Supplementary Materials

Table S1: Crystal data and structure refinement for complex **1**

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Empirical formula	$C_{24}H_{23}Fe_2NO_6P_2$
Formula weight	595.07
Temperature	100 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbcn
Unit cell dimension	a = 27.4929(5)Å
	b= 13.2772(2) Å
	c= 13.9398(2) Å
Volume	5088.43(14) Å^3
Z, Calculated density	8, 1.554 Mg/m^3
Absorption coefficient	1.306 mm^{-1}
F(000)	2432
Crystal size	0.52 x 0.30 x 0.28 mm
Crystal color	Yellow
Theta range	1.48 to 25.02 °
Limiting indices	-32 ≤ h ≤ 32, -15 ≤ k ≤ 15, -14 ≤ l ≤ 16
Reflections collected/unique	20152 / 4265 [R(int) = 0.0733]
Completeness to θ= 26.37	94.7%
Absorption correction	Semi-empirical from equivalents
Max and min. transmission	0.7113 and 0.5500
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4265 / 0 / 319
Goodness-of-fit on F^2	1.039
Final R indices [I>2σ(I)]	R1 = 0.0356, wR2 = 0.0947
R indices (all data)	R1 = 0.0403, wR2 = 0.0988
Largest diff. peak and hole	0.581 and -0.424 e.Å^{-3}

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Table S2: Crystal data and structure refinement for complex **2**

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Empirical formula	$C_{28}H_{34}Fe_2N_2O_6P_2$
Formula weight	668.21
Temperature	120 (2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	a = 9.3120(2) Å
	b = 18.7523(3) Å ß = 99.9740(10) (°)
	c = 17.9380(4) Å
Volume	3085.02(11) Å^3
Z, Calculated density	4, 1.439 Mg/m^3
Absorption coefficient	1.086 mm^{-1}
F(000)	1384
Crystal size	0.48 x 0.27 x 0.21 mm
Crystal color	Orange
Theta range	1.58 to 26.37 °
Limiting indices	$-11 \leq h \leq 11, -23 \leq k \leq 23, -22 \leq l \leq 22$
Reflections collected / unique	29959 / 6303 [R(int) = 0.1045]
Completeness to theta = 28.28	99.8%
Absorption correction	None
Max. and min. transmission	0.8040 and 0.6237
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6303 / 0 / 375
Goodness-of-fit on F^2	1.022
Final R indices [I>2σ (I)]	R1 = 0.0381, wR2 = 0.0826
R indices (all data)	R1 = 0.0645, wR2 = 0.0910
Largest diff. peak and hole	0.538 and -0.325 e. Å^{-3}

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Table S3: Crystal data and structure refinement for complex **3**

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Empirical formula	$C_{24}H_{26}BF_4Fe_2NO_7P_2$
Formula weight	700.91
Temperature	293 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	a = 8.8855 (4) Å
	b = 33.1855(18) Å ß =97.782 (4) (°)
	c = 10.2437(5) Å
Volume	2992.7(3) Å^3
Z, Calculated density	4, 1.556 Mg/m^3
Absorption coefficient	1.143 mm^{-1}
F(000)	1424
Crystal size	0.37 x 0.17 x 0.06 mm
Crystal color	Light orange
Theta range	2.85 to 26.37 °
Limiting indices	-11 ≤ h ≤ 10, -38 ≤ k ≤ 41, -12 ≤ l ≤ 12
Reflections collected / unique	25067 / 6105 [R(int) = 0.0669]
Completeness to theta = 28.28	99.9%
Absorption correction	Analytical
Max. and min. transmission	0.9346 and 0.6771
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6105 / 4 / 383
Goodness-of-fit on F^2	0.824
Final R indices [I>2σ(I)]	R1 = 0.0465, wR2 = 0.0952
R indices (all data)	R1 = 0. 1062, wR2 = 0.1070
Largest diff. peak and hole	0.456 and -0.293 e.Å^{-3}

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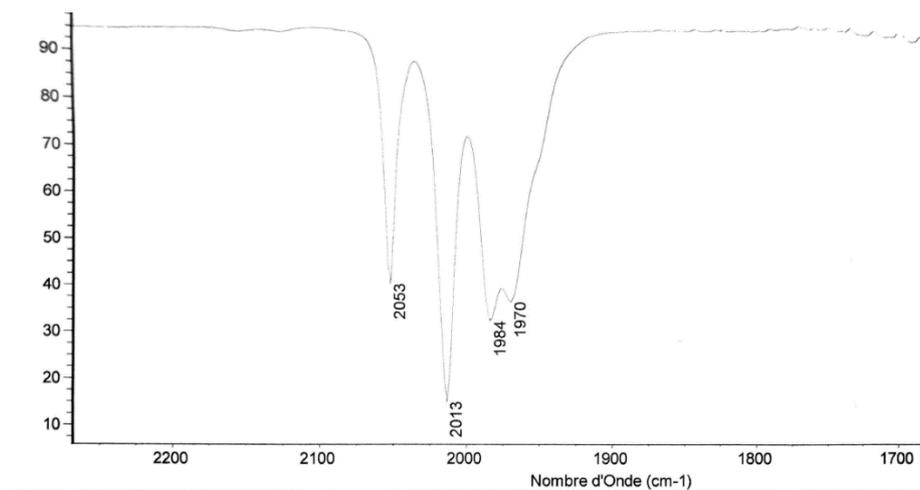
Figure S1 : IR spectrum in CH$_2$Cl$_2$ of **1**
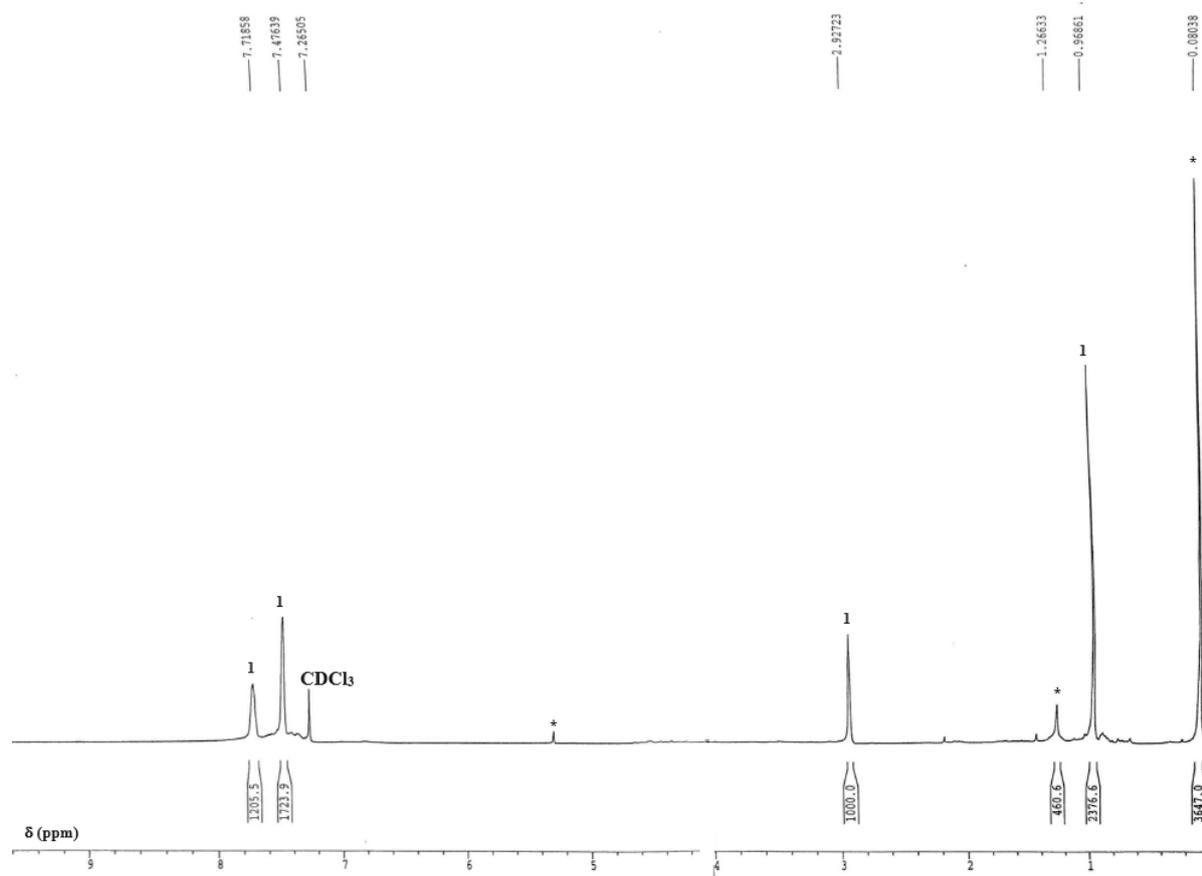
Figure S2 : ^{1}H NMR spectrum (CDCl$_3$) of **1**
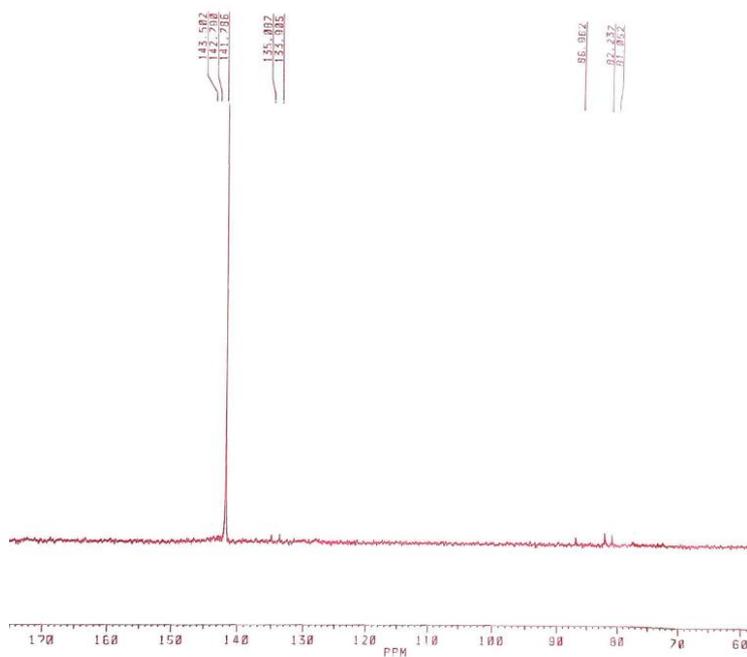
Figure S3 : ^{31}P-{^1H} NMR spectrum (CDCl$_3$) of **1**
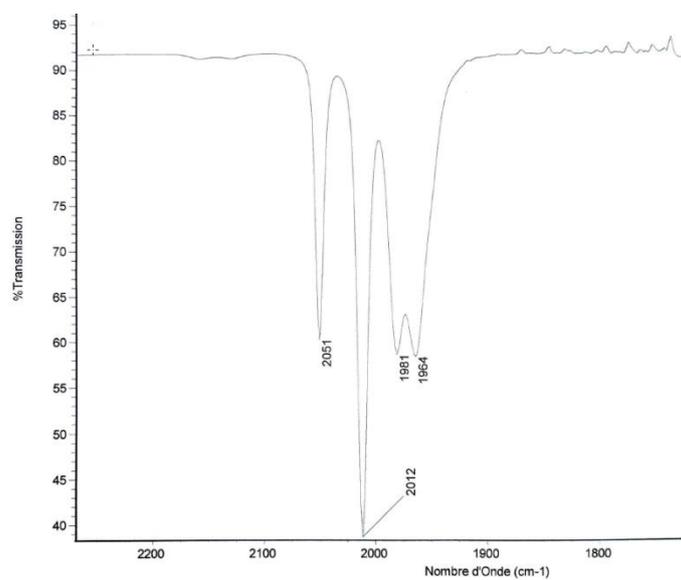
Figure S4 : IR spectrum in CH$_2$Cl$_2$ of **2-anti**
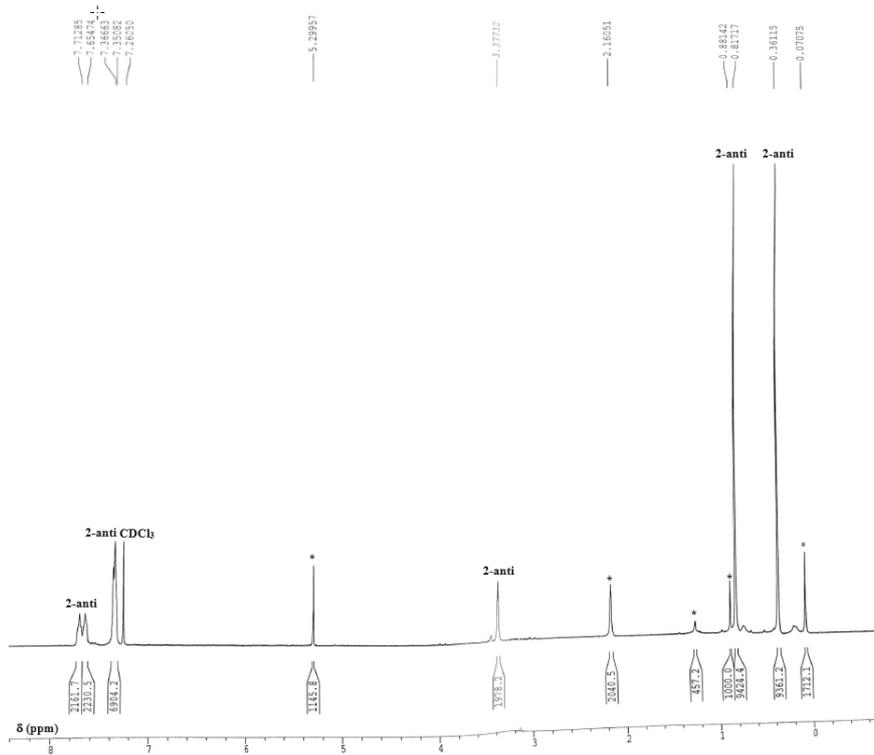
**Figure S5** : ¹H NMR spectrum (CDCl₃) of **2-anti**
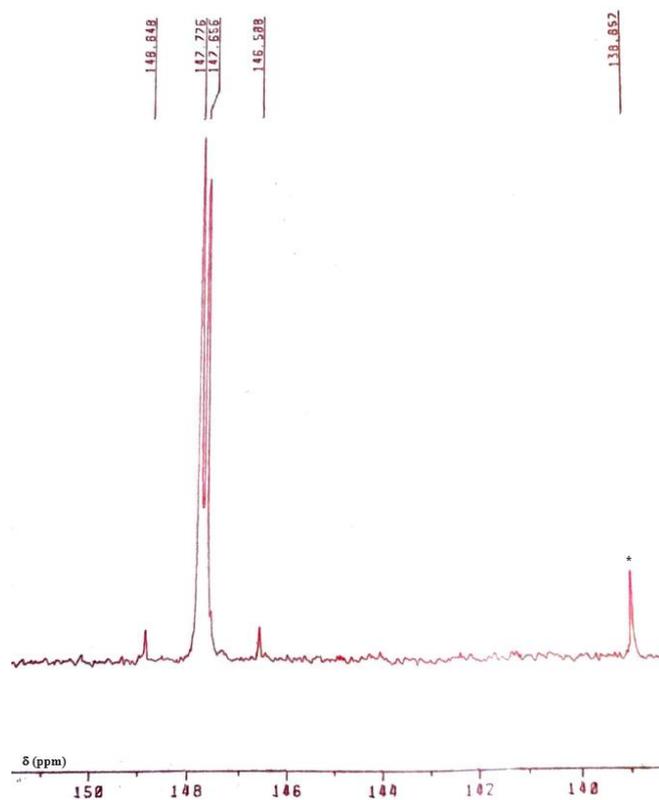
Figure S6 : ^{31}P-$\{^{1}H\}$ NMR spectrum (CDCl$_3$) of **2-anti**
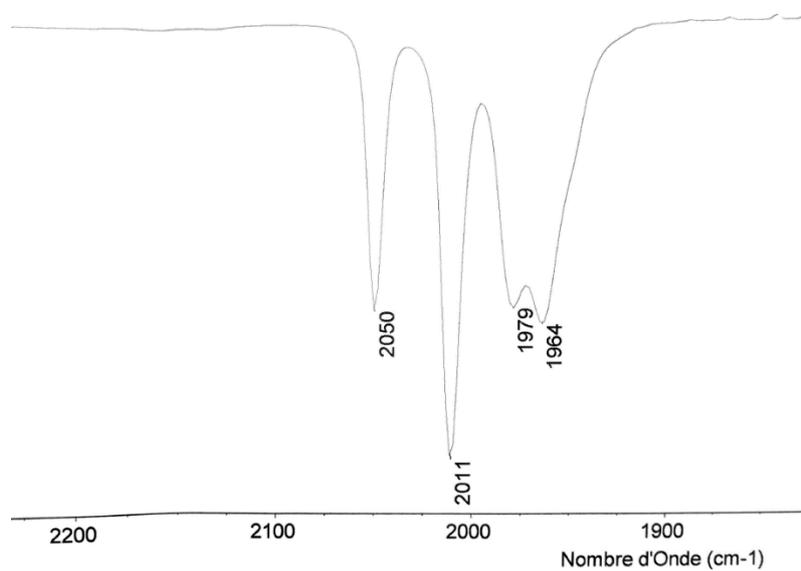
Figure S7 : IR spectrum in CH$_2$Cl$_2$ of **2-syn**

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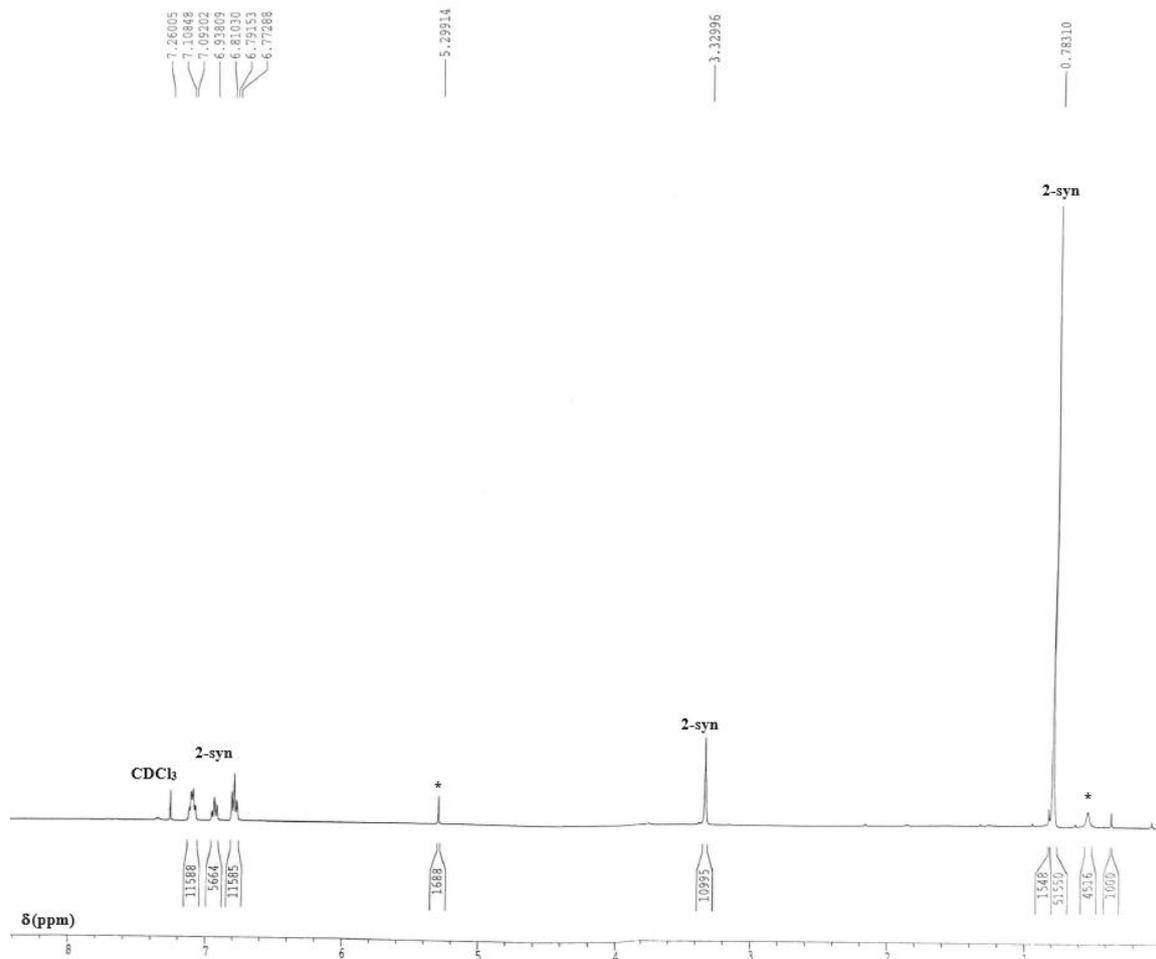
Figure S8 : ^{1}H NMR spectrum (CDCl$_3$) of **2-syn**.
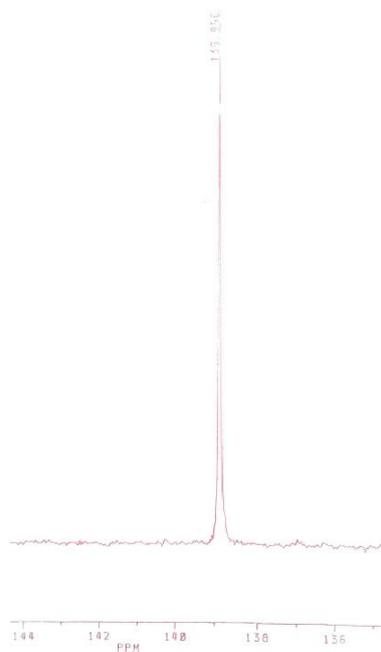
Figure S9 : ^{31}P-{^{1}H} NMR spectrum (CDCl$_3$) of **2-syn**
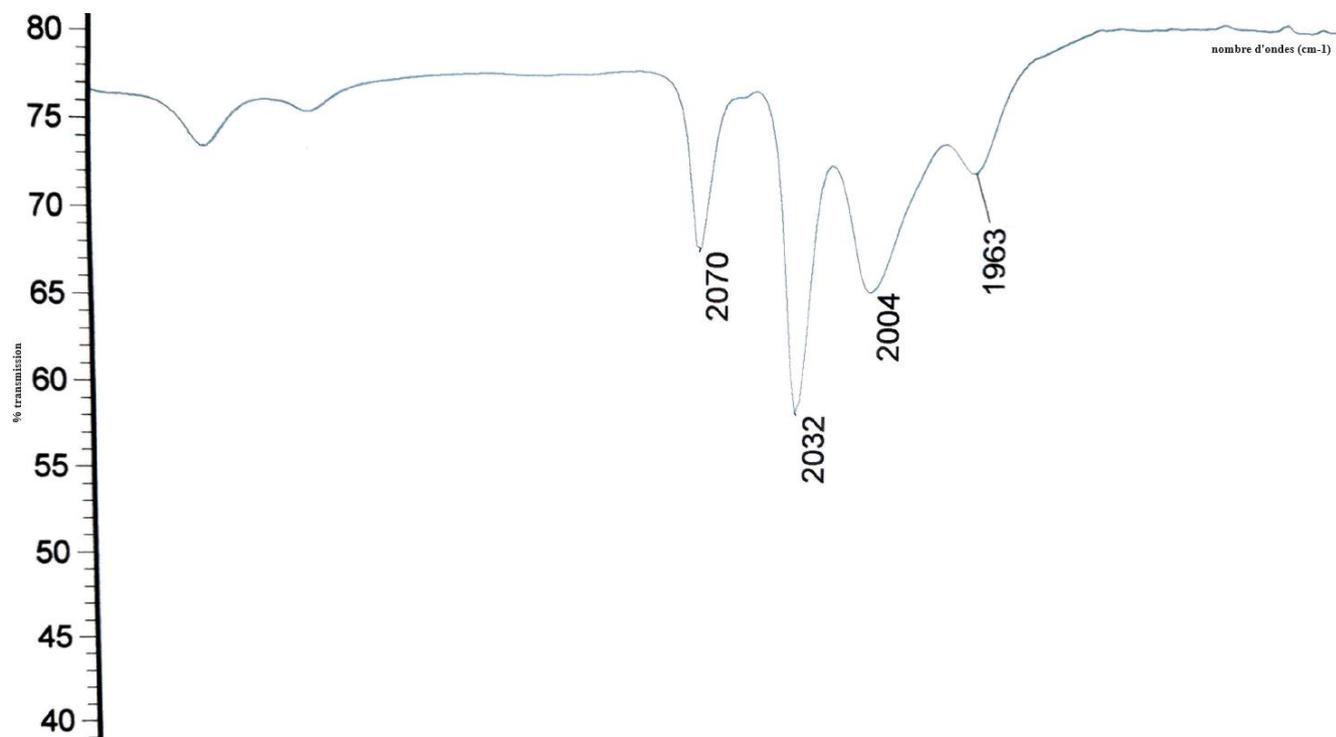
**Figure S10 :** IR spectrum in CH$_2$Cl$_2$ of **3**
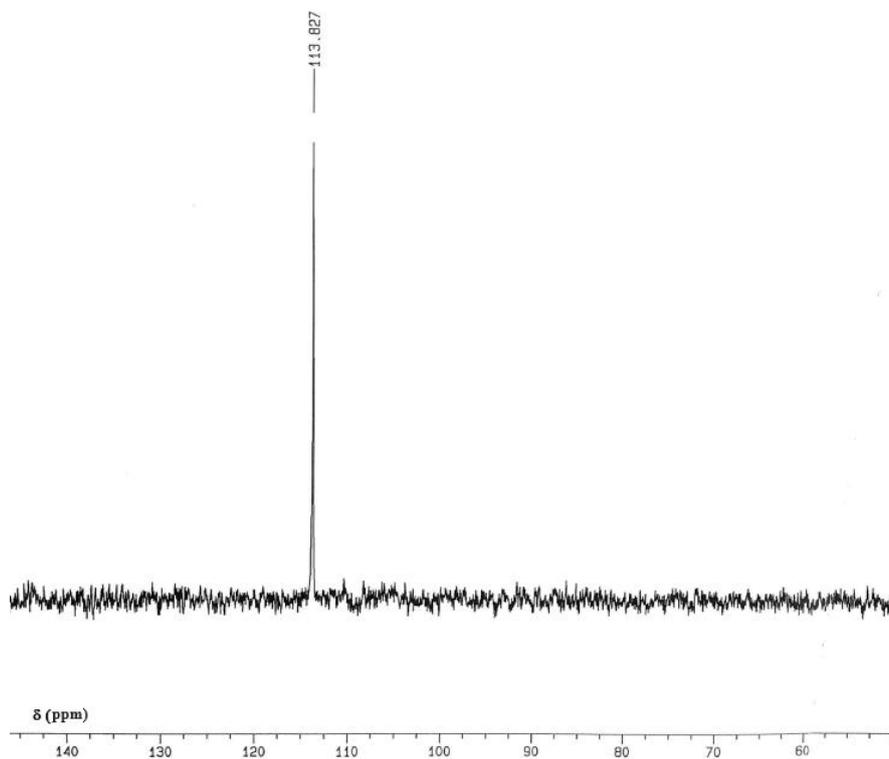
Figure S11 : ^{31}P-{^{1}H} NMR spectrum (CDCl$_3$) of **3**
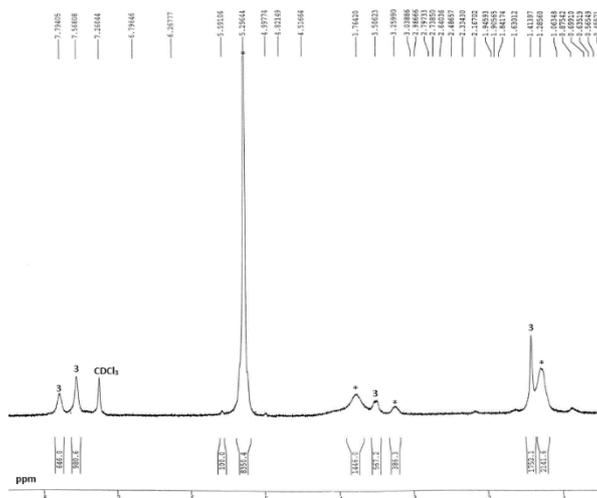
Figure S12 : ^{1}H NMR spectrum (CDCl$_3$) of **3**

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