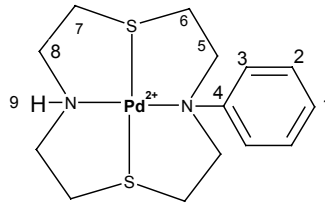


APÈNDIX II:
ESPECTRES DELS COMPLEXOS

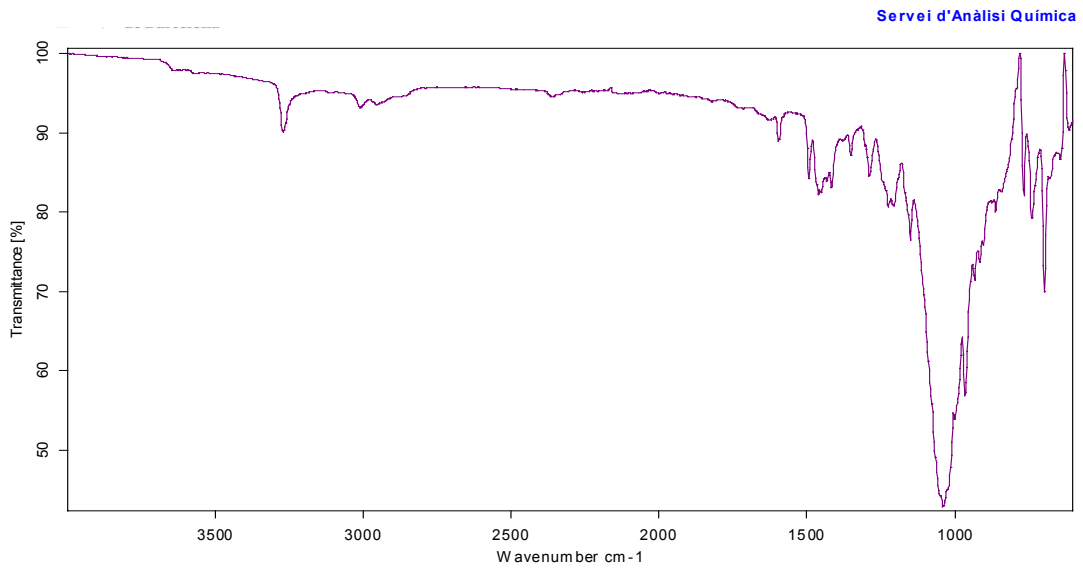
1	Complexos de Pd(II)	121
	▪ [Pd(L1)](BF ₄) ₂	121
	▪ [Pd(L2)](BF ₄) ₂	123
	▪ [Pd(L4)](BF ₄) ₂	126
	▪ [Pd(L5)](BF ₄) ₂	128
	▪ [Pd(L15)](BF ₄) ₂	131
	▪ [Pd ₂ (Bi-L15)](BF ₄) ₄	133
	▪ [Pd(L17)](BF ₄) ₂	137
2	Complexos de Cu(II)	140
	▪ [Cu(ClO ₄)(L1)]ClO ₄	140
	▪ [Cu(L2)](BF ₄) ₂	141
	▪ [Cu(L15)](BF ₄) ₂	142
3	Complexos de Ni(II)	143
	▪ [Ni(L4)](ClO ₄) ₂	143
	▪ [Ni(L17)](ClO ₄) ₂	147
	▪ [NiCl(L17)]ClO ₄	150
	▪ [NiBr(L17)]ClO ₄	153
	▪ [NiI(L17)]ClO ₄	156

1 Complexos de Pd(II)

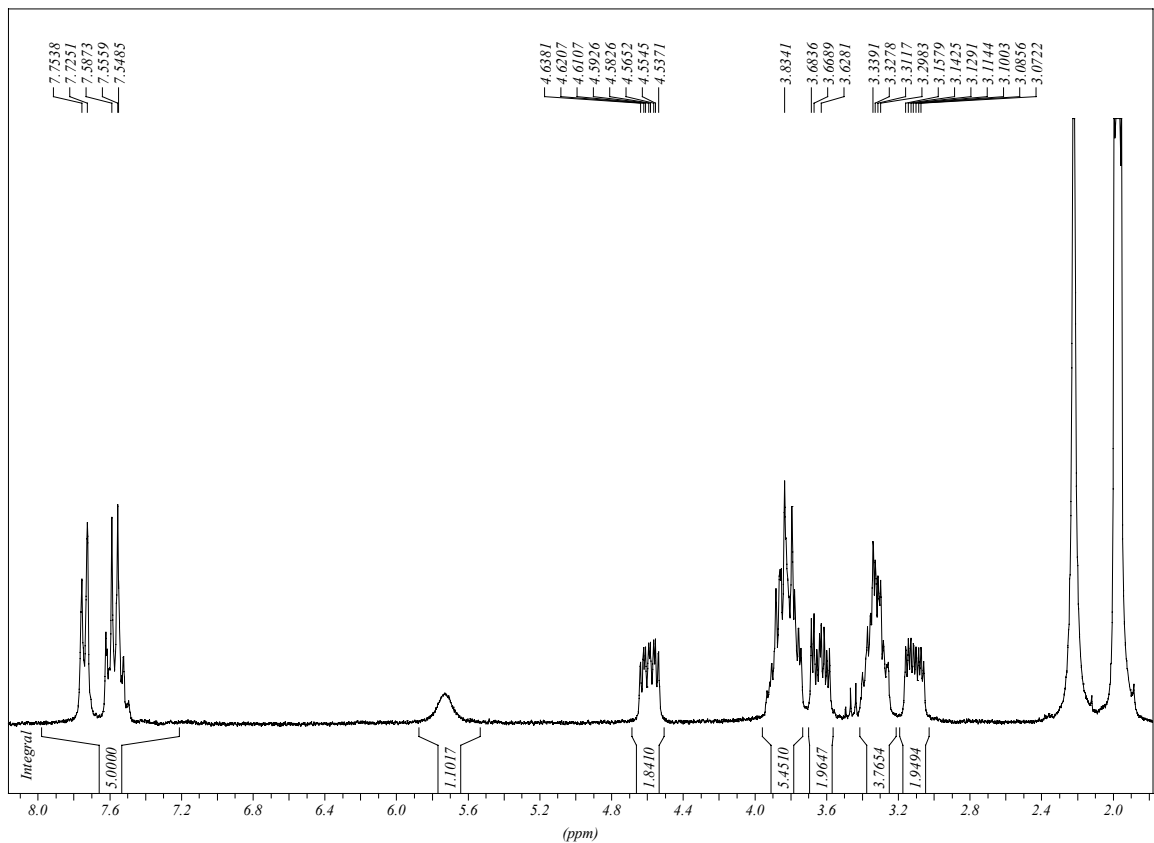
- $[\text{Pd}(\text{L1})](\text{BF}_4)_2$



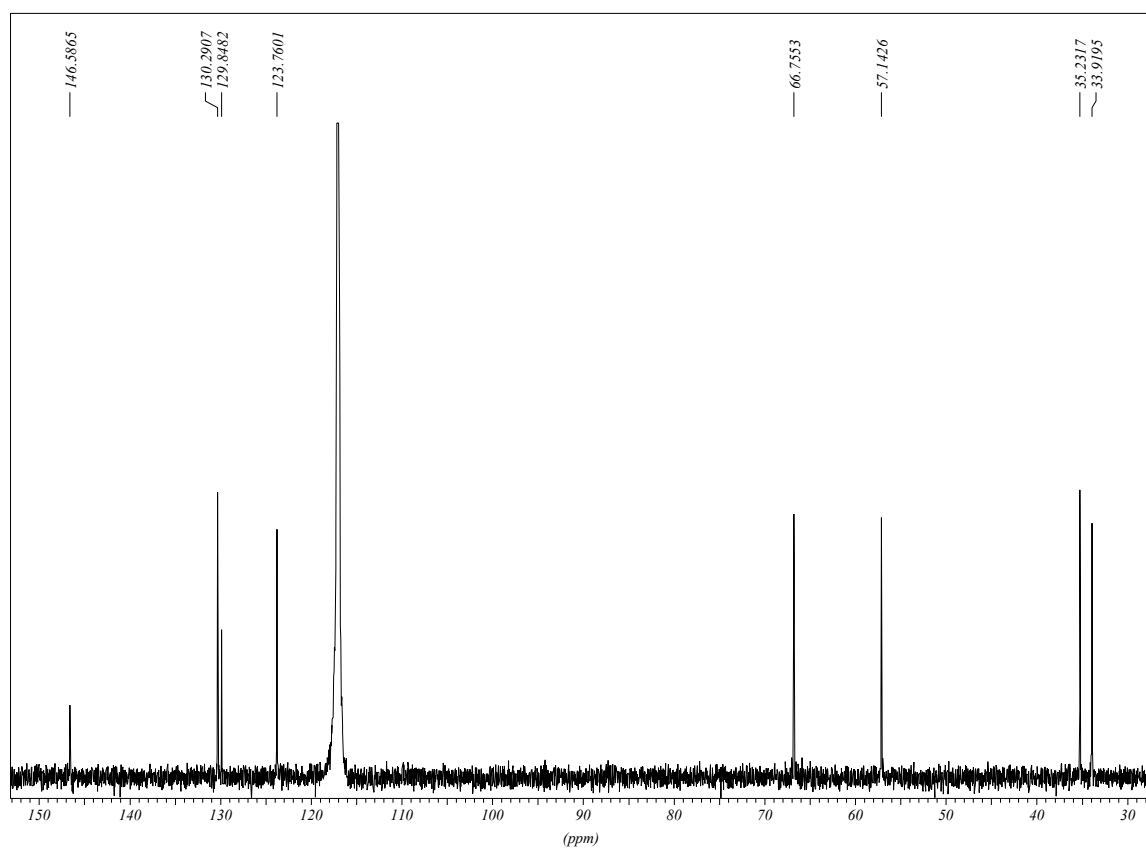
IR (ATR)



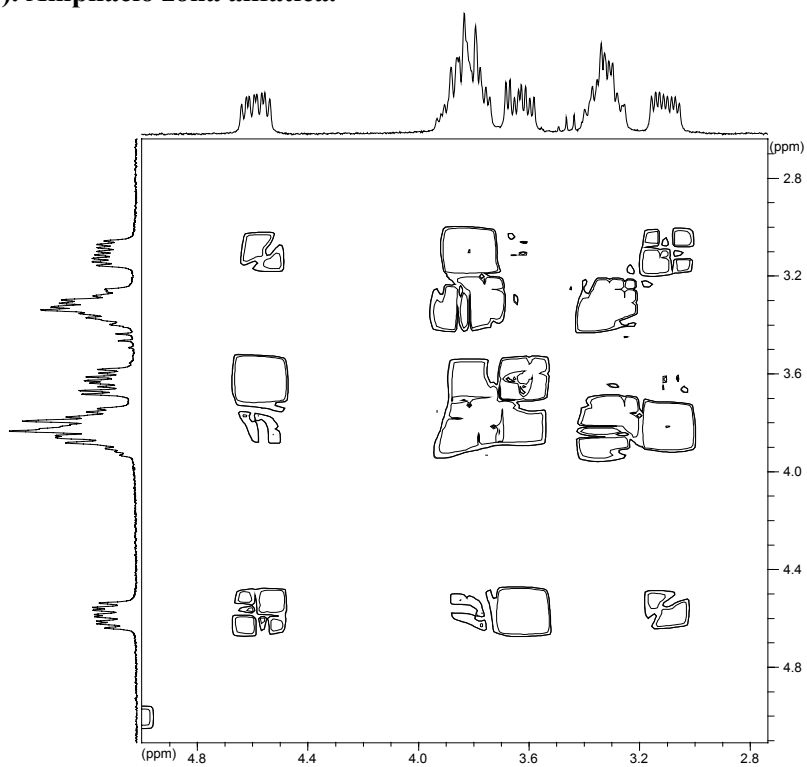
^1H RMN (CD_3CN)



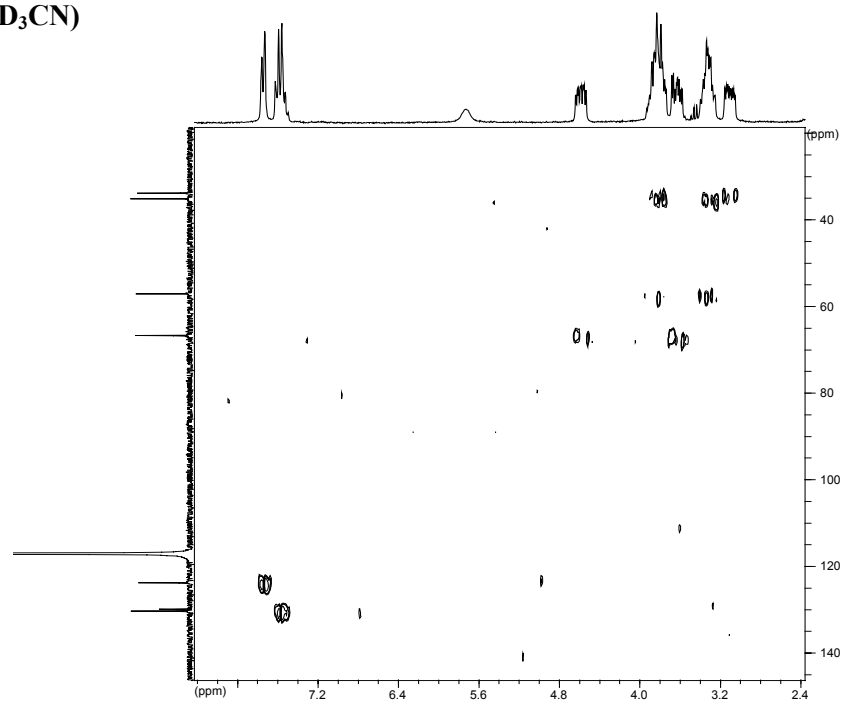
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



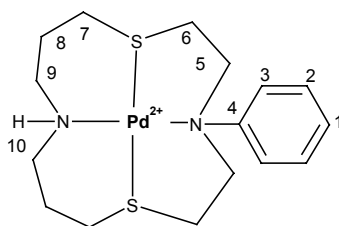
COSY (CD_3CN). Ampliació zona alifàtica.



HMQC (CD₃CN)

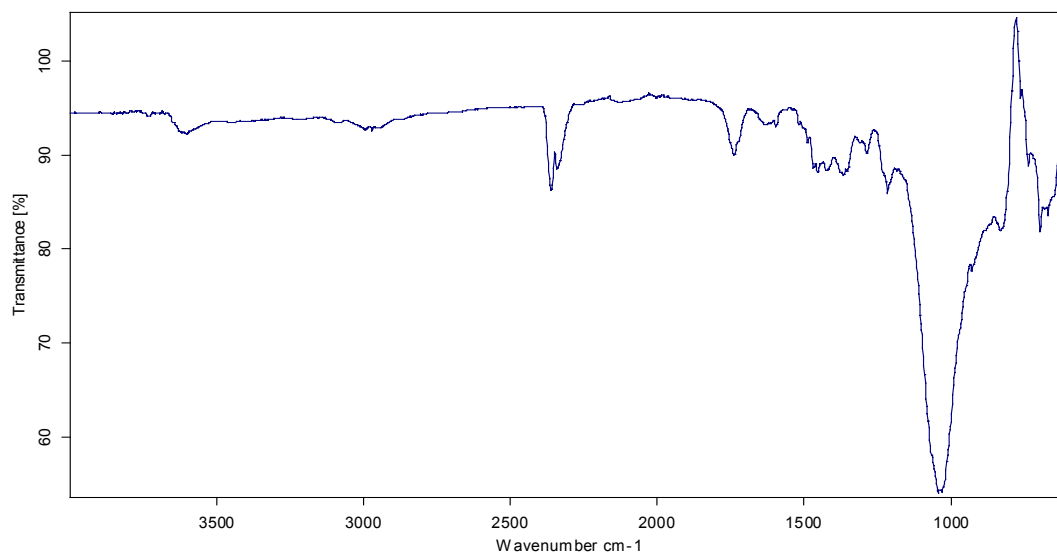


▪ [Pd(L2)](BF₄)₂

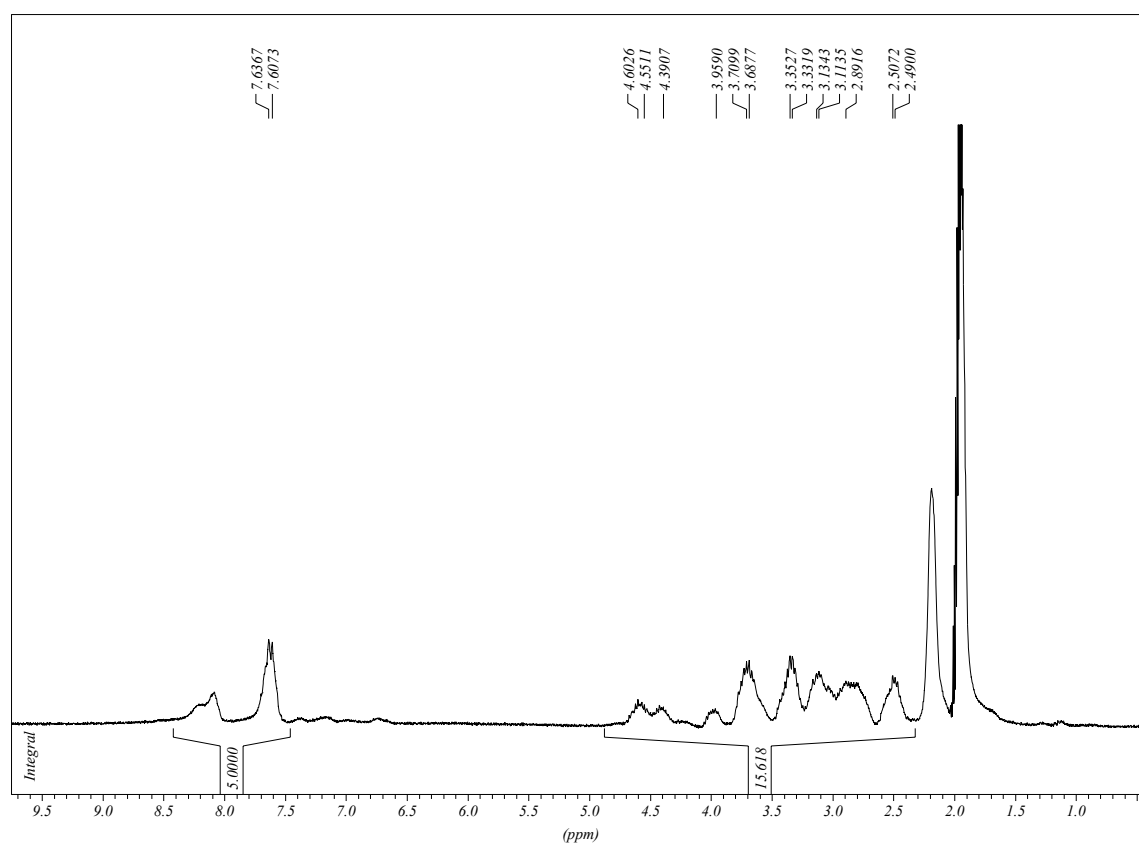


IR (ATR)

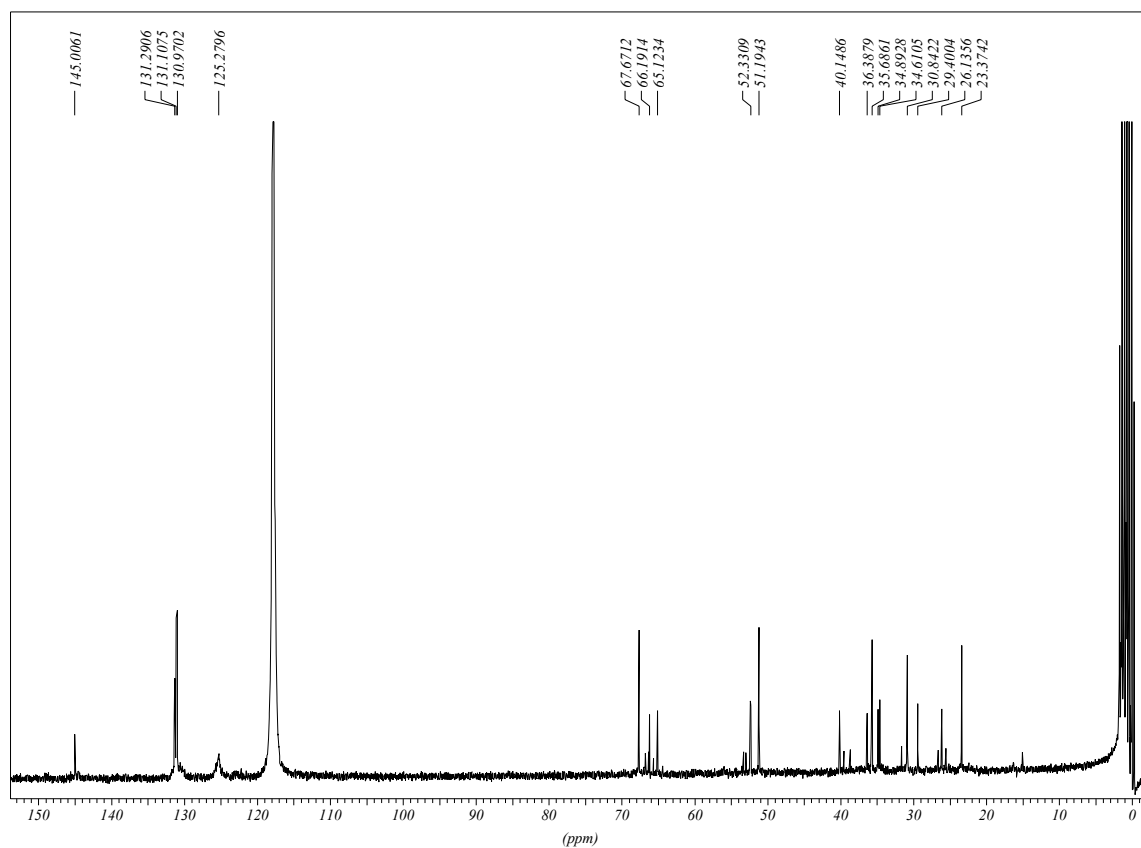
Servei d'Anàlisi Química



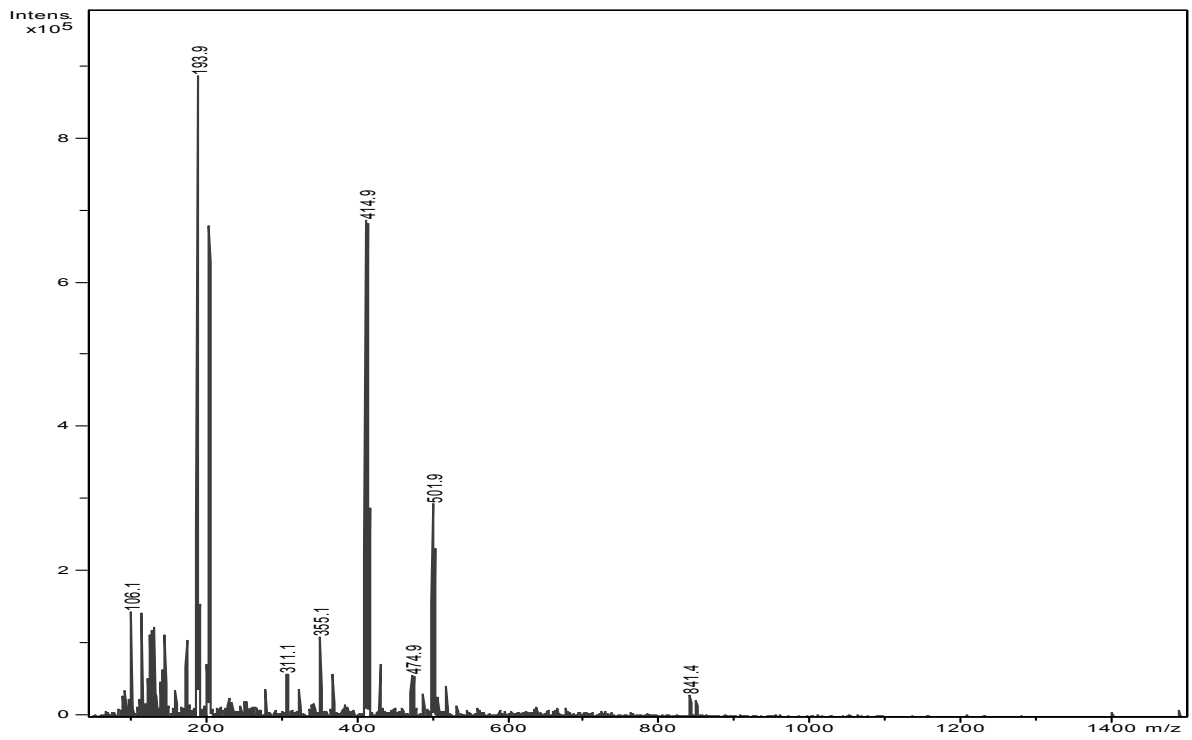
^1H RMN (CD_3CN)



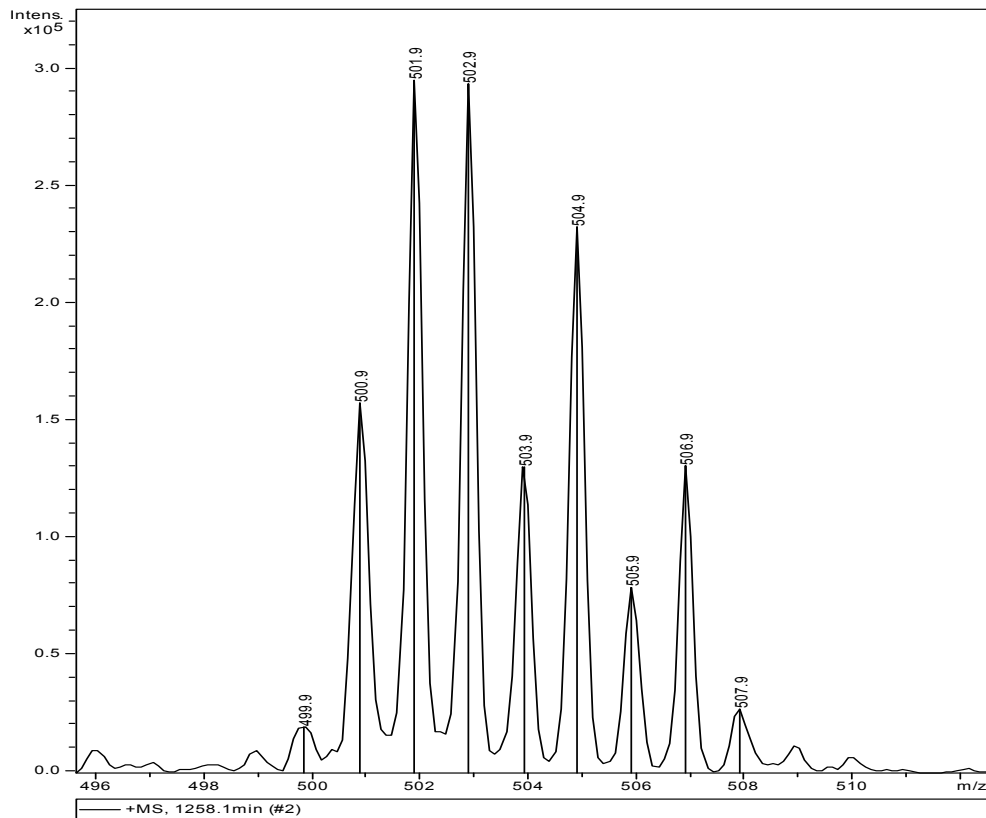
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



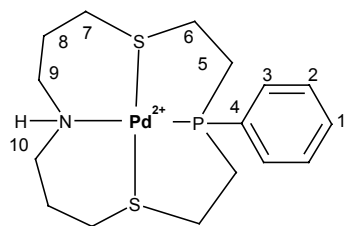
ESPECTROSCÒPIA DE MASSES (ESI(+)-IT) (20 ppm en MeOH)



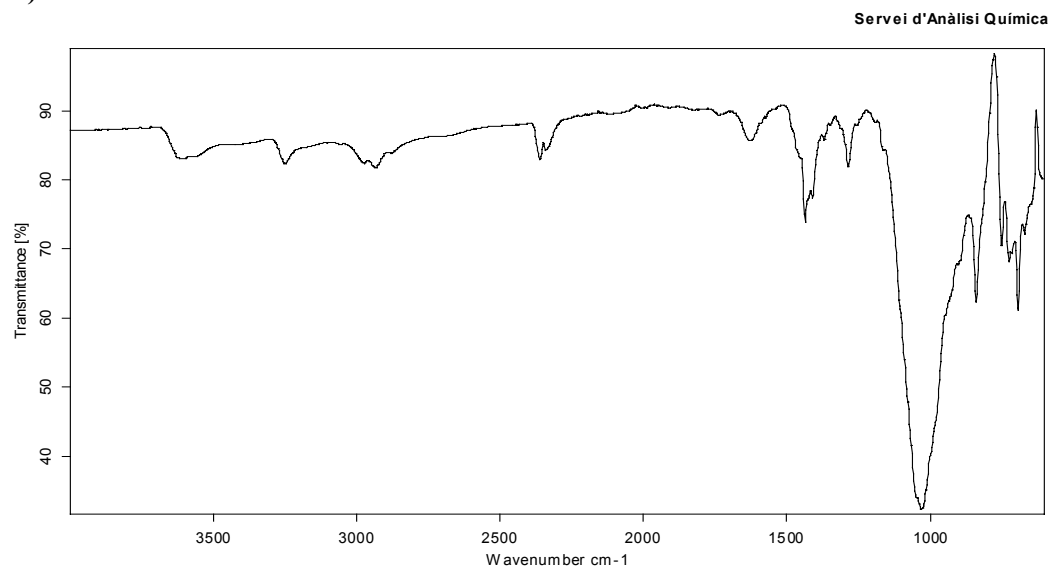
Ampliació pic 501.09 m/z



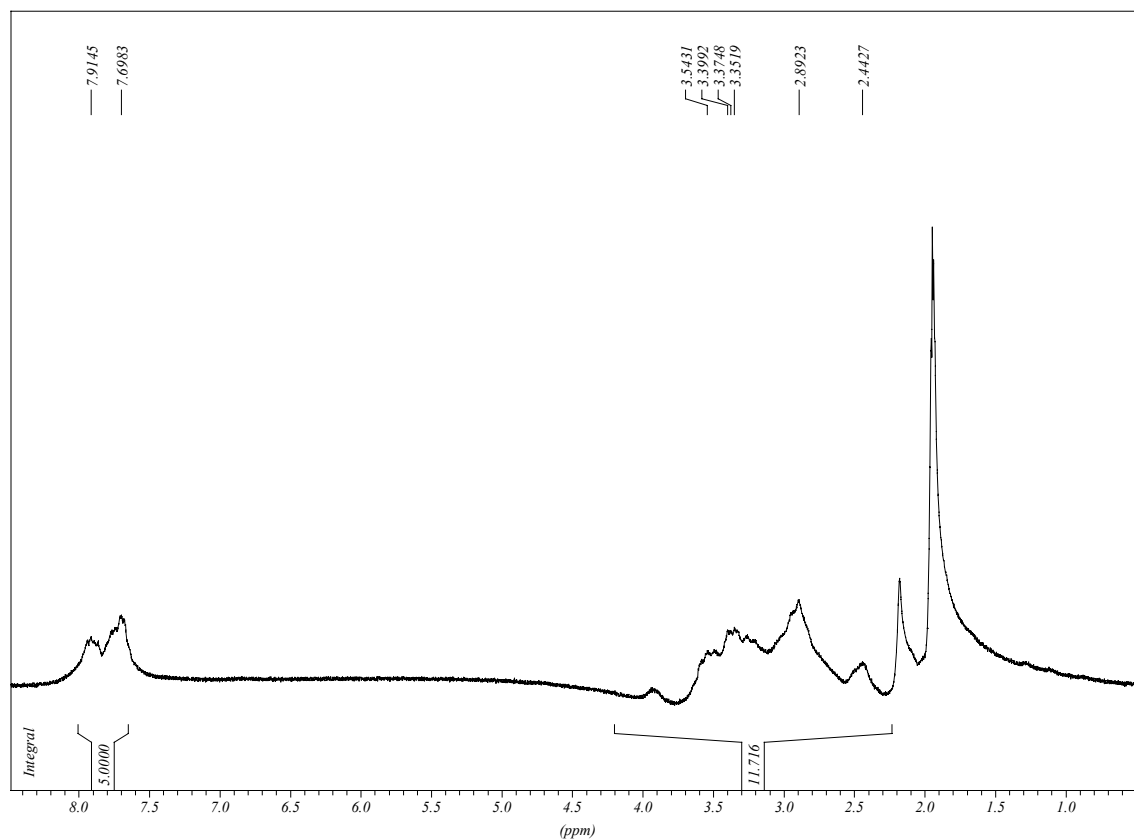
▪ $[\text{Pd}(\text{L4})](\text{BF}_4)_2$



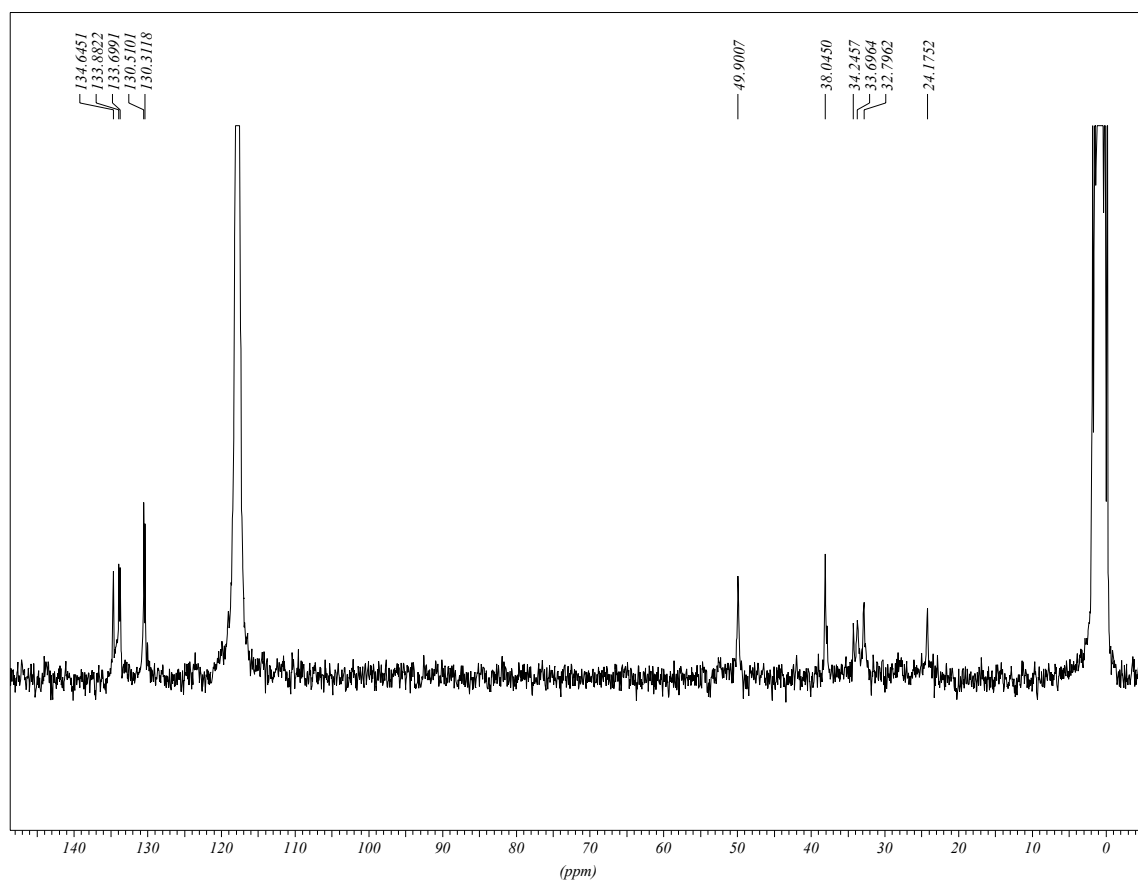
IR (ATR)



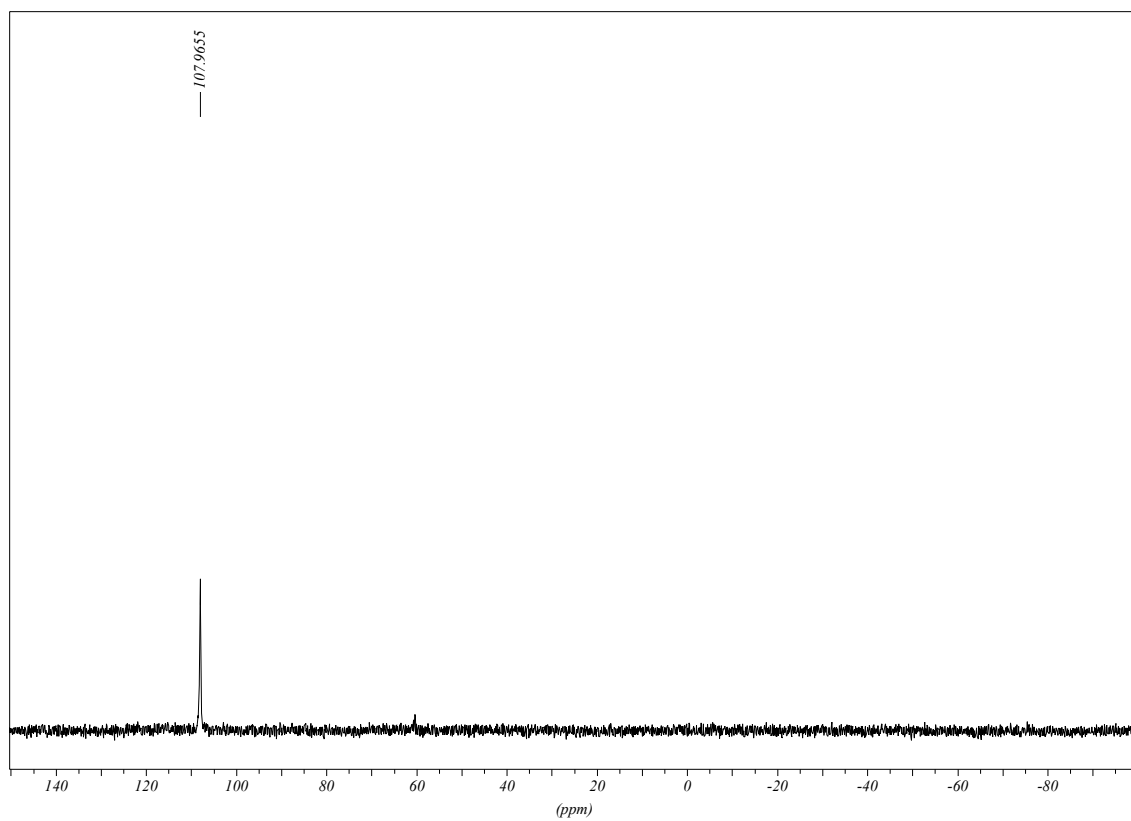
^1H RMN (CD_3CN)



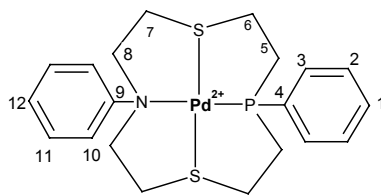
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)

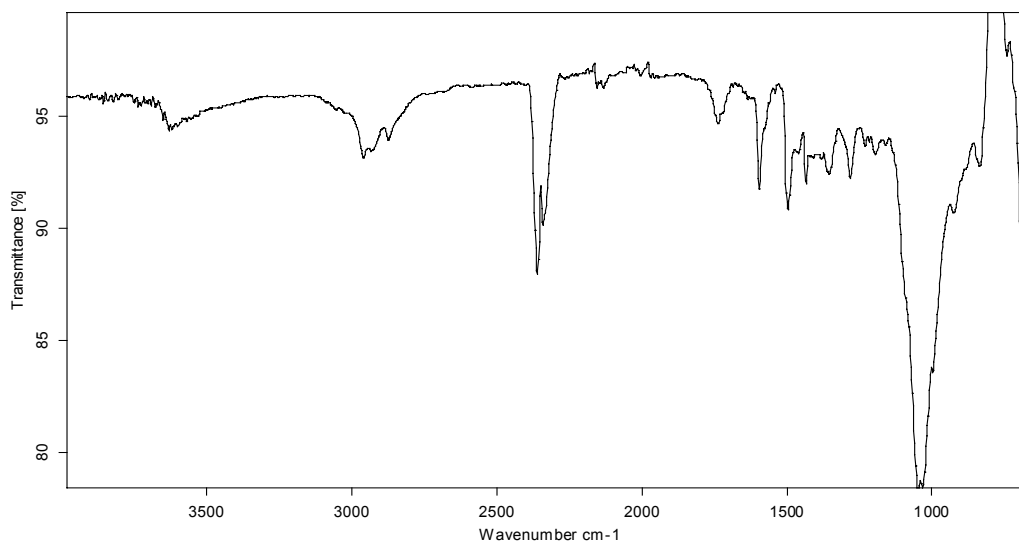


▪ [Pd(L5)](BF₄)₂

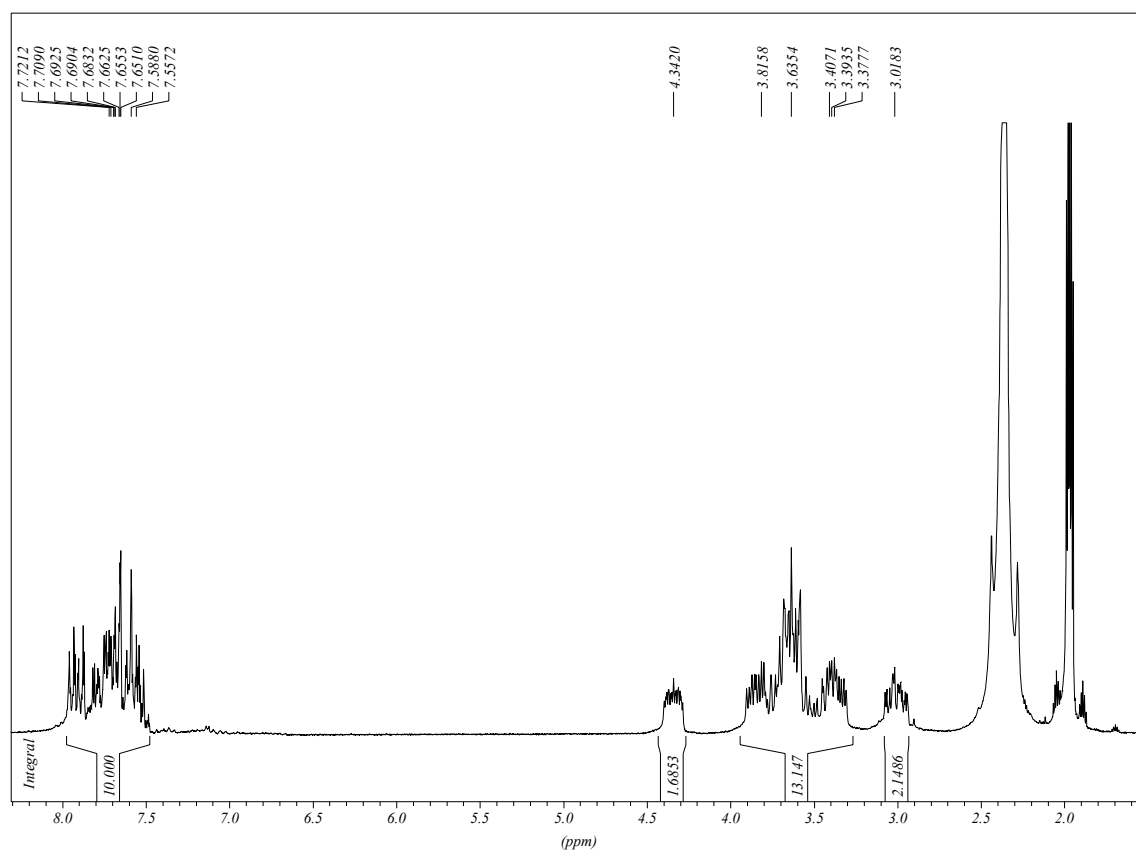


IR (ATR)

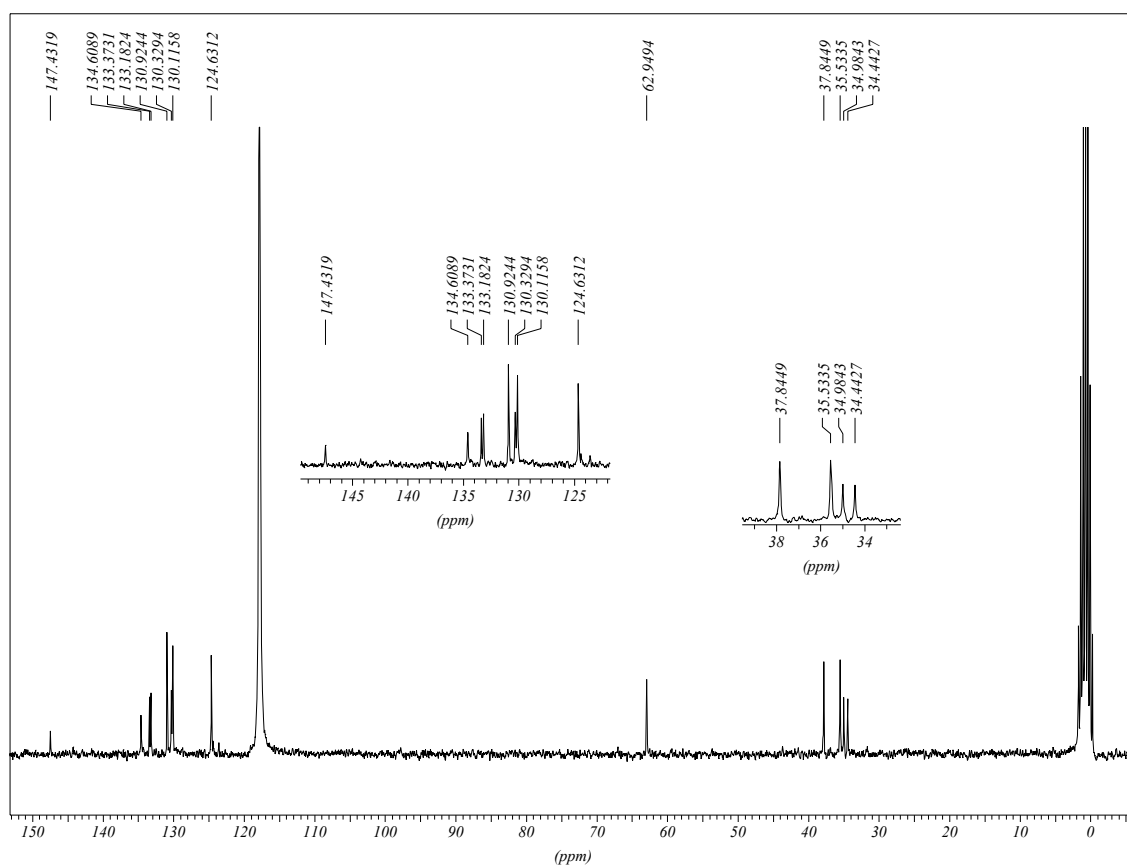
Servei d'Anàlisi Química



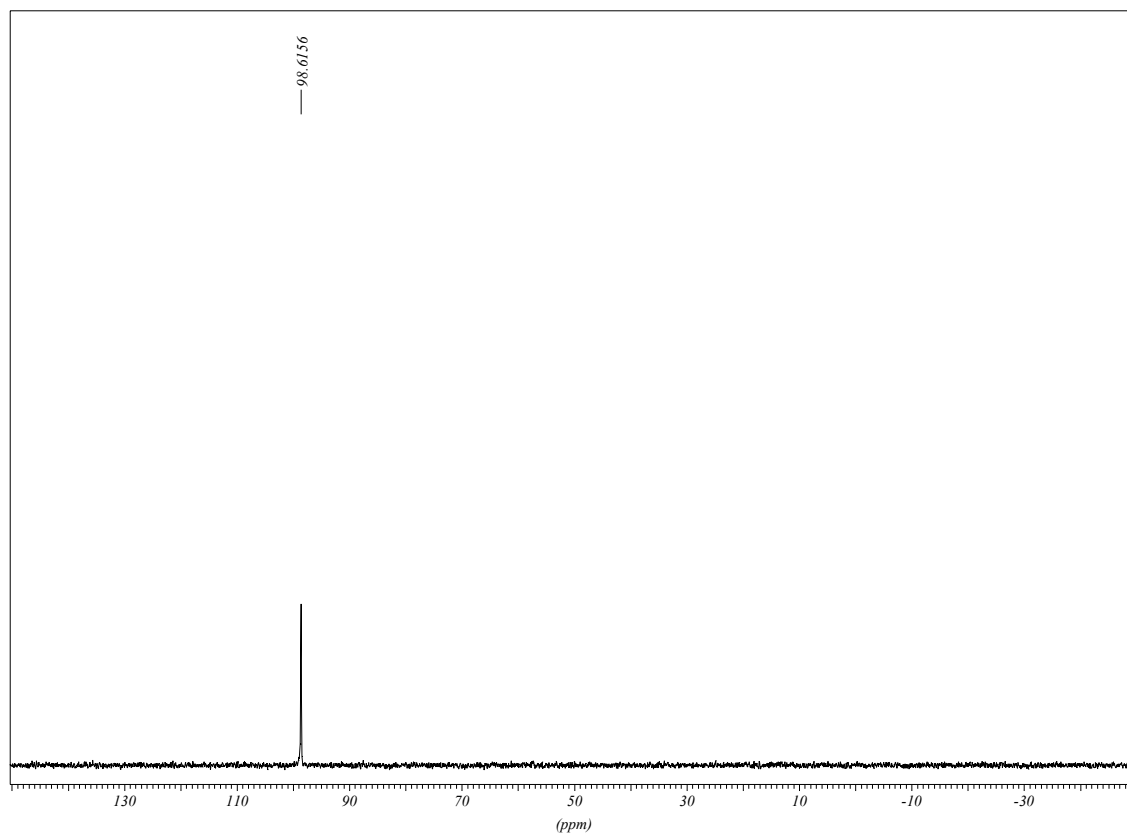
¹H RMN (CD₃CN)



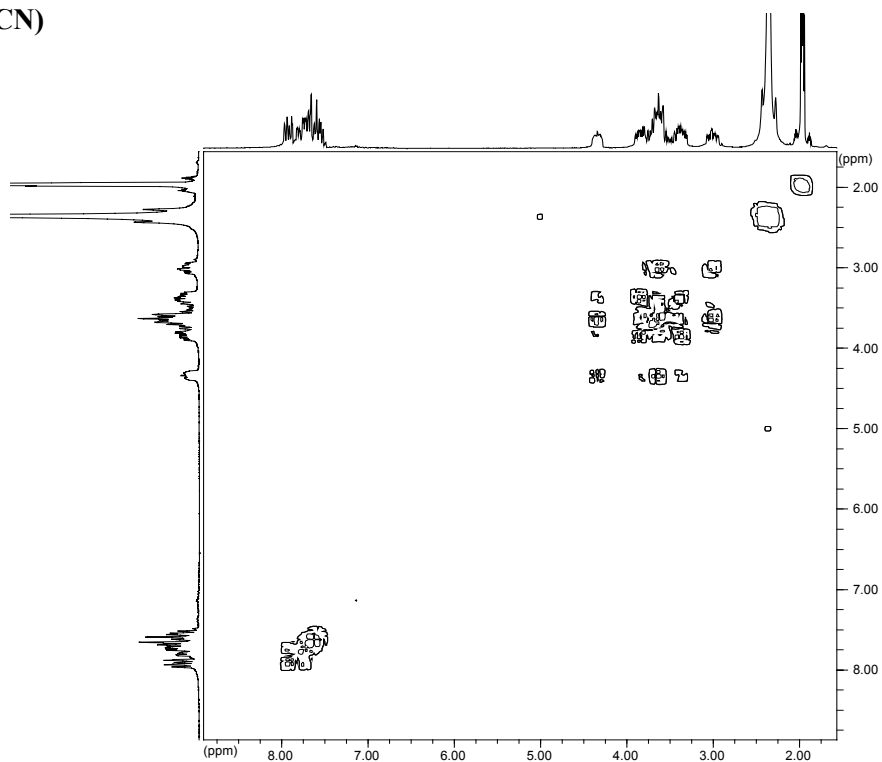
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



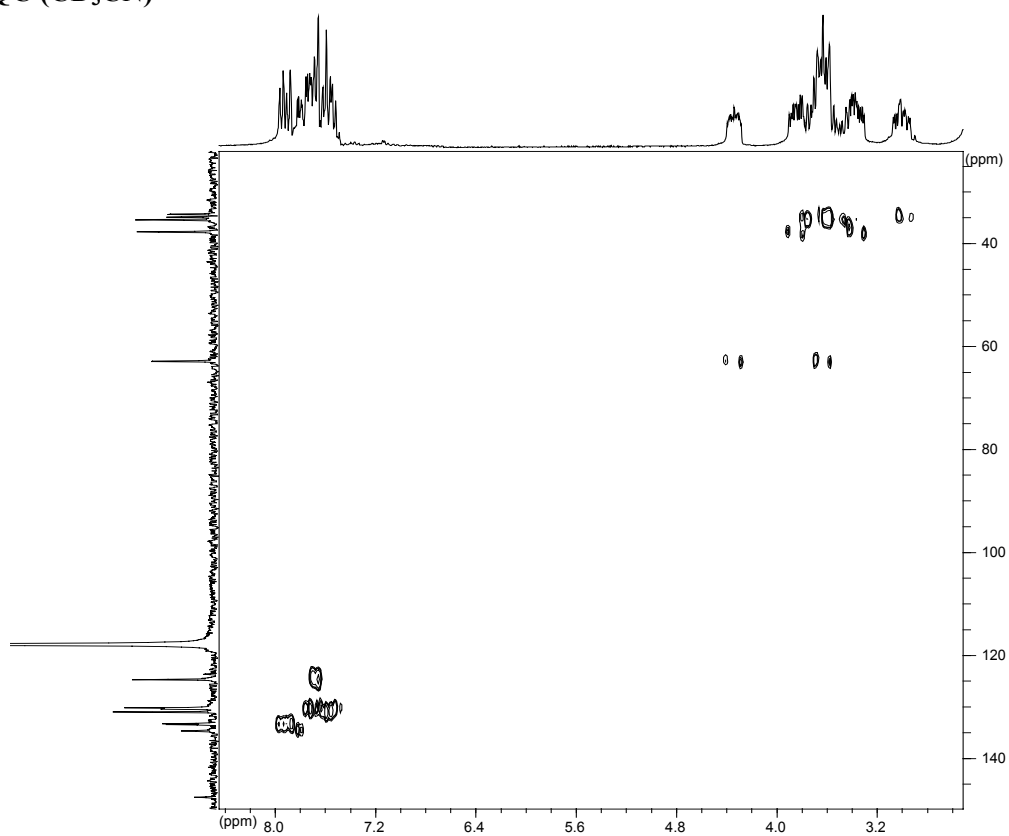
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



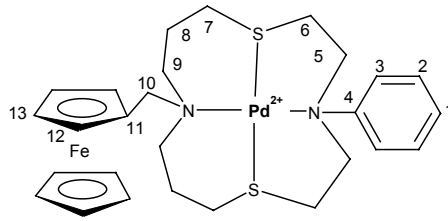
COSY (CD₃CN)



HMQC (CD₃CN)

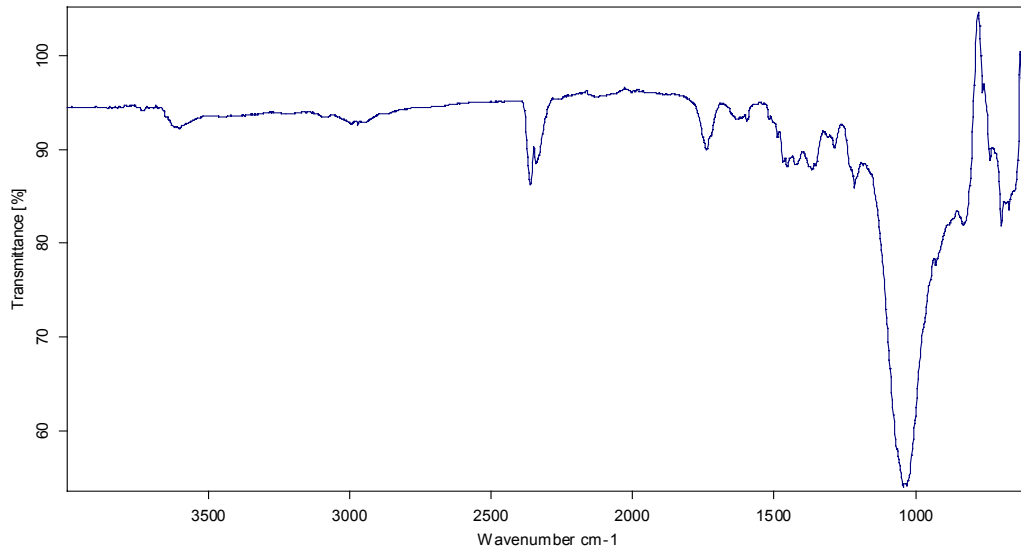


▪ [Pd(L15)](BF₄)₂

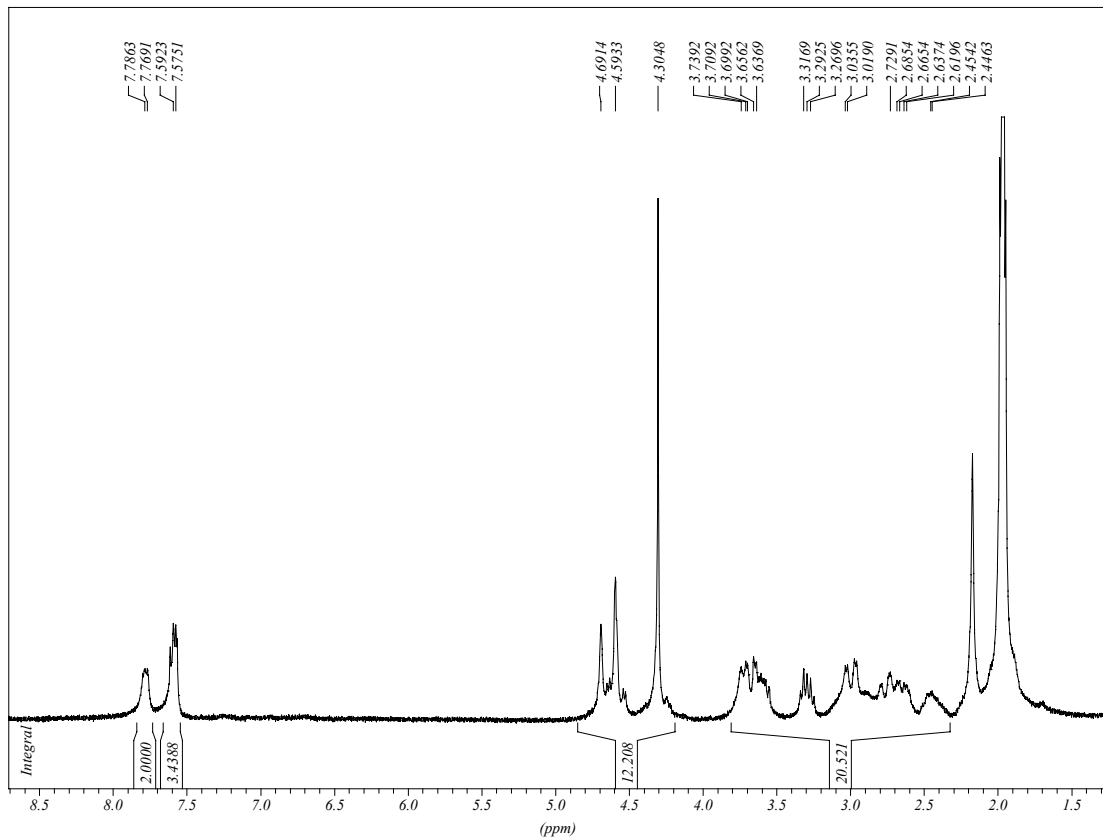


IR (ATR)

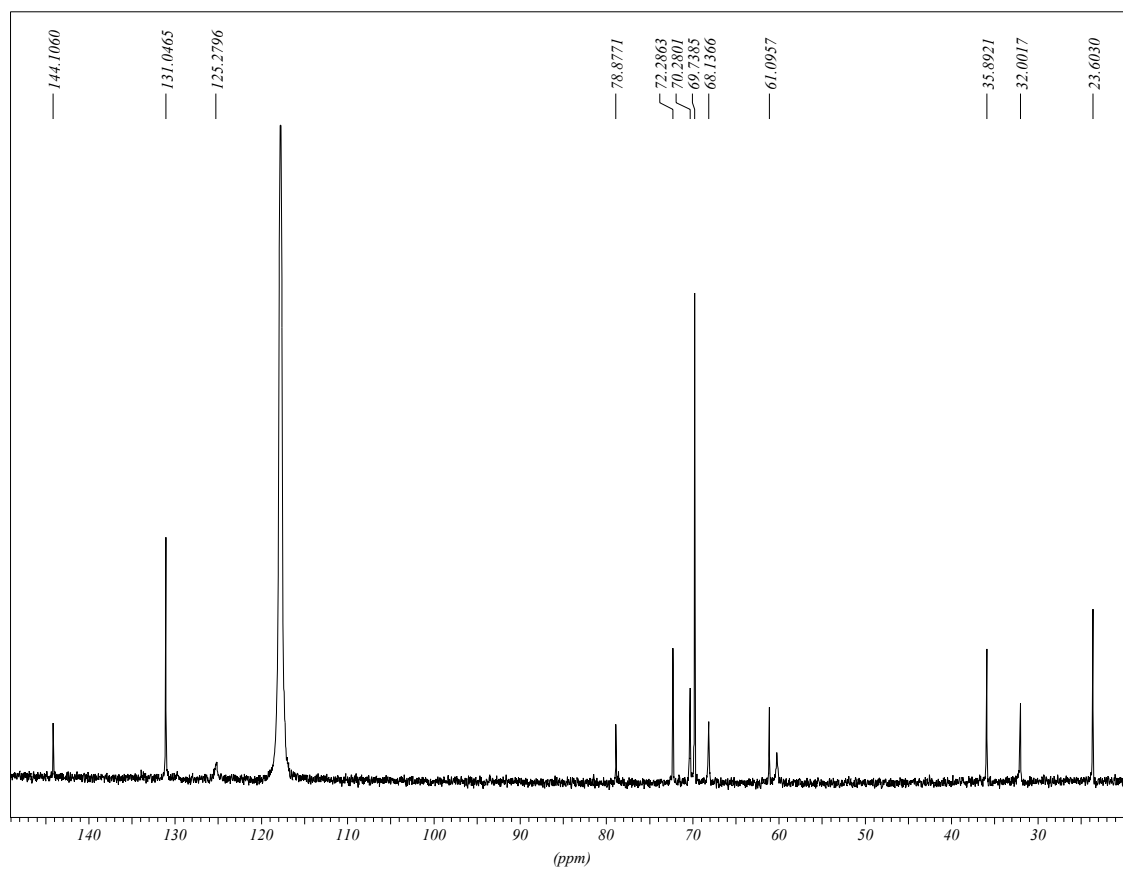
Servei d'Anàlisi Química



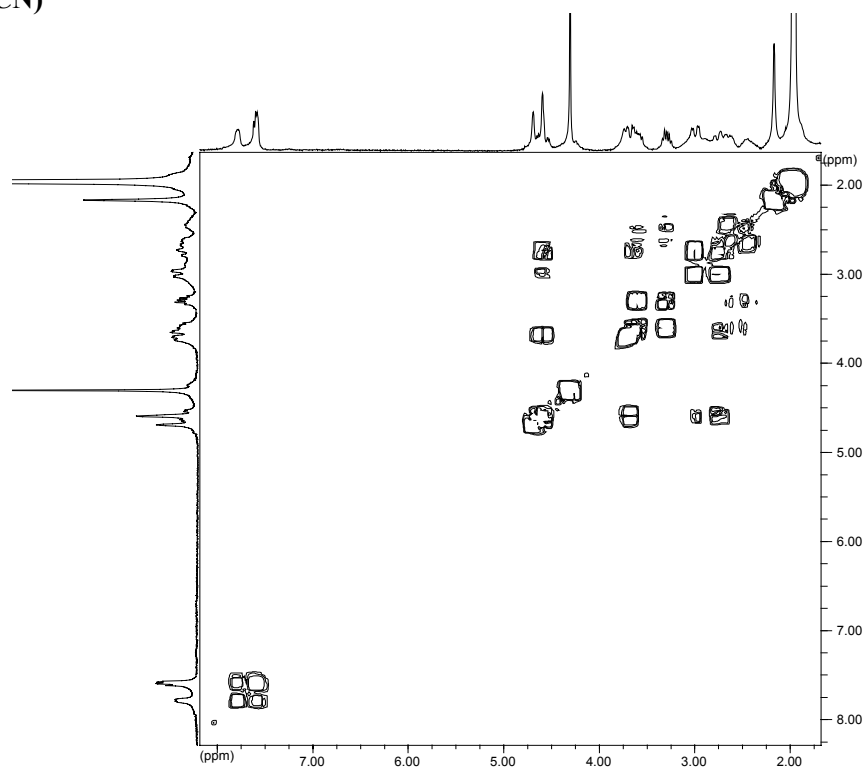
¹H RMN (CD₃CN)



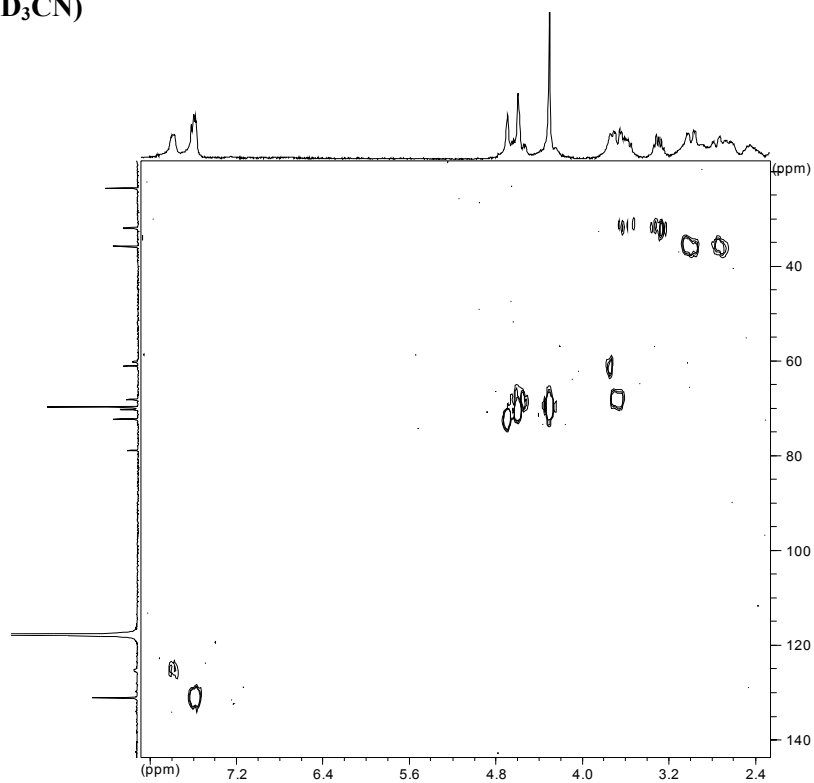
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



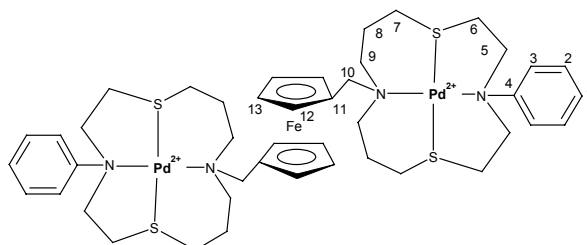
COSY (CD_3CN)



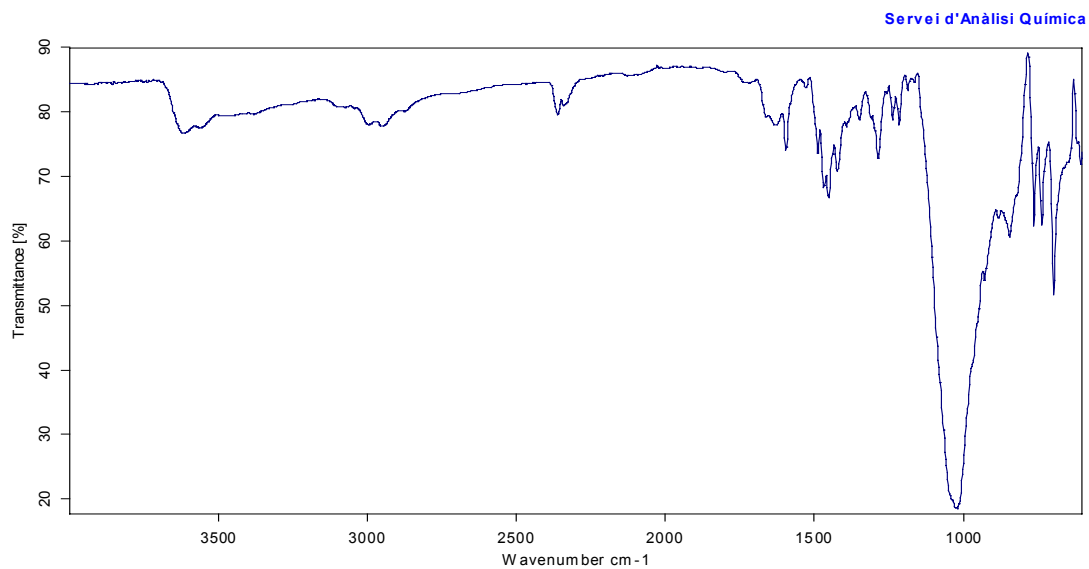
HMQC (CD₃CN)



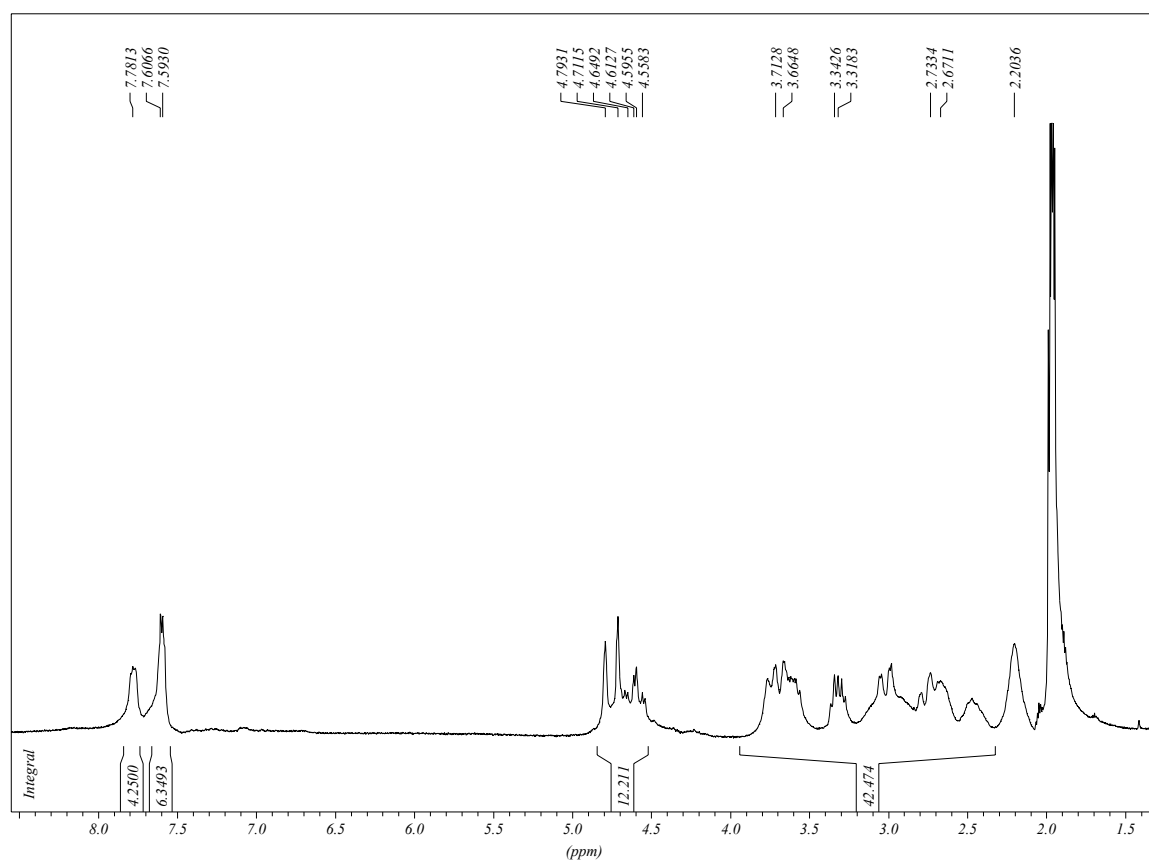
▪ [Pd₂(Bi-L15)](BF₄)₄



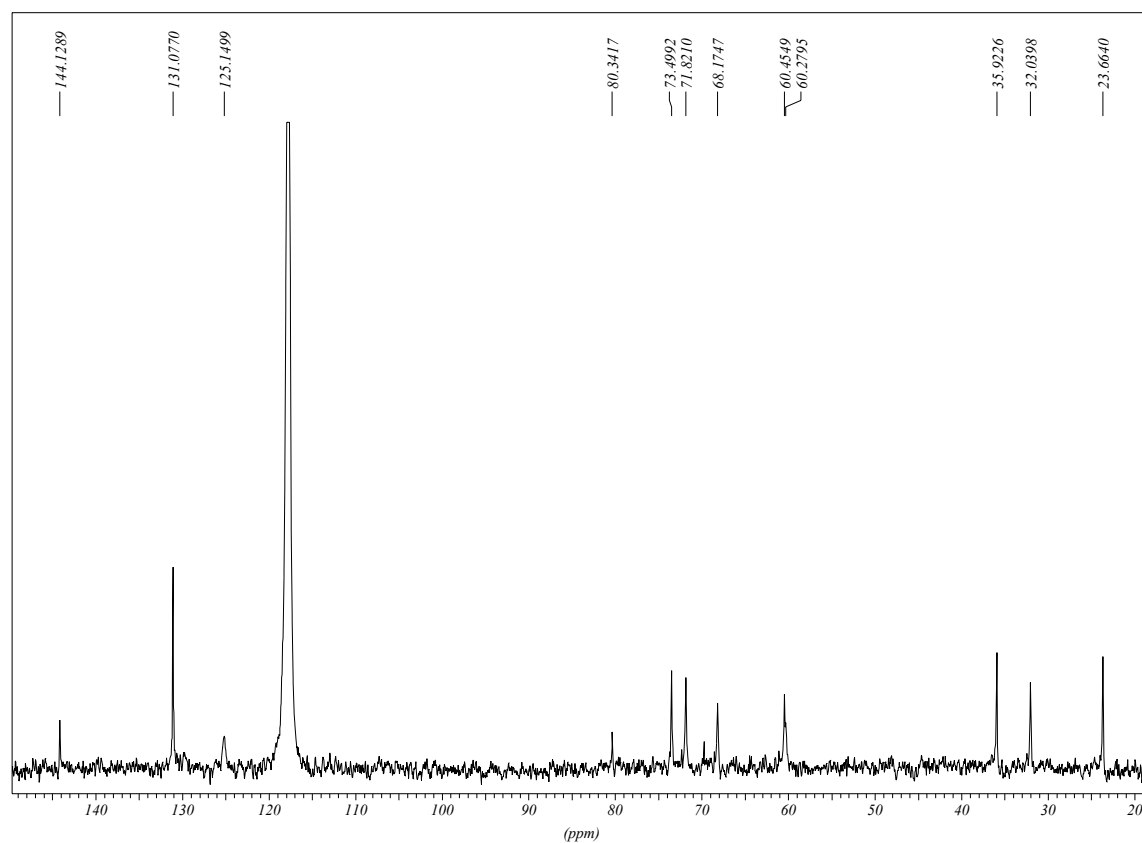
IR (ATR)



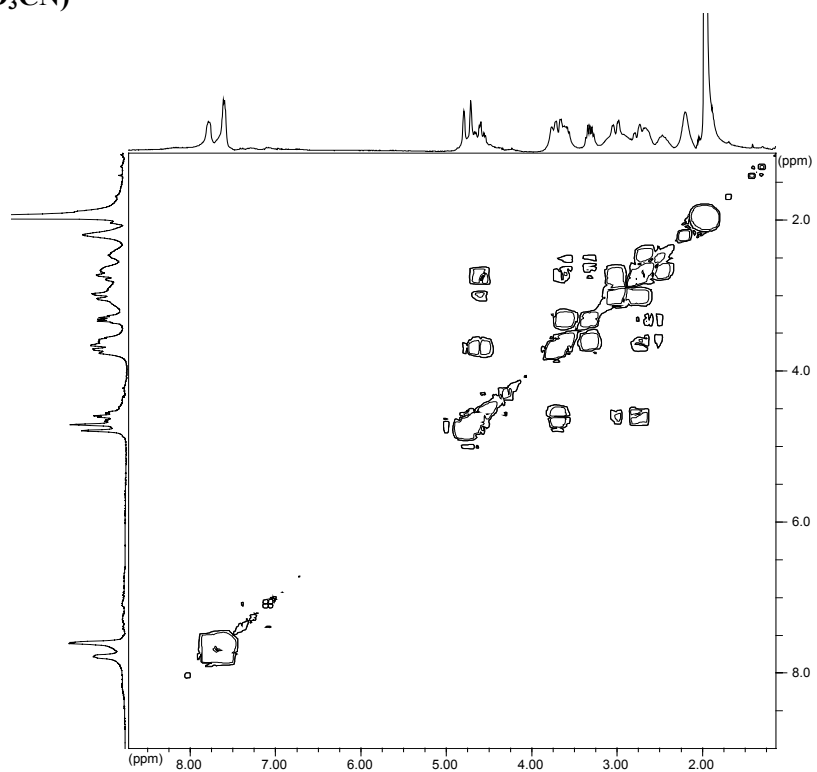
^1H RMN (CD_3CN)



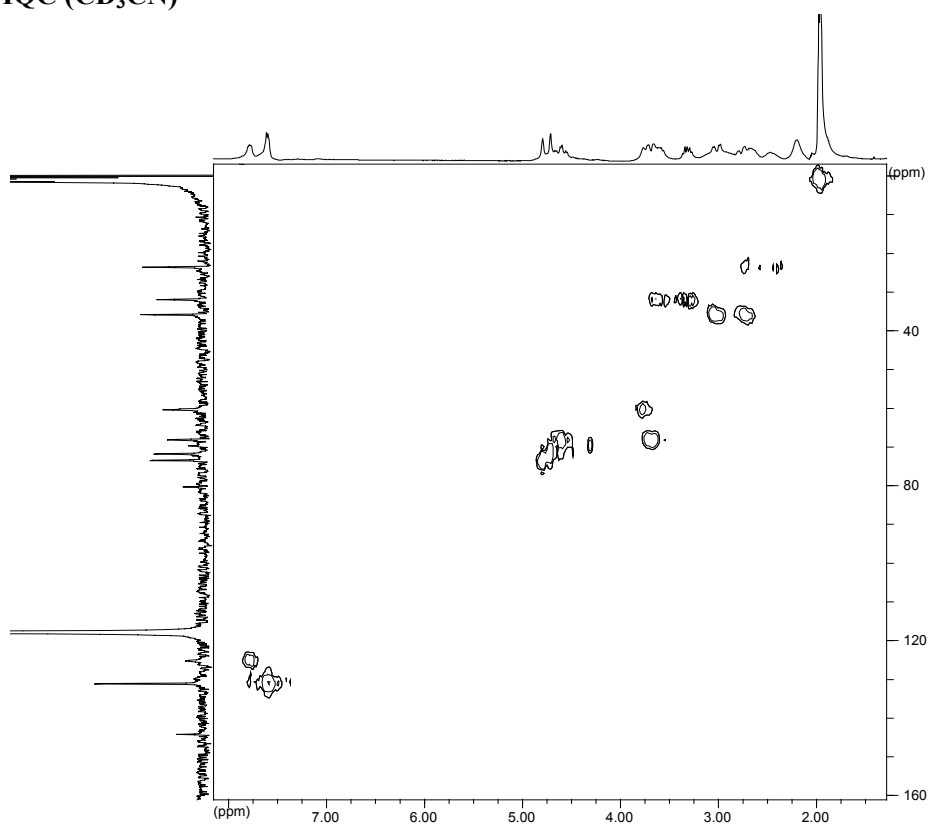
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



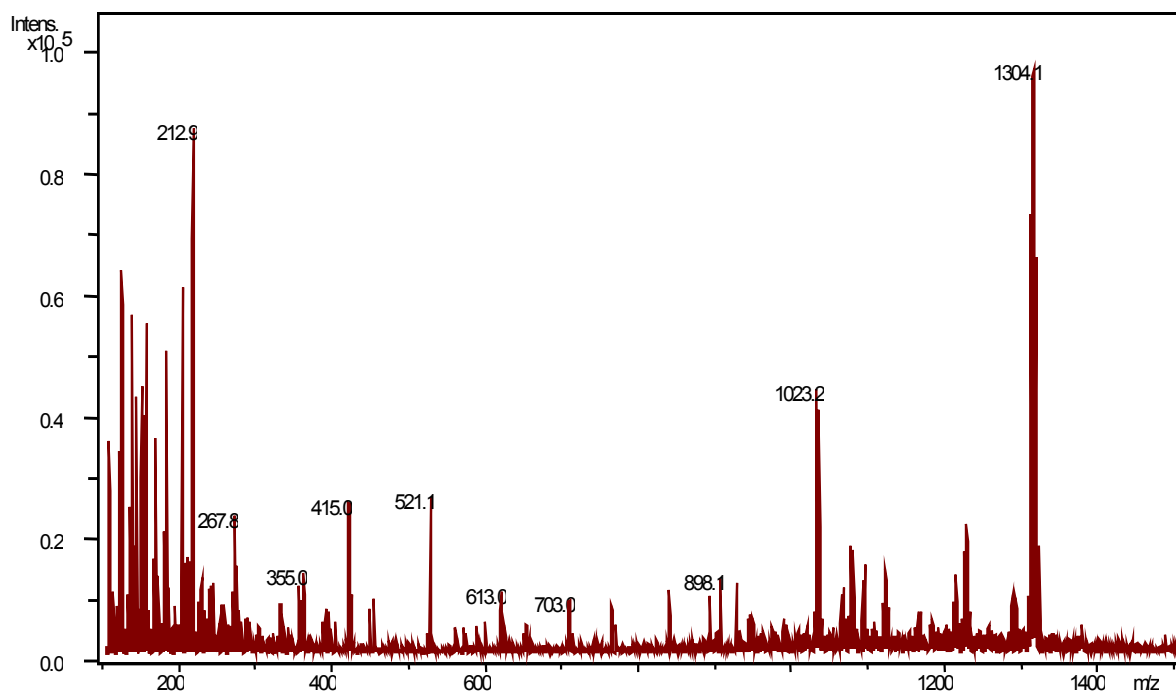
COSY (CD₃CN)



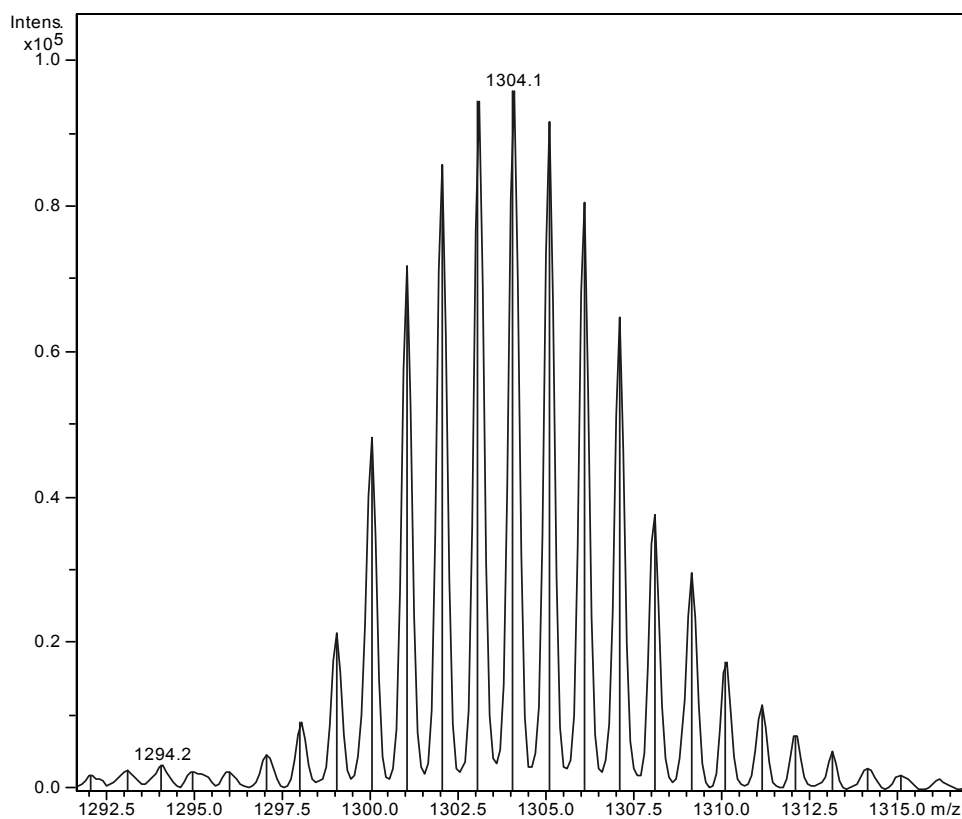
HMQC (CD₃CN)



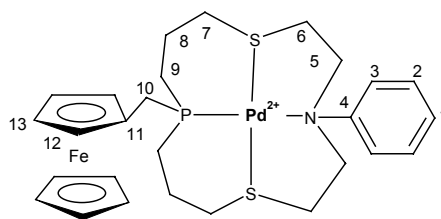
ESPECTROSCÒPIA DE MASSES (ESI(+)-IT) (10 ppm en CH₃CN)



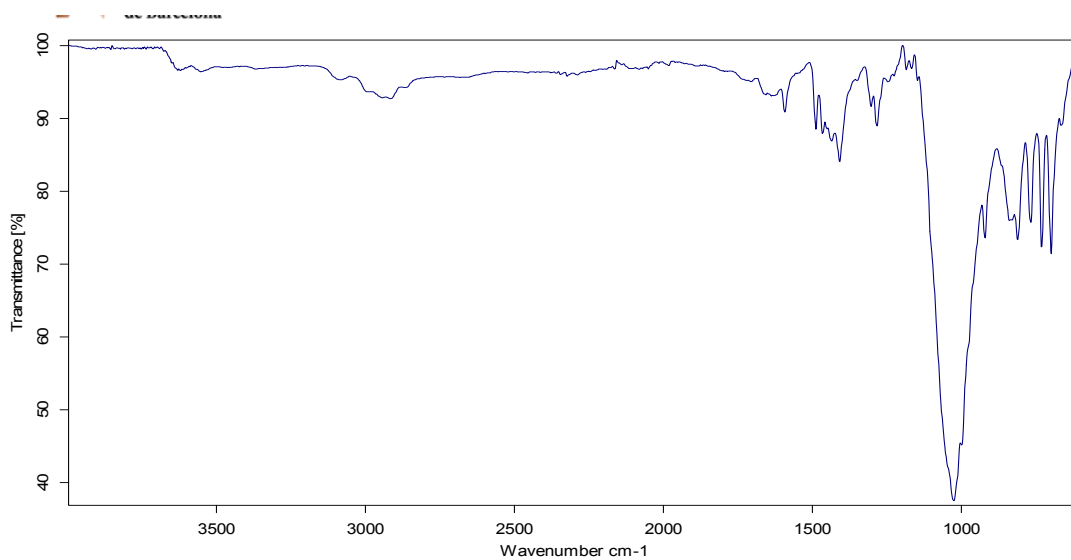
Ampliació pic 1304.1 m/z



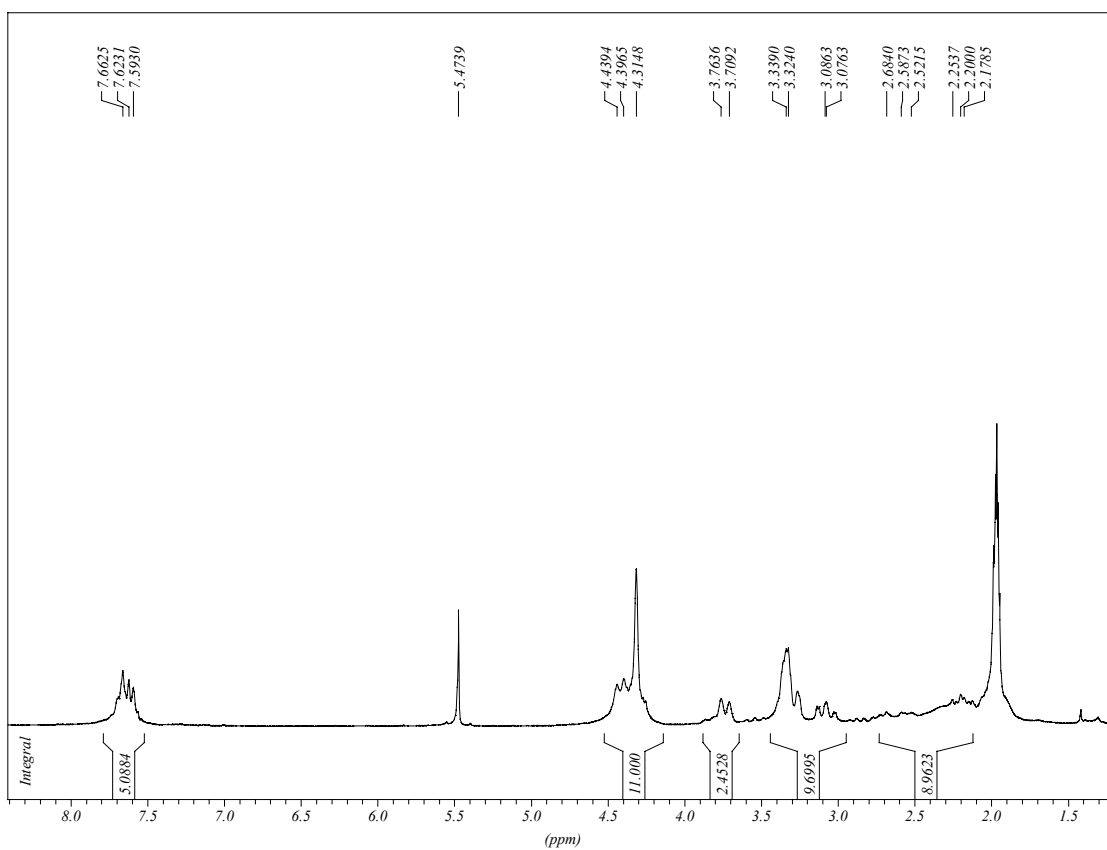
▪ [Pd(L17)](BF₄)₂



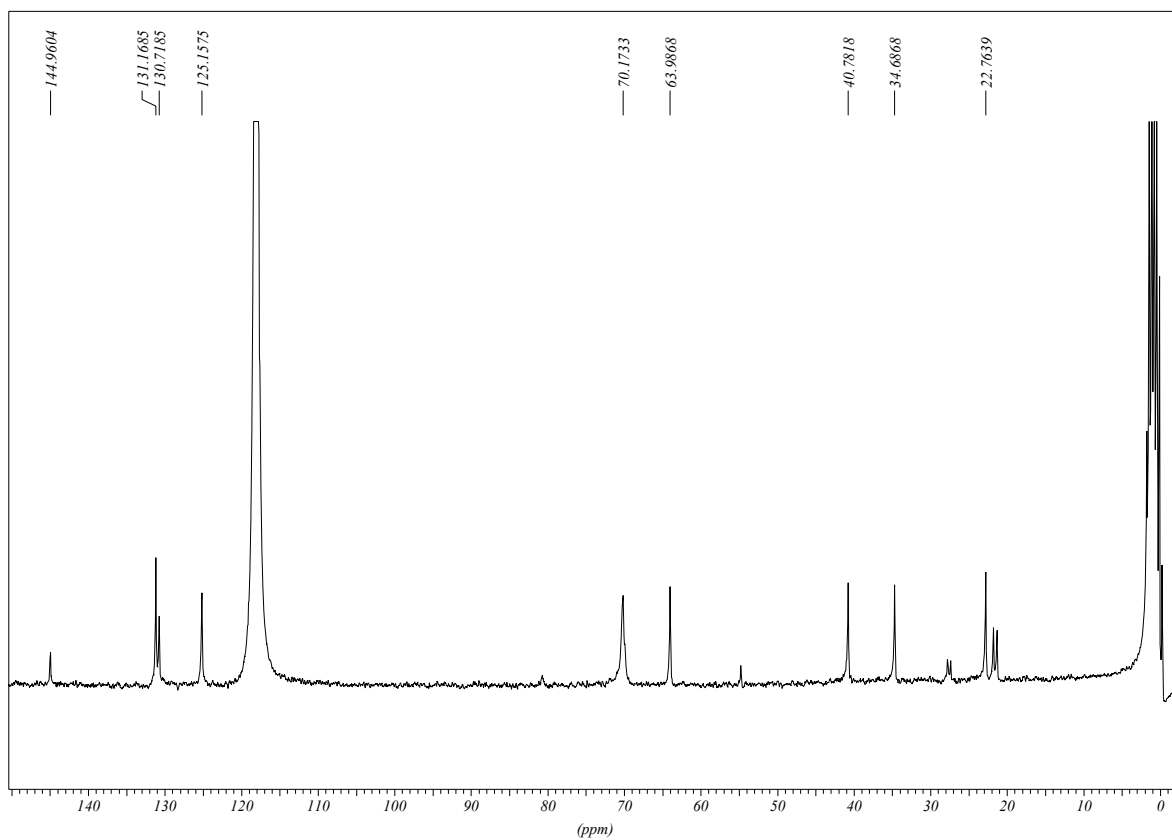
IR (ATR)



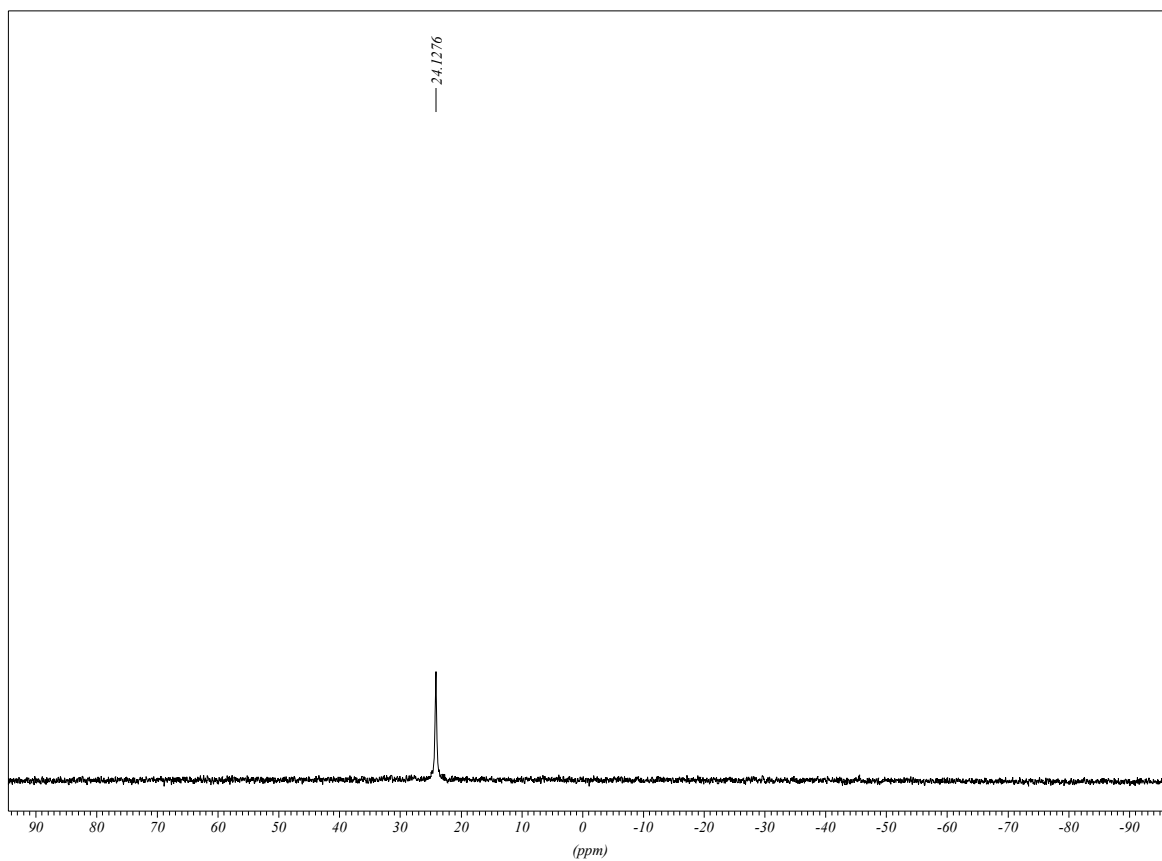
¹H RMN (CD₃CN)



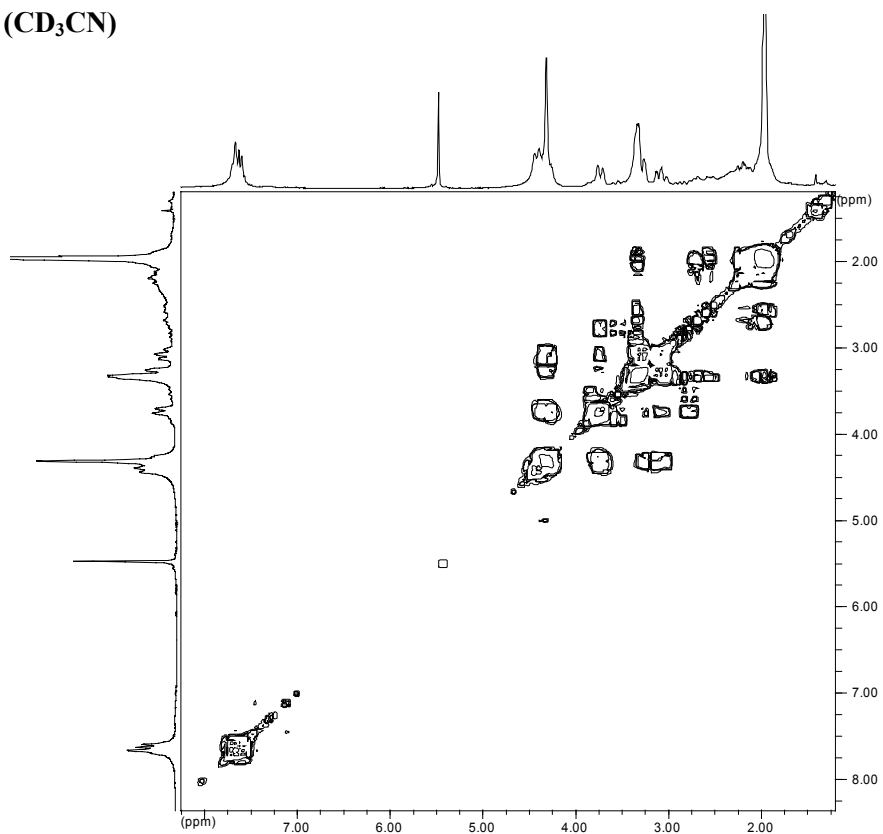
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



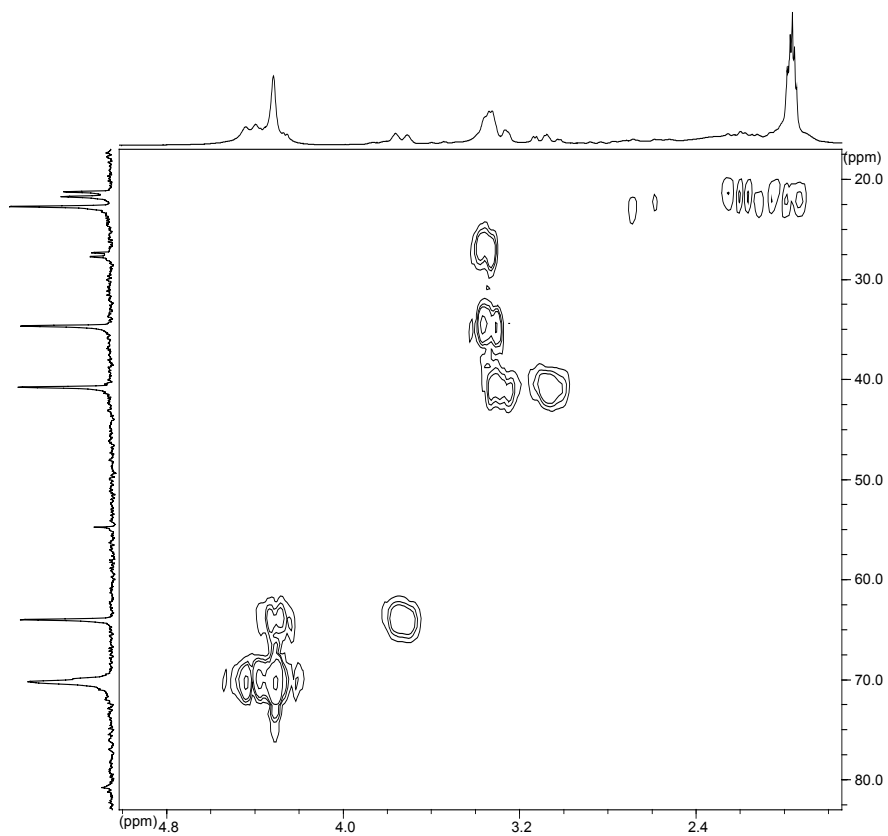
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



COSY (CD₃CN)

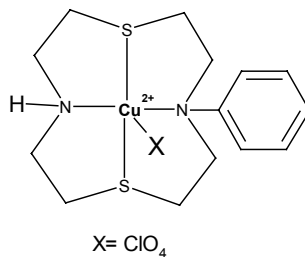


HMQC (CD₃CN). Ampliació zona alifàtica.

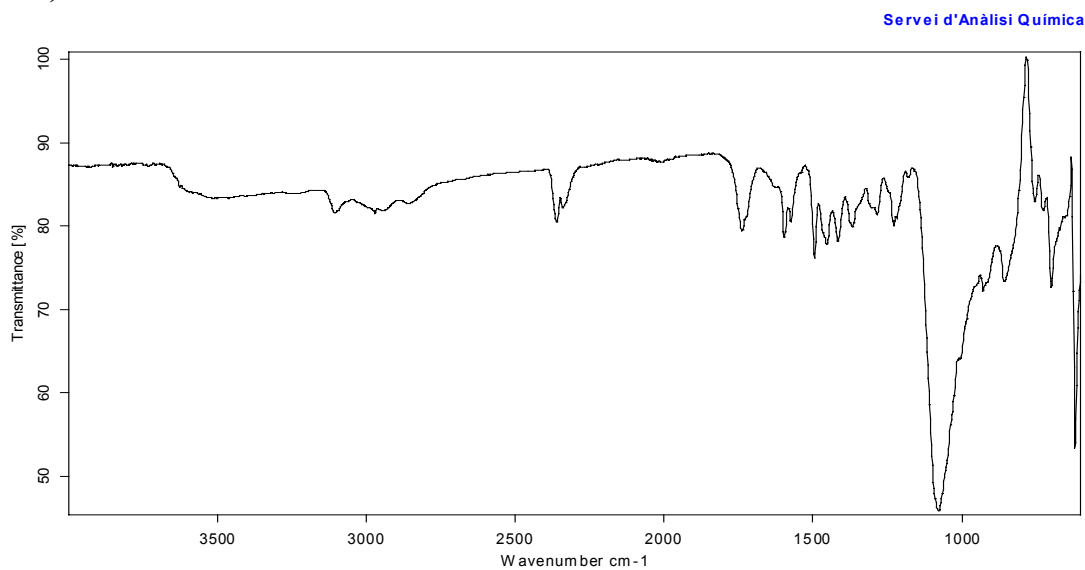


2 Complexos de Cu(II)

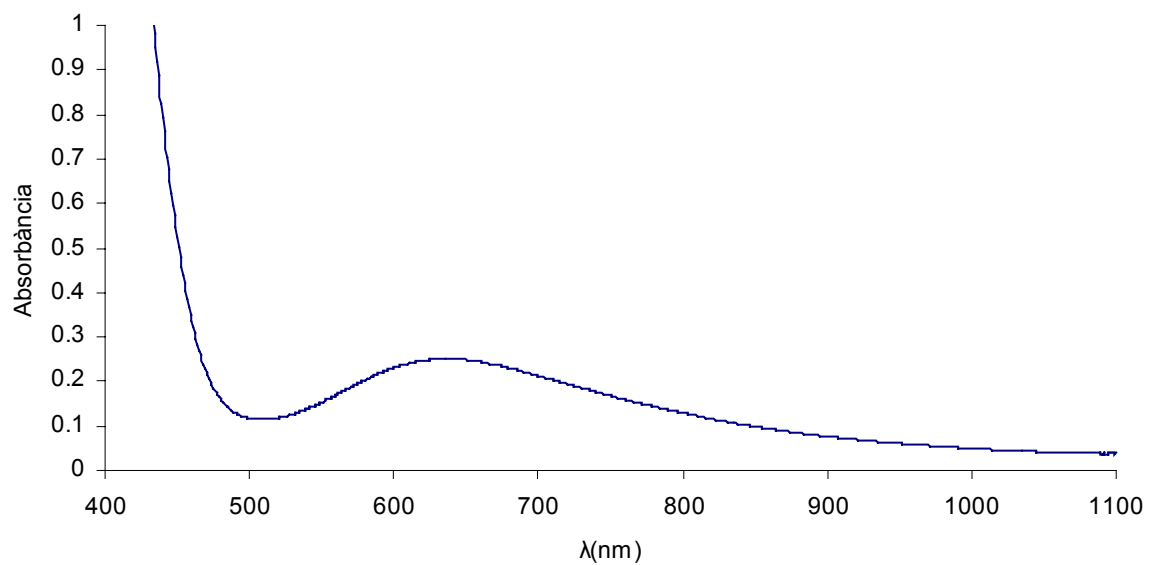
▪ $[\text{Cu}(\text{ClO}_4)(\text{L1})]\text{ClO}_4$



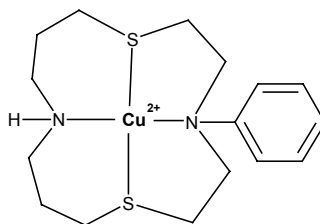
IR (ATR)



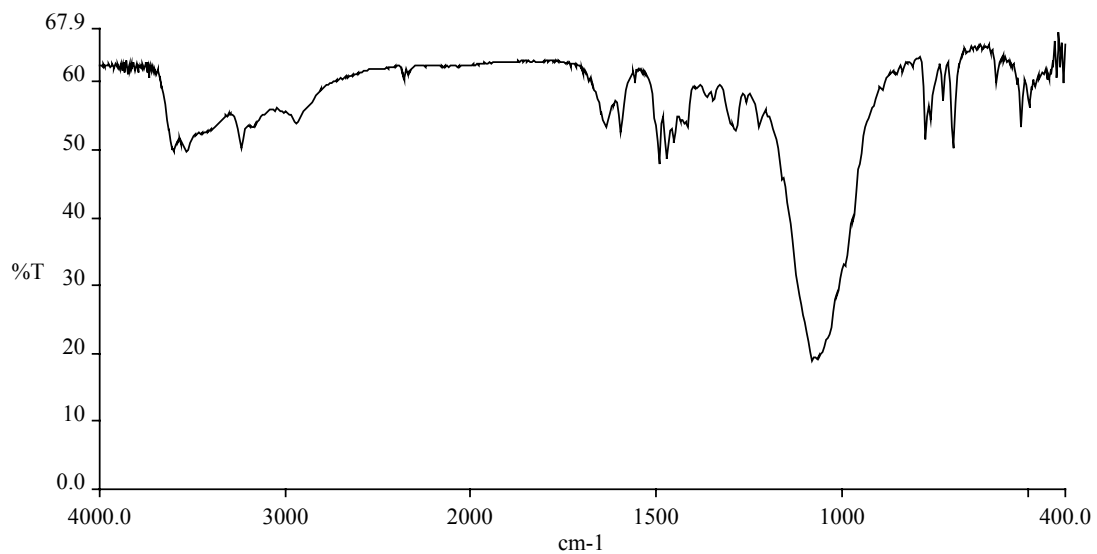
UV-VIS (CH₃COCH₃, 1 mM)



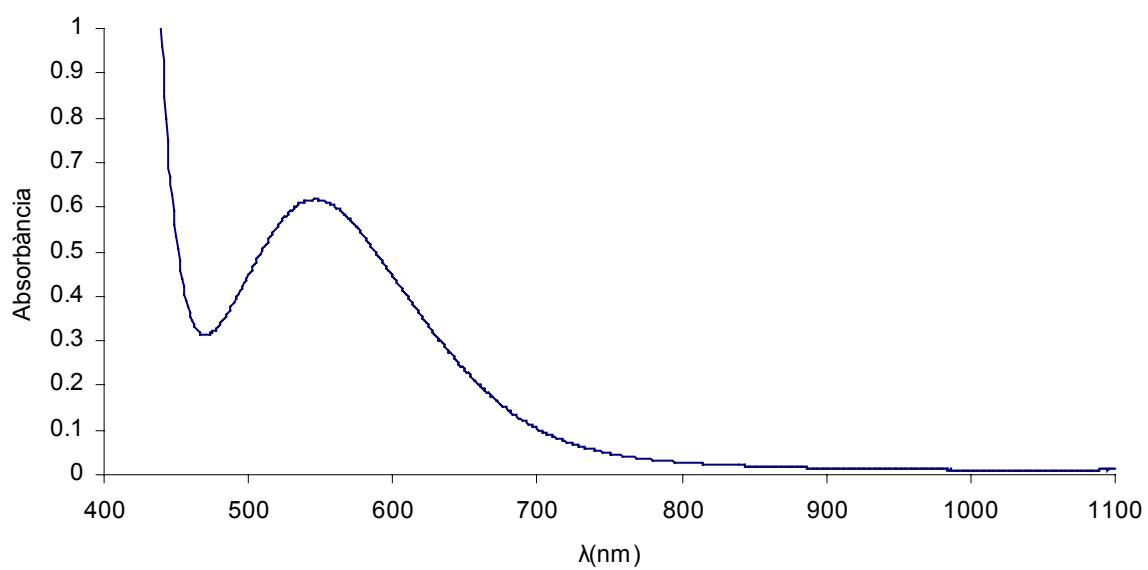
▪ $[\text{Cu}(\text{L2})](\text{BF}_4)_2$



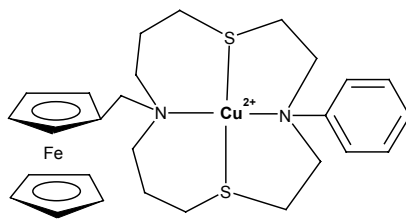
IR (KBr)



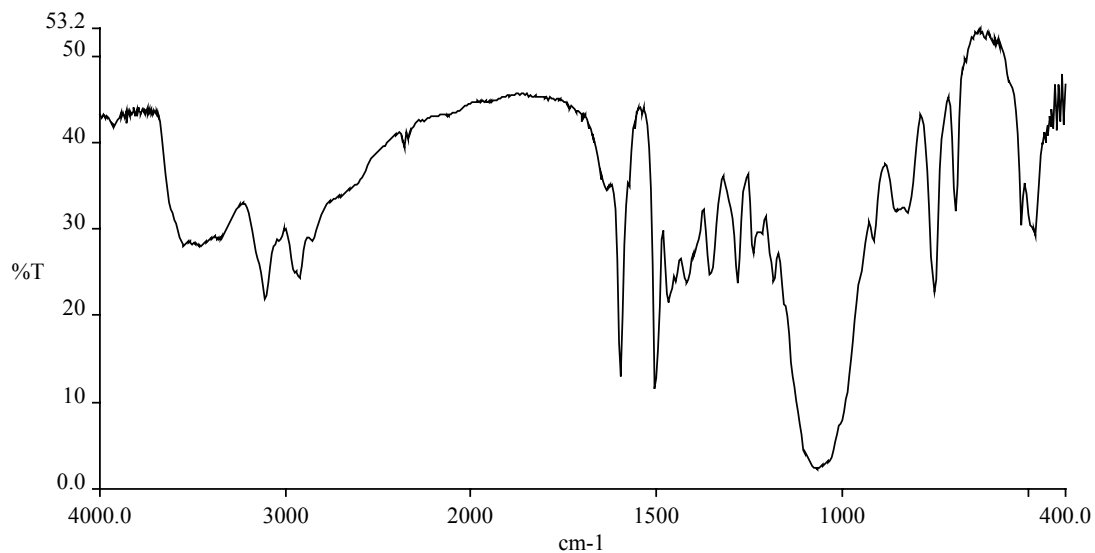
UV-VIS (CH_3COCH_3 , 1 mM)



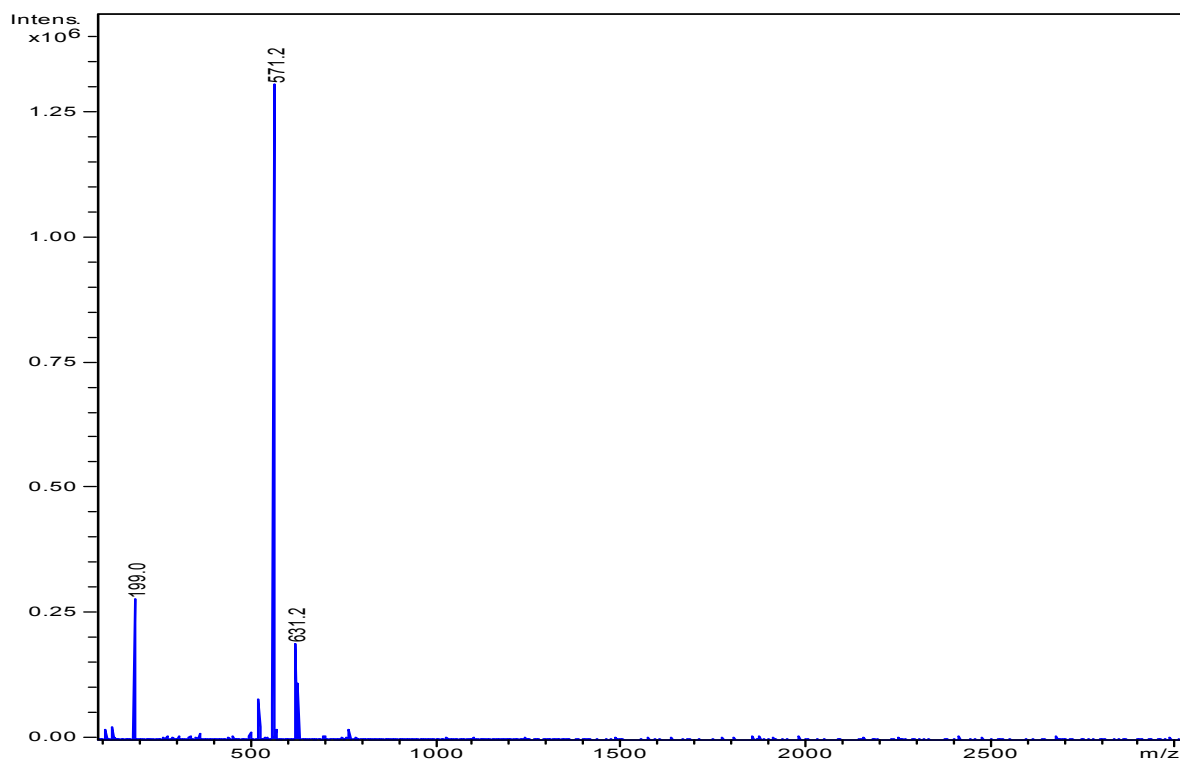
▪ [Cu(L15)](BF₄)₂



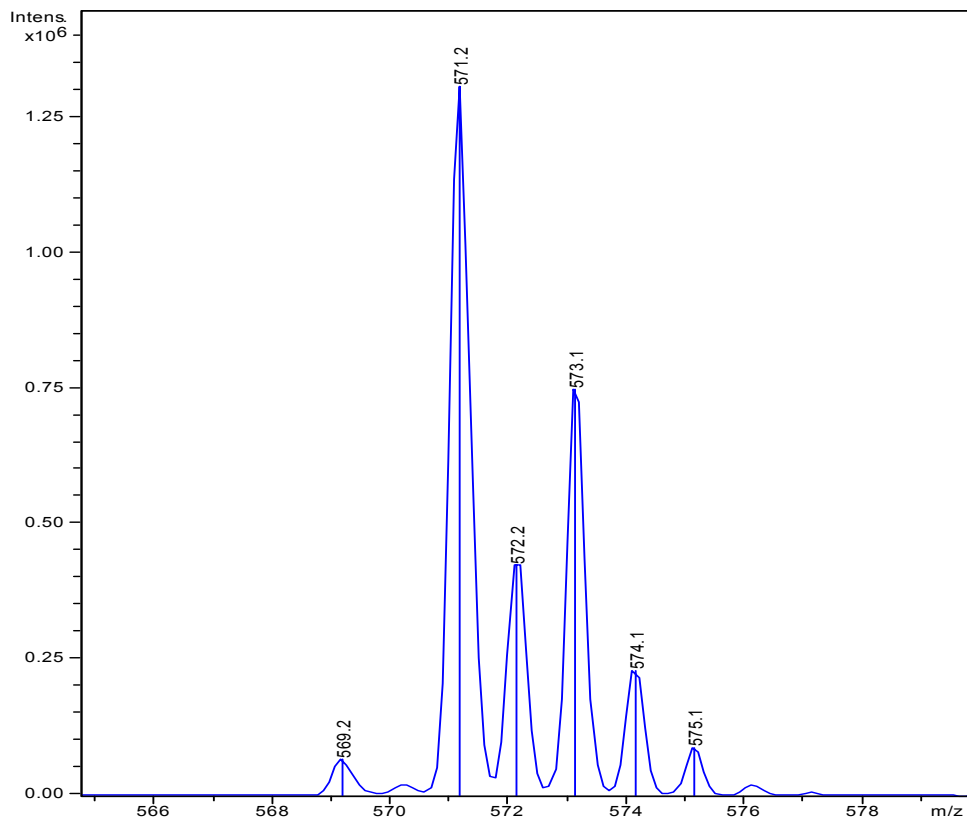
IR (KBr)



ESPECTROSCÒPIA DE MASSES (ESI(+)-IT) (10 ppm en MeOH)

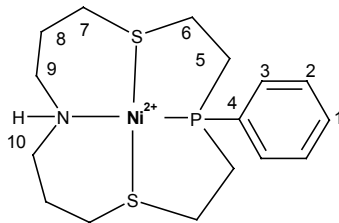


Ampliació pic 571.2 m/z

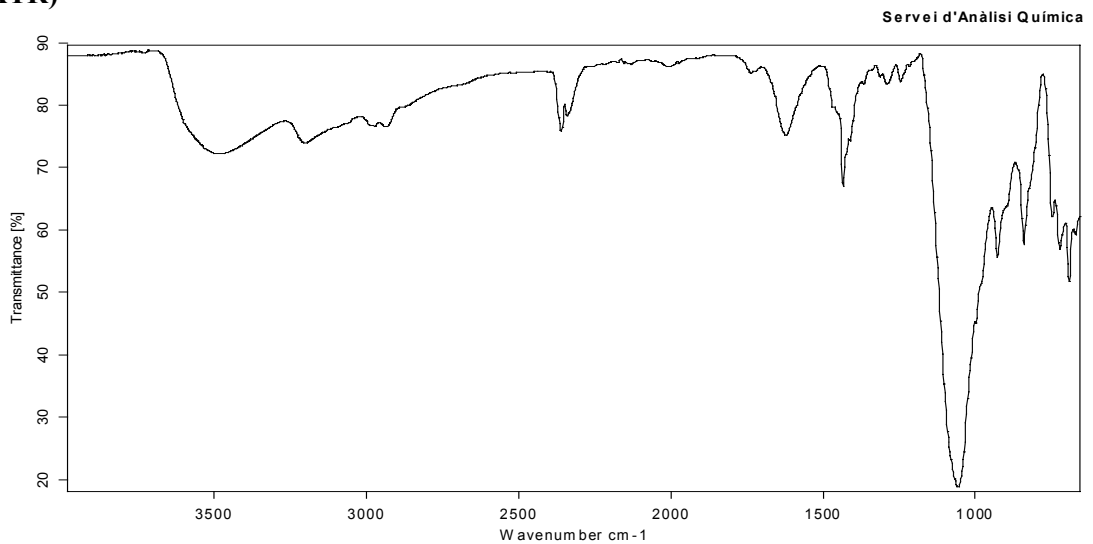


3 Complexos de Ni(II)

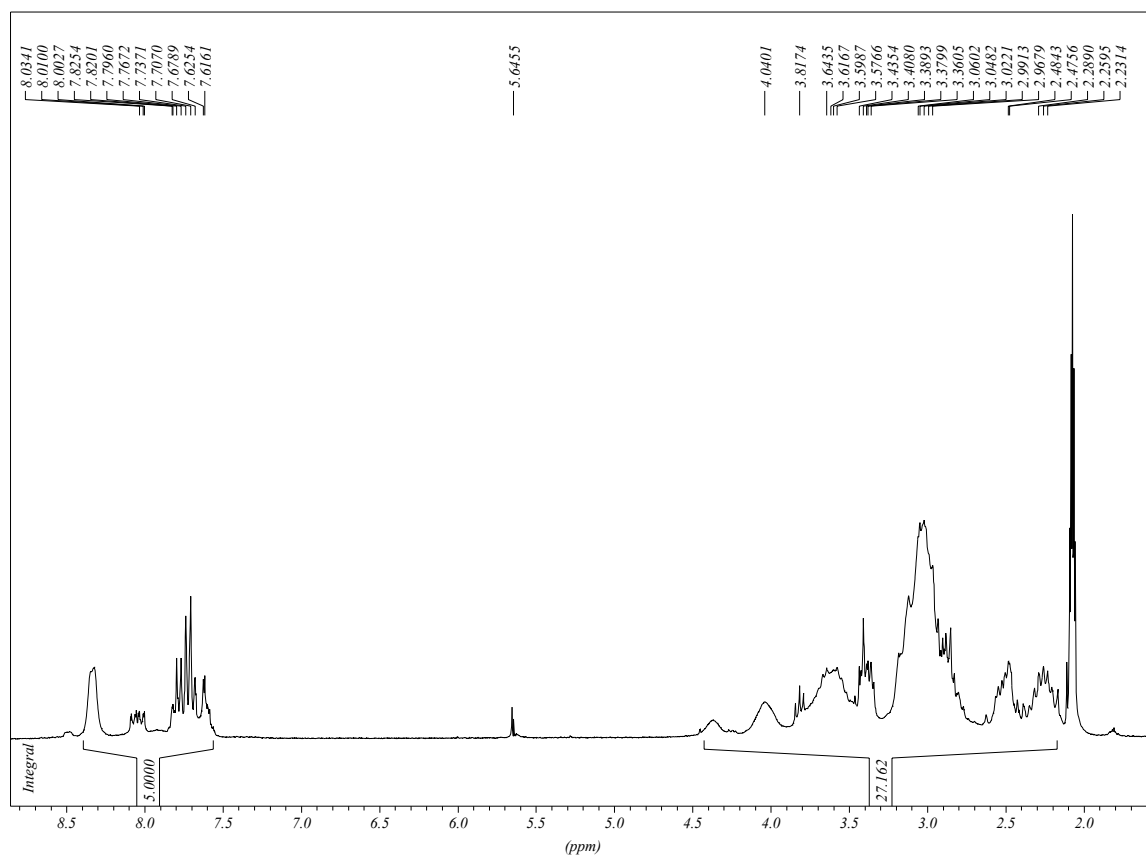
- $[\text{Ni}(\text{L}4)](\text{ClO}_4)_2$



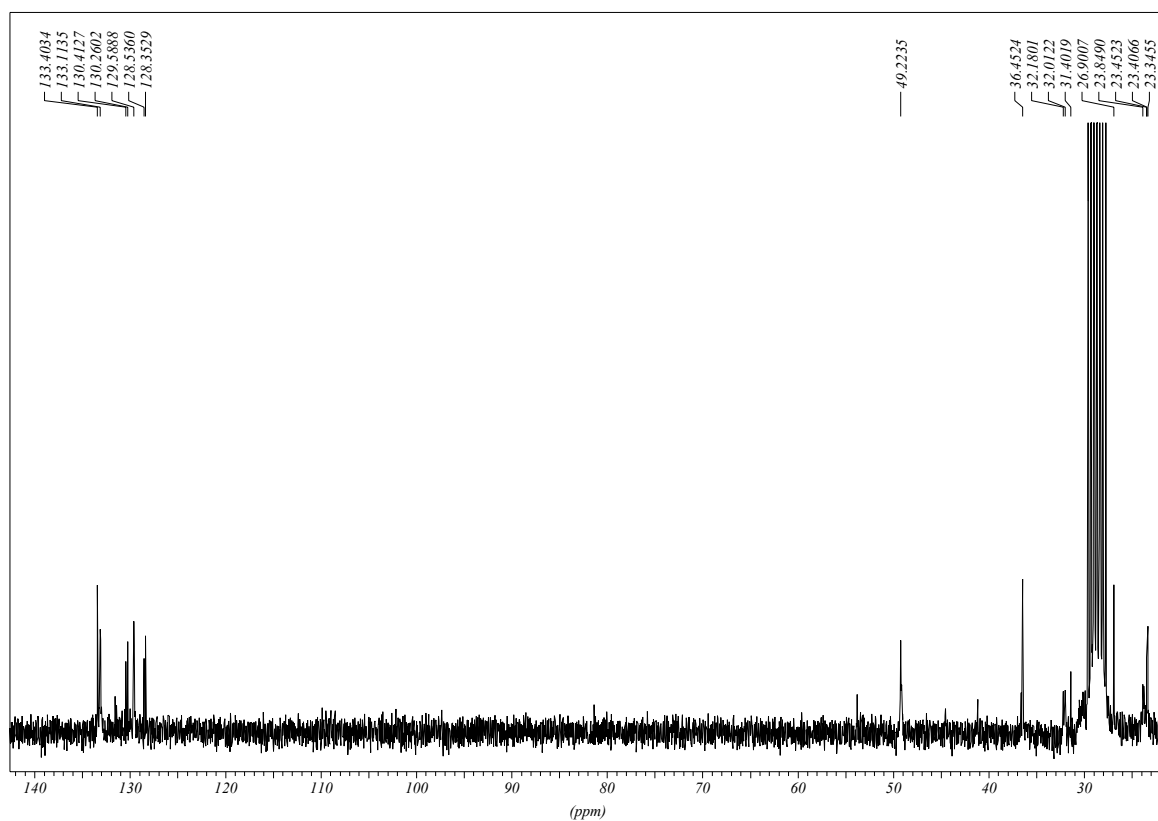
IR (ATR)



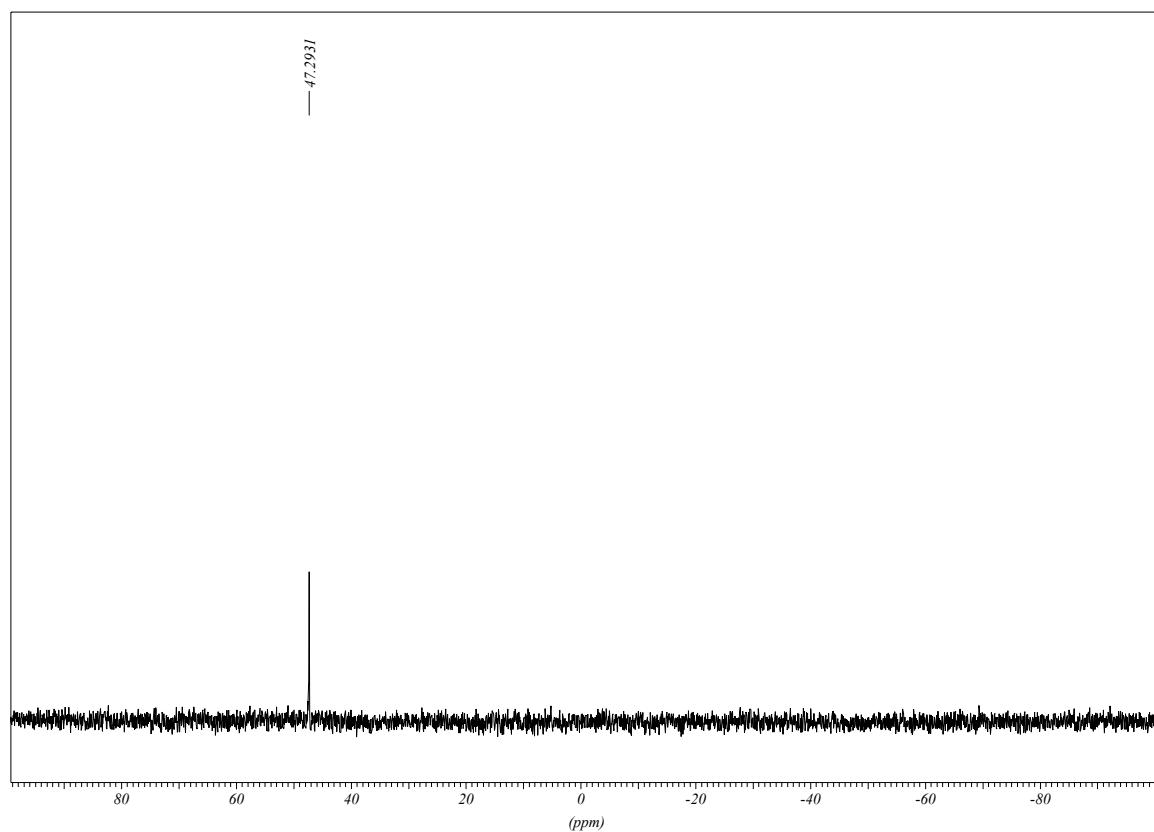
^1H RMN (CD_3COCD_3)



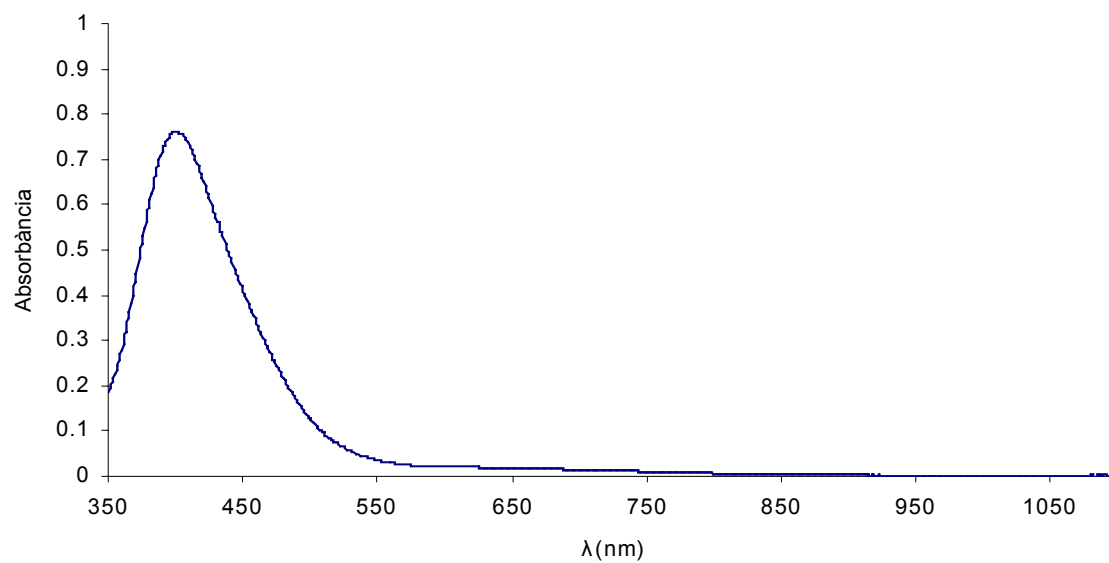
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3COCD_3)



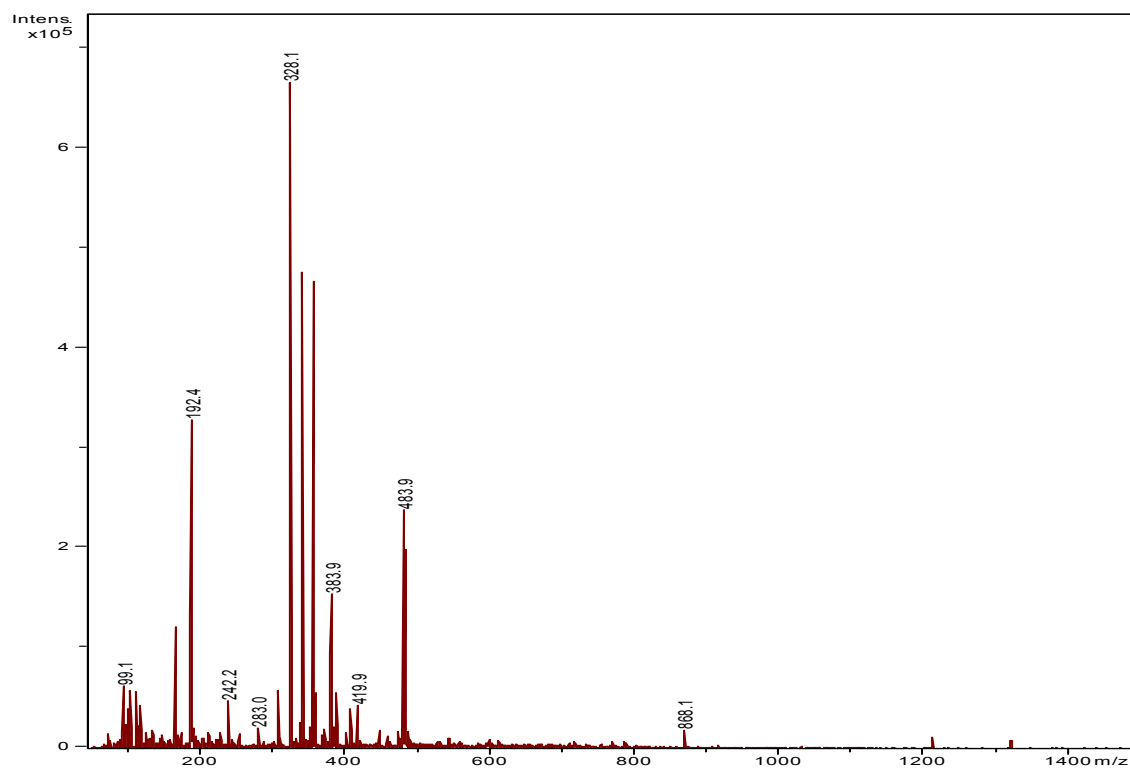
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3COCD_3)



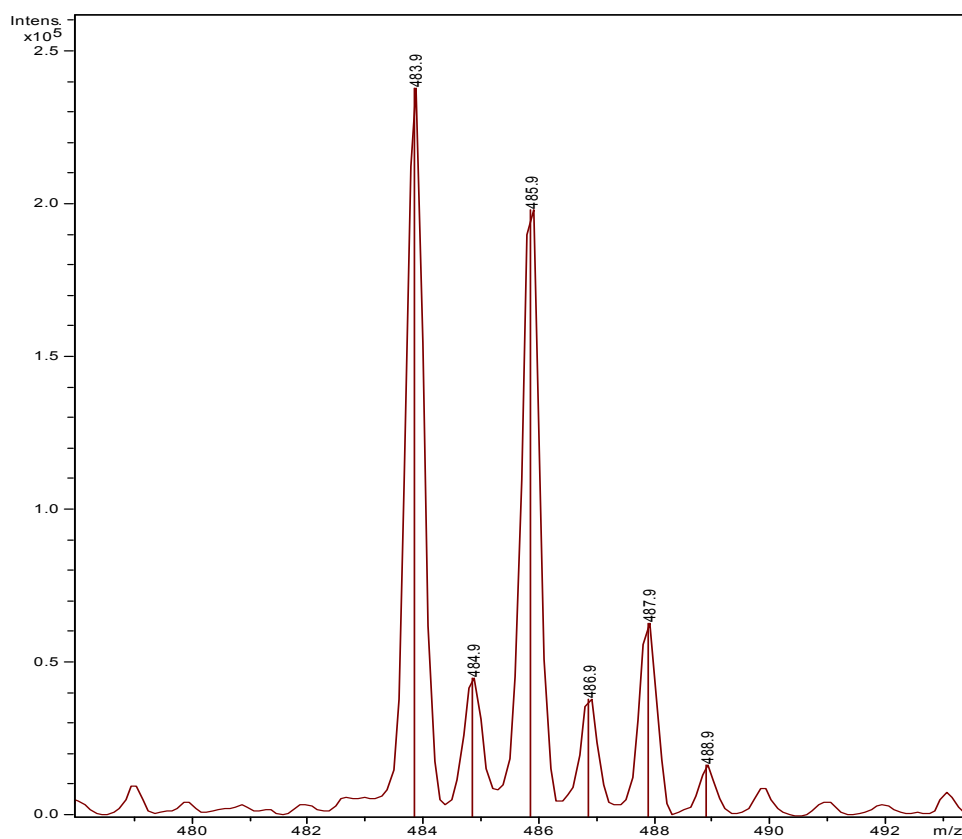
UV-VIS (CH_3COCH_3 , 1 mM)



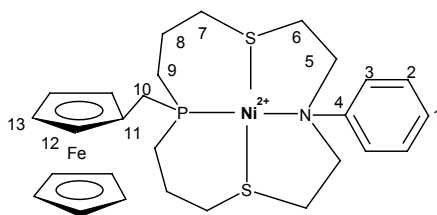
ESPECTROSCÒPIA DE MASSES (ESI(+)-IT) (20 ppm en MeOH)



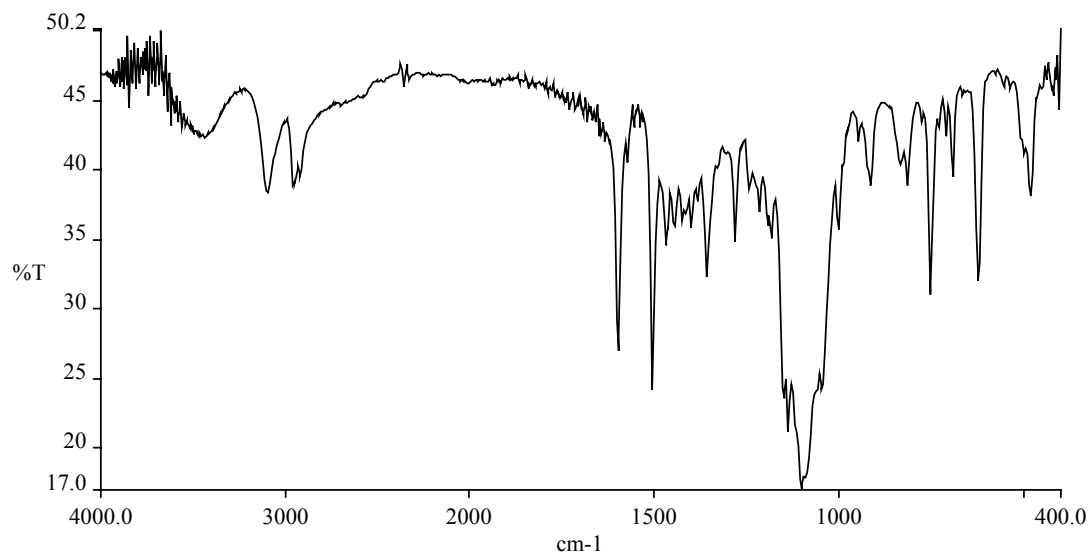
Ampliació del pic a 483.9 m/z



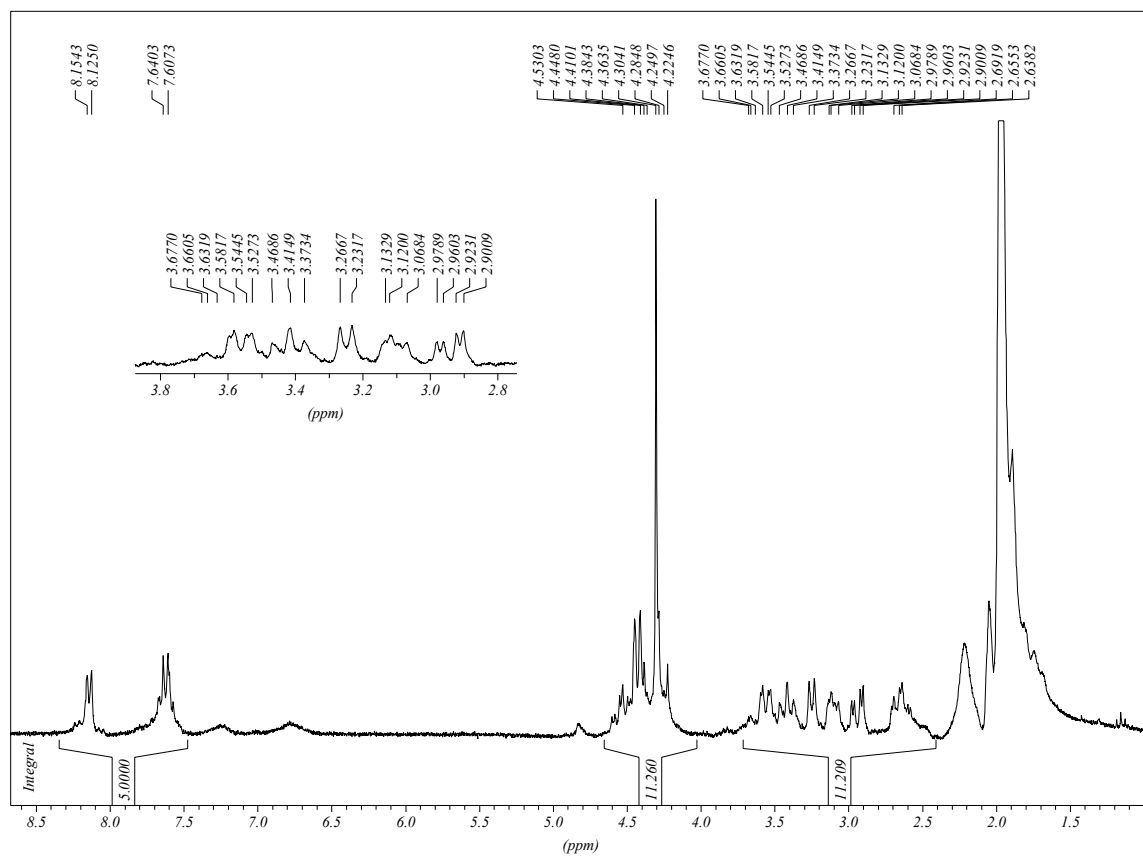
▪ $[\text{Ni}(\text{L17})](\text{ClO}_4)_2$



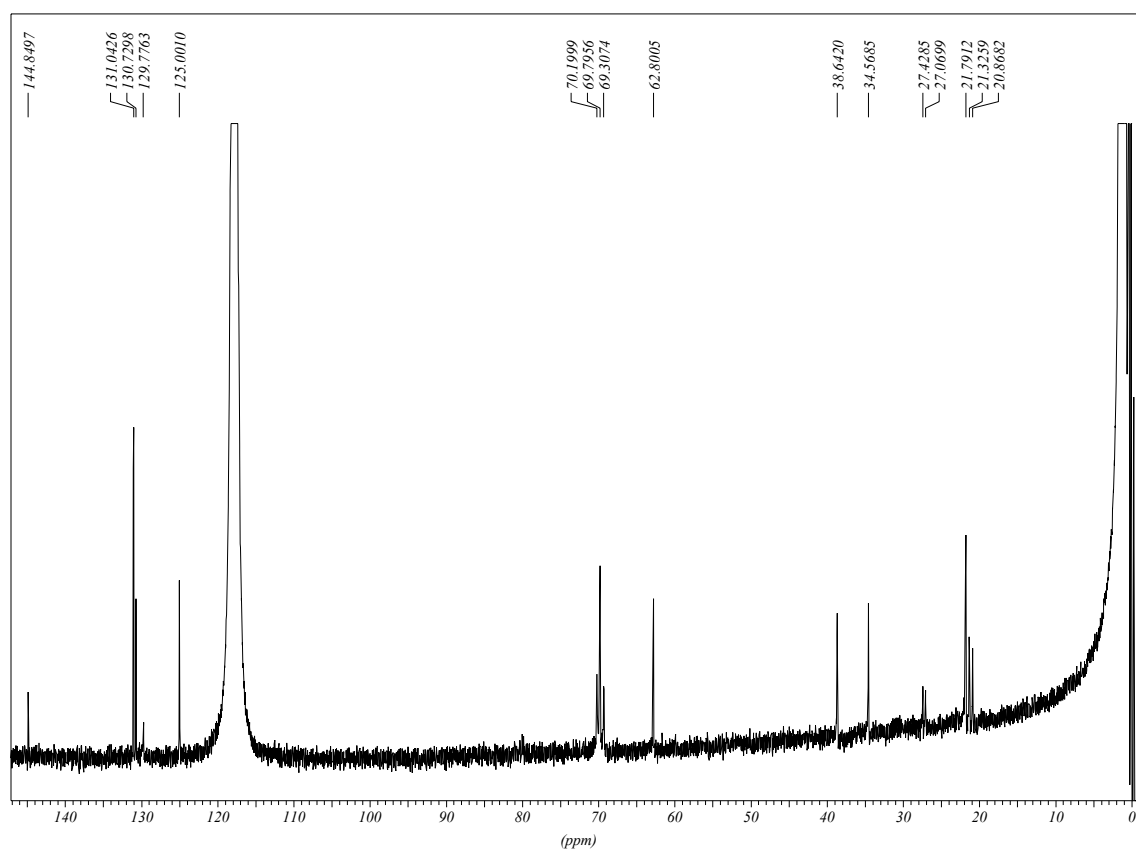
IR (ATR)



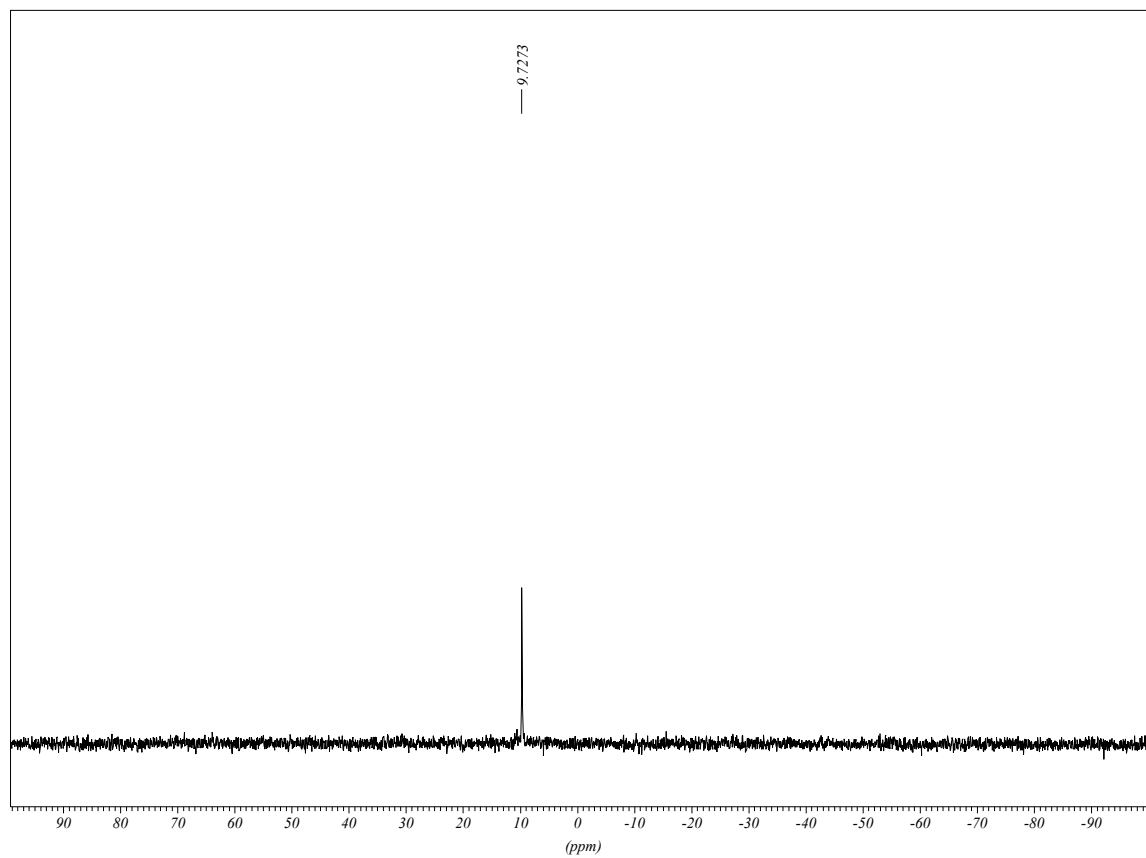
^1H RMN (CD_3CN)



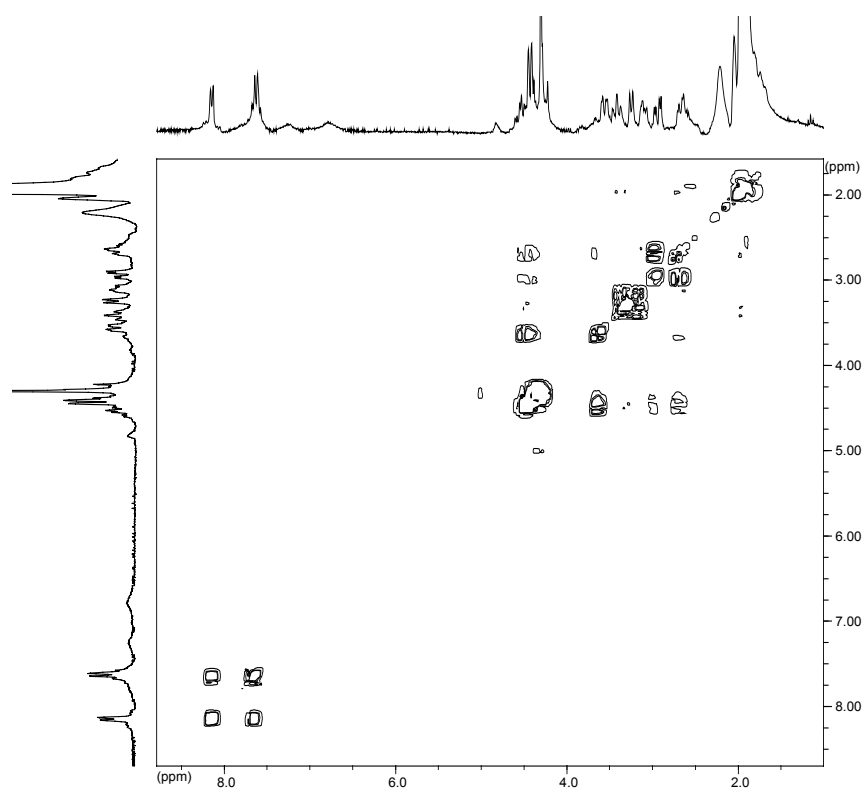
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



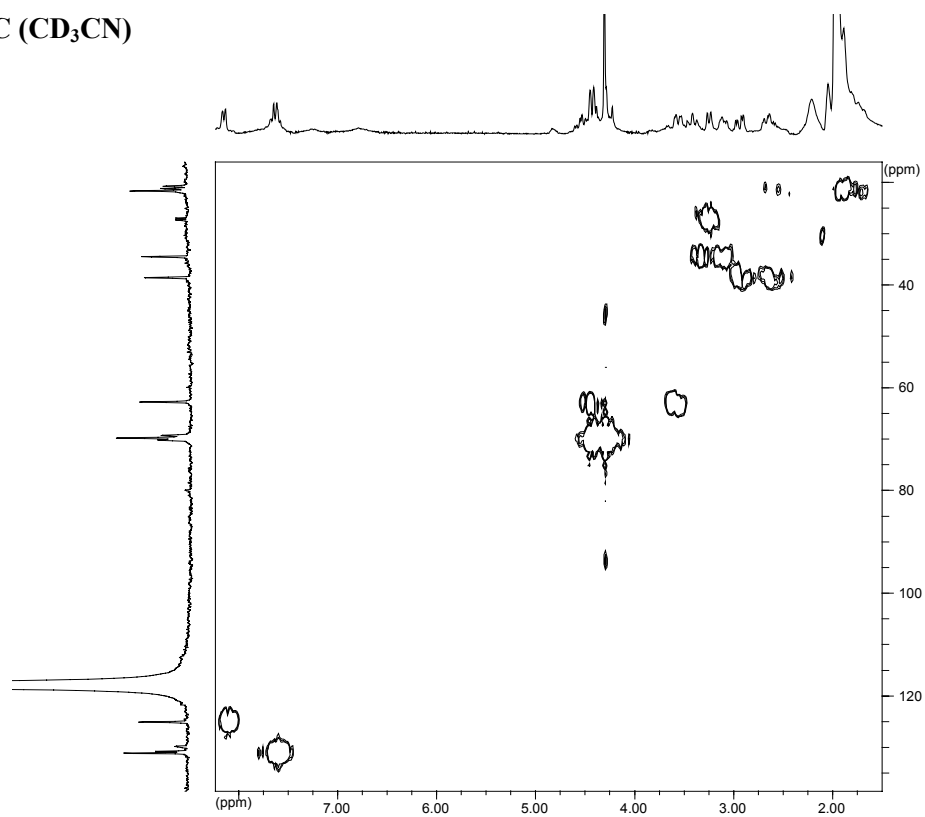
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



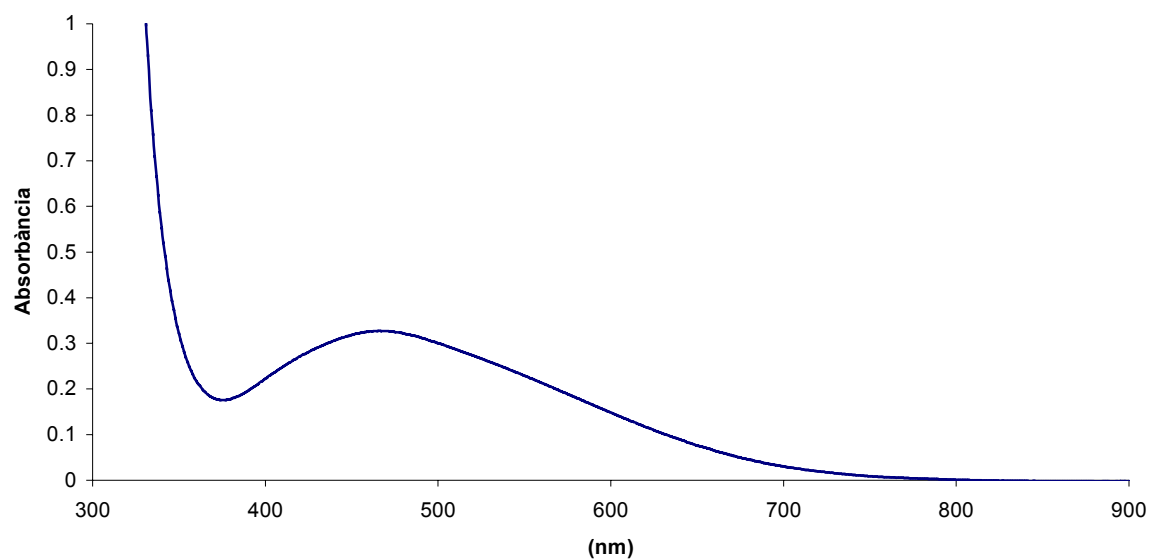
COSY (CD₃CN)



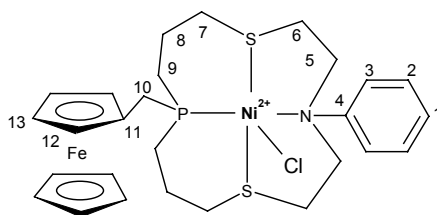
HMQC (CD₃CN)



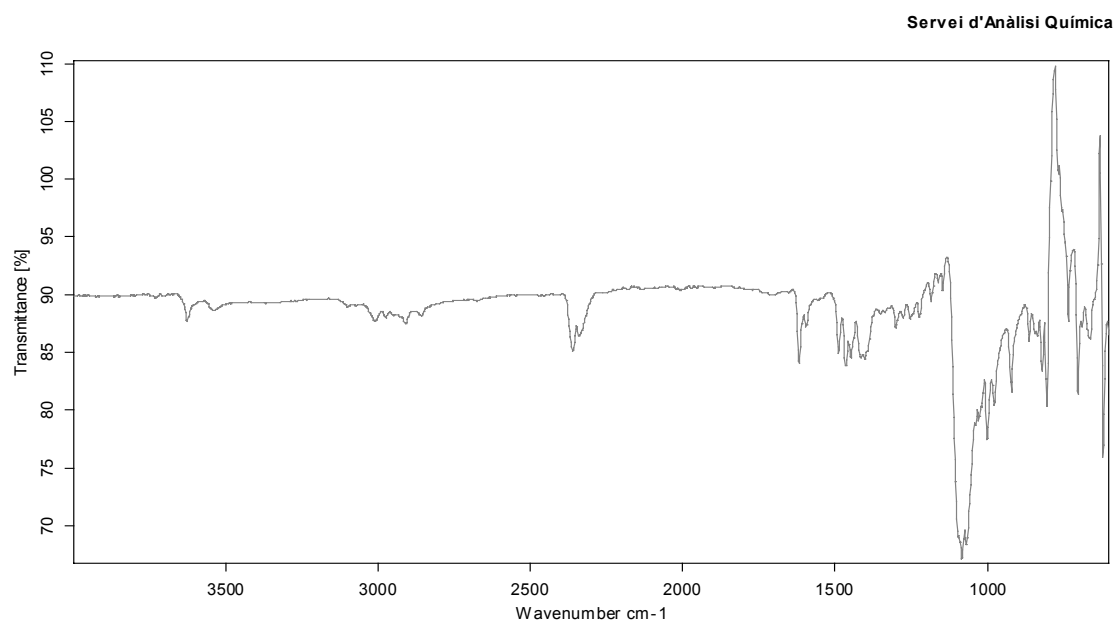
UV-VIS (CH₃CN, 1 mM)



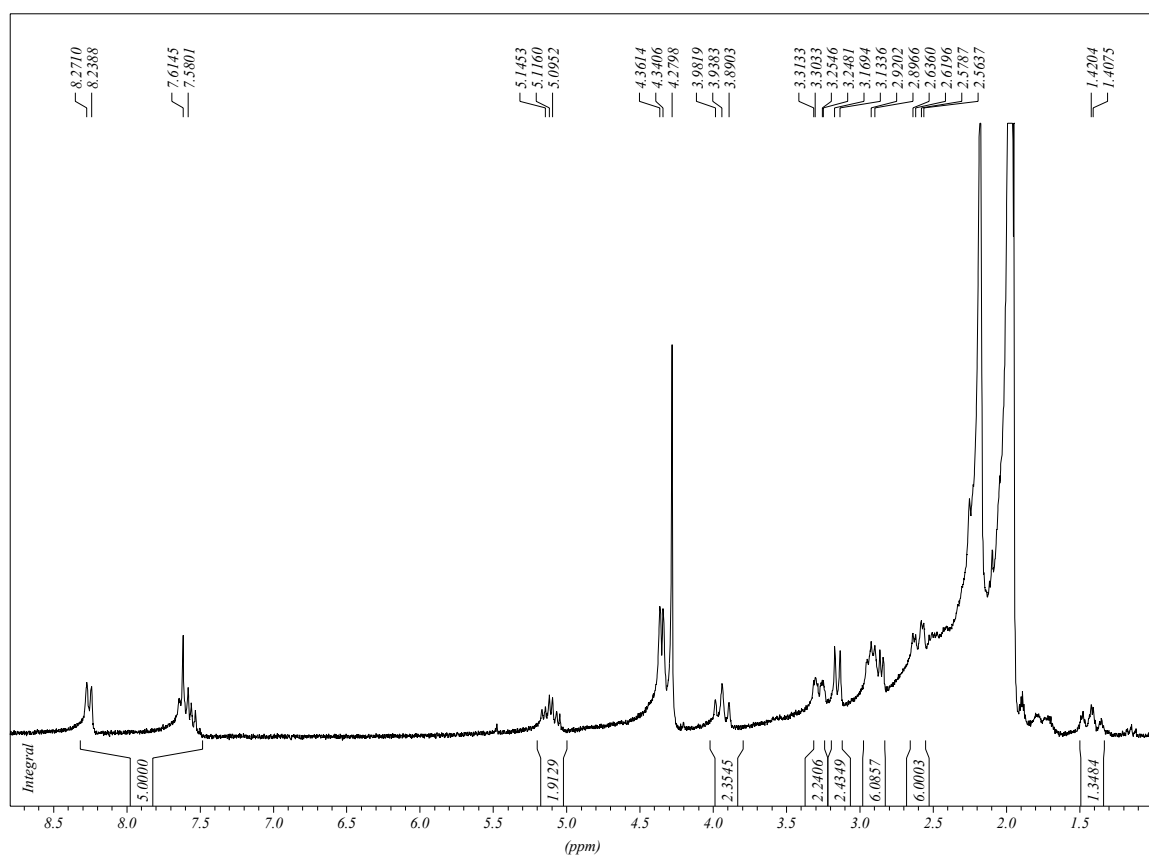
▪ [NiCl(L17)]ClO₄



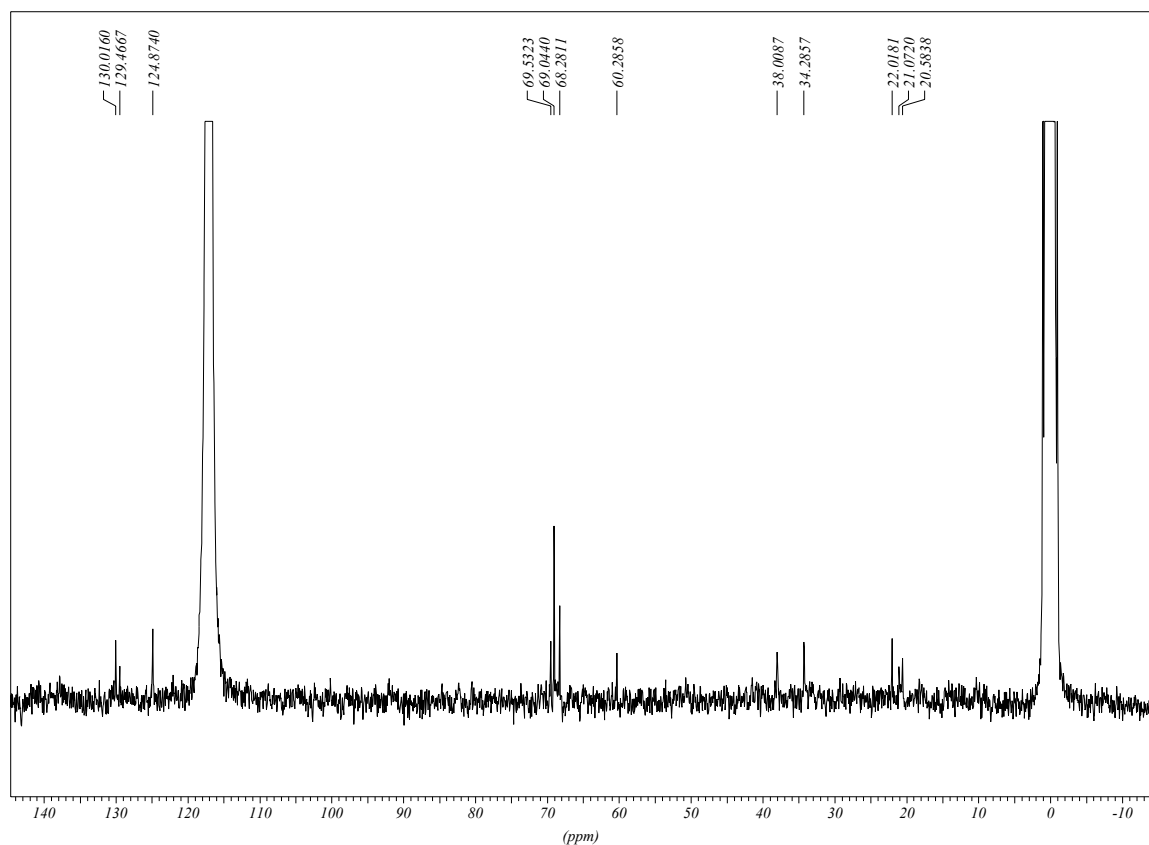
IR (ATR)



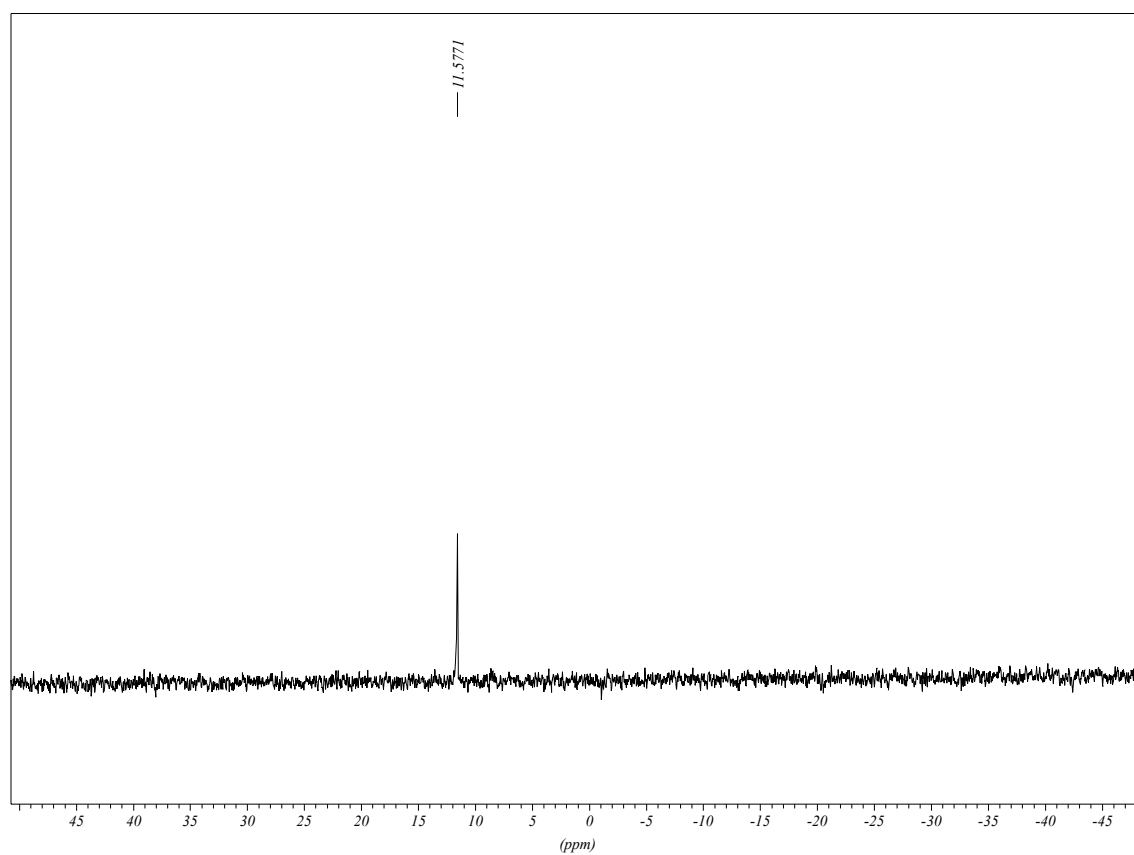
^1H RMN (CD_3CN)



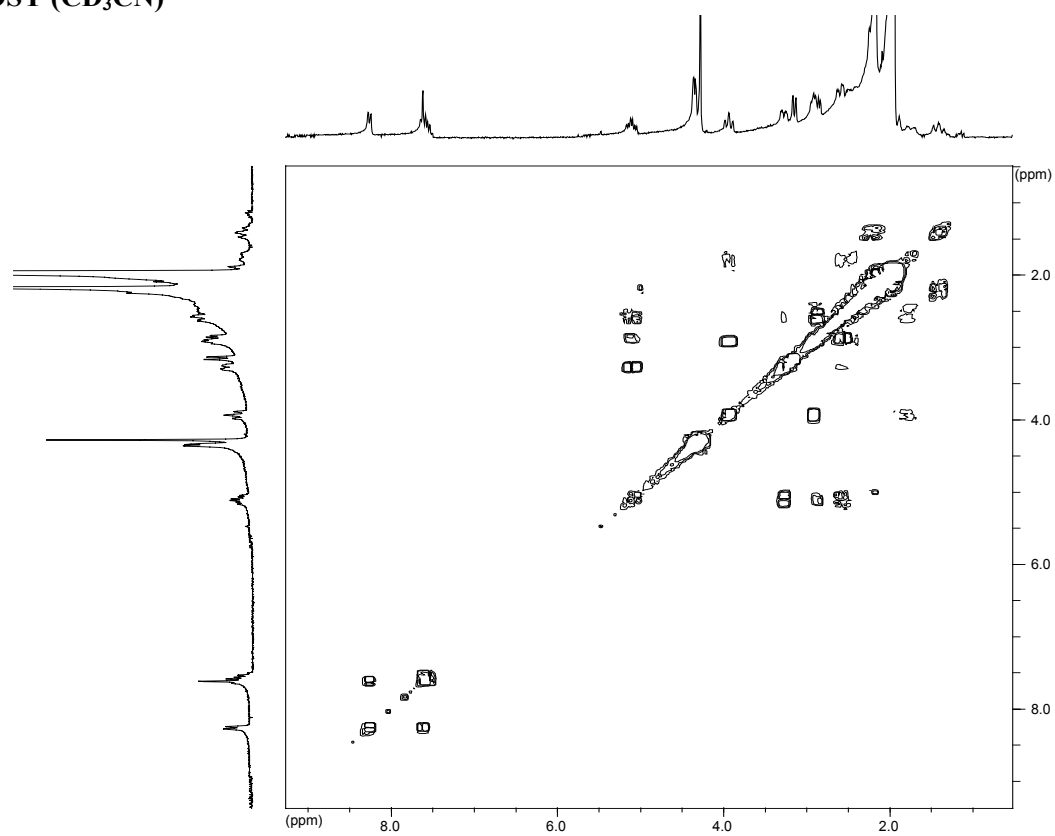
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



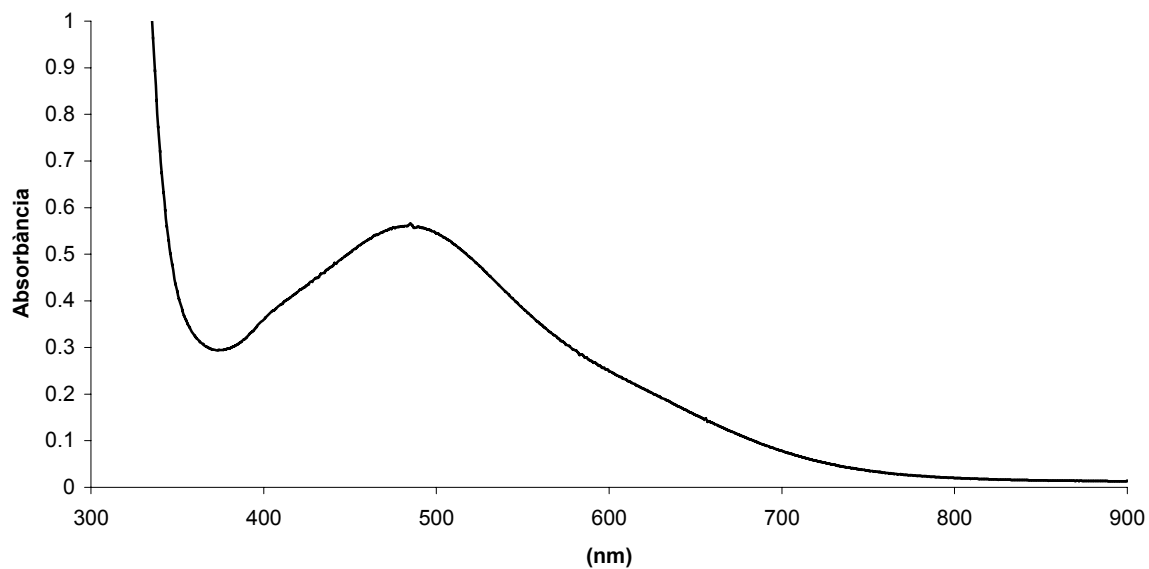
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



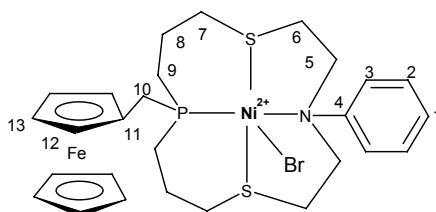
COSY (CD_3CN)



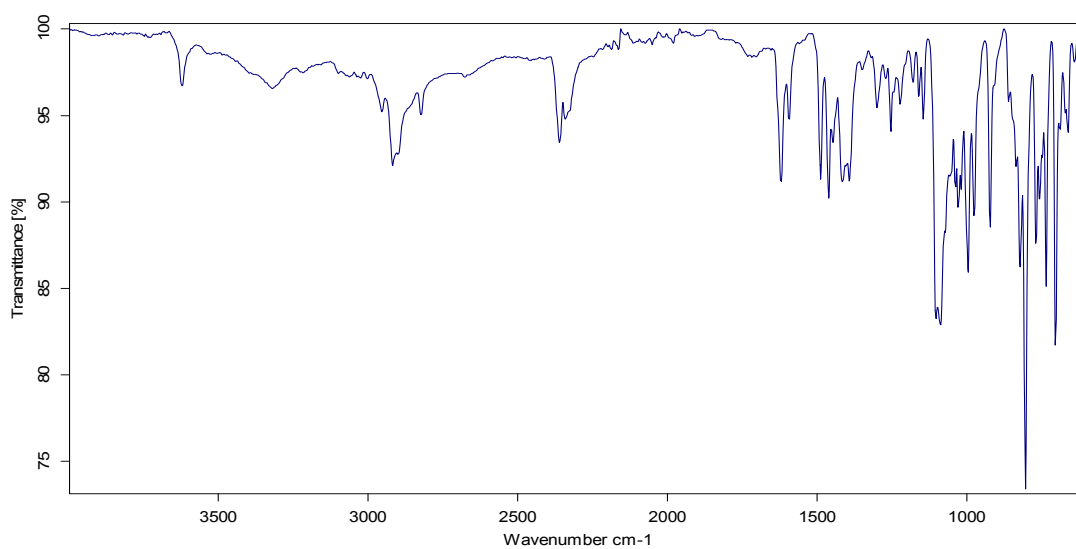
UV-VIS (CH₃CN, 1 mM)



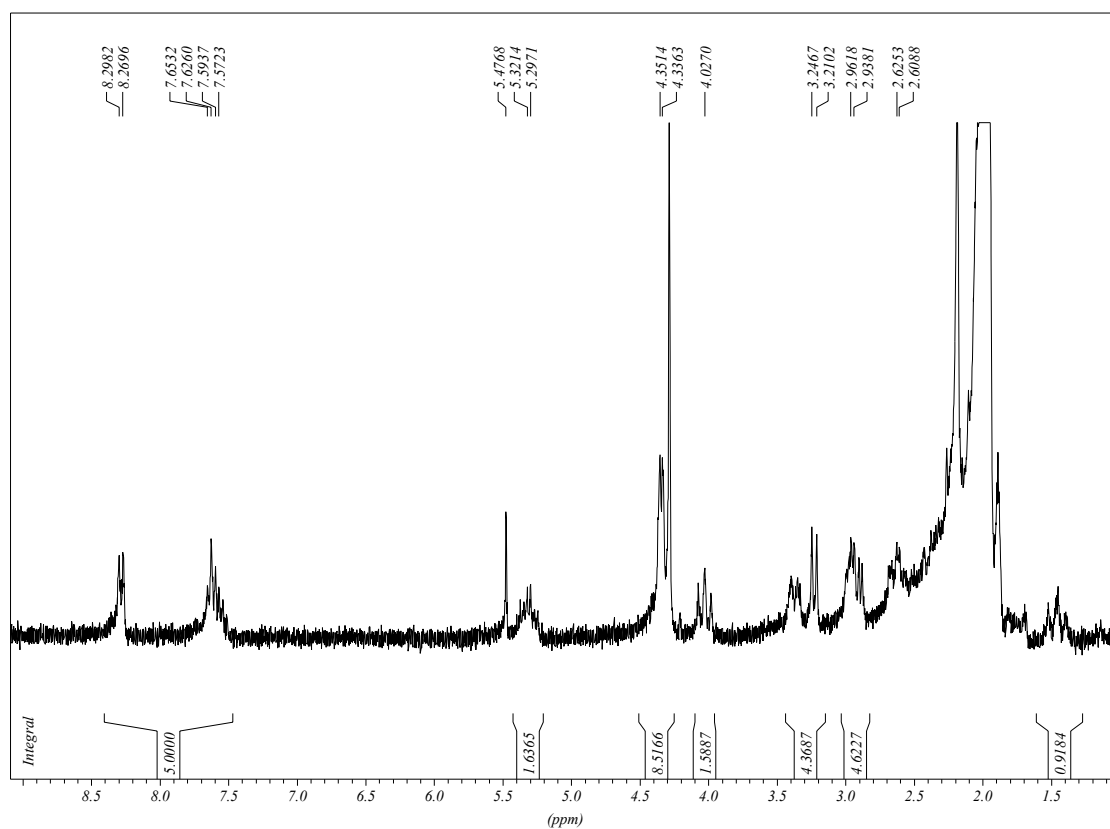
▪ [NiBr(L17)]ClO₄



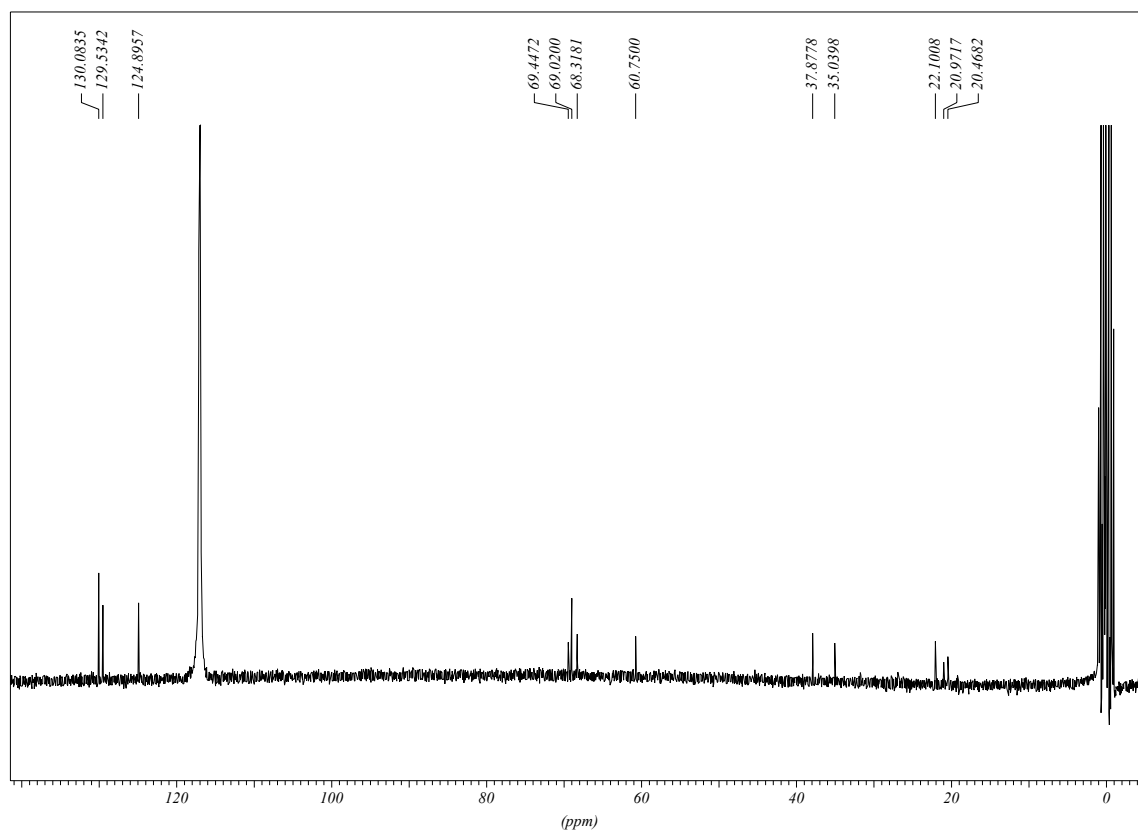
IR (ATR)



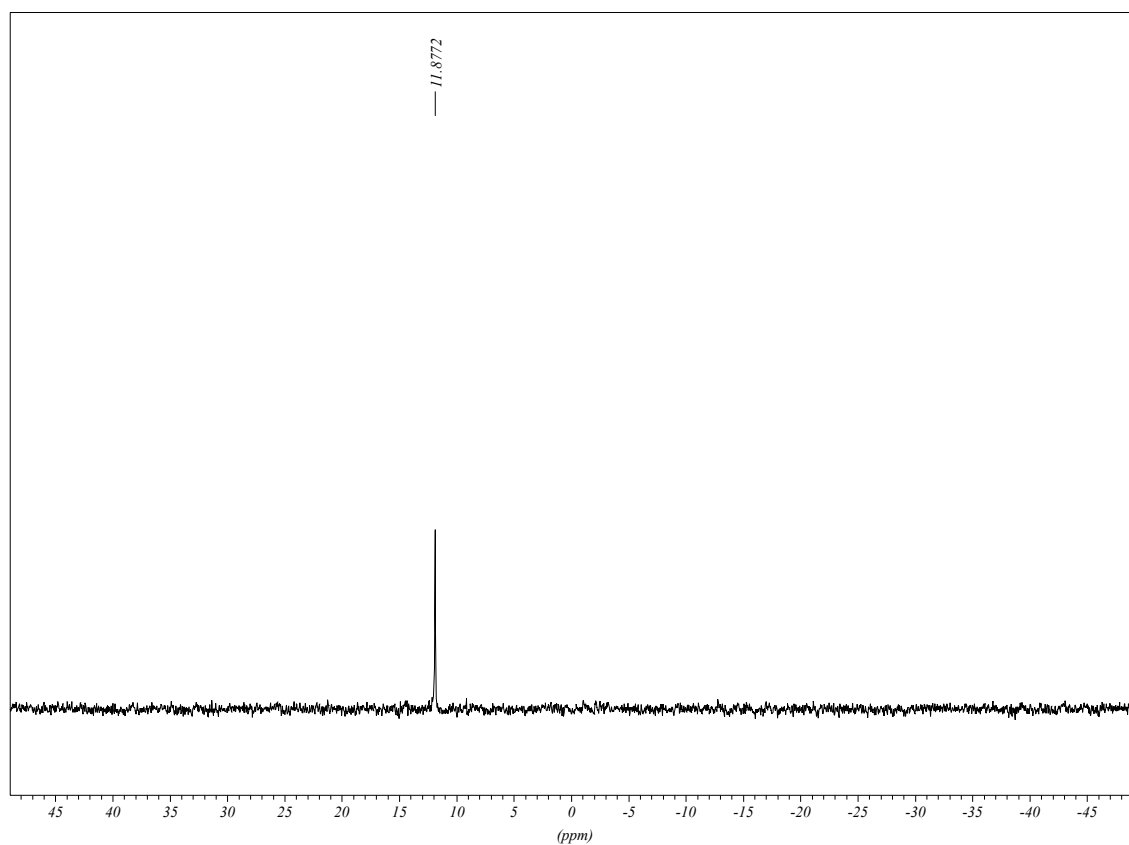
^1H RMN (CD_3CN)



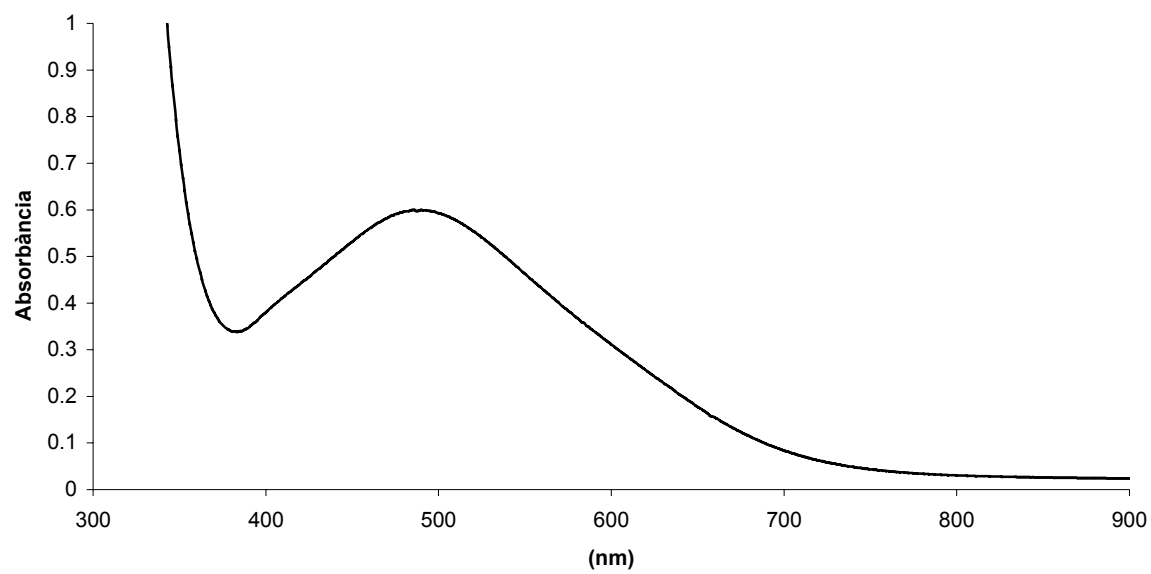
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



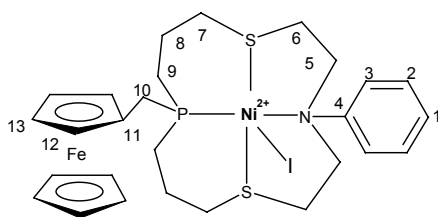
$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



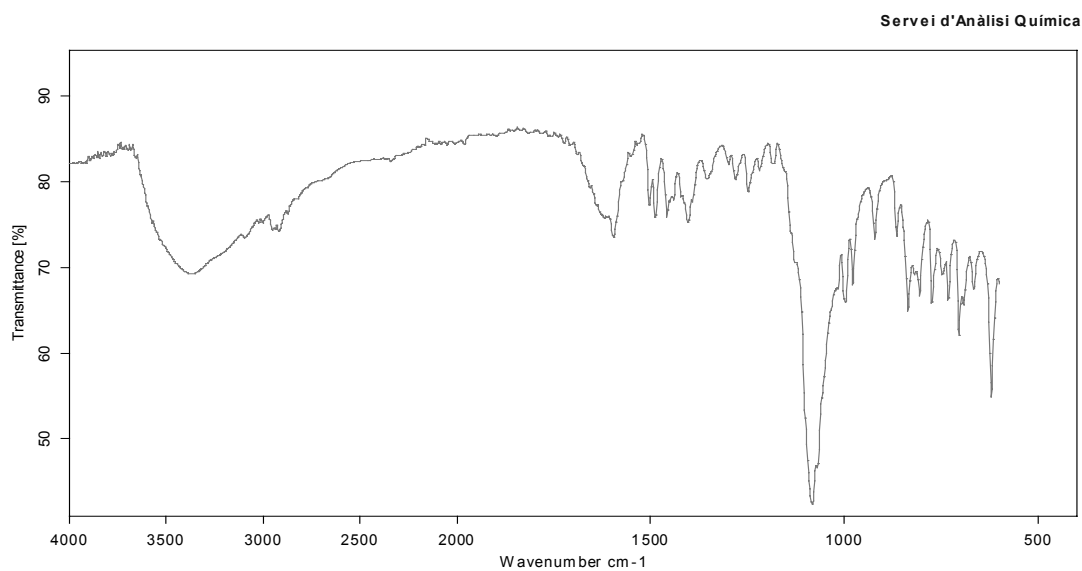
UV-VIS (CH_3CN , 1 mM)



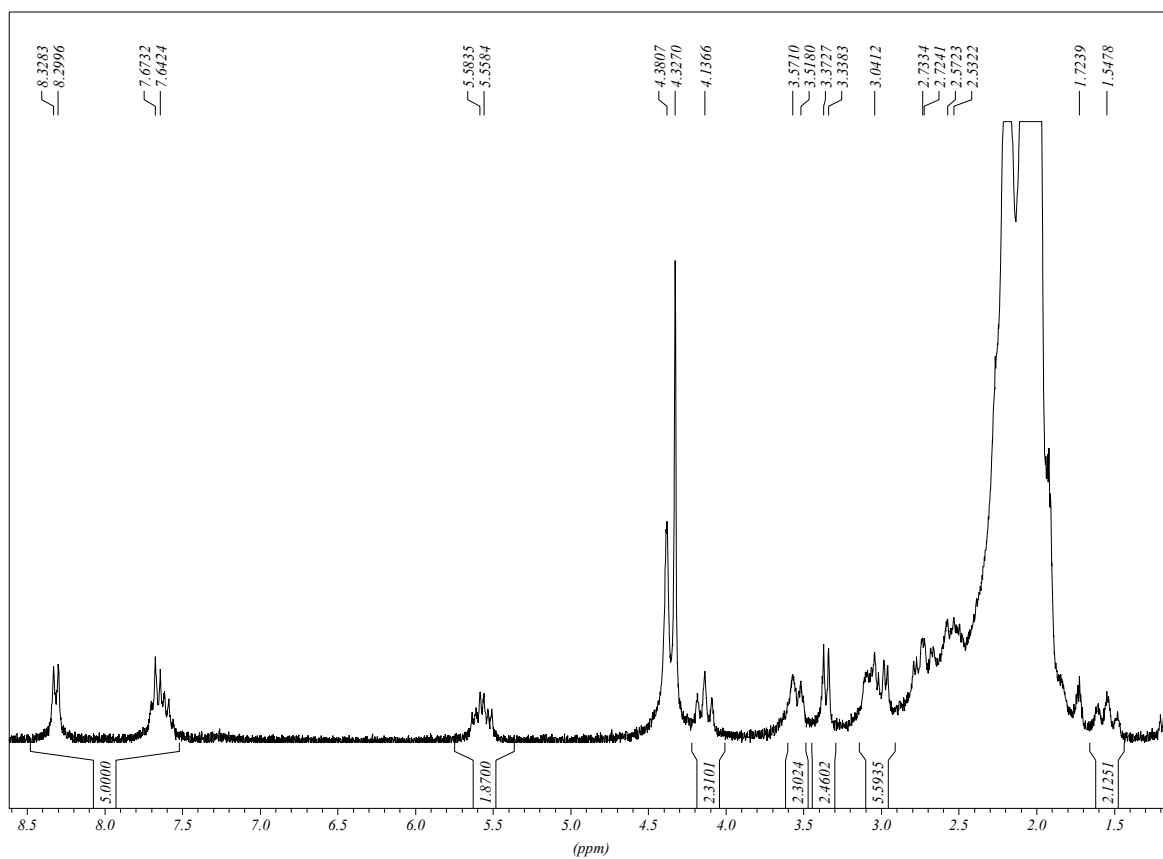
▪ $[\text{Ni}(\text{L17})]\text{ClO}_4$



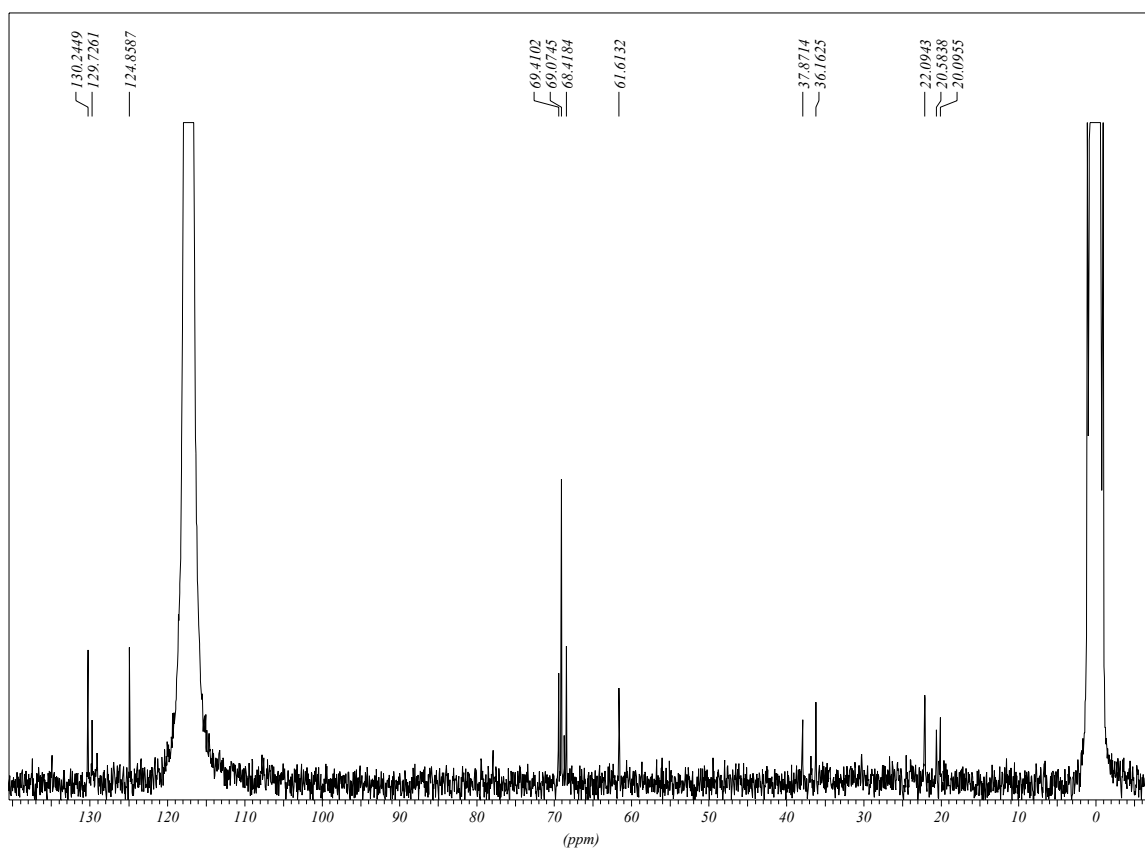
IR (ATR)



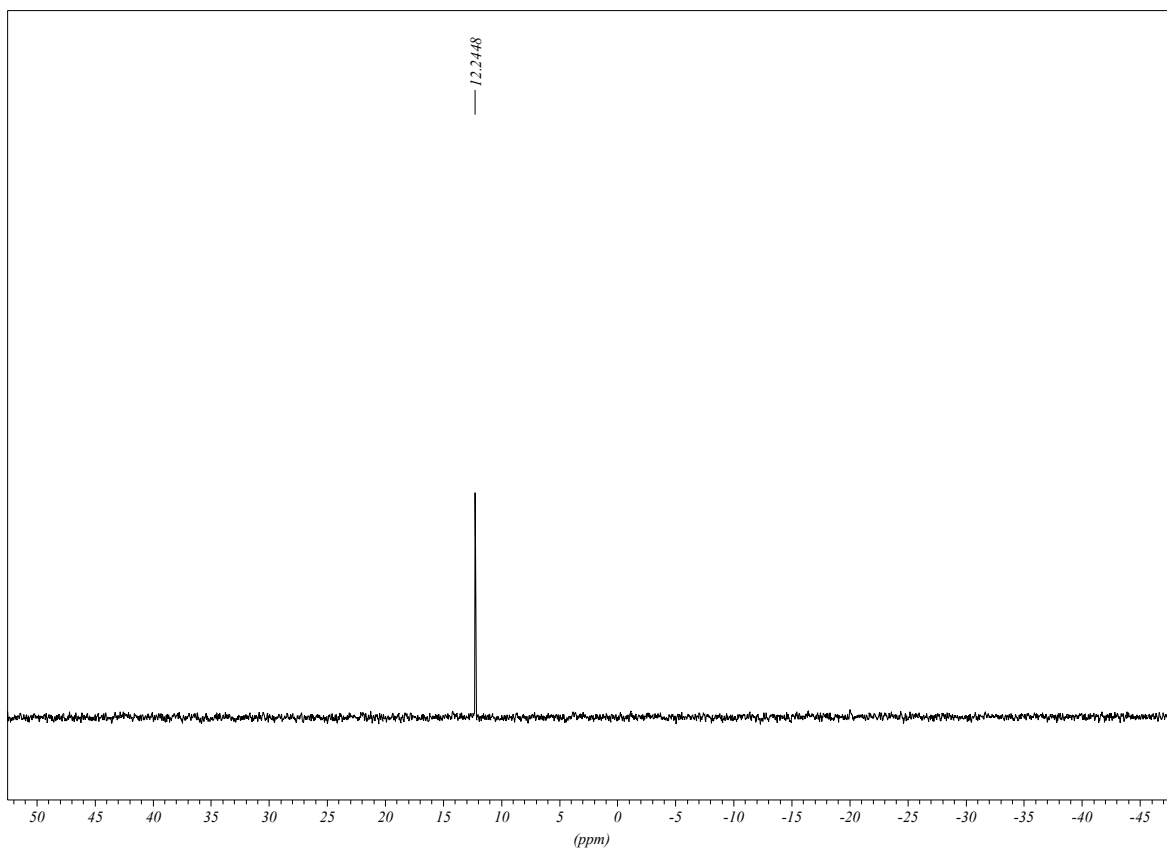
^1H RMN (CD_3CN)



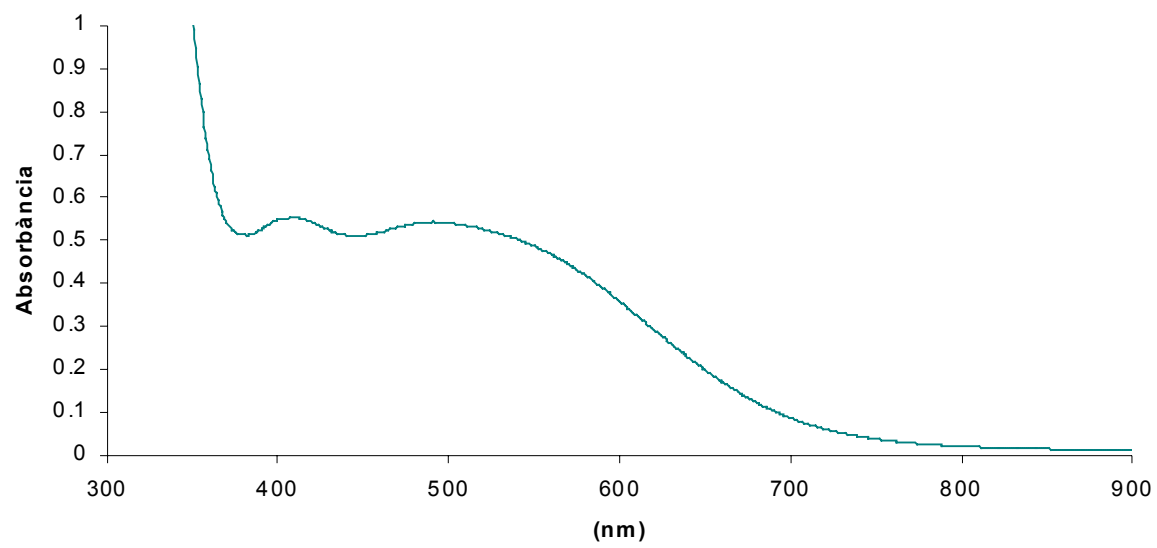
$^{13}\text{C}\{^1\text{H}\}$ RMN (CD_3CN)



$^{31}\text{P}\{^1\text{H}\}$ RMN (CD_3CN)



UV-VIS (CH₃CN, 1 mM)



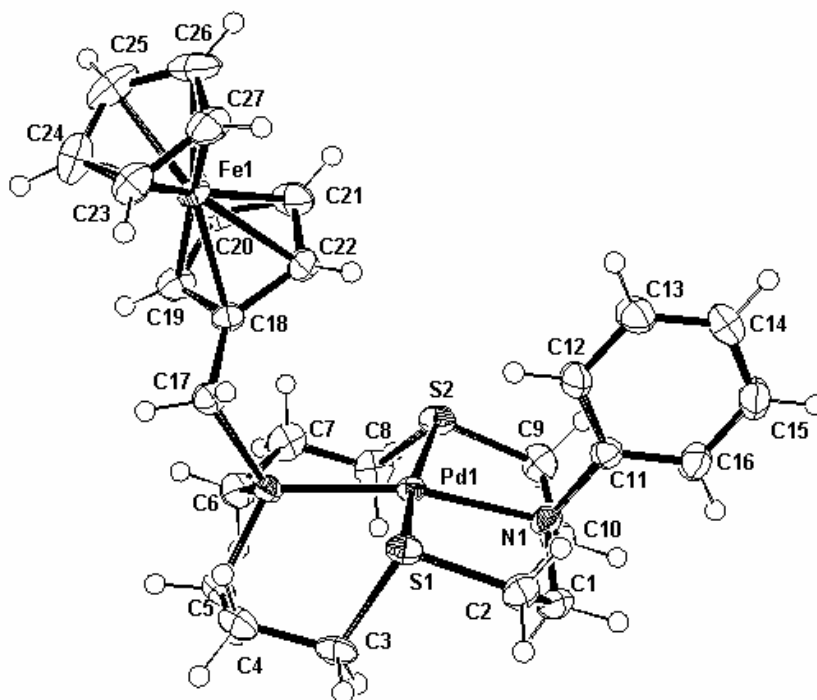
APÈNDIX III:
ESTRUCTURES CRISTAL·LINES
(DADES REFINADES)

1	Estructura cristalina del complex [Pd(L17)](BF₄)₂	163
2	Estructura cristalina del complex [Ni(L17)](ClO₄)₂	170
3	Estructura cristalina del complex [NiBr(L17)]ClO₄	176

1 Estructura cristal·lina del complex [Pd(L17)](BF₄)₂

- Paràmetres cristal·logràfics

	[Pd(L17)](BF ₄) ₂ ·CH ₃ COCH ₃ C ₃₀ H ₄₂ B ₂ F ₈ FeNPPdOS ₂
fórmula química	C ₃₀ H ₄₂ B ₂ F ₈ FeNPPdOS ₂
pes molecular, g/mol	863.64
T(K)	173(2)
λ (Å)	0.71073
sistema cristal·lí	Triclínic
grup espacial	P-1
a, Å	12.4272(2)
b, Å	12.8400 (2)
c, Å	12.9154(10)
a, deg	116.531(10)
b, deg	99.548 (10)
γ, deg	102.029(10)
V, Å ³	1722.56(5)
ρ _{calc} , g/cm ³	1.665
Z	2
mida del cristall, mm	0.30 x 0.28 x 0.22
R1 [I > 2σ(I)]	0.0390
wR2 [I > 2σ(I)]	0.0921



- Coordenades fraccionàries i desplaçaments isotròpics per $[\text{Pd}(\text{L17})](\text{BF}_4)_2 \cdot \text{CH}_3\text{COCH}_3$

	x	y	z	U(eq)
Pd(1)	7217(1)	9168(1)	7502(1)	19(1)
Fe(1)	10287(1)	7702(1)	4746(1)	23(1)
S(1)	6323(1)	10076(1)	6601(1)	24(1)
S(2)	8358(1)	8613(1)	8625(1)	27(1)
P(1)	6767(1)	7412(1)	5725(1)	22(1)
O(1)	7078(4)	14244(4)	8151(4)	67(1)
N(1)	7249(3)	10620(3)	9209(3)	24(1)
C(1)	6171(4)	10931(4)	8934(4)	32(1)
C(2)	6158(4)	11278(4)	7960(4)	32(1)
C(3)	4871(3)	9035(4)	5752(4)	29(1)
C(4)	4908(4)	7950(4)	4618(4)	33(1)
C(5)	5287(3)	6989(4)	4833(4)	31(1)
C(6)	6729(4)	6069(4)	5892(4)	33(1)
C(7)	7620(4)	6185(4)	6935(4)	36(1)
C(8)	7577(4)	7054(4)	8192(4)	34(1)
C(9)	8145(4)	9542(4)	10093(4)	34(1)
C(10)	7129(4)	9988(4)	9948(4)	30(1)
C(11)	8272(3)	11723(4)	9813(4)	25(1)
C(12)	9038(4)	11882(4)	9188(4)	32(1)
C(13)	9975(4)	12953(4)	9748(4)	37(1)
C(14)	10152(4)	13846(4)	10924(4)	36(1)
C(15)	9397(4)	13673(4)	11550(4)	36(1)
C(16)	8457(4)	12617(4)	11000(4)	33(1)
C(17)	7682(3)	7445(4)	4767(4)	26(1)
C(18)	8858(3)	7451(4)	5290(4)	23(1)
C(19)	9224(4)	6393(4)	4933(4)	33(1)
C(20)	10367(4)	6768(5)	5666(5)	40(1)
C(21)	10714(4)	8041(5)	6481(4)	38(1)
C(22)	9777(3)	8476(4)	6264(4)	27(1)
C(23)	9963(4)	8157(4)	3423(4)	35(1)
C(24)	10215(5)	7045(5)	2971(4)	45(1)
C(25)	11329(5)	7272(5)	3662(5)	52(1)
C(26)	11762(4)	8526(5)	4556(5)	49(1)
C(27)	10920(4)	9073(4)	4403(4)	38(1)
C(28)	6626(5)	14594(4)	8909(5)	50(1)
C(29)	5589(5)	14924(5)	8724(5)	55(1)
C(30)	7120(6)	14747(6)	10144(6)	75(2)
B(1)	3251(5)	11539(6)	7996(6)	46(1)
F(1)	3371(3)	10456(4)	7932(4)	88(1)
F(2)	2279(4)	11694(7)	8240(6)	149(3)
F(3)	4172(5)	12374(5)	8921(6)	170(3)
F(4)	3355(5)	11501(6)	6986(5)	126(2)
B(2)	3972(4)	6878(6)	7362(5)	45(2)
F(5A)	4951(7)	6797(8)	7185(7)	82(3)
F(5B)	4988(7)	7725(8)	7574(7)	74(2)
F(6A)	3292(5)	6772(6)	6221(6)	49(2)
F(6B)	3032(9)	6617(9)	6644(9)	96(3)

F(7A)	3259(8)	6017(9)	7462(9)	101(3)
F(7B)	4380(6)	5806(7)	6919(6)	64(2)
F(8A)	4031(7)	8030(7)	8220(7)	78(2)
F(8B)	3869(9)	6920(10)	8471(10)	104(3)

• Distàncies (Å) i angles (°) d'enllaç

Pd(1)-N(1) 2.146(3)	C(10)-H(10B) 0.9900
Pd(1)-P(1) 2.2561(10)	C(11)-C(12) 1.385(6)
Pd(1)-S(1) 2.2954(10)	C(11)-C(16) 1.387(6)
Pd(1)-S(2) 2.2983(10)	C(12)-C(13) 1.391(6)
Fe(1)-C(26) 2.029(5)	C(12)-H(12) 0.9500
Fe(1)-C(21) 2.032(4)	C(13)-C(14) 1.377(6)
Fe(1)-C(18) 2.032(4)	C(13)-H(13) 0.9500
Fe(1)-C(27) 2.036(4)	C(14)-C(15) 1.382(7)
Fe(1)-C(20) 2.036(4)	C(14)-H(14) 0.9500
Fe(1)-C(24) 2.037(5)	C(15)-C(16) 1.383(6)
Fe(1)-C(25) 2.038(5)	C(15)-H(15) 0.9500
Fe(1)-C(22) 2.041(4)	C(16)-H(16) 0.9500
Fe(1)-C(19) 2.043(4)	C(17)-C(18) 1.502(5)
Fe(1)-C(23) 2.046(4)	C(17)-H(17A) 0.9900
S(1)-C(3) 1.808(4)	C(17)-H(17B) 0.9900
S(1)-C(2) 1.827(4)	C(18)-C(19) 1.426(6)
S(2)-C(8) 1.809(4)	C(18)-C(22) 1.427(6)
S(2)-C(9) 1.835(4)	C(19)-C(20) 1.417(7)
P(1)-C(17) 1.822(4)	C(19)-H(19) 0.9500
P(1)-C(5) 1.824(4)	C(20)-C(21) 1.409(7)
P(1)-C(6) 1.824(4)	C(20)-H(20) 0.9500
O(1)-C(28) 1.171(6)	C(21)-C(22) 1.432(6)
N(1)-C(11) 1.471(5)	C(21)-H(21) 0.9500
N(1)-C(1) 1.507(5)	C(22)-H(22) 0.9500
N(1)-C(10) 1.510(5)	C(23)-C(24) 1.408(7)
C(1)-C(2) 1.509(6)	C(23)-C(27) 1.410(7)
C(1)-H(1A) 0.9900	C(23)-H(23) 0.9500
C(1)-H(1B) 0.9900	C(24)-C(25) 1.409(8)
C(2)-H(2A) 0.9900	C(24)-H(24) 0.9500
C(2)-H(2B) 0.9900	C(25)-C(26) 1.410(8)
C(3)-C(4) 1.521(6)	C(25)-H(25) 0.9500
C(3)-H(3A) 0.9900	C(26)-C(27) 1.410(7)
C(3)-H(3B) 0.9900	C(26)-H(26) 0.9500
C(4)-C(5) 1.525(6)	C(27)-H(27) 0.9500
C(4)-H(4A) 0.9900	C(28)-C(29) 1.454(8)
C(4)-H(4B) 0.9900	C(28)-C(30) 1.518(9)
C(5)-H(5A) 0.9900	C(29)-H(29A) 0.9800
C(5)-H(5B) 0.9900	C(29)-H(29B) 0.9800
C(6)-C(7) 1.523(6)	C(29)-H(29C) 0.9800
C(6)-H(6A) 0.9900	C(30)-H(30A) 0.9800
C(6)-H(6B) 0.9900	C(30)-H(30B) 0.9800
C(7)-C(8) 1.523(6)	C(30)-H(30C) 0.9800
C(7)-H(7A) 0.9900	B(1)-F(4) 1.312(7)
C(7)-H(7B) 0.9900	B(1)-F(2) 1.330(7)
C(8)-H(8A) 0.9900	B(1)-F(3) 1.333(8)
C(8)-H(8B) 0.9900	B(1)-F(1) 1.395(7)
C(9)-C(10) 1.508(6)	B(2)-F(6B) 1.240(10)
C(9)-H(9A) 0.9900	B(2)-F(5A) 1.291(10)
C(9)-H(9B) 0.9900	B(2)-F(7A) 1.335(11)
C(10)-H(10A) 0.9900	B(2)-F(8A) 1.373(9)

B(2)-F(5B) 1.378(10)	C(3)-S(1)-Pd(1) 106.51(14)
B(2)-F(8B) 1.437(12)	C(2)-S(1)-Pd(1) 97.72(14)
B(2)-F(7B) 1.470(9)	C(8)-S(2)-C(9) 103.7(2)
B(2)-F(6A) 1.504(8)	C(8)-S(2)-Pd(1) 106.37(15)
F(5B)-F(8A) 1.579(11)	C(9)-S(2)-Pd(1) 97.90(14)
F(6B)-F(7A) 1.584(13)	C(17)-P(1)-C(5) 107.2(2)
F(7A)-F(8B) 1.254(12)	C(17)-P(1)-C(6) 107.4(2)
	C(5)-P(1)-C(6) 101.6(2)
N(1)-Pd(1)-P(1) 166.02(9)	C(17)-P(1)-Pd(1) 115.41(14)
N(1)-Pd(1)-S(1) 87.45(9)	C(5)-P(1)-Pd(1) 110.56(14)
P(1)-Pd(1)-S(1) 92.53(4)	C(6)-P(1)-Pd(1) 113.61(15)
N(1)-Pd(1)-S(2) 85.99(9)	C(11)-N(1)-C(1) 110.9(3)
P(1)-Pd(1)-S(2) 95.82(4)	C(11)-N(1)-C(10) 112.2(3)
S(1)-Pd(1)-S(2) 169.46(4)	C(1)-N(1)-C(10) 109.9(3)
C(26)-Fe(1)-C(21) 105.1(2)	C(11)-N(1)-Pd(1) 116.1(2)
C(26)-Fe(1)-C(18) 161.5(2)	C(1)-N(1)-Pd(1) 104.7(2)
C(21)-Fe(1)-C(18) 69.12(17)	C(10)-N(1)-Pd(1) 102.5(2)
C(26)-Fe(1)-C(27) 40.6(2)	N(1)-C(1)-C(2) 110.3(3)
C(21)-Fe(1)-C(27) 119.0(2)	N(1)-C(1)-H(1A) 109.6
C(18)-Fe(1)-C(27) 125.61(17)	C(2)-C(1)-H(1A) 109.6
C(26)-Fe(1)-C(20) 118.8(2)	N(1)-C(1)-H(1B) 109.6
C(21)-Fe(1)-C(20) 40.5(2)	C(2)-C(1)-H(1B) 109.6
C(18)-Fe(1)-C(20) 68.85(17)	H(1A)-C(1)-H(1B) 108.1
C(27)-Fe(1)-C(20) 153.7(2)	C(1)-C(2)-S(1) 111.5(3)
C(26)-Fe(1)-C(24) 68.2(2)	C(1)-C(2)-H(2A) 109.3
C(21)-Fe(1)-C(24) 161.5(2)	S(1)-C(2)-H(2A) 109.3
C(18)-Fe(1)-C(24) 122.6(2)	C(1)-C(2)-H(2B) 109.3
C(27)-Fe(1)-C(24) 67.9(2)	S(1)-C(2)-H(2B) 109.3
C(20)-Fe(1)-C(24) 126.2(2)	H(2A)-C(2)-H(2B) 108.0
C(26)-Fe(1)-C(25) 40.6(2)	C(4)-C(3)-S(1) 108.9(3)
C(21)-Fe(1)-C(25) 123.4(2)	C(4)-C(3)-H(3A) 109.9
C(18)-Fe(1)-C(25) 157.1(2)	S(1)-C(3)-H(3A) 109.9
C(27)-Fe(1)-C(25) 68.0(2)	C(4)-C(3)-H(3B) 109.9
C(20)-Fe(1)-C(25) 107.2(2)	S(1)-C(3)-H(3B) 109.9
C(24)-Fe(1)-C(25) 40.5(2)	H(3A)-C(3)-H(3B) 108.3
C(26)-Fe(1)-C(22) 123.3(2)	C(3)-C(4)-C(5) 114.4(4)
C(21)-Fe(1)-C(22) 41.16(17)	C(3)-C(4)-H(4A) 108.6
C(18)-Fe(1)-C(22) 41.00(16)	C(5)-C(4)-H(4A) 108.6
C(27)-Fe(1)-C(22) 106.73(18)	C(3)-C(4)-H(4B) 108.6
C(20)-Fe(1)-C(22) 68.68(18)	C(5)-C(4)-H(4B) 108.6
C(24)-Fe(1)-C(22) 156.94(19)	H(4A)-C(4)-H(4B) 107.6
C(25)-Fe(1)-C(22) 160.4(2)	C(4)-C(5)-P(1) 118.6(3)
C(26)-Fe(1)-C(19) 154.9(2)	C(4)-C(5)-H(5A) 107.7
C(21)-Fe(1)-C(19) 68.54(19)	P(1)-C(5)-H(5A) 107.7
C(18)-Fe(1)-C(19) 40.97(16)	C(4)-C(5)-H(5B) 107.7
C(27)-Fe(1)-C(19) 163.85(19)	P(1)-C(5)-H(5B) 107.7
C(20)-Fe(1)-C(19) 40.66(19)	H(5A)-C(5)-H(5B) 107.1
C(24)-Fe(1)-C(19) 109.8(2)	C(7)-C(6)-P(1) 119.7(3)
C(25)-Fe(1)-C(19) 121.4(2)	C(7)-C(6)-H(6A) 107.4
C(22)-Fe(1)-C(19) 68.74(17)	P(1)-C(6)-H(6A) 107.4
C(26)-Fe(1)-C(23) 68.2(2)	C(7)-C(6)-H(6B) 107.4
C(21)-Fe(1)-C(23) 155.1(2)	P(1)-C(6)-H(6B) 107.4
C(18)-Fe(1)-C(23) 109.26(17)	H(6A)-C(6)-H(6B) 106.9
C(27)-Fe(1)-C(23) 40.41(19)	C(8)-C(7)-C(6) 114.8(4)
C(20)-Fe(1)-C(23) 163.9(2)	C(8)-C(7)-H(7A) 108.6
C(24)-Fe(1)-C(23) 40.34(19)	C(6)-C(7)-H(7A) 108.6
C(25)-Fe(1)-C(23) 68.0(2)	C(8)-C(7)-H(7B) 108.6
C(22)-Fe(1)-C(23) 121.10(17)	C(6)-C(7)-H(7B) 108.6
C(19)-Fe(1)-C(23) 127.56(19)	H(7A)-C(7)-H(7B) 107.5
C(3)-S(1)-C(2) 104.1(2)	C(7)-C(8)-S(2) 109.0(3)

C(7)-C(8)-H(8A) 109.9	C(20)-C(21)-Fe(1) 69.9(3)
S(2)-C(8)-H(8A) 109.9	C(22)-C(21)-Fe(1) 69.8(2)
C(7)-C(8)-H(8B) 109.9	C(20)-C(21)-H(21) 125.9
S(2)-C(8)-H(8B) 109.9	C(22)-C(21)-H(21) 125.9
H(8A)-C(8)-H(8B) 108.3	Fe(1)-C(21)-H(21) 126.0
C(10)-C(9)-S(2) 111.4(3)	C(18)-C(22)-C(21) 107.5(4)
C(10)-C(9)-H(9A) 109.3	C(18)-C(22)-Fe(1) 69.2(2)
S(2)-C(9)-H(9A) 109.3	C(21)-C(22)-Fe(1) 69.1(2)
C(10)-C(9)-H(9B) 109.3	C(18)-C(22)-H(22) 126.2
S(2)-C(9)-H(9B) 109.3	C(21)-C(22)-H(22) 126.2
H(9A)-C(9)-H(9B) 108.0	Fe(1)-C(22)-H(22) 127.1
C(9)-C(10)-N(1) 109.7(3)	C(24)-C(23)-C(27) 107.7(4)
C(9)-C(10)-H(10A) 109.7	C(24)-C(23)-Fe(1) 69.5(3)
N(1)-C(10)-H(10A) 109.7	C(27)-C(23)-Fe(1) 69.4(3)
C(9)-C(10)-H(10B) 109.7	C(24)-C(23)-H(23) 126.1
N(1)-C(10)-H(10B) 109.7	C(27)-C(23)-H(23) 126.1
H(10A)-C(10)-H(10B) 108.2	Fe(1)-C(23)-H(23) 126.5
C(12)-C(11)-C(16) 119.9(4)	C(23)-C(24)-C(25) 108.3(5)
C(12)-C(11)-N(1) 120.1(3)	C(23)-C(24)-Fe(1) 70.2(3)
C(16)-C(11)-N(1) 119.9(4)	C(25)-C(24)-Fe(1) 69.8(3)
C(11)-C(12)-C(13) 119.7(4)	C(23)-C(24)-H(24) 125.9
C(11)-C(12)-H(12) 120.1	C(25)-C(24)-H(24) 125.9
C(13)-C(12)-H(12) 120.1	Fe(1)-C(24)-H(24) 125.7
C(14)-C(13)-C(12) 120.3(4)	C(24)-C(25)-C(26) 107.9(4)
C(14)-C(13)-H(13) 119.8	C(24)-C(25)-Fe(1) 69.7(3)
C(12)-C(13)-H(13) 119.8	C(26)-C(25)-Fe(1) 69.4(3)
C(13)-C(14)-C(15) 119.7(4)	C(24)-C(25)-H(25) 126.0
C(13)-C(14)-H(14) 120.1	C(26)-C(25)-H(25) 126.0
C(15)-C(14)-H(14) 120.1	Fe(1)-C(25)-H(25) 126.4
C(14)-C(15)-C(16) 120.5(4)	C(25)-C(26)-C(27) 107.8(5)
C(14)-C(15)-H(15) 119.7	C(25)-C(26)-Fe(1) 70.1(3)
C(16)-C(15)-H(15) 119.7	C(27)-C(26)-Fe(1) 70.0(3)
C(15)-C(16)-C(11) 119.8(4)	C(25)-C(26)-H(26) 126.1
C(15)-C(16)-H(16) 120.1	C(27)-C(26)-H(26) 126.1
C(11)-C(16)-H(16) 120.1	Fe(1)-C(26)-H(26) 125.5
C(18)-C(17)-P(1) 110.9(3)	C(23)-C(27)-C(26) 108.2(4)
C(18)-C(17)-H(17A) 109.5	C(23)-C(27)-Fe(1) 70.2(2)
P(1)-C(17)-H(17A) 109.5	C(26)-C(27)-Fe(1) 69.4(3)
C(18)-C(17)-H(17B) 109.5	C(23)-C(27)-H(27) 125.9
P(1)-C(17)-H(17B) 109.5	C(26)-C(27)-H(27) 125.9
H(17A)-C(17)-H(17B) 108.0	Fe(1)-C(27)-H(27) 126.1
C(19)-C(18)-C(22) 107.8(4)	O(1)-C(28)-C(29) 121.9(6)
C(19)-C(18)-C(17) 125.0(4)	O(1)-C(28)-C(30) 121.0(6)
C(22)-C(18)-C(17) 127.1(4)	C(29)-C(28)-C(30) 117.1(5)
C(19)-C(18)-Fe(1) 69.9(2)	C(28)-C(29)-H(29A) 109.5
C(22)-C(18)-Fe(1) 69.8(2)	C(28)-C(29)-H(29B) 109.5
C(17)-C(18)-Fe(1) 128.5(3)	H(29A)-C(29)-H(29B) 109.5
C(20)-C(19)-C(18) 108.0(4)	C(28)-C(29)-H(29C) 109.5
C(20)-C(19)-Fe(1) 69.4(2)	H(29A)-C(29)-H(29C) 109.5
C(18)-C(19)-Fe(1) 69.1(2)	H(29B)-C(29)-H(29C) 109.5
C(20)-C(19)-H(19) 126.0	C(28)-C(30)-H(30A) 109.5
C(18)-C(19)-H(19) 126.0	C(28)-C(30)-H(30B) 109.5
Fe(1)-C(19)-H(19) 127.0	H(30A)-C(30)-H(30B) 109.5
C(21)-C(20)-C(19) 108.6(4)	C(28)-C(30)-H(30C) 109.5
C(21)-C(20)-Fe(1) 69.6(2)	H(30A)-C(30)-H(30C) 109.5
C(19)-C(20)-Fe(1) 69.9(2)	H(30B)-C(30)-H(30C) 109.5
C(21)-C(20)-H(20) 125.7	F(4)-B(1)-F(2) 115.0(5)
C(19)-C(20)-H(20) 125.7	F(4)-B(1)-F(3) 110.3(6)
Fe(1)-C(20)-H(20) 126.4	F(2)-B(1)-F(3) 111.4(6)
C(20)-C(21)-C(22) 108.1(4)	F(4)-B(1)-F(1) 107.3(6)

F(2)-B(1)-F(1) 110.9(5)	F(7A)-B(2)-F(7B) 73.4(6)
F(3)-B(1)-F(1) 101.0(5)	F(8A)-B(2)-F(7B) 152.8(6)
F(6B)-B(2)-F(5A) 131.0(8)	F(5B)-B(2)-F(7B) 96.3(5)
F(6B)-B(2)-F(7A) 75.9(7)	F(8B)-B(2)-F(7B) 96.5(6)
F(5A)-B(2)-F(7A) 121.5(8)	F(6B)-B(2)-F(6A) 30.0(5)
F(6B)-B(2)-F(8A) 98.0(7)	F(5A)-B(2)-F(6A) 104.3(6)
F(5A)-B(2)-F(8A) 113.6(7)	F(7A)-B(2)-F(6A) 102.3(6)
F(7A)-B(2)-F(8A) 110.5(6)	F(8A)-B(2)-F(6A) 101.7(6)
F(6B)-B(2)-F(5B) 125.9(8)	F(5B)-B(2)-F(6A) 98.6(6)
F(5A)-B(2)-F(5B) 46.4(5)	F(8B)-B(2)-F(6A) 142.3(6)
F(7A)-B(2)-F(5B) 158.3(8)	F(7B)-B(2)-F(6A) 103.7(5)
F(8A)-B(2)-F(5B) 70.1(5)	B(2)-F(5B)-F(8A) 54.8(5)
F(6B)-B(2)-F(8B) 113.1(8)	B(2)-F(6B)-F(7A) 54.8(6)
F(5A)-B(2)-F(8B) 113.1(7)	F(8B)-F(7A)-B(2) 67.4(7)
F(7A)-B(2)-F(8B) 53.6(6)	F(8B)-F(7A)-F(6B) 103.4(9)
F(8A)-B(2)-F(8B) 68.3(6)	B(2)-F(7A)-F(6B) 49.4(5)
F(5B)-B(2)-F(8B) 110.5(7)	B(2)-F(8A)-F(5B) 55.1(5)
F(6B)-B(2)-F(7B) 108.9(7)	F(7A)-F(8B)-B(2) 59.0(7)
F(5A)-B(2)-F(7B) 50.1(5)	

• Angles (°) de torsió

N(1)-Pd(1)-S(1)-C(3) -112.48(17)	Pd(1)-S(1)-C(2)-C(1) -23.4(3)
P(1)-Pd(1)-S(1)-C(3) 53.52(15)	C(2)-S(1)-C(3)-C(4) -177.1(3)
S(2)-Pd(1)-S(1)-C(3) -164.0(2)	Pd(1)-S(1)-C(3)-C(4) -74.5(3)
N(1)-Pd(1)-S(1)-C(2) -5.23(17)	S(1)-C(3)-C(4)-C(5) 78.4(4)
P(1)-Pd(1)-S(1)-C(2) 160.78(15)	C(3)-C(4)-C(5)-P(1) -66.9(5)
S(2)-Pd(1)-S(1)-C(2) -56.7(3)	C(17)-P(1)-C(5)-C(4) -74.9(4)
N(1)-Pd(1)-S(2)-C(8) 120.56(18)	C(6)-P(1)-C(5)-C(4) 172.6(3)
P(1)-Pd(1)-S(2)-C(8) -45.53(16)	Pd(1)-P(1)-C(5)-C(4) 51.7(4)
S(1)-Pd(1)-S(2)-C(8) 172.2(2)	C(17)-P(1)-C(6)-C(7) 90.1(4)
N(1)-Pd(1)-S(2)-C(9) 13.71(17)	C(5)-P(1)-C(6)-C(7) -157.5(4)
P(1)-Pd(1)-S(2)-C(9) -152.38(15)	Pd(1)-P(1)-C(6)-C(7) -38.7(4)
S(1)-Pd(1)-S(2)-C(9) 65.3(3)	P(1)-C(6)-C(7)-C(8) 62.9(5)
N(1)-Pd(1)-P(1)-C(17) 169.0(4)	C(6)-C(7)-C(8)-S(2) -82.6(4)
S(1)-Pd(1)-P(1)-C(17) 79.36(15)	C(9)-S(2)-C(8)-C(7) 176.3(3)
S(2)-Pd(1)-P(1)-C(17) -94.21(15)	Pd(1)-S(2)-C(8)-C(7) 73.7(3)
N(1)-Pd(1)-P(1)-C(5) 47.1(4)	C(8)-S(2)-C(9)-C(10) -93.8(3)
S(1)-Pd(1)-P(1)-C(5) -42.50(16)	Pd(1)-S(2)-C(9)-C(10) 15.3(3)
S(2)-Pd(1)-P(1)-C(5) 143.93(16)	S(2)-C(9)-C(10)-N(1) -52.4(4)
N(1)-Pd(1)-P(1)-C(6) -66.4(4)	C(11)-N(1)-C(10)-C(9) -62.9(4)
S(1)-Pd(1)-P(1)-C(6) -156.00(16)	C(1)-N(1)-C(10)-C(9) 173.2(3)
S(2)-Pd(1)-P(1)-C(6) 30.43(16)	Pd(1)-N(1)-C(10)-C(9) 62.3(4)
P(1)-Pd(1)-N(1)-C(11) 179.8(3)	C(1)-N(1)-C(11)-C(12) -107.2(4)
S(1)-Pd(1)-N(1)-C(11) -90.0(3)	C(10)-N(1)-C(11)-C(12) 129.4(4)
S(2)-Pd(1)-N(1)-C(11) 81.8(2)	Pd(1)-N(1)-C(11)-C(12) 12.0(5)
P(1)-Pd(1)-N(1)-C(1) -57.6(5)	C(1)-N(1)-C(11)-C(16) 71.3(5)
S(1)-Pd(1)-N(1)-C(1) 32.6(2)	C(10)-N(1)-C(11)-C(16) -52.0(5)
S(2)-Pd(1)-N(1)-C(1) -155.6(2)	Pd(1)-N(1)-C(11)-C(16) -169.4(3)
P(1)-Pd(1)-N(1)-C(10) 57.2(5)	C(16)-C(11)-C(12)-C(13) -1.5(7)
S(1)-Pd(1)-N(1)-C(10) 147.4(2)	N(1)-C(11)-C(12)-C(13) 177.1(4)
S(2)-Pd(1)-N(1)-C(10) -40.8(2)	C(11)-C(12)-C(13)-C(14) 0.8(7)
C(11)-N(1)-C(1)-C(2) 68.9(4)	C(12)-C(13)-C(14)-C(15) 0.3(7)
C(10)-N(1)-C(1)-C(2) -166.5(3)	C(13)-C(14)-C(15)-C(16) -0.8(7)
Pd(1)-N(1)-C(1)-C(2) -57.0(4)	C(14)-C(15)-C(16)-C(11) 0.2(7)
N(1)-C(1)-C(2)-S(1) 55.1(4)	C(12)-C(11)-C(16)-C(15) 1.0(6)
C(3)-S(1)-C(2)-C(1) 85.8(3)	N(1)-C(11)-C(16)-C(15) -177.6(4)

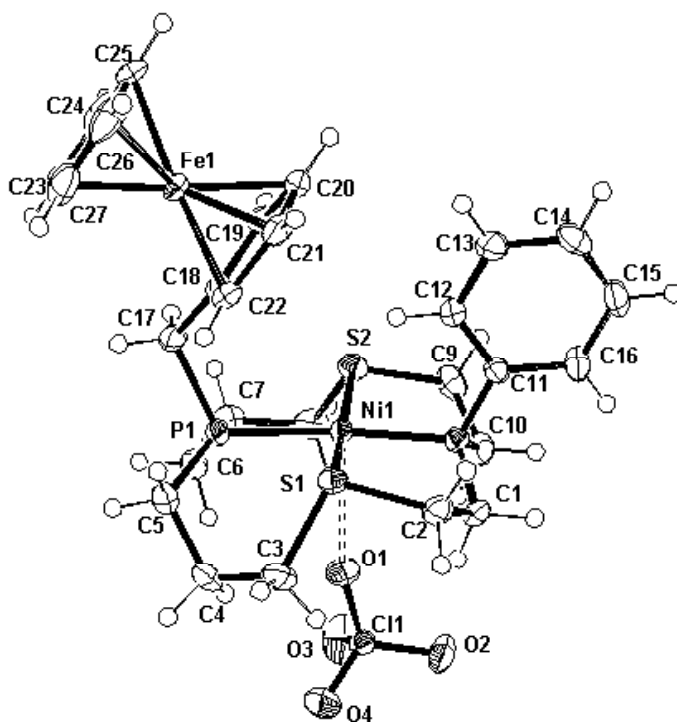
C(5)-P(1)-C(17)-C(18) -164.9(3)
C(6)-P(1)-C(17)-C(18) -56.3(3)
Pd(1)-P(1)-C(17)-C(18) 71.5(3)
P(1)-C(17)-C(18)-C(19) 97.4(4)
P(1)-C(17)-C(18)-C(22) -78.6(4)
P(1)-C(17)-C(18)-Fe(1) -171.4(2)
C(22)-C(18)-C(19)-C(20) -1.1(5)
C(17)-C(18)-C(19)-C(20) -177.7(4)
C(18)-C(19)-C(20)-C(21) 0.5(5)

C(19)-C(20)-C(21)-C(22) 0.3(5)
C(20)-C(21)-C(22)-C(18) -1.0(5)
C(27)-C(23)-C(24)-C(25) -0.5(5)
C(23)-C(24)-C(25)-C(26) 0.8(6)
C(24)-C(25)-C(26)-C(27) -0.8(6)
C(24)-C(23)-C(27)-C(26) 0.1(5)
C(25)-C(26)-C(27)-C(23) 0.4(5)

2 Estructura cristal·lina del complex [Ni(L17)](ClO₄)₂

- Paràmetres cristal·logràfics

	[Ni(L17)](ClO ₄) ₂ · CHCl ₃
fórmula química	C ₂₈ H ₃₇ Cl ₃ FeNNiPO ₈ S ₂
pes molecular, g/mol	902.49
T(K)	173(2)
λ (Å)	0.71073
sistema cristal·lí	Monoclinic
grup espacial	P 2 ₁ /C
a, Å	16.5998(2)
b, Å	9.50850(10)
c, Å	22.7476(3)
a, deg	90.00
b, deg	102.1330(10)
γ, deg	90.00
V, Å ³	3510.26(7)
ρ _{calc} , g/cm ³	1.708
Z	4
mida del cristall, mm	0.28 x 0.26 x 0.16
R1 [I > 2σ(I)]	0.0391
wR2 [I > 2σ(I)]	0.0777



- Coordenades fraccionàries i desplaçaments isotròpics per $[\text{Ni(L17)}](\text{ClO}_4)_2 \cdot \text{CHCl}_3$

	x	y	z	U(eq)
Ni(1)	2337(1)	2308(1)	858(1)	18(1)
Fe(1)	5494(1)	2074(1)	1949(1)	21(1)
P(1)	3249(1)	2450(1)	305(1)	21(1)
S(1)	2466(1)	4522(1)	1076(1)	22(1)
S(2)	2339(1)	24(1)	792(1)	25(1)
N(1)	1418(1)	2197(2)	1302(1)	20(1)
C(1)	955(2)	3568(3)	1196(1)	26(1)
C(2)	1547(2)	4763(3)	1388(1)	28(1)
C(3)	2260(2)	5641(3)	404(1)	33(1)
C(4)	2626(2)	5079(3)	-112(1)	33(1)
C(5)	3418(2)	4233(3)	72(1)	32(1)
C(6)	2946(2)	1441(3)	-388(1)	30(1)
C(7)	2760(2)	-108(3)	-310(1)	33(1)
C(8)	2042(2)	-383(3)	-6(1)	32(1)
C(9)	1392(2)	-311(3)	1051(1)	32(1)
C(10)	880(2)	1012(3)	1004(1)	29(1)
C(11)	1687(2)	1934(3)	1955(1)	22(1)
C(12)	2516(2)	2007(3)	2222(1)	24(1)
C(13)	2760(2)	1780(3)	2838(1)	31(1)
C(14)	2181(2)	1456(3)	3170(1)	32(1)
C(15)	1362(2)	1393(3)	2906(1)	34(1)
C(16)	1110(2)	1640(3)	2296(1)	30(1)
C(17)	4263(2)	1823(3)	688(1)	27(1)
C(18)	4390(2)	2008(3)	1357(1)	22(1)
C(19)	4441(2)	890(3)	1777(1)	23(1)
C(20)	4571(2)	1473(3)	2363(1)	24(1)
C(21)	4588(2)	2959(3)	2309(1)	25(1)
C(22)	4478(2)	3301(3)	1690(1)	24(1)
C(23)	6364(2)	1945(4)	1449(1)	40(1)
C(24)	6445(2)	821(3)	1855(2)	39(1)
C(25)	6591(2)	1393(4)	2438(2)	48(1)
C(26)	6596(2)	2874(4)	2384(2)	50(1)
C(27)	6454(2)	3191(3)	1775(2)	43(1)
Cl(1)	408(1)	2998(1)	-617(1)	24(1)
O(1)	1155(1)	2746(2)	-177(1)	42(1)
O(2)	-277(1)	2992(2)	-321(1)	39(1)
O(3)	310(2)	1901(2)	-1056(1)	53(1)
O(4)	472(1)	4326(2)	-896(1)	48(1)
Cl(2)	4740(1)	-2672(1)	792(1)	34(1)
O(5)	5224(2)	-3901(3)	914(1)	74(1)
O(6)	5238(2)	-1463(3)	914(2)	91(1)
O(7)	4130(2)	-2683(3)	1145(1)	74(1)
O(8)	4344(2)	-2686(3)	171(1)	79(1)
C(28)	1482(2)	-3109(3)	3021(1)	30(1)
Cl(3)	1275(1)	-2131(1)	3629(1)	44(1)
Cl(4)	887(1)	-2472(1)	2338(1)	41(1)
Cl(5)	1271(1)	-4896(1)	3105(1)	53(1)

• Distàncies (Å) i angles (°) d'enllaç

Ni(1)-N(1) 2.001(2)	C(14)-H(14) 0.9500
Ni(1)-S(1) 2.1636(7)	C(15)-C(16) 1.383(4)
Ni(1)-P(1) 2.1669(8)	C(15)-H(15) 0.9500
Ni(1)-S(2) 2.1763(7)	C(16)-H(16) 0.9500
Fe(1)-C(23) 2.020(3)	C(17)-C(18) 1.503(4)
Fe(1)-C(27) 2.023(3)	C(17)-H(17A) 0.9900
Fe(1)-C(24) 2.025(3)	C(17)-H(17B) 0.9900
Fe(1)-C(25) 2.029(3)	C(18)-C(19) 1.420(4)
Fe(1)-C(22) 2.034(3)	C(18)-C(22) 1.435(4)
Fe(1)-C(18) 2.034(3)	C(19)-C(20) 1.419(4)
Fe(1)-C(26) 2.035(3)	C(19)-H(19) 0.9500
Fe(1)-C(21) 2.039(3)	C(20)-C(21) 1.419(4)
Fe(1)-C(20) 2.042(3)	C(20)-H(20) 0.9500
Fe(1)-C(19) 2.047(3)	C(21)-C(22) 1.418(4)
P(1)-C(5) 1.815(3)	C(21)-H(21) 0.9500
P(1)-C(6) 1.824(3)	C(22)-H(22) 0.9500
P(1)-C(17) 1.825(3)	C(23)-C(27) 1.389(5)
S(1)-C(2) 1.826(3)	C(23)-C(24) 1.400(4)
S(1)-C(3) 1.834(3)	C(23)-H(23) 0.9500
S(2)-C(9) 1.819(3)	C(24)-C(25) 1.406(5)
S(2)-C(8) 1.821(3)	C(24)-H(24) 0.9500
N(1)-C(11) 1.480(3)	C(25)-C(26) 1.414(5)
N(1)-C(10) 1.507(3)	C(25)-H(25) 0.9500
N(1)-C(1) 1.507(3)	C(26)-C(27) 1.389(5)
C(1)-C(2) 1.505(4)	C(26)-H(26) 0.9500
C(1)-H(1A) 0.9900	C(27)-H(27) 0.9500
C(1)-H(1B) 0.9900	Cl(1)-O(4) 1.427(2)
C(2)-H(2A) 0.9900	Cl(1)-O(3) 1.429(2)
C(2)-H(2B) 0.9900	Cl(1)-O(2) 1.437(2)
C(3)-C(4) 1.528(4)	Cl(1)-O(1) 1.440(2)
C(3)-H(3A) 0.9900	Cl(2)-O(6) 1.409(2)
C(3)-H(3B) 0.9900	Cl(2)-O(5) 1.413(2)
C(4)-C(5) 1.524(4)	Cl(2)-O(7) 1.418(3)
C(4)-H(4A) 0.9900	Cl(2)-O(8) 1.428(3)
C(4)-H(4B) 0.9900	C(28)-Cl(5) 1.754(3)
C(5)-H(5A) 0.9900	C(28)-Cl(3) 1.759(3)
C(5)-H(5B) 0.9900	C(28)-Cl(4) 1.764(3)
C(6)-C(7) 1.523(4)	C(28)-H(28) 1.0000
C(6)-H(6A) 0.9900	
C(6)-H(6B) 0.9900	N(1)-Ni(1)-S(1) 89.17(6)
C(7)-C(8) 1.520(4)	N(1)-Ni(1)-P(1) 174.90(6)
C(7)-H(7A) 0.9900	S(1)-Ni(1)-P(1) 91.38(3)
C(7)-H(7B) 0.9900	N(1)-Ni(1)-S(2) 89.71(6)
C(8)-H(8A) 0.9900	S(1)-Ni(1)-S(2) 170.17(3)
C(8)-H(8B) 0.9900	P(1)-Ni(1)-S(2) 90.60(3)
C(9)-C(10) 1.509(4)	C(23)-Fe(1)-C(27) 40.18(13)
C(9)-H(9A) 0.9900	C(23)-Fe(1)-C(24) 40.49(13)
C(9)-H(9B) 0.9900	C(27)-Fe(1)-C(24) 67.94(12)
C(10)-H(10A) 0.9900	C(23)-Fe(1)-C(25) 67.92(13)
C(10)-H(10B) 0.9900	C(27)-Fe(1)-C(25) 67.78(14)
C(11)-C(16) 1.382(4)	C(24)-Fe(1)-C(25) 40.60(13)
C(11)-C(12) 1.384(4)	C(23)-Fe(1)-C(22) 121.26(12)
C(12)-C(13) 1.390(4)	C(27)-Fe(1)-C(22) 106.35(12)
C(12)-H(12) 0.9500	C(24)-Fe(1)-C(22) 157.60(13)
C(13)-C(14) 1.376(4)	C(25)-Fe(1)-C(22) 159.34(14)
C(13)-H(13) 0.9500	C(23)-Fe(1)-C(18) 106.05(12)
C(14)-C(15) 1.368(4)	C(27)-Fe(1)-C(18) 121.58(13)

C(24)-Fe(1)-C(18)	121.73(12)	C(1)-C(2)-H(2B)	109.7
C(25)-Fe(1)-C(18)	158.82(14)	S(1)-C(2)-H(2B)	109.7
C(22)-Fe(1)-C(18)	41.30(10)	H(2A)-C(2)-H(2B)	108.2
C(23)-Fe(1)-C(26)	67.72(14)	C(4)-C(3)-S(1)	113.78(19)
C(27)-Fe(1)-C(26)	40.03(14)	C(4)-C(3)-H(3A)	108.8
C(24)-Fe(1)-C(26)	68.32(13)	S(1)-C(3)-H(3A)	108.8
C(25)-Fe(1)-C(26)	40.72(14)	C(4)-C(3)-H(3B)	108.8
C(22)-Fe(1)-C(26)	122.15(13)	S(1)-C(3)-H(3B)	108.8
C(18)-Fe(1)-C(26)	157.77(14)	H(3A)-C(3)-H(3B)	107.7
C(23)-Fe(1)-C(21)	157.73(12)	C(5)-C(4)-C(3)	115.7(2)
C(27)-Fe(1)-C(21)	122.67(12)	C(5)-C(4)-H(4A)	108.4
C(24)-Fe(1)-C(21)	160.52(13)	C(3)-C(4)-H(4A)	108.4
C(25)-Fe(1)-C(21)	124.37(13)	C(5)-C(4)-H(4B)	108.4
C(22)-Fe(1)-C(21)	40.75(10)	C(3)-C(4)-H(4B)	108.4
C(18)-Fe(1)-C(21)	68.90(11)	H(4A)-C(4)-H(4B)	107.4
C(26)-Fe(1)-C(21)	108.30(12)	C(4)-C(5)-P(1)	113.3(2)
C(23)-Fe(1)-C(20)	159.56(12)	C(4)-C(5)-H(5A)	108.9
C(27)-Fe(1)-C(20)	159.38(13)	P(1)-C(5)-H(5A)	108.9
C(24)-Fe(1)-C(20)	124.18(12)	C(4)-C(5)-H(5B)	108.9
C(25)-Fe(1)-C(20)	109.37(12)	P(1)-C(5)-H(5B)	108.9
C(22)-Fe(1)-C(20)	68.71(11)	H(5A)-C(5)-H(5B)	107.7
C(18)-Fe(1)-C(20)	68.77(11)	C(7)-C(6)-P(1)	115.70(19)
C(26)-Fe(1)-C(20)	124.41(14)	C(7)-C(6)-H(6A)	108.4
C(21)-Fe(1)-C(20)	40.70(11)	P(1)-C(6)-H(6A)	108.4
C(23)-Fe(1)-C(19)	122.79(12)	C(7)-C(6)-H(6B)	108.4
C(27)-Fe(1)-C(19)	158.10(13)	P(1)-C(6)-H(6B)	108.4
C(24)-Fe(1)-C(19)	108.05(11)	H(6A)-C(6)-H(6B)	107.4
C(25)-Fe(1)-C(19)	124.15(13)	C(8)-C(7)-C(6)	114.6(2)
C(22)-Fe(1)-C(19)	68.70(11)	C(8)-C(7)-H(7A)	108.6
C(18)-Fe(1)-C(19)	40.70(10)	C(6)-C(7)-H(7A)	108.6
C(26)-Fe(1)-C(19)	160.55(14)	C(8)-C(7)-H(7B)	108.6
C(21)-Fe(1)-C(19)	68.36(11)	C(6)-C(7)-H(7B)	108.6
C(20)-Fe(1)-C(19)	40.61(10)	H(7A)-C(7)-H(7B)	107.6
C(5)-P(1)-C(6)	105.64(13)	C(7)-C(8)-S(2)	110.0(2)
C(5)-P(1)-C(17)	105.10(14)	C(7)-C(8)-H(8A)	109.7
C(6)-P(1)-C(17)	107.43(13)	S(2)-C(8)-H(8A)	109.7
C(5)-P(1)-Ni(1)	113.46(10)	C(7)-C(8)-H(8B)	109.7
C(6)-P(1)-Ni(1)	111.68(10)	S(2)-C(8)-H(8B)	109.7
C(17)-P(1)-Ni(1)	112.97(9)	H(8A)-C(8)-H(8B)	108.2
C(2)-S(1)-C(3)	103.06(13)	C(10)-C(9)-S(2)	110.04(19)
C(2)-S(1)-Ni(1)	99.19(9)	C(10)-C(9)-H(9A)	109.7
C(3)-S(1)-Ni(1)	112.44(10)	S(2)-C(9)-H(9A)	109.7
C(9)-S(2)-C(8)	102.36(14)	C(10)-C(9)-H(9B)	109.7
C(9)-S(2)-Ni(1)	97.95(9)	S(2)-C(9)-H(9B)	109.7
C(8)-S(2)-Ni(1)	106.10(9)	H(9A)-C(9)-H(9B)	108.2
C(11)-N(1)-C(10)	110.6(2)	N(1)-C(10)-C(9)	108.7(2)
C(11)-N(1)-C(1)	110.06(19)	N(1)-C(10)-H(10A)	110.0
C(10)-N(1)-C(1)	109.9(2)	C(9)-C(10)-H(10A)	110.0
C(11)-N(1)-Ni(1)	114.44(16)	N(1)-C(10)-H(10B)	110.0
C(10)-N(1)-Ni(1)	104.75(16)	C(9)-C(10)-H(10B)	110.0
C(1)-N(1)-Ni(1)	106.90(16)	H(10A)-C(10)-H(10B)	108.3
C(2)-C(1)-N(1)	109.0(2)	C(16)-C(11)-C(12)	120.5(3)
C(2)-C(1)-H(1A)	109.9	C(16)-C(11)-N(1)	119.9(2)
N(1)-C(1)-H(1A)	109.9	C(12)-C(11)-N(1)	119.7(2)
C(2)-C(1)-H(1B)	109.9	C(11)-C(12)-C(13)	119.1(3)
N(1)-C(1)-H(1B)	109.9	C(11)-C(12)-H(12)	120.4
H(1A)-C(1)-H(1B)	108.3	C(13)-C(12)-H(12)	120.4
C(1)-C(2)-S(1)	109.94(19)	C(14)-C(13)-C(12)	119.9(3)
C(1)-C(2)-H(2A)	109.7	C(14)-C(13)-H(13)	120.0
S(1)-C(2)-H(2A)	109.7	C(12)-C(13)-H(13)	120.0

C(15)-C(14)-C(13)	120.9(3)	C(24)-C(23)-Fe(1)	69.93(18)
C(15)-C(14)-H(14)	119.6	C(27)-C(23)-H(23)	125.8
C(13)-C(14)-H(14)	119.6	C(24)-C(23)-H(23)	125.8
C(14)-C(15)-C(16)	119.8(3)	Fe(1)-C(23)-H(23)	125.8
C(14)-C(15)-H(15)	120.1	C(23)-C(24)-C(25)	107.4(3)
C(16)-C(15)-H(15)	120.1	C(23)-C(24)-Fe(1)	69.58(17)
C(11)-C(16)-C(15)	119.8(3)	C(25)-C(24)-Fe(1)	69.86(17)
C(11)-C(16)-H(16)	120.1	C(23)-C(24)-H(24)	126.3
C(15)-C(16)-H(16)	120.1	C(25)-C(24)-H(24)	126.3
C(18)-C(17)-P(1)	111.30(19)	Fe(1)-C(24)-H(24)	125.9
C(18)-C(17)-H(17A)	109.4	C(24)-C(25)-C(26)	107.9(3)
P(1)-C(17)-H(17A)	109.4	C(24)-C(25)-Fe(1)	69.54(17)
C(18)-C(17)-H(17B)	109.4	C(26)-C(25)-Fe(1)	69.87(18)
P(1)-C(17)-H(17B)	109.4	C(24)-C(25)-H(25)	126.1
H(17A)-C(17)-H(17B)	108.0	C(26)-C(25)-H(25)	126.1
C(19)-C(18)-C(22)	107.6(2)	Fe(1)-C(25)-H(25)	126.1
C(19)-C(18)-C(17)	124.7(2)	C(27)-C(26)-C(25)	107.4(3)
C(22)-C(18)-C(17)	127.7(2)	C(27)-C(26)-Fe(1)	69.53(18)
C(19)-C(18)-Fe(1)	70.15(15)	C(25)-C(26)-Fe(1)	69.41(17)
C(22)-C(18)-Fe(1)	69.33(14)	C(27)-C(26)-H(26)	126.3
C(17)-C(18)-Fe(1)	126.08(19)	C(25)-C(26)-H(26)	126.3
C(20)-C(19)-C(18)	108.4(2)	Fe(1)-C(26)-H(26)	126.4
C(20)-C(19)-Fe(1)	69.50(15)	C(26)-C(27)-C(23)	108.9(3)
C(18)-C(19)-Fe(1)	69.14(15)	C(26)-C(27)-Fe(1)	70.45(19)
C(20)-C(19)-H(19)	125.8	C(23)-C(27)-Fe(1)	69.79(18)
C(18)-C(19)-H(19)	125.8	C(26)-C(27)-H(27)	125.6
Fe(1)-C(19)-H(19)	127.1	C(23)-C(27)-H(27)	125.6
C(19)-C(20)-C(21)	108.0(2)	Fe(1)-C(27)-H(27)	125.8
C(19)-C(20)-Fe(1)	69.89(15)	O(4)-Cl(1)-O(3)	110.09(15)
C(21)-C(20)-Fe(1)	69.54(15)	O(4)-Cl(1)-O(2)	110.59(13)
C(19)-C(20)-H(20)	126.0	O(3)-Cl(1)-O(2)	109.85(13)
C(21)-C(20)-H(20)	126.0	O(4)-Cl(1)-O(1)	108.79(13)
Fe(1)-C(20)-H(20)	126.1	O(3)-Cl(1)-O(1)	108.60(14)
C(22)-C(21)-C(20)	108.3(2)	O(2)-Cl(1)-O(1)	108.87(13)
C(22)-C(21)-Fe(1)	69.41(15)	O(6)-Cl(2)-O(5)	110.5(2)
C(20)-C(21)-Fe(1)	69.77(15)	O(6)-Cl(2)-O(7)	110.68(17)
C(22)-C(21)-H(21)	125.8	O(5)-Cl(2)-O(7)	109.10(18)
C(20)-C(21)-H(21)	125.8	O(6)-Cl(2)-O(8)	109.4(2)
Fe(1)-C(21)-H(21)	126.6	O(5)-Cl(2)-O(8)	108.10(18)
C(21)-C(22)-C(18)	107.8(2)	O(7)-Cl(2)-O(8)	109.08(19)
C(21)-C(22)-Fe(1)	69.84(15)	Cl(5)-C(28)-Cl(3)	110.53(16)
C(18)-C(22)-Fe(1)	69.37(14)	Cl(5)-C(28)-Cl(4)	109.91(16)
C(21)-C(22)-H(22)	126.1	Cl(3)-C(28)-Cl(4)	110.27(15)
C(18)-C(22)-H(22)	126.1	Cl(5)-C(28)-H(28)	108.7
Fe(1)-C(22)-H(22)	126.2	Cl(3)-C(28)-H(28)	108.7
C(27)-C(23)-C(24)	108.4(3)	Cl(4)-C(28)-H(28)	108.7
C(27)-C(23)-Fe(1)	70.02(18)		

• Angles (°) de torsió

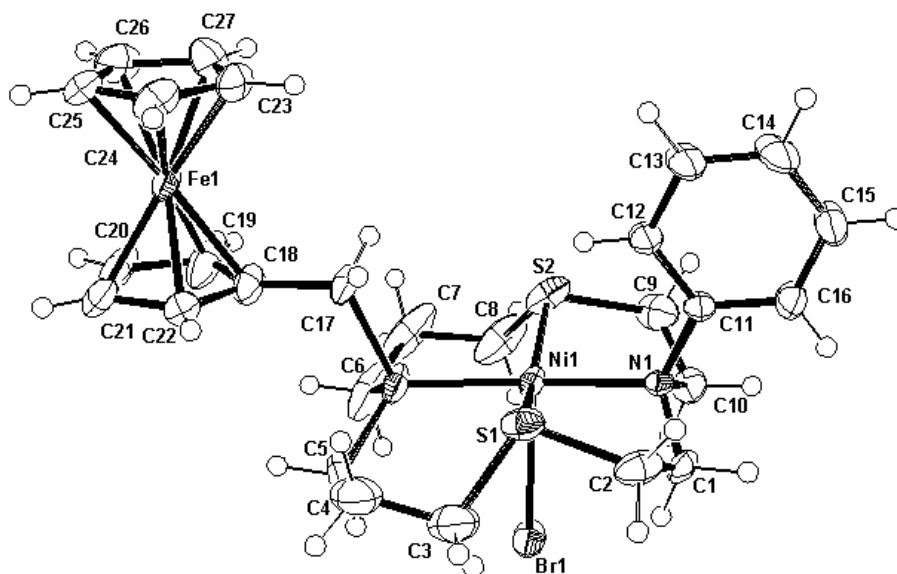
N(1)-Ni(1)-P(1)-C(5)	76.7(7)	S(2)-Ni(1)-P(1)-C(17)	-70.21(11)
S(1)-Ni(1)-P(1)-C(5)	-19.34(11)	N(1)-Ni(1)-S(1)-C(2)	-9.24(11)
S(2)-Ni(1)-P(1)-C(5)	170.29(11)	P(1)-Ni(1)-S(1)-C(2)	165.69(9)
N(1)-Ni(1)-P(1)-C(6)	-42.5(7)	S(2)-Ni(1)-S(1)-C(2)	-92.7(2)
S(1)-Ni(1)-P(1)-C(6)	-138.60(10)	N(1)-Ni(1)-S(1)-C(3)	-117.56(12)
S(2)-Ni(1)-P(1)-C(6)	51.03(10)	P(1)-Ni(1)-S(1)-C(3)	57.36(11)
N(1)-Ni(1)-P(1)-C(17)	-163.8(7)	S(2)-Ni(1)-S(1)-C(3)	158.9(2)
S(1)-Ni(1)-P(1)-C(17)	100.16(10)	N(1)-Ni(1)-S(2)-C(9)	10.39(12)

S(1)-Ni(1)-S(2)-C(9) 93.9(2)	Ni(1)-S(2)-C(9)-C(10) 18.3(2)
P(1)-Ni(1)-S(2)-C(9) -164.51(10)	C(11)-N(1)-C(10)-C(9) -65.3(3)
N(1)-Ni(1)-S(2)-C(8) 115.78(12)	C(1)-N(1)-C(10)-C(9) 173.0(2)
S(1)-Ni(1)-S(2)-C(8) -160.8(2)	Ni(1)-N(1)-C(10)-C(9) 58.4(2)
P(1)-Ni(1)-S(2)-C(8) -59.13(11)	S(2)-C(9)-C(10)-N(1) -50.5(3)
S(1)-Ni(1)-N(1)-C(11) -86.60(15)	C(10)-N(1)-C(11)-C(16) -53.0(3)
P(1)-Ni(1)-N(1)-C(11) 177.2(6)	C(1)-N(1)-C(11)-C(16) 68.7(3)
S(2)-Ni(1)-N(1)-C(11) 83.64(15)	Ni(1)-N(1)-C(11)-C(16) -170.94(19)
S(1)-Ni(1)-N(1)-C(10) 152.18(15)	C(10)-N(1)-C(11)-C(12) 128.0(2)
P(1)-Ni(1)-N(1)-C(10) 56.0(8)	C(1)-N(1)-C(11)-C(12) -110.3(3)
S(2)-Ni(1)-N(1)-C(10) -37.58(15)	Ni(1)-N(1)-C(11)-C(12) 10.0(3)
S(1)-Ni(1)-N(1)-C(1) 35.53(15)	C(16)-C(11)-C(12)-C(13) 0.0(4)
P(1)-Ni(1)-N(1)-C(1) -60.7(8)	N(1)-C(11)-C(12)-C(13) 179.0(2)
S(2)-Ni(1)-N(1)-C(1) -154.24(15)	C(11)-C(12)-C(13)-C(14) 1.5(4)
C(11)-N(1)-C(1)-C(2) 69.1(3)	C(12)-C(13)-C(14)-C(15) -1.9(4)
C(10)-N(1)-C(1)-C(2) -168.9(2)	C(13)-C(14)-C(15)-C(16) 0.8(4)
Ni(1)-N(1)-C(1)-C(2) -55.7(2)	C(12)-C(11)-C(16)-C(15) -1.1(4)
N(1)-C(1)-C(2)-S(1) 47.8(3)	N(1)-C(11)-C(16)-C(15) 179.9(2)
C(3)-S(1)-C(2)-C(1) 97.7(2)	C(14)-C(15)-C(16)-C(11) 0.7(4)
Ni(1)-S(1)-C(2)-C(1) -18.05(19)	C(5)-P(1)-C(17)-C(18) 96.1(2)
C(2)-S(1)-C(3)-C(4) -147.4(2)	C(6)-P(1)-C(17)-C(18) -151.76(19)
Ni(1)-S(1)-C(3)-C(4) -41.5(2)	Ni(1)-P(1)-C(17)-C(18) -28.1(2)
S(1)-C(3)-C(4)-C(5) -30.7(3)	P(1)-C(17)-C(18)-C(19) 111.1(3)
C(3)-C(4)-C(5)-P(1) 77.4(3)	P(1)-C(17)-C(18)-C(22) -68.6(3)
C(6)-P(1)-C(5)-C(4) 81.4(2)	P(1)-C(17)-C(18)-Fe(1) -159.23(15)
C(17)-P(1)-C(5)-C(4) -165.2(2)	C(22)-C(18)-C(19)-C(20) -0.9(3)
Ni(1)-P(1)-C(5)-C(4) -41.3(2)	C(18)-C(19)-C(20)-C(21) 1.0(3)
C(5)-P(1)-C(6)-C(7) -179.5(2)	C(19)-C(20)-C(21)-C(22) -0.7(3)
C(17)-P(1)-C(6)-C(7) 68.7(2)	C(20)-C(21)-C(22)-C(18) 0.1(3)
Ni(1)-P(1)-C(6)-C(7) -55.7(2)	C(19)-C(18)-C(22)-C(21) 0.5(3)
P(1)-C(6)-C(7)-C(8) 62.2(3)	C(27)-C(23)-C(24)-C(25) -0.2(3)
C(6)-C(7)-C(8)-S(2) -72.9(3)	C(23)-C(24)-C(25)-C(26) 0.1(3)
C(9)-S(2)-C(8)-C(7) 177.91(19)	C(24)-C(25)-C(26)-C(27) 0.0(4)
Ni(1)-S(2)-C(8)-C(7) 75.74(19)	C(25)-C(26)-C(27)-C(23) -0.1(4)
C(8)-S(2)-C(9)-C(10) -90.2(2)	C(24)-C(23)-C(27)-C(26) 0.2(4)

3 Estructura cristal·lina del complex [NiBr(L17)]ClO₄

- Paràmetres cristal·logràfics

	[Ni(Br)(L17)]ClO ₄ · 1 H ₂ O
fórmula química	C₂₇H₃₈BrClFeNNiO₅PS₂
pes molecular, g/mol	781.59
T(K)	173 (2)
λ (Å)	0.71073
sistema cristal·lí	Monoclínic
grup espacial	C2
a, Å	17.8907(5)
b, Å	10.7310(4)
c, Å	17.7475(5)
a, deg	90
b, deg	-
γ, deg	90
V, Å ³	3055.77(17)
ρ _{calc} , g/cm ³	1.699
Z	4
mida del cristall, mm	0.20 x 0.14 x 0.12
R1 [I > 2σ(I)]	0.0393
wR2 [I > 2σ(I)]	0.0800



- Coordenades fraccionàries i desplaçaments isotròpics per [NiBr(L17)]ClO₄

	x	y	z	U(eq)
Br(1)	6628(1)	1874(1)	4998(1)	37(1)
Ni(1)	7541(1)	1407(1)	6771(1)	22(1)
Fe(1)	7415(1)	5599(1)	9332(1)	29(1)
P(1)	7053(1)	3189(2)	6917(1)	37(1)
S(1)	6632(1)	366(2)	7025(1)	34(1)
S(2)	8752(1)	2214(2)	7060(1)	38(1)
O(7)	10258(5)	4354(8)	7946(5)	115(3)
N(1)	7975(3)	-219(5)	6604(3)	22(1)
C(1)	7213(4)	-985(6)	6081(4)	31(2)
C(2)	6686(4)	-1120(7)	6545(4)	37(2)
C(3)	5597(4)	916(8)	6371(4)	56(2)
C(4)	5490(5)	2194(10)	6682(5)	67(3)
C(5)	5915(5)	3228(9)	6461(4)	63(3)
C(6)	7313(7)	4470(7)	6421(5)	66(3)
C(7)	8213(7)	4608(7)	6622(5)	77(3)
C(8)	8601(6)	3513(7)	6347(5)	59(2)
C(9)	9152(4)	963(7)	6632(4)	42(2)
C(10)	8470(4)	77(6)	6127(4)	33(2)
C(11)	8514(4)	-907(6)	7389(3)	27(1)
C(12)	8702(4)	-369(6)	8157(3)	31(2)
C(13)	9229(4)	-1009(7)	8882(4)	44(2)
C(14)	9571(5)	-2118(8)	8838(4)	50(2)
C(15)	9387(4)	-2652(7)	8072(4)	41(2)
C(16)	8853(4)	-2044(6)	7339(4)	33(2)
C(17)	7439(4)	3577(6)	8043(3)	31(1)
C(18)	7086(4)	4768(6)	8190(4)	35(2)
C(19)	7398(6)	5993(7)	8209(4)	61(2)
C(20)	6879(6)	6844(8)	8372(4)	59(2)
C(21)	6265(6)	6174(9)	8471(4)	66(3)
C(22)	6376(4)	4884(8)	8351(4)	49(2)
C(23)	8185(4)	4411(6)	10248(4)	36(2)
C(24)	7511(5)	4750(7)	10402(4)	42(2)
C(25)	7522(4)	6058(7)	10491(4)	41(2)
C(26)	8202(4)	6515(7)	10390(4)	48(2)
C(27)	8611(4)	5491(7)	10229(4)	46(2)
Cl(1)	10000	2656(3)	10000	64(1)
O(1)	9309(4)	1955(8)	9898(6)	137(4)
O(2)	9727(5)	3482(10)	9295(4)	123(3)
Cl(2)	5000	6554(2)	5000	38(1)
O(3)	4478(5)	6532(10)	4036(5)	44(2)
O(4)	4701(6)	7628(9)	5283(6)	44(2)
O(5)	4763(7)	5394(10)	5254(6)	58(3)
O(6)	5832(5)	6585(12)	5155(6)	64(3)

• Distàncies (Å) i angles (°) d'enllaç

Br(1)-Ni(1) 2.8769(8)	C(14)-H(14) 0.9500
Ni(1)-N(1) 1.985(5)	C(15)-C(16) 1.389(8)
Ni(1)-P(1) 2.1645(18)	C(15)-H(15) 0.9500
Ni(1)-S(2) 2.1746(17)	C(16)-H(16) 0.9500
Ni(1)-S(1) 2.1773(17)	C(17)-C(18) 1.499(9)
Fe(1)-C(19) 2.025(6)	C(17)-H(17A) 0.9900
Fe(1)-C(27) 2.028(7)	C(17)-H(17B) 0.9900
Fe(1)-C(26) 2.034(6)	C(18)-C(19) 1.423(10)
Fe(1)-C(25) 2.040(6)	C(18)-C(22) 1.425(9)
Fe(1)-C(20) 2.041(7)	C(19)-C(20) 1.421(11)
Fe(1)-C(21) 2.042(8)	C(19)-H(19) 0.9500
Fe(1)-C(24) 2.043(7)	C(20)-C(21) 1.388(12)
Fe(1)-C(23) 2.045(6)	C(20)-H(20) 0.9500
Fe(1)-C(18) 2.048(6)	C(21)-C(22) 1.428(11)
Fe(1)-C(22) 2.052(7)	C(21)-H(21) 0.9500
P(1)-C(6) 1.801(8)	C(22)-H(22) 0.9500
P(1)-C(5) 1.830(8)	C(23)-C(27) 1.395(10)
P(1)-C(17) 1.849(6)	C(23)-C(24) 1.397(9)
S(1)-C(3) 1.795(7)	C(23)-H(23) 0.9500
S(1)-C(2) 1.831(7)	C(24)-C(25) 1.411(10)
S(2)-C(8) 1.822(8)	C(24)-H(24) 0.9500
S(2)-C(9) 1.836(7)	C(25)-C(26) 1.395(10)
N(1)-C(11) 1.493(7)	C(25)-H(25) 0.9500
N(1)-C(10) 1.505(7)	C(26)-C(27) 1.417(10)
N(1)-C(1) 1.507(7)	C(26)-H(26) 0.9500
C(1)-C(2) 1.510(8)	C(27)-H(27) 0.9500
C(1)-H(1A) 0.9900	Cl(1)-O(1) 1.388(7)
C(1)-H(1B) 0.9900	Cl(1)-O(1) 1 1.388(7)
C(2)-H(2A) 0.9900	Cl(1)-O(2) 1 1.432(8)
C(2)-H(2B) 0.9900	Cl(1)-O(2) 1.432(8)
C(3)-C(4) 1.522(12)	Cl(2)-O(6) 1.390(9)
C(3)-H(3A) 0.9900	Cl(2)-O(5) 1.449(10)
C(3)-H(3B) 0.9900	Cl(2)-O(4) 1.451(9)
C(4)-C(5) 1.491(13)	Cl(2)-O(3) 1.545(8)
C(4)-H(4A) 0.9900	
C(4)-H(4B) 0.9900	N(1)-Ni(1)-P(1) 178.41(13)
C(5)-H(5A) 0.9900	N(1)-Ni(1)-S(2) 88.28(14)
C(5)-H(5B) 0.9900	P(1)-Ni(1)-S(2) 91.85(8)
C(6)-C(7) 1.494(13)	N(1)-Ni(1)-S(1) 87.56(14)
C(6)-H(6A) 0.9900	P(1)-Ni(1)-S(1) 92.96(7)
C(6)-H(6B) 0.9900	S(2)-Ni(1)-S(1) 155.94(6)
C(7)-C(8) 1.549(12)	N(1)-Ni(1)-Br(1) 93.41(12)
C(7)-H(7A) 0.9900	P(1)-Ni(1)-Br(1) 85.01(5)
C(7)-H(7B) 0.9900	S(2)-Ni(1)-Br(1) 102.29(5)
C(8)-H(8A) 0.9900	S(1)-Ni(1)-Br(1) 101.61(5)
C(8)-H(8B) 0.9900	C(19)-Fe(1)-C(27) 109.7(3)
C(9)-C(10) 1.493(9)	C(19)-Fe(1)-C(26) 120.7(3)
C(9)-H(9A) 0.9900	C(27)-Fe(1)-C(26) 40.8(3)
C(9)-H(9B) 0.9900	C(19)-Fe(1)-C(25) 153.6(3)
C(10)-H(10A) 0.9900	C(27)-Fe(1)-C(25) 68.0(3)
C(10)-H(10B) 0.9900	C(26)-Fe(1)-C(25) 40.0(3)
C(11)-C(12) 1.378(8)	C(19)-Fe(1)-C(20) 40.9(3)
C(11)-C(16) 1.382(9)	C(27)-Fe(1)-C(20) 129.5(4)
C(12)-C(13) 1.393(8)	C(26)-Fe(1)-C(20) 109.4(3)
C(12)-H(12) 0.9500	C(25)-Fe(1)-C(20) 118.9(3)
C(13)-C(14) 1.356(10)	C(19)-Fe(1)-C(21) 68.2(4)
C(13)-H(13) 0.9500	C(27)-Fe(1)-C(21) 165.6(4)
C(14)-C(15) 1.375(9)	C(26)-Fe(1)-C(21) 127.0(3)

C(25)-Fe(1)-C(21)	107.2(3)	S(1)-C(2)-H(2B)	109.6
C(20)-Fe(1)-C(21)	39.7(3)	H(2A)-C(2)-H(2B)	108.1
C(19)-Fe(1)-C(24)	165.1(3)	C(4)-C(3)-S(1)	108.7(5)
C(27)-Fe(1)-C(24)	67.6(3)	C(4)-C(3)-H(3A)	109.9
C(26)-Fe(1)-C(24)	67.6(3)	S(1)-C(3)-H(3A)	109.9
C(25)-Fe(1)-C(24)	40.4(3)	C(4)-C(3)-H(3B)	109.9
C(20)-Fe(1)-C(24)	152.0(3)	S(1)-C(3)-H(3B)	109.9
C(21)-Fe(1)-C(24)	118.2(4)	H(3A)-C(3)-H(3B)	108.3
C(19)-Fe(1)-C(23)	128.6(3)	C(5)-C(4)-C(3)	114.5(6)
C(27)-Fe(1)-C(23)	40.1(3)	C(5)-C(4)-H(4A)	108.6
C(26)-Fe(1)-C(23)	67.7(3)	C(3)-C(4)-H(4A)	108.6
C(25)-Fe(1)-C(23)	67.6(3)	C(5)-C(4)-H(4B)	108.6
C(20)-Fe(1)-C(23)	167.0(3)	C(3)-C(4)-H(4B)	108.6
C(21)-Fe(1)-C(23)	152.2(4)	H(4A)-C(4)-H(4B)	107.6
C(24)-Fe(1)-C(23)	40.0(3)	C(4)-C(5)-P(1)	117.7(5)
C(19)-Fe(1)-C(18)	40.9(3)	C(4)-C(5)-H(5A)	107.9
C(27)-Fe(1)-C(18)	119.6(3)	P(1)-C(5)-H(5A)	107.9
C(26)-Fe(1)-C(18)	154.5(3)	C(4)-C(5)-H(5B)	107.9
C(25)-Fe(1)-C(18)	163.9(3)	P(1)-C(5)-H(5B)	107.9
C(20)-Fe(1)-C(18)	68.6(3)	H(5A)-C(5)-H(5B)	107.2
C(21)-Fe(1)-C(18)	68.7(3)	C(7)-C(6)-P(1)	116.3(6)
C(24)-Fe(1)-C(18)	126.5(3)	C(7)-C(6)-H(6A)	108.2
C(23)-Fe(1)-C(18)	108.3(3)	P(1)-C(6)-H(6A)	108.2
C(19)-Fe(1)-C(22)	68.2(3)	C(7)-C(6)-H(6B)	108.2
C(27)-Fe(1)-C(22)	152.9(3)	P(1)-C(6)-H(6B)	108.2
C(26)-Fe(1)-C(22)	164.0(3)	H(6A)-C(6)-H(6B)	107.4
C(25)-Fe(1)-C(22)	126.3(3)	C(6)-C(7)-C(8)	115.8(7)
C(20)-Fe(1)-C(22)	67.7(4)	C(6)-C(7)-H(7A)	108.3
C(21)-Fe(1)-C(22)	40.8(3)	C(8)-C(7)-H(7A)	108.3
C(24)-Fe(1)-C(22)	107.1(3)	C(6)-C(7)-H(7B)	108.3
C(23)-Fe(1)-C(22)	118.7(3)	C(8)-C(7)-H(7B)	108.3
C(18)-Fe(1)-C(22)	40.7(3)	H(7A)-C(7)-H(7B)	107.4
C(6)-P(1)-C(5)	104.2(5)	C(7)-C(8)-S(2)	108.1(5)
C(6)-P(1)-C(17)	107.6(3)	C(7)-C(8)-H(8A)	110.1
C(5)-P(1)-C(17)	106.4(3)	S(2)-C(8)-H(8A)	110.1
C(6)-P(1)-Ni(1)	114.3(3)	C(7)-C(8)-H(8B)	110.1
C(5)-P(1)-Ni(1)	113.3(3)	S(2)-C(8)-H(8B)	110.1
C(17)-P(1)-Ni(1)	110.5(2)	H(8A)-C(8)-H(8B)	108.4
C(3)-S(1)-C(2)	103.7(3)	C(10)-C(9)-S(2)	110.5(4)
C(3)-S(1)-Ni(1)	110.4(3)	C(10)-C(9)-H(9A)	109.6
C(2)-S(1)-Ni(1)	98.8(2)	S(2)-C(9)-H(9A)	109.6
C(8)-S(2)-C(9)	103.7(3)	C(10)-C(9)-H(9B)	109.6
C(8)-S(2)-Ni(1)	108.3(3)	S(2)-C(9)-H(9B)	109.6
C(9)-S(2)-Ni(1)	98.1(2)	H(9A)-C(9)-H(9B)	108.1
C(11)-N(1)-C(10)	109.3(4)	C(9)-C(10)-N(1)	109.0(5)
C(11)-N(1)-C(1)	109.9(5)	C(9)-C(10)-H(10A)	109.9
C(10)-N(1)-C(1)	111.4(4)	N(1)-C(10)-H(10A)	109.9
C(11)-N(1)-Ni(1)	115.4(3)	C(9)-C(10)-H(10B)	109.9
C(10)-N(1)-Ni(1)	105.4(4)	N(1)-C(10)-H(10B)	109.9
C(1)-N(1)-Ni(1)	105.3(3)	H(10A)-C(10)-H(10B)	108.3
N(1)-C(1)-C(2)	109.2(5)	C(12)-C(11)-C(16)	120.7(5)
N(1)-C(1)-H(1A)	109.8	C(12)-C(11)-N(1)	119.4(5)
C(2)-C(1)-H(1A)	109.8	C(16)-C(11)-N(1)	119.8(5)
N(1)-C(1)-H(1B)	109.8	C(11)-C(12)-C(13)	118.4(6)
C(2)-C(1)-H(1B)	109.8	C(11)-C(12)-H(12)	120.8
H(1A)-C(1)-H(1B)	108.3	C(13)-C(12)-H(12)	120.8
C(1)-C(2)-S(1)	110.2(4)	C(14)-C(13)-C(12)	121.2(6)
C(1)-C(2)-H(2A)	109.6	C(14)-C(13)-H(13)	119.4
S(1)-C(2)-H(2A)	109.6	C(12)-C(13)-H(13)	119.4
C(1)-C(2)-H(2B)	109.6	C(13)-C(14)-C(15)	120.4(6)

C(13)-C(14)-H(14)	119.8	Fe(1)-C(22)-H(22)	126.9
C(15)-C(14)-H(14)	119.8	C(27)-C(23)-C(24)	108.4(6)
C(14)-C(15)-C(16)	119.6(6)	C(27)-C(23)-Fe(1)	69.3(4)
C(14)-C(15)-H(15)	120.2	C(24)-C(23)-Fe(1)	69.9(4)
C(16)-C(15)-H(15)	120.2	C(27)-C(23)-H(23)	125.8
C(11)-C(16)-C(15)	119.6(6)	C(24)-C(23)-H(23)	125.8
C(11)-C(16)-H(16)	120.2	Fe(1)-C(23)-H(23)	126.6
C(15)-C(16)-H(16)	120.2	C(23)-C(24)-C(25)	108.1(6)
C(18)-C(17)-P(1)	113.3(4)	C(23)-C(24)-Fe(1)	70.1(4)
C(18)-C(17)-H(17A)	108.9	C(25)-C(24)-Fe(1)	69.7(4)
P(1)-C(17)-H(17A)	108.9	C(23)-C(24)-H(24)	126.0
C(18)-C(17)-H(17B)	108.9	C(25)-C(24)-H(24)	126.0
P(1)-C(17)-H(17B)	108.9	Fe(1)-C(24)-H(24)	125.9
H(17A)-C(17)-H(17B)	107.7	C(26)-C(25)-C(24)	107.8(6)
C(19)-C(18)-C(22)	106.8(6)	C(26)-C(25)-Fe(1)	69.7(4)
C(19)-C(18)-C(17)	126.9(6)	C(24)-C(25)-Fe(1)	69.9(4)
C(22)-C(18)-C(17)	126.2(7)	C(26)-C(25)-H(25)	126.1
C(19)-C(18)-Fe(1)	68.7(4)	C(24)-C(25)-H(25)	126.1
C(22)-C(18)-Fe(1)	69.8(4)	Fe(1)-C(25)-H(25)	125.8
C(17)-C(18)-Fe(1)	125.8(4)	C(25)-C(26)-C(27)	108.0(7)
C(20)-C(19)-C(18)	108.3(8)	C(25)-C(26)-Fe(1)	70.2(4)
C(20)-C(19)-Fe(1)	70.1(4)	C(27)-C(26)-Fe(1)	69.3(4)
C(18)-C(19)-Fe(1)	70.4(4)	C(25)-C(26)-H(26)	126.0
C(20)-C(19)-H(19)	125.9	C(27)-C(26)-H(26)	126.0
C(18)-C(19)-H(19)	125.9	Fe(1)-C(26)-H(26)	126.1
Fe(1)-C(19)-H(19)	125.1	C(23)-C(27)-C(26)	107.7(6)
C(21)-C(20)-C(19)	108.6(8)	C(23)-C(27)-Fe(1)	70.6(4)
C(21)-C(20)-Fe(1)	70.2(5)	C(26)-C(27)-Fe(1)	69.8(4)
C(19)-C(20)-Fe(1)	68.9(4)	C(23)-C(27)-H(27)	126.2
C(21)-C(20)-H(20)	125.7	C(26)-C(27)-H(27)	126.2
C(19)-C(20)-H(20)	125.7	Fe(1)-C(27)-H(27)	125.0
Fe(1)-C(20)-H(20)	126.7	O(1)-Cl(1)-O(1)#1	114.4(7)
C(20)-C(21)-C(22)	108.2(8)	O(1)-Cl(1)-O(2)#1	112.9(5)
C(20)-C(21)-Fe(1)	70.1(5)	O(1)#1-Cl(1)-O(2)#1	106.3(5)
C(22)-C(21)-Fe(1)	69.9(4)	O(1)-Cl(1)-O(2)	106.3(5)
C(20)-C(21)-H(21)	125.9	O(1)#1-Cl(1)-O(2)	112.9(5)
C(22)-C(21)-H(21)	125.9	O(2)#1-Cl(1)-O(2)	103.5(8)
Fe(1)-C(21)-H(21)	125.7	O(6)-Cl(2)-O(5)	113.2(7)
C(18)-C(22)-C(21)	108.1(8)	O(6)-Cl(2)-O(4)	116.0(6)
C(18)-C(22)-Fe(1)	69.5(4)	O(5)-Cl(2)-O(4)	111.8(5)
C(21)-C(22)-Fe(1)	69.2(5)	O(6)-Cl(2)-O(3)	106.9(5)
C(18)-C(22)-H(22)	126.0	O(5)-Cl(2)-O(3)	102.4(6)
C(21)-C(22)-H(22)	126.0	O(4)-Cl(2)-O(3)	105.1(5)

• Angles (°) de torsió

N(1)-Ni(1)-P(1)-C(6)	-50(5)	N(1)-Ni(1)-S(1)-C(3)	-127.2(3)
S(2)-Ni(1)-P(1)-C(6)	44.7(3)	P(1)-Ni(1)-S(1)-C(3)	51.3(3)
S(1)-Ni(1)-P(1)-C(6)	-158.9(3)	S(2)-Ni(1)-S(1)-C(3)	152.5(3)
Br(1)-Ni(1)-P(1)-C(6)	-57.5(3)	Br(1)-Ni(1)-S(1)-C(3)	-34.2(3)
N(1)-Ni(1)-P(1)-C(5)	69(5)	N(1)-Ni(1)-S(1)-C(2)	-19.0(2)
S(2)-Ni(1)-P(1)-C(5)	163.8(3)	P(1)-Ni(1)-S(1)-C(2)	159.5(2)
S(1)-Ni(1)-P(1)-C(5)	-39.8(3)	S(2)-Ni(1)-S(1)-C(2)	-99.3(3)
Br(1)-Ni(1)-P(1)-C(5)	61.6(3)	Br(1)-Ni(1)-S(1)-C(2)	74.0(2)
N(1)-Ni(1)-P(1)-C(17)	-172(5)	N(1)-Ni(1)-S(2)-C(8)	123.7(3)
S(2)-Ni(1)-P(1)-C(17)	-76.9(3)	P(1)-Ni(1)-S(2)-C(8)	-54.7(3)
S(1)-Ni(1)-P(1)-C(17)	79.5(3)	S(1)-Ni(1)-S(2)-C(8)	-156.2(3)
Br(1)-Ni(1)-P(1)-C(17)	-179.1(3)	Br(1)-Ni(1)-S(2)-C(8)	30.6(3)

N(1)-Ni(1)-S(2)-C(9) 16.2(2)	C(8)-S(2)-C(9)-C(10) -99.9(5)
P(1)-Ni(1)-S(2)-C(9) -162.2(2)	Ni(1)-S(2)-C(9)-C(10) 11.3(5)
S(1)-Ni(1)-S(2)-C(9) 96.3(3)	S(2)-C(9)-C(10)-N(1) -45.0(6)
Br(1)-Ni(1)-S(2)-C(9) -76.9(2)	C(11)-N(1)-C(10)-C(9) -65.4(6)
P(1)-Ni(1)-N(1)-C(11) 174.(63)	C(1)-N(1)-C(10)-C(9) 173.0(5)
S(2)-Ni(1)-N(1)-C(11) 78.8(4)	Ni(1)-N(1)-C(10)-C(9) 59.2(5)
S(1)-Ni(1)-N(1)-C(11) -77.5(4)	C(10)-N(1)-C(11)-C(12) 115.9(6)
Br(1)-Ni(1)-N(1)-C(11) -179.0(4)	C(1)-N(1)-C(11)-C(12) -121.5(6)
P(1)-Ni(1)-N(1)-C(10) 53(5)	Ni(1)-N(1)-C(11)-C(12) -2.6(7)
S(2)-Ni(1)-N(1)-C(10) -41.9(3)	C(10)-N(1)-C(11)-C(16) -60.9(7)
S(1)-Ni(1)-N(1)-C(10) 161.8(3)	C(1)-N(1)-C(11)-C(16) 61.6(7)
Br(1)-Ni(1)-N(1)-C(10) 60.3(3)	Ni(1)-N(1)-C(11)-C(16) -179.5(5)
P(1)-Ni(1)-N(1)-C(1) -65(5)	C(16)-C(11)-C(12)-C(13) -1.0(10)
S(2)-Ni(1)-N(1)-C(1) -159.8(3)	N(1)-C(11)-C(12)-C(13) -177.8(6)
S(1)-Ni(1)-N(1)-C(1) 43.9(3)	C(11)-C(12)-C(13)-C(14) 1.7(11)
Br(1)-Ni(1)-N(1)-C(1) -57.6(3)	C(12)-C(13)-C(14)-C(15) -1.5(12)
C(11)-N(1)-C(1)-C(2) 65.6(6)	C(13)-C(14)-C(15)-C(16) 0.5(12)
C(10)-N(1)-C(1)-C(2) -173.1(5)	C(12)-C(11)-C(16)-C(15) 0.1(10)
Ni(1)-N(1)-C(1)-C(2) -59.3(5)	N(1)-C(11)-C(16)-C(15) 176.9(6)
N(1)-C(1)-C(2)-S(1) 42.3(6)	C(14)-C(15)-C(16)-C(11) 0.2(10)
C(3)-S(1)-C(2)-C(1) 105.8(5)	C(6)-P(1)-C(17)-C(18) 57.9(6)
Ni(1)-S(1)-C(2)-C(1) -7.8(4)	C(5)-P(1)-C(17)-C(18) -53.3(6)
C(2)-S(1)-C(3)-C(4) -177.0(5)	Ni(1)-P(1)-C(17)-C(18) -176.7(4)
Ni(1)-S(1)-C(3)-C(4) -72.1(6)	P(1)-C(17)-C(18)-C(19) -86.2(7)
S(1)-C(3)-C(4)-C(5) 75.3(7)	P(1)-C(17)-C(18)-C(22) 94.9(7)
C(3)-C(4)-C(5)-P(1) -64.5(8)	C(22)-C(18)-C(19)-C(20) -0.6(7)
C(6)-P(1)-C(5)-C(4) 174.0(6)	C(18)-C(19)-C(20)-C(21) 1.2(8)
C(17)-P(1)-C(5)-C(4) -72.4(6)	C(19)-C(20)-C(21)-C(22) -1.4(8)
Ni(1)-P(1)-C(5)-C(4) 49.2(6)	C(19)-C(18)-C(22)-C(21) -0.3(7)
C(5)-P(1)-C(6)-C(7) -175.1(5)	C(20)-C(21)-C(22)-C(18) 1.0(8)
C(17)-P(1)-C(6)-C(7) 72.2(6)	C(27)-C(23)-C(24)-C(25) -0.8(7)
Ni(1)-P(1)-C(6)-C(7) -51.0(6)	C(23)-C(24)-C(25)-C(26) 0.1(7)
P(1)-C(6)-C(7)-C(8) 62.8(8)	C(24)-C(25)-C(26)-C(27) 0.6(7)
C(6)-C(7)-C(8)-S(2) -74.3(8)	C(24)-C(23)-C(27)-C(26) 1.1(7)
C(9)-S(2)-C(8)-C(7) 176.8(6)	C(25)-C(26)-C(27)-C(23) -1.0(7)
Ni(1)-S(2)-C(8)-C(7) 73.2(6)	

APÈNDIX IV:

ARXIUS DE LES ESTRUCTURES CRISTAL·LINES

Al CD s'inclouen els arxius de les dades estructurals refinades (extensió cif) i de les dades estructurals no refinades (extensió res).

Els arxius són:

PdL17.cif corresponent al complex $[\text{Pd}(\text{L17})](\text{BF}_4)_2$

NiL17.cif corresponent al complex $[\text{Ni}(\text{L17})](\text{ClO}_4)_2$

NiBrL17.cif corresponent al complex $[\text{NiBr}(\text{L17})]\text{ClO}_4$

Bi-L15.res corresponent al lligand bimaqurocíclic **Bi-L15**

PdL2.res corresponent al complex $[\text{Pd}(\text{L12})](\text{BF}_4)_2$

PdL4.res corresponent al complex $[\text{Pd}(\text{L4})](\text{BF}_4)_2$

PdL5.res corresponent al complex $[\text{Pd}(\text{L5})](\text{BF}_4)_2$

CuL1.res corresponent al complex $[\text{Cu}(\text{ClO}_4)(\text{L1})]\text{ClO}_4$

CuL2.res corresponent al complex $[\text{Cu}(\text{L2})](\text{BF}_4)_2$

NiL17.res corresponent al complex $[\text{Ni}(\text{L17})]\text{ClO}_4$

També s'ha inclòs el programa ORTEP, versió 1.076, per poder visualitzar-les. Per instal·lar-lo només cal clicar la icona corresponent i seguir les instruccions.