Pyrazine-Based Donor Tectons: Synthesis, Self-Assembly and Characterization

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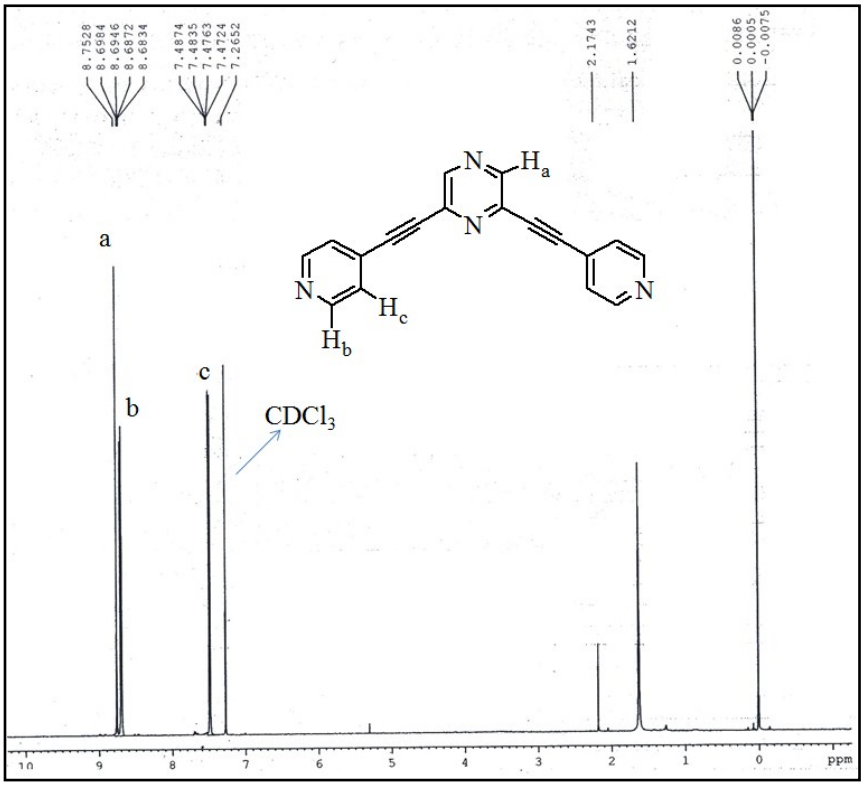
^{1}H NMR spectrum of 1:



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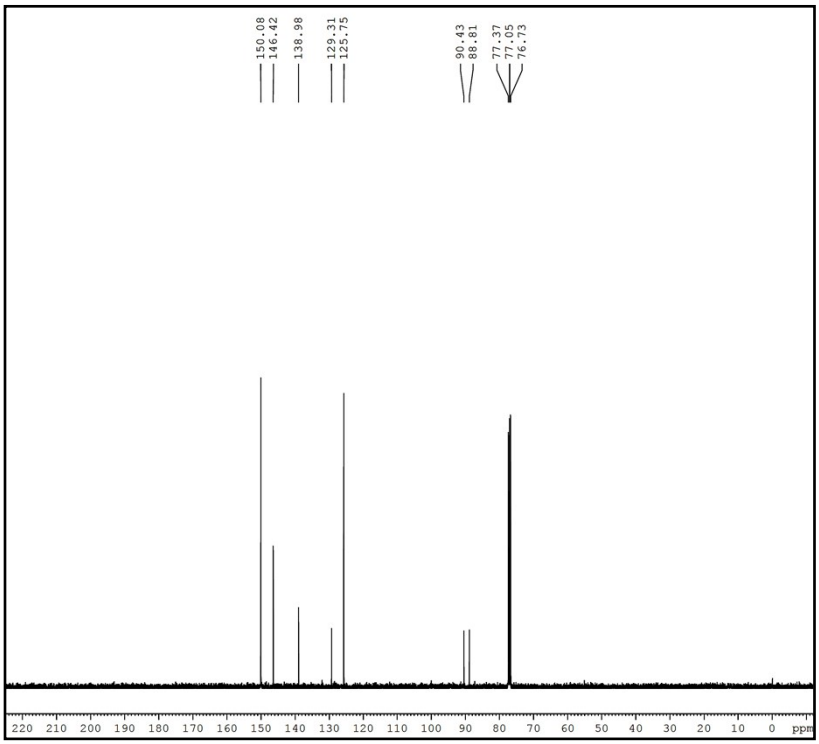

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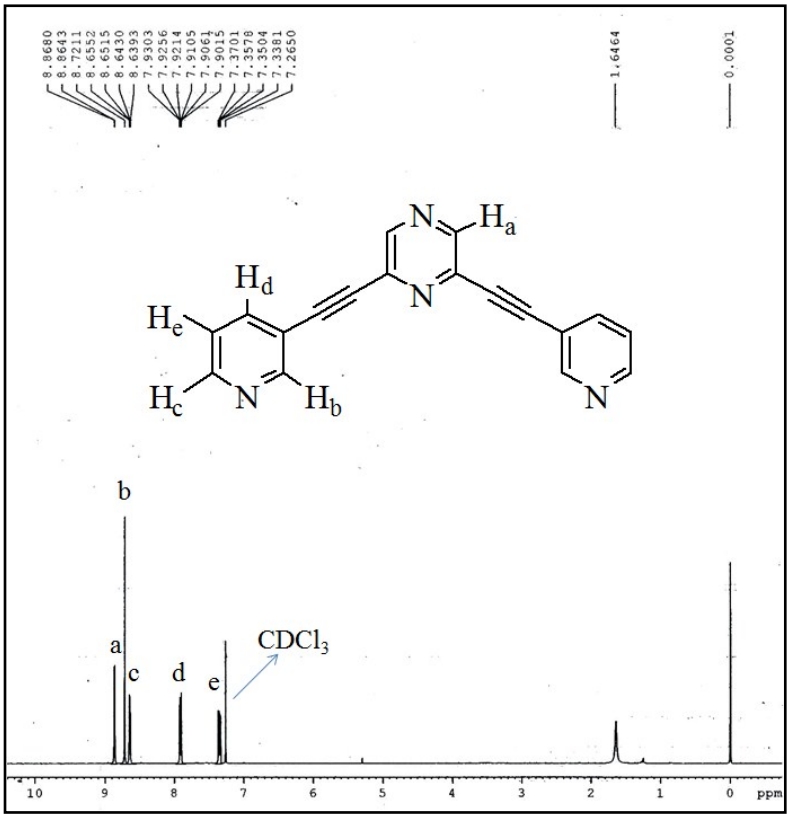

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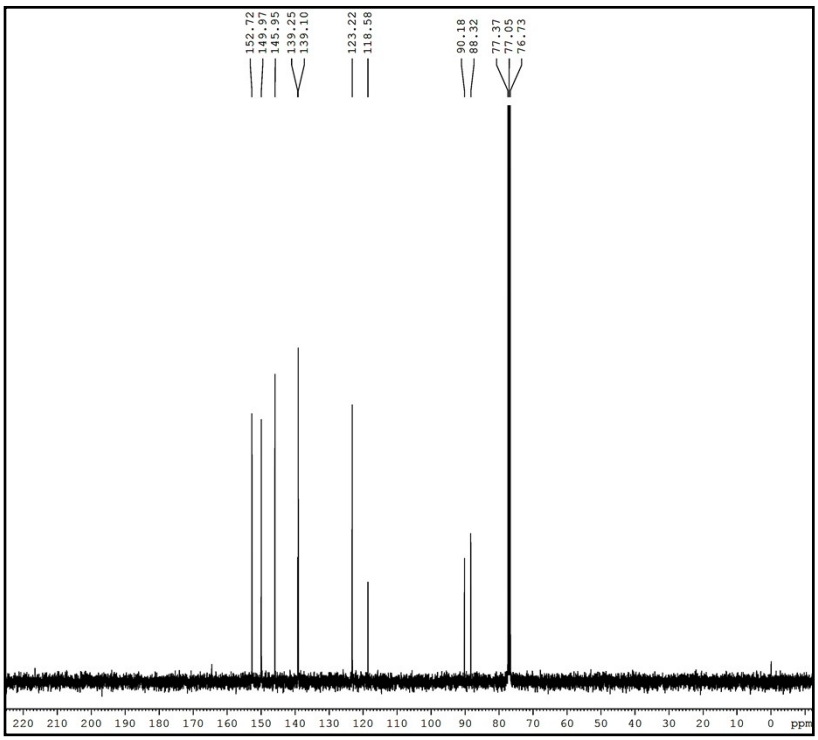

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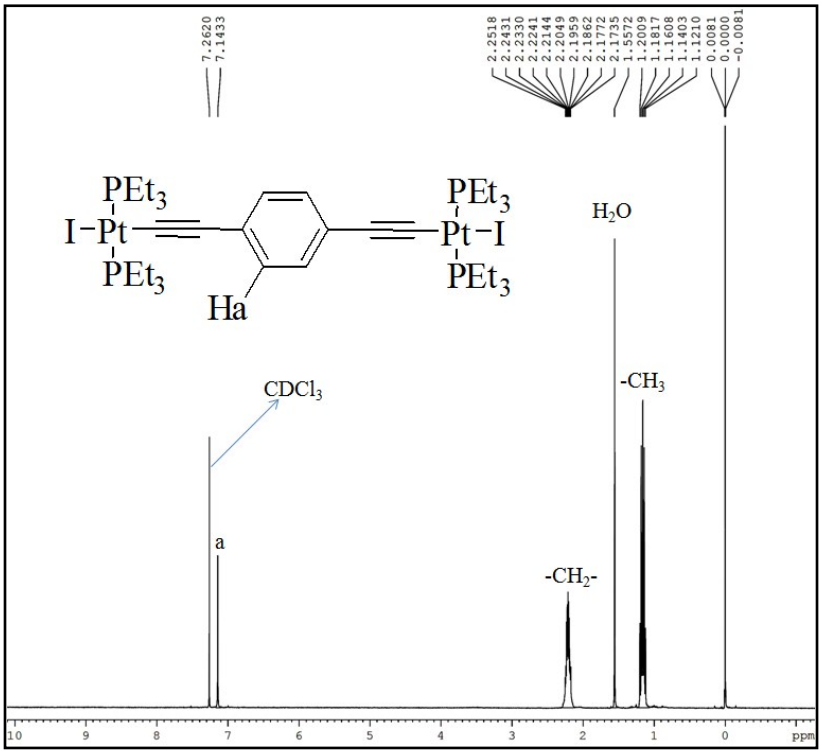

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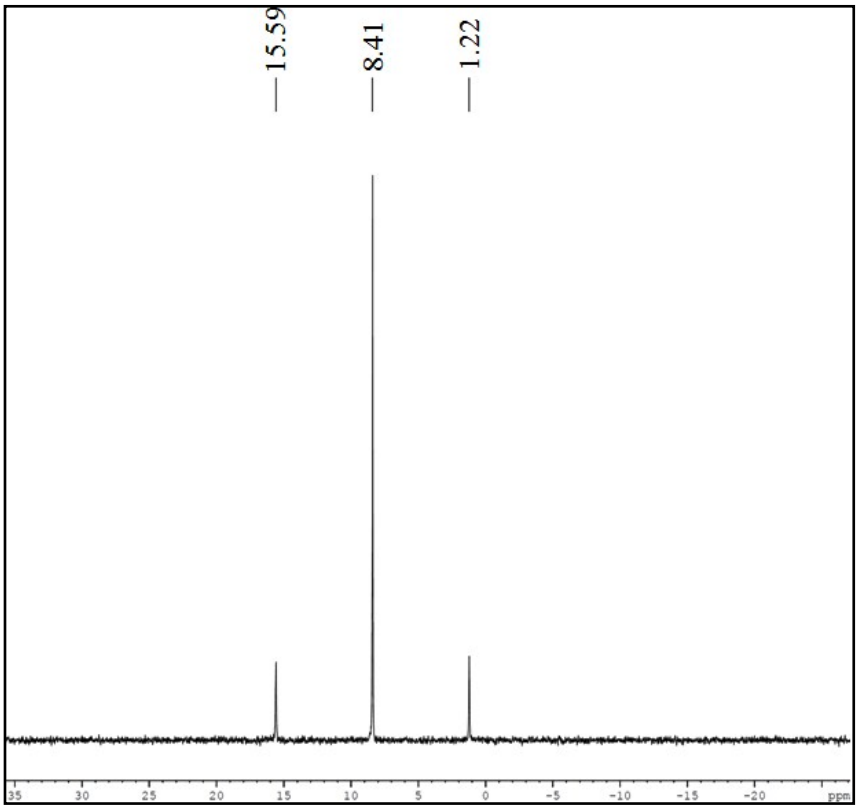

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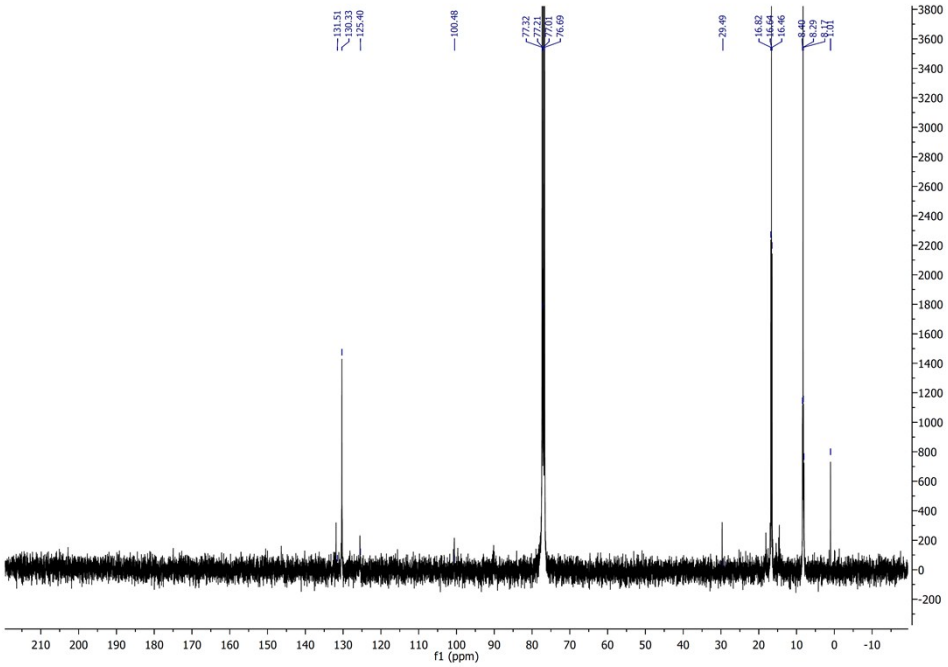

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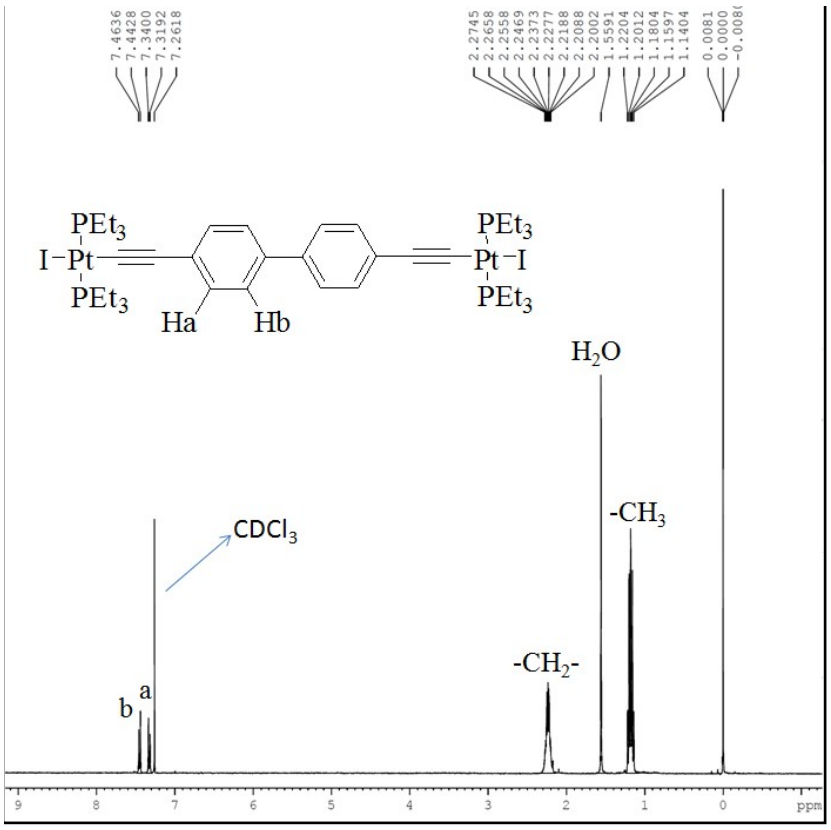

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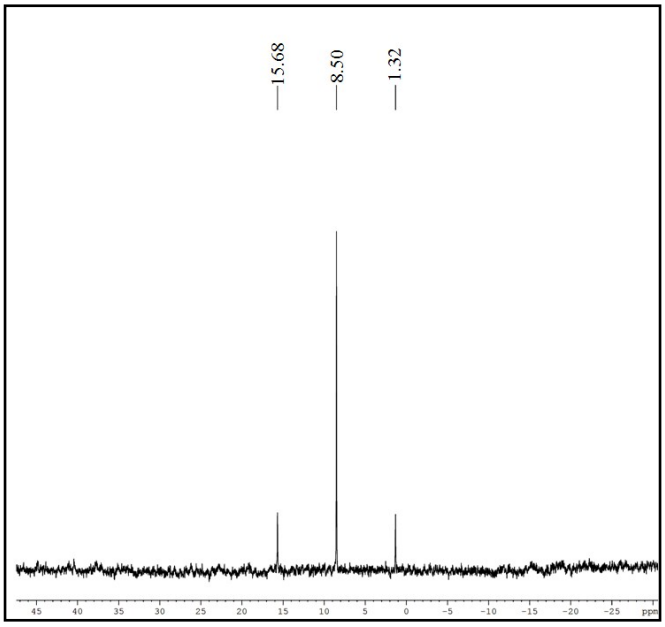

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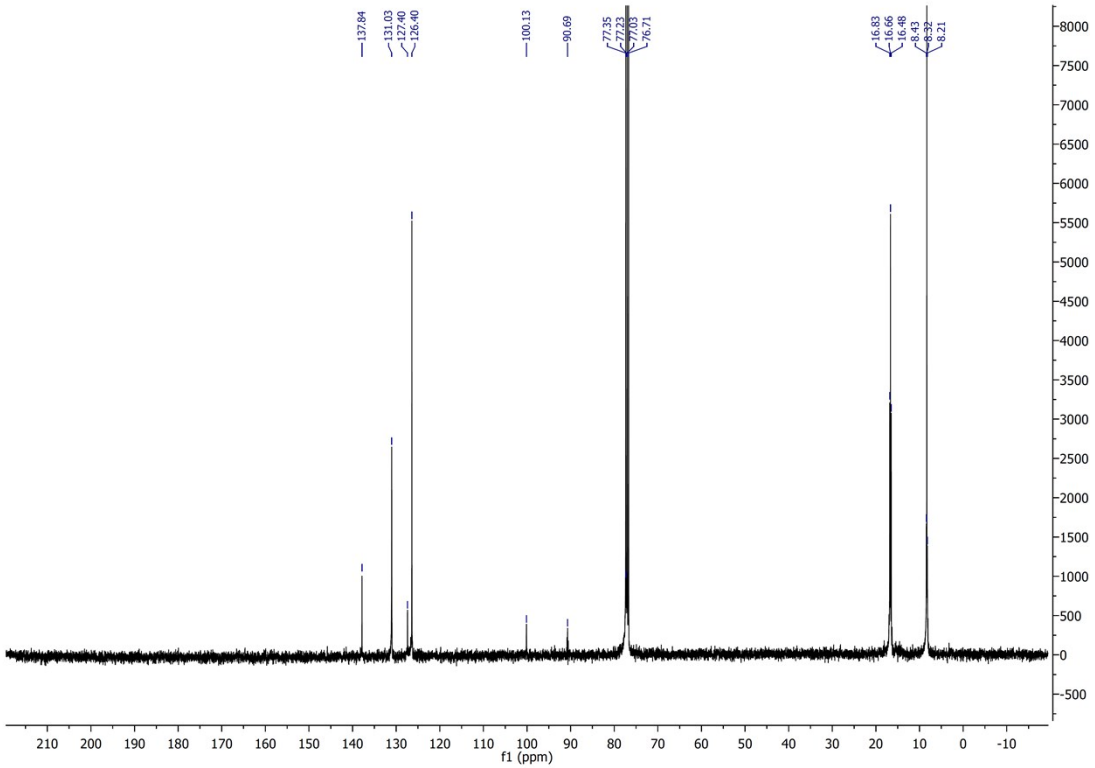

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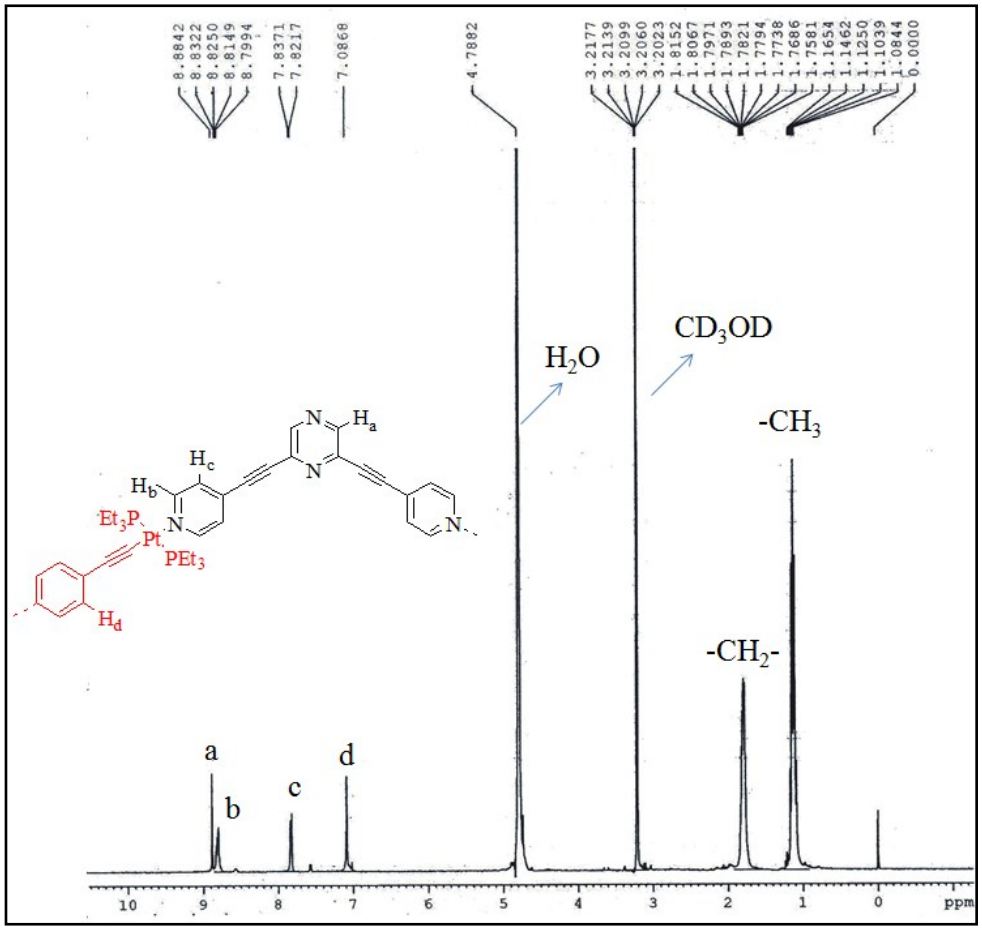

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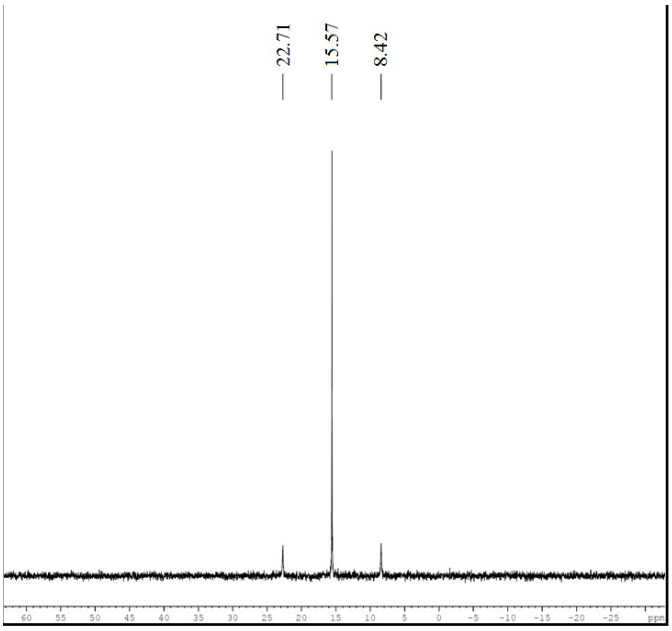

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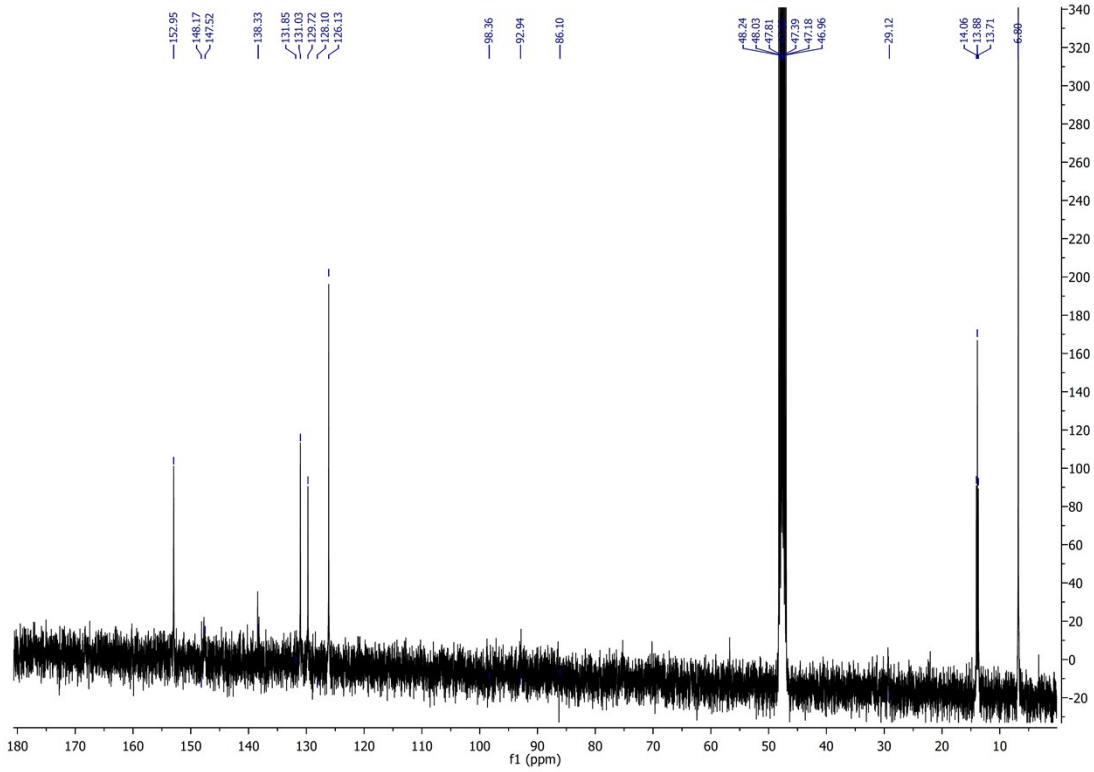

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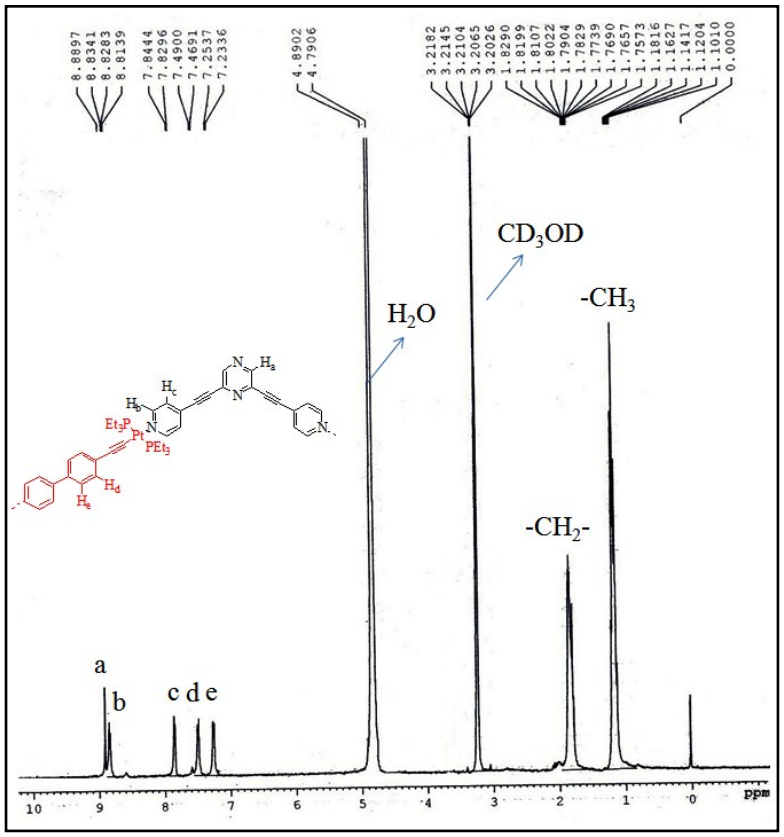

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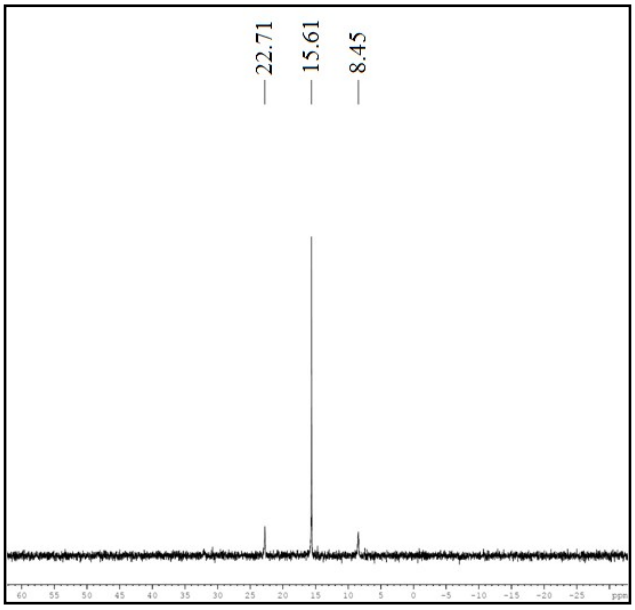

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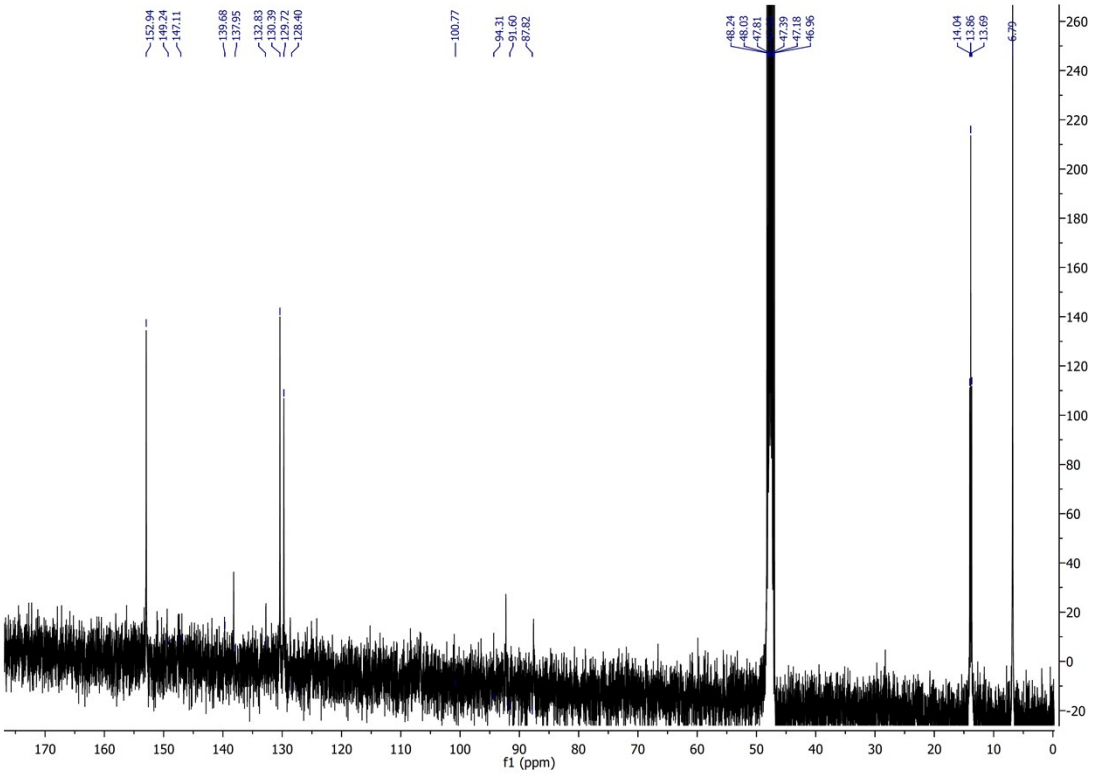

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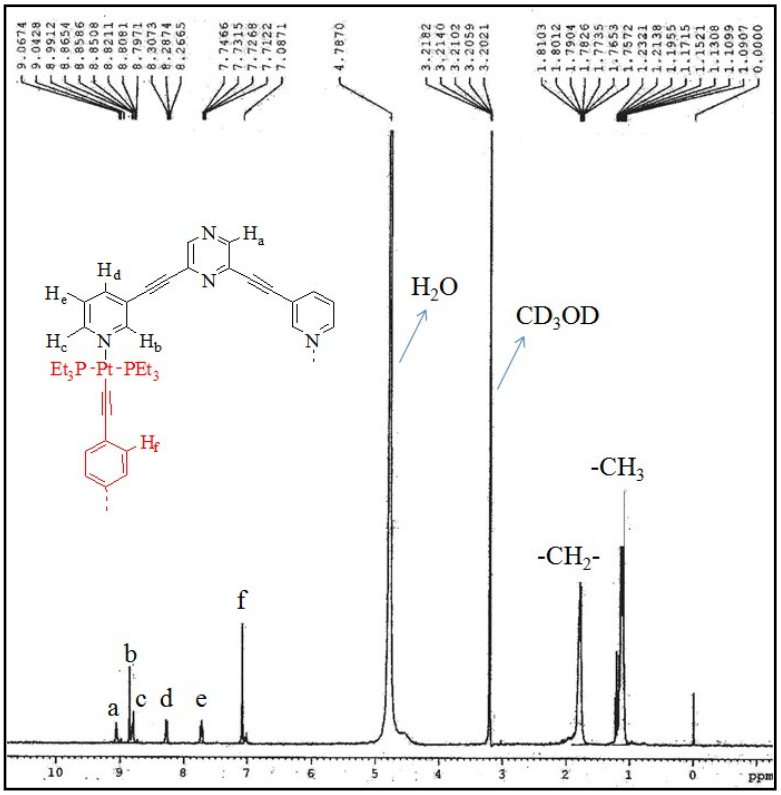

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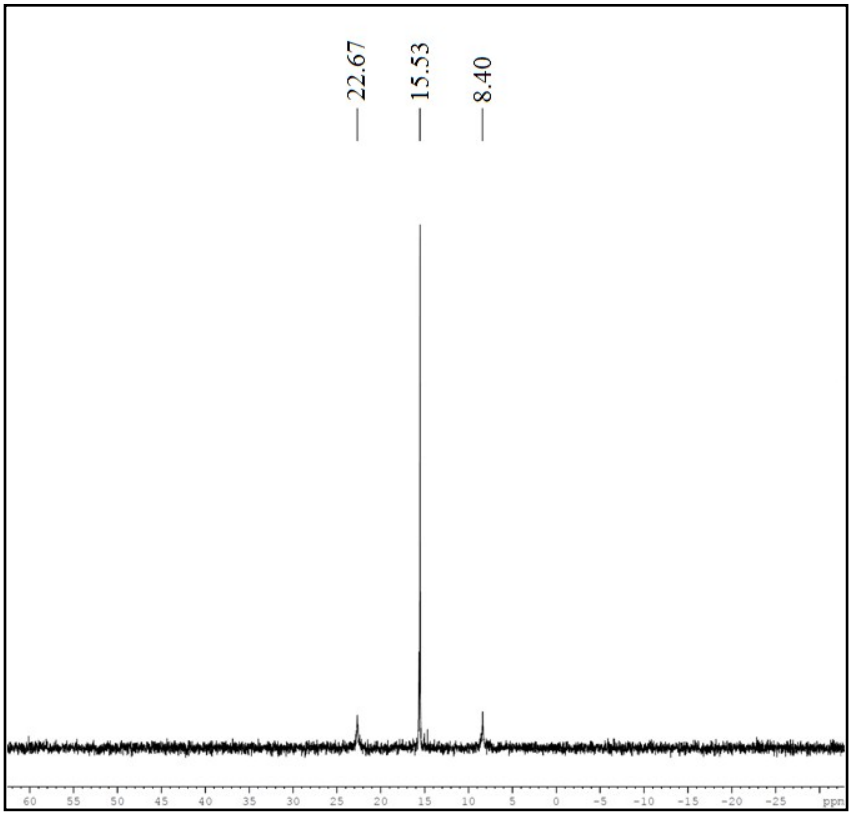

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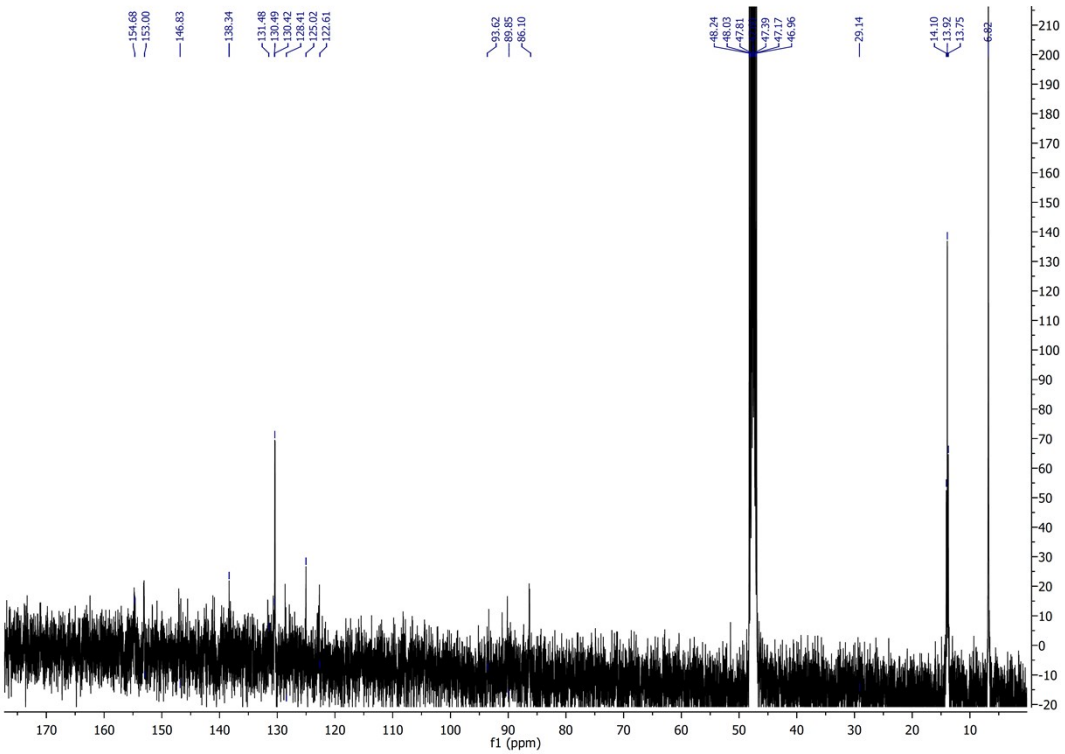

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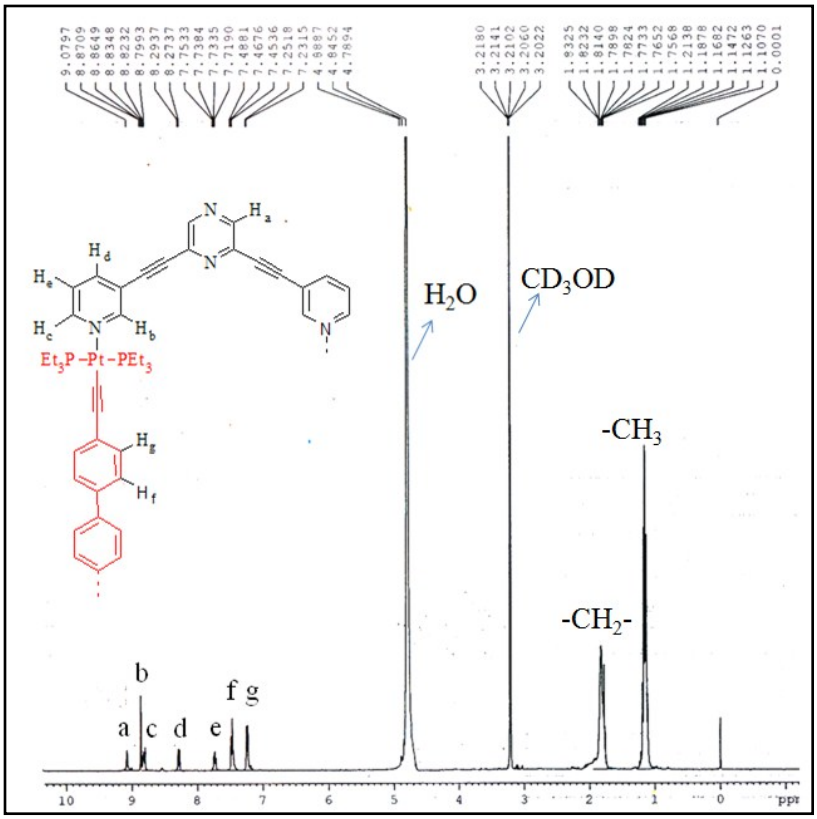

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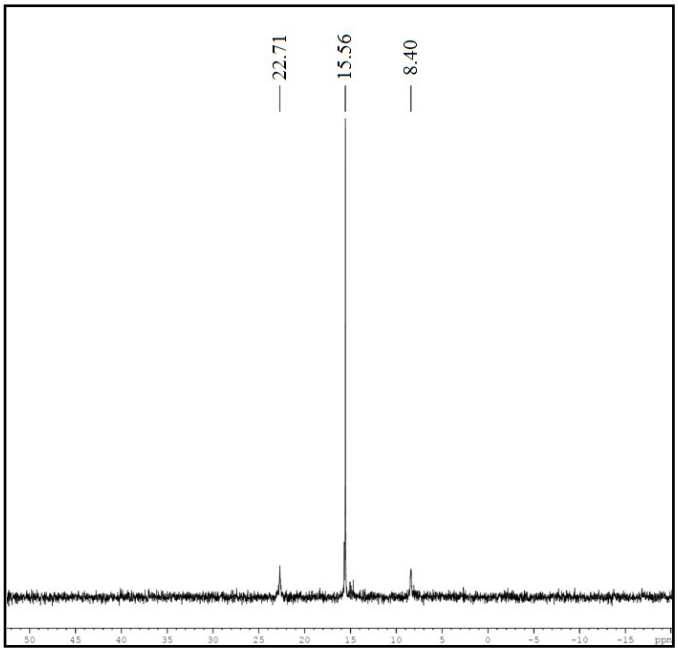

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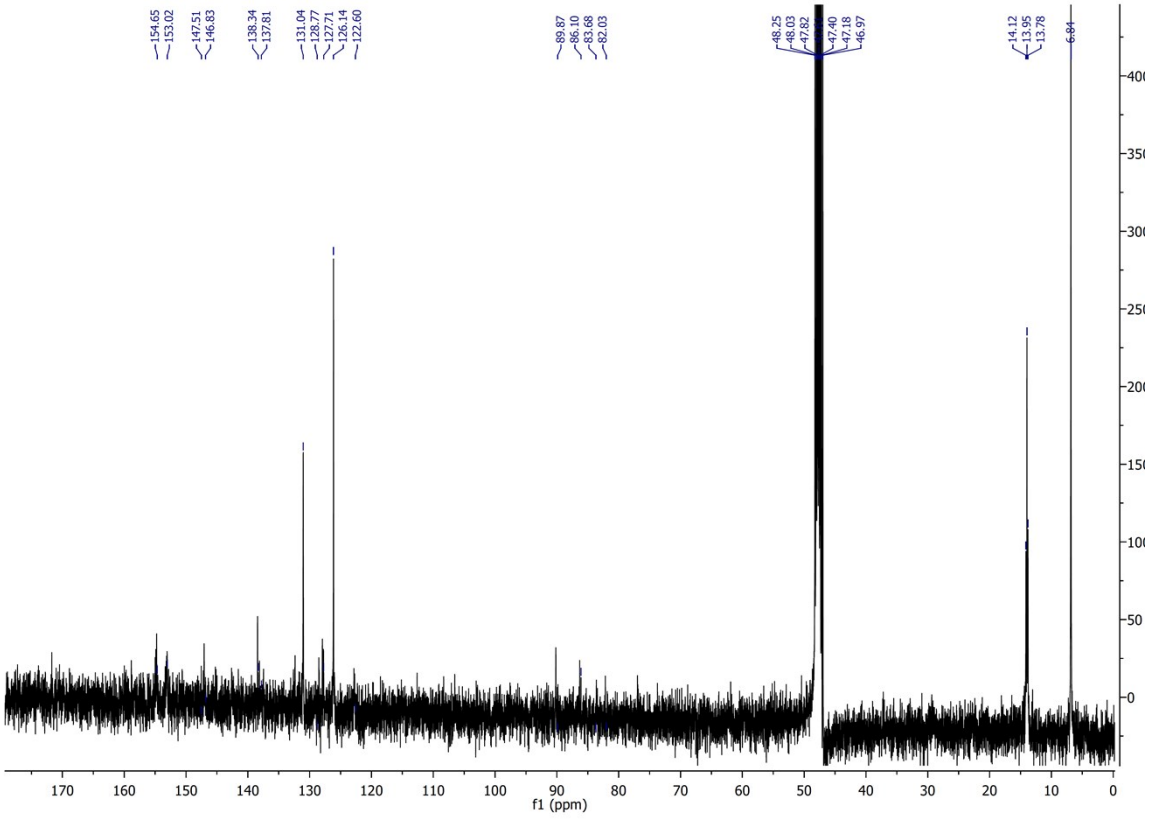

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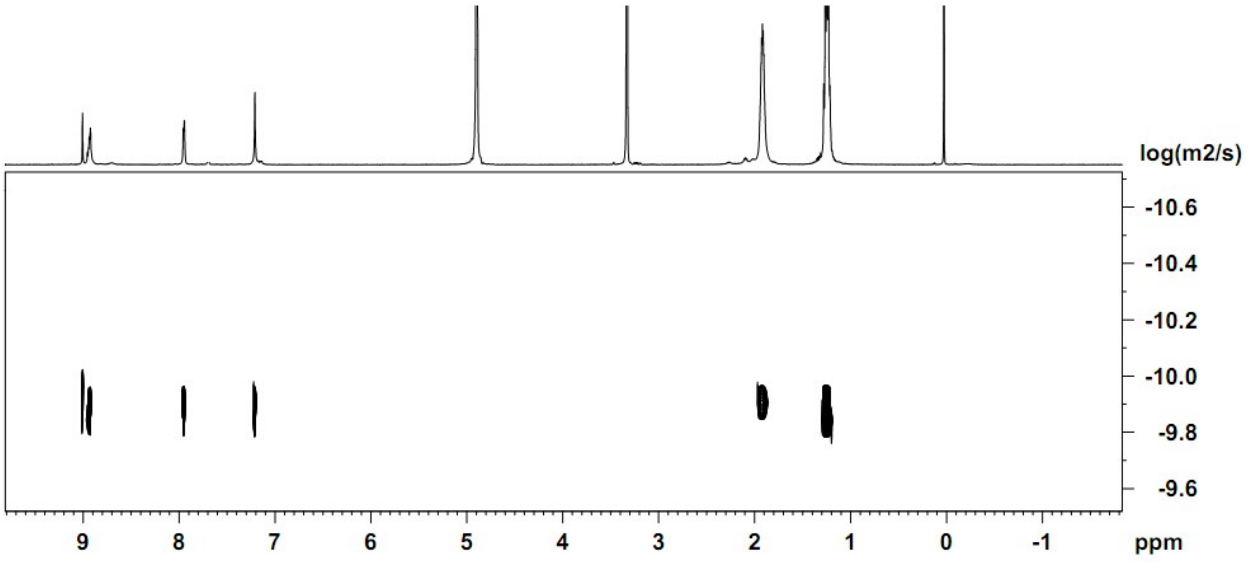

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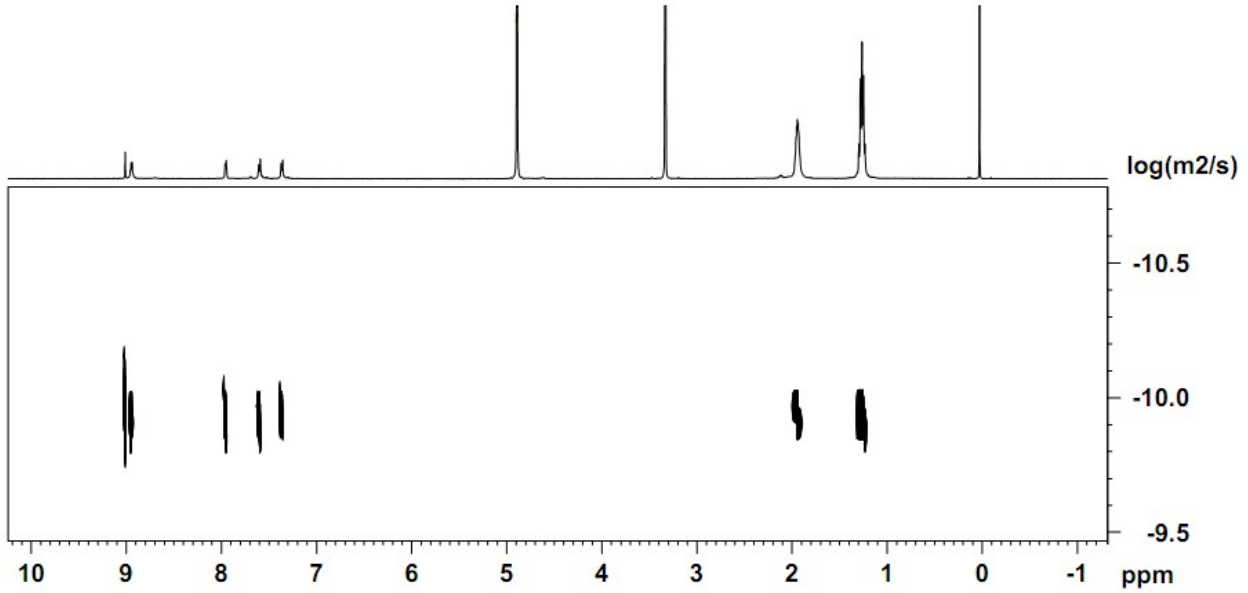

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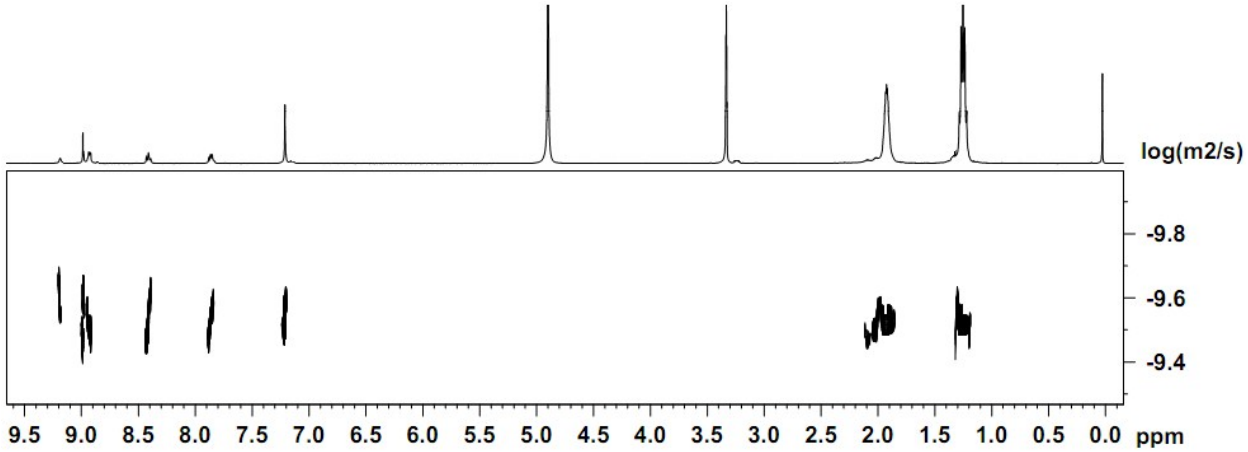

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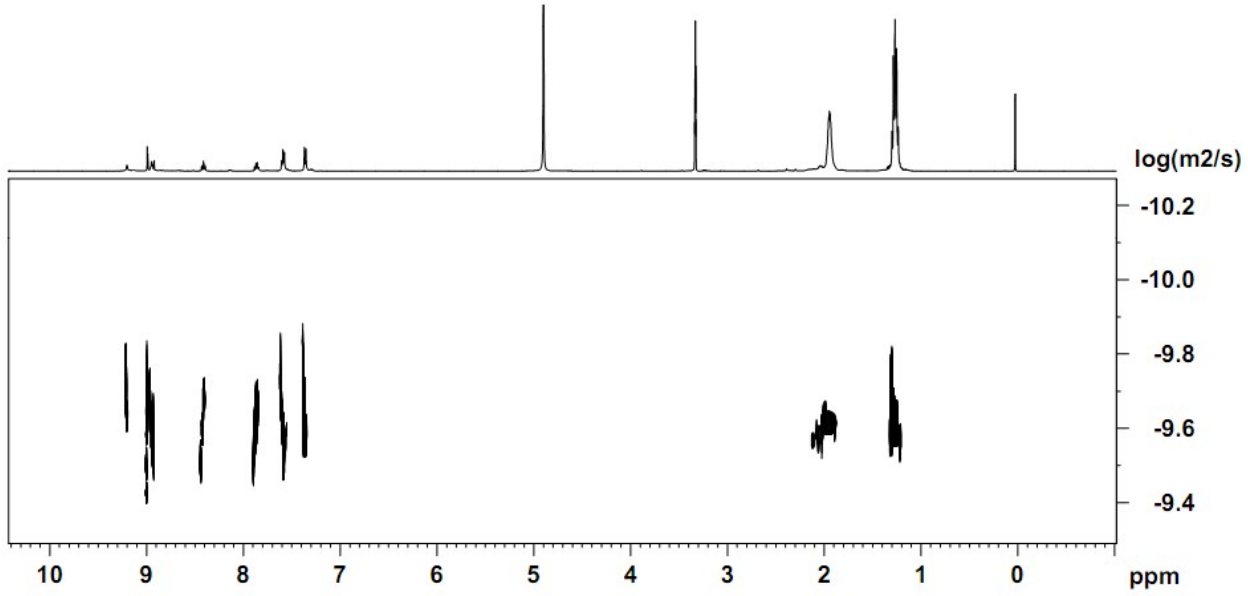

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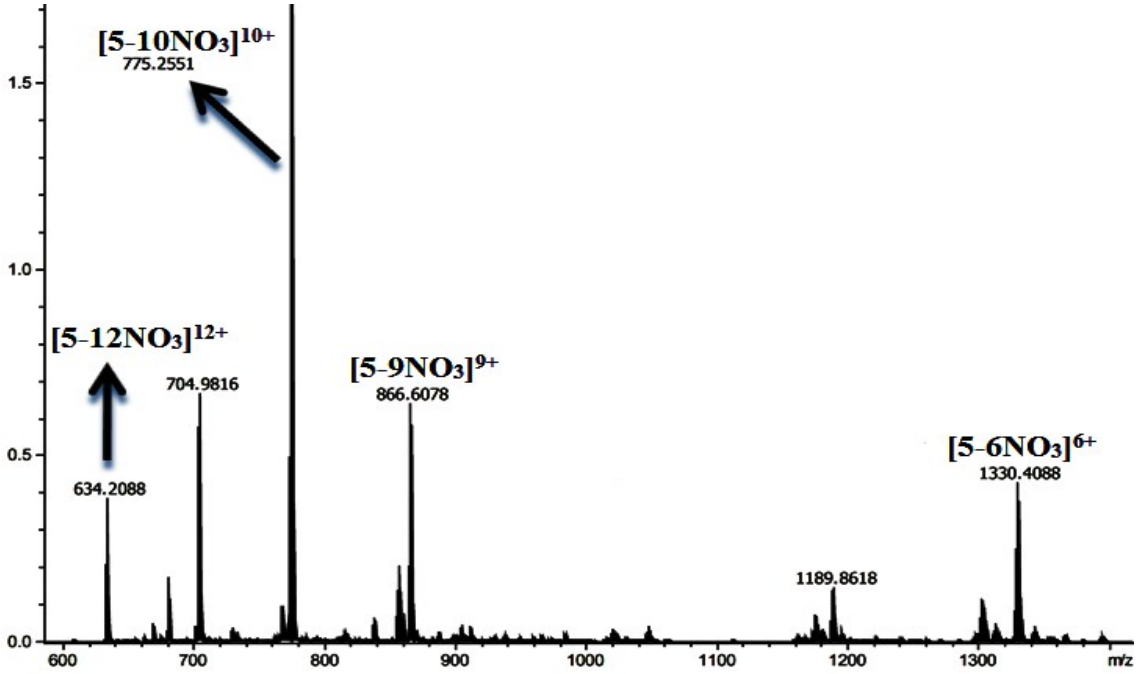

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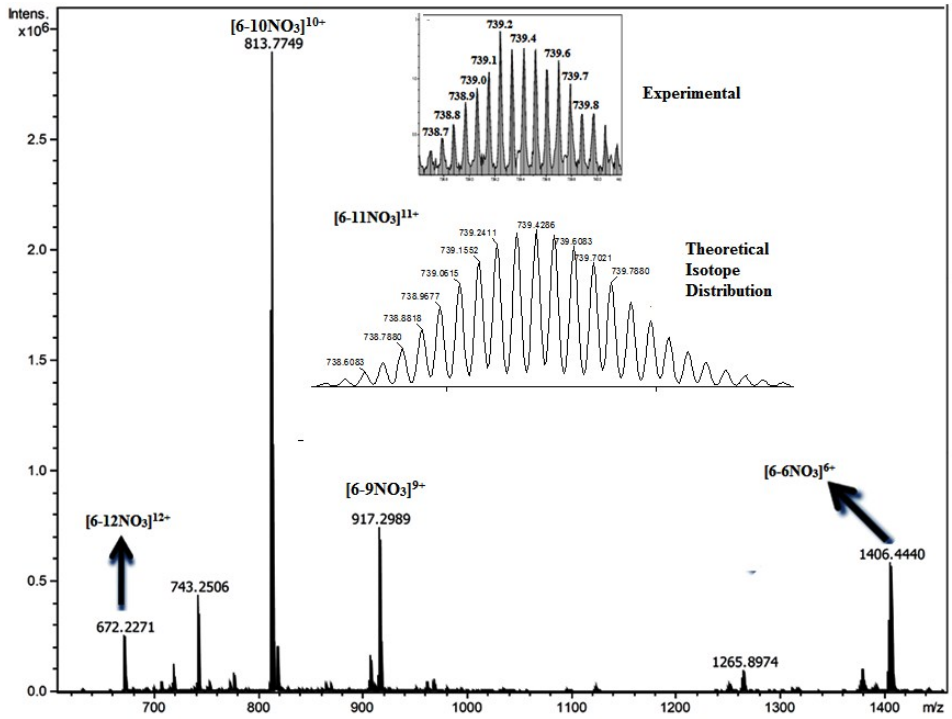

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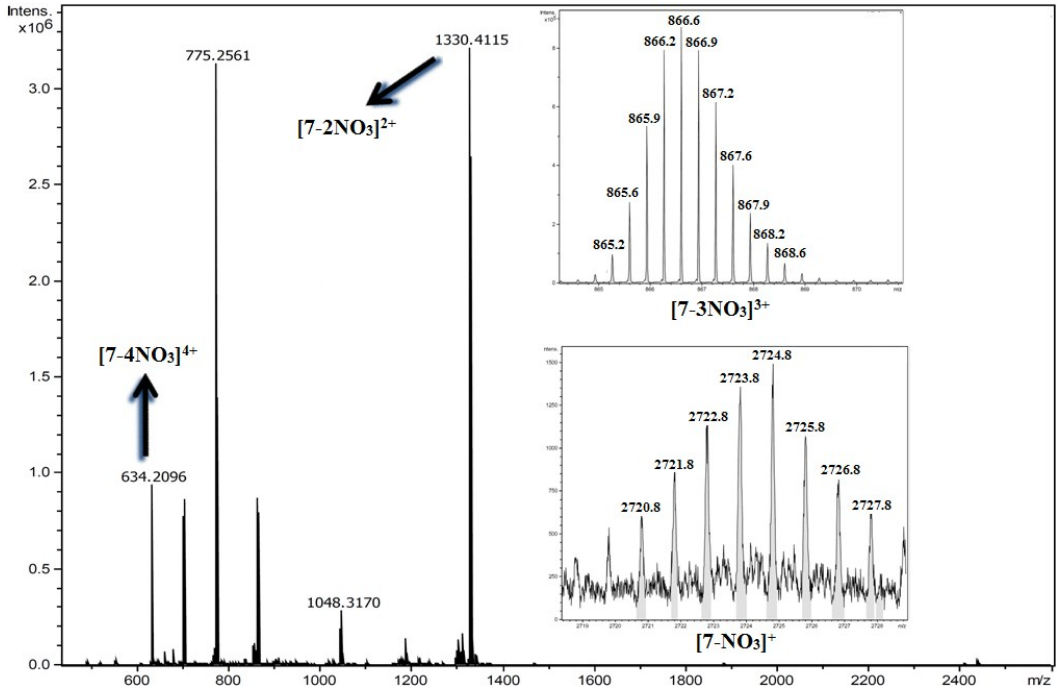

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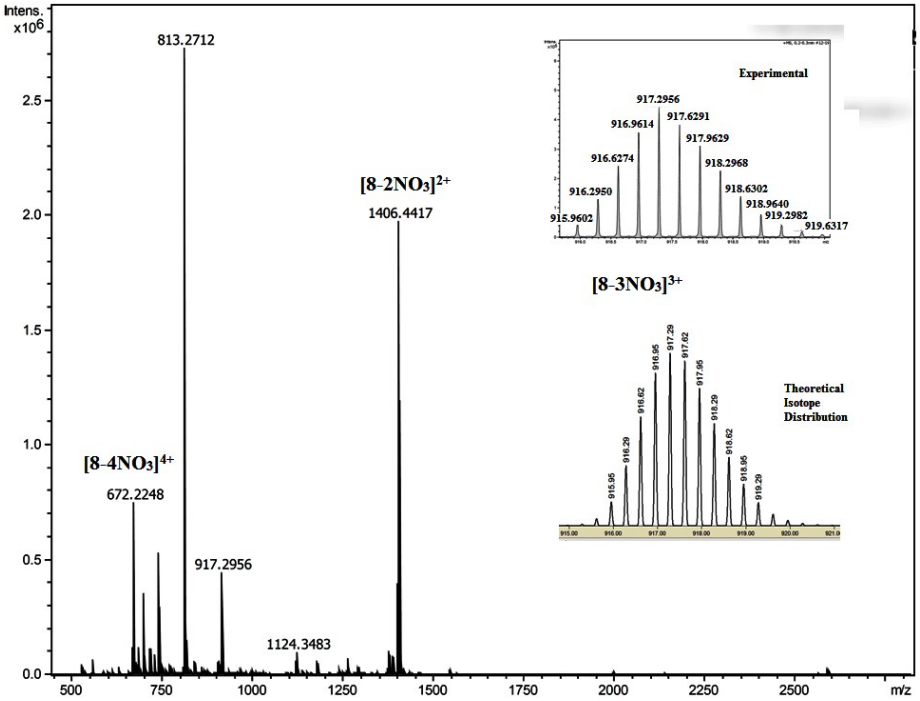

X-ray crystallography analysis of ligand 1.

The crystal lattice of **1** is shown in Figure 1. It consists of various C─H···N short interactions which are less than the sum of their van der Waals radii (2.74 Å). Both the pyrazine nitrogens are engendering weak interactions towards aromatic C-H hydrogens which are 2.64 and 2.69 Å and there extends in the lattice along *a*-axis as shown in Figure 1a. Additionally, one of the terminal nitrogen of pyridine moiety shows hydrogen bonding interaction with aromatic C-H ortho to the pyridine nitrogen of adjacent molecule as shown in Figure 1b with fragmented bond to generate a 1D polymer along *b*-axis (C─H17···N2=2.60 Å). The other terminal pyridine nitrogen shows very weak interaction with one of the aromatic hydrogen present in the pyrazine ring with C─H10···N1 length of 2.72 Å. These two interactions extend the lattice in *bc*-plane. We also observed the π-π stacking interaction as an additional crystal stabilizing interaction which is highlighted in Figure 1b with a distance of 3.91 Å. Crystal data and structure refinement parameters for compound **1** are listed in S15. Selected bond distances and angles are listed in S16.

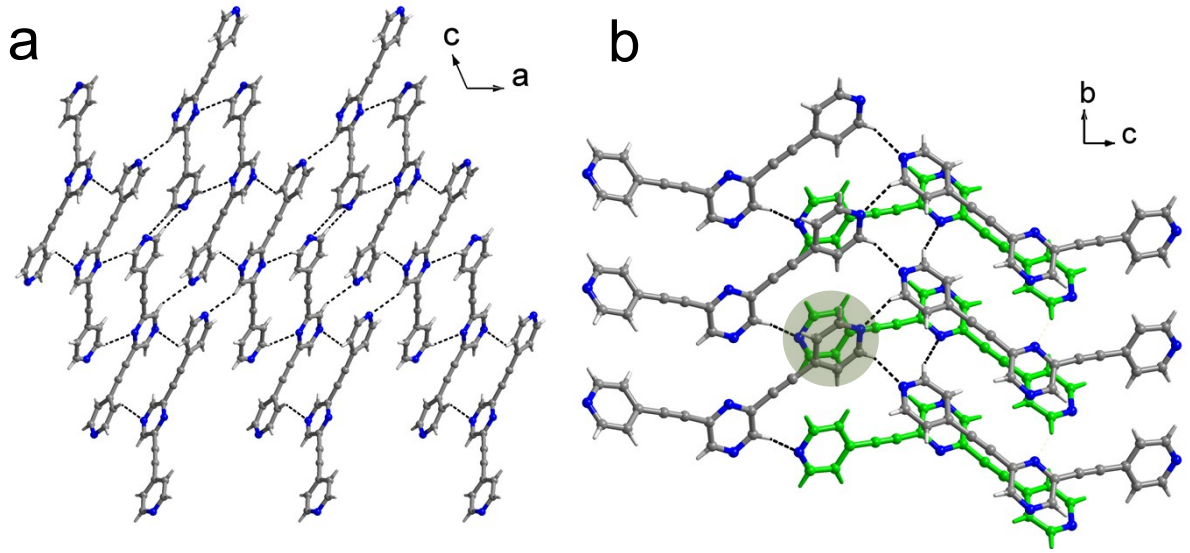

Figure 1: Non-classical interactions (fragmented bonds) in the crystal lattice of **1** as viewed along *b*-axis (a) and *a*-axis (b). Color code: C-gray, N-blue and H-light gray. π-π stacking interactions are highlighted with gray circle.

Crystal Data and structure refinement parameters of 1:

Parameters	Compound **1**
Empirical formula	$C_{18}H_{10}N_4$
a (Å)	22.8914(8)
b (Å)	5.7531(2)
c (Å)	23.2380(7)
α(^{0})	90
β(^{0})	113.464(4)
γ(^{0})	90
V (Å^3)	2807.30(16)
Z	8
Formula weight	282.30
Space group	C2/c
T (^{o}C)	23
λ(MoKα) Å	0.71073
ρ_{calc}(gcm^{-3})	1.336
μ (mm^{-1})	0.083
R[I.>2σ(I)]	R1 = 0.0431 wR2 = 0.1097
R (all data)	R1 = 0.0626 wR2 = 0.1214

$^aR_1=\sum|F_0| - |F_c|$; $^bwR_2=\{[w(F_0^2-F_c^2)^2] / [w(F_0^2)^2]\}^{1/2}$, $w=1/[\sigma^2(F_0)^2+(aP)^2+bP]$,

$P= [F_0^2+2Fc^2] / 3$; where a= 0.0537,b= 0.7386

Bond distances and angles for 1:

Moiety	Distance(A^o)	Moiety	Angle(deg)
C(1)-N(1)	1.3290(17)	C(1)-C(2)-C(3)	118.46(11)
C(1)-C(2)	1.3785(15)	C(4)-C(3)-C(2)	117.73(10)
C(2)-C(3)	1.3843(15)	C(4)-C(3)-C(6)	121.26(10)
C(3)-C(4)	1.3819(16)	C(2)-C(3)-C(6)	120.95(10)
C(4)-C(5)	1.3772(16)	C(7)-C(6)-C(3)	178.37(12)
C(5)-N(1)	1.3287(16)	C(6)-C(7)-C(8)	175.49(12)
C(3)-C(6)	1.4365(14)	N(4)-C(8)-C(9)	121.83(9)
C(6)-C(7)	1.1913(14)	N(4)-C(8)-C(7)	118.61(10)
C(7)-C(8)	1.4361(14)	C(9)-C(8)-C(7)	119.56(10)
C(8)-C(9)	1.3917(16)	N(3)-C(9)-C(8)	122.40(10)
C(8)-N(4)	1.3360(13)	N(3)-C(10)-C(11)	122.31(10)
C(9)-N(3)	1.3250(14)	N(4)-C(11)-C(10)	121.63(9)
C(10)-N(3)	1.3252(14)	N(4)-C(11)-C(12)	118.17(10)
C(10)-C(11)	1.3933(15)	C(10)-C(11)-C(12)	120.19(9)
C(11)-N(4)	1.3433(13)	C(13)-C(12)-C(11)	176.08(13)
C(11)-C(12)	1.4349(15)	C(12)-C(13)-C(14)	178.61(13)
C(12)-C(13)	1.1900(15)	C(15)-C(14)-C(18)	117.30(10)
C(13)-C(14)	1.4355(15)	C(15)-C(14)-C(13)	121.91(10)
C(14)-C(15)	1.3865(16)	C(18)-C(14)-C(13)	120.79(10)
C(14)-C(18)	1.3874(15)	C(16)-C(15)-C(14)	118.88(11)
C(15)-C(16)	1.3751(17)	N(2)-C(16)-C(15)	124.35(11)
C(16)-N(2)	1.3293(16)	N(2)-C(17)-C(18)	123.86(11)
C(17)-N(2)	1.3335(16)	C(17)-C(18)-C(14)	119.32(11)
C(17)-C(18)	1.3727(16)	C(16)-N(2)-C(17)	116.27(10)
Moiety	**Angle(deg)**	C(5)-N(1)-C(1)	116.16(10)
N(1)-C(1)-C(2)	124.54(11)	C(9)-N(3)-C(10)	116.07(10)
N(1)-C(5)-C(4)	123.96(11)	C(8)-N(4)-C(11)	115.68(9)
C(5)-C(4)-C(3)	119.14(11)		