

Supplimentary Materials

Mono- and Dinitro BN-Naphthalenes: Formation and Characterization

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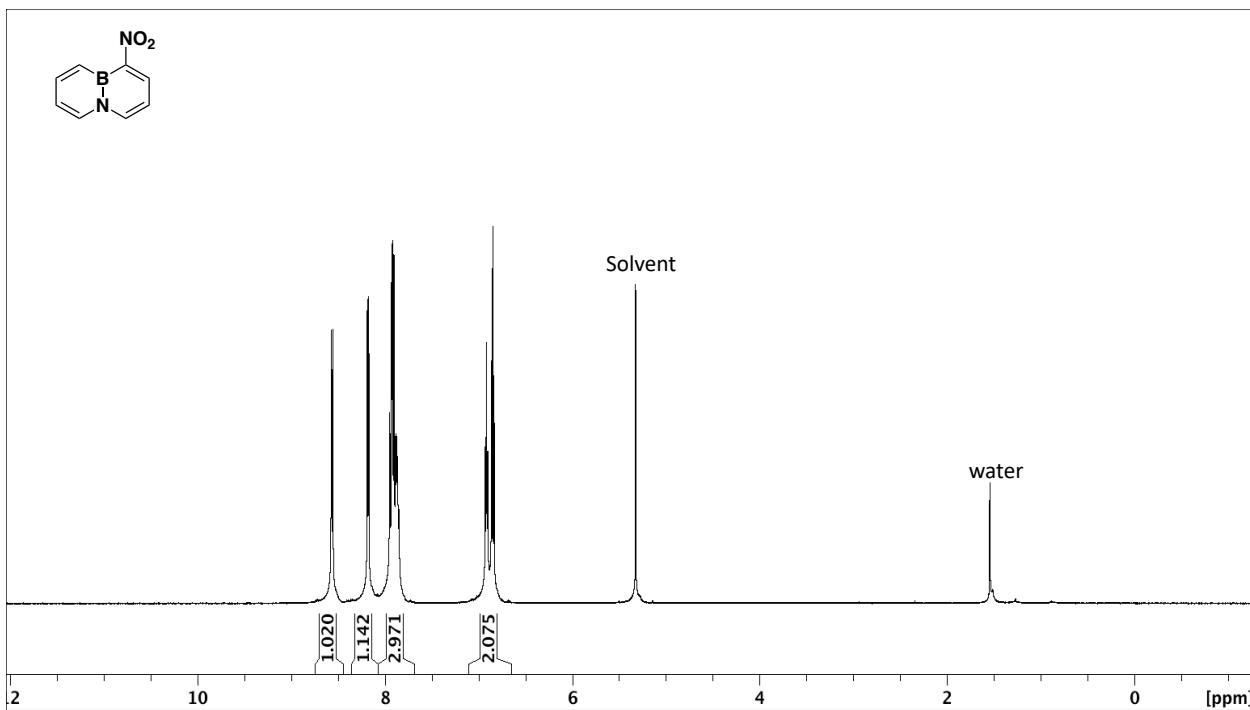
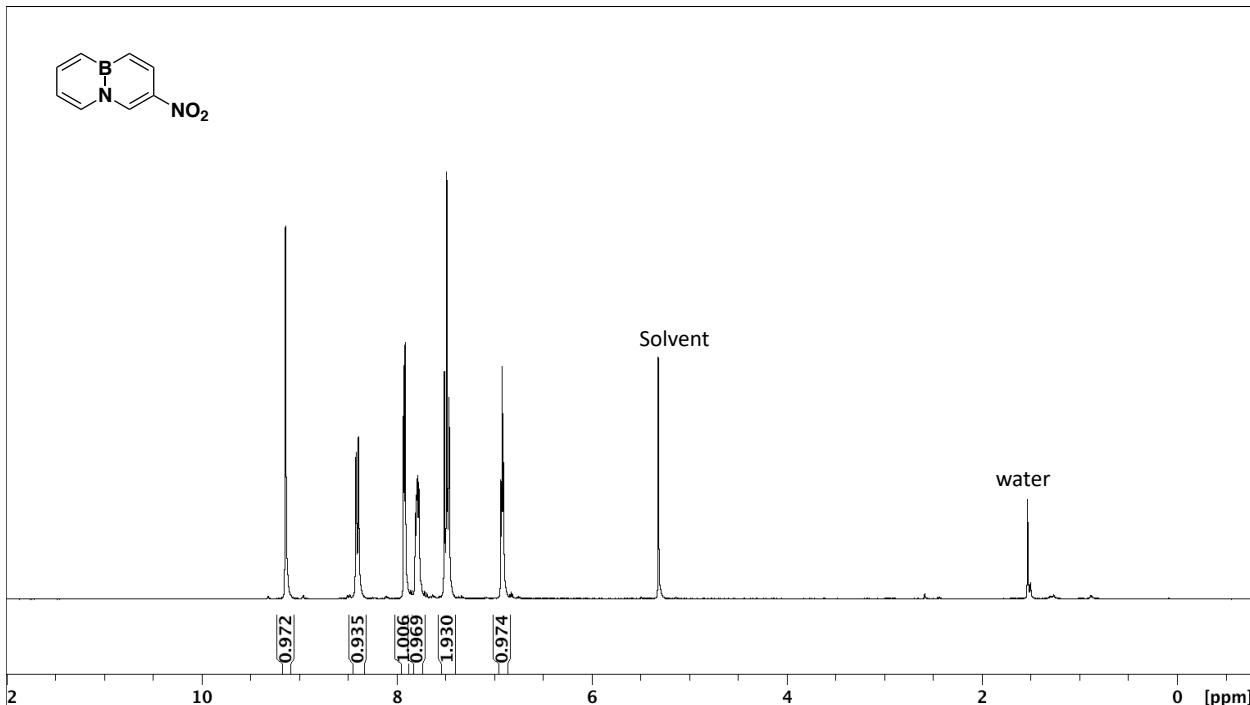
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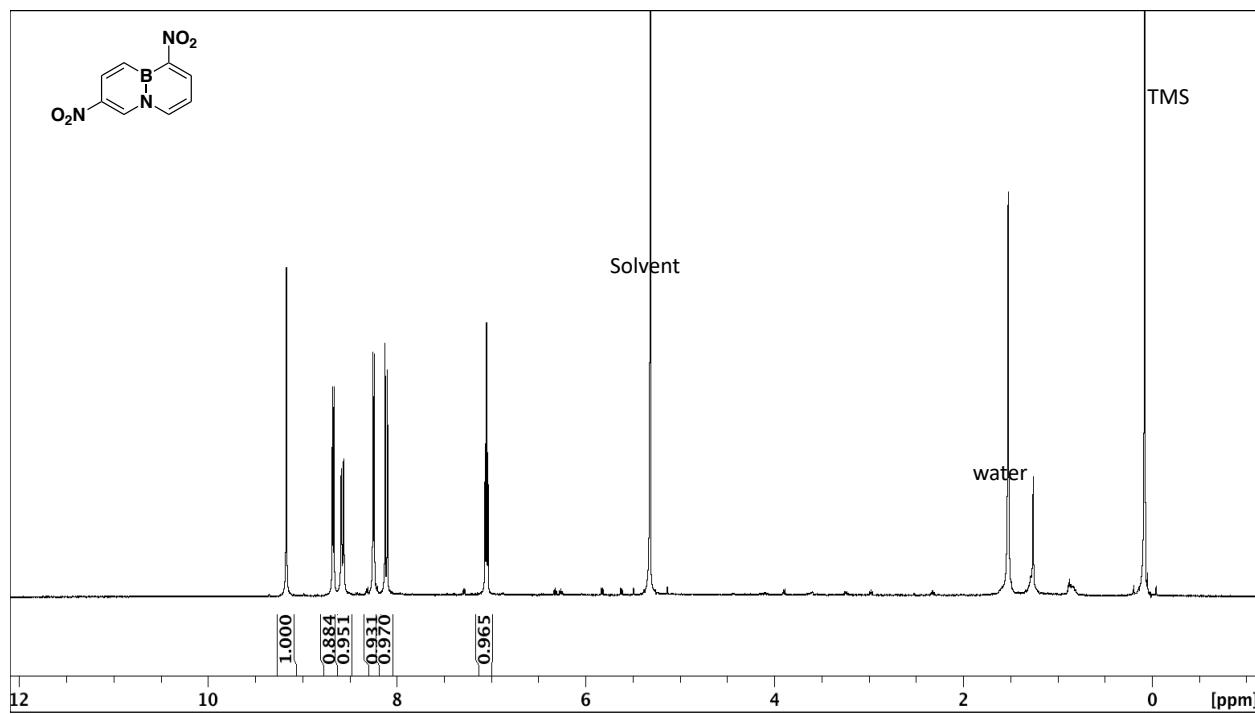
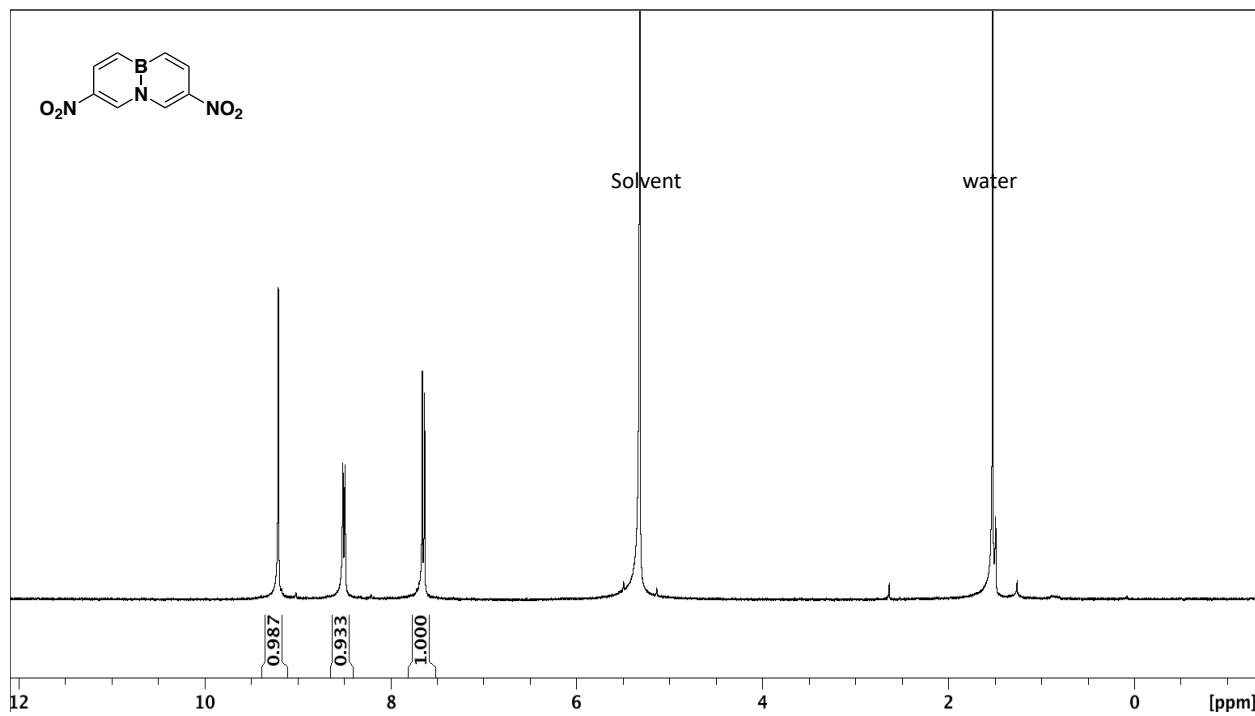
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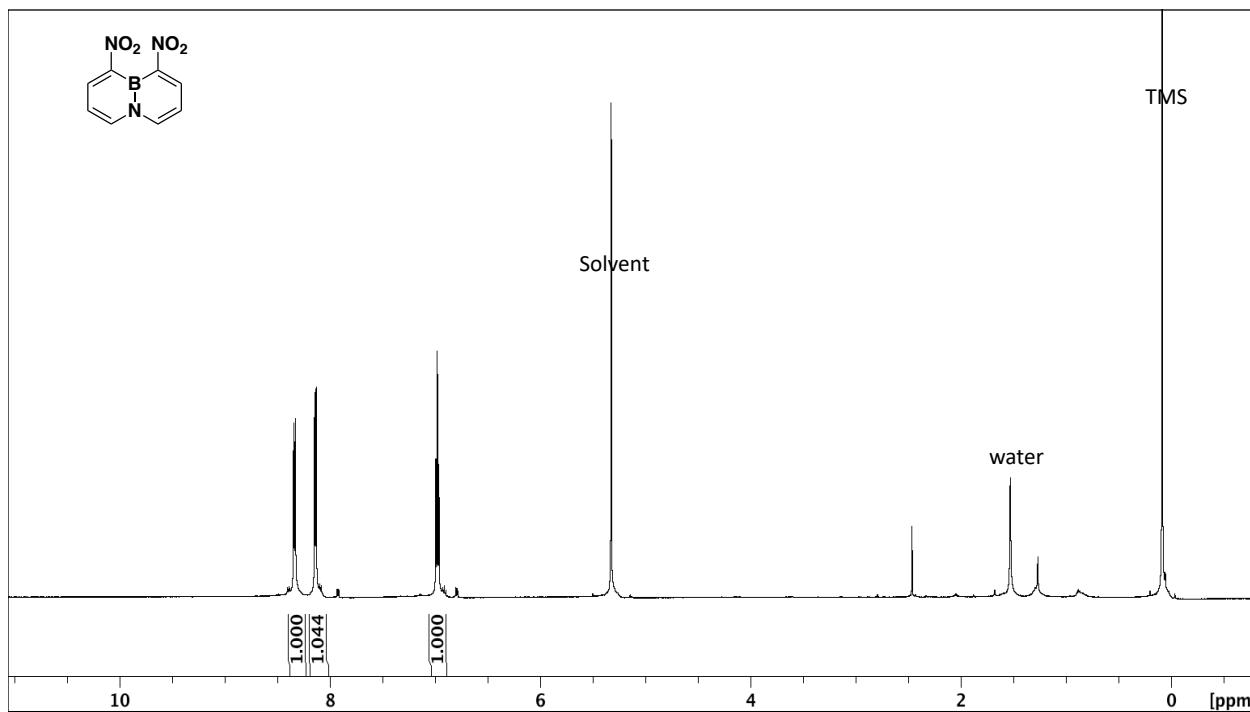
Content

1. Proton NMR of nitro-BNNs
2. Carbon-13 NMR of nitro-BNNs
3. B-11 NMR of nitro-BNNs
4. Infrared spectra of nitro-BNNs
5. X-ray crystallography of BNNs

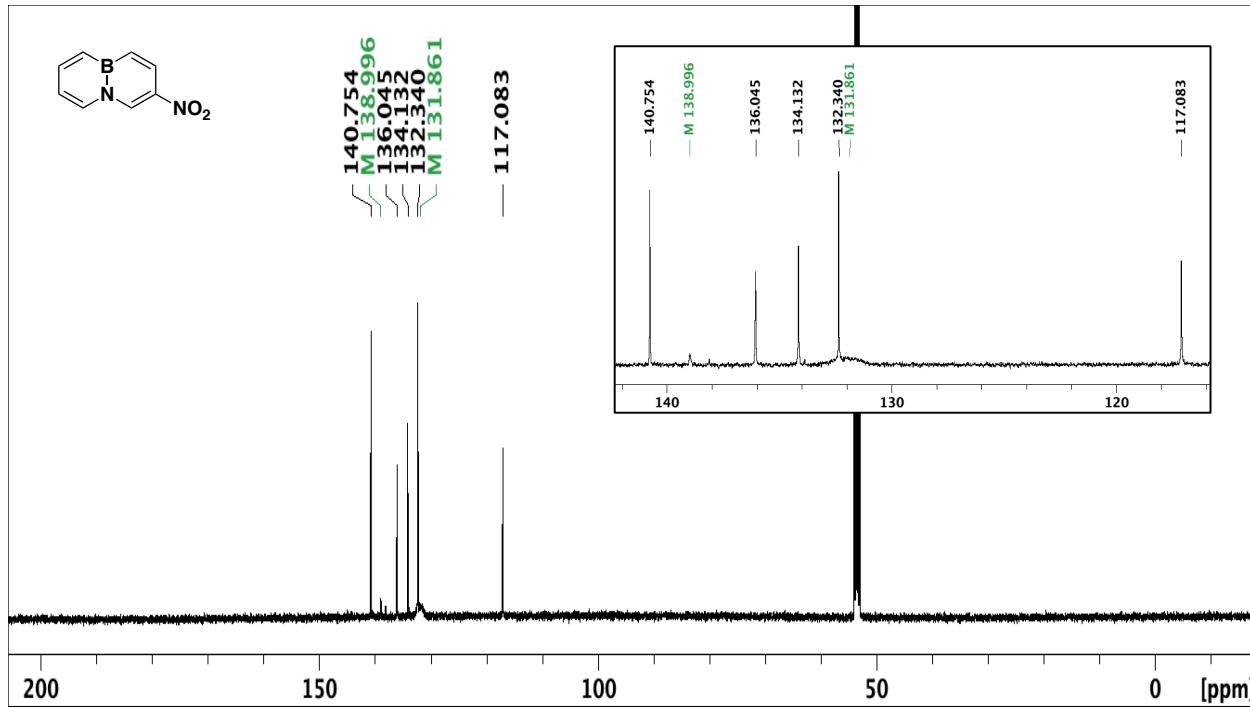
1. Proton NMR spectra of compound 3, 4, 5, 6, and 7.

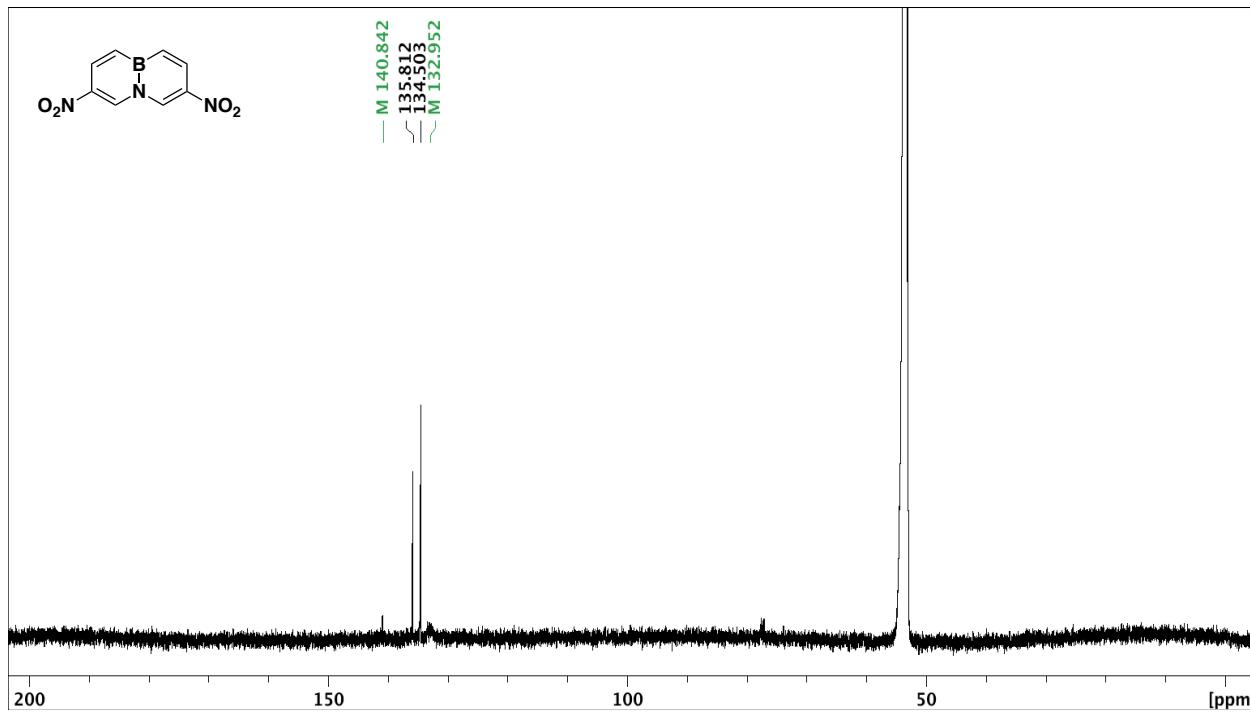
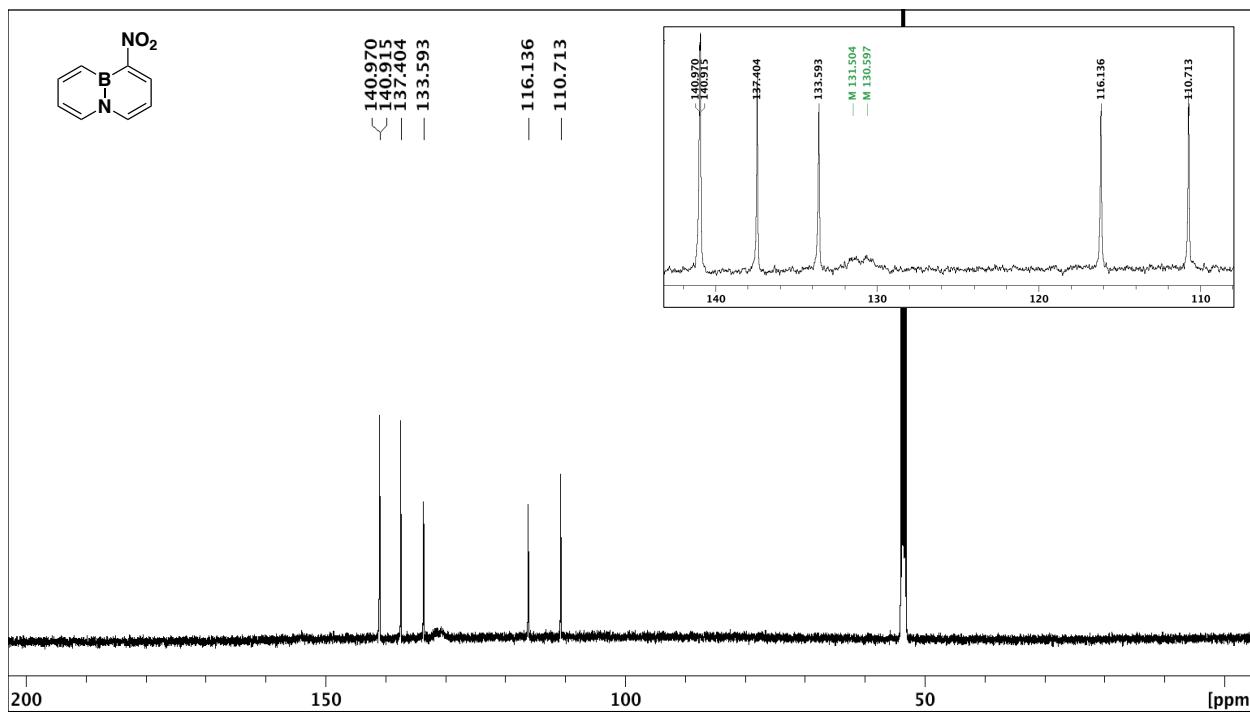


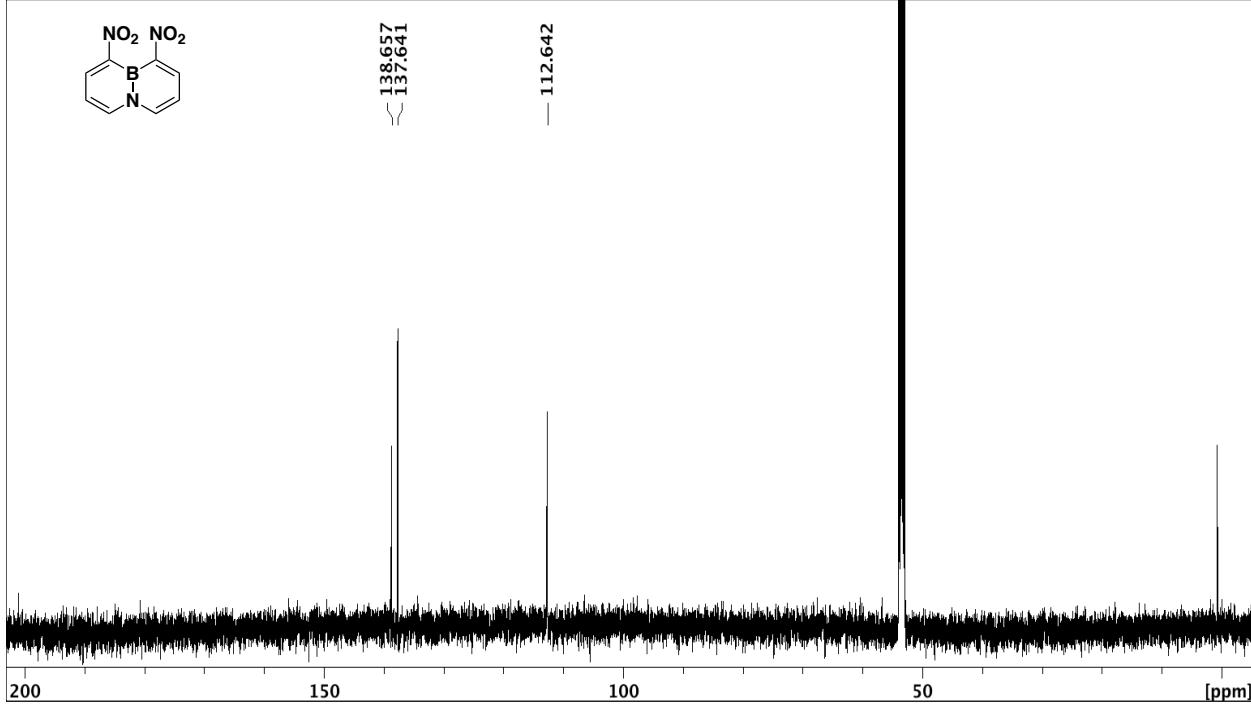
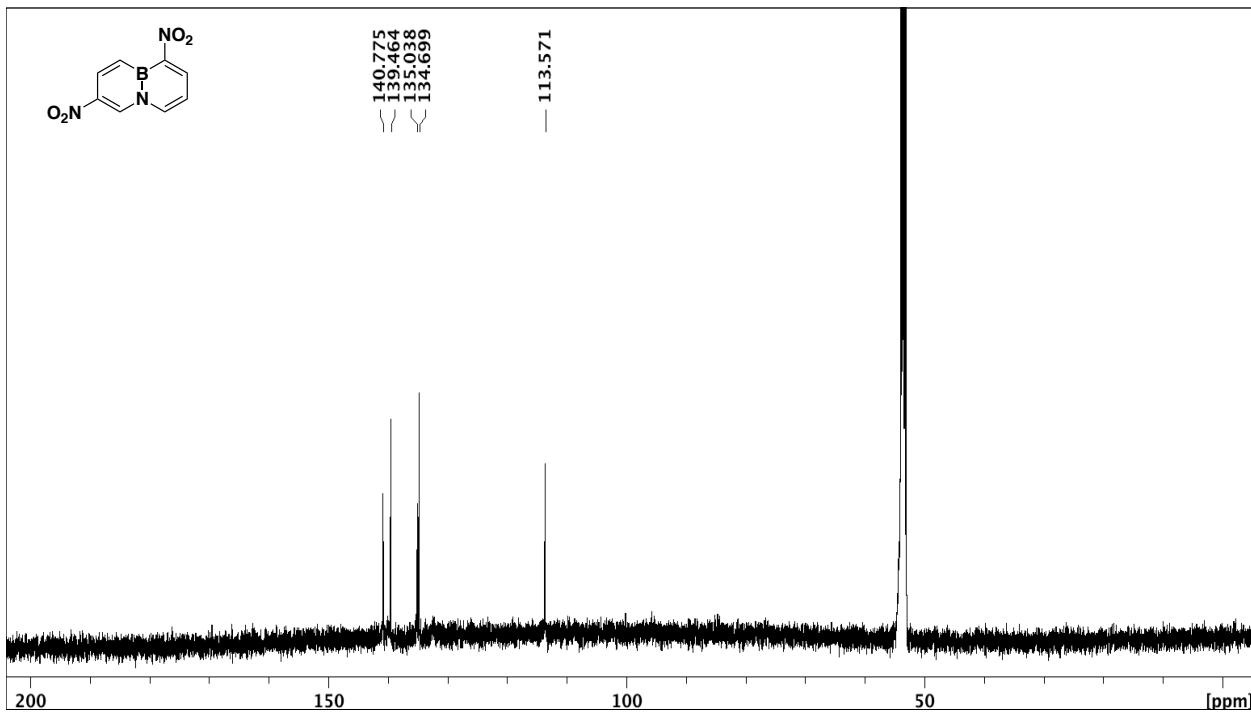




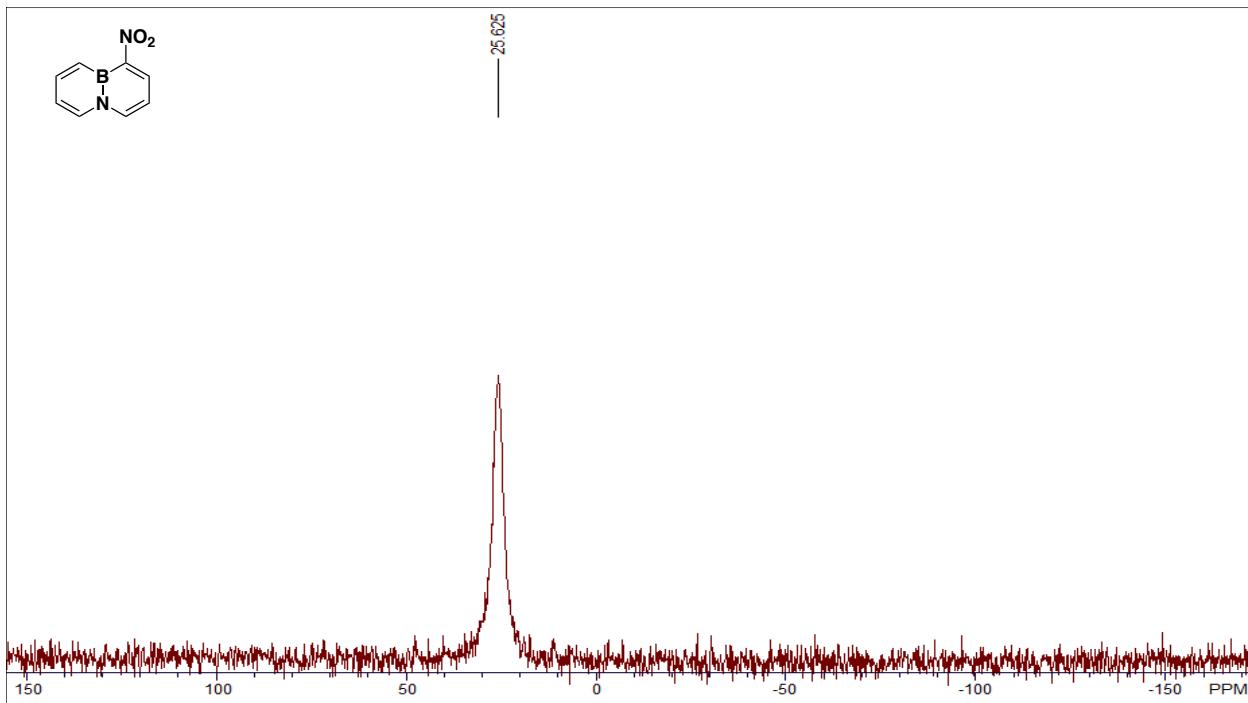
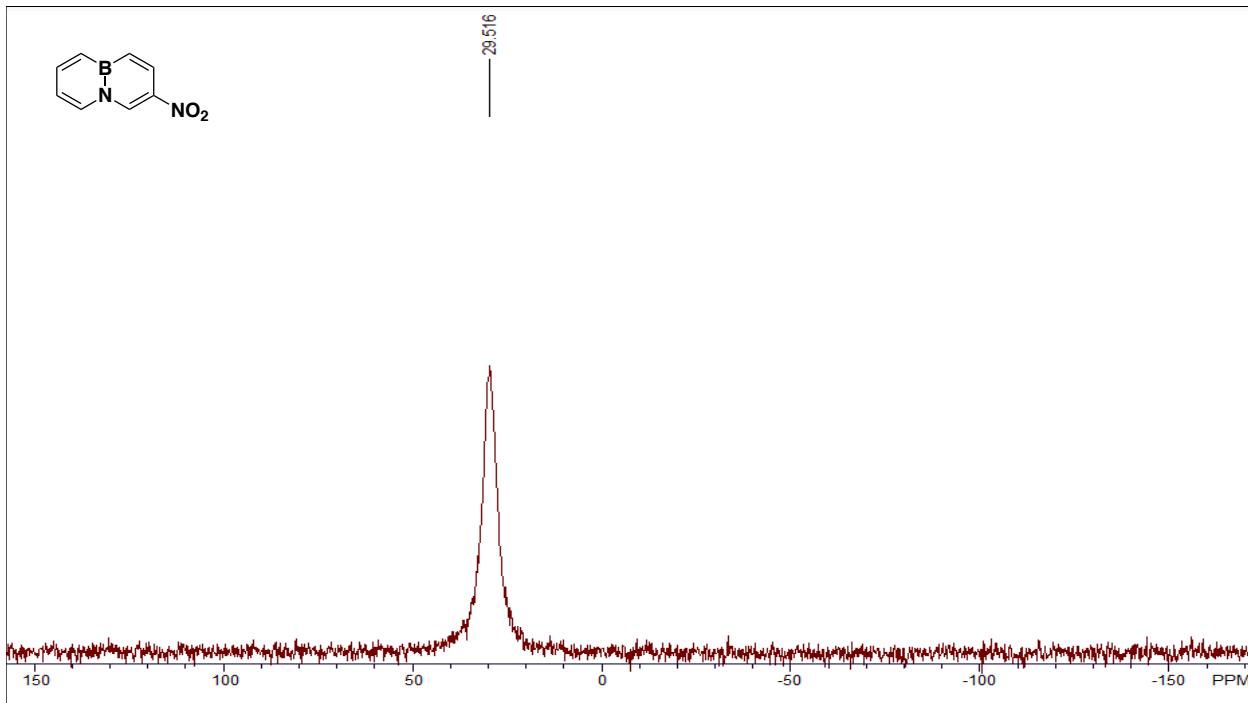
2. C-13 NMR spectra of compound 3, 4, 5, 6, and 7.

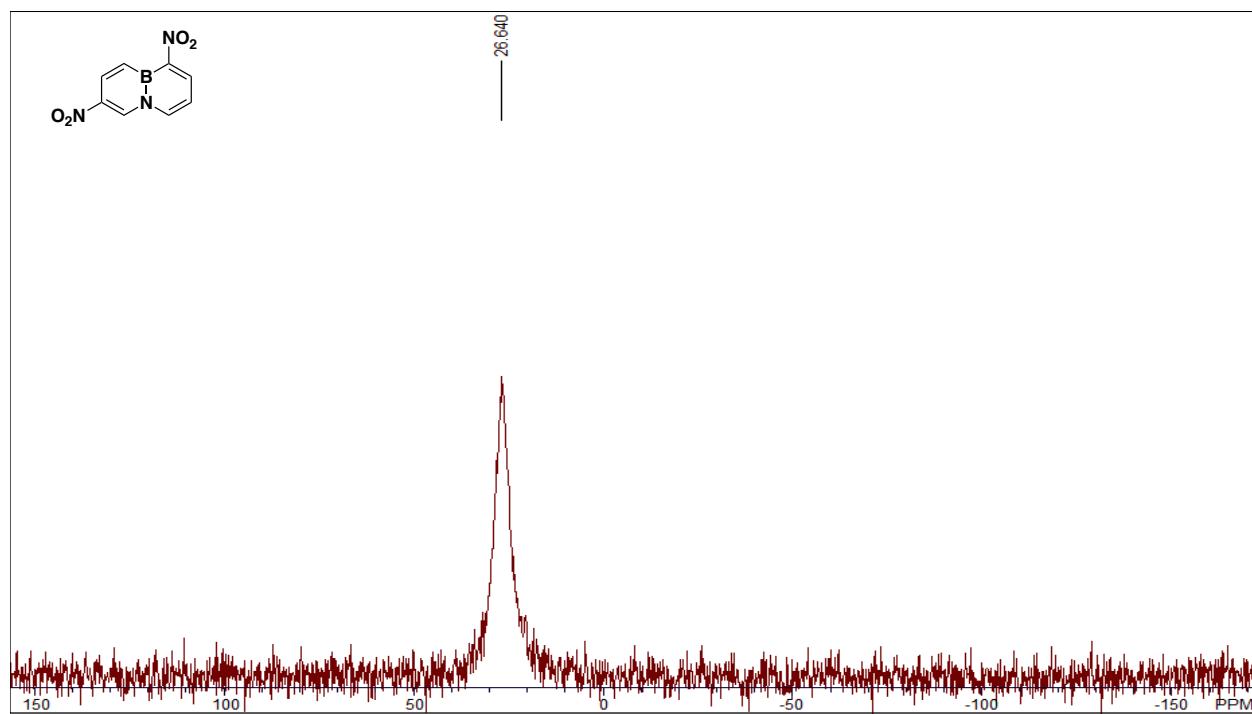
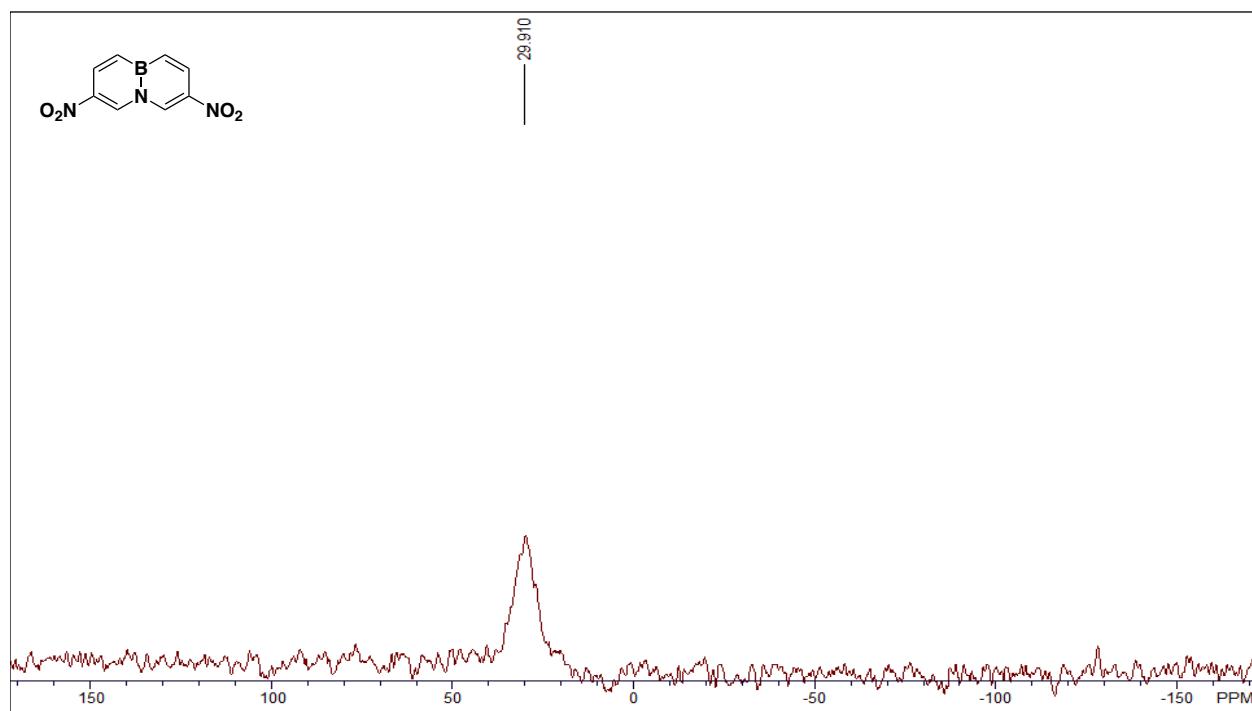


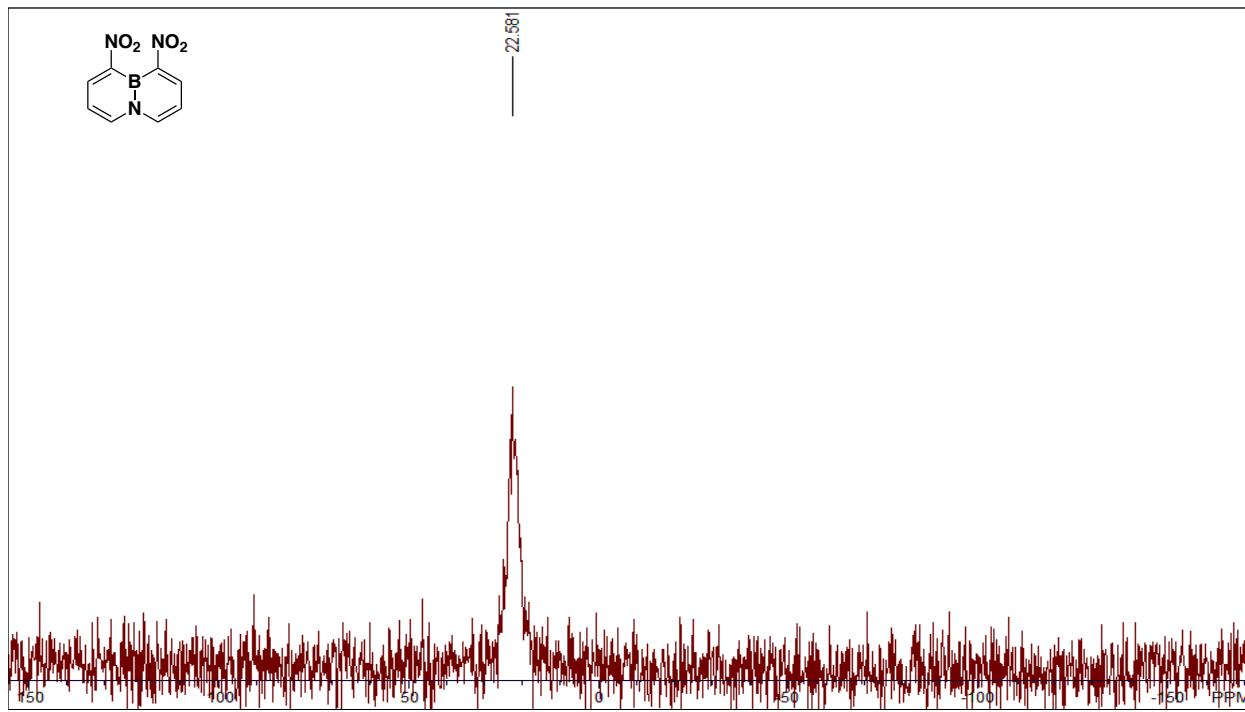




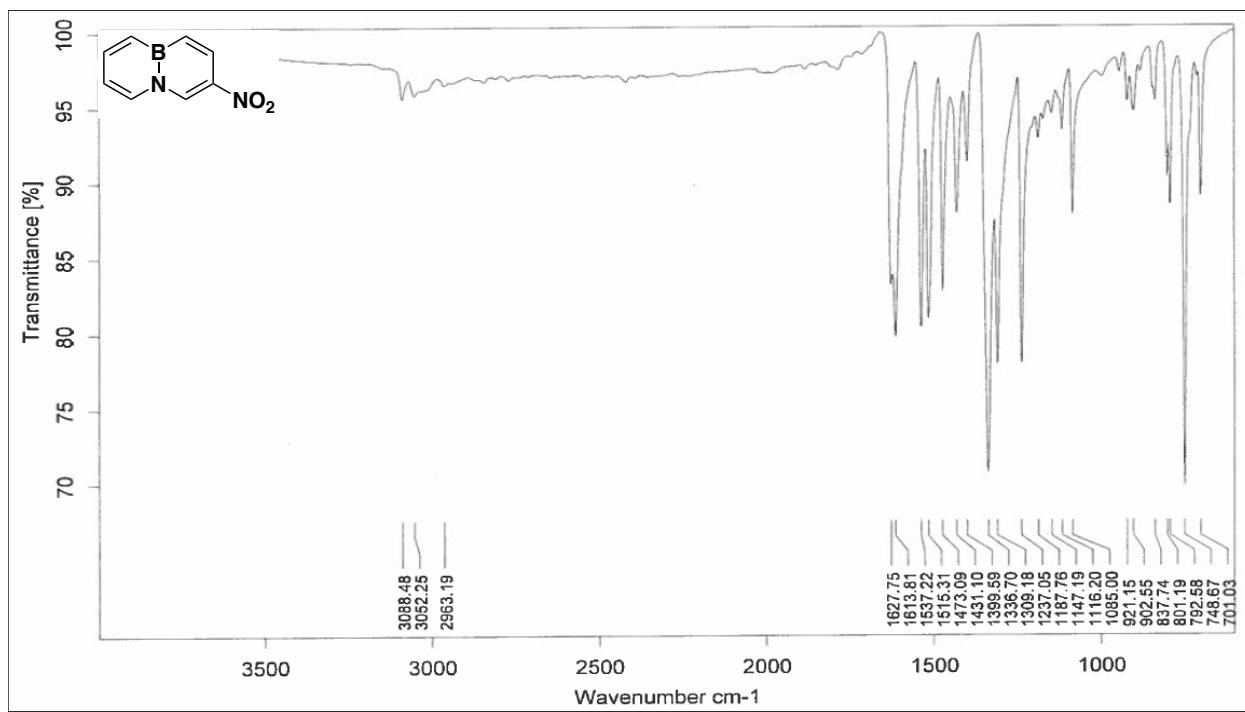
3. B-11 NMR spectra of compound 3, 4, 5, 6, and 7.

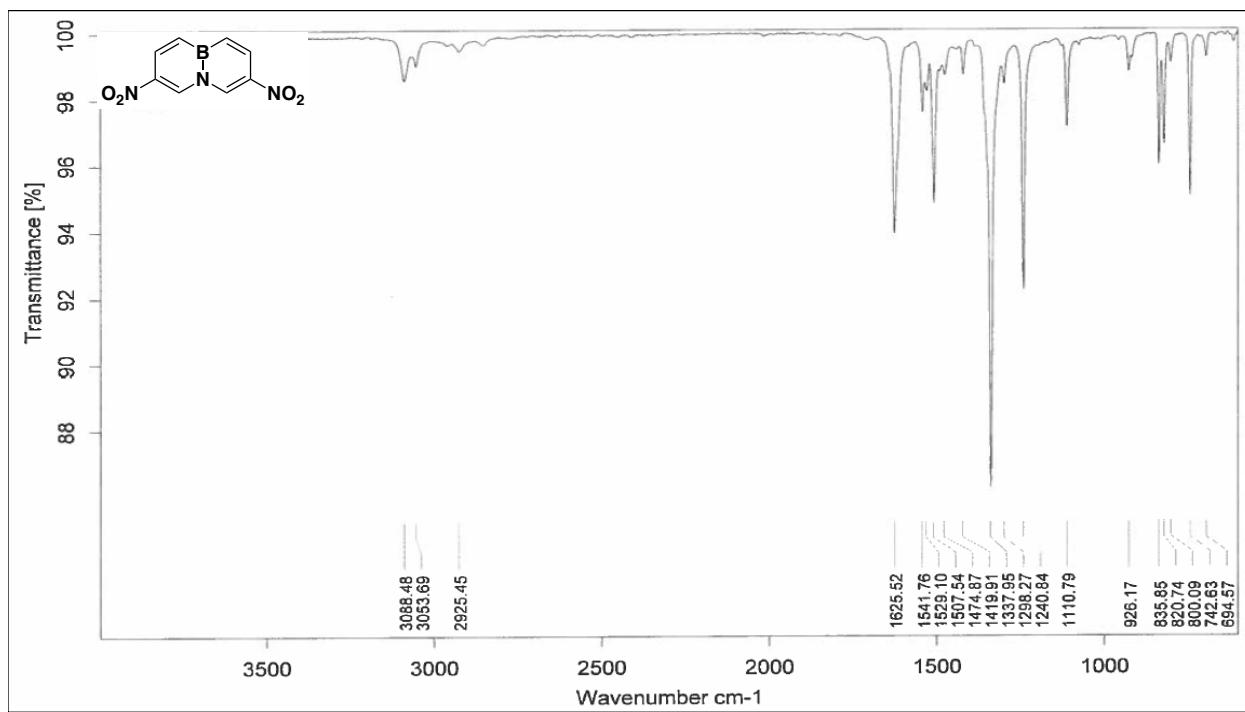
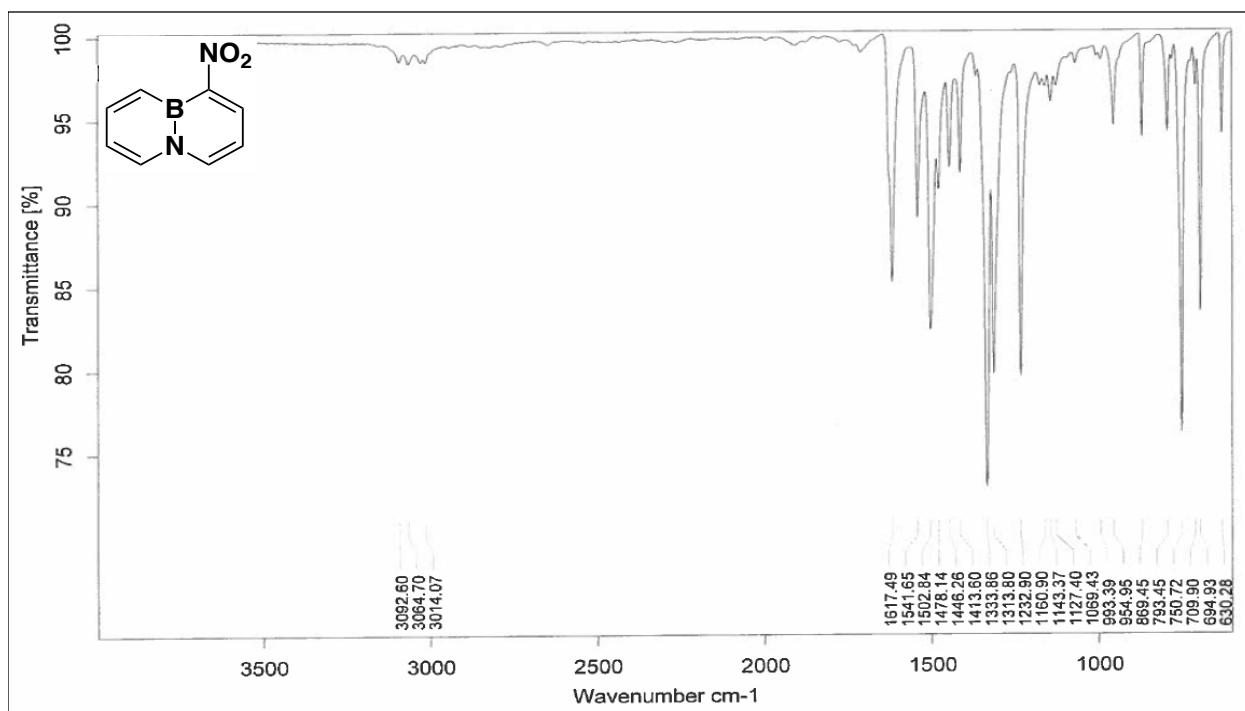


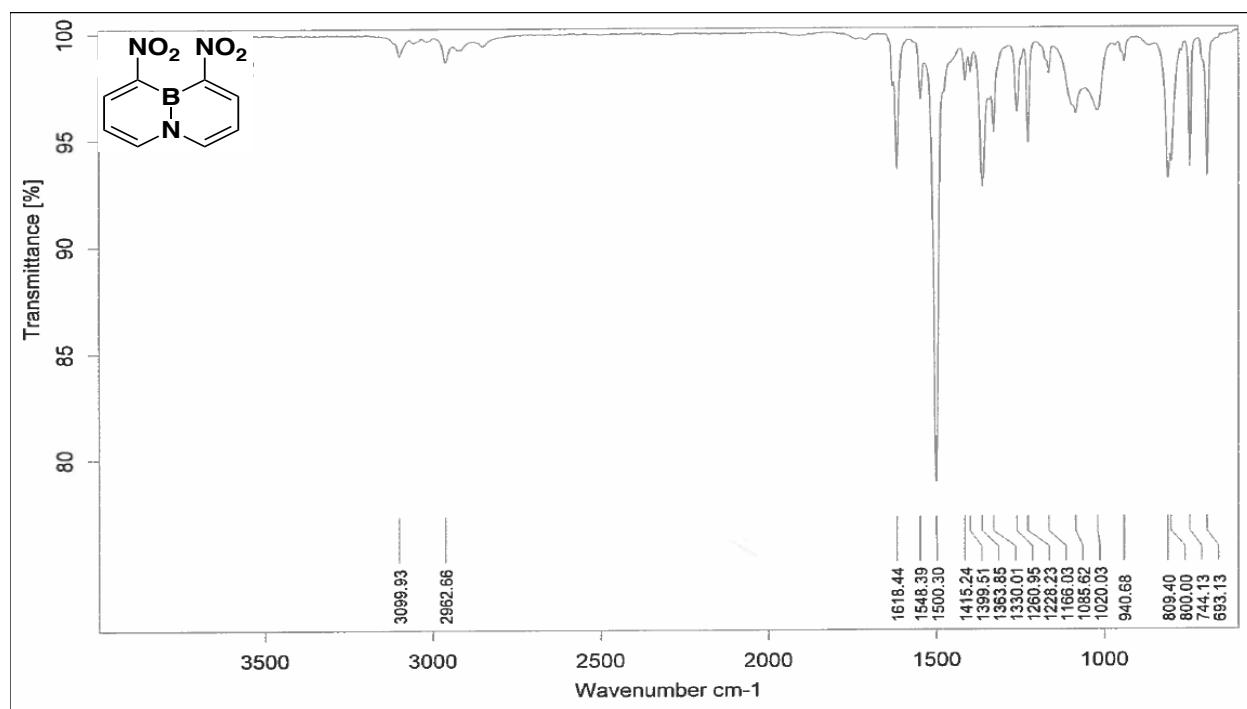
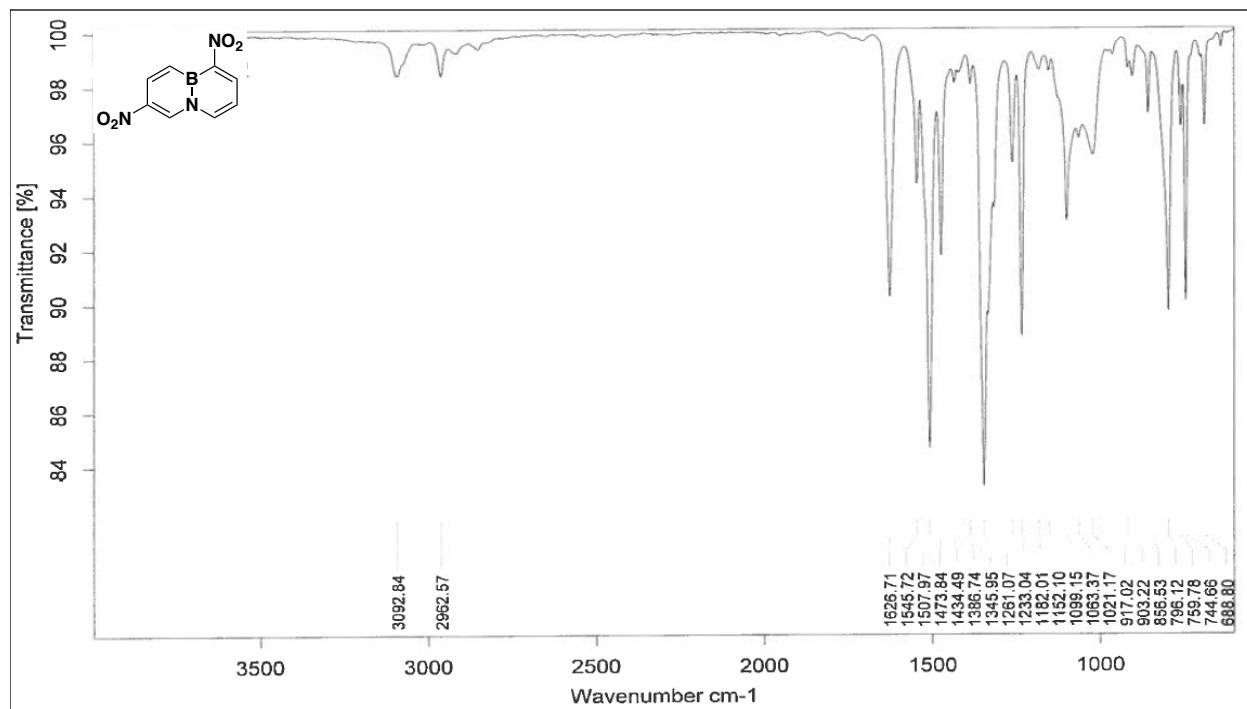




4. Infrared spectrum of compound 3, 4, 5, 6, and 7.

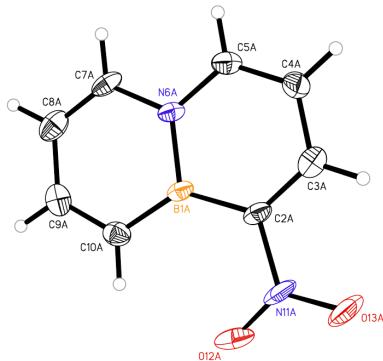






5. X-ray crystallographic analysis data for 1-nitro-BNN, 1,6-dinitro-BNN and 1,8-dinitro-BNN
 6.

Table S1, Crystal data and structure refinement for 1-nitro-BNN **1-nitro-BNN**.



Empirical formula	$C_8H_7BN_2O_2$	
Formula weight	173.97	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	$a = 16.722(2)$ Å	$\alpha = 90^\circ$.
	$b = 3.7994(5)$ Å	$\beta = 90^\circ$.
	$c = 25.070(3)$ Å	$\gamma = 90^\circ$.
Volume	$1592.8(4)$ Å ³	
Z	8	
Density (-123°C)	1.451 Mg/m ³	
Density (20°C)	1.406 Mg/m ³	
Absorption coefficient	0.104 mm ⁻¹	
F(000)	720	
Crystal size	0.62 x 0.14 x 0.08 mm ³	
Theta range for data collection	2.44 to 26.52°.	
Index ranges	$-20 \leq h \leq 20, -4 \leq k \leq 4, -31 \leq l \leq 27$	
Reflections collected	12754	
Independent reflections	3068 [$R_{int} = 0.0652$]	
Completeness to theta = 26.52°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9917 and 0.9383	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3068 / 1 / 235	
Goodness-of-fit on F^2	1.101	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0546, wR_2 = 0.1352$	
R indices (all data)	$R_1 = 0.0628, wR_2 = 0.1416$	
Largest diff. peak and hole	0.363 and -0.275 e.Å ⁻³	

Table S2. Bond lengths [\AA] and angles [$^\circ$] for 1-nitro-BNN **1-nitro-BNN**.

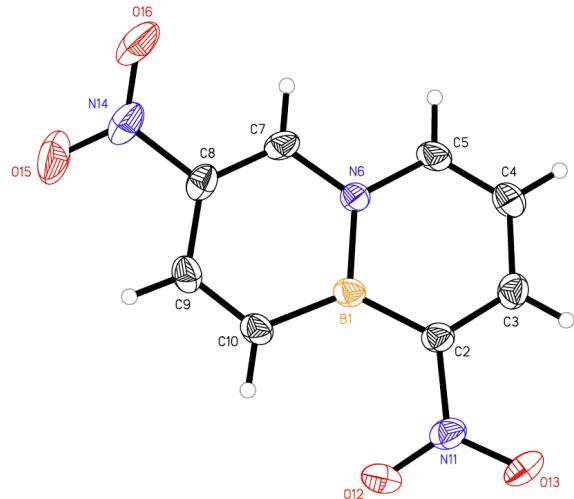
B(1A)-N(6A)	1.472(3)	B(1A)-C(10A)	1.510(5)
B(1A)-C(2A)	1.525(4)	C(2A)-C(3A)	1.358(5)
C(2A)-N(11A)	1.474(3)	C(3A)-C(4A)	1.415(4)
C(3A)-H(3A)	0.9500	C(4A)-C(5A)	1.359(4)
C(4A)-H(4A)	0.9500	C(5A)-N(6A)	1.382(4)
C(5A)-H(5A)	0.9500	N(6A)-C(7A)	1.395(3)
C(7A)-C(8A)	1.343(5)	C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.427(4)	C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.364(5)	C(9A)-H(9A)	0.9500
C(10A)-H(10A)	0.9500	N(11A)-O(12A)	1.226(4)
N(11A)-O(13A)	1.231(4)	B(1B)-N(6B)	1.473(4)
B(1B)-C(10B)	1.521(5)	B(1B)-C(2B)	1.531(4)
C(2B)-C(3B)	1.372(5)	C(2B)-N(11B)	1.453(3)
C(3B)-C(4B)	1.410(4)	C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.351(5)	C(4B)-H(4B)	0.9500
C(5B)-N(6B)	1.372(4)	C(5B)-H(5B)	0.9500
N(6B)-C(7B)	1.392(3)	C(7B)-C(8B)	1.346(5)
C(7B)-H(7B)	0.9500	C(8B)-C(9B)	1.420(5)
C(8B)-H(8B)	0.9500	C(9B)-C(10B)	1.347(5)
C(9B)-H(9B)	0.9500	C(10B)-H(10B)	0.9500
N(11B)-O(13B)	1.235(4)	N(11B)-O(12B)	1.235(4)
N(6A)-B(1A)-C(10A)	115.5(2)	N(6A)-B(1A)-C(2A)	112.0(2)
C(10A)-B(1A)-C(2A)	132.5(2)	C(3A)-C(2A)-N(11A)	115.8(2)
C(3A)-C(2A)-B(1A)	122.4(2)	N(11A)-C(2A)-B(1A)	121.8(2)
C(2A)-C(3A)-C(4A)	120.4(3)	C(2A)-C(3A)-H(3A)	119.8
C(4A)-C(3A)-H(3A)	119.8	C(5A)-C(4A)-C(3A)	120.9(3)
C(5A)-C(4A)-H(4A)	119.6	C(3A)-C(4A)-H(4A)	119.6
C(4A)-C(5A)-N(6A)	121.8(2)	C(4A)-C(5A)-H(5A)	119.1
N(6A)-C(5A)-H(5A)	119.1	C(5A)-N(6A)-C(7A)	117.1(2)
C(5A)-N(6A)-B(1A)	122.5(2)	C(7A)-N(6A)-B(1A)	120.3(2)
C(8A)-C(7A)-N(6A)	121.6(2)	C(8A)-C(7A)-H(7A)	119.2
N(6A)-C(7A)-H(7A)	119.2	C(7A)-C(8A)-C(9A)	121.9(3)
C(7A)-C(8A)-H(8A)	119.0	C(9A)-C(8A)-H(8A)	119.0
C(10A)-C(9A)-C(8A)	120.6(3)	C(10A)-C(9A)-H(9A)	119.7
C(8A)-C(9A)-H(9A)	119.7	C(9A)-C(10A)-B(1A)	120.0(3)
C(9A)-C(10A)-H(10A)	120.0	B(1A)-C(10A)-H(10A)	120.0
O(12A)-N(11A)-O(13A)	122.6(3)	O(12A)-N(11A)-C(2A)	118.0(2)
O(13A)-N(11A)-C(2A)	119.4(3)	N(6B)-B(1B)-C(10B)	115.6(3)
N(6B)-B(1B)-C(2B)	112.3(3)	C(10B)-B(1B)-C(2B)	132.1(3)

C(3B)-C(2B)-N(11B)	116.0(3)	C(3B)-C(2B)-B(1B)	121.9(2)
N(11B)-C(2B)-B(1B)	122.1(3)	C(2B)-C(3B)-C(4B)	119.7(3)
C(2B)-C(3B)-H(3B)	120.2	C(4B)-C(3B)-H(3B)	120.2

Table S2. Continued

C(5B)-C(4B)-C(3B)	121.5(3)	C(5B)-C(4B)-H(4B)	119.2
C(3B)-C(4B)-H(4B)	119.2	C(4B)-C(5B)-N(6B)	122.3(3)
C(4B)-C(5B)-H(5B)	118.8	N(6B)-C(5B)-H(5B)	118.8
C(5B)-N(6B)-C(7B)	117.3(2)	C(5B)-N(6B)-B(1B)	122.2(2)
C(7B)-N(6B)-B(1B)	120.5(3)	C(8B)-C(7B)-N(6B)	121.2(3)
C(8B)-C(7B)-H(7B)	119.4	N(6B)-C(7B)-H(7B)	119.4
C(7B)-C(8B)-C(9B)	121.7(3)	C(7B)-C(8B)-H(8B)	119.2
C(9B)-C(8B)-H(8B)	119.2	C(10B)-C(9B)-C(8B)	122.1(4)
C(10B)-C(9B)-H(9B)	119.0	C(8B)-C(9B)-H(9B)	119.0
C(9B)-C(10B)-B(1B)	118.9(3)	C(9B)-C(10B)-H(10B)	120.5
B(1B)-C(10B)-H(10B)	120.5	O(13B)-N(11B)-O(12B)	121.6(3)
O(13B)-N(11B)-C(2B)	120.1(3)	O(12B)-N(11B)-C(2B)	118.3(3)

Table S3. Crystal data and structure refinement for 1,6-dinitro-BNN **1,6-dinitro-BNN**.



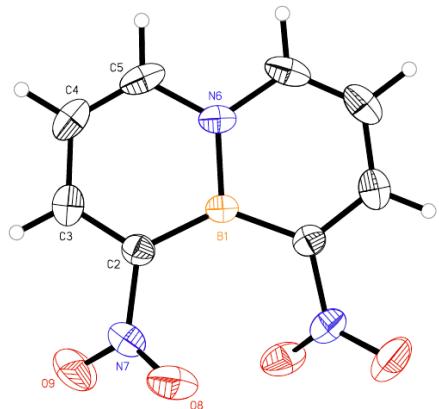
Empirical formula	$C_8H_6BN_3O_4$	
Formula weight	218.97	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna ₂ 1	
Unit cell dimensions	$a = 15.0780(17)$ Å	$\alpha = 90^\circ$.
	$b = 16.2287(18)$ Å	$\beta = 90^\circ$.
	$c = 3.7551(5)$ Å	$\gamma = 90^\circ$.
Volume	$918.86(19)$ Å ³	
Z	4	
Density (calculated)	1.583 Mg/m ³	
Absorption coefficient	0.127 mm ⁻¹	
F(000)	448	
Crystal size	0.41 x 0.05 x 0.04 mm ³	
Theta range for data collection	1.84 to 26.51°.	
Index ranges	$-18 \leq h \leq 18, -14 \leq k \leq 20, -4 \leq l \leq 4$	
Reflections collected	6470	
Independent reflections	1879 [$R_{\text{int}} = 0.0505$]	
Completeness to theta = 26.51°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9949 and 0.9499	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1879 / 1 / 145	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	$R_1 = 0.0467, wR_2 = 0.1133$	
R indices (all data)	$R_1 = 0.0632, wR_2 = 0.1241$	

Largest diff. peak and hole 0.237 and -0.195 e. \AA^{-3}

Table S4. Bond lengths [\AA] and angles [$^\circ$] for 1,6-dinitro-BNN **1,6-dinitro-BNN**.

B(1)-N(6)	1.469(3)	B(1)-C(2)	1.517(4)
B(1)-C(10)	1.520(4)	C(2)-C(3)	1.368(4)
C(2)-N(11)	1.460(3)	C(3)-C(4)	1.412(4)
C(3)-H(3)	0.9300	C(4)-C(5)	1.344(4)
C(4)-H(4)	0.9300	C(5)-N(6)	1.395(3)
C(5)-H(5)	0.9300	N(6)-C(7)	1.381(3)
C(7)-C(8)	1.353(4)	C(7)-H(7)	0.9300
C(8)-C(9)	1.423(4)	C(8)-N(14)	1.468(3)
C(9)-C(10)	1.350(4)	C(9)-H(9)	0.9300
C(10)-H(10)	0.9300	N(11)-O(12)	1.228(3)
N(11)-O(13)	1.234(3)	N(14)-O(15)	1.225(3)
N(14)-O(16)	1.225(3)		
N(6)-B(1)-C(2)	113.2(2)	N(6)-B(1)-C(10)	115.4(2)
C(2)-B(1)-C(10)	131.3(2)	C(3)-C(2)-N(11)	116.3(2)
C(3)-C(2)-B(1)	121.6(2)	N(11)-C(2)-B(1)	122.1(2)
C(2)-C(3)-C(4)	120.0(2)	C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0	C(5)-C(4)-C(3)	122.0(2)
C(5)-C(4)-H(4)	119.0	C(3)-C(4)-H(4)	119.0
C(4)-C(5)-N(6)	121.5(2)	C(4)-C(5)-H(5)	119.2
N(6)-C(5)-H(5)	119.2	C(7)-N(6)-C(5)	117.2(2)
C(7)-N(6)-B(1)	121.2(2)	C(5)-N(6)-B(1)	121.6(2)
C(8)-C(7)-N(6)	119.5(2)	C(8)-C(7)-H(7)	120.2
N(6)-C(7)-H(7)	120.2	C(7)-C(8)-C(9)	124.4(2)
C(7)-C(8)-N(14)	116.9(2)	C(9)-C(8)-N(14)	118.7(2)
C(10)-C(9)-C(8)	119.1(2)	C(10)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5	C(9)-C(10)-B(1)	120.3(2)
C(9)-C(10)-H(10)	119.9	B(1)-C(10)-H(10)	119.9
O(12)-N(11)-O(13)	121.9(2)	O(12)-N(11)-C(2)	118.5(2)
O(13)-N(11)-C(2)	119.6(2)	O(15)-N(14)-O(16)	123.9(2)
O(15)-N(14)-C(8)	117.4(2)	O(16)-N(14)-C(8)	118.7(2)

Table S5. Crystal data and structure refinement for 1,8-dinitro-BNN **1,8-dinitro-BNN**



Empirical formula	$C_8H_6BN_3O_4$	
Formula weight	218.97	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	$a = 14.541(5)$ Å	$\alpha = 90^\circ.$
	$b = 8.153(2)$ Å	$\beta = 117.709(15)^\circ.$
	$c = 8.923(2)$ Å	$\gamma = 90^\circ.$
Volume	$936.6(5)$ Å ³	
Z	4	
Density (calculated)	1.553 Mg/m ³	
Absorption coefficient	0.124 mm ⁻¹	
F(000)	448	
Crystal size	0.80 x 0.18 x 0.08 mm ³	
Theta range for data collection	2.96 to 26.13°.	
Index ranges	$-17 \leq h \leq 17, -10 \leq k \leq 9, -10 \leq l \leq 10$	
Reflections collected	4108	
Independent reflections	917 [$R_{int} = 0.0184$]	
Completeness to theta = 26.13°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9901 and 0.9071	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	917 / 0 / 74	
Goodness-of-fit on F^2	1.108	
Final R indices [I>2sigma(I)]	$R_1 = 0.0448, wR_2 = 0.1222$	
R indices (all data)	$R_1 = 0.0514, wR_2 = 0.1283$	
Largest diff. peak and hole	0.189 and -0.206 e.Å ⁻³	

Table S6. Bond lengths [Å] and angles [°] for 1,8-dinitro-BNN **1,8-dinitro-BNN**

B(1)-N(6)	1.460(3)
B(1)-C(2)	1.5195(19)
B(1)-C(2)#1	1.5195(19)
C(2)-C(3)	1.356(3)
C(2)-N(7)	1.457(2)
C(3)-C(4)	1.396(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.337(3)
C(4)-H(4)	0.9500
C(5)-N(6)	1.387(2)
C(5)-H(5)	0.9500
N(6)-C(5)#1	1.387(2)
N(7)-O(9)	1.216(2)
N(7)-O(8)	1.226(2)
N(6)-B(1)-C(2)	113.14(11)
N(6)-B(1)-C(2)#1	113.14(11)
C(2)-B(1)-C(2)#1	133.7(2)
C(3)-C(2)-N(7)	115.39(16)
C(3)-C(2)-B(1)	121.47(18)
N(7)-C(2)-B(1)	123.04(16)
C(2)-C(3)-C(4)	120.26(18)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	121.79(18)
C(5)-C(4)-H(4)	119.1
C(3)-C(4)-H(4)	119.1
C(4)-C(5)-N(6)	122.04(18)
C(4)-C(5)-H(5)	119.0
N(6)-C(5)-H(5)	119.0
C(5)-N(6)-C(5)#1	117.6(2)
C(5)-N(6)-B(1)	121.20(12)
C(5)#1-N(6)-B(1)	121.20(12)
O(9)-N(7)-O(8)	122.79(18)
O(9)-N(7)-C(2)	119.85(17)
O(8)-N(7)-C(2)	117.30(15)