10.1071/CH15381_AC

Australian Journal of Chemistry 2015, 68(11), 1750-1758

Supplementary Material

Aryl-substituted boron subphthalocyanines and their application in organic photovoltaics.

Catherine Bonnier,[A] *David S. Josey,*[A] *and Timothy P. Bender*[A,B,C,*]

[A] Department of Chemical Engineering and Applied Chemistry, University of Toronto, 200 College St., Toronto, Ontario, Canada M5S 3E5

[B] Department of Materials Science and Engineering, University of Toronto, 184 College St., Toronto, Ontario, Canada M5S 3E4

[C] Department of Chemistry, University of Toronto, 80 St. George St., Toronto, Ontario, Canada, M5S 3H6

* - Corresponding author. Email: tim.bender@utoronto.ca

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Cyclic Voltammograms

Table S1. Reversibility of the electrochemical processes of aryl-BSubPc ***3a-e***.

	$BSubPc^{\bullet+}$/BSubPc		BSubPc/$BSubPc^{\bullet-}$		$BSubPc^{\bullet-}$/$BSubPc^{2-}$		$Cp^*_2Fe^{\bullet+}$/Cp^*_2Fe	
	ΔE (mV)	i_a/i_c	ΔE (mV)	i_a/i_c	ΔE (mV)	i_a/i_c	ΔE (mV)	i_a/i_c
3a	65	0.85	60	0.90	59	0.44	59	0.97
3b	85	0.68	85	0.79	69	0.28	72	0.99
3c	60	0.93	58	0.73	60	0.24	81	0.96
3d	75	0.91	72	0.76	69	0.22	55	0.96
3e	55	0.85	52	0.66	71	0.14	67	0.98

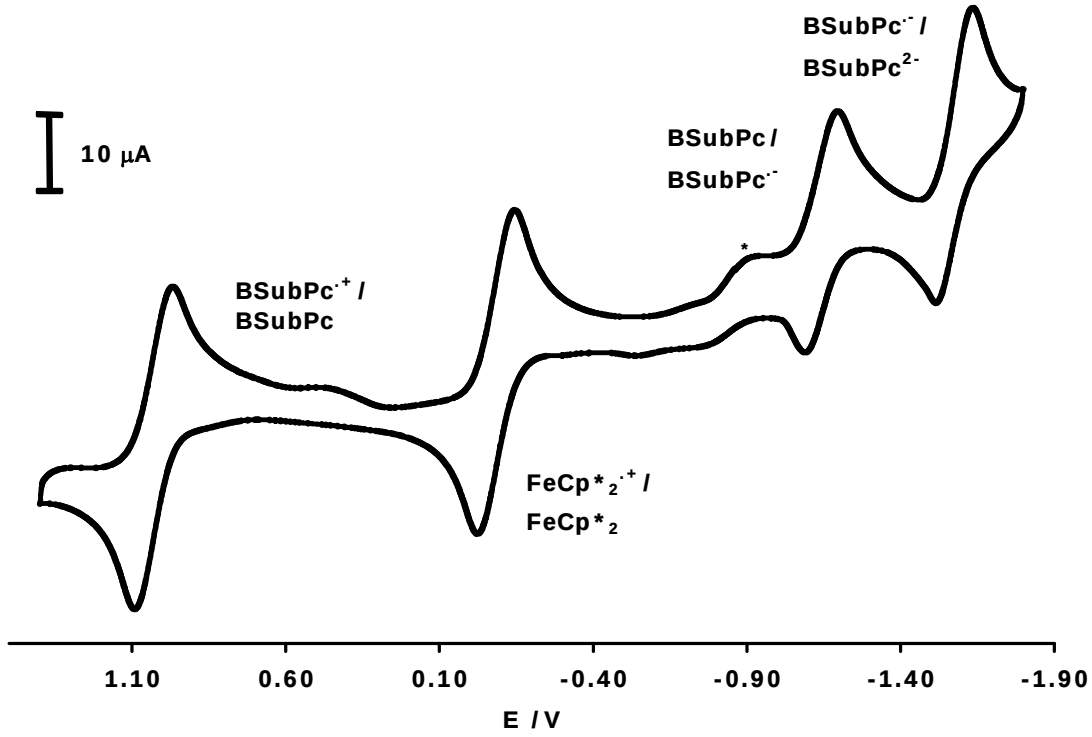


Figure S1. Cyclic voltammogram of ***3a*** recorded in CH_2Cl_2 at 100 mV/s containing $[n\text{Bu}_4\text{N}]^+[PF_6]^-$ as supporting electrolyte. * denotes the reduction of residual dissolved oxygen.

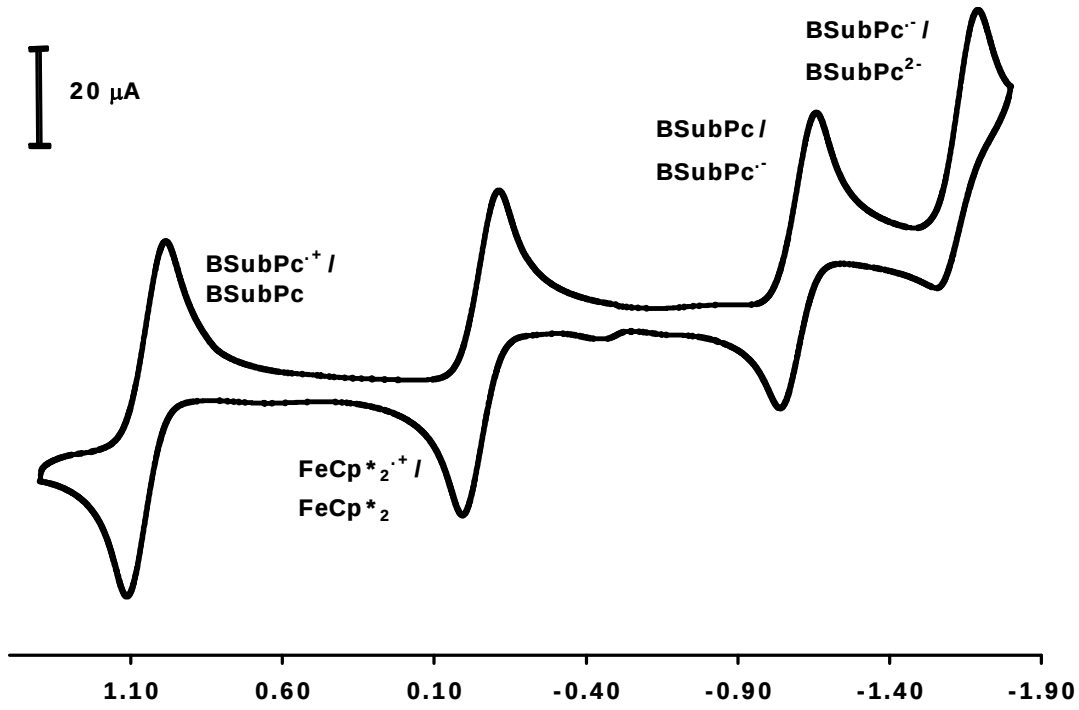


Figure S2. Cyclic voltammogram of ***3c*** recorded in CH_2Cl_2 at 100 mV/s containing $[n\text{Bu}_4\text{N}]^+[PF_6]^-$ as supporting electrolyte.

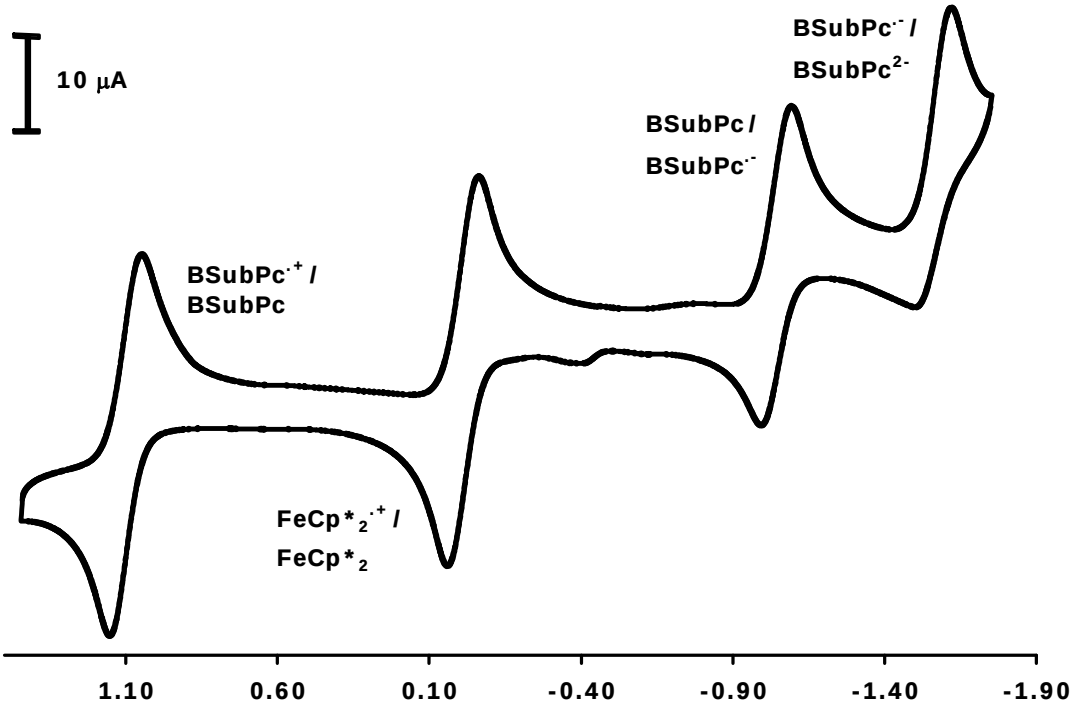


Figure S3. Cyclic voltammogram of ***3d*** recorded in CH_2Cl_2 at 100 mV/s containing $[n\text{Bu}_4\text{N}]^+[PF_6]^-$ as supporting electrolyte.

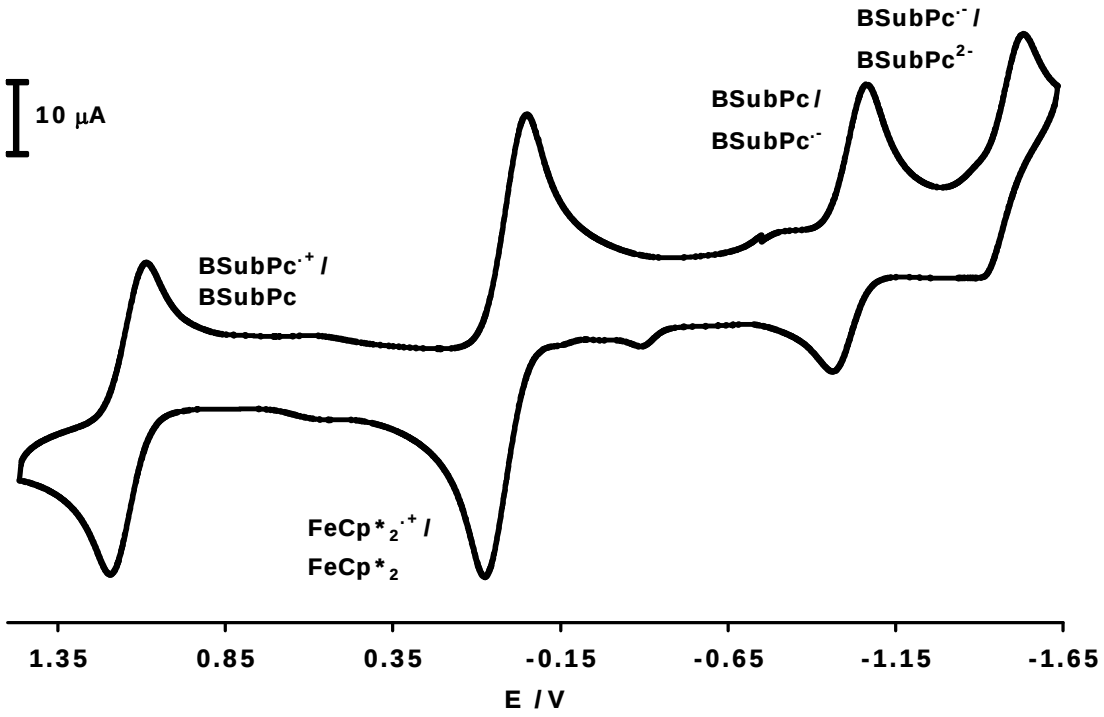


Figure S4. Cyclic voltammogram of ***3e*** recorded in CH_2Cl_2 at 100 mV/s containing $[n\text{Bu}_4\text{N}]^+[PF_6]^-$ as supporting electrolyte.

X-Ray Crystallographic Information

Table S2. Crystal data and structure refinement for ***3b***.

Empirical formula	C_{31} H_{19} B N_6	
Formula weight	486.33	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.4071(7) Å	a= 90º.
	b = 17.2712(8) Å	b= 90º.
	c = 18.7280(9) Å	g = 90º.
Volume	4660.0(4) $Å^3$	
Z	8	
Density (calculated)	1.386 Mg/m^3	
Absorption coefficient	0.666 mm^{-1}	
F(000)	2016	
Crystal size	0.14 x 0.12 x 0.10 mm^3	
Theta range for data collection	4.64 to 66.41º.	
Index ranges	-16<=h<=13, -20<=k<=17, -21<=l<=18	
Reflections collected	17504	
Independent reflections	4047 [R(int) = 0.0353]	
Completeness to theta = 66.41º	98.8%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6683	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4047 / 0 / 344	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0823	
R indices (all data)	R1 = 0.0375, wR2 = 0.0863	
Largest difference peak and hole	0.200 and -0.208 e. $Å^{-3}$	

Table S3. Crystal data and structure refinement for ***3c***.

Empirical formula	C_{31} H_{19} B N_6 O	
Formula weight	502.33	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.8152(7) Å	α = 90º.
	b = 16.5992(8) Å	β = 90º.
	c = 19.3422(10) Å	γ = 90º.
Volume	4756.6(4) $Å^3$	
Z	8	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.703 mm^{-1}	
F(000)	2080	
Crystal size	0.23 x 0.17 x 0.06 mm^3	
Theta range for data collection	4.57 to 66.52º.	
Index ranges	-16<=h<=17, -19<=k<=12, -22<=l<=23	
Reflections collected	17322	
Independent reflections	4064 [R(int) = 0.0329]	
Completeness to theta = 66.52º	97.0%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6670	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4064 / 0 / 353	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0877	
R indices (all data)	R1 = 0.0375, wR2 = 0.0899	
Largest difference peak and hole	0.212 and -0.236 e. $Å^{-3}$	

Table S4. Crystal data and structure refinement for ***3d***.

Empirical formula	C_{36} H_{21} B N_6	
Formula weight	548.40	
Temperature	147(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 17.8366(12) Å	α = 90°.
	b = 16.8762(11) Å	β = 104.773(2)°.
	c = 18.1163(11) Å	γ = 90°.
Volume	5273.0(6) $Å^3$	
Z	8	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	0.084 mm^{-1}	
F(000)	2272	
Crystal size	0.41 x 0.14 x 0.11 mm^3	
Theta range for data collection	1.69 to 27.53°.	
Index ranges	-23<=h<=22, -21<=k<=21, -23<=l<=17	
Reflections collected	23503	
Independent reflections	6039 [R(int) = 0.0326]	
Completeness to theta = 27.53°	99.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7079	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6039 / 0 / 388	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0391, wR2 = 0.0918	
R indices (all data)	R1 = 0.0532, wR2 = 0.1002	
Largest difference peak and hole	0.346 and -0.203 e. $Å^{-3}$	

Table S5. Crystal data and structure refinement for ***3e***.

Empirical formula	C_{30} H_{16} B F N_6	
Formula weight	490.30	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.8117(12) Å	α = 90°.
	b = 16.3101(14) Å	β = 90°.
	c = 18.9126(15) Å	γ = 90°.
Volume	4568.9(6) $Å^3$	
Z	8	
Density (calculated)	1.426 Mg/m^3	
Absorption coefficient	0.750 mm^{-1}	
F(000)	2016	
Crystal size	0.14 x 0.10 x 0.04 mm^3	
Theta range for data collection	4.66 to 66.62°.	
Index ranges	-12<=h<=17, -19<=k<=19, -22<=l<=21	
Reflections collected	28159	
Independent reflections	3966 [R(int) = 0.0366]	
Completeness to theta = 66.62°	98.1%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6934	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3966 / 0 / 343	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0804	
R indices (all data)	R1 = 0.0356, wR2 = 0.0829	
Largest diff. peak and hole	0.236 and -0.218 e. $Å^{-3}$	

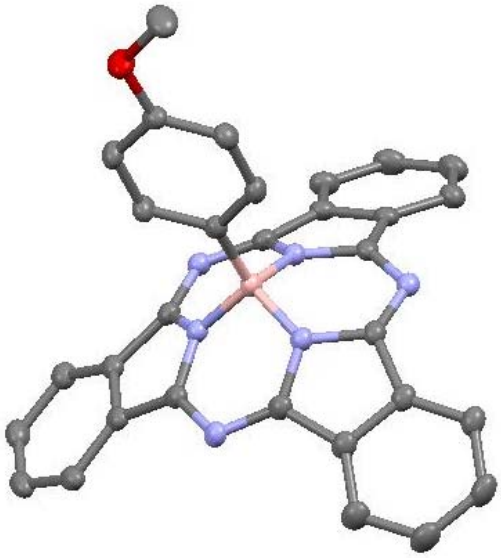


Figure S9. Thermal ellipsoid diagram (left, 35% probability. Hydrogen atoms were omitted for clarity purposes. Centroids are illustrated in red.

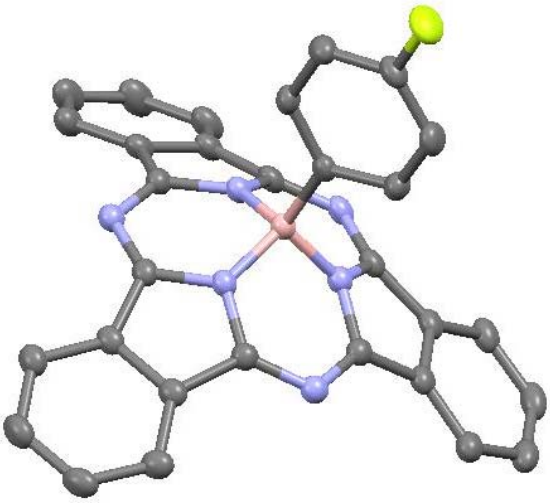


Figure S10. Thermal ellipsoid diagram (left, 35% probability). Hydrogen atoms were omitted for clarity purposes. Centroids are illustrated in red.

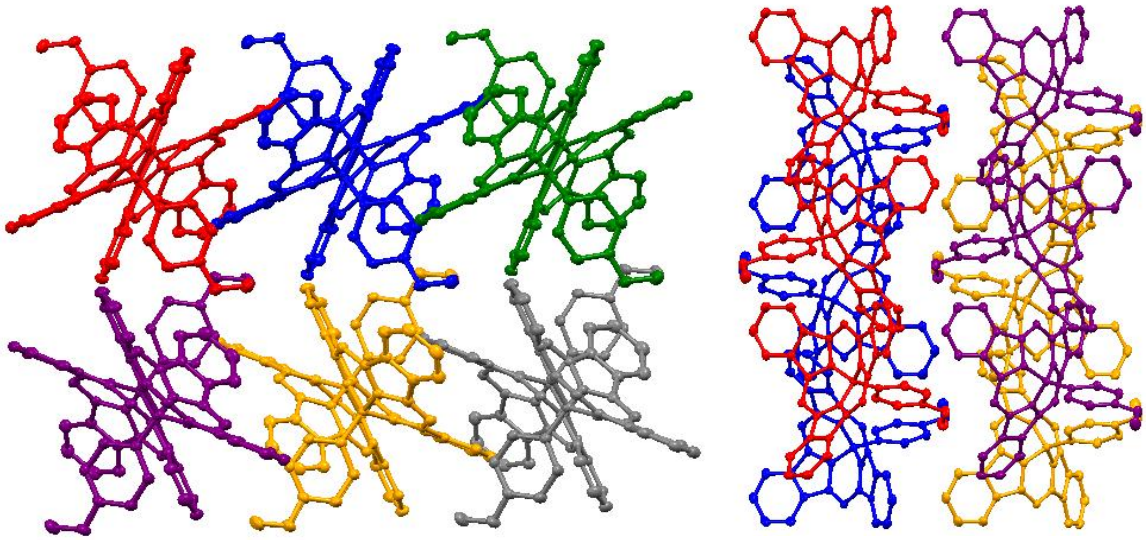
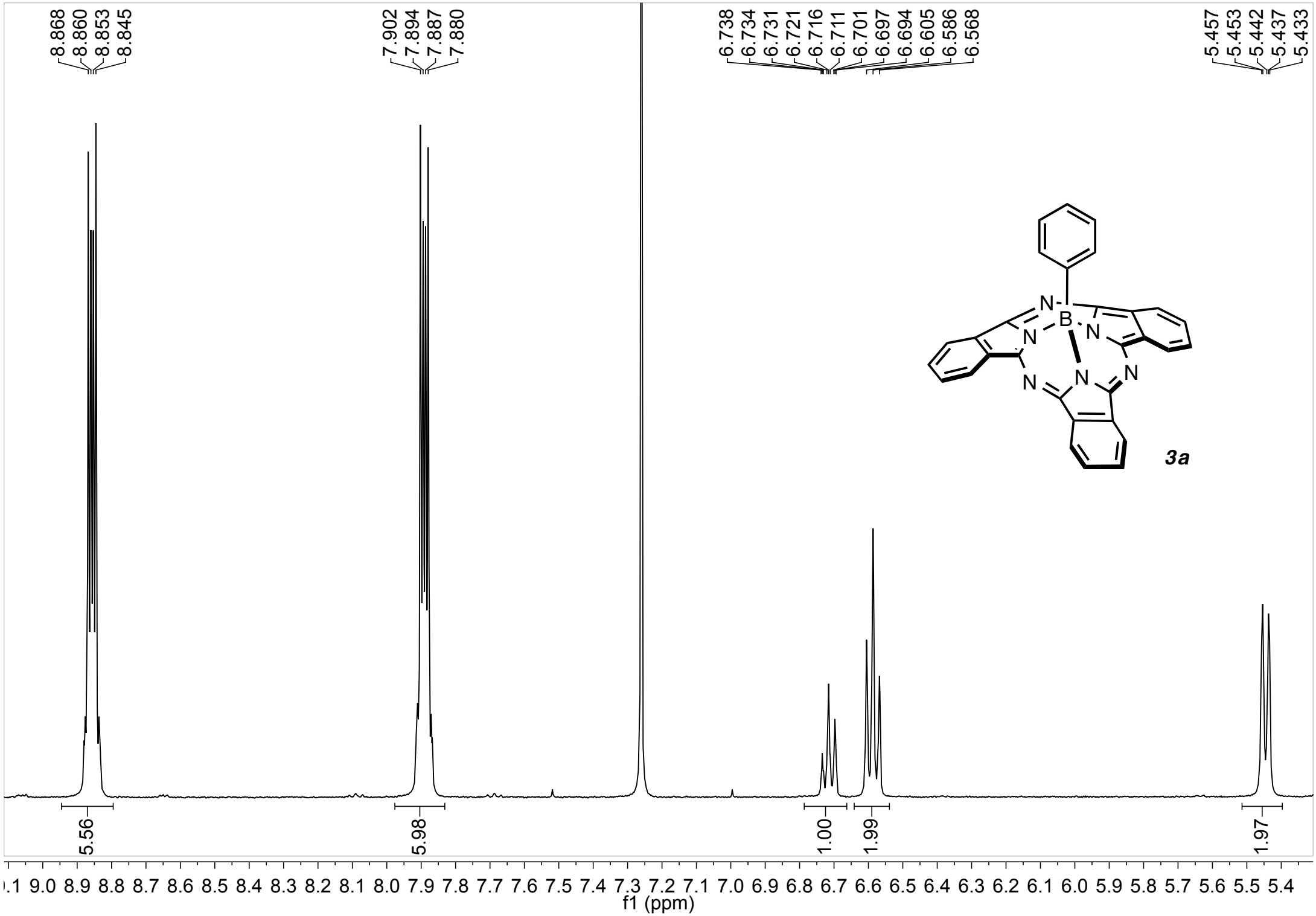


Figure S11. Packing structure of ***3c*** displaying the interactions generating ribbons (top), the ribbon – ribbon interactions along the a axis (bottom left) and the b axis (bottom right). Each ribbon is represented by a different color. Thermal ellipsoids were generated with 35% probability. Hydrogen atoms were omitted for clarity purposes. Centroids are illustrated in red.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6.697
6.694
6.605
6.586
6.568
5.457
5.453
5.442
5.437
5.433
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B
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N
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N
N
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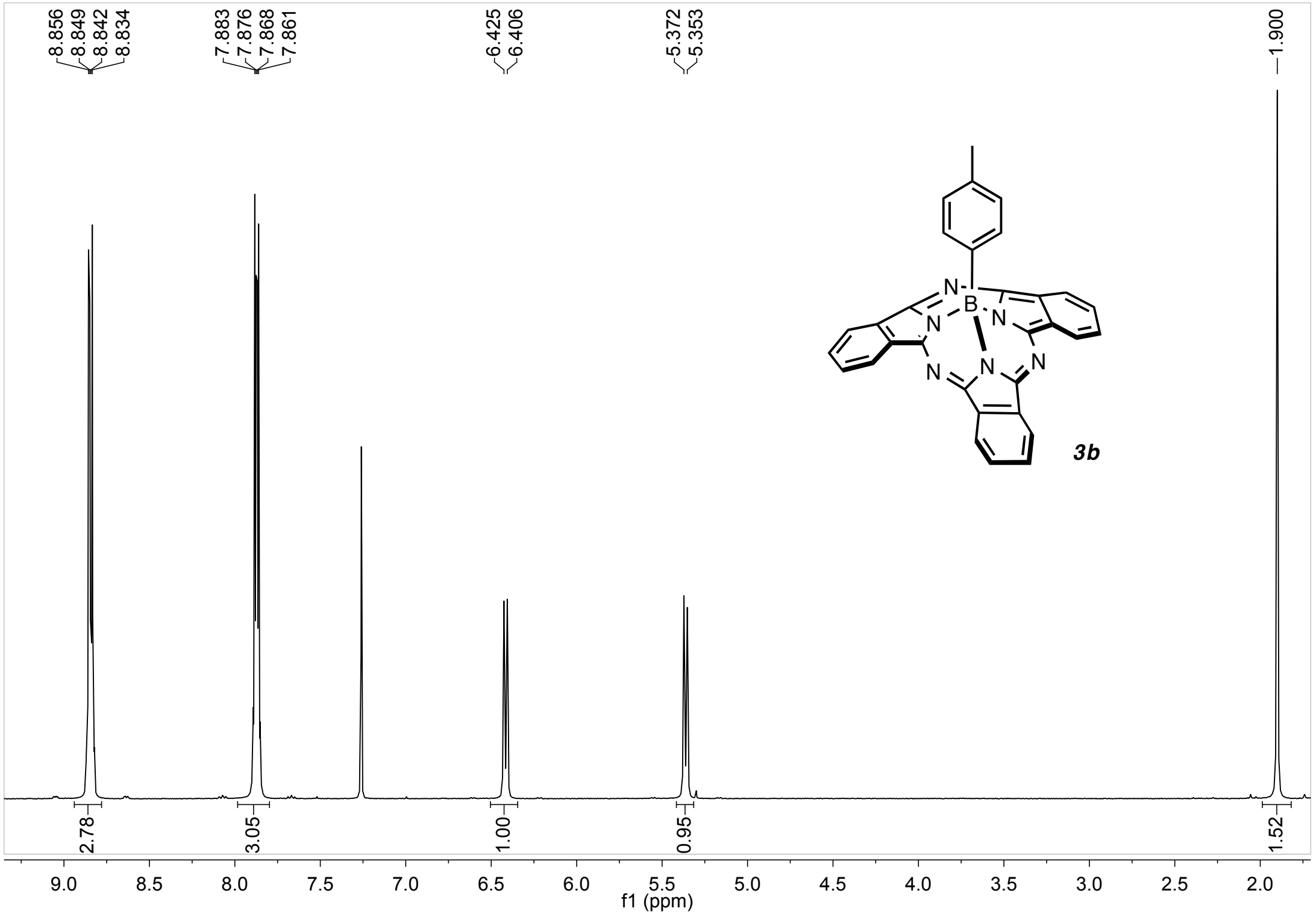
1.00
1.99
1.97
f1 (ppm)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N
B
N
N
N
N
N
3b
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3.05
1.00
0.95
1.52
9.0
8.5
8.0
7.5
7.0
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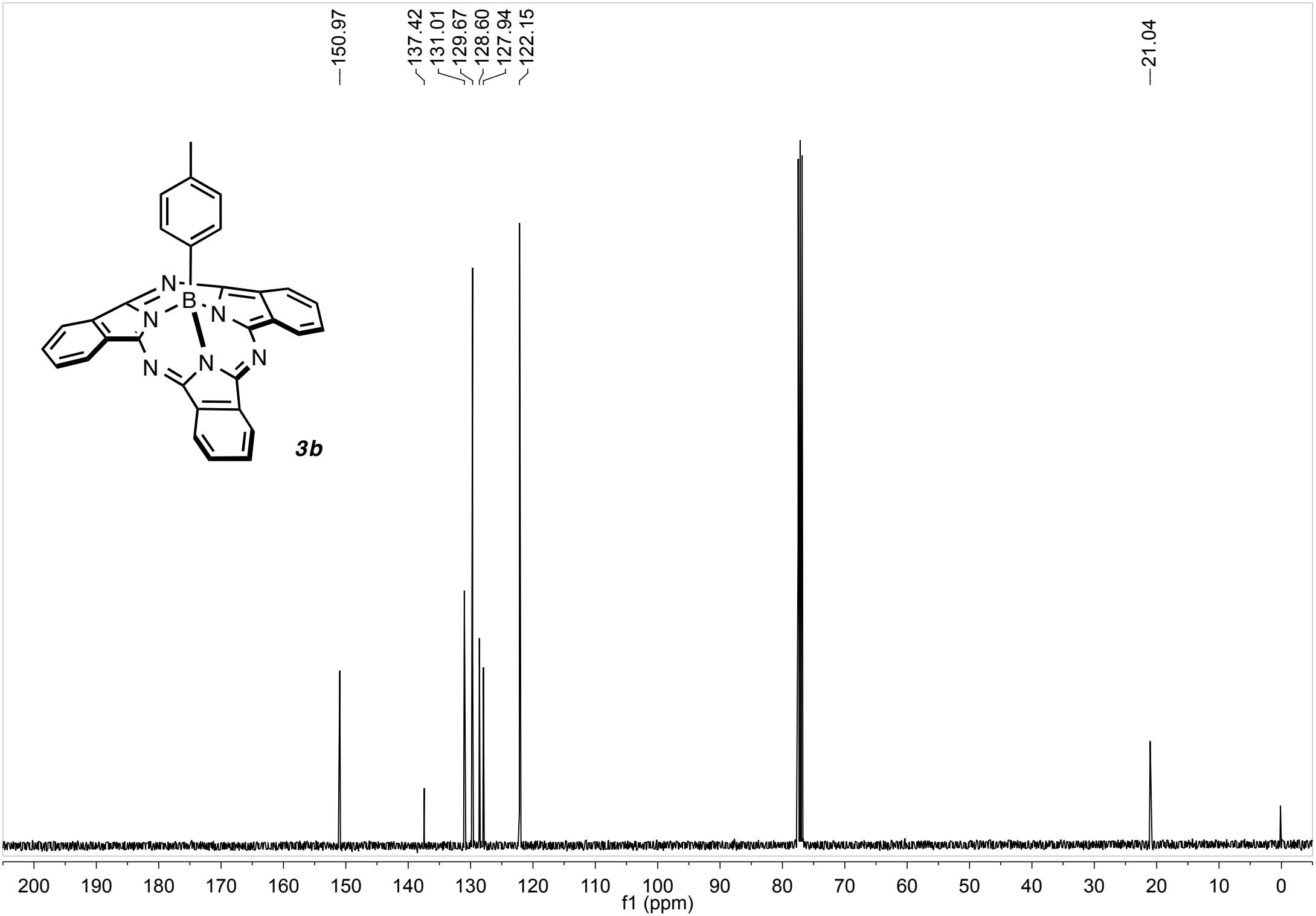
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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127.94
122.15
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B
N
N
N
N
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200
190
180
170
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110
100
90
80
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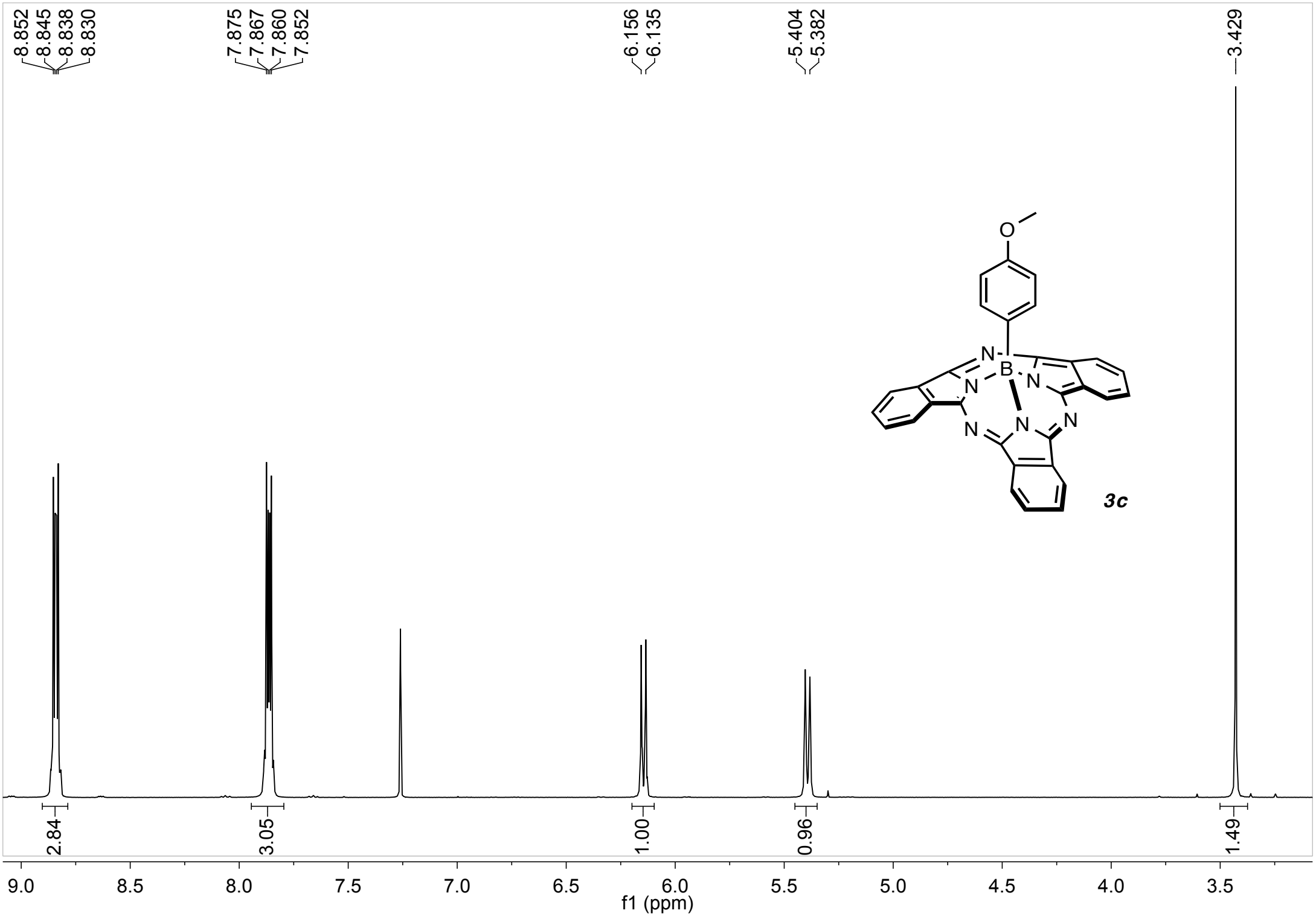
60
50
40
30
20
10
0
f1 (ppm)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O
N
B
N
N
N
N
N
3c
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0.96
1.49
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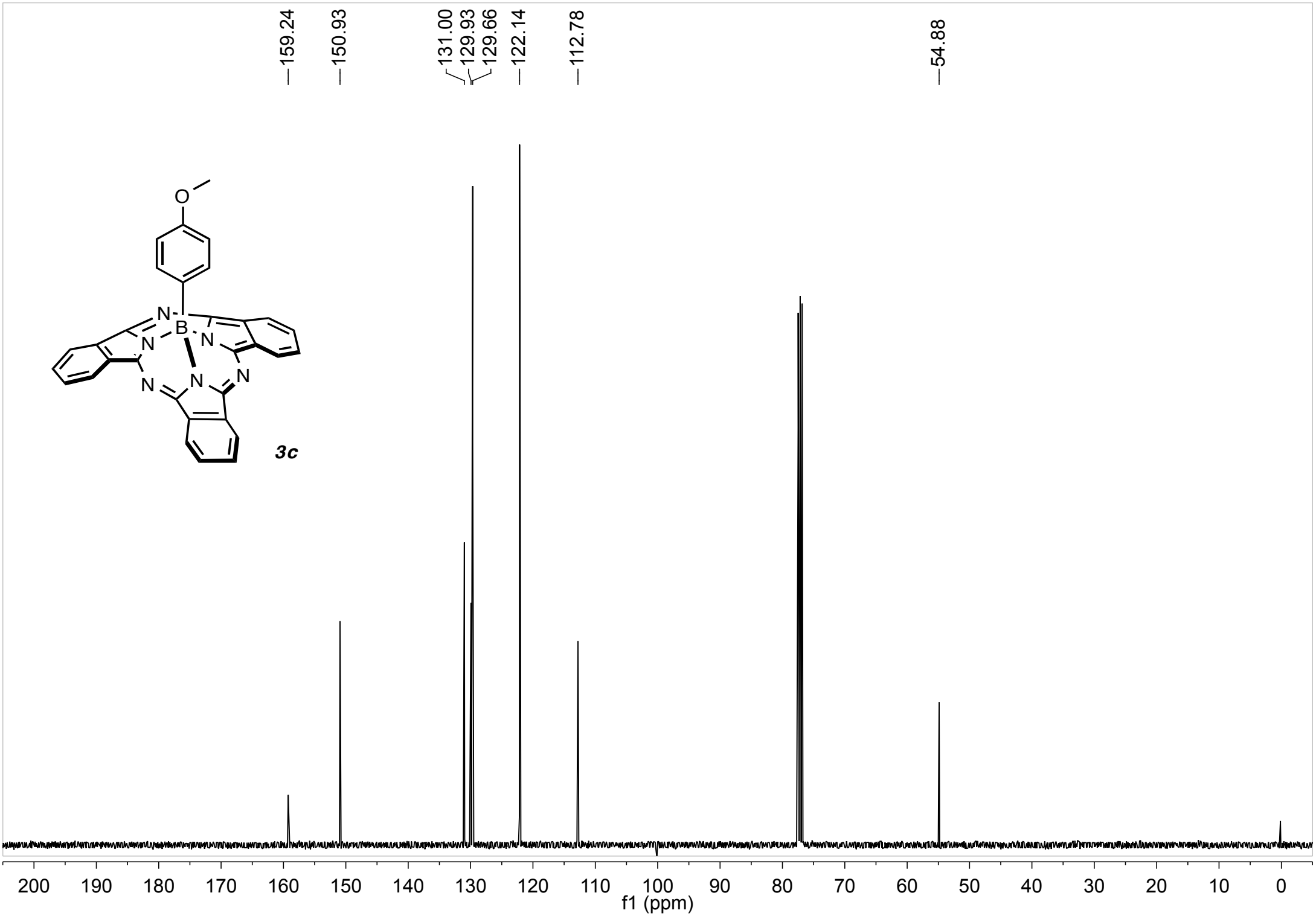
4.5
4.0
3.5
f1 (ppm)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180
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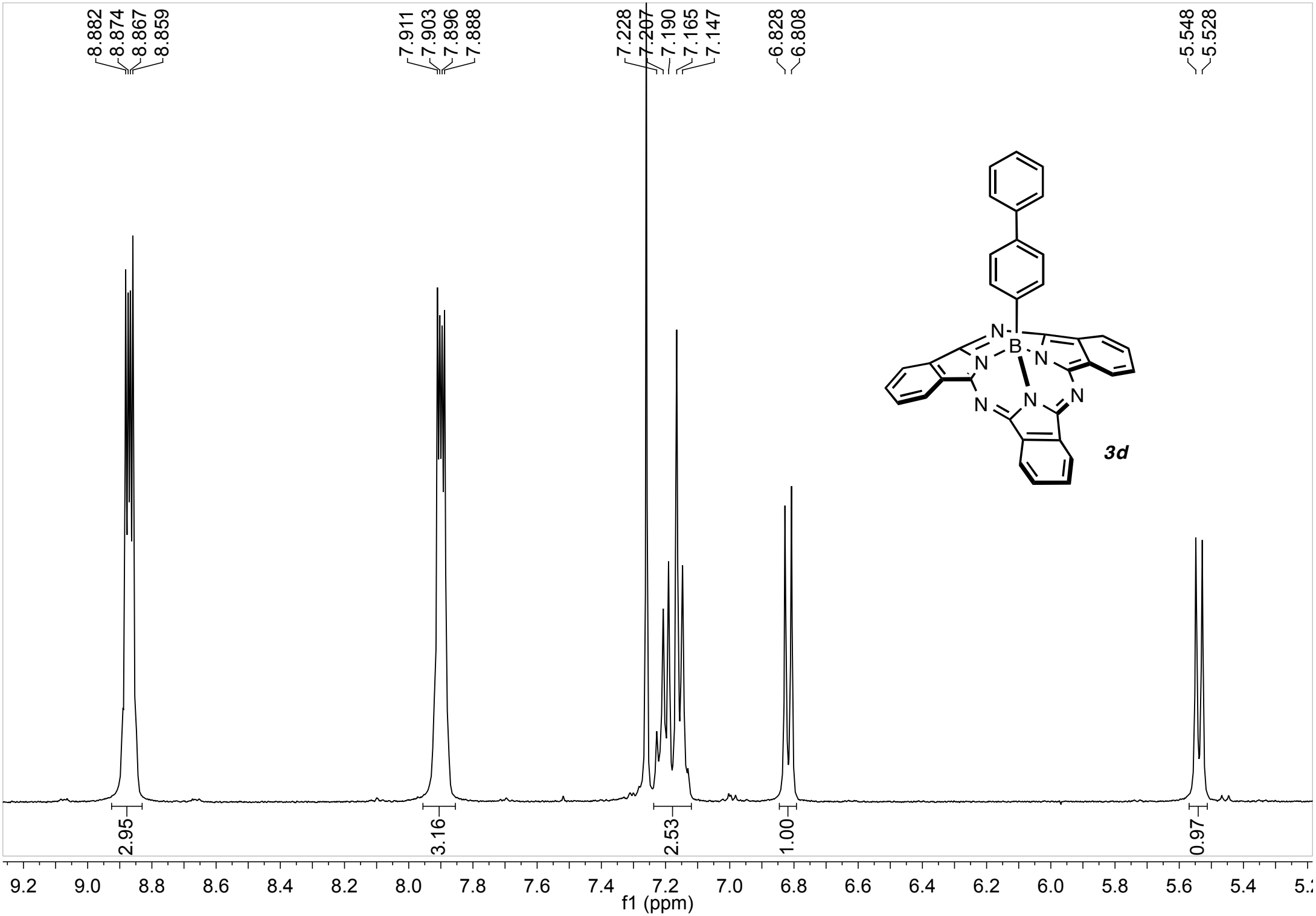
60
50
40
30
20
10
0
f1 (ppm)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9.0
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8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
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5.6
5.4
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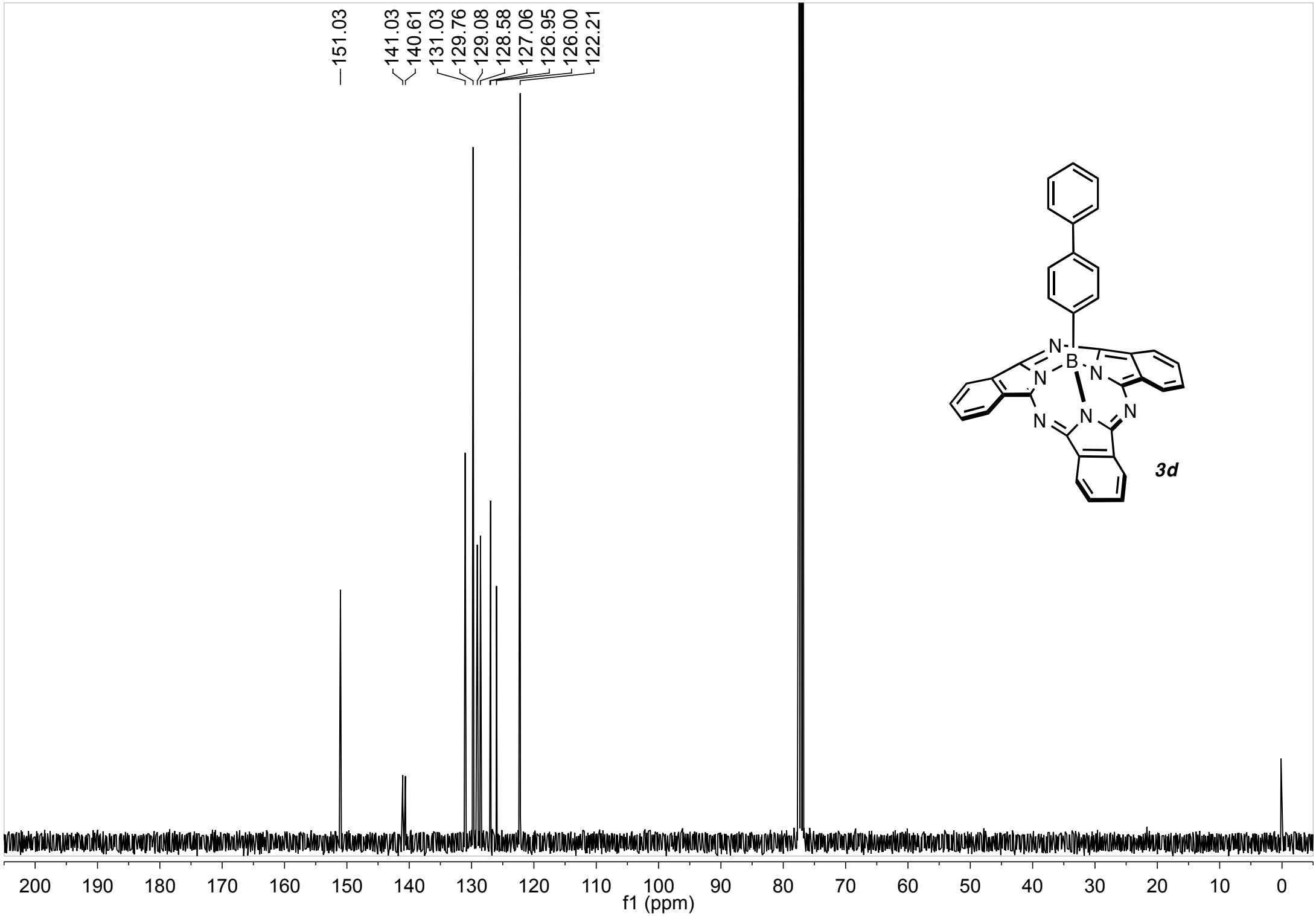
B
N
N
N
N
N
3d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126.00
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180
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100
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40
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20
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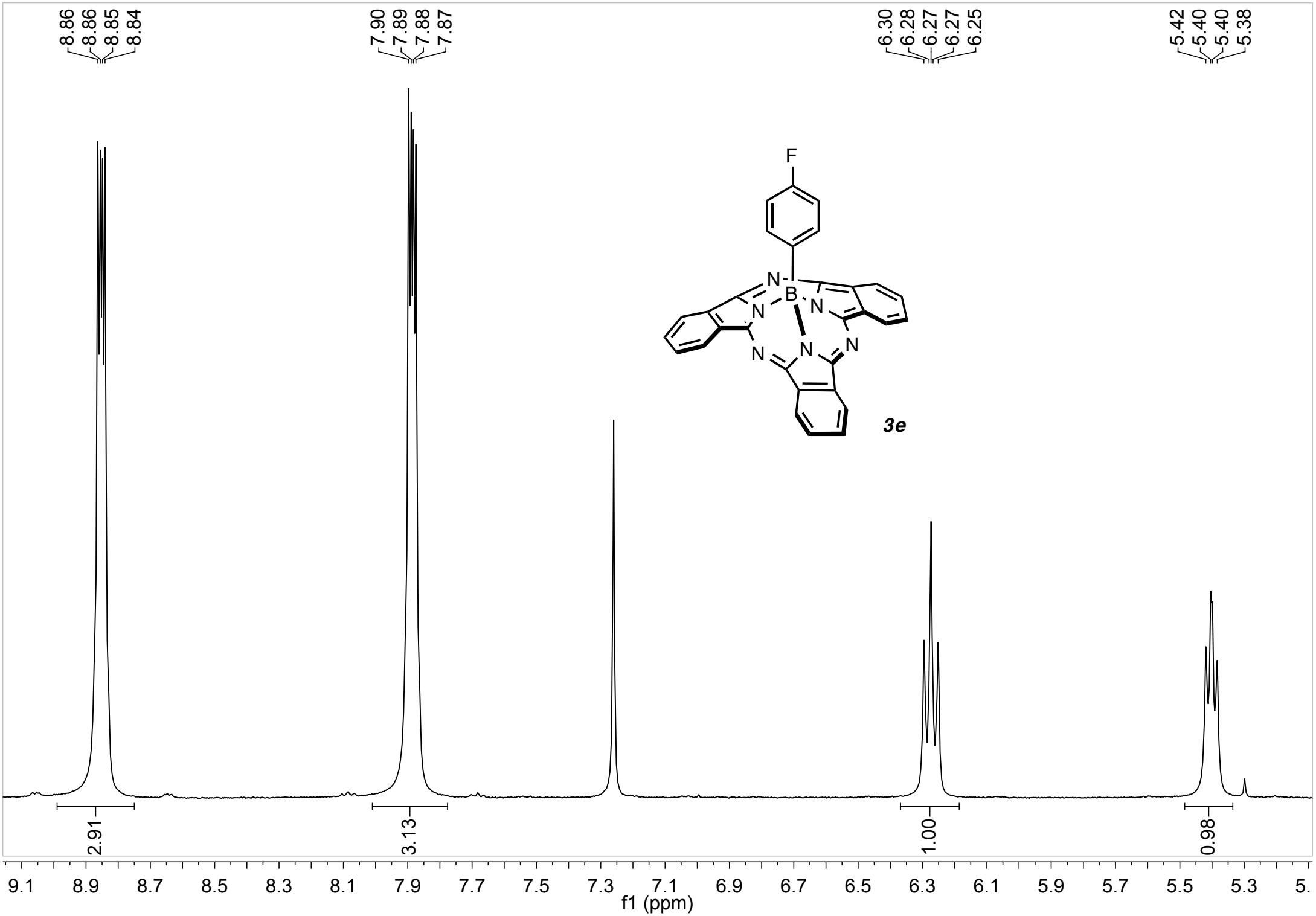
f1 (ppm)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5.40
5.40
5.38
F
N
B
N
N
N
N
N
N
3e
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3.13
1.00
0.98
9.1
8.9
8.7
8.5
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
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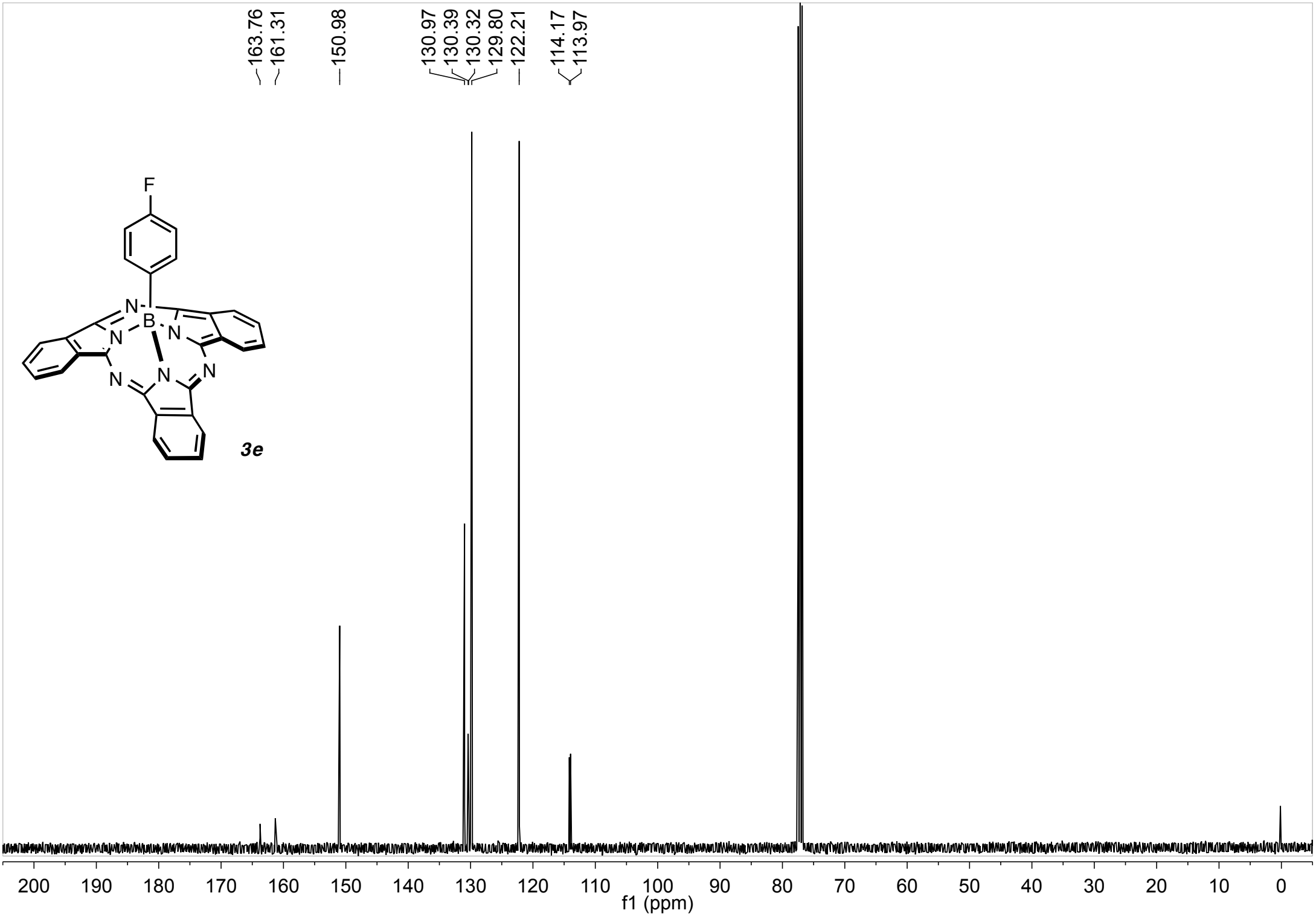
5.5
5.3
5.
f1 (ppm)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130.97
130.39
130.32
129.80
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114.17
113.97
F
N
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N
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180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)