Supporting Information for:

A Boron-Complexation Strategy for Use with 1-Acyldipyrromethanes

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General Experimental Section. ^{1}H NMR (400 MHz), and ^{13}C NMR (100 MHz) were collected routinely in $CDCl_3$ unless noted otherwise. $BF_3{\cdot}O(Et_2)$ in $CDCl_3$ was used as external standard (referenced to δ = 0.00 ppm) for ^{11}B NMR (128 MHz) spectroscopy. Melting points are uncorrected. Absorption spectra were collected in toluene unless noted otherwise. Silica gel (40 μm average particle size) was used for column chromatography. THF was distilled from sodium under argon with benzophenone/ketyl as indicator. Diethyl ether was anhydrous. Toluene and CH_2Cl_2 (reagent grade) were used as received. The dipyrromethanes and 1-acyldipyrromethanes are easily detected in TLC upon exposure to Br_2 vapor. All other chemicals were reagent grade and were used as received.

X-ray Structural Determination for 6a-BBN.

Data Collection. Crystals of **6a-BBN** were examined under a light hydrocarbon oil. The specimen crystal was mounted to the tip of a thin glass fiber attached to a tapered copper mounting-pin and transferred to the goniometer of a Bruker D8-Apex diffractometer equipped with an Oxford Cryosystems Series 700 low-temperature apparatus operating at 100 K. Cell parameters were determined using reflections harvested from a series of three orthogonal sets of 20 0.3° ω scans and refined using 7 763 reflections chosen with I>10σ(I) from the entire data collection. Scan series were calculated with COSMO to collect a complete data set with an average 4-fold redundancy. 44 186 Reflections, were measured to 0.65 Å with 99.4 % coverage of the 10 383 unique reflections, [R(int) = 0.0345]. All data were corrected for Lorentz and polarization effects, as well as for absorption.

Structure Solution and Refinement. The data were reduced using the SHELXTL suite of programs. The initial solution via direct methods in centrosymmetric space group $P\bar{1}$ returned most of the atomic positions. A subsequent difference Fourier map revealed the remaining non-hydrogen atoms. The asymmetric unit consists of one

molecule of **6a-BBN** and 1/2 molecule of diethyl ether. Most hydrogen atoms were placed at calculated geometries and allowed to ride on the position of the parent atom. Parameters for isotropic thermal motion of these hydrogens were set to 1.2 × the equivalent isotropic U of the parent atom, 1.5 × for methyl hydrogens. Hydrogen bound to N(2) and C(23) were readily located by difference map and freely refined in subsequent cycles of least-squares refinement. Disorder is present in the tolyl group, in positions for atoms C(16), C(17) and C(20) and their hydrogens. Site occupancy is refined with a complementary model. No minor position was found for H(15). Rotational disorder is present in the group containing the phenyl ring and the pyrrole ring, defined by atoms C(22) to C(28). Site occupancy is refined with a complementary model. The location of the minor position of the pyrrole nitrogen was not determined. The diethyl ether molecule is disordered across a crystallographic inversion center and is modeled at half-occupancy.

Crystal data and structure refinement for 6a-BBN.

Empirical formula	C33 H38 B N2 O1.50	
Formula weight	497.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.0785(2) Å	α = 92.295(1)°.
	b = 10.5821(3) Å	β = 98.991(1)°.
	c = 13.3436(3) Å	γ = 102.113(1)°.
Volume	1370.42(6) Å^3	
Z	2	
Density (calculated)	1.206 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	534	
Crystal size	0.36 x 0.34 x 0.25 mm^3	
Crystal color and habit	orange block	
Diffractometer	CCD area detector	
Theta range for data collection	1.55 to 33.14°.	
Index ranges	-15<=h<=15, -14<=k<=16, -20<=l<=20	
Reflections collected	44186	
Independent reflections	10383 [R(int) = 0.0345]	
Observed reflections (I > 2sigma(I))	7899	
Completeness to theta = 33.14°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9824 and 0.9741	
Solution method	SHELXS-97 (Sheldrick, 1990)	
Refinement method	SHELXL-97 (Sheldrick, 1997)	
Data / restraints / parameters	10383 / 0 / 438	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0634, wR2 = 0.1750	
R indices (all data)	R1 = 0.0810, wR2 = 0.1910	
Largest diff. peak and hole	0.582 and -0.465 e. Å^{-3}	

Atomic coordinates and equivalent isotropic displacement parameters (Å²) for 6a-BBN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
B(1)	0.42081(11)	0.40962(12)	0.17077(9)	0.0246(2)
N(1)	0.27103(9)	0.43748(9)	0.16477(6)	0.02363(17)
O(1)	0.38644(8)	0.30749(8)	0.07763(6)	0.02695(16)
C(1)	0.46988(11)	0.33747(11)	0.26980(8)	0.0270(2)
C(2)	0.59561(12)	0.28239(12)	0.25210(9)	0.0322(2)
C(3)	0.71342(12)	0.37761(13)	0.21533(9)	0.0339(2)
C(4)	0.66414(11)	0.46230(13)	0.13256(9)	0.0315(2)
C(5)	0.54685(10)	0.52528(11)	0.15743(8)	0.0262(2)
C(6)	0.59292(11)	0.61960(12)	0.25367(8)	0.0291(2)
C(7)	0.60578(12)	0.55834(13)	0.35731(8)	0.0325(2)
C(8)	0.49867(12)	0.43335(12)	0.36405(8)	0.0302(2)
C(9)	0.25522(10)	0.27484(10)	0.04330(7)	0.02424(19)
C(10)	0.17979(10)	0.34662(10)	0.09358(8)	0.02479(19)
C(11)	0.04545(11)	0.36550(12)	0.09051(9)	0.0313(2)
C(12)	0.05636(11)	0.46921(12)	0.16030(10)	0.0322(2)
C(13)	0.19647(11)	0.51287(10)	0.20432(8)	0.02577(19)
C(14)	0.20523(11)	0.17529(10)	-0.04094(8)	0.02586(19)
C(15)	0.29961(12)	0.13271(11)	-0.09370(8)	0.0301(2)
C(16)	0.2573(6)	0.0362(5)	-0.1751(4)	0.0246(8)
C(17)	0.1164(13)	-0.0195(10)	-0.2042(8)	0.0315(12)
C(18)	0.02029(14)	0.02452(13)	-0.14921(10)	0.0363(3)
C(19)	0.06471(12)	0.12010(12)	-0.06965(9)	0.0314(2)
C(20)	0.0680(8)	-0.1177(5)	-0.2894(5)	0.0370(11)
C(21)	0.25653(11)	0.63646(11)	0.27092(8)	0.0283(2)
C(22)	0.15982(11)	0.66344(11)	0.34220(8)	0.0286(2)
C(23)	0.05471(12)	0.72764(12)	0.31108(9)	0.0317(2)
C(24)	-0.03110(13)	0.74844(14)	0.37842(10)	0.0374(3)
C(25)	-0.0166(2)	0.7094(2)	0.47314(15)	0.0368(4)
C(26)	0.0886(2)	0.6458(2)	0.50509(14)	0.0427(5)
C(27)	0.17229(16)	0.62437(15)	0.44042(10)	0.0434(3)
C(28)	0.29115(11)	0.74665(11)	0.20405(9)	0.0308(2)
N(2)	0.28133(12)	0.73669(12)	0.09969(10)	0.0416(3)
C(30)	0.32026(15)	0.85789(18)	0.06269(15)	0.0543(4)
C(31)	0.3534(2)	0.9476(2)	0.1515(3)	0.0637(12)
C(33)	0.3357(5)	0.8750(4)	0.2329(3)	0.0501(9)
C(16')	0.2410(19)	0.0425(15)	-0.1700(11)	0.049(4)
C(17')	0.105(3)	-0.013(2)	-0.1992(16)	0.038(4)
C(20')	0.050(2)	-0.1234(16)	-0.2925(13)	0.072(5)
C(26')	0.0330(10)	0.6765(9)	0.4727(7)	0.048(3)
C(31')	0.3716(7)	0.9585(8)	0.1089(4)	0.0303(15)
C(32')	0.3871(7)	0.9749(6)	0.2191(5)	0.0348(15)
C(33')	0.3460(12)	0.8692(11)	0.2645(6)	0.0215(13)
O(1S)	0.4512(3)	0.9792(2)	0.45690(18)	0.0506(5)
C(1S)	0.6695(5)	0.9286(5)	0.4551(4)	0.0735(12)
C(2S)	0.5383(5)	0.8981(5)	0.4982(3)	0.0686(11)
C(3S)	0.3390(5)	0.9824(5)	0.5114(3)	0.0638(9)
C(4S)	0.2519(4)	1.0653(4)	0.4628(4)	0.0677(11)

Bond lengths [Å] and angles [deg] for 6a-BBN.

B(1)-O(1)	1.5599(13)
B(1)-N(1)	1.5884(14)
B(1)-C(5)	1.6059(16)
B(1)-C(1)	1.6152(16)
N(1)-C(13)	1.3496(13)
N(1)-C(10)	1.3983(13)
O(1)-C(9)	1.2979(12)
C(1)-C(8)	1.5348(16)
C(1)-C(2)	1.5472(15)
C(1)-H(1)	1.0000
C(2)-C(3)	1.5444(18)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5376(17)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.5450(15)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.5418(15)
C(5)-H(5)	1.0000
C(6)-C(7)	1.5494(16)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.5374(18)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.4021(14)
C(9)-C(14)	1.4603(14)
C(10)-C(11)	1.4042(15)
C(11)-C(12)	1.3854(16)
C(11)-H(11)	0.9500
C(12)-C(13)	1.4134(15)
C(12)-H(12)	0.9500
C(13)-C(21)	1.5077(15)
C(14)-C(19)	1.3997(16)
C(14)-C(15)	1.4025(15)
C(15)-C(16')	1.339(14)
C(15)-C(16)	1.410(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.405(13)
C(16)-H(16)	0.9500
C(17)-C(18)	1.442(14)
C(17)-C(20)	1.459(12)
C(18)-C(17')	1.28(3)
C(18)-C(19)	1.3878(16)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

C(21)-C(28)	1.5125(17)
C(21)-C(22)	1.5235(15)
C(21)-H(21)	1.0000
C(22)-C(27)	1.3849(18)
C(22)-C(23)	1.3940(15)
C(23)-C(24)	1.3823(17)
C(23)-H(2')	0.884(19)
C(24)-C(25)	1.341(2)
C(24)-C(26')	1.616(12)
C(24)-H(24)	0.9500
C(25)-C(26)	1.392(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.342(2)
C(26)-H(26)	0.9500
C(27)-C(26')	1.718(11)
C(27)-H(27)	0.9500
C(28)-C(33)	1.358(5)
C(28)-N(2)	1.3787(18)
C(28)-C(33')	1.454(11)
N(2)-C(30)	1.394(2)
N(2)-H(2)	1.061(18)
C(30)-C(31')	1.182(8)
C(30)-C(31)	1.438(4)
C(30)-H(30)	0.9500
C(31)-C(33)	1.369(6)
C(31)-H(31)	0.9500
C(33)-H(33)	0.9500
C(16')-C(17')	1.36(3)
C(16')-H(16')	0.9500
C(17')-C(20')	1.62(3)
C(20')-H(20D)	0.9800
C(20')-H(20E)	0.9800
C(20')-H(20F)	0.9800
C(26')-H(26')	0.9500
C(31')-C(32')	1.454(7)
C(31')-H(31')	0.9500
C(32')-C(33')	1.314(13)
C(32')-H(32')	0.9500
C(33')-H(33')	0.9500
O(1S)-C(2S)	1.420(5)
O(1S)-C(3S)	1.442(5)
C(1S)-C(2S)	1.501(6)
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
C(2S)-H(2S1)	0.9900
C(2S)-H(2S2)	0.9900
C(3S)-C(4S)	1.467(6)
C(3S)-H(3S1)	0.9900
C(3S)-H(3S2)	0.9900
C(4S)-H(4S1)	0.9800
C(4S)-H(4S2)	0.9800
C(4S)-H(4S3)	0.9800

O(1)-B(1)-N(1)	97.04(7)
O(1)-B(1)-C(5)	110.43(8)
N(1)-B(1)-C(5)	119.43(9)
O(1)-B(1)-C(1)	107.20(9)
N(1)-B(1)-C(1)	114.16(9)
C(5)-B(1)-C(1)	107.59(8)
C(13)-N(1)-C(10)	107.27(8)
C(13)-N(1)-B(1)	144.17(9)
C(10)-N(1)-B(1)	108.52(8)
C(9)-O(1)-B(1)	111.96(8)
C(8)-C(1)-C(2)	113.70(9)
C(8)-C(1)-B(1)	108.82(9)
C(2)-C(1)-B(1)	108.75(9)
C(8)-C(1)-H(1)	108.5
C(2)-C(1)-H(1)	108.5
B(1)-C(1)-H(1)	108.5
C(3)-C(2)-C(1)	116.05(10)
C(3)-C(2)-H(2A)	108.3
C(1)-C(2)-H(2A)	108.3
C(3)-C(2)-H(2B)	108.3
C(1)-C(2)-H(2B)	108.3
H(2A)-C(2)-H(2B)	107.4
C(4)-C(3)-C(2)	114.00(9)
C(4)-C(3)-H(3A)	108.8
C(2)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3B)	108.8
C(2)-C(3)-H(3B)	108.8
H(3A)-C(3)-H(3B)	107.6
C(3)-C(4)-C(5)	113.54(9)
C(3)-C(4)-H(4A)	108.9
C(5)-C(4)-H(4A)	108.9
C(3)-C(4)-H(4B)	108.9
C(5)-C(4)-H(4B)	108.9
H(4A)-C(4)-H(4B)	107.7
C(6)-C(5)-C(4)	111.95(9)
C(6)-C(5)-B(1)	111.31(8)
C(4)-C(5)-B(1)	107.10(9)
C(6)-C(5)-H(5)	108.8
C(4)-C(5)-H(5)	108.8
B(1)-C(5)-H(5)	108.8
C(5)-C(6)-C(7)	116.79(10)
C(5)-C(6)-H(6A)	108.1
C(7)-C(6)-H(6A)	108.1
C(5)-C(6)-H(6B)	108.1
C(7)-C(6)-H(6B)	108.1
H(6A)-C(6)-H(6B)	107.3
C(8)-C(7)-C(6)	115.84(9)
C(8)-C(7)-H(7A)	108.3
C(6)-C(7)-H(7A)	108.3
C(8)-C(7)-H(7B)	108.3
C(6)-C(7)-H(7B)	108.3
H(7A)-C(7)-H(7B)	107.4
C(1)-C(8)-C(7)	114.02(9)
C(1)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8A)	108.7

C(1)-C(8)-H(8B)	108.7
C(7)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
O(1)-C(9)-C(10)	112.58(9)
O(1)-C(9)-C(14)	118.80(9)
C(10)-C(9)-C(14)	128.60(9)
N(1)-C(10)-C(9)	108.97(9)
N(1)-C(10)-C(11)	109.53(9)
C(9)-C(10)-C(11)	141.19(10)
C(12)-C(11)-C(10)	105.85(10)
C(12)-C(11)-H(11)	127.1
C(10)-C(11)-H(11)	127.1
C(11)-C(12)-C(13)	108.30(10)
C(11)-C(12)-H(12)	125.8
C(13)-C(12)-H(12)	125.8
N(1)-C(13)-C(12)	109.03(9)
N(1)-C(13)-C(21)	124.78(9)
C(12)-C(13)-C(21)	125.45(9)
C(19)-C(14)-C(15)	119.07(10)
C(19)-C(14)-C(9)	121.34(10)
C(15)-C(14)-C(9)	119.59(10)
C(16')-C(15)-C(14)	113.9(9)
C(14)-C(15)-C(16)	122.0(3)
C(16')-C(15)-H(15)	127.1
C(14)-C(15)-H(15)	119.0
C(16)-C(15)-H(15)	119.0
C(17)-C(16)-C(15)	119.1(7)
C(17)-C(16)-H(16)	120.4
C(15)-C(16)-H(16)	120.4
C(16)-C(17)-C(18)	118.4(8)
C(16)-C(17)-C(20)	120.9(10)
C(18)-C(17)-C(20)	120.7(9)
C(17')-C(18)-C(19)	121.3(8)
C(19)-C(18)-C(17)	121.3(4)
C(17')-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(18)-C(19)-C(14)	120.09(11)
C(18)-C(19)-H(19)	120.0
C(14)-C(19)-H(19)	120.0
C(13)-C(21)-C(28)	108.95(9)
C(13)-C(21)-C(22)	111.59(9)
C(28)-C(21)-C(22)	111.92(9)
C(13)-C(21)-H(21)	108.1
C(28)-C(21)-H(21)	108.1
C(22)-C(21)-H(21)	108.1
C(27)-C(22)-C(23)	117.30(11)
C(27)-C(22)-C(21)	121.28(11)
C(23)-C(22)-C(21)	121.42(10)
C(24)-C(23)-C(22)	119.08(12)
C(24)-C(23)-H(2')	120.2(12)
C(22)-C(23)-H(2')	120.7(12)
C(25)-C(24)-C(23)	122.30(15)
C(23)-C(24)-C(26')	98.5(3)
C(25)-C(24)-H(24)	118.8

C(23)-C(24)-H(24)	118.8
C(26')-C(24)-H(24)	142.6
C(24)-C(25)-C(26)	119.02(19)
C(24)-C(25)-H(25)	120.5
C(26)-C(25)-H(25)	120.5
C(27)-C(26)-C(25)	119.37(17)
C(27)-C(26)-H(26)	120.3
C(25)-C(26)-H(26)	120.3
C(26)-C(27)-C(22)	122.93(15)
C(22)-C(27)-C(26')	96.8(4)
C(26)-C(27)-H(27)	118.5
C(22)-C(27)-H(27)	118.5
C(26')-C(27)-H(27)	144.6
C(33)-C(28)-N(2)	105.7(2)
N(2)-C(28)-C(33')	122.1(4)
C(33)-C(28)-C(21)	127.8(2)
N(2)-C(28)-C(21)	126.51(10)
C(33')-C(28)-C(21)	111.3(4)
C(28)-N(2)-C(30)	111.24(13)
C(28)-N(2)-H(2)	126.7(9)
C(30)-N(2)-H(2)	122.1(9)
C(31')-C(30)-N(2)	128.6(3)
N(2)-C(30)-C(31)	104.63(17)
C(31')-C(30)-H(30)	103.1
N(2)-C(30)-H(30)	127.7
C(31)-C(30)-H(30)	127.7
C(33)-C(31)-C(30)	106.5(2)
C(33)-C(31)-H(31)	126.7
C(30)-C(31)-H(31)	126.7
C(28)-C(33)-C(31)	111.9(3)
C(28)-C(33)-H(33)	124.0
C(31)-C(33)-H(33)	124.0
C(15)-C(16')-C(17')	128.1(17)
C(15)-C(16')-H(16')	115.9
C(17')-C(16')-H(16')	115.9
C(18)-C(17')-C(16')	117.5(15)
C(18)-C(17')-C(20')	120.2(16)
C(16')-C(17')-C(20')	122(2)
C(17')-C(20')-H(20D)	109.5
C(17')-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20E)	109.5
C(17')-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20F)	109.5
H(20E)-C(20')-H(20F)	109.5
C(24)-C(26')-C(27)	108.2(4)
C(24)-C(26')-H(26')	125.9
C(27)-C(26')-H(26')	125.9
C(30)-C(31')-C(32')	122.2(6)
C(30)-C(31')-H(31')	118.9
C(32')-C(31')-H(31')	118.9
C(33')-C(32')-C(31')	115.6(7)
C(33')-C(32')-H(32')	122.2
C(31')-C(32')-H(32')	122.2
C(32')-C(33')-C(28)	119.6(6)
C(32')-C(33')-H(33')	120.2

C(28)-C(33')-H(33')	120.2
C(2S)-O(1S)-C(3S)	113.3(3)
O(1S)-C(2S)-C(1S)	108.7(4)
O(1S)-C(2S)-H(2S1)	109.9
C(1S)-C(2S)-H(2S1)	109.9
O(1S)-C(2S)-H(2S2)	109.9
C(1S)-C(2S)-H(2S2)	109.9
H(2S1)-C(2S)-H(2S2)	108.3
O(1S)-C(3S)-C(4S)	110.0(4)
O(1S)-C(3S)-H(3S1)	109.7
C(4S)-C(3S)-H(3S1)	109.7
O(1S)-C(3S)-H(3S2)	109.7
C(4S)-C(3S)-H(3S2)	109.7
H(3S1)-C(3S)-H(3S2)	108.2

Anisotropic displacement parameters (Å²) for 6a-BBN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

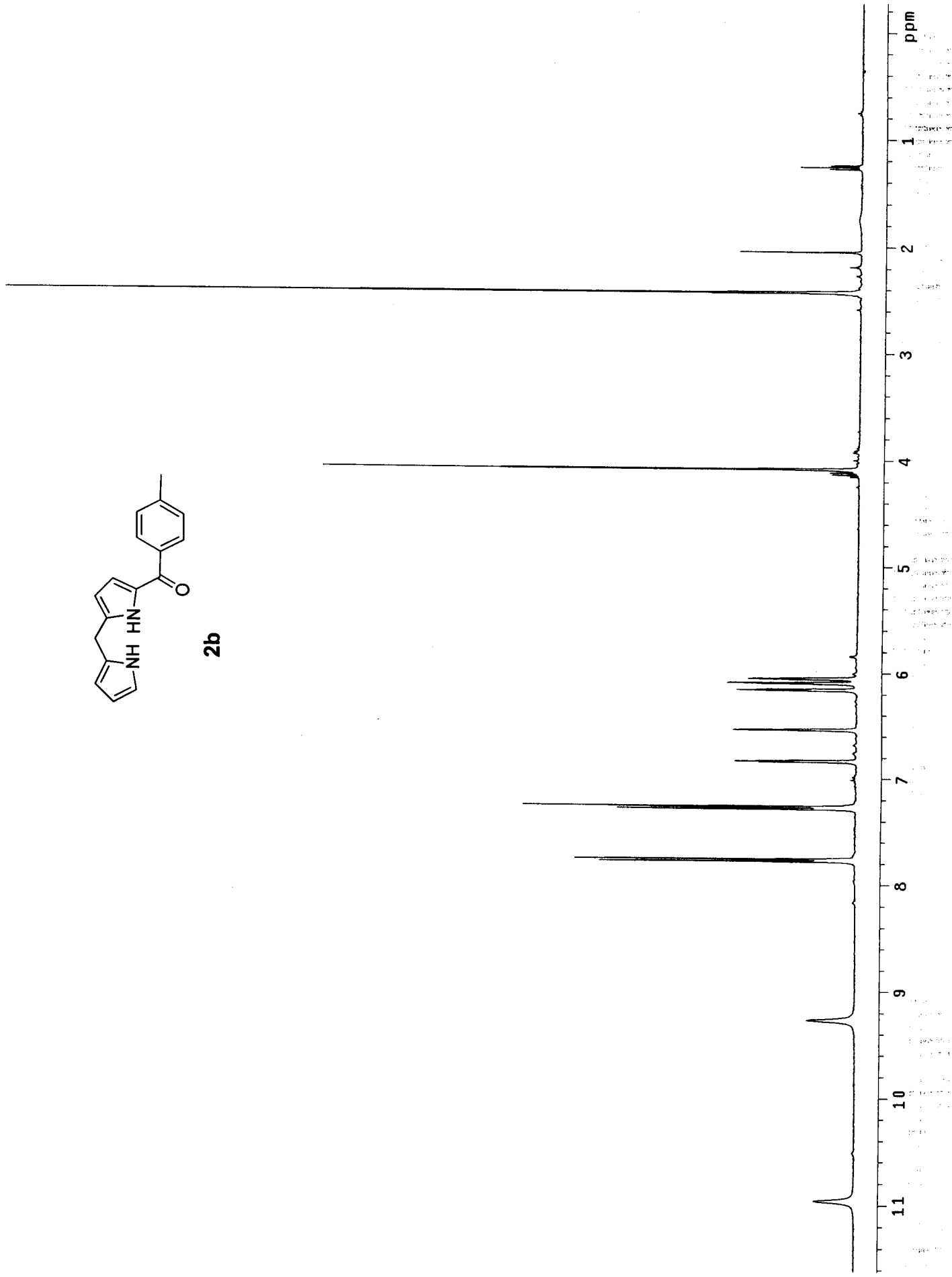
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B(1)	0.0212(4)	0.0302(5)	0.0233(4)	-0.0005(4)	0.0021(4)	0.0093(4)
N(1)	0.0210(4)	0.0259(4)	0.0243(4)	0.0001(3)	0.0023(3)	0.0074(3)
O(1)	0.0224(3)	0.0331(4)	0.0260(3)	-0.0021(3)	0.0026(3)	0.0095(3)
C(1)	0.0244(4)	0.0317(5)	0.0268(4)	0.0047(4)	0.0038(3)	0.0103(4)
C(2)	0.0283(5)	0.0376(6)	0.0344(5)	0.0062(4)	0.0042(4)	0.0154(4)
C(3)	0.0244(5)	0.0457(7)	0.0349(5)	0.0063(5)	0.0044(4)	0.0153(4)
C(4)	0.0237(5)	0.0455(6)	0.0275(5)	0.0050(4)	0.0059(4)	0.0114(4)
C(5)	0.0213(4)	0.0344(5)	0.0231(4)	0.0040(4)	0.0013(3)	0.0082(4)
C(6)	0.0240(4)	0.0341(5)	0.0277(5)	0.0013(4)	0.0014(4)	0.0057(4)
C(7)	0.0301(5)	0.0413(6)	0.0241(4)	-0.0003(4)	-0.0001(4)	0.0071(4)
C(8)	0.0293(5)	0.0392(6)	0.0236(4)	0.0042(4)	0.0038(4)	0.0107(4)
C(9)	0.0240(4)	0.0259(4)	0.0233(4)	0.0021(3)	0.0027(3)	0.0075(3)
C(10)	0.0217(4)	0.0255(4)	0.0267(4)	-0.0007(3)	0.0019(3)	0.0062(3)
C(11)	0.0214(4)	0.0313(5)	0.0398(6)	-0.0056(4)	0.0017(4)	0.0066(4)
C(12)	0.0218(4)	0.0314(5)	0.0430(6)	-0.0065(4)	0.0036(4)	0.0081(4)
C(13)	0.0230(4)	0.0269(5)	0.0283(4)	-0.0009(4)	0.0032(3)	0.0087(3)
C(14)	0.0280(5)	0.0258(5)	0.0240(4)	0.0004(3)	0.0025(3)	0.0080(4)
C(15)	0.0324(5)	0.0311(5)	0.0281(5)	-0.0001(4)	0.0052(4)	0.0104(4)
C(16)	0.0297(13)	0.0258(13)	0.0201(12)	-0.0033(8)	0.0032(11)	0.0114(11)
C(17)	0.0405(19)	0.030(2)	0.027(2)	0.0013(19)	0.0037(15)	0.0163(16)
C(18)	0.0355(6)	0.0334(6)	0.0357(6)	-0.0046(4)	-0.0025(4)	0.0056(4)
C(19)	0.0295(5)	0.0306(5)	0.0328(5)	-0.0024(4)	0.0026(4)	0.0067(4)
C(20)	0.0462(18)	0.0299(17)	0.0317(18)	-0.0067(13)	-0.0053(12)	0.0115(11)
C(21)	0.0245(4)	0.0296(5)	0.0305(5)	-0.0041(4)	0.0002(4)	0.0100(4)
C(22)	0.0265(5)	0.0314(5)	0.0278(4)	-0.0047(4)	-0.0004(4)	0.0112(4)
C(23)	0.0310(5)	0.0371(6)	0.0298(5)	-0.0020(4)	0.0015(4)	0.0168(4)
C(24)	0.0282(5)	0.0435(7)	0.0396(6)	-0.0130(5)	0.0025(4)	0.0111(5)
C(25)	0.0327(9)	0.0465(10)	0.0313(8)	-0.0106(7)	0.0020(6)	0.0140(7)
C(26)	0.0457(11)	0.0626(12)	0.0250(7)	0.0003(7)	0.0013(7)	0.0273(9)
C(27)	0.0512(8)	0.0499(8)	0.0295(5)	-0.0002(5)	-0.0030(5)	0.0200(6)
C(28)	0.0228(4)	0.0268(5)	0.0416(6)	-0.0029(4)	0.0032(4)	0.0057(4)
N(2)	0.0356(5)	0.0422(6)	0.0447(6)	0.0087(5)	0.0012(4)	0.0063(4)

C(30)	0.0317(6)	0.0640(10)	0.0674(10)	0.0386(9)	0.0050(6)	0.0067(6)
C(31)	0.0380(11)	0.0321(10)	0.127(4)	0.0153(17)	0.0267(18)	0.0099(8)
C(33)	0.0394(14)	0.0338(14)	0.074(2)	-0.0172(18)	0.0164(18)	-0.0009(10)
C(16')	0.064(7)	0.055(5)	0.045(4)	0.006(3)	0.027(4)	0.034(4)
C(17')	0.052(8)	0.029(4)	0.025(3)	-0.013(3)	-0.008(5)	0.006(5)
C(20')	0.077(8)	0.082(8)	0.045(5)	-0.032(5)	-0.013(5)	0.018(6)
C(26')	0.047(5)	0.054(5)	0.042(4)	-0.014(4)	0.025(4)	0.000(4)
C(31')	0.031(3)	0.053(4)	0.0131(18)	0.0101(19)	0.0088(16)	0.018(3)
C(32')	0.037(3)	0.032(3)	0.033(3)	-0.004(2)	0.003(2)	0.005(2)
C(33')	0.023(2)	0.013(2)	0.028(3)	-0.004(2)	0.001(2)	0.0036(16)
O(1S)	0.0572(13)	0.0493(12)	0.0513(12)	0.0056(9)	0.0161(10)	0.0196(10)
C(1S)	0.060(2)	0.080(3)	0.086(3)	-0.008(2)	0.018(2)	0.027(2)
C(2S)	0.070(2)	0.096(3)	0.0463(17)	0.0012(19)	0.0028(16)	0.040(2)
C(3S)	0.076(3)	0.071(2)	0.0513(18)	-0.0014(17)	0.0175(17)	0.028(2)
C(4S)	0.058(2)	0.064(2)	0.085(3)	-0.018(2)	0.0118(19)	0.0274(18)

Hydrogen coordinates and isotropic displacement parameters (Å²) for 6a-BBN.

	x	y	z	U(eq)
H(1)	0.3932	0.2636	0.2780	0.032
H(2A)	0.6336	0.2501	0.3166	0.039
H(2B)	0.5631	0.2071	0.2013	0.039
H(3A)	0.7686	0.4348	0.2744	0.041
H(3B)	0.7745	0.3274	0.1885	0.041
H(4A)	0.6319	0.4083	0.0675	0.038
H(4B)	0.7431	0.5316	0.1231	0.038
H(5)	0.5168	0.5742	0.0986	0.031
H(6A)	0.5266	0.6766	0.2535	0.035
H(6B)	0.6834	0.6754	0.2488	0.035
H(7A)	0.6986	0.5394	0.3729	0.039
H(7B)	0.5990	0.6233	0.4106	0.039
H(8A)	0.5313	0.3898	0.4244	0.036
H(8B)	0.4114	0.4567	0.3743	0.036
H(11)	-0.0362	0.3171	0.0491	0.038
H(12)	-0.0176	0.5049	0.1759	0.039
H(15)	0.3950	0.1700	-0.0740	0.036
H(16)	0.3233	0.0093	-0.2098	0.030
H(18)	-0.0753	-0.0126	-0.1678	0.044
H(19)	-0.0004	0.1481	-0.0346	0.038
H(20A)	0.0173	-0.0816	-0.3459	0.055
H(20B)	0.0071	-0.1930	-0.2680	0.055
H(20C)	0.1470	-0.1443	-0.3114	0.055
H(21)	0.3441	0.6264	0.3134	0.034
H(2')	0.044(2)	0.7564(18)	0.2497(15)	0.047(5)
H(24)	-0.1028	0.7919	0.3569	0.045
H(25)	-0.0773	0.7248	0.5178	0.044
H(26)	0.1010	0.6179	0.5720	0.051
H(27)	0.2433	0.5804	0.4630	0.052
H(2)	0.2511(18)	0.6502(17)	0.0511(13)	0.041(4)
H(30)	0.3240	0.8770	-0.0059	0.065
H(31)	0.3821	1.0392	0.1532	0.076

H(33)	0.3524	0.9103	0.3015	0.060
H(16')	0.3021	0.0135	-0.2085	0.059
H(20D)	0.0970	-0.1949	-0.2807	0.108
H(20E)	0.0688	-0.0863	-0.3563	0.108
H(20F)	-0.0495	-0.1559	-0.2971	0.108
H(26')	-0.0004	0.6649	0.5352	0.057
H(31')	0.4037	1.0311	0.0727	0.036
H(32')	0.4246	1.0566	0.2558	0.042
H(33')	0.3521	0.8729	0.3364	0.026
H(1S1)	0.6477	0.9314	0.3812	0.110
H(1S2)	0.7216	0.8614	0.4709	0.110
H(1S3)	0.7247	1.0129	0.4852	0.110
H(2S1)	0.4920	0.8059	0.4805	0.082
H(2S2)	0.5588	0.9131	0.5732	0.082
H(3S1)	0.3760	1.0164	0.5828	0.077
H(3S2)	0.2834	0.8935	0.5120	0.077
H(4S1)	0.3091	1.1505	0.4556	0.102
H(4S2)	0.1828	1.0754	0.5048	0.102
H(4S3)	0.2057	1.0253	0.3954	0.102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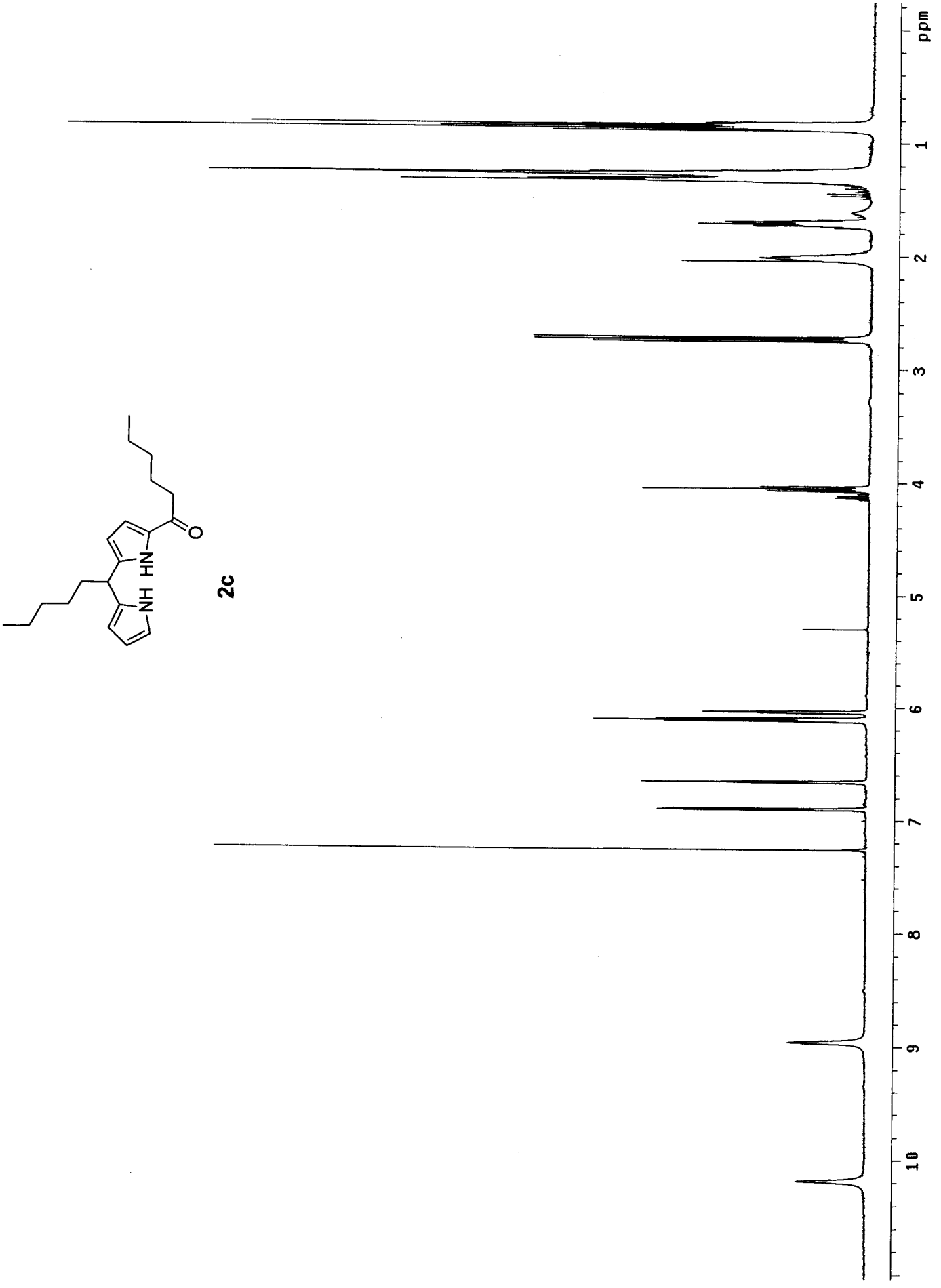
2
3
4
5
6
7
8
9
10
11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HN
O
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ppm
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3
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7
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9
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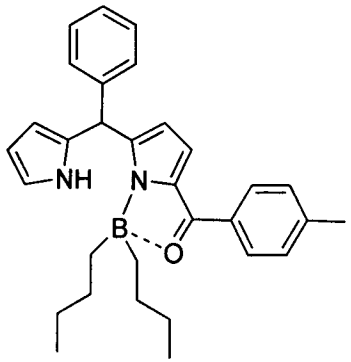

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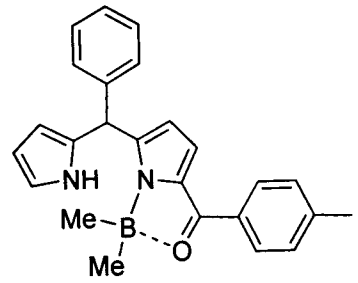

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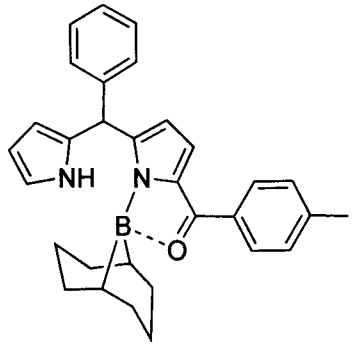

6a-BBN
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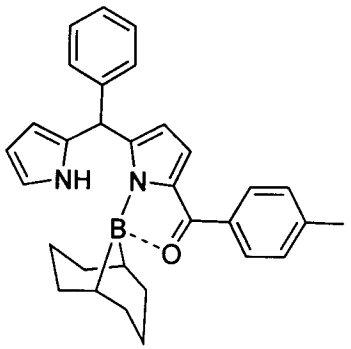

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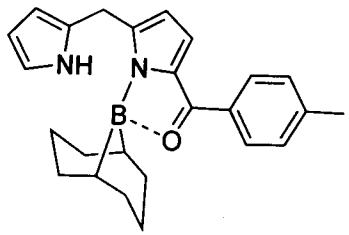

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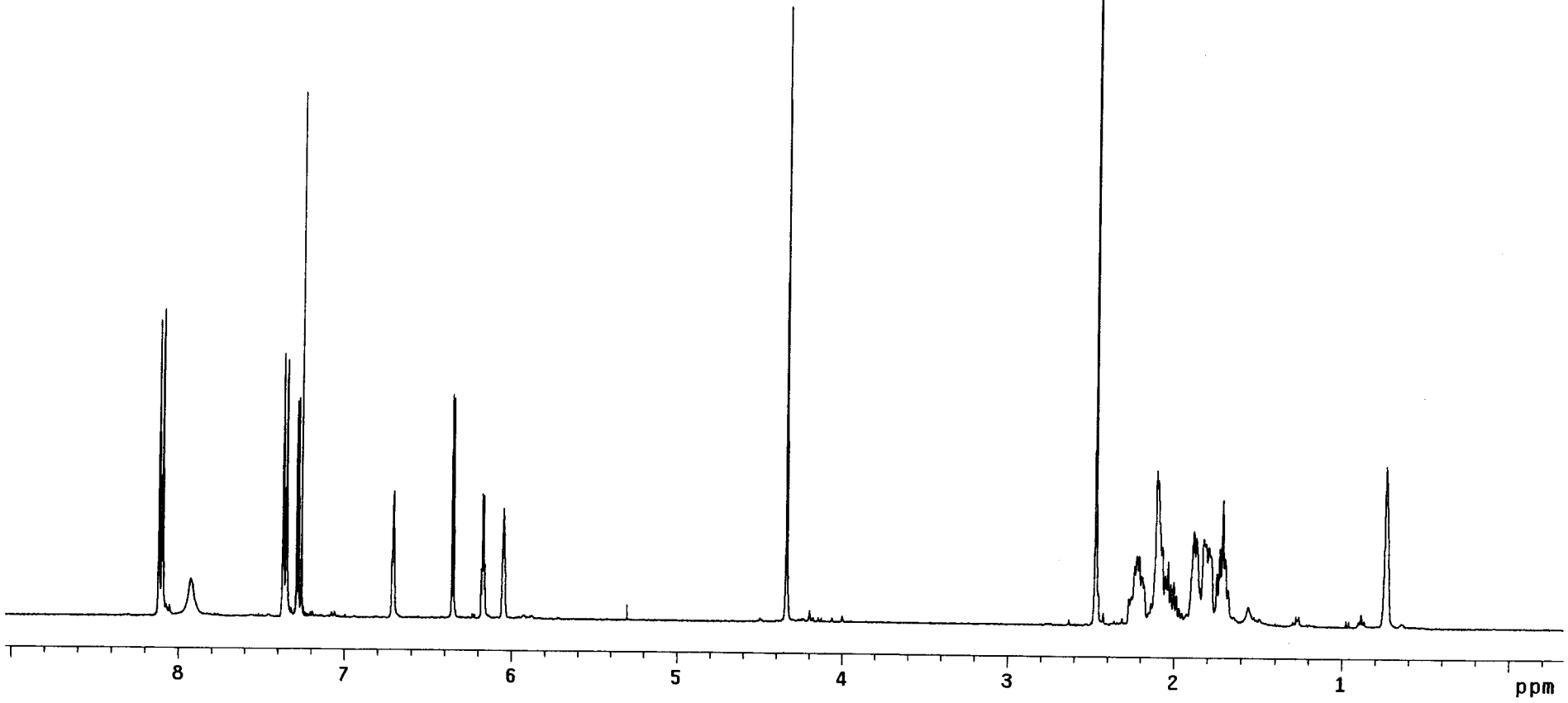

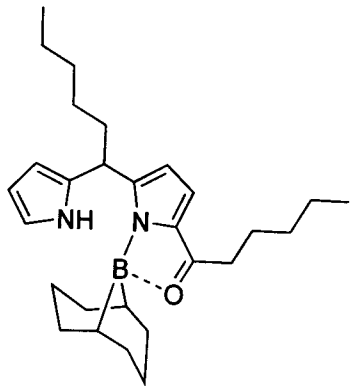

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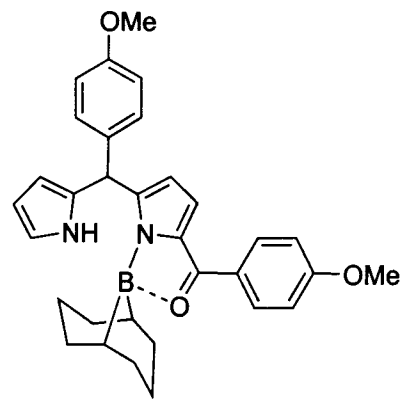

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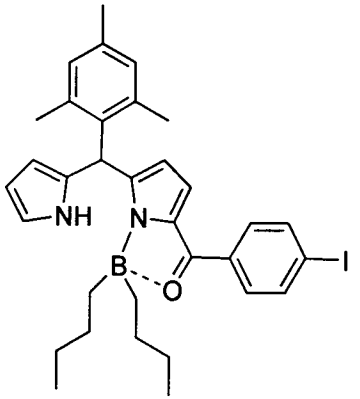

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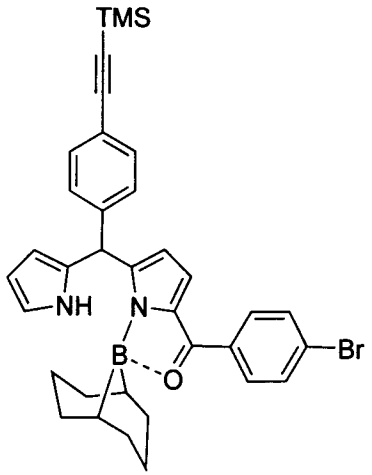

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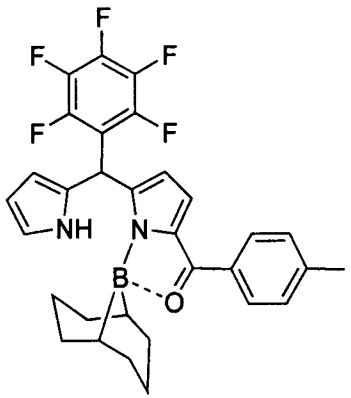

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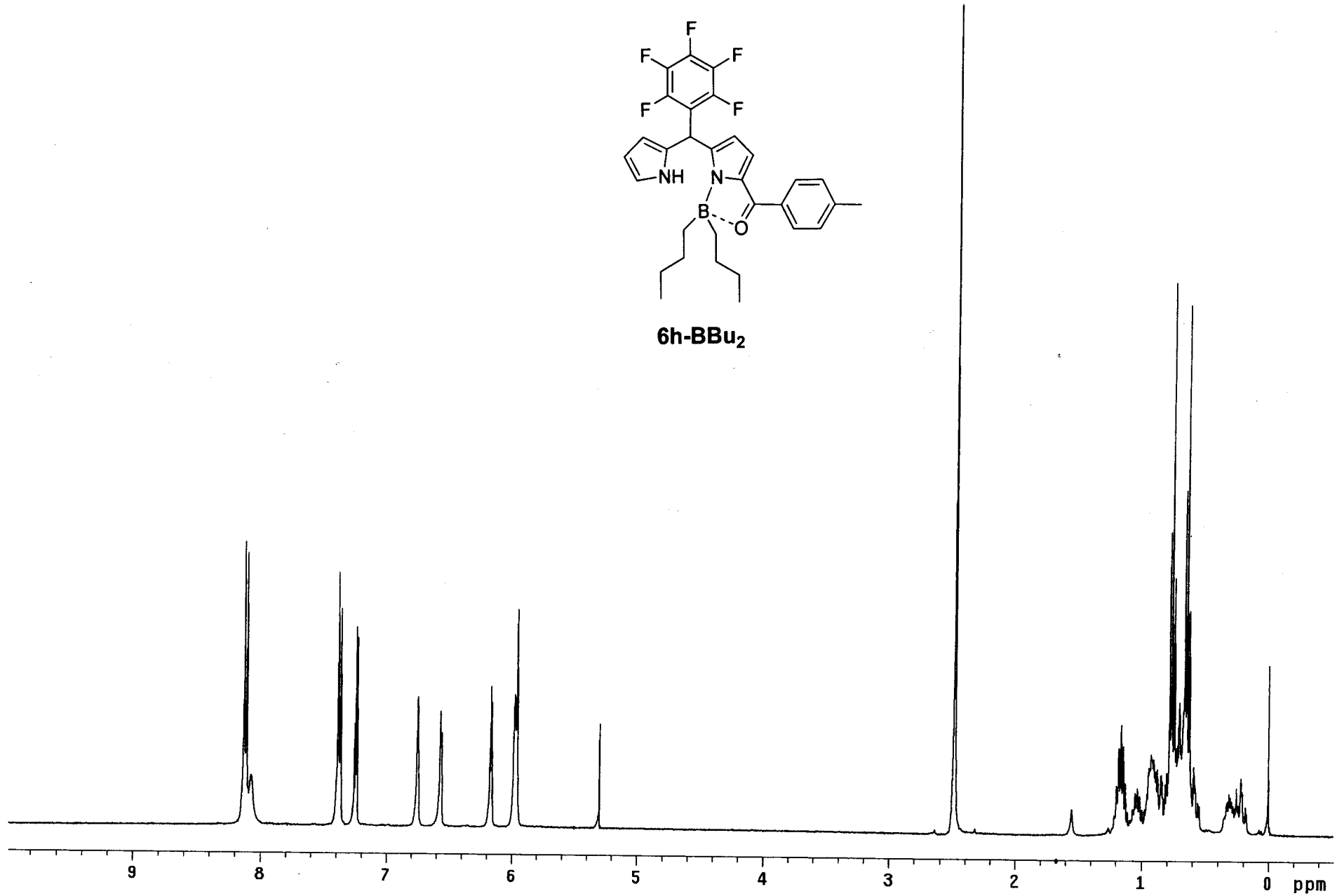

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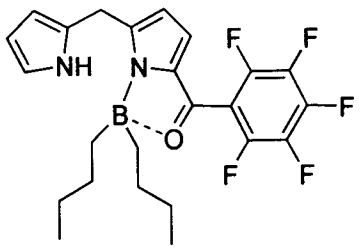

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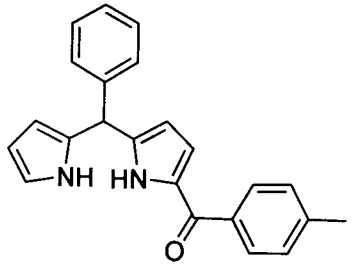

2a
(from decomplexation of **6a-BBN**)