Supporting Information for:

Electrochemistry and Electrochemiluminescence of a Homologous set of BODIPY Appended Bipyridine Derivatives

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Index

Table S1. Coordinates for the energy optimized structure of **BB1.**

Atom	X	Y	Z
F	0.42115700	-0.27828000	7.86683800
F	-1.01641700	-2.05665400	8.03013300
C	-1.53038500	-0.47585100	4.89729100
C	0.36671700	-2.01350800	4.76225500
C	-0.33400700	-0.48688500	0.45474500
N	-1.41391200	-0.41697200	6.29055400
C	-2.36719100	0.40010800	6.77174400
N	0.51628700	-1.98875300	6.15344800
N	-1.09328800	-1.43223000	-0.11905700
C	-1.59003100	-2.30682100	2.06244300
H	-2.10728200	-3.04864300	2.66063200
C	-0.80086700	-1.32407300	2.66417700
C	-0.16290300	-0.39957200	1.84133500
H	0.46179500	0.38429400	2.24926500
C	-1.70050100	-2.31337400	0.67424700
H	-2.30767200	-3.06453200	0.17517400
C	1.55329300	-2.77462800	6.49281700
C	1.38622800	-2.87081300	4.22978200
B	-0.36768200	-1.18411200	7.14916900
C	-2.62851200	0.36493500	4.51591400
C	-0.64896400	-1.26761300	4.14871500
C	1.68294600	-3.23693200	2.80654100
H	0.84966200	-3.75727300	2.32801300
H	2.55093100	-3.89798500	2.76910200
H	1.90499200	-2.36181300	2.19109500
C	-3.17582700	0.66512500	3.15294300
H	-2.44700500	1.17718600	2.51952000
H	-4.05063800	1.31220500	3.24088900
H	-3.48115700	-0.23720000	2.61823300
C	-3.12949700	0.89589700	5.69547900
H	-3.96414400	1.57722600	5.78635600
C	2.10709200	-3.33008200	5.32242700
H	2.95539100	-3.99989000	5.29323700
C	-2.53656900	0.68357600	8.22587600
H	-2.76085700	-0.23434500	8.77508500
H	-3.34479500	1.39796700	8.38545000
H	-1.61486800	1.08528000	8.65260400
C	1.99116300	-2.97879100	7.90357800
H	2.28313700	-2.02994000	8.36000200
H	2.83508700	-3.66797600	7.94676900
H	1.17375100	-3.37785100	8.50880600

F	-0.42115700	0.27828000	-7.86683800
F	1.01641700	2.05665400	-8.03013300
C	1.53038500	0.47585100	-4.89729100
C	-0.36671700	2.01350800	-4.76225500
C	0.33400700	0.48688500	-0.45474500
N	1.41391200	0.41697200	-6.29055400
C	2.36719100	-0.40010800	-6.77174400
N	-0.51628700	1.98875300	-6.15344800
N	1.09328800	1.43223000	0.11905700
C	1.59003100	2.30682100	-2.06244300
H	2.10728200	3.04864300	-2.66063200
C	0.80086700	1.32407300	-2.66417700
C	0.16290300	0.39957200	-1.84133500
H	-0.46179500	-0.38429400	-2.24926500
C	1.70050100	2.31337400	-0.67424700
H	2.30767200	3.06453200	-0.17517400
C	-1.55329300	2.77462800	-6.49281700
C	-1.38622800	2.87081300	-4.22978200
B	0.36768200	1.18411200	-7.14916900
C	2.62851200	-0.36493500	-4.51591400
C	0.64896400	1.26761300	-4.14871500
C	-1.68294600	3.23693200	-2.80654100
H	-0.84966200	3.75727300	-2.32801300
H	-2.55093100	3.89798500	-2.76910200
H	-1.90499200	2.36181300	-2.19109500
C	3.17582700	-0.66512500	-3.15294300
H	2.44700500	-1.17718600	-2.51952000
H	4.05063800	-1.31220500	-3.24088900
H	3.48115700	0.23720000	-2.61823300
C	3.12949700	-0.89589700	-5.69547900
H	3.96414400	-1.57722600	-5.78635600
C	-2.10709200	3.33008200	-5.32242700
H	-2.95539100	3.99989000	-5.29323700
C	2.53656900	-0.68357600	-8.22587600
H	2.76085700	0.23434500	-8.77508500
H	3.34479500	-1.39796700	-8.38545000
H	1.61486800	-1.08528000	-8.65260400
C	-1.99116300	2.97879100	-7.90357800
H	-2.28313700	2.02994000	-8.36000200
H	-2.83508700	3.66797600	-7.94676900
H	-1.17375100	3.37785100	-8.50880600

Table S2. Coordinates for the energy optimized structure of **BB2.**

Atom	X	Y	Z
F	5.50889000	-3.37622400	5.29812200
F	4.97182000	-4.86433700	3.63794300
N	5.08242800	-2.51032900	3.07515300
N	3.22864000	-3.40649700	4.47927600
C	0.37100900	0.12824900	0.63351600
C	2.85048100	-1.57107300	2.93994700
C	1.91624900	-0.56880200	2.34530500
C	2.36761900	-2.47180700	3.90119000
C	4.19190400	-1.58376700	2.52927800
N	0.16852300	1.31411000	1.22721800
C	1.23541800	-0.83815600	1.16079500
H	1.35985500	-1.77786700	0.63873700
C	0.82286100	1.56516500	2.36007100
H	0.63537300	2.53551400	2.81330400
C	1.06894100	-2.66441100	4.47820500
C	1.18717800	-3.71237300	5.39278600
C	4.92199500	-0.78295600	1.59007300
C	6.23462700	-1.25717200	1.59293400
C	3.18210400	-5.22775500	6.16452900
H	3.70025900	-5.93139200	5.50984400
H	2.44816000	-5.77067200	6.75929700
H	3.93845300	-4.81331300	6.83618300
C	1.70218000	0.66689300	2.95959700
H	2.20962100	0.92470200	3.88253800
C	4.42028400	0.34961800	0.74368700
H	3.96028500	1.14021300	1.34045400
H	3.66888000	0.02297500	0.02009000
H	5.23975300	0.80071300	0.18324400
C	6.29516700	-2.32258800	2.52673800
C	2.53808700	-4.14301000	5.36650500
B	4.73677900	-3.58061700	4.14743400
C	-0.19945500	4.18498700	-1.91889200
H	-1.03776800	4.72191400	-2.36428200
H	-0.44827200	3.12180100	-1.92695500
H	-0.14205200	4.48781600	-0.87002100
C	0.11205700	-4.28413900	6.27603500
H	0.28588600	-5.35532200	6.41973800
H	-0.85643800	-4.21671100	5.77124700
C	7.47248000	-3.15780500	2.90687200
H	7.69921700	-3.04033900	3.96941600
H	8.35436600	-2.88495100	2.32817600
H	7.25919900	-4.21760200	2.75060700

C	7.39794400	-0.73745200	0.79224200
H	7.04305900	-0.35210900	-0.16832000
H	8.06766200	-1.56534700	0.53817100
C	0.01436500	-3.60013500	7.65051900
H	0.95342800	-3.68722800	8.20352400
H	-0.77640800	-4.04879100	8.25900900
H	-0.20522400	-2.53420300	7.54586900
C	8.20215200	0.35866700	1.51198300
H	7.57356800	1.22337000	1.74118900
H	9.03769500	0.70364600	0.89569000
H	8.61146900	-0.00628700	2.45778200
F	-5.50889000	3.37622400	-5.29812200
F	-4.97182000	4.86433700	-3.63794300
N	-5.08242800	2.51032900	-3.07515300
N	-3.22864000	3.40649700	-4.47927600
C	-0.37100900	-0.12824900	-0.63351600
C	-2.85048100	1.57107300	-2.93994700
C	-1.91624900	0.56880200	-2.34530500
C	-2.36761900	2.47180700	-3.90119000
C	-4.19190400	1.58376700	-2.52927800
N	-0.16852300	-1.31411000	-1.22721800
C	-1.23541800	0.83815600	-1.16079500
H	-1.35985500	1.77786700	-0.63873700
C	-0.82286100	-1.56516500	-2.36007100
H	-0.63537300	-2.53551400	-2.81330400
C	-1.06894100	2.66441100	-4.47820500
C	-1.18717800	3.71237300	-5.39278600
C	-4.92199500	0.78295600	-1.59007300
C	-6.23462700	1.25717200	-1.59293400
C	-3.18210400	5.22775500	-6.16452900
H	-3.70025900	5.93139200	-5.50984400
H	-2.44816000	5.77067200	-6.75929700
H	-3.93845300	4.81331300	-6.83618300
C	-1.70218000	-0.66689300	-2.95959700
H	-2.20962100	-0.92470200	-3.88253800
C	-4.42028400	-0.34961800	-0.74368700
H	-3.96028500	-1.14021300	-1.34045400
H	-3.66888000	-0.02297500	-0.02009000
H	-5.23975300	-0.80071300	-0.18324400
C	-6.29516700	2.32258800	-2.52673800
C	-2.53808700	4.14301000	-5.36650500
B	-4.73677900	3.58061700	-4.14743400
C	0.19945500	1.91889200	-4.18498700
H	1.03776800	2.36428200	-4.72191400

H	0.44827200	1.92695500	-3.12180100
H	0.14205200	0.87002100	-4.48781600
C	-0.11205700	4.28413900	-6.27603500
H	-0.28588600	5.35532200	-6.41973800
H	0.85643800	4.21671100	-5.77124700
C	-7.47248000	3.15780500	-2.90687200
H	-7.69921700	3.04033900	-3.96941600
H	-8.35436600	2.88495100	-2.32817600
H	-7.25919900	4.21760200	-2.75060700
C	-7.39794400	0.73745200	-0.79224200
H	-7.04305900	0.35210900	0.16832000
H	-8.06766200	1.56534700	-0.53817100
C	-0.01436500	3.60013500	-7.65051900
H	-0.95342800	3.68722800	-8.20352400
H	0.77640800	4.04879100	-8.25900900
H	0.20522400	2.53420300	-7.54586900
C	-8.20215200	-0.35866700	-1.51198300
H	-7.57356800	-1.22337000	-1.74118900
H	-9.03769500	-0.70364600	-0.89569000
H	-8.61146900	0.00628700	-2.45778200

Figure S1. Fully labeled thermal ellipsoid plot of the solid-state structure of **BB1**. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity.

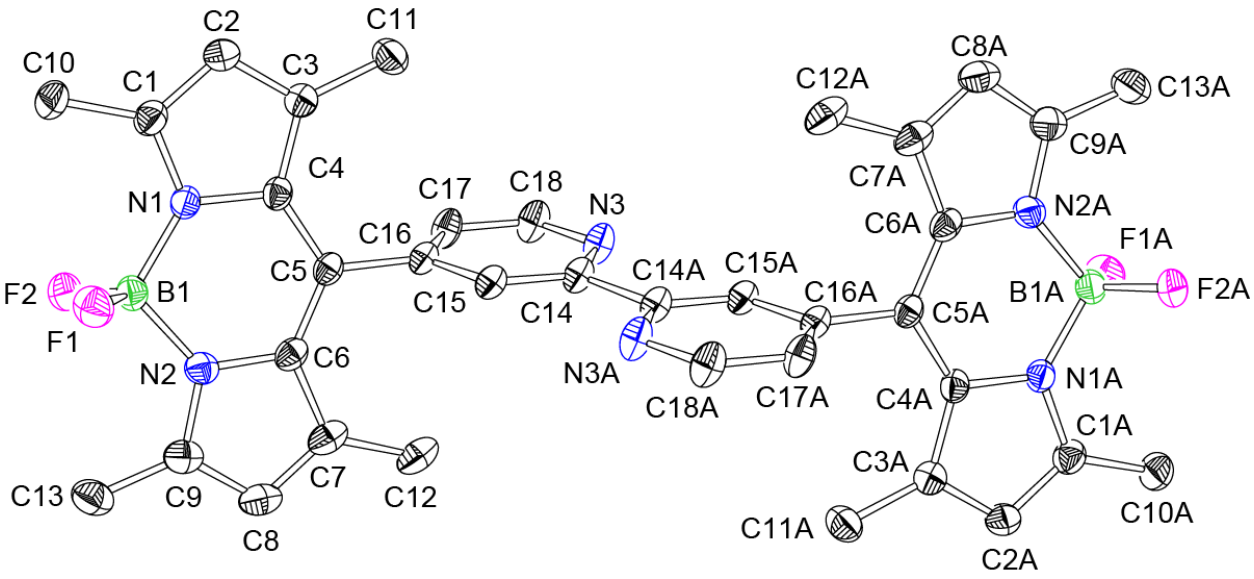

Figure S2. Fully labeled thermal ellipsoid plot of the solid-state structure of **BB2**. Ellipsoids are shown at the 50% probability level and hydrogen atoms are omitted for clarity.

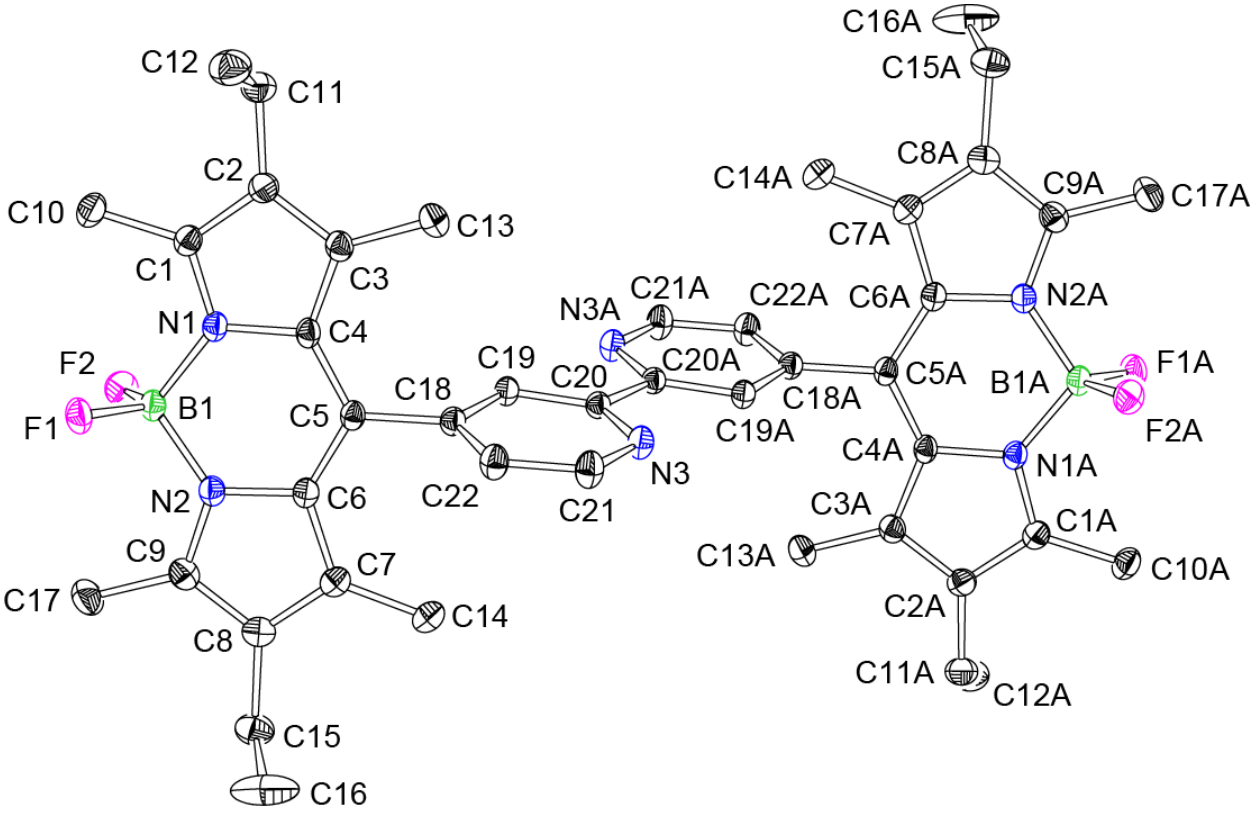

Table S3. Summary of X-Ray Crystallography Data of **BB1** and **BB2**.

	BB1	**BB2**
Empirical formula	$C_{36}H_{34}B_2F_4N_6$	$C_{44}H_{50}B_2F_4N_6$
Formula weight	648.31	760.52
Temperature (K)	110(2)	100(2)
Radiation (λ, Å)	0.71073	0.71073
μ (Mo Kα), (mm^{-1})	0.098	0.088
Crystal size (mm^3)	0.40 x 0.08 x 0.08	0.40 x 0.20 x 0.10
Crystal system	Monoclinic	Monoclinic
Space group	*P2$_1$/n*	*C2/c*
a (Å)	6.640(2)	20.6867(13)
b (Å)	12.269(4)	7.4167(5)
c (Å)	19.584(6)	27.0419(17)
β (deg)	98.055(6)	106.4180(10)
V ($Å^3$)	1579.6(9)	3979.8(4)
Z	2	4
ρ_{calc} (g/cm^3)	1.363	1.269
θ range (deg)	1.96 – 30.57	1.57 – 31.73
Reflections collected	35900	40861
Independent reflections	4836 [R(int) = 0.0792]	6304 [R(int) = 0.0378]
Completeness to θ (%)	99.8	99.9
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.127	1.050
Final R indices [R > 2σ (I)]		
R_1 (%)[a]	8.58	4.83
wR_2 (%)[b]	16.65	12.09
R indices (all data)		
R_1 (%)[a]	0.1214	0.0618
wR_2 (%)[b]	0.1821	0.1341
Max, min peaks ($e/Å^3$)	0.460 and –0.231	0.524 and –0.390

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

Table S4. Bond lengths (Å) of **BB1**.

F(1)-B(1)	1.385(3)
F(2)-B(1)	1.387(3)
C(4)-C(5)	1.397(3)
C(4)-N(1)	1.397(3)
C(4)-C(3)	1.429(3)
C(6)-N(2)	1.395(3)
C(6)-C(5)	1.395(3)
C(6)-C(7)	1.433(3)
C(14)-N(3)	1.342(3)
C(14)-C(15)	1.388(3)
C(14)-C(14)A	1.495(4)
N(1)-C(1)	1.357(3)
N(1)-B(1)	1.553(3)
C(1)-C(2)	1.403(3)
C(1)-C(10)	1.482(3)
N(2)-C(9)	1.350(3)
N(2)-B(1)	1.553(3)
N(3)-C(18)	1.337(3)
C(17)-C(16)	1.387(3)
C(17)-C(18)	1.389(3)
C(16)-C(15)	1.383(3)
C(16)-C(5)	1.488(3)
C(9)-C(8)	1.402(3)
C(9)-C(13)	1.484(3)
C(7)-C(8)	1.382(4)
C(7)-C(12)	1.508(3)
C(3)-C(2)	1.379(3)
C(3)-C(11)	1.494(3)

Table S5. Bond angles (°) of **BB1**.

C(5)-C(4)-N(1)	119.9(2)
C(5)-C(4)-C(3)	131.7(2)
N(1)-C(4)-C(3)	108.43(18)
N(2)-C(6)-C(5)	120.22(19)
N(2)-C(6)-C(7)	108.0(2)
C(5)-C(6)-C(7)	131.8(2)
N(3)-C(14)-C(15)	123.2(2)
N(3)-C(14)-C(14)A	116.1(2)
C(15)-C(14)-C(14)A	120.7(3)
C(1)-N(1)-C(4)	107.98(19)
C(1)-N(1)-B(1)	126.27(19)
C(4)-N(1)-B(1)	125.70(18)
N(1)-C(1)-C(2)	108.6(2)
N(1)-C(1)-C(10)	123.3(2)
C(2)-C(1)-C(10)	128.0(2)
C(9)-N(2)-C(6)	108.27(19)
C(9)-N(2)-B(1)	126.1(2)
C(6)-N(2)-B(1)	125.50(19)
C(18)-N(3)-C(14)	117.0(2)
C(16)-C(17)-C(18)	118.4(2)
C(15)-C(16)-C(17)	118.5(2)
C(15)-C(16)-C(5)	120.4(2)
C(17)-C(16)-C(5)	121.0(2)
C(16)-C(15)-C(14)	119.1(2)
N(3)-C(18)-C(17)	123.8(2)
N(2)-C(9)-C(8)	109.1(2)
N(2)-C(9)-C(13)	123.2(2)
C(8)-C(9)-C(13)	127.7(2)
C(8)-C(7)-C(6)	105.9(2)
C(8)-C(7)-C(12)	125.6(2)
C(6)-C(7)-C(12)	128.5(2)
F(1)-B(1)-F(2)	110.0(2)
F(1)-B(1)-N(2)	110.6(2)
F(2)-B(1)-N(2)	110.0(2)
F(1)-B(1)-N(1)	109.7(2)

F(2)-B(1)-N(1)	109.8(2)
N(2)-B(1)-N(1)	106.64(18)
C(2)-C(3)-C(4)	105.59(19)
C(2)-C(3)-C(11)	124.6(2)
C(4)-C(3)-C(11)	129.8(2)
C(6)-C(5)-C(4)	121.8(2)
C(6)-C(5)-C(16)	118.63(19)
C(4)-C(5)-C(16)	119.5(2)
C(3)-C(2)-C(1)	109.3(2)
C(7)-C(8)-C(9)	108.7(2)

Table S6. Bond lengths (Å) of **BB2**.

F(1)-B(1)	1.3916(14)
F(2)-B(1)	1.3968(14)
N(2)-C(9)	1.3464(15)
N(2)-C(6)	1.3977(14)
N(2)-B(1)	1.5442(16)
N(1)-C(1)	1.3471(14)
N(1)-C(4)	1.3986(13)
N(1)-B(1)	1.5503(16)
C(20)-N(3)	1.3481(13)
C(20)-C(19)	1.3932(14)
C(20)-C(20)A	1.484(2)
C(5)-C(6)	1.3968(16)
C(5)-C(4)	1.3996(15)
C(5)-C(18)	1.4886(15)
C(18)-C(19)	1.3878(15)
C(18)-C(22)	1.3899(15)
C(4)-C(3)	1.4250(16)
C(6)-C(7)	1.4301(16)
N(3)-C(21)	1.3361(15)
C(21)-C(22)	1.3895(16)
C(3)-C(2)	1.3937(15)
C(3)-C(13)	1.5020(16)
C(2)-C(1)	1.4137(17)
C(2)-C(11)	1.4995(17)
C(7)-C(8)	1.3876(17)
C(7)-C(14)	1.4959(16)
C(8)-C(9)	1.4137(17)
C(8)-C(15)	1.4987(18)
C(10)-C(1)	1.4867(16)
C(9)-C(17)	1.4948(17)
C(11)-C(12)	1.529(2)
C(15)-C(16)	1.525(2)

Table S7. Bond angles (°) of **BB2**.

C(9)-N(2)-C(6)	108.14(10)
C(9)-N(2)-B(1)	126.30(10)
C(6)-N(2)-B(1)	125.27(10)
C(1)-N(1)-C(4)	108.01(9)
C(1)-N(1)-B(1)	126.19(9)
C(4)-N(1)-B(1)	125.70(9)
N(3)-C(20)-C(19)	122.72(10)
N(3)-C(20)-C(20)A	116.59(12)
C(19)-C(20)-C(20)A	120.69(12)
C(6)-C(5)-C(4)	121.80(10)
C(6)-C(5)-C(18)	118.30(10)
C(4)-C(5)-C(18)	119.89(10)
C(19)-C(18)-C(22)	118.51(10)
C(19)-C(18)-C(5)	120.14(9)
C(22)-C(18)-C(5)	121.28(10)
N(1)-C(4)-C(5)	119.63(10)
N(1)-C(4)-C(3)	108.12(9)
C(5)-C(4)-C(3)	132.24(10)
C(5)-C(6)-N(2)	119.98(10)
C(5)-C(6)-C(7)	132.00(10)
N(2)-C(6)-C(7)	107.94(10)
C(21)-N(3)-C(20)	117.36(10)
C(18)-C(19)-C(20)	119.03(10)
N(3)-C(21)-C(22)	123.74(10)
C(2)-C(3)-C(4)	106.71(10)
C(2)-C(3)-C(13)	125.11(11)
C(4)-C(3)-C(13)	128.04(10)
C(3)-C(2)-C(1)	107.19(10)
C(3)-C(2)-C(11)	128.25(11)
C(1)-C(2)-C(11)	124.51(11)
C(8)-C(7)-C(6)	106.62(10)
C(8)-C(7)-C(14)	124.58(11)
C(6)-C(7)-C(14)	128.80(11)
C(7)-C(8)-C(9)	107.51(11)
C(7)-C(8)-C(15)	126.69(11)

C(9)-C(8)-C(15)	125.74(12)
C(21)-C(22)-C(18)	118.50(11)
N(2)-C(9)-C(8)	109.75(10)
N(2)-C(9)-C(17)	122.87(11)
C(8)-C(9)-C(17)	127.38(12)
N(1)-C(1)-C(2)	109.94(10)
N(1)-C(1)-C(10)	122.75(11)
C(2)-C(1)-C(10)	127.26(11)
F(1)-B(1)-F(2)	109.27(9)
F(1)-B(1)-N(2)	110.58(10)
F(2)-B(1)-N(2)	109.88(10)
F(1)-B(1)-N(1)	110.17(10)
F(2)-B(1)-N(1)	110.16(10)
N(2)-B(1)-N(1)	106.77(9)
C(2)-C(11)-C(12)	113.05(11)
C(8)-C(15)-C(16)	112.16(12)