Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for:

PNPCB Heterocycles via Thermal and Lewis Acid Catalyzed *trans*-Hydroborations

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1. NMR Spectra

Figure 1 ^{1}H NMR spectrum of **8** (400 MHz, d_6-benzene, 298K).

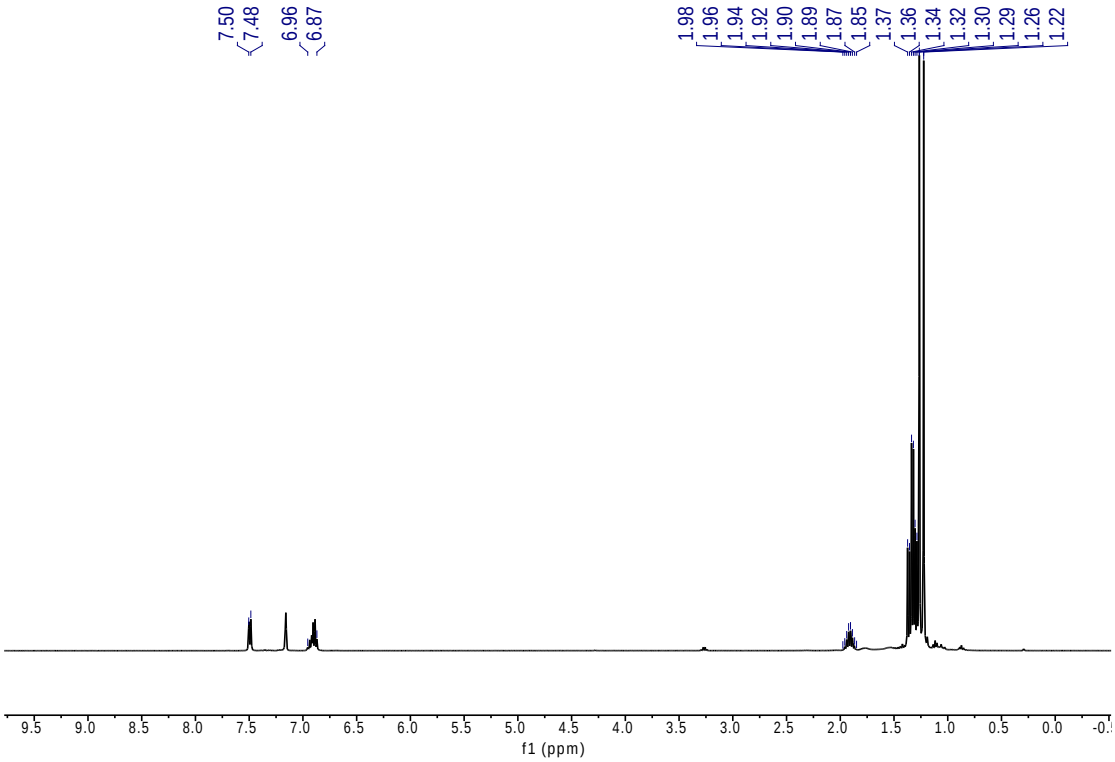


Figure 2 ^{13}C NMR spectrum of **8** (100 MHz, d_6-benzene, 298K)

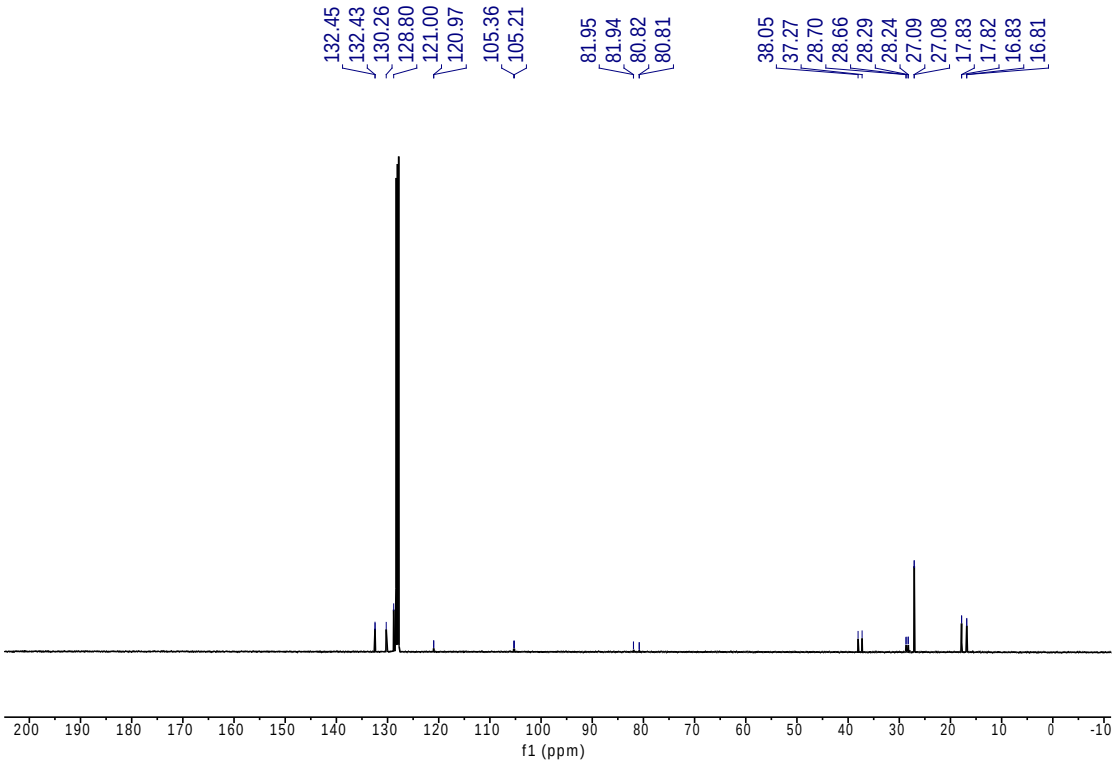


Figure 3 ^{31}P NMR spectrum of **8** (162 MHz, d_6-benzene, 298K).

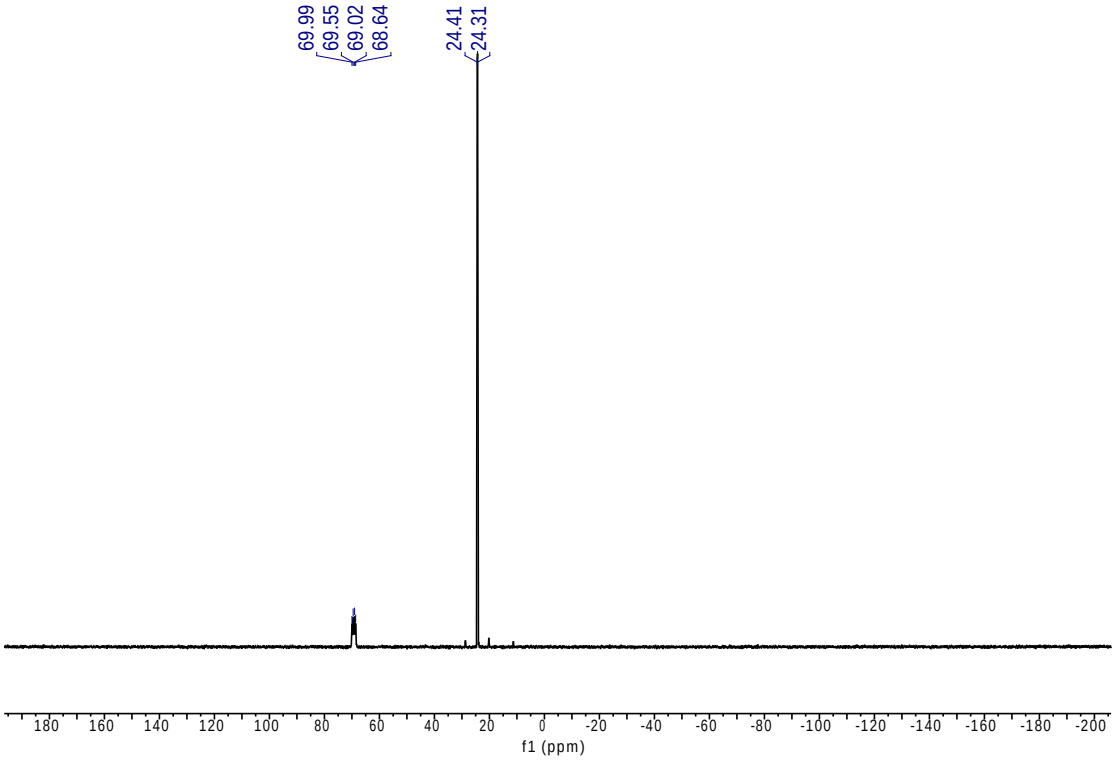


Figure 4 ^{11}B NMR spectrum of **8** (128 MHz, d_6-benzene, 298K)

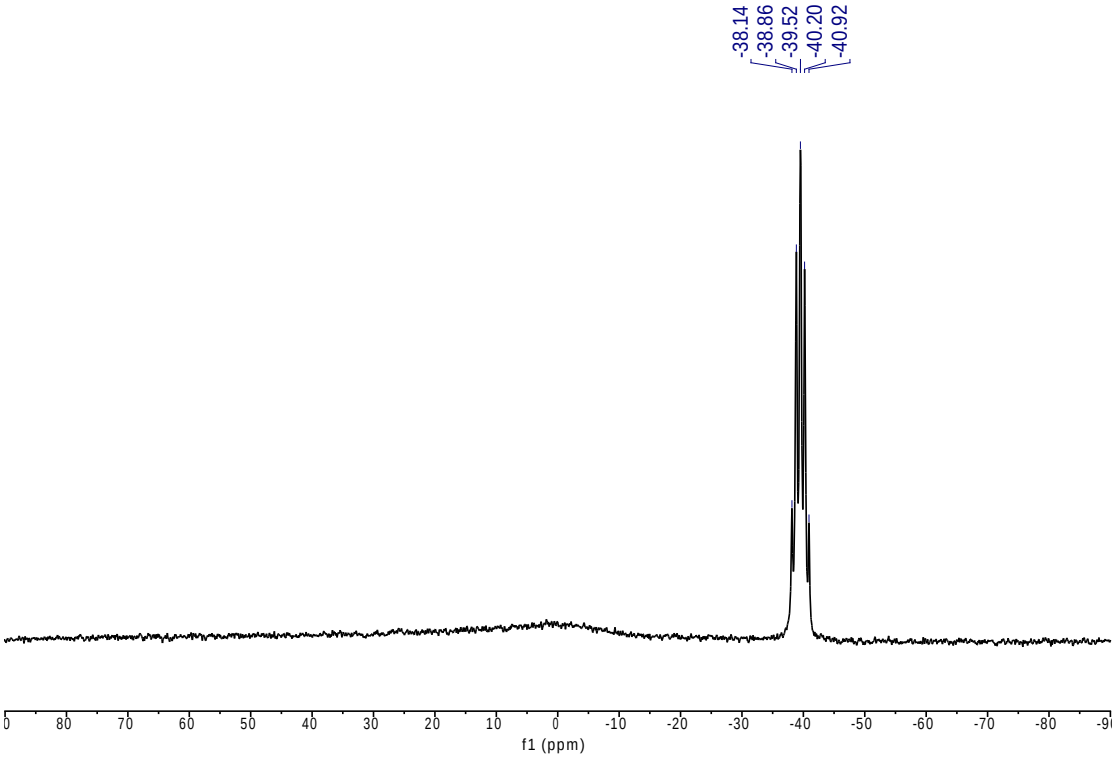


Figure 5 ^{1}H NMR spectrum of **9** (400 MHz, d_6-benzene, 298K)

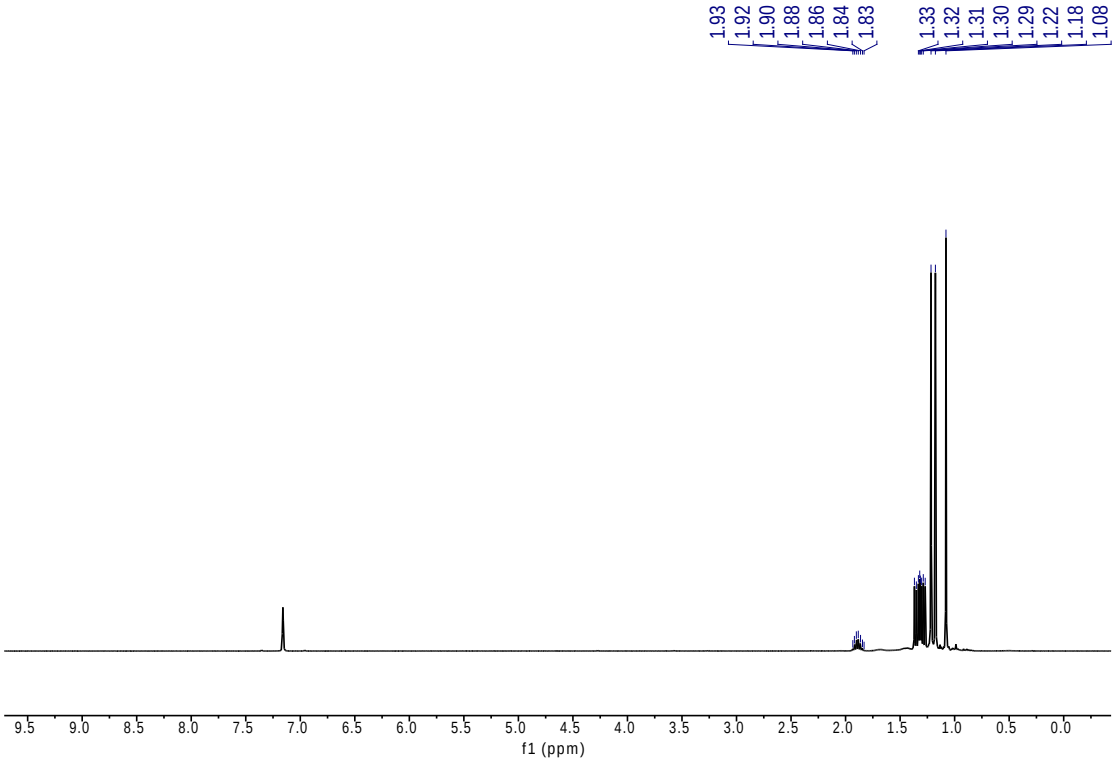


Figure 6 ^{13}C NMR spectrum of **9** (100 MHz, d_6-benzene, 298K)

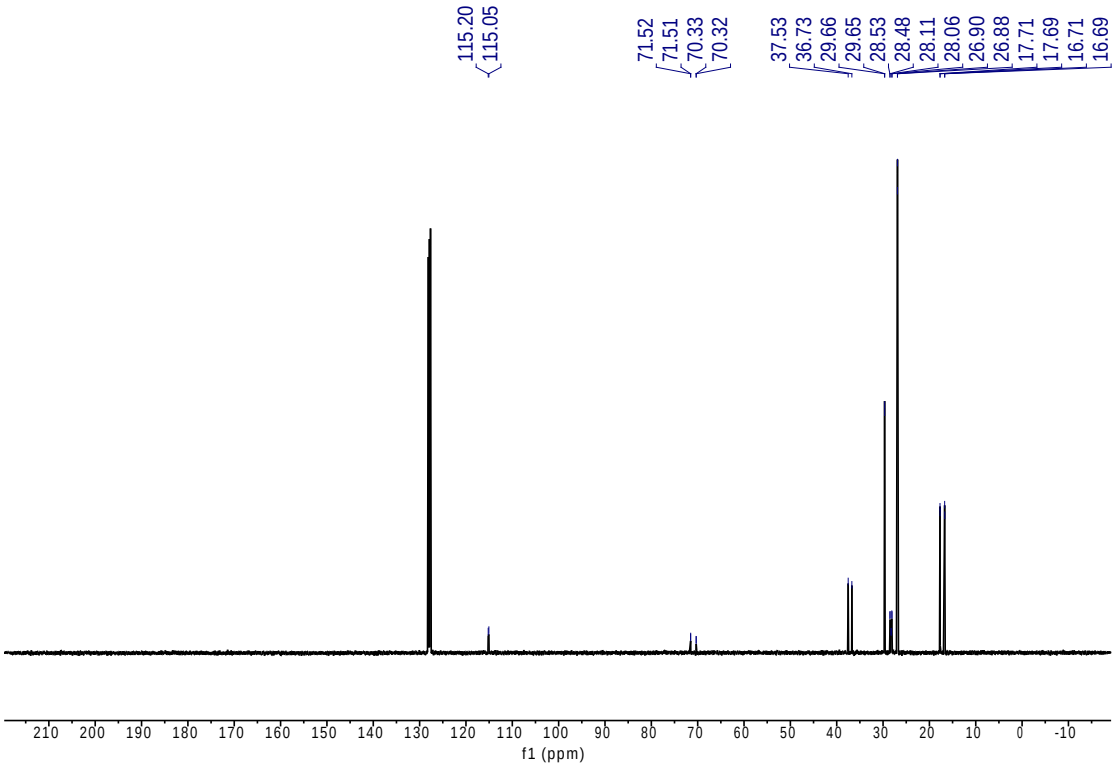


Figure 7 ^{31}P NMR spectrum of **9** (162 MHz, d_6-benzene, 298K)

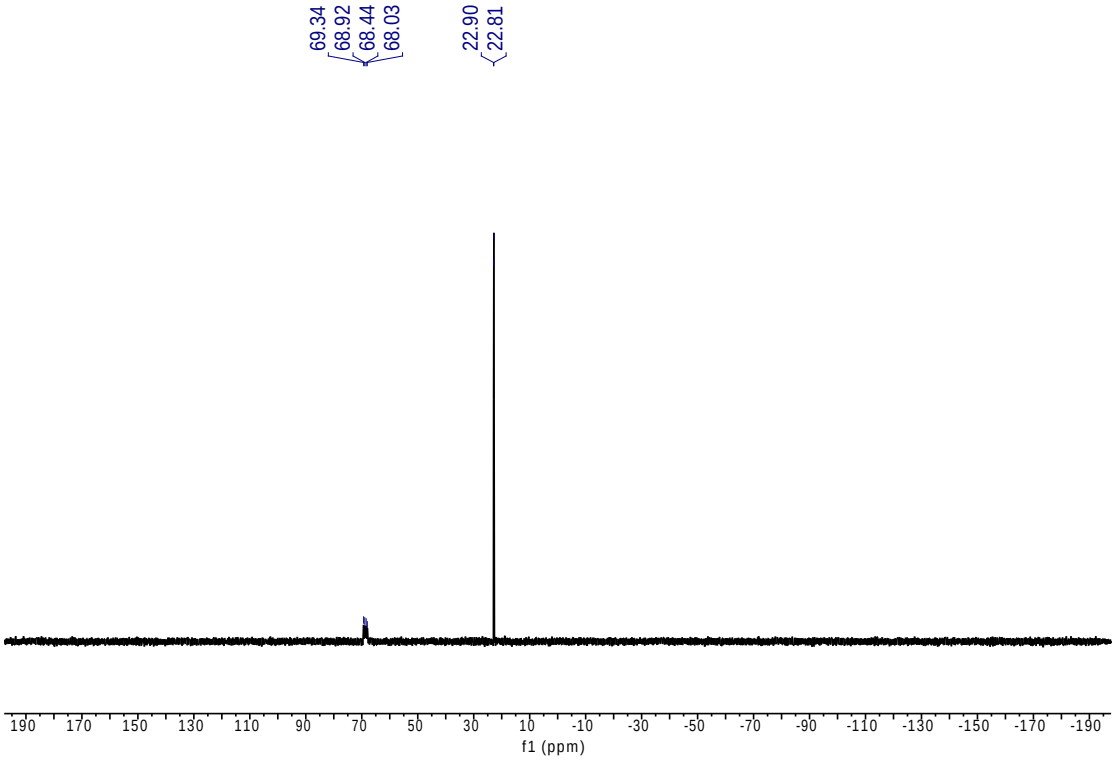


Figure 8 ^{11}B NMR spectrum of **9** (128 MHz, d_6-benzene, 298K)

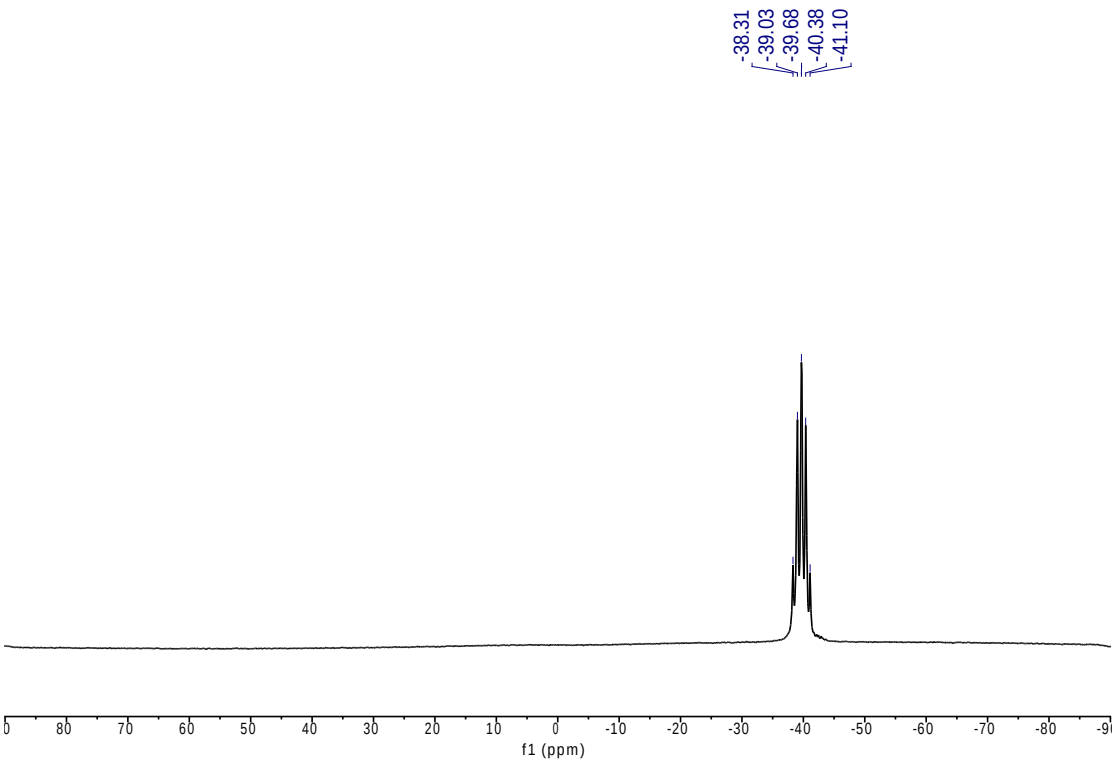


Figure 9 ^{1}H NMR spectrum of **10** (400MHz, d_6-benzene, 298K)

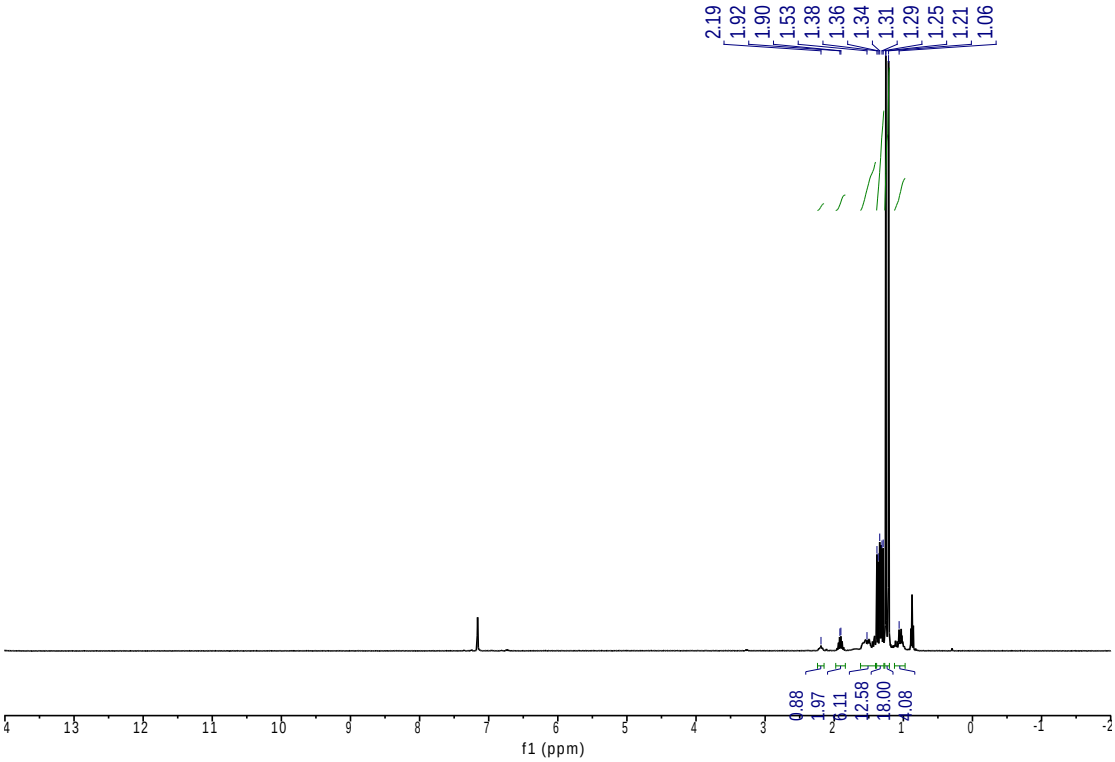


Figure 10 ^{13}C NMR spectrum of **10** (100 MHz, d_6-benzene, 298K)

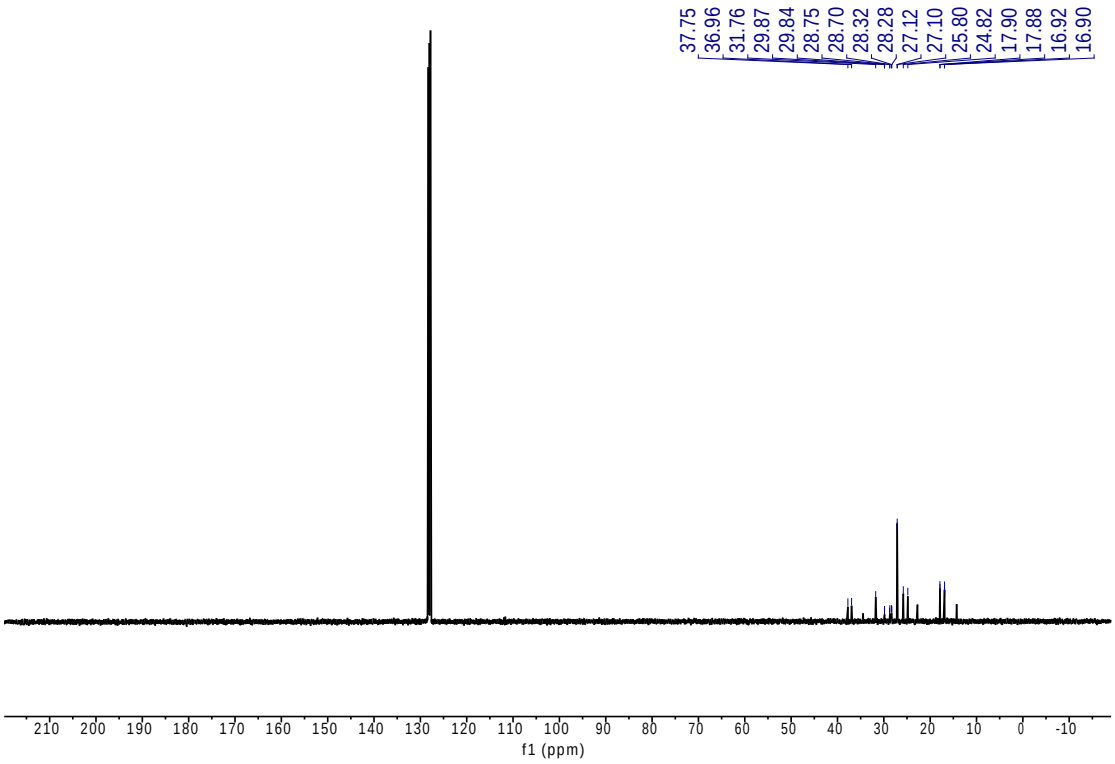


Figure 11 ^{31}P NMR spectrum of **10** (162 MHz, d_6-benzene, 298K)

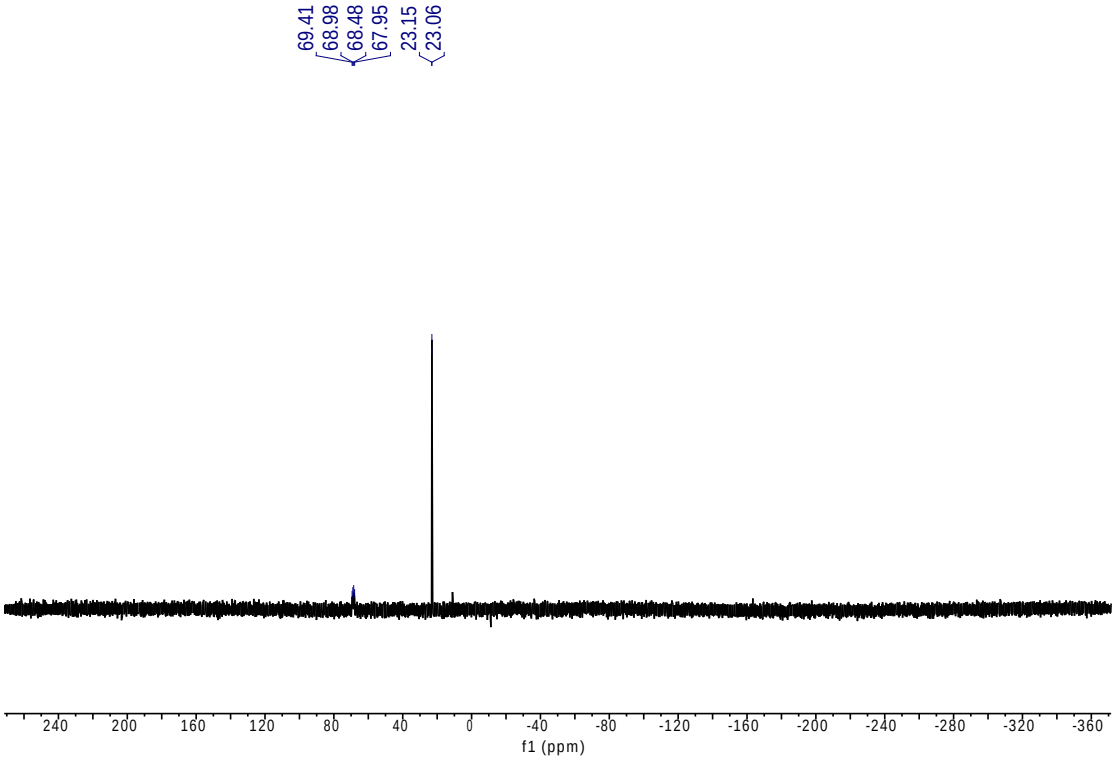


Figure 12 ^{11}B NMR spectrum of **10** (128MHz, d_6-benzene, 298K)

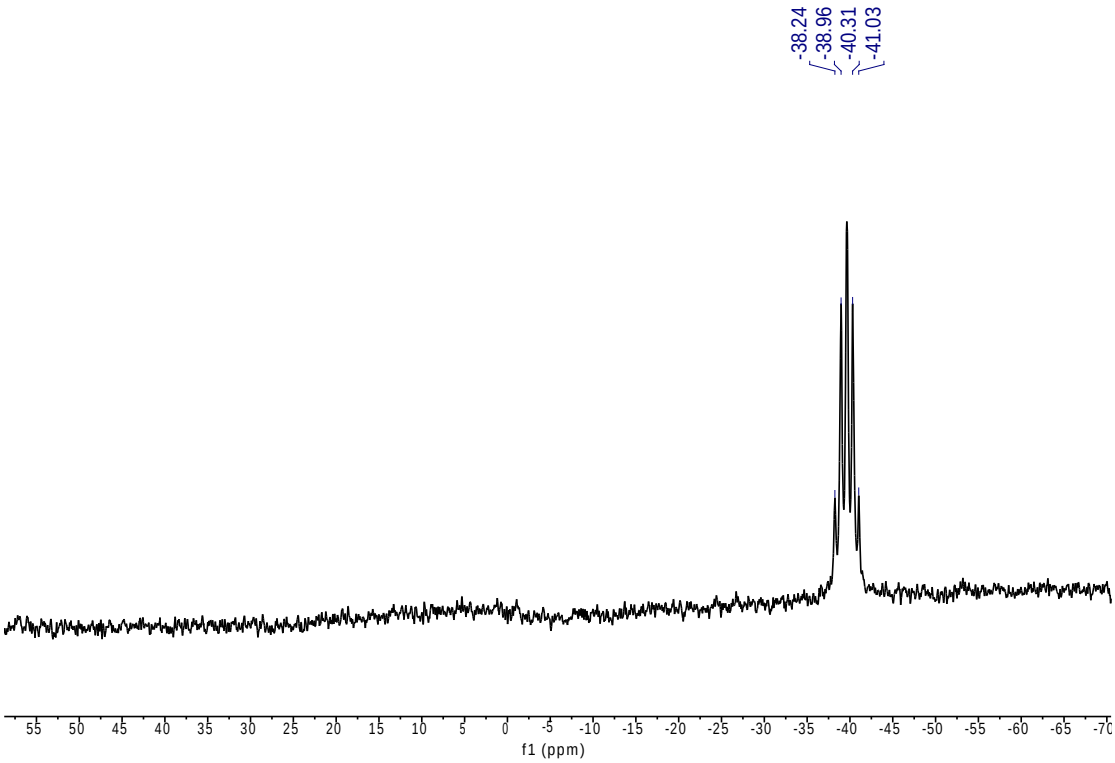


Figure 13 ^{1}H NMR spectrum of **11** (400MHz, d_6-benzene, 298K)

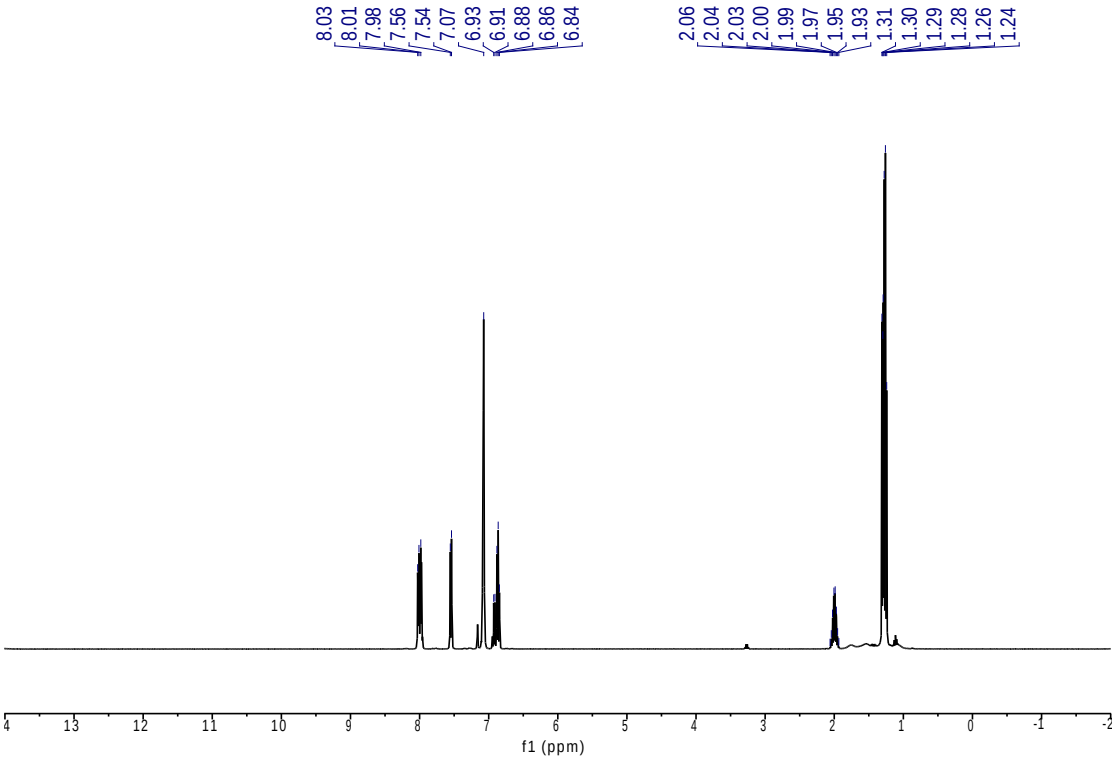


Figure 14 ^{13}C NMR spectrum of **11** (100 MHz, d_6-benzene, 298K)

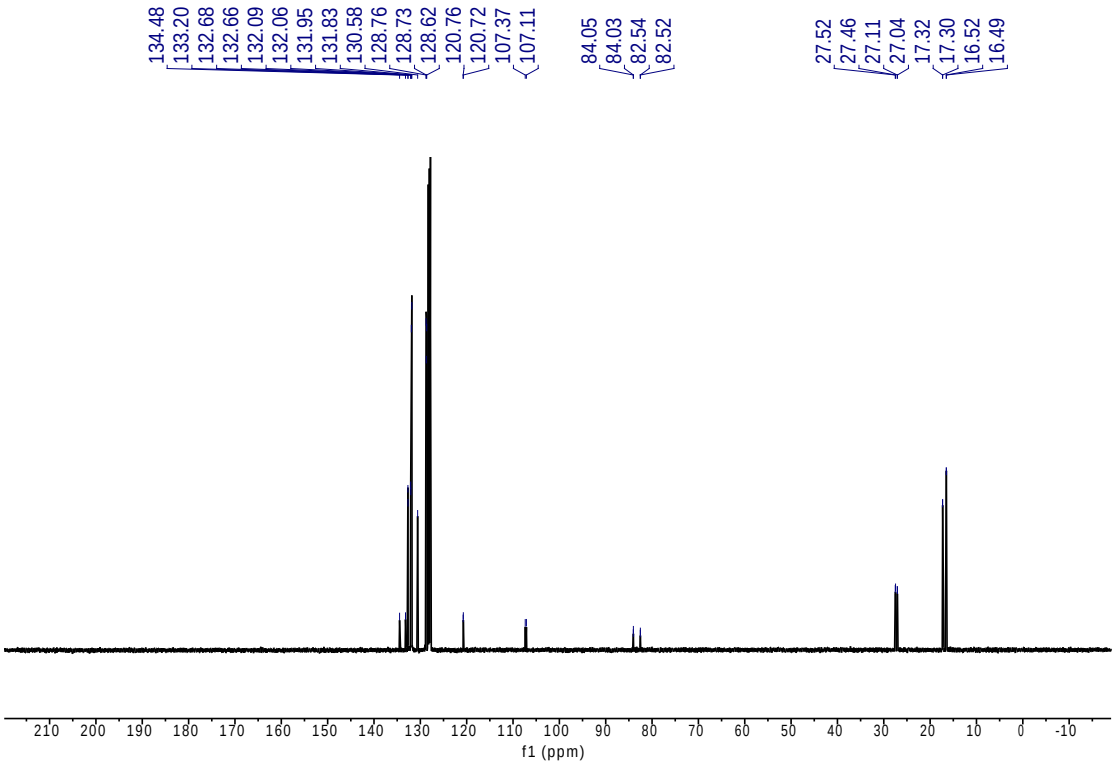


Figure 15 ^{31}P NMR spectrum of **11** (162 MHz, d_6-benzene, 298K)

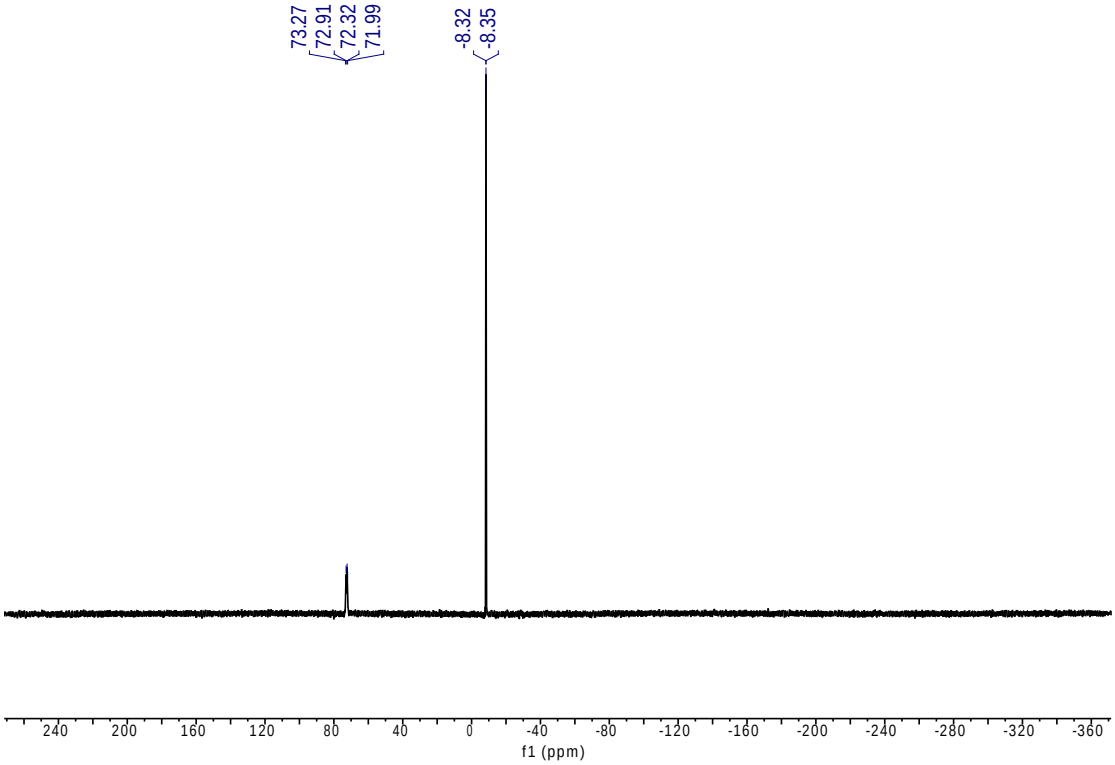


Figure 16 ^{11}B NMR spectrum of **11** (128MHz, d_6-benzene, 298K)

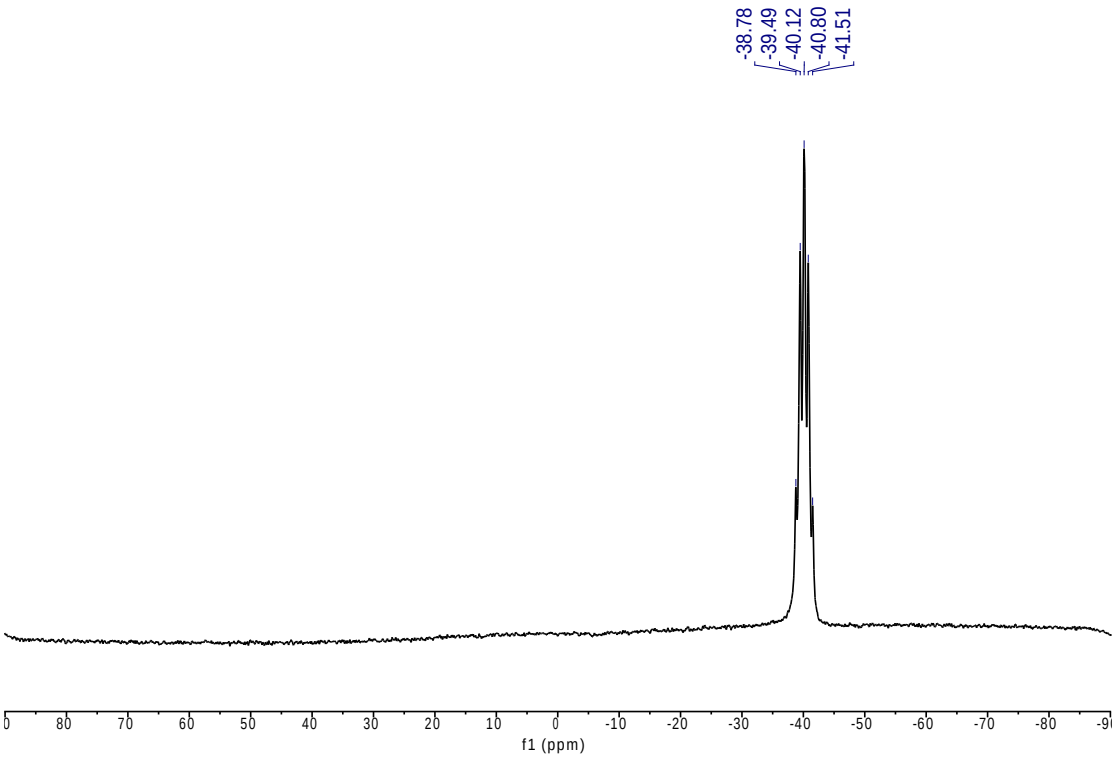


Figure 17 ^{1}H NMR spectrum of **12** (400MHz, d_6-benzene, 298K)

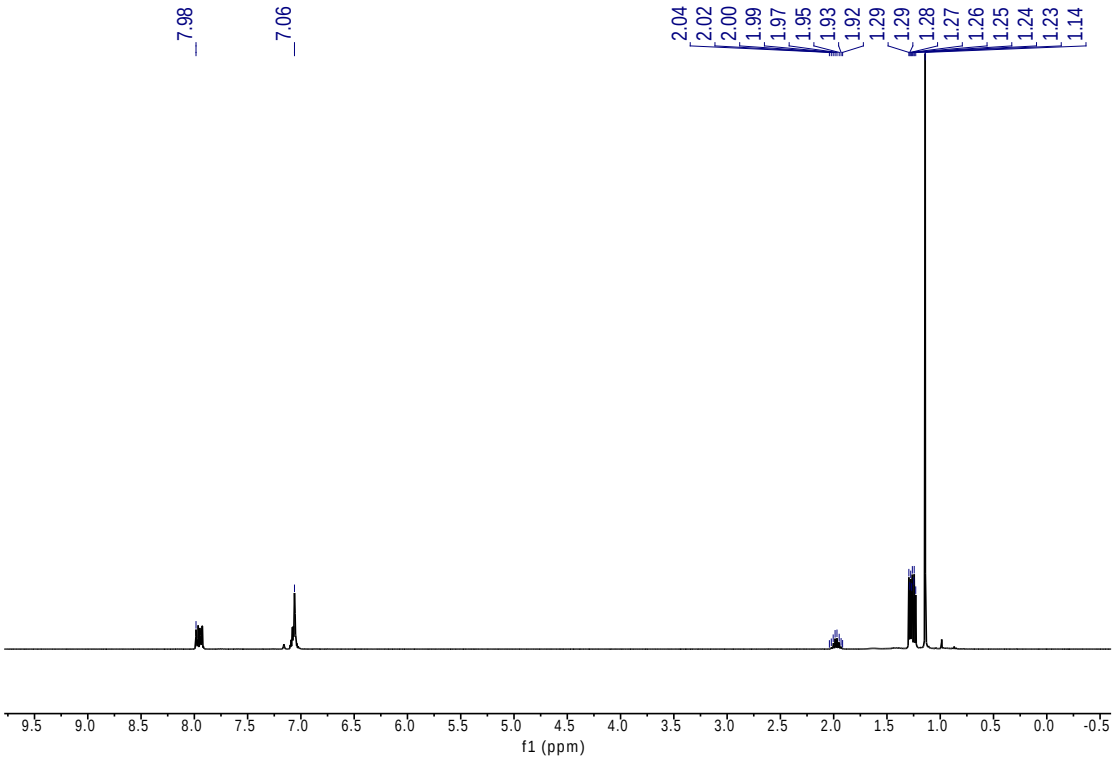


Figure 18 ^{13}C NMR spectrum of **12** (100 MHz, d_6-benzene, 298K)

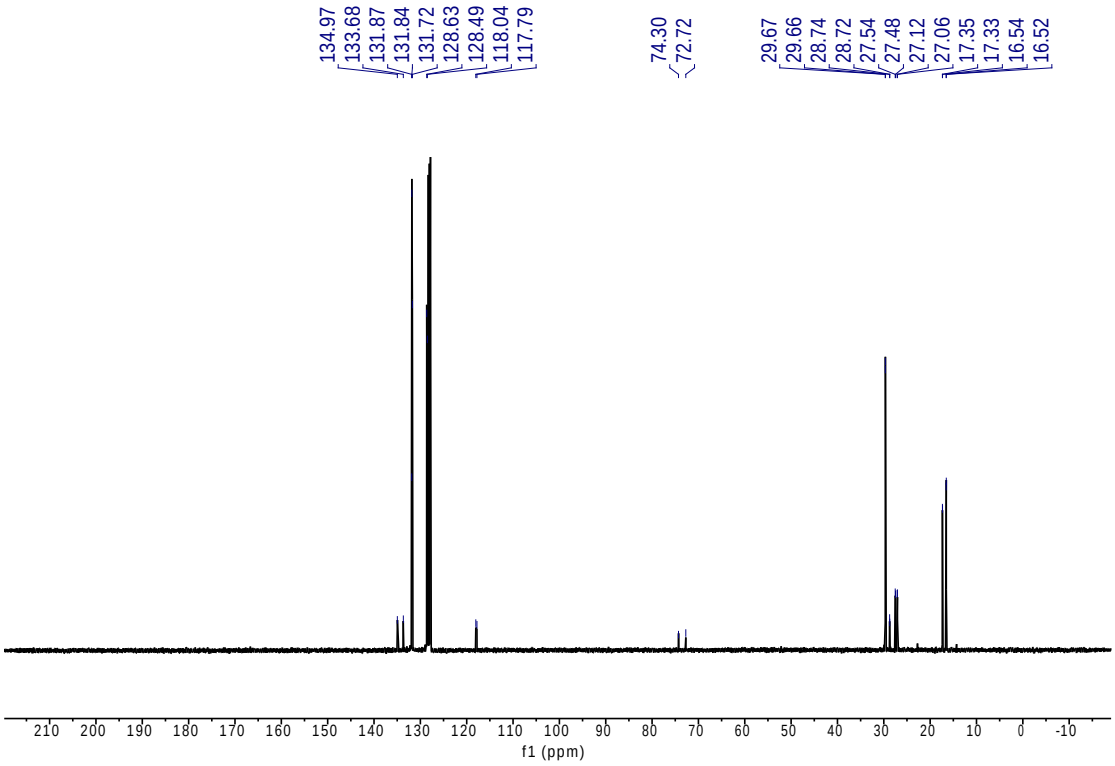


Figure 19 ^{31}P NMR spectrum of **12** (162 MHz, d_6-benzene, 298K)

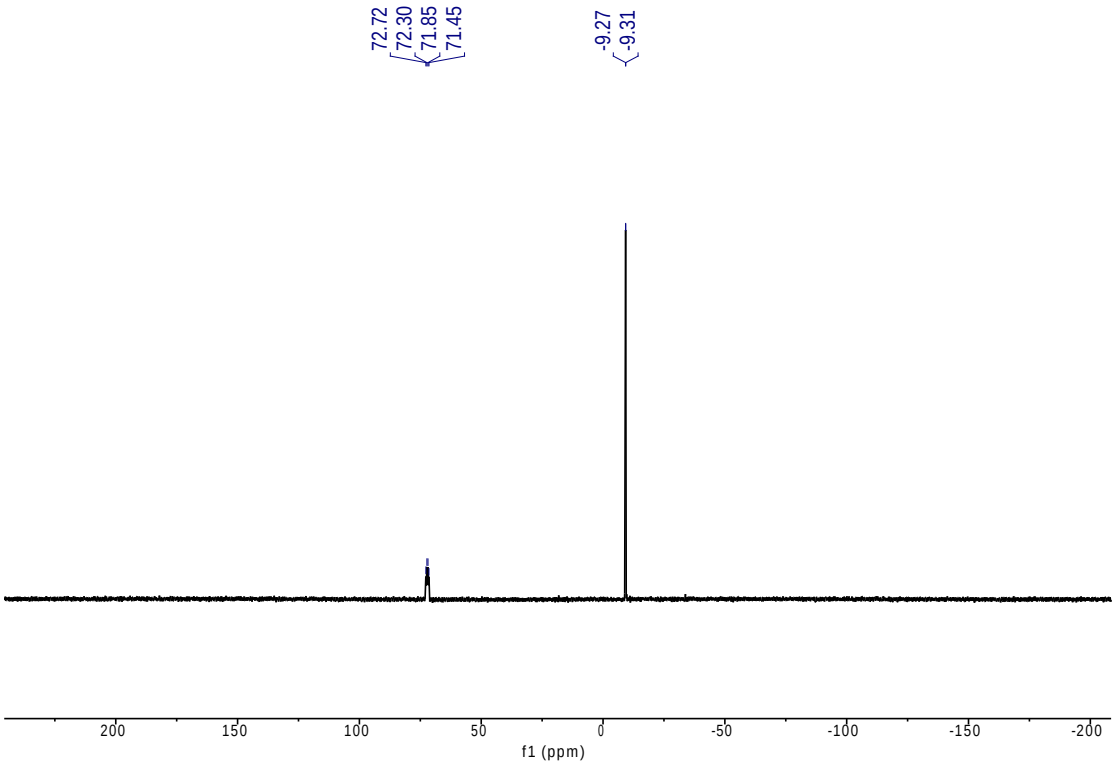


Figure 20 ^{11}B NMR spectrum of **12** (128MHz, d_6-benzene, 298K)

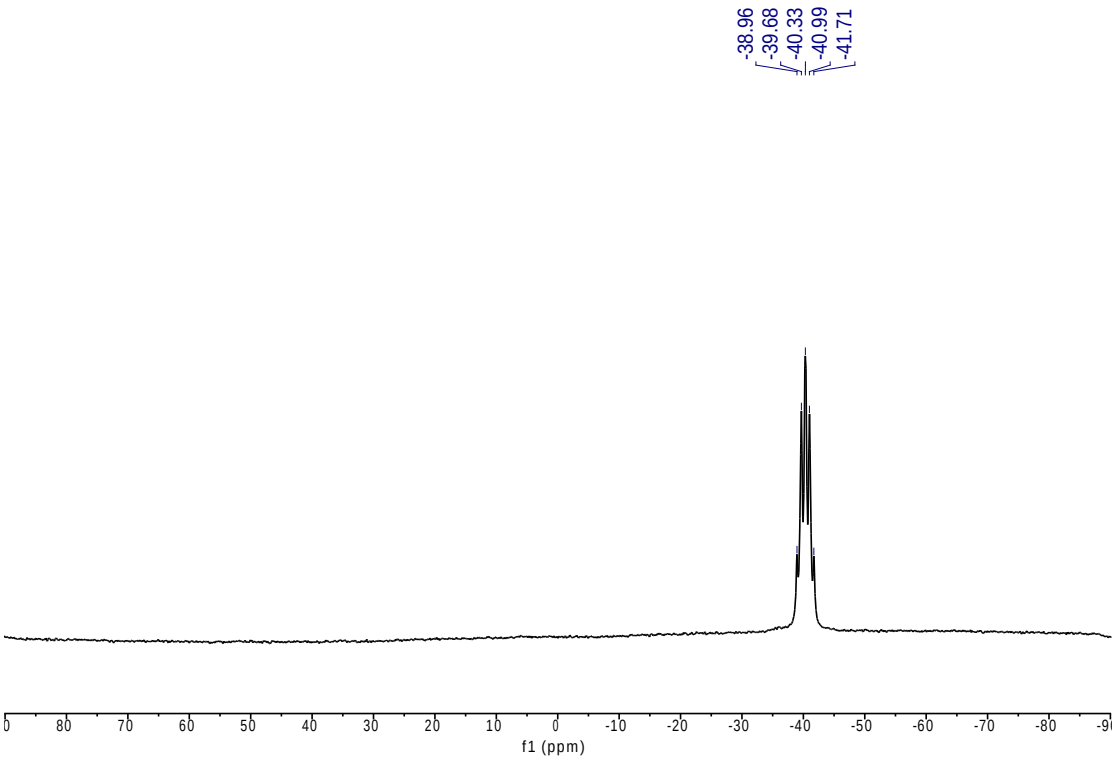


Figure 21 ^{1}H NMR spectrum of **13** (400MHz, d_6-benzene, 298K)

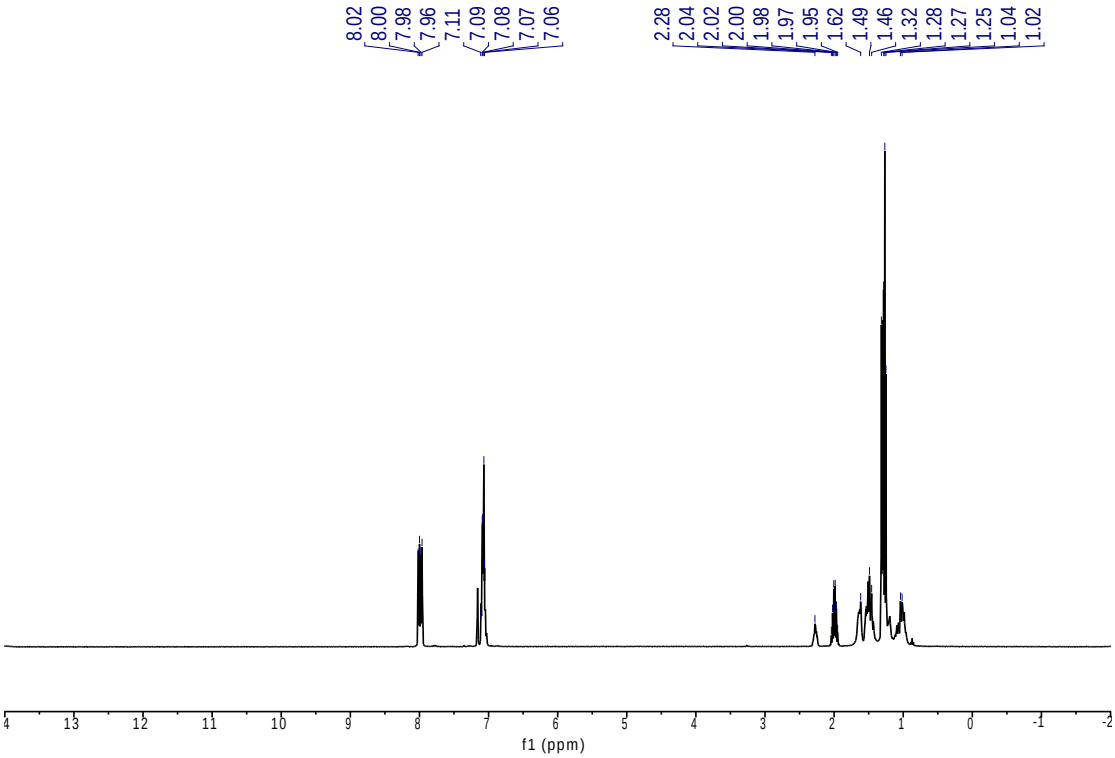


Figure 22 ^{13}C NMR spectrum of **13**(100 MHz, d_6-benzene, 298K)

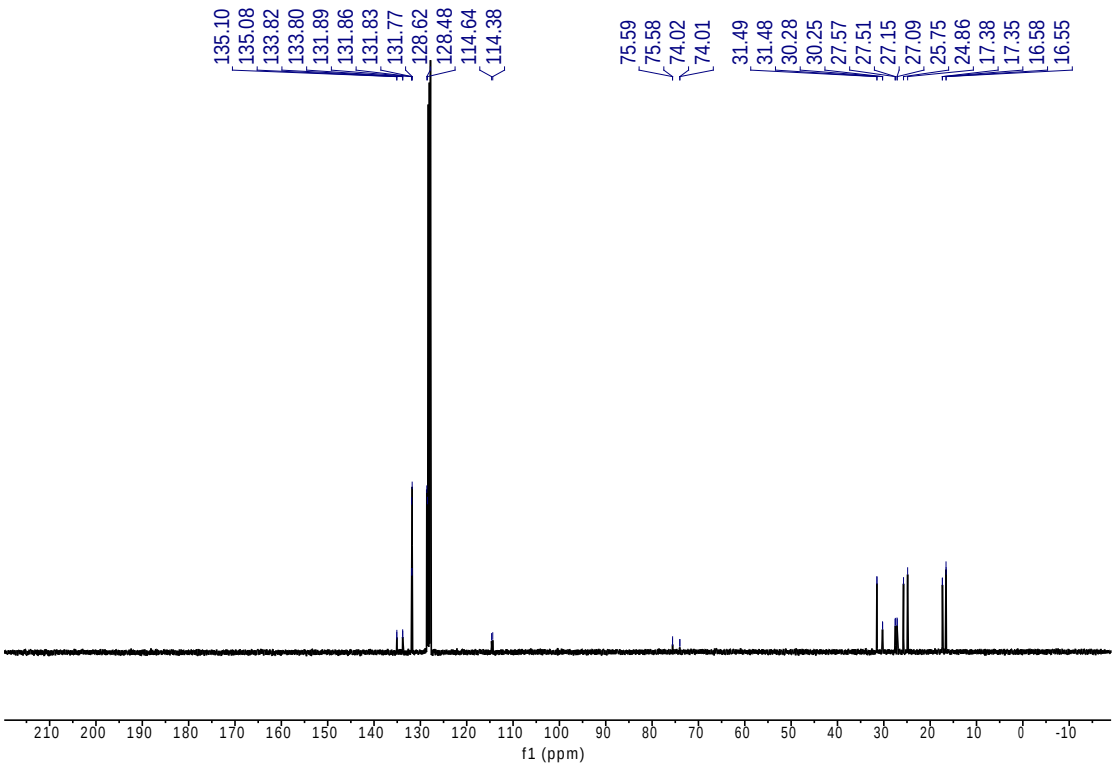


Figure 23 ^{31}P NMR spectrum of **13** (162 MHz, d_6-benzene, 298K)

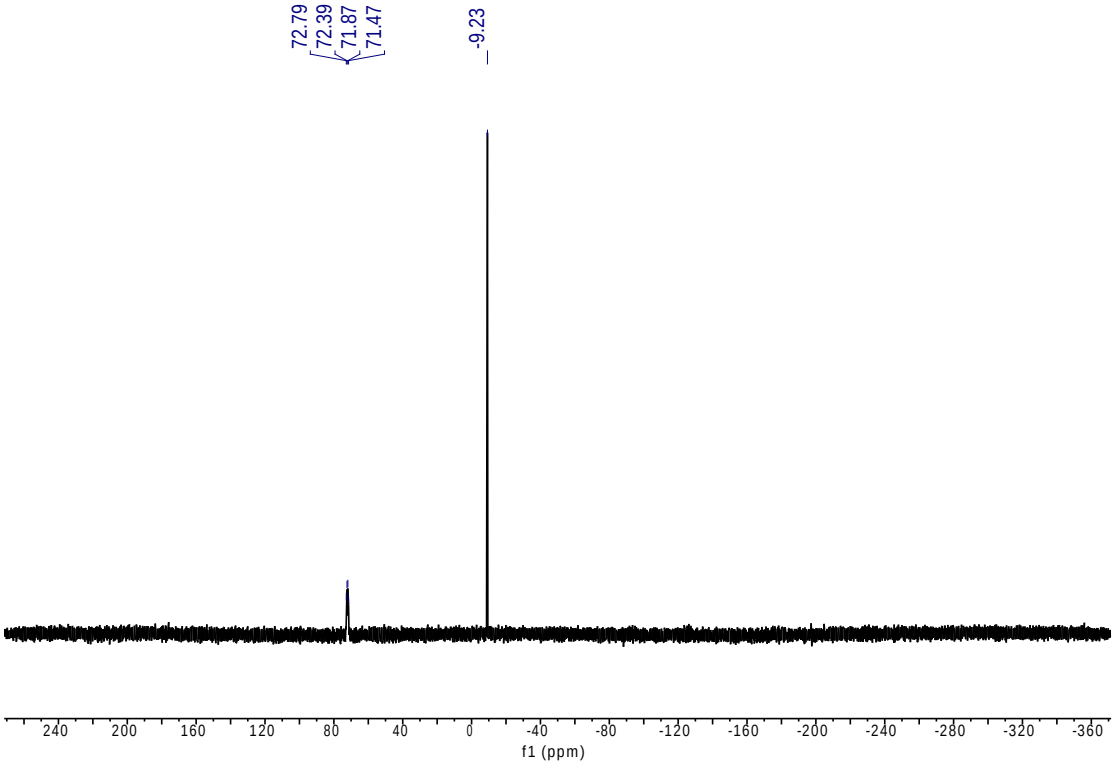


Figure 24 ^{11}B NMR spectrum of **13** (128MHz, d_6-benzene, 298K)

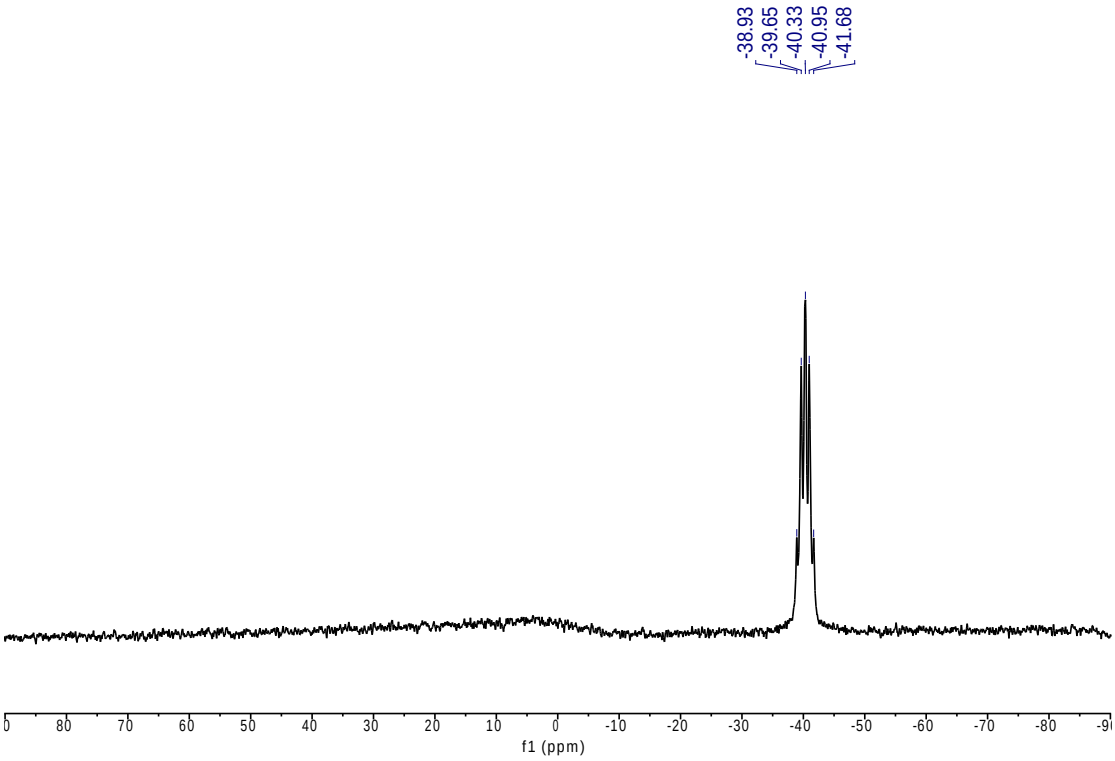


Figure 25 ^{1}H NMR spectrum of **14** (100 MHz, d_6-benzene, 298K)

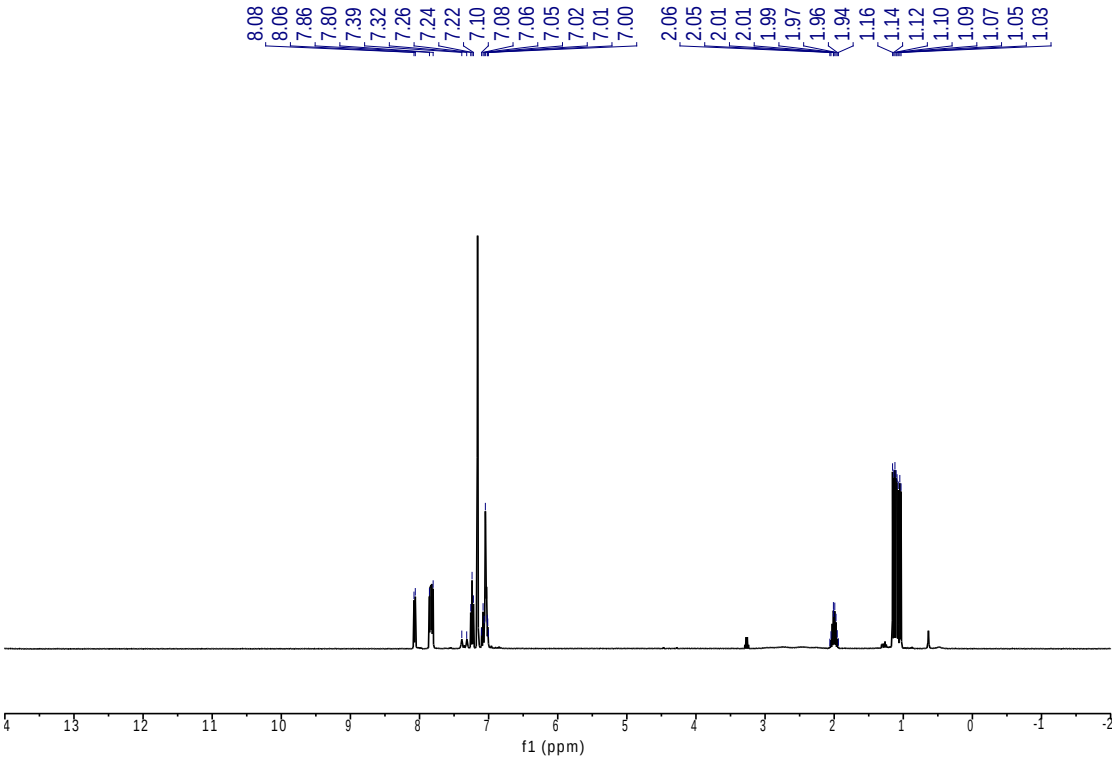


Figure 26 ^{13}C NMR spectrum of **14** (100 MHz, d_6-benzene, 298K)

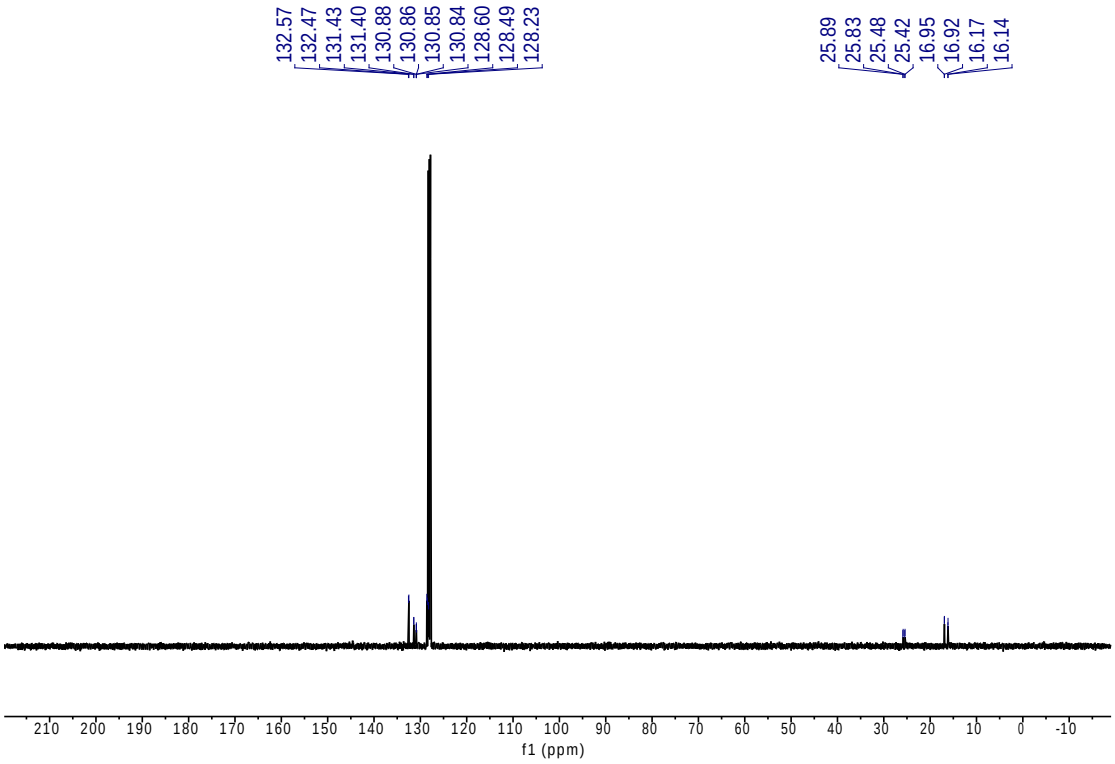


Figure 27 ^{31}P NMR spectrum of **14** (100 MHz, d_6-benzene, 298K)

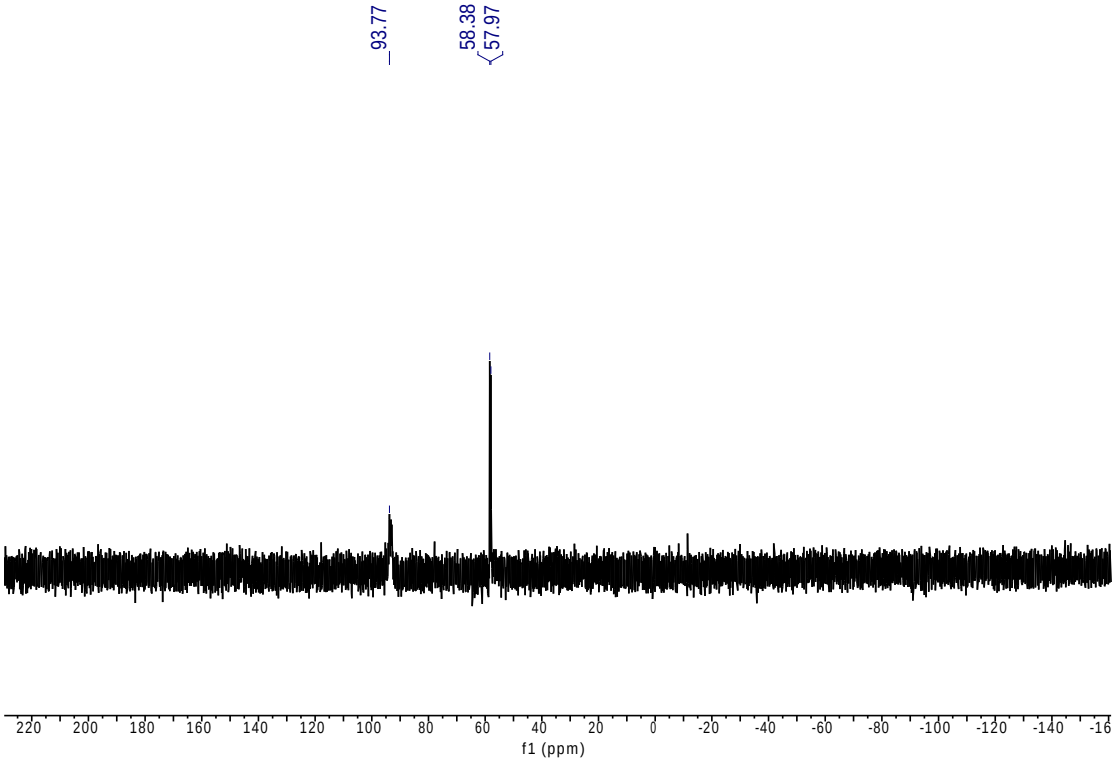


Figure 28 ^{11}B NMR spectrum of **14** (100 MHz, d_6-benzene, 298K)

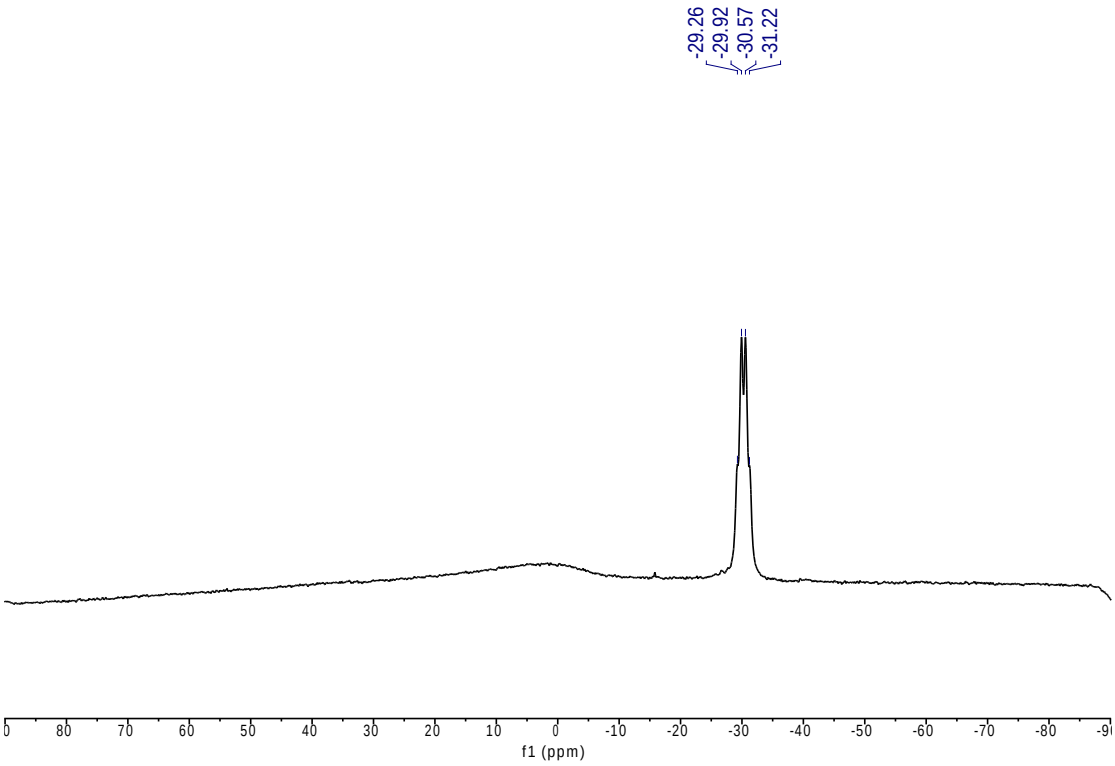


Figure 29 ^{1}H NMR spectrum of **15** (100 MHz, d_6-benzene, 298K)

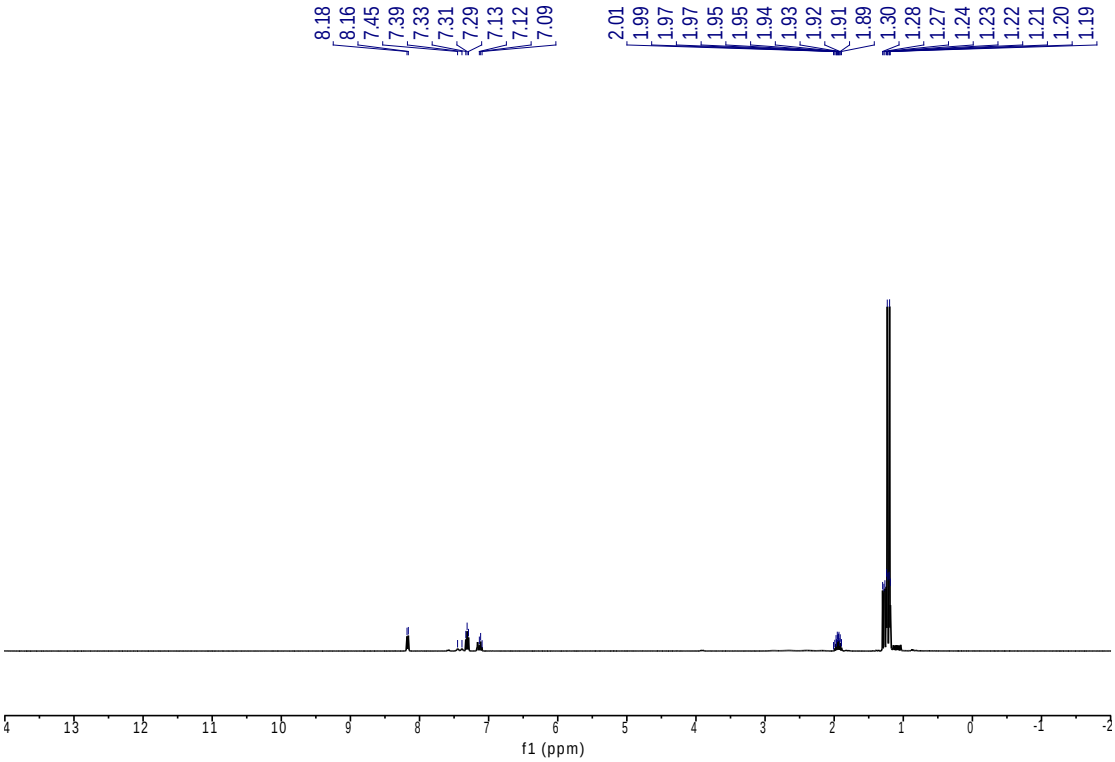


Figure 30 ^{13}C NMR spectrum of **15** (100 MHz, d_6-benzene, 298K)

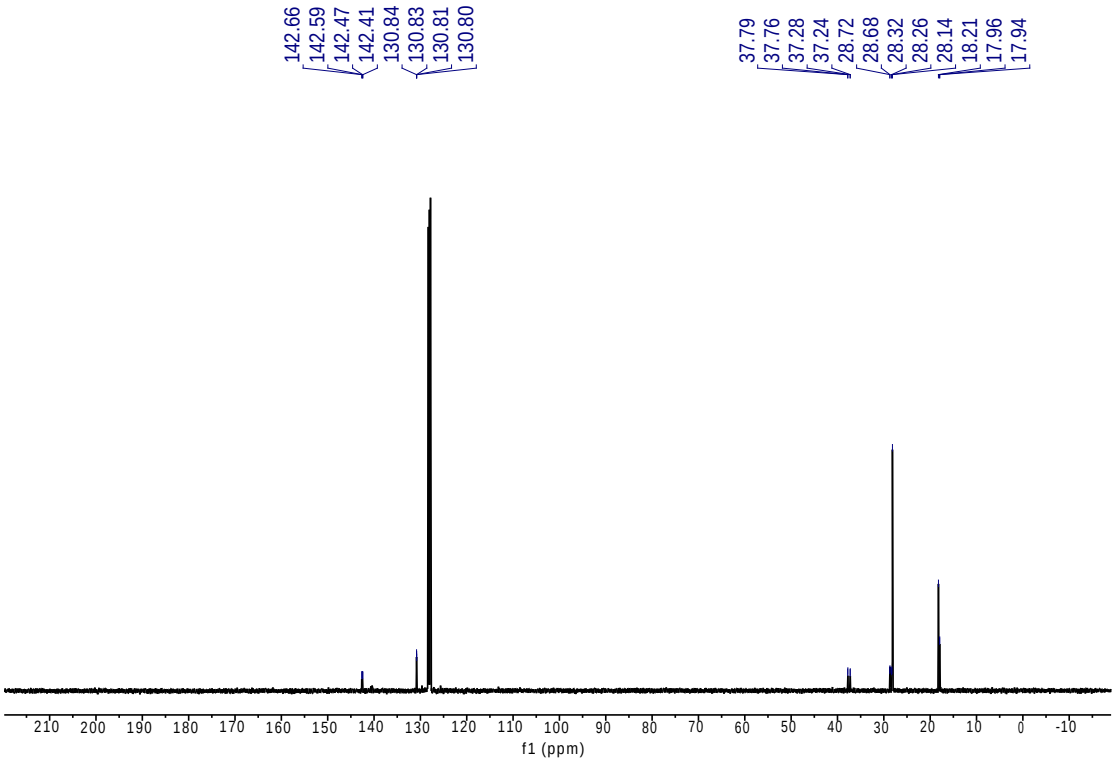


Figure 31 ^{31}P NMR spectrum of **15** (100 MHz, d_6-benzene, 298K)

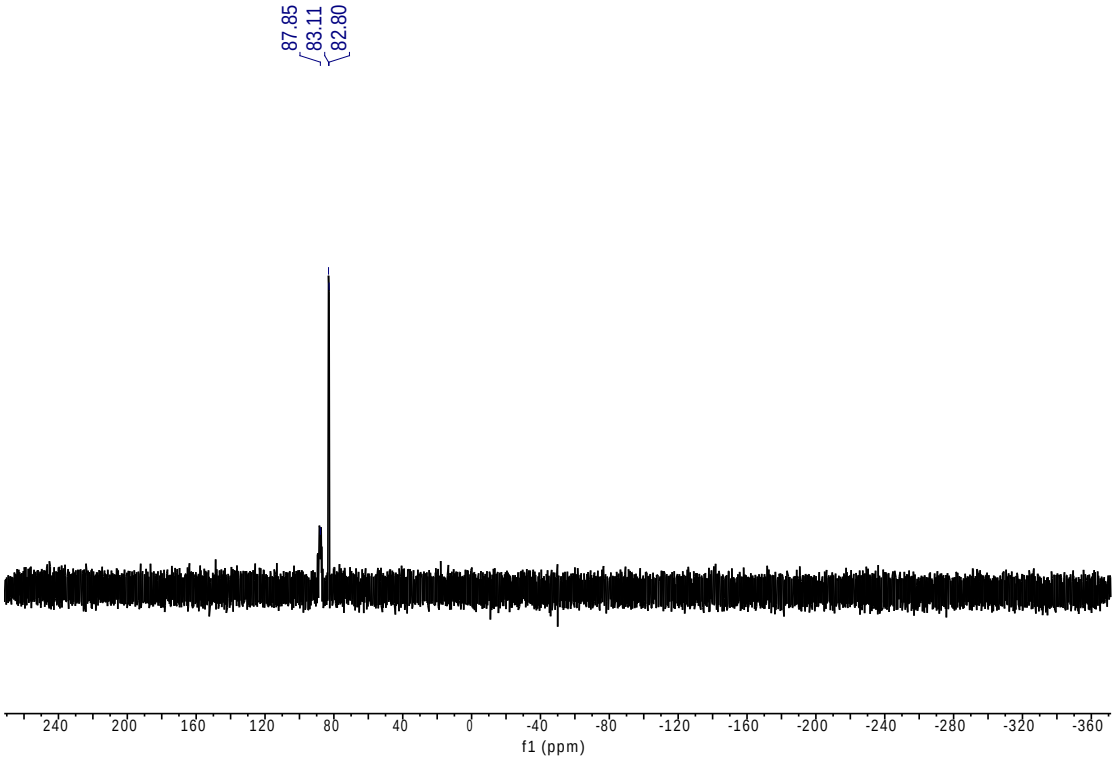
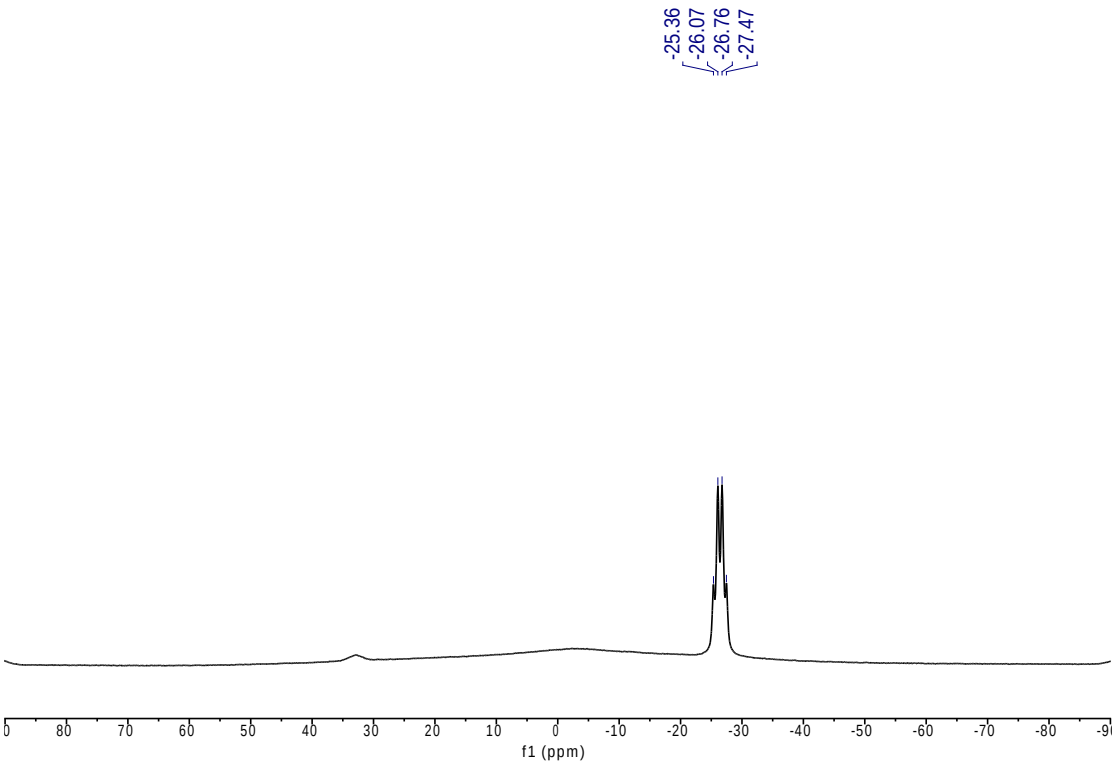


Figure 32 ^{11}B NMR spectrum of **15** (100 MHz, d_6-benzene, 298K)



2. Crystallographic Details:

Table 1 Geometric Parameters for Compounds 8-10, 11, 13-15

Coumpound	**8**	**9**	**10**	**11**
Emperical Formula	$C_{22}H_{40}BNP_2$	$C_{20}H_{44}BNP_2$	$C_{22}H_{46}BNP_2$	$C_{26}H_{32}BNP_2$
Crystal System	Monoclinic	Triclinic	Triclinic	Monoclinic
Space Group	C2/c	P-1	P-1	P2(1)/n
a/ Å	16.6512(13)	8.8873(4)	8.3977(8)	17.1910(12)
b/ Å	8.7599(5)	9.6687(5)	9.8974(8)	9.0756(8)
c/ Å	32.962(2)	15.5632(8)	17.1444(14)	17.2932(13)
α/ °	90	85.608(2)	86.080(5)	90
β/ °	97.279(6)	88.203(2)	78.918(4)	111.777(4)
γ/ °	90	65.678(2)	65.594(4)	90
V/ $Å^3$	4769.2(6)	1215.05(10)	1273.34(19)	2505.3
Z	8	2	2	4
T/ K	150	150	150	150
D_c/ $g.cm^{-3}$	1.090	1.015	1.036	1.143
Total data	5453	5573	5791	5713
Unique data	3775	4675	4840	3823
R_{int}	0.0699	0.0297	0.0348	0.0915
$R_1[F^2>2\ \sigma(F^2)]$	0.0457(3775)	0.0348(4675)	0.0363(4840)	0.0463(3823)
wR2 (all data)	0.1148(5453)	0.1319(5573)	0.1316(5791)	0.1061(5713)
GoF	1.013	1.009	0.985	1.009
min/ max/ $eÅ^{-3}$	0.396/-0.340	0.354/-0.295	0.0329/-0.267	0.396/ -0.340

	13	**14**	**15**
Emperical Formula	$C_{26}H_{38}BNP_2$	$C_{26}H_{32}BNP_2$	$C_{22}H_{40}BNP_2$
Crystal System	Monoclinic	Triclinic	Monoclinic
Space Group	P2(1)/n	P-1	P21/c
a/ Å	8.9183(5)	10.3495(7)	9.7047(7)
b/ Å	16.6266(8)	15.2609(11)	16.3976(9)
c/ Å	17.4581(10)	16.9887(12)	15.2998(10)
α/ °	90	108.455(3)	90
β/ °	91.698(2)	104.696(3)	105.659(4)
γ/ °	90	92.445(4)	90
V/ $Å^3$	2587.6(2)	2439.8(3)	2344.4(3)
Z	4	2	4
T/ K	150	150	150
D_c/ $g.cm^{-3}$	1.123	1.174	1.109
Total data	5962	11157	5738
Unique data	4443	9548	3064
R_{int}	0.0494	0.0380	
$R_1[F^2>2\ \sigma(F^2)]$	0.0418(4443)	0.0395(9548)	0.0846(3064)
wR2 (all data)	0.1102(5962)	0.1455(11157)	0.1711(5738)
GoF	1.010	1.148	1.034
min/max/$eÅ^{-3}$	0.422/-0.267	0.468/-0.359	0.750/-0.579