9(3)
C(10)-Cr(1)-N(1)-B(1)	29.3(3)
C(2)-Cr(1)-N(1)-Si(1)	-149.3(6)
C(3)-Cr(1)-N(1)-Si(1)	-29.9(3)
C(1)-Cr(1)-N(1)-Si(1)	60.0(3)
C(7)-Cr(1)-N(1)-Si(1)	-106.1(3)
C(8)-Cr(1)-N(1)-Si(1)	-134.8(3)
C(9)-Cr(1)-N(1)-Si(1)	-171.3(3)
C(10)-Cr(1)-N(1)-Si(1)	153.1(3)
B(1)-Cr(1)-N(1)-Si(1)	123.9(4)
C(23)-Si(2)-N(2)-C(19)	-147.4(3)
C(24)-Si(2)-N(2)-C(19)	-29.6(4)
C(25)-Si(2)-N(2)-C(19)	89.3(3)
C(23)-Si(2)-N(2)-B(2)	36.5(4)
C(24)-Si(2)-N(2)-B(2)	154.3(4)
C(25)-Si(2)-N(2)-B(2)	-86.7(4)
C(23)-Si(2)-N(2)-Cr(2)	-64.2(3)
C(24)-Si(2)-N(2)-Cr(2)	53.6(3)
C(25)-Si(2)-N(2)-Cr(2)	172.5(2)
C(4)-Cr(2)-N(2)-C(19)	166.5(3)
C(5)-Cr(2)-N(2)-C(19)	-57.0(8)
C(6)-Cr(2)-N(2)-C(19)	75.2(3)
C(20)-Cr(2)-N(2)-C(19)	-29.0(3)
C(21)-Cr(2)-N(2)-C(19)	-65.0(3)
C(22)-Cr(2)-N(2)-C(19)	-100.7(3)
B(2)-Cr(2)-N(2)-C(19)	-129.4(4)
C(4)-Cr(2)-N(2)-B(2)	-64.2(3)
C(5)-Cr(2)-N(2)-B(2)	72.4(8)
C(6)-Cr(2)-N(2)-B(2)	-155.4(3)
C(19)-Cr(2)-N(2)-B(2)	129.4(4)
C(20)-Cr(2)-N(2)-B(2)	100.4(3)
C(21)-Cr(2)-N(2)-B(2)	64.4(3)
C(22)-Cr(2)-N(2)-B(2)	28.7(3)
C(4)-Cr(2)-N(2)-Si(2)	60.0(3)

C(5)-Cr(2)-N(2)-Si(2)	-163.5(6)
C(6)-Cr(2)-N(2)-Si(2)	-31.2(3)
C(19)-Cr(2)-N(2)-Si(2)	-106.5(3)
C(20)-Cr(2)-N(2)-Si(2)	-135.5(3)
C(21)-Cr(2)-N(2)-Si(2)	-171.5(3)
C(22)-Cr(2)-N(2)-Si(2)	152.8(3)
B(2)-Cr(2)-N(2)-Si(2)	124.1(4)
C(7)-N(1)-B(1)-C(10)	6.3(6)
Si(1)-N(1)-B(1)-C(10)	-178.2(3)
Cr(1)-N(1)-B(1)-C(10)	-48.4(4)
C(7)-N(1)-B(1)-C(17)	-174.2(4)
Si(1)-N(1)-B(1)-C(17)	1.4(6)
Cr(1)-N(1)-B(1)-C(17)	131.1(5)
C(7)-N(1)-B(1)-Cr(1)	54.7(3)
Si(1)-N(1)-B(1)-Cr(1)	-129.8(3)
C(2)-Cr(1)-B(1)-N(1)	-156.0(3)
C(3)-Cr(1)-B(1)-N(1)	37.0(4)
C(1)-Cr(1)-B(1)-N(1)	118.7(3)
C(7)-Cr(1)-B(1)-N(1)	-30.3(2)
C(8)-Cr(1)-B(1)-N(1)	-67.3(3)
C(9)-Cr(1)-B(1)-N(1)	-104.5(3)
C(10)-Cr(1)-B(1)-N(1)	-132.8(4)
C(2)-Cr(1)-B(1)-C(10)	-23.2(4)
C(3)-Cr(1)-B(1)-C(10)	169.8(3)
C(1)-Cr(1)-B(1)-C(10)	-108.5(3)
C(7)-Cr(1)-B(1)-C(10)	102.5(3)
C(8)-Cr(1)-B(1)-C(10)	65.5(3)
C(9)-Cr(1)-B(1)-C(10)	28.3(3)
N(1)-Cr(1)-B(1)-C(10)	132.8(4)
C(2)-Cr(1)-B(1)-C(17)	88.5(6)
C(3)-Cr(1)-B(1)-C(17)	-78.6(6)
C(1)-Cr(1)-B(1)-C(17)	3.2(5)
C(7)-Cr(1)-B(1)-C(17)	-145.8(6)
C(8)-Cr(1)-B(1)-C(17)	177.2(5)
C(9)-Cr(1)-B(1)-C(17)	140.0(5)
N(1)-Cr(1)-B(1)-C(17)	-115.5(6)
C(10)-Cr(1)-B(1)-C(17)	111.7(6)
C(19)-N(2)-B(2)-C(22)	7.6(6)
Si(2)-N(2)-B(2)-C(22)	-176.4(3)
Cr(2)-N(2)-B(2)-C(22)	-48.2(4)

C(19)-N(2)-B(2)-C(18)	-171.8(4)
Si(2)-N(2)-B(2)-C(18)	4.2(6)
Cr(2)-N(2)-B(2)-C(18)	132.4(5)
C(19)-N(2)-B(2)-Cr(2)	55.8(3)
Si(2)-N(2)-B(2)-Cr(2)	-128.2(3)
C(4)-Cr(2)-B(2)-N(2)	116.9(3)
C(5)-Cr(2)-B(2)-N(2)	-161.1(3)
C(6)-Cr(2)-B(2)-N(2)	35.6(4)
C(19)-Cr(2)-B(2)-N(2)	-30.6(2)
C(20)-Cr(2)-B(2)-N(2)	-67.7(3)
C(21)-Cr(2)-B(2)-N(2)	-104.9(3)
C(22)-Cr(2)-B(2)-N(2)	-133.7(4)
C(4)-Cr(2)-B(2)-C(22)	-109.4(3)
C(5)-Cr(2)-B(2)-C(22)	-27.4(4)
C(6)-Cr(2)-B(2)-C(22)	169.3(3)
C(19)-Cr(2)-B(2)-C(22)	103.1(3)
N(2)-Cr(2)-B(2)-C(22)	133.7(4)
C(20)-Cr(2)-B(2)-C(22)	66.0(3)
C(21)-Cr(2)-B(2)-C(22)	28.8(3)
C(4)-Cr(2)-B(2)-C(18)	2.3(5)
C(5)-Cr(2)-B(2)-C(18)	84.2(6)
C(6)-Cr(2)-B(2)-C(18)	-79.0(6)
C(19)-Cr(2)-B(2)-C(18)	-145.3(6)
N(2)-Cr(2)-B(2)-C(18)	-114.6(6)
C(20)-Cr(2)-B(2)-C(18)	177.7(5)
C(21)-Cr(2)-B(2)-C(18)	140.5(6)
C(22)-Cr(2)-B(2)-C(18)	111.7(6)
C(2)-Cr(1)-C(1)-O(1)	74(20)
C(3)-Cr(1)-C(1)-O(1)	-12(20)
C(7)-Cr(1)-C(1)-O(1)	-101(20)
C(8)-Cr(1)-C(1)-O(1)	-167(19)
C(9)-Cr(1)-C(1)-O(1)	158(20)
N(1)-Cr(1)-C(1)-O(1)	-113(20)
C(10)-Cr(1)-C(1)-O(1)	177(100)
B(1)-Cr(1)-C(1)-O(1)	-147(20)
C(3)-Cr(1)-C(2)-O(2)	-79(33)
C(1)-Cr(1)-C(2)-O(2)	-167(100)
C(7)-Cr(1)-C(2)-O(2)	9(34)
C(8)-Cr(1)-C(2)-O(2)	28(33)
C(9)-Cr(1)-C(2)-O(2)	63(33)

N(1)-Cr(1)-C(2)-O(2)	42(34)
C(10)-Cr(1)-C(2)-O(2)	95(33)
B(1)-Cr(1)-C(2)-O(2)	110(33)
C(2)-Cr(1)-C(3)-O(3)	-25(8)
C(1)-Cr(1)-C(3)-O(3)	66(8)
C(7)-Cr(1)-C(3)-O(3)	-155(8)
C(8)-Cr(1)-C(3)-O(3)	-122(8)
C(9)-Cr(1)-C(3)-O(3)	-102(8)
N(1)-Cr(1)-C(3)-O(3)	169(8)
C(10)-Cr(1)-C(3)-O(3)	-175(100)
B(1)-Cr(1)-C(3)-O(3)	146(8)
C(5)-Cr(2)-C(4)-O(4)	38(25)
C(6)-Cr(2)-C(4)-O(4)	-48(25)
C(19)-Cr(2)-C(4)-O(4)	-139(25)
N(2)-Cr(2)-C(4)-O(4)	-151(25)
C(20)-Cr(2)-C(4)-O(4)	162(100)
C(21)-Cr(2)-C(4)-O(4)	123(25)
C(22)-Cr(2)-C(4)-O(4)	139(25)
B(2)-Cr(2)-C(4)-O(4)	175(100)
C(4)-Cr(2)-C(5)-O(5)	-19(17)
C(6)-Cr(2)-C(5)-O(5)	70(17)
C(19)-Cr(2)-C(5)-O(5)	159(17)
N(2)-Cr(2)-C(5)-O(5)	-156(17)
C(20)-Cr(2)-C(5)-O(5)	178(100)
C(21)-Cr(2)-C(5)-O(5)	-148(17)
C(22)-Cr(2)-C(5)-O(5)	-115(17)
B(2)-Cr(2)-C(5)-O(5)	-98(17)
C(4)-Cr(2)-C(6)-O(6)	73(7)
C(5)-Cr(2)-C(6)-O(6)	-17(7)
C(19)-Cr(2)-C(6)-O(6)	-151(7)
N(2)-Cr(2)-C(6)-O(6)	173(6)
C(20)-Cr(2)-C(6)-O(6)	-118(6)
C(21)-Cr(2)-C(6)-O(6)	-97(6)
C(22)-Cr(2)-C(6)-O(6)	-163(6)
B(2)-Cr(2)-C(6)-O(6)	152(6)
B(1)-N(1)-C(7)-C(8)	-0.8(6)
Si(1)-N(1)-C(7)-C(8)	-176.8(4)
Cr(1)-N(1)-C(7)-C(8)	57.4(4)
B(1)-N(1)-C(7)-Cr(1)	-58.2(4)
Si(1)-N(1)-C(7)-Cr(1)	125.9(2)

C(2)-Cr(1)-C(7)-C(8)	33.5(4)
C(3)-Cr(1)-C(7)-C(8)	119.7(3)
C(1)-Cr(1)-C(7)-C(8)	-153.5(3)
C(9)-Cr(1)-C(7)-C(8)	-28.2(3)
N(1)-Cr(1)-C(7)-C(8)	-132.6(4)
C(10)-Cr(1)-C(7)-C(8)	-63.9(3)
B(1)-Cr(1)-C(7)-C(8)	-102.0(3)
C(2)-Cr(1)-C(7)-N(1)	166.1(3)
C(3)-Cr(1)-C(7)-N(1)	-107.8(3)
C(1)-Cr(1)-C(7)-N(1)	-20.9(4)
C(8)-Cr(1)-C(7)-N(1)	132.6(4)
C(9)-Cr(1)-C(7)-N(1)	104.3(3)
C(10)-Cr(1)-C(7)-N(1)	68.6(2)
B(1)-Cr(1)-C(7)-N(1)	30.6(2)
N(1)-C(7)-C(8)-C(9)	-4.8(7)
Cr(1)-C(7)-C(8)-C(9)	52.9(4)
N(1)-C(7)-C(8)-Cr(1)	-57.7(4)
C(2)-Cr(1)-C(8)-C(7)	-154.9(3)
C(3)-Cr(1)-C(8)-C(7)	-66.0(3)
C(1)-Cr(1)-C(8)-C(7)	87.6(7)
C(9)-Cr(1)-C(8)-C(7)	133.8(4)
N(1)-Cr(1)-C(8)-C(7)	29.0(2)
C(10)-Cr(1)-C(8)-C(7)	105.0(3)
B(1)-Cr(1)-C(8)-C(7)	66.8(3)
C(2)-Cr(1)-C(8)-C(9)	71.3(3)
C(3)-Cr(1)-C(8)-C(9)	160.2(3)
C(1)-Cr(1)-C(8)-C(9)	-46.2(8)
C(7)-Cr(1)-C(8)-C(9)	-133.8(4)
N(1)-Cr(1)-C(8)-C(9)	-104.8(3)
C(10)-Cr(1)-C(8)-C(9)	-28.8(3)
B(1)-Cr(1)-C(8)-C(9)	-67.0(3)
C(7)-C(8)-C(9)-C(10)	4.3(7)
Cr(1)-C(8)-C(9)-C(10)	56.0(4)
C(7)-C(8)-C(9)-Cr(1)	-51.7(4)
C(2)-Cr(1)-C(9)-C(10)	118.9(3)
C(3)-Cr(1)-C(9)-C(10)	-163.2(3)
C(1)-Cr(1)-C(9)-C(10)	32.4(4)
C(7)-Cr(1)-C(9)-C(10)	-103.5(3)
C(8)-Cr(1)-C(9)-C(10)	-131.6(4)
N(1)-Cr(1)-C(9)-C(10)	-66.9(3)

B(1)-Cr(1)-C(9)-C(10)	-29.9(3)
C(2)-Cr(1)-C(9)-C(8)	-109.5(3)
C(3)-Cr(1)-C(9)-C(8)	-31.6(4)
C(1)-Cr(1)-C(9)-C(8)	164.1(3)
C(7)-Cr(1)-C(9)-C(8)	28.1(3)
N(1)-Cr(1)-C(9)-C(8)	64.7(3)
C(10)-Cr(1)-C(9)-C(8)	131.6(4)
B(1)-Cr(1)-C(9)-C(8)	101.7(3)
C(8)-C(9)-C(10)-B(1)	1.6(7)
Cr(1)-C(9)-C(10)-B(1)	56.4(4)
C(8)-C(9)-C(10)-Cr(1)	-54.7(4)
N(1)-B(1)-C(10)-C(9)	-6.8(7)
C(17)-B(1)-C(10)-C(9)	173.7(4)
Cr(1)-B(1)-C(10)-C(9)	-54.7(4)
N(1)-B(1)-C(10)-Cr(1)	48.0(3)
C(17)-B(1)-C(10)-Cr(1)	-131.6(4)
C(2)-Cr(1)-C(10)-C(9)	-63.2(3)
C(3)-Cr(1)-C(10)-C(9)	86.4(11)
C(1)-Cr(1)-C(10)-C(9)	-155.4(3)
C(7)-Cr(1)-C(10)-C(9)	66.0(3)
C(8)-Cr(1)-C(10)-C(9)	29.7(3)
N(1)-Cr(1)-C(10)-C(9)	103.4(3)
B(1)-Cr(1)-C(10)-C(9)	132.2(4)
C(2)-Cr(1)-C(10)-B(1)	164.6(3)
C(3)-Cr(1)-C(10)-B(1)	-45.8(11)
C(1)-Cr(1)-C(10)-B(1)	72.4(3)
C(7)-Cr(1)-C(10)-B(1)	-66.2(3)
C(8)-Cr(1)-C(10)-B(1)	-102.5(3)
C(9)-Cr(1)-C(10)-B(1)	-132.2(4)
N(1)-Cr(1)-C(10)-B(1)	-28.8(2)
N(1)-Si(1)-C(13)-C(16)	-59.0(4)
C(11)-Si(1)-C(13)-C(16)	-179.0(3)
C(12)-Si(1)-C(13)-C(16)	57.8(4)
N(1)-Si(1)-C(13)-C(15)	-179.0(3)
C(11)-Si(1)-C(13)-C(15)	61.0(4)
C(12)-Si(1)-C(13)-C(15)	-62.2(4)
N(1)-Si(1)-C(13)-C(14)	61.9(4)
C(11)-Si(1)-C(13)-C(14)	-58.1(4)
C(12)-Si(1)-C(13)-C(14)	178.7(3)
N(1)-B(1)-C(17)-C(18)	160(3)

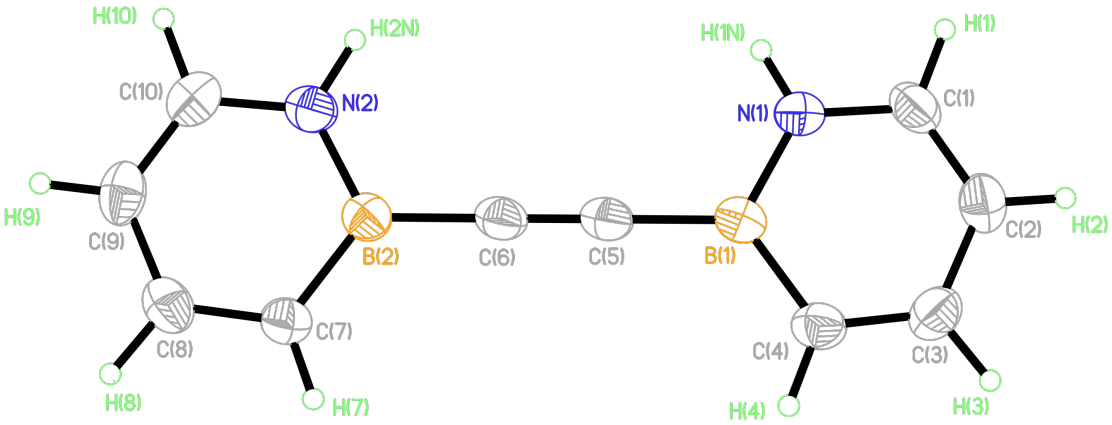
C(10)-B(1)-C(17)-C(18)	-20(3)
Cr(1)-B(1)-C(17)-C(18)	-109(3)
B(1)-C(17)-C(18)-B(2)	-44(5)
N(2)-B(2)-C(18)-C(17)	153(3)
C(22)-B(2)-C(18)-C(17)	-26(3)
Cr(2)-B(2)-C(18)-C(17)	-116(3)
B(2)-N(2)-C(19)-C(20)	-1.0(7)
Si(2)-N(2)-C(19)-C(20)	-177.3(4)
Cr(2)-N(2)-C(19)-C(20)	58.0(4)
B(2)-N(2)-C(19)-Cr(2)	-59.0(4)
Si(2)-N(2)-C(19)-Cr(2)	124.7(2)
C(4)-Cr(2)-C(19)-C(20)	-151.5(3)
C(5)-Cr(2)-C(19)-C(20)	32.1(4)
C(6)-Cr(2)-C(19)-C(20)	118.7(3)
N(2)-Cr(2)-C(19)-C(20)	-132.0(4)
C(21)-Cr(2)-C(19)-C(20)	-27.5(3)
C(22)-Cr(2)-C(19)-C(20)	-63.2(3)
B(2)-Cr(2)-C(19)-C(20)	-101.0(3)
C(4)-Cr(2)-C(19)-N(2)	-19.5(4)
C(5)-Cr(2)-C(19)-N(2)	164.1(3)
C(6)-Cr(2)-C(19)-N(2)	-109.3(3)
C(20)-Cr(2)-C(19)-N(2)	132.0(4)
C(21)-Cr(2)-C(19)-N(2)	104.6(3)
C(22)-Cr(2)-C(19)-N(2)	68.9(3)
B(2)-Cr(2)-C(19)-N(2)	31.0(2)
N(2)-C(19)-C(20)-C(21)	-6.3(7)
Cr(2)-C(19)-C(20)-C(21)	51.5(4)
N(2)-C(19)-C(20)-Cr(2)	-57.8(4)
C(4)-Cr(2)-C(20)-C(19)	81.1(7)
C(5)-Cr(2)-C(20)-C(19)	-157.1(3)
C(6)-Cr(2)-C(20)-C(19)	-67.1(3)
N(2)-Cr(2)-C(20)-C(19)	29.3(3)
C(21)-Cr(2)-C(20)-C(19)	135.0(4)
C(22)-Cr(2)-C(20)-C(19)	105.7(3)
B(2)-Cr(2)-C(20)-C(19)	67.4(3)
C(4)-Cr(2)-C(20)-C(21)	-53.8(7)
C(5)-Cr(2)-C(20)-C(21)	67.9(3)
C(6)-Cr(2)-C(20)-C(21)	158.0(3)
C(19)-Cr(2)-C(20)-C(21)	-135.0(4)
N(2)-Cr(2)-C(20)-C(21)	-105.7(3)

C(22)-Cr(2)-C(20)-C(21)	-29.2(3)
B(2)-Cr(2)-C(20)-C(21)	-67.6(3)
C(19)-C(20)-C(21)-C(22)	6.1(7)
Cr(2)-C(20)-C(21)-C(22)	56.4(4)
C(19)-C(20)-C(21)-Cr(2)	-50.3(4)
C(4)-Cr(2)-C(21)-C(22)	28.5(4)
C(5)-Cr(2)-C(21)-C(22)	114.6(3)
C(6)-Cr(2)-C(21)-C(22)	-165.6(3)
C(19)-Cr(2)-C(21)-C(22)	-103.7(3)
N(2)-Cr(2)-C(21)-C(22)	-67.3(3)
C(20)-Cr(2)-C(21)-C(22)	-131.1(4)
B(2)-Cr(2)-C(21)-C(22)	-30.3(3)
C(4)-Cr(2)-C(21)-C(20)	159.6(3)
C(5)-Cr(2)-C(21)-C(20)	-114.3(3)
C(6)-Cr(2)-C(21)-C(20)	-34.5(5)
C(19)-Cr(2)-C(21)-C(20)	27.4(3)
N(2)-Cr(2)-C(21)-C(20)	63.9(3)
C(22)-Cr(2)-C(21)-C(20)	131.1(4)
B(2)-Cr(2)-C(21)-C(20)	100.8(3)
C(20)-C(21)-C(22)-B(2)	1.1(7)
Cr(2)-C(21)-C(22)-B(2)	56.7(4)
C(20)-C(21)-C(22)-Cr(2)	-55.6(4)
N(2)-B(2)-C(22)-C(21)	-7.8(7)
C(18)-B(2)-C(22)-C(21)	171.7(4)
Cr(2)-B(2)-C(22)-C(21)	-55.3(4)
N(2)-B(2)-C(22)-Cr(2)	47.6(4)
C(18)-B(2)-C(22)-Cr(2)	-133.0(4)
C(4)-Cr(2)-C(22)-C(21)	-158.2(3)
C(5)-Cr(2)-C(22)-C(21)	-67.5(3)
C(6)-Cr(2)-C(22)-C(21)	77.5(13)
C(19)-Cr(2)-C(22)-C(21)	65.8(3)
N(2)-Cr(2)-C(22)-C(21)	103.0(3)
C(20)-Cr(2)-C(22)-C(21)	29.8(3)
B(2)-Cr(2)-C(22)-C(21)	131.4(4)
C(4)-Cr(2)-C(22)-B(2)	70.4(3)
C(5)-Cr(2)-C(22)-B(2)	161.1(3)
C(6)-Cr(2)-C(22)-B(2)	-53.9(13)
C(19)-Cr(2)-C(22)-B(2)	-65.6(3)
N(2)-Cr(2)-C(22)-B(2)	-28.3(3)
C(20)-Cr(2)-C(22)-B(2)	-101.6(3)

C(21)-Cr(2)-C(22)-B(2)	-131.4(4)
N(2)-Si(2)-C(25)-C(26)	53.0(4)
C(23)-Si(2)-C(25)-C(26)	-67.6(4)
C(24)-Si(2)-C(25)-C(26)	170.5(4)
N(2)-Si(2)-C(25)-C(28)	-68.5(4)
C(23)-Si(2)-C(25)-C(28)	170.9(4)
C(24)-Si(2)-C(25)-C(28)	48.9(5)
N(2)-Si(2)-C(25)-C(27)	173.0(3)
C(23)-Si(2)-C(25)-C(27)	52.4(4)
C(24)-Si(2)-C(25)-C(27)	-69.5(4)

Symmetry transformations used to generate equivalent atoms:

X-ray Crystal Structure Determination of 2. Crystals of **2** suitable for X-ray diffraction were obtained by slow evaporation of a solution of **2** in Et_2O.



Diffraction intensity data were collected with a Bruker Smart Apex CCD diffractometer at 173(2) K using MoKα - radiation (0.71073 Å). The structure was solved using direct methods, completed by subsequent difference Fourier syntheses, and refined by full matrix least-squares procedures on F^2. All non-H atoms were refined with anisotropic thermal parameters. H atoms were found on the residual density map and refined with isotropic thermal parameters. The Flack parameter is 0.00(8). All software and sources scattering factors are contained in the SHELXTL (6.10) program package (G.Sheldrick, Bruker XRD, Madison, WI). Crystallographic data and some details of data collection and crystal structure refinement for $C_{10}H_{10}B_2N_2$ are given in the following tables.

Table S19. Crystal data and structure refinement for **2** (liu60).

Identification code	liu60	
Empirical formula	$C_{10}\ H_{10}\ B_2\ N_2$	
Formula weight	179.82	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 19.076(6) Å	α= 90°.
	b = 9.301(3) Å	β= 90°.
	c = 10.997(3) Å	γ = 90°.
Volume	1951.1(10) $Å^3$	
Z	8	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.071 mm^{-1}	
F(000)	752	
Crystal size	0.34 x 0.16 x 0.12 mm^3	
Theta range for data collection	2.14 to 27.00°.	
Index ranges	-24<=h<=24, -11<=k<=11, -13<=l<=12	
Reflections collected	9364	
Independent reflections	2125 [R(int) = 0.0438]	
Completeness to theta = 27.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9915 and 0.9762	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2125 / 0 / 167	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1012	
R indices (all data)	R1 = 0.0743, wR2 = 0.1157	
Largest diff. peak and hole	0.170 and -0.151 e.$Å^{-3}$	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3774(1)	901(2)	1950(1)	35(1)
N(2)	5752(1)	-3060(2)	3802(1)	36(1)
B(1)	3698(1)	407(2)	3169(2)	31(1)
B(2)	5190(1)	-2612(2)	4578(2)	31(1)
C(1)	3358(1)	1931(2)	1452(2)	40(1)
C(2)	2829(1)	2524(2)	2098(2)	41(1)
C(3)	2697(1)	2082(2)	3305(2)	41(1)
C(4)	3096(1)	1060(2)	3855(2)	37(1)
C(5)	4221(1)	-706(2)	3669(1)	34(1)
C(6)	4645(1)	-1550(2)	4070(1)	34(1)
C(7)	5196(1)	-3249(2)	5831(2)	35(1)
C(8)	5707(1)	-4201(2)	6136(2)	39(1)
C(9)	6235(1)	-4587(2)	5302(2)	41(1)
C(10)	6253(1)	-4018(2)	4164(2)	40(1)

Table S21. Bond lengths [Å] and angles [°] for **2**.

N(1)-C(1)	1.359(2)
N(1)-B(1)	1.425(2)
N(2)-C(10)	1.367(2)
N(2)-B(2)	1.431(2)
B(1)-C(4)	1.502(3)
B(1)-C(5)	1.539(3)
B(2)-C(7)	1.500(2)
B(2)-C(6)	1.539(2)
C(1)-C(2)	1.352(3)
C(2)-C(3)	1.413(3)
C(3)-C(4)	1.360(2)
C(5)-C(6)	1.210(2)
C(7)-C(8)	1.359(2)
C(8)-C(9)	1.410(3)
C(9)-C(10)	1.359(3)
C(1)-N(1)-B(1)	123.22(16)
C(10)-N(2)-B(2)	122.66(15)
N(1)-B(1)-C(4)	114.79(15)
N(1)-B(1)-C(5)	119.16(15)
C(4)-B(1)-C(5)	126.04(15)

N(2)-B(2)-C(7)	115.34(16)
N(2)-B(2)-C(6)	118.39(15)
C(7)-B(2)-C(6)	126.27(16)
C(2)-C(1)-N(1)	120.72(17)
C(1)-C(2)-C(3)	120.60(17)
C(4)-C(3)-C(2)	121.37(17)
C(3)-C(4)-B(1)	119.24(16)
C(6)-C(5)-B(1)	178.17(18)
C(5)-C(6)-B(2)	179.45(18)
C(8)-C(7)-B(2)	119.27(17)
C(7)-C(8)-C(9)	121.25(17)
C(10)-C(9)-C(8)	121.18(17)
C(9)-C(10)-N(2)	120.30(17)

Symmetry transformations used to generate equivalent atoms:

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. 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}
N(1)	38(1)	39(1)	28(1)	0(1)	4(1)	3(1)
N(2)	41(1)	37(1)	30(1)	0(1)	2(1)	-1(1)
B(1)	34(1)	31(1)	28(1)	0(1)	0(1)	-5(1)
B(2)	36(1)	29(1)	30(1)	-2(1)	-2(1)	-2(1)
C(1)	45(1)	46(1)	29(1)	7(1)	-4(1)	1(1)
C(2)	38(1)	40(1)	45(1)	8(1)	-6(1)	3(1)
C(3)	34(1)	42(1)	47(1)	1(1)	7(1)	4(1)
C(4)	40(1)	39(1)	32(1)	3(1)	6(1)	-2(1)
C(5)	40(1)	36(1)	26(1)	-1(1)	4(1)	-1(1)
C(6)	43(1)	35(1)	24(1)	-2(1)	2(1)	0(1)
C(7)	39(1)	36(1)	29(1)	-1(1)	1(1)	1(1)
C(8)	46(1)	38(1)	34(1)	3(1)	-8(1)	-1(1)
C(9)	35(1)	36(1)	53(1)	-2(1)	-12(1)	5(1)
C(10)	34(1)	38(1)	46(1)	-7(1)	2(1)	0(1)

Table S23. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **2**.

	x	y	z	U(eq)
H(1N)	4117(10)	596(19)	1497(17)	42(5)
H(2N)	5797(10)	-2700(20)	2985(19)	56(6)
H(1)	3465(9)	2187(19)	586(18)	53(5)
H(2)	2539(10)	3290(20)	1738(17)	54(5)

H(3)	2307(10)	2560(19)	3723(17)	46(5)
H(4)	2994(10)	819(18)	4694(17)	48(5)
H(7)	4856(10)	-3024(19)	6422(18)	50(5)
H(8)	5720(10)	-4656(19)	6964(17)	51(5)
H(9)	6606(9)	-5242(19)	5534(15)	42(5)
H(10)	6624(9)	-4290(18)	3529(17)	49(5)

Table S24. Torsion angles [°] for **2**.

C(1)-N(1)-B(1)-C(4)	2.9(2)
C(1)-N(1)-B(1)-C(5)	-176.74(15)
C(10)-N(2)-B(2)-C(7)	1.0(2)
C(10)-N(2)-B(2)-C(6)	-178.84(15)
B(1)-N(1)-C(1)-C(2)	-1.6(3)
N(1)-C(1)-C(2)-C(3)	-0.2(3)
C(1)-C(2)-C(3)-C(4)	0.5(3)
C(2)-C(3)-C(4)-B(1)	1.0(3)
N(1)-B(1)-C(4)-C(3)	-2.6(2)
C(5)-B(1)-C(4)-C(3)	177.05(16)
N(1)-B(1)-C(5)-C(6)	83(5)
C(4)-B(1)-C(5)-C(6)	-96(5)
B(1)-C(5)-C(6)-B(2)	-18(22)
N(2)-B(2)-C(6)-C(5)	-64(19)
C(7)-B(2)-C(6)-C(5)	116(19)
N(2)-B(2)-C(7)-C(8)	-1.3(2)
C(6)-B(2)-C(7)-C(8)	178.56(15)
B(2)-C(7)-C(8)-C(9)	0.7(3)
C(7)-C(8)-C(9)-C(10)	0.2(3)
C(8)-C(9)-C(10)-N(2)	-0.5(3)
B(2)-N(2)-C(10)-C(9)	-0.1(3)

Symmetry transformations used to generate equivalent atoms:

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