

**Carbon-Carbon Bond Formation between the Adjacent Alkenyl
Ligands: η^3 -Allyl Ir(III) and η^4 -Butadiene Ir(I) Complexes from *cis*-
Bis(Alkenyl) Ir(III) Complex**

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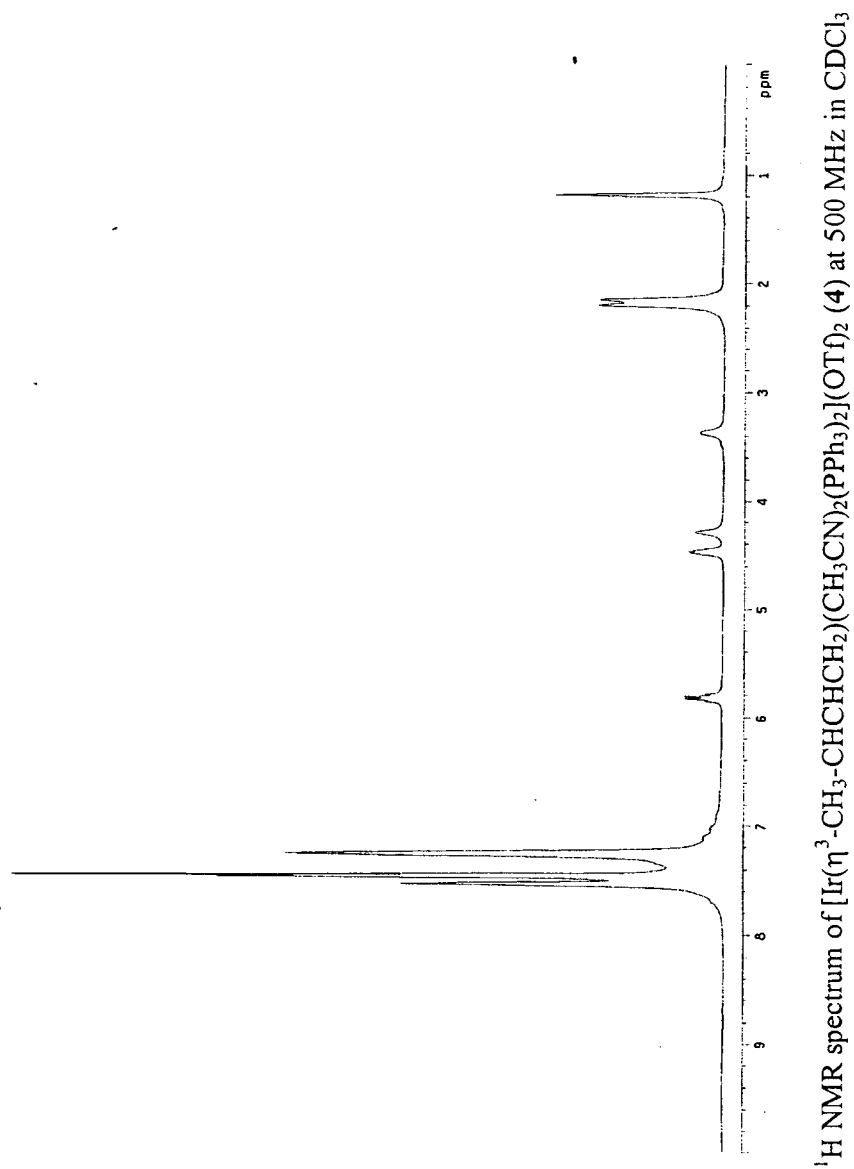
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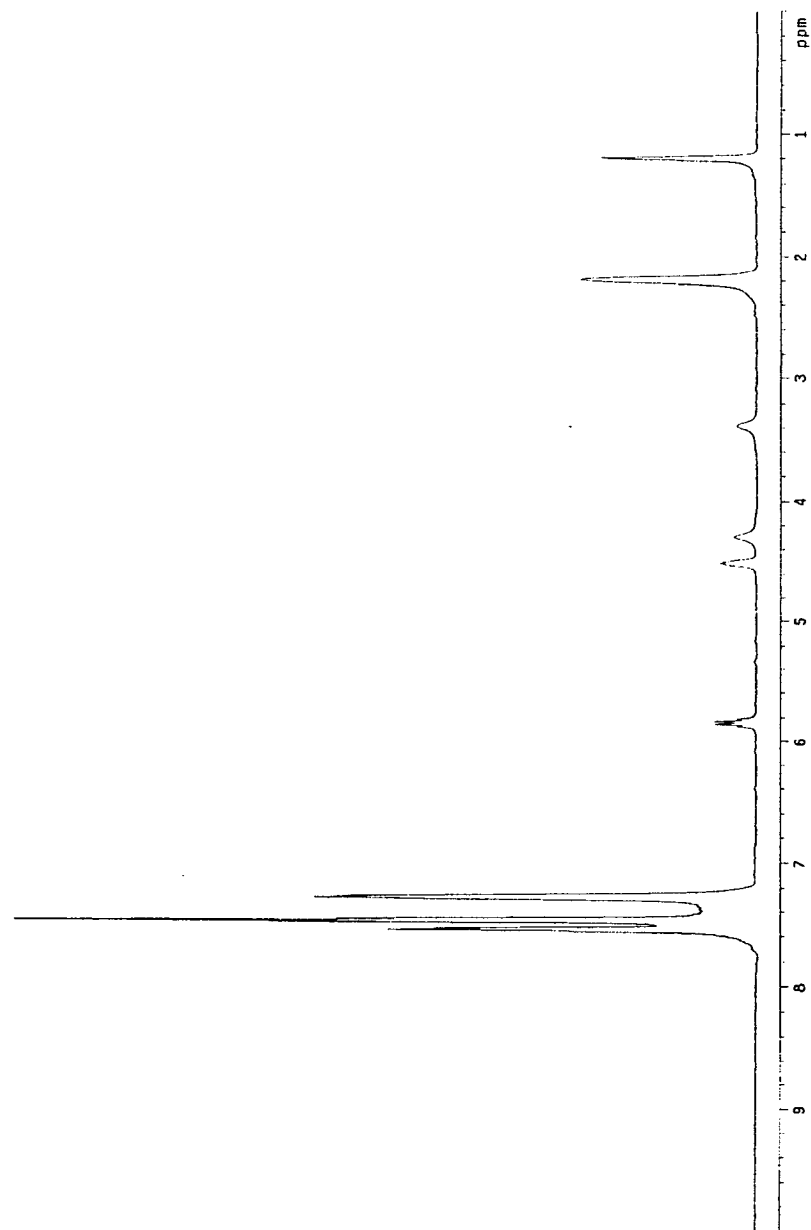
SUPPORTING INFORMATION

Table of Contents

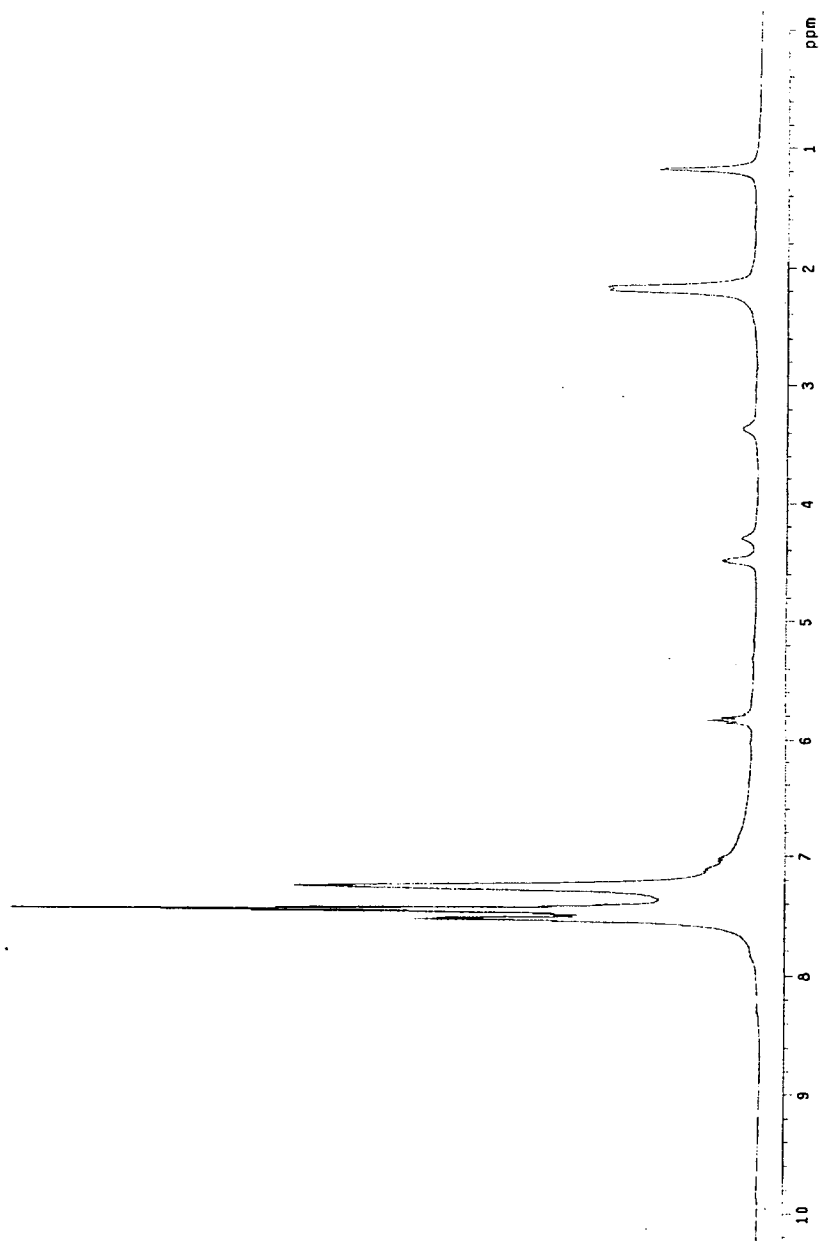
^1H NMR spectrum of 4 at 500 MHz in CDCl_3	S3
^1H NMR spectrum of 4-d_1 at 500 MHz in CDCl_3	S4
^1H NMR spectrum of 4-d_2 at 500 MHz in CDCl_3	S5
^{13}C NMR spectrum of 4 at 125.7 MHz in CDCl_3	S6
^1H , ^{13}C -2D HETCOR spectrum of 4 at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3 ..	S7
^1H NMR spectrum of 5 at 500 MHz in CDCl_3	S8
^{13}C NMR spectrum of 5 at 125.7 MHz in CDCl_3	S9
^{31}P NMR spectrum of 5 at 81 MHz in CDCl_3	S10
^1H NMR spectrum of 6 at 500 MHz in CDCl_3	S11
^{13}C NMR spectrum of 6 at 125.7 MHz in CDCl_3	S12
^1H , ^{13}C -2D HETCOR spectrum of 6 at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3 ..	S13

^{31}P NMR spectrum of 6 at 121.3 MHz in CDCl_3	S14
^1H NMR spectrum of 8 at 500 MHz in CDCl_3	S15
^{13}C NMR spectrum of 8 at 125.7 MHz in CDCl_3	S16
^1H , ^{13}C -2D HETCOR spectrum of 8 at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3 ..	S17
^1H NMR spectrum of 10a at 500 MHz in CDCl_3	S18
^1H NMR spectrum of 10a-<i>d</i>₁ at 500 MHz in CDCl_3	S19
^{13}C NMR spectrum of 10a at 125.7 MHz in CDCl_3	S20
^1H , ^{13}C -2D HETCOR spectrum of 10a at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3	S21

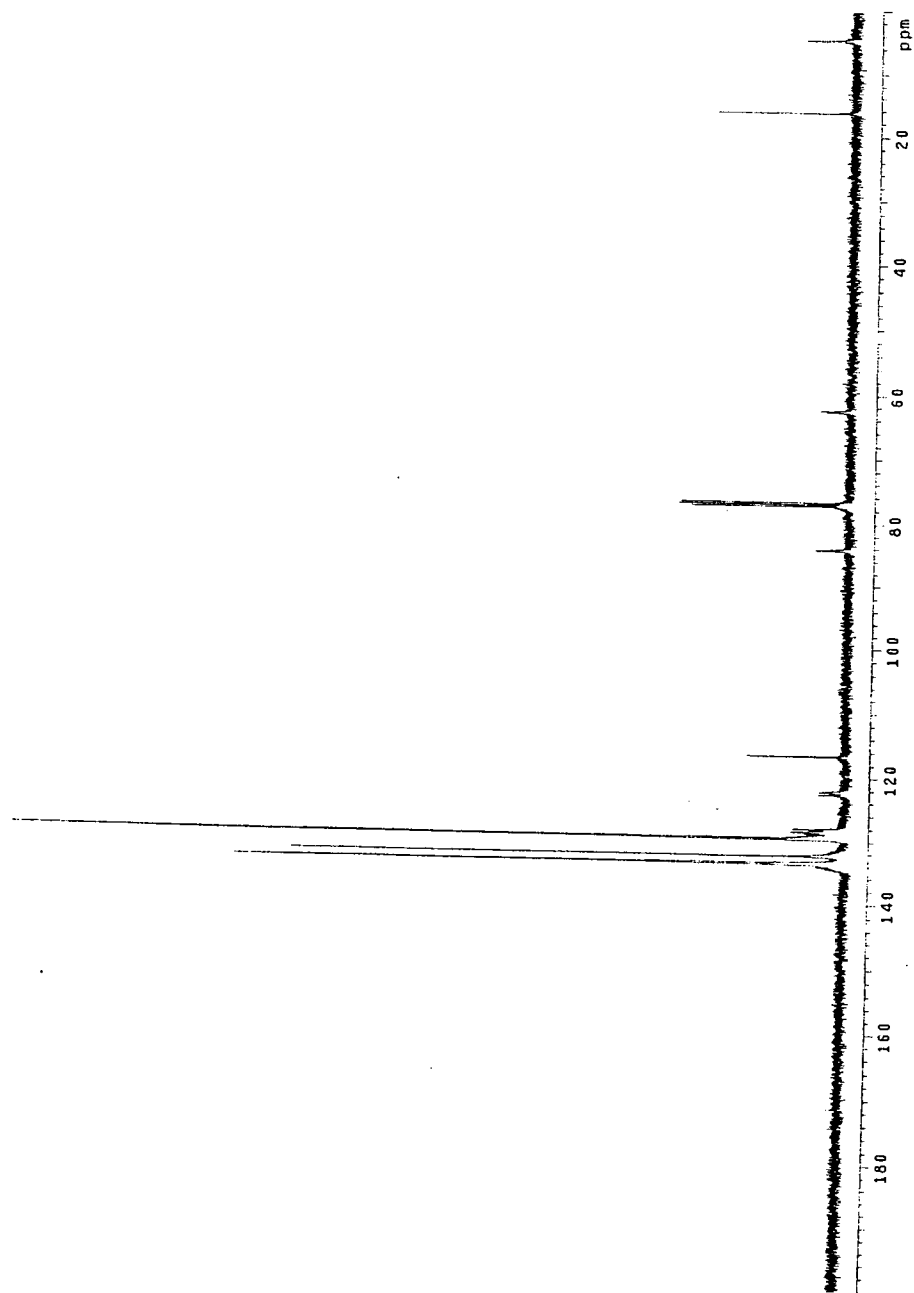




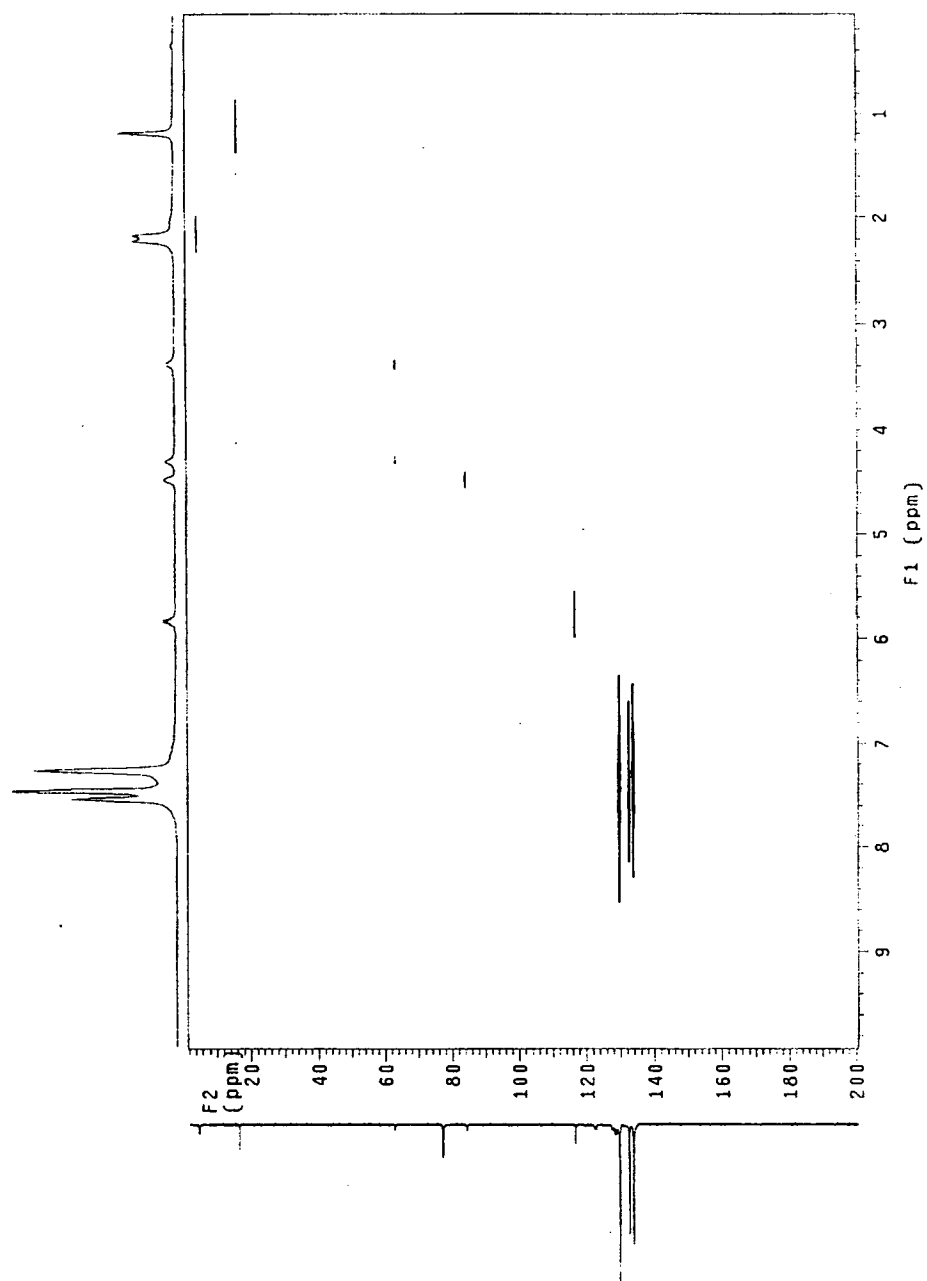
^1H NMR spectrum of $[\text{Ir}(\eta^3\text{-CH}_2\text{D-CHCHCH}_2)(\text{CH}_3\text{CN})_2(\text{PPh}_3)_2](\text{OTf})_2$ (**4-d₁**) at 500 MHz in CDCl_3



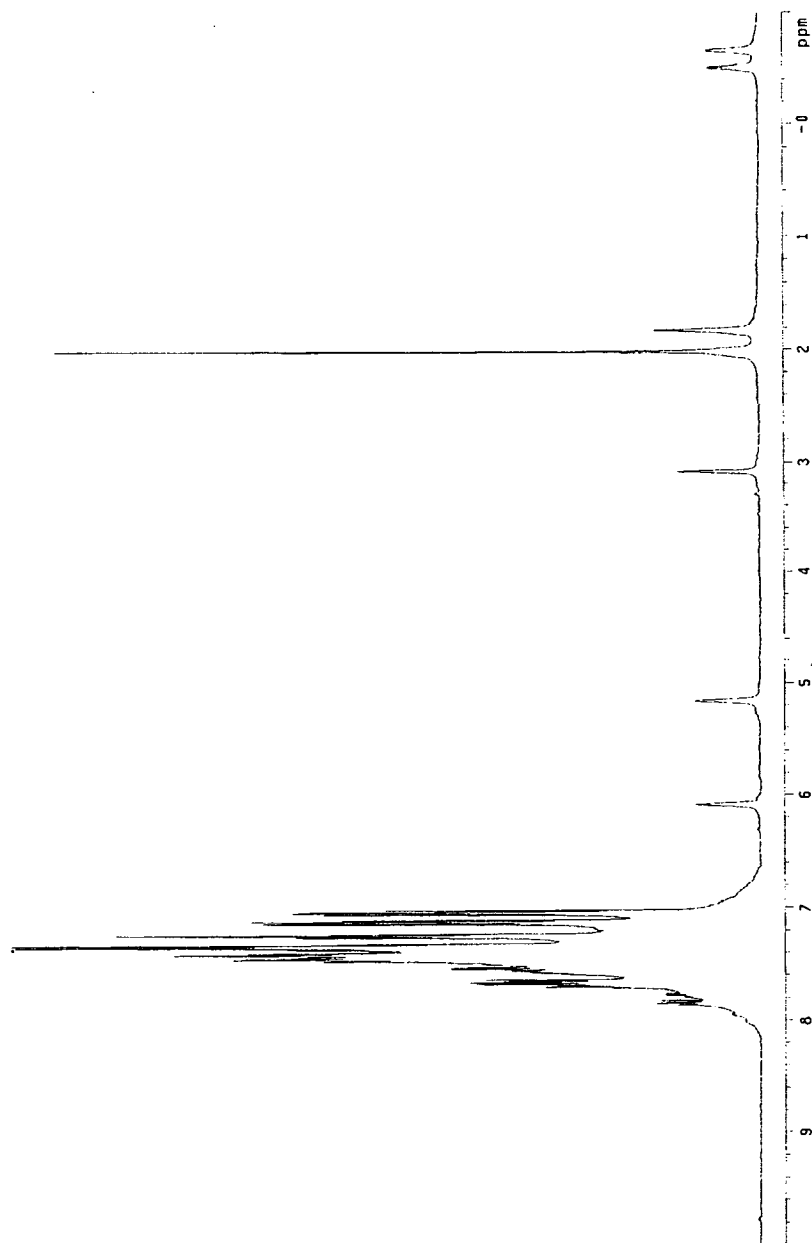
^1H NMR spectrum of $[\text{Ir}(\eta^3\text{-CH}_2\text{D-CHCHCHD})(\text{CH}_3\text{CN})_2(\text{PPh}_3)_2](\text{OTf})_2$ (**4-d₂**) at 500 MHz in CDCl_3



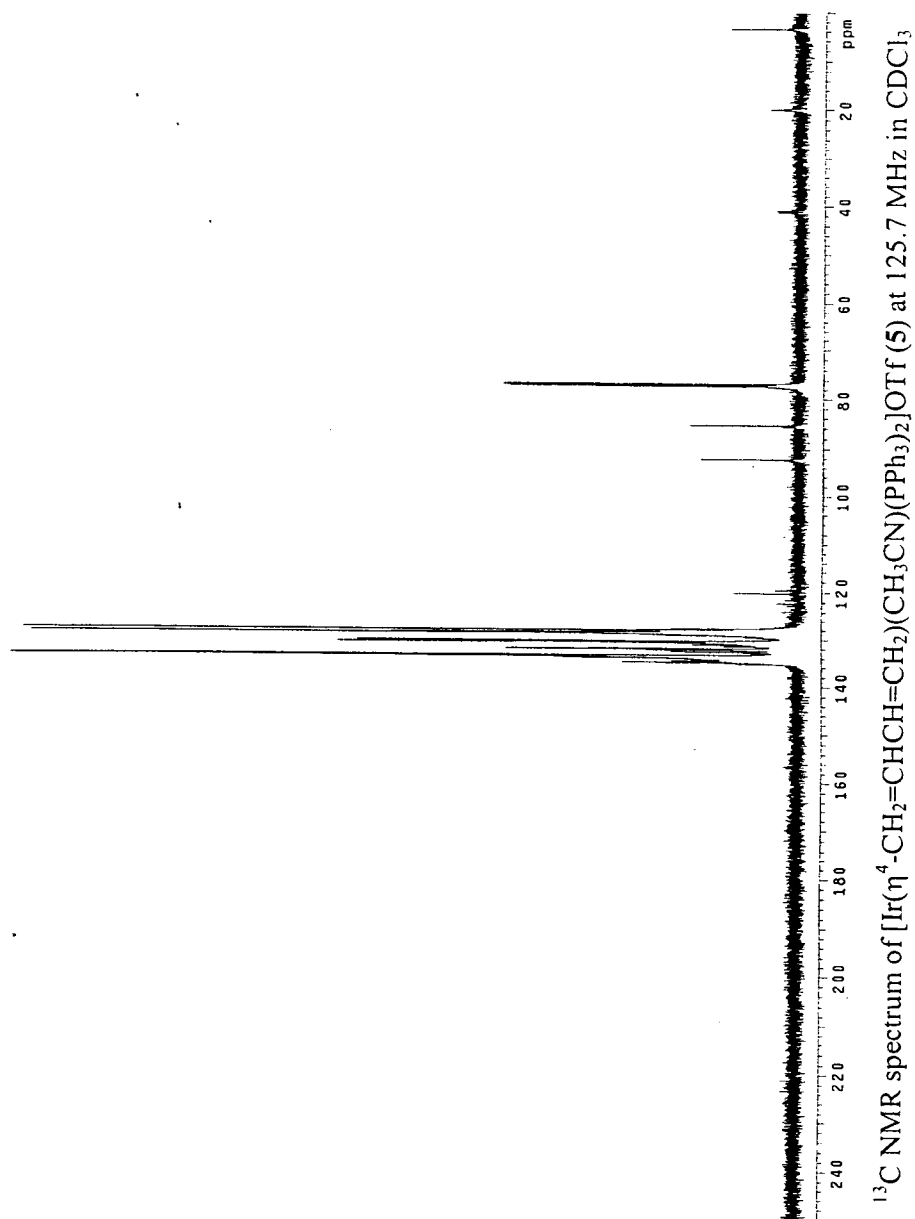
^{13}C NMR spectrum of $[\text{Ir}(\eta^3\text{-CH}_3\text{-CHCHCH}_2)(\text{CH}_3\text{CN})_2(\text{PPh}_3)_2](\text{OTf})_2$ (**4**) at 125.7 MHz in CDCl_3

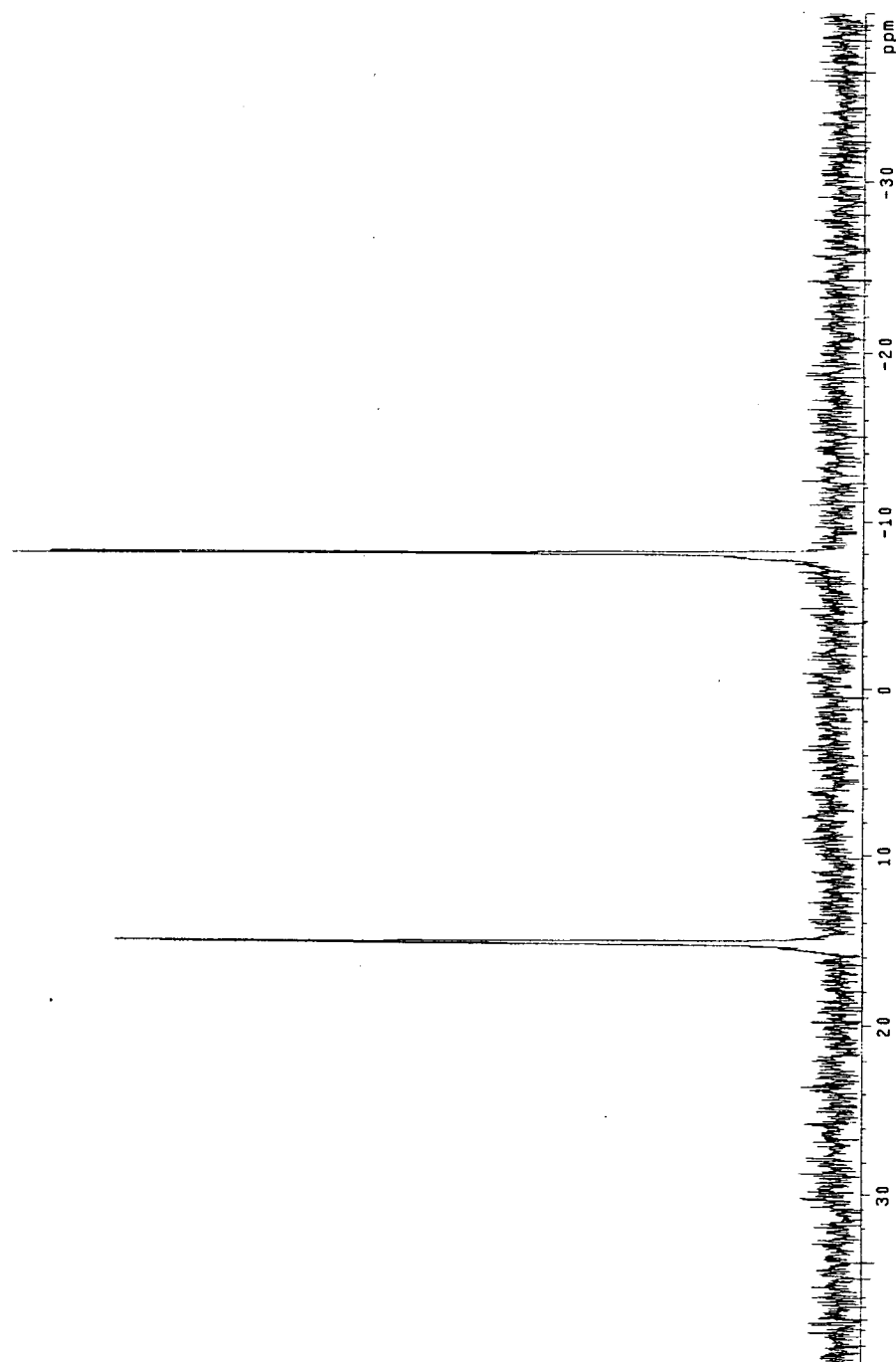


^1H , ^{13}C -2D HETCOR spectrum of $[\text{Ir}(\eta^3\text{-CH}_3\text{-CHCHCH}_2)(\text{CH}_3\text{CN})_2(\text{PPh}_3)_2](\text{OTf})_2$ (**4**) at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3

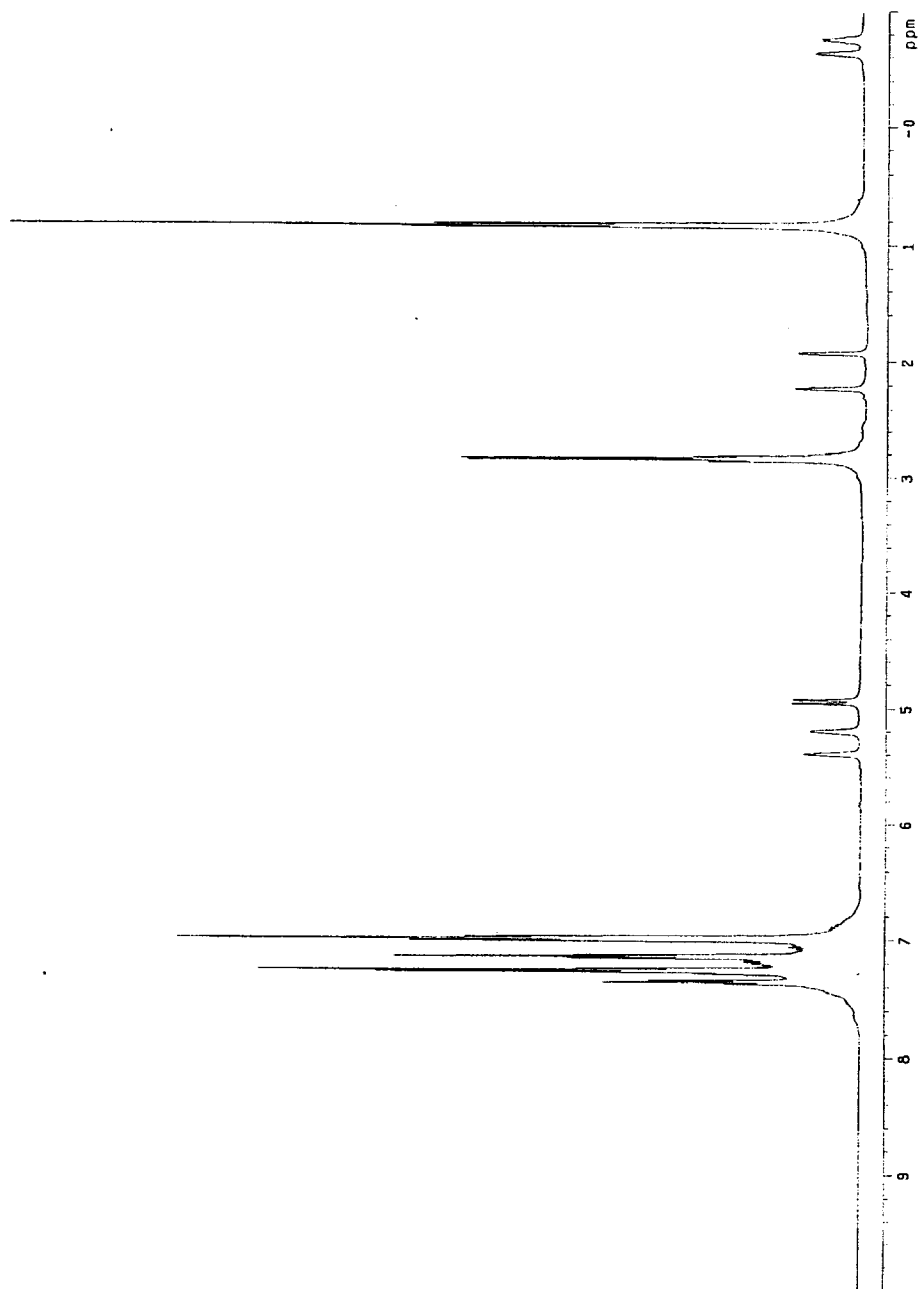


^1H NMR spectrum of $[\text{Ir}(\eta^4\text{-CH}_2\text{=CHCH=CH}_2)(\text{CH}_3\text{CN})(\text{PPh}_3)_2]\text{OTf}$ (5) at 500 MHz in CDCl_3

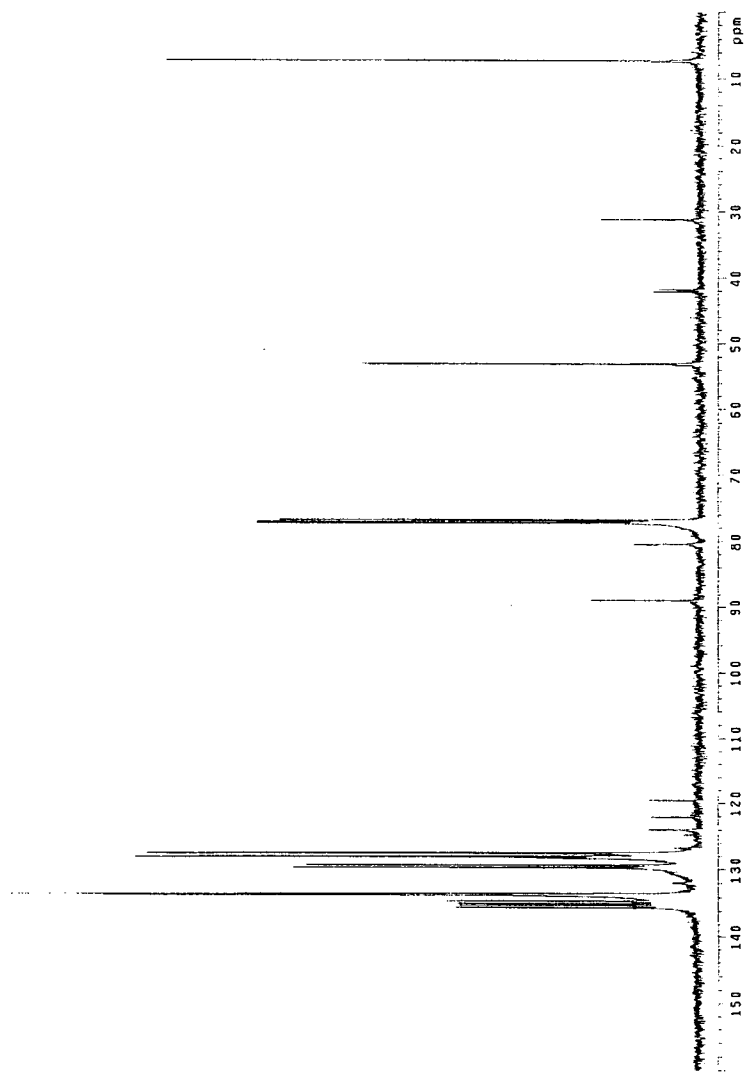




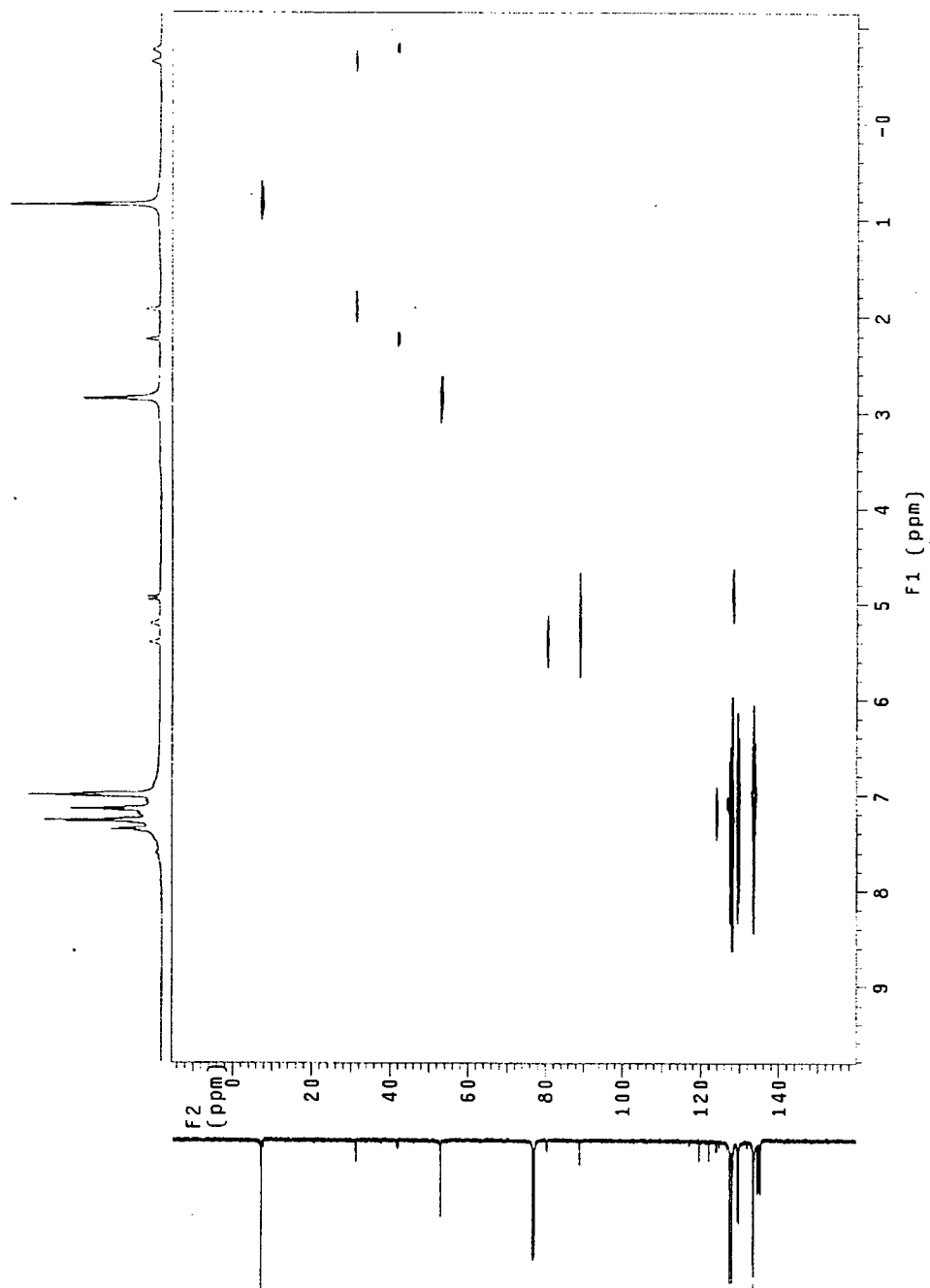
^{31}P NMR spectrum of $[\text{Ir}(\eta^4\text{-CH}_2\text{=CHCH=CH}_2)(\text{CH}_3\text{CN})(\text{PPh}_3)_2]\text{OTf}(\mathbf{5})$ at 81 MHz in CDCl_3



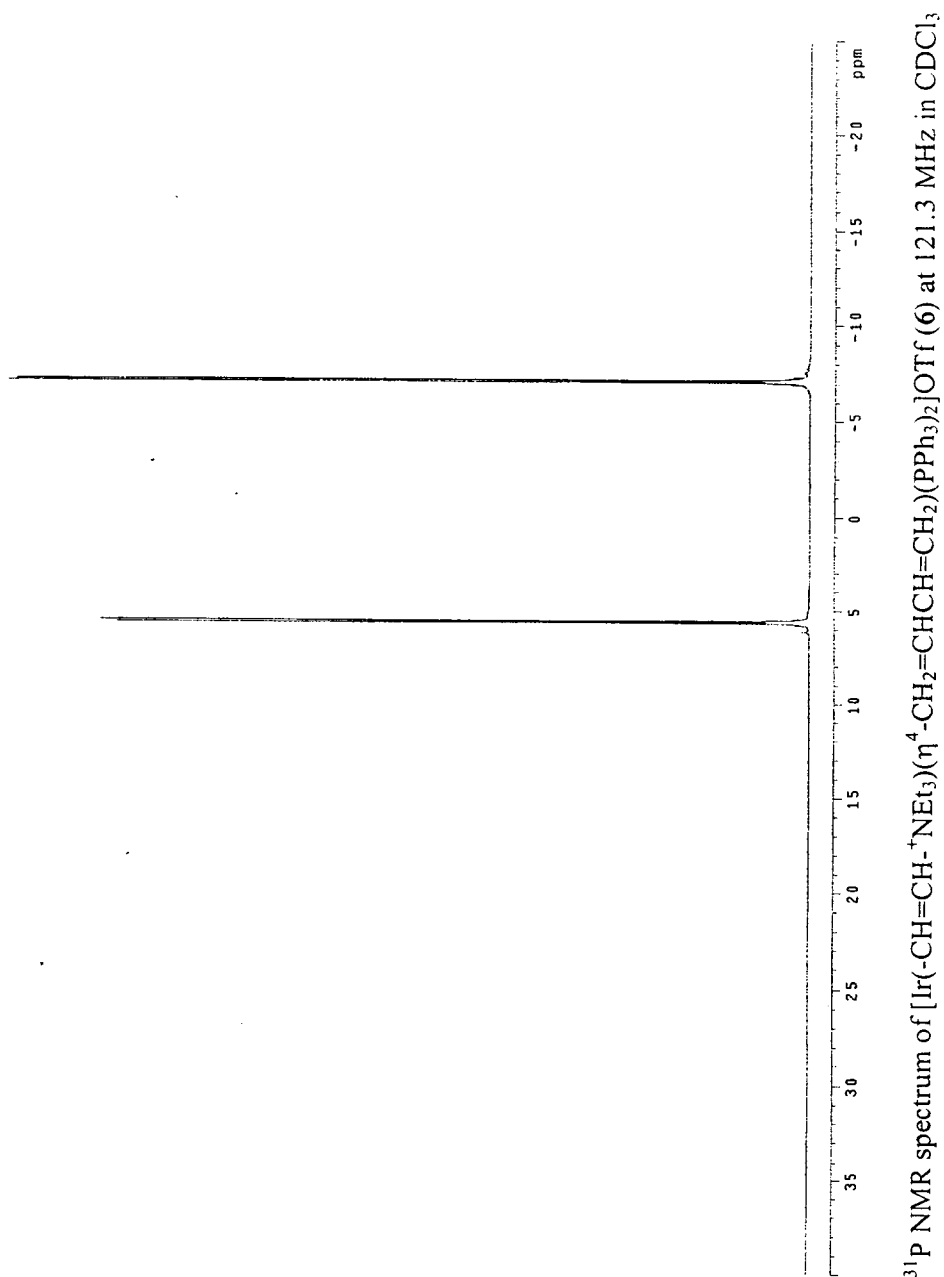
^1H NMR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-\text{NEt}_3)(\eta^4-\text{CH}_2=\text{CHCH}=\text{CH}_2)(\text{PPh}_3)_2]\text{OTf}$ (6) at 500 MHz in CDCl_3

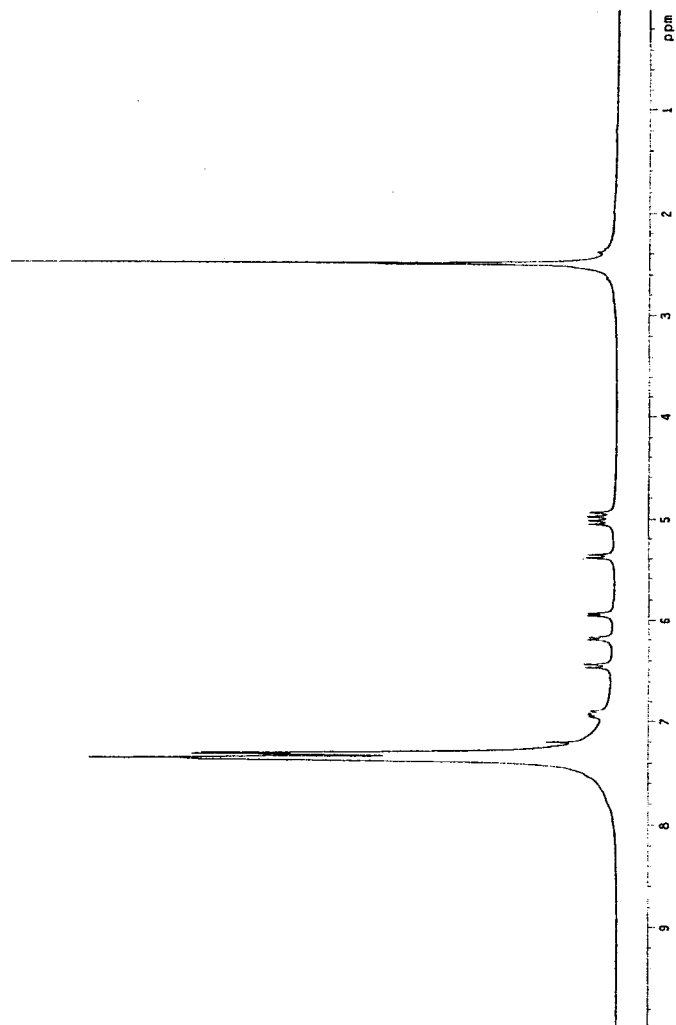


^{13}C NMR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-\text{CH}-\text{NEt}_3)(\eta^4-\text{CH}_2=\text{CHCH}=\text{CH}_2)(\text{PPh}_3)_2]\text{OTf}$ (6) at 125.7 MHz in CDCl_3

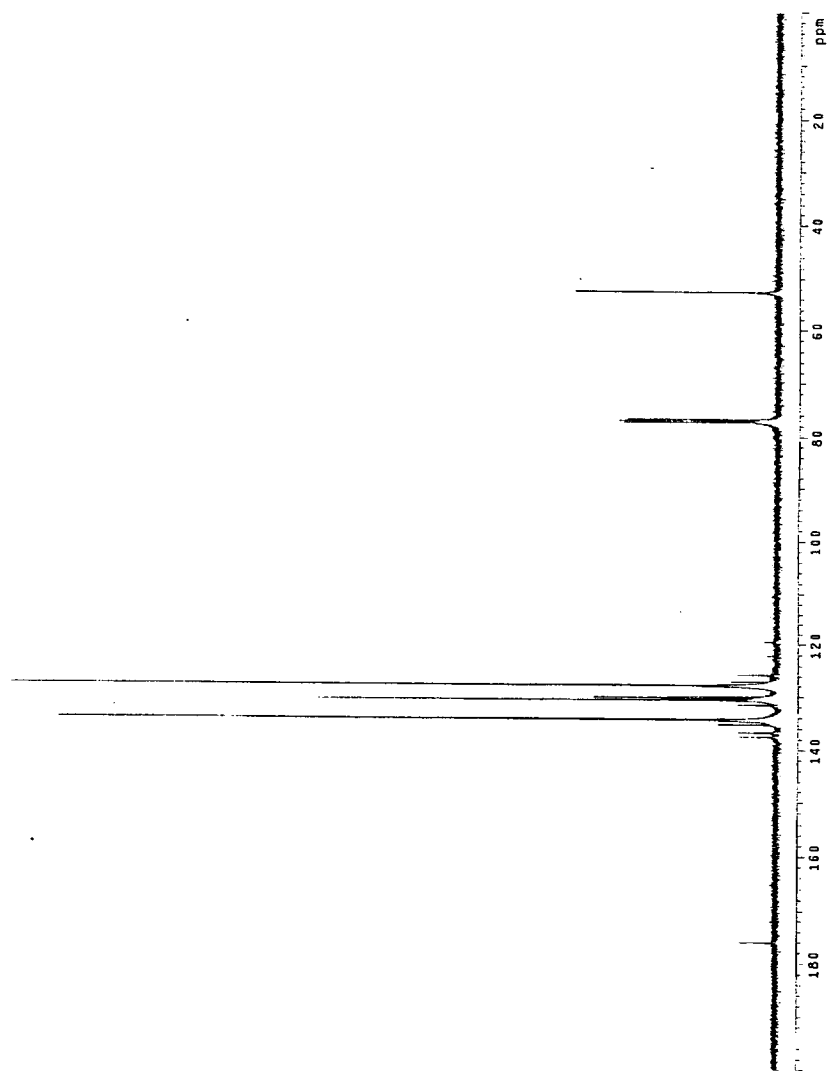


^1H , ^{13}C -2D HETCOR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-\text{CH}-^+\text{NEt}_3)(\eta^4-\text{CH}_2=\text{CHCH}=\text{CH}_2)(\text{PPh}_3)_2]\text{OTf}$ (**6**) at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3

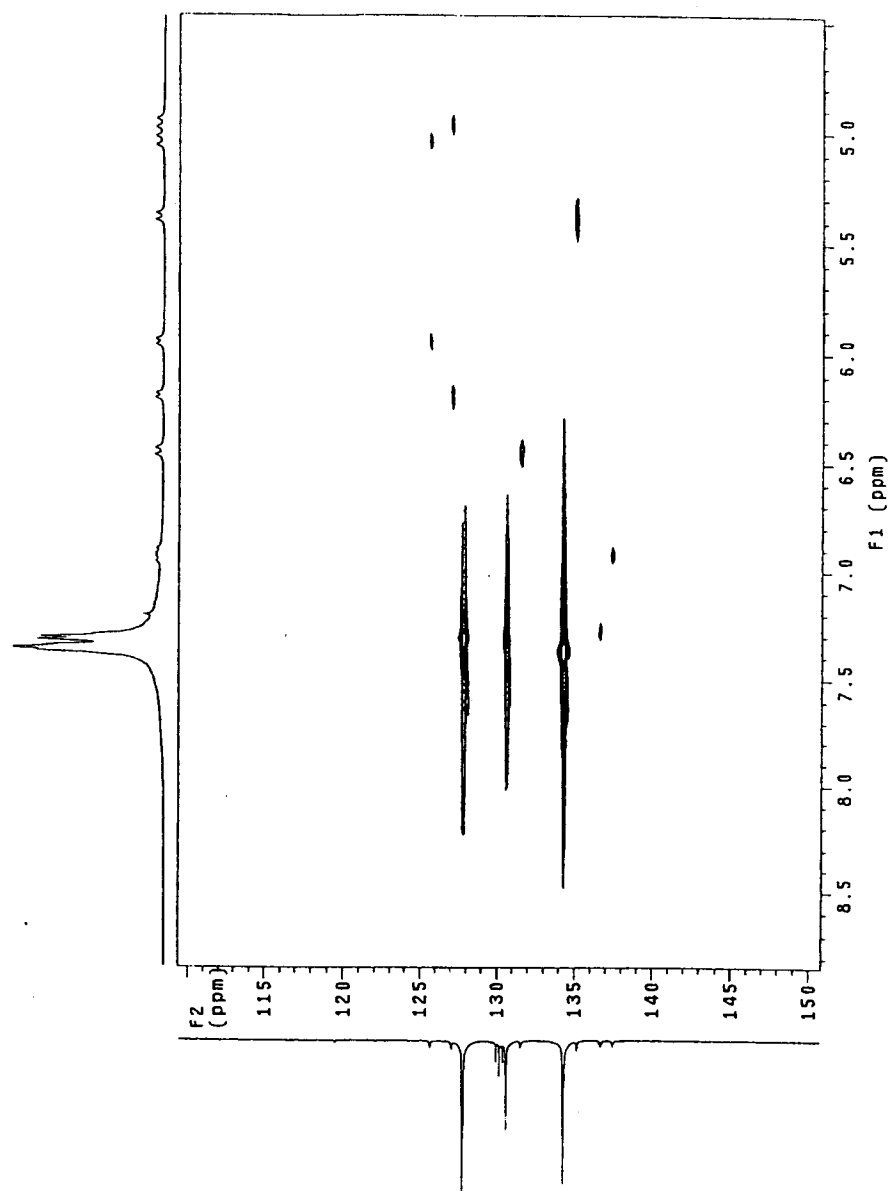




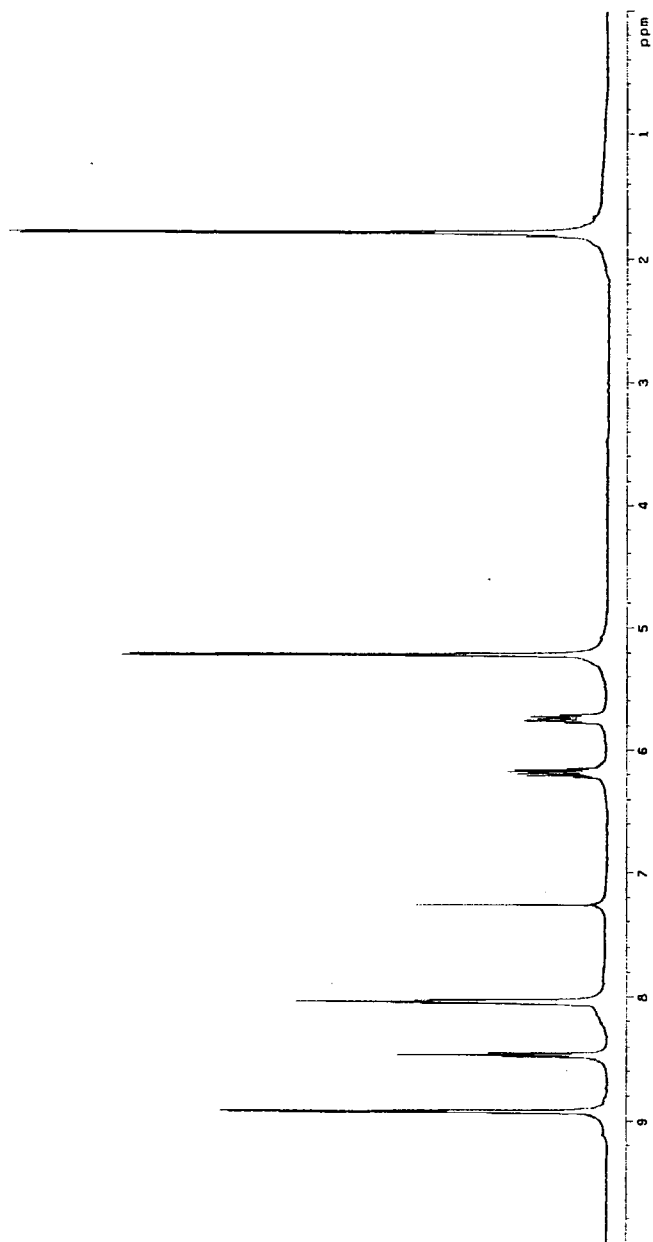
^1H NMR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-\text{CH}_2-\text{NMe}_3)(-\text{CH}=\text{CH}_2)_2(\text{CO})(\text{PPh}_3)_2]\text{OTf}$ (8) at 500 MHz in CDCl_3



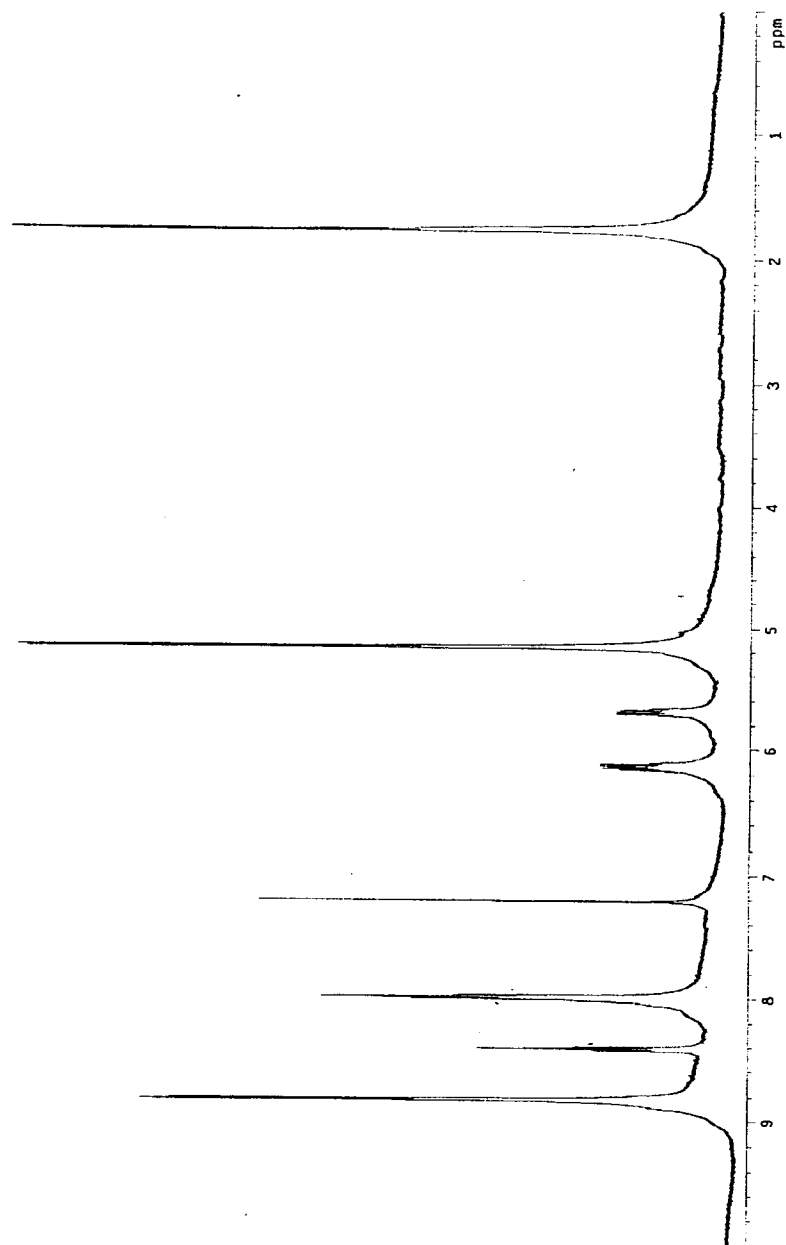
^{13}C NMR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-^+\text{NMe}_3)(-\text{CH}=\text{CH}_2)_2(\text{CO})(\text{PPh}_3)_2]\text{OTf}$ (**8**) at 125.7 MHz in CDCl_3



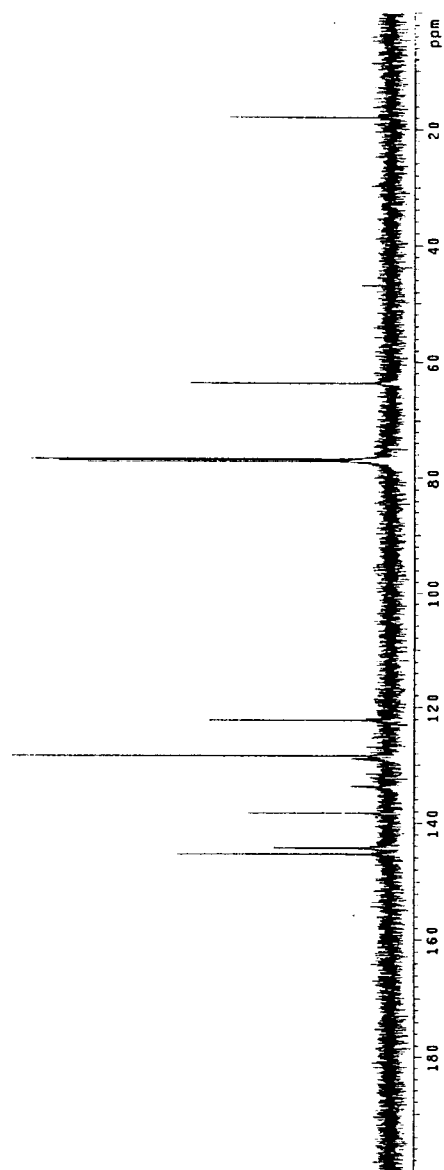
^1H , ^{13}C -2D HETCOR spectrum of $[\text{Ir}(-\text{CH}=\text{CH}-\text{NMe}_3)(-\text{CH}=\text{CH}_2)_2(\text{CO})(\text{PPh}_3)_2]\text{OTf}$ (**8**) at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3



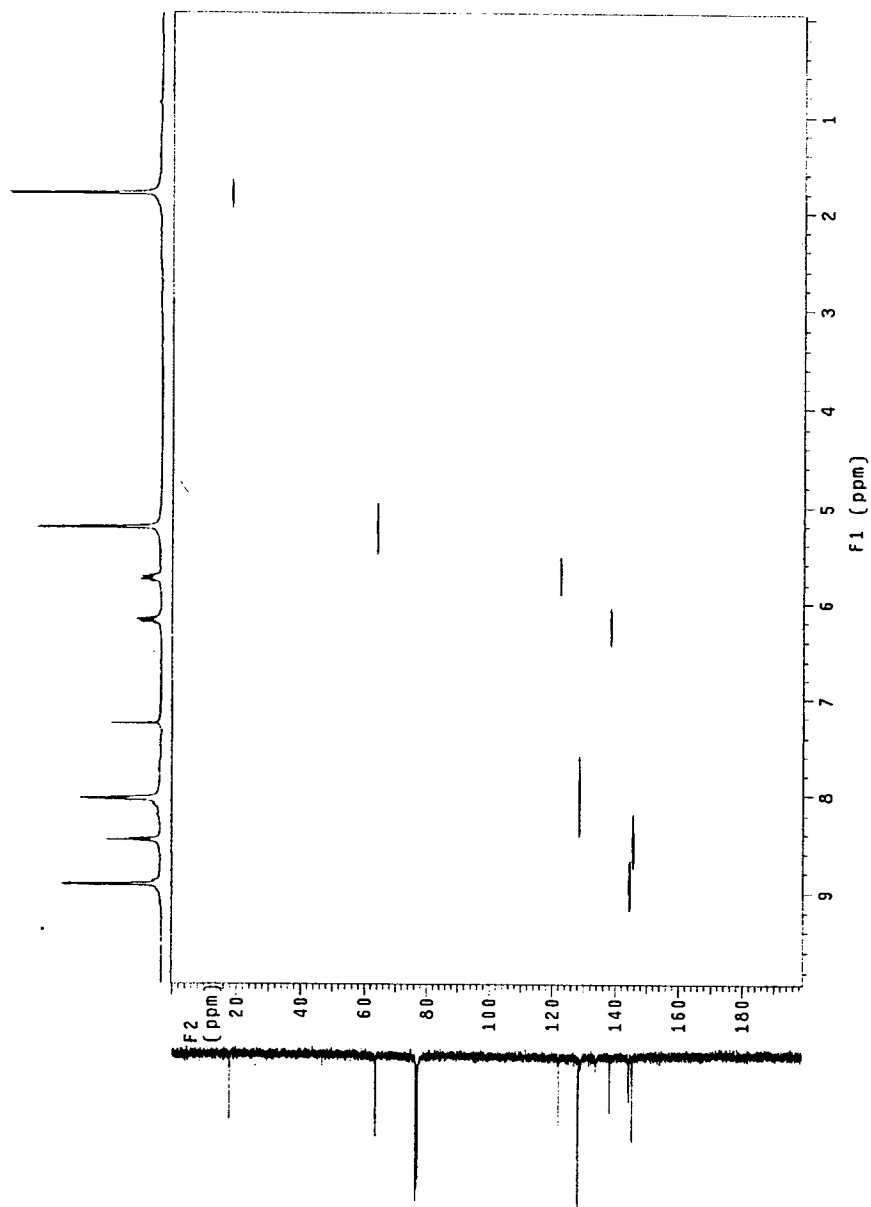
^1H NMR spectrum of $[\text{trans-CH}_3\text{CH=CHCH}_2\text{-NC}_5\text{H}_5]\text{OTf}$ (10a) at 500 MHz in CDCl_3



^1H NMR spectrum of $[\text{trans-CH}_2\text{DCH=CHCH}_2\text{NC}_5\text{H}_5]\text{OTf}$ (10a-d₁) at 500 MHz in CDCl_3



^{13}C NMR spectrum of $[\text{trans-CH}_3\text{CH=CHCH}_2\text{-NC}_5\text{H}_5]\text{OTf}$ (10a) at 125.7 MHz in CDCl_3



^1H , ^{13}C -2D HETCOR spectrum of [*trans*- $\text{CH}_3\text{CH}=\text{CHCH}_2\text{-NC}_5\text{H}_5$]OTf (**10a**) at ^1H 500 MHz, ^{13}C 125.7 MHz in CDCl_3