VI. Annexos

Annex I.

Determinacions cristal·logràfiques

	Complex 5	Complex 6	Compost 9	Compost 40b
Fòrmula empírica	C_{12} H_{24} Cl_4 N_2 Pt	C_{10} H_{19} Cl_2 N Pt	C_{12} H_{22} Cl_4 N_2 Pt	C_8 H_{10} N_2 O
Pes molecular (g/mol)	533.22	419.25	531.21	150.18
T (K)	293(2)	293(2)	293(2)	293(2)
λ (Mo-K_α) (Å)	0.71069	0.71069	0.71069	0.71069
Sistema cristal·lí	Ortoròmbic	Monoclinic	Triclínic	Ortoròmbic
Grup espacial	$P2_12_12_1$	$P2_1/m$	P1	Pnab
a (Å)	10.8650(10)	8.4980(10)	7.372(9)	9.094(8)
b (Å)	12.1680(10)	16.5210(10)	10.261(5)	10.420(3)
c (Å)	13.2060(10)	9.5350(10)	12.3310(10)	17.854(4)
α (º)	90	90	68.5210(10)	90
β (º)	90	113.106(10)	86.8400(10)	90
γ (º)	90	90	82.8590(10)	90
V (Å^3)	1745.9(3)	1231.3(2)	861.2(11)	1691.8(16)
Z	4	4	2	8
D_{calc} (Mg m^{-3})	2.029	2.262	2.048	1.179
μ (mm^{-1})	8.638	11.793	8.756	0.080
F (000)	1024	792	508	640
Rang Θ (º)	2.51-31.60	2.47-33.40	2.23-31.71	2.26-29.93
h, k, l ranges	$0\leq h\leq 13$, $0\leq k\leq 16$, $0\leq l\leq 19$	$-11\leq h\leq 10$, $0\leq k\leq 24$, $0\leq l\leq 13$	$-9\leq h\leq 9$, $-13\leq k\leq 14$, $0\leq l\leq 18$	$0\leq h\leq 12$, $0\leq k\leq 14$, $0\leq l\leq 25$
Nre. reflexions enregistrades	11617	7247	6209	2467
Nre. reflexions independents	2587	2960	3949	2467
[R_{int} (on F)]	0.0490	0.0355	0.0258	0.0544
Mètode de refinament	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	*Full-matrix least-squares on* F^2	Full-matrix least-squares on F^2
No. of data	2587	2960	3949	2467

Nre. de paràmetres	173	127	188	116
Goodness-of-fit on F^2	1.089	1.117	1.059	0.704
R final [$I>2\sigma(I)$]	R_1 = 0.0377, wR_2 = 0.0889	R_1 = 0.0317, wR_2 = 0.0987	R_1 = 0.0404, wR_2 = 0.1016	R_1 = 0.0294, wR_2 = 0.0428
R indices (all data)	R_1 = 0.0464, wR_2 = 0.1008	R_1 = 0.0365, wR_2 = 0.1021	R_1 = 0.0404, wR_2 = 0.1016	R_1 = 0.2800, wR_2 = 0.0757
Largest difference peak and hole (e Å^3)	0.847 and –0.877	0.787 and –0.886	0.797 and –0.551	0.098 and –0.092

Taula I. 1.- *Dades cristal·logràfiques i de refinament d'estructura dels compostos **5**, **6**, **9** i **40b**.*

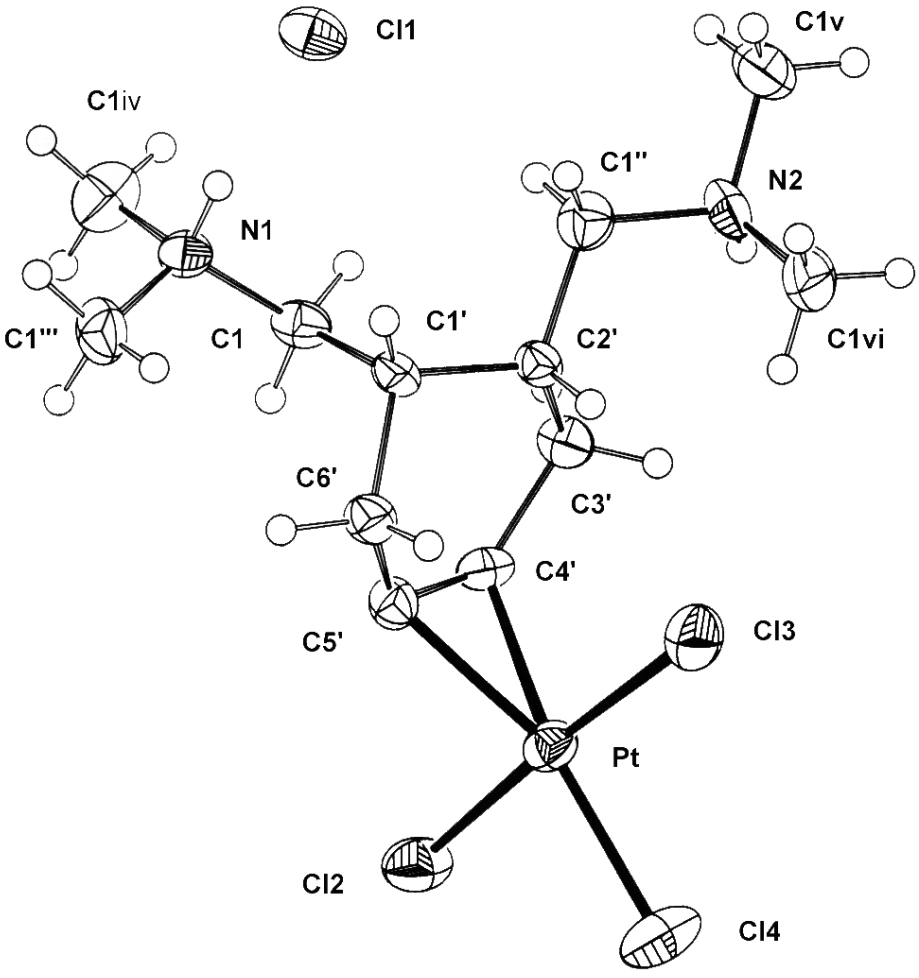

Figura I. 1.- *Estructura molecular del complex **5**.*

Complex 5			
Distàncies d'enllaç (Å)		**Angles d'enllaç (º)**	
		C(4')-Pt-C(3')	37.3(3)
		C(4')-Pt-Cl(3)	93.4(3)
		C(3')-Pt-Cl(3)	98.5(3)
		C(4')-Pt-Cl(2)	89.2(3)
		C(3')-Pt-Cl(2)	85.4(3)
		Cl(3)-Pt-Cl(2)	176.10(12)
		C(4')-Pt-Cl(4)	163.5(3)
		C(3')-Pt-Cl(4)	158.4(2)
Pt-C(4')	2.167(10)	Cl(3)-Pt-Cl(4)	87.94(13)
Pt-C(3')	2.180(10)	Cl(2)-Pt-Cl(4)	88.74(12)
Pt-Cl(3)	2.298(3)	C(4')-C(3')-Pt	70.8(6)
Pt-Cl(2)	2.304(3)	C(2')-C(3')-Pt	120.0(7)
Pt-Cl(4)	2.316(3)	C(3')-C(4')-Pt	71.9(6)
N(1)-C(1''')	1.484(13)	C(5')-C(4')-Pt	120.9(8)
N(1)-C(1^{iv})	1.49(2)	C(1''')-N(1)-C(1^{iv})	110.2(9)
N(1)-C(1)	1.494(13)	C(1''')-N(1)-C(1)	115.8(8)
N(2)-C(1^{v})	1.476(13)	C(1)-N(1)-C(1^{iv})	111.1(8)
N(1)-C(1^{vi})	1.48(2)	C(1''')-N(1)-H (N1)	106.4(5)
N(1)-C(1'')	1.494(13)	C(1^{iv})-N(1)-H (N1)	106.4(6)
C(3')-C(4')	1.390(13)	C(1)-N(1)-H (N1)	106.4(5)
C(3')-C(2')	1.513(13)	C(1^{v})-N(2)-C(1^{vi})	112.3(9)
C(4')-C(5')	1.528(13)	C(1^{v})-N(2)-C(1'')	109.3(9)
C(5')-C(6')	1.545(12)	C(1^{vi})-N(2)-C(1'')	112.3(8)
C(1')-C(6')	1.519(13)	C(4')-C(3')-C(2')	121.4(8)
C(6')-C(1'')	1.531(14)	C(4')-C(5')-C(6')	113.8(8)
C(1')-C(1)	1.55(2)	C(1')-C(6')-C(1''')	112.1(8)
C(1')-C(2')	1.552(12)	C(3')-C(4')-C(5')	121.5(8)
		C(1)-C(1')-C-(2')	111.9(8)
		C(1'')-C(6')-C(5')	112.1(7)
		C(6')-C(1')-C(1)	112.8(7)
		C(6')-C(1')-C(2')	106.4(8)
		C(1)-C(1')-C(2')	111.9(8)
		C(3')-C(2')-C(1')	109.5(7)
		N(2)-C(1'')-C(6')	112.8(9)
		N(1)-C(1)-C(1')	113.5(7)

Taula I. 2.- *Distàncies i angles d'enllaç del complex **5**.*

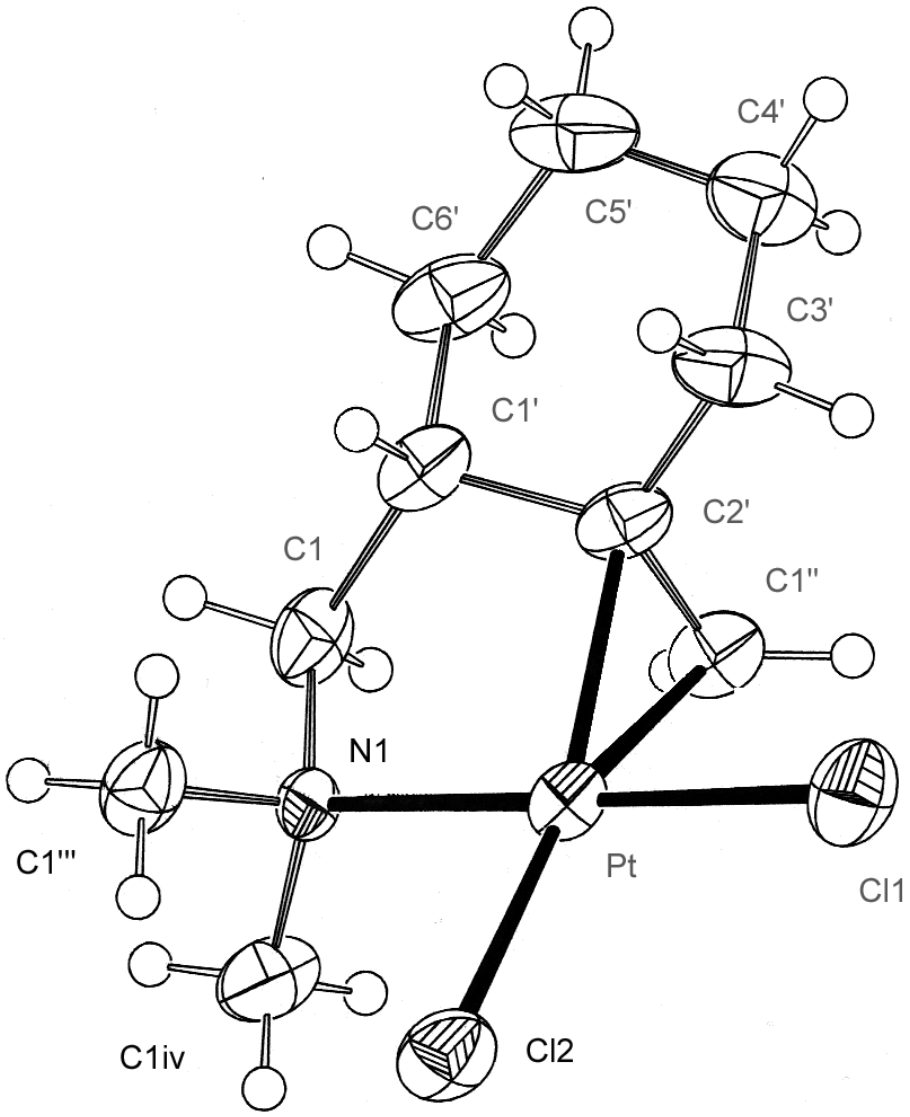

Figura I. 2.- *Estructura molecular del complex* ***6****.*

Complex 6			
Distàncies d'enllaç (Å)		**Angles d'enllaç (º)**	
		N(1)-Pt-C(1'')	97.12(18)
		N(1)-Pt-C(6')	91.0(2)
		C(1'')-Pt-C(6')	37.79(16)
		N(1)-Pt-Cl(1)	179.19(11)
		C(1'')-Pt-Cl(1)	82.63(14)
		C(6')-Pt-Cl(1)	88.35(17)
		N(1)-Pt-Cl(2)	84.67(14)
		C(1'')-Pt-Cl(2)	158.98(13)
Pt-N(1)	2.077(4)	C(6')-Pt-Cl(2)	163.12(12)
Pt-C(1'')	2.120(4)	Cl(1)-Pt-Cl(2)	95.84(6)
Pt-C(6')	2.149(6)	C(1)-N(1)-Pt	104.2(3)
Pt-Cl(1)	2.2876(18)	C(1^{iv})-N(1)-Pt	114.0(3)
Pt-Cl(2)	2.3409(14)	C(1''')-N(1)-Pt	115.4(3)
N(1)-C(1)	1.463(8)	C(1'')-C(6')-Pt	70.0(3)
N(1)-C(1''')	1.520(6)	C(1')-C(6')-Pt	98.2(4)
N(1)-C(1^{iv})	1.526(6)	C(5')-C(6')-Pt	124.1(4)
C(6')-C(1'')	1.383(6)	C(6')-C(1'')-Pt	72.3(3)
C(1)-C(1')	1.586(8)	C(1)-N(1)-C(1''')	108.5(4)
C(1')-C(2')	1.485(8)	C(1)-N(1)-C(1^{iv})	108.9(4)
C(1')-C(6')	1.529(7)	C(1''')-N(1)-C(1^{iv})	105.6(5)
C(2')-C(3')	1.624(10)	N(1)-C(1)-C(1')	111.4(4)
C(3')-C(4')	1.484(10)	C(1'')-C(6')-C(1')	118.3(5)
C(4')-C(5')	1.488(8)	C(1'')-C(6')-C(5')	122.0(5)
C(5')-C(6')	1.550(8)	C(2')-C(1')-C(6')	103.1(5)
		C(2')-C(1')-C(1)	115.2(4)
		C(1')-C(6')-C(5')	114.5(4)
		C(6')-C(1')-C(1)	113.0(4)
		C(1')-C(2')-C(3')	113.1(5)
		C(4')-C(3')-C(2')	113.3(5)
		C(3')-C(4')-C(5')	107.4(6)
		C(4')-C(5')-C(6')	109.3(5)

Taula I. 3.- *Distàncies i angles d'enllaç del complex **6**.*

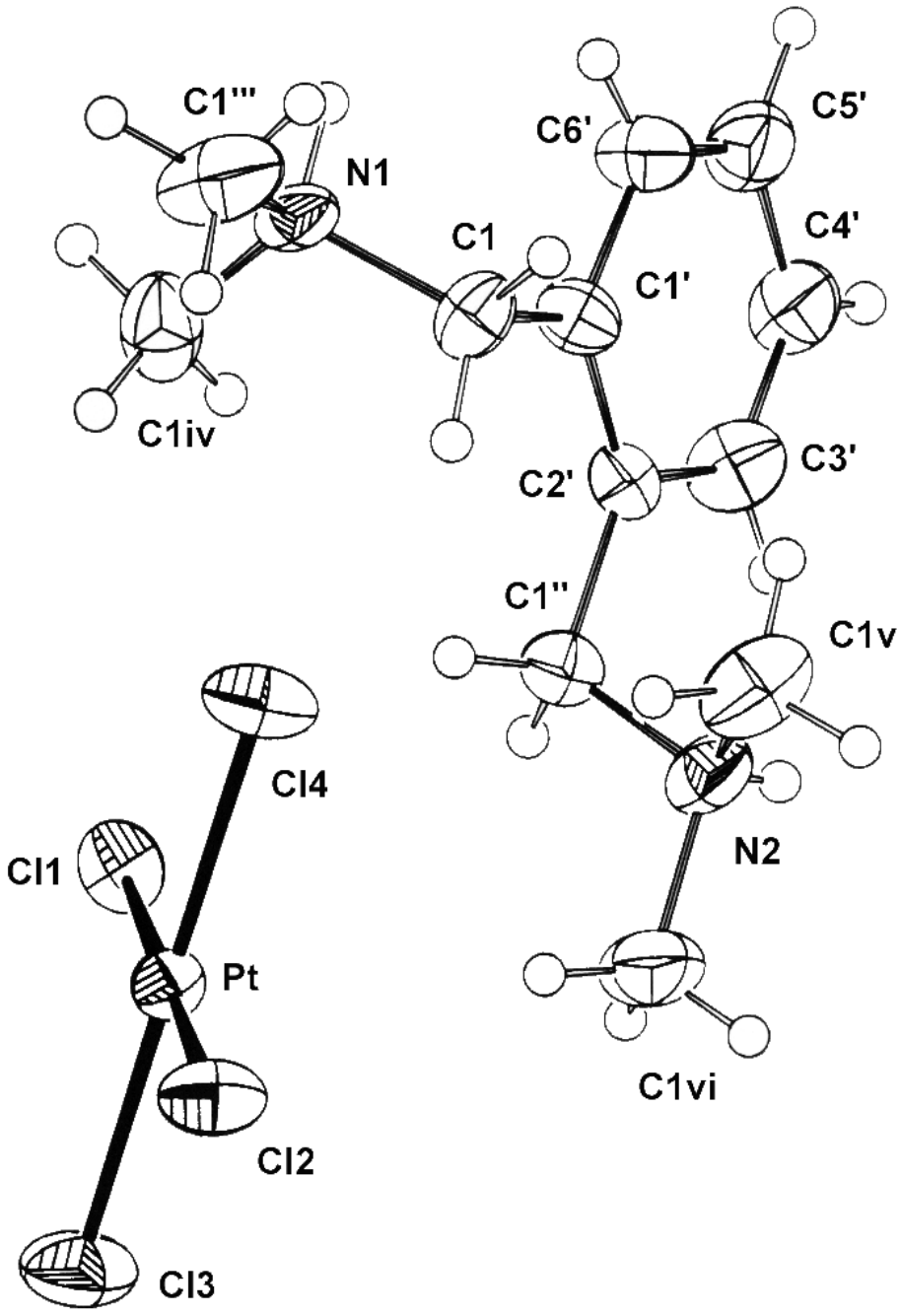

Figura I. 3.- *Estructura molecular del compost* ***9****.*

Compost 9			
Distàncies d'enllaç (Å)		**Angles d'enllaç (º)**	
		Cl3-Pt-Cl4	179.20(4)
		Cl3-Pt-Cl2	89.17(6)
		Cl4-Pt-Cl2	90.15(6)
Pt-Cl3	2.2935(13)	Cl3-Pt-Cl1	90.30(6)
Pt-Cl4	2.2962(14)	Cl4-Pt-Cl1	90.39(6)
Pt-Cl2	2.3032(15)	Cl2-Pt-Cl1	179.11(4)
Pt-Cl1	2.3139(15)	C1'''-N1-C1	110.5(5)
N1-C1'''	1.473(7)	C1'''-N1-C^{iv}	110.5(5)
N1-C1	1.490(6)	C1-N1-C1'''	111.0(4)
N1-C1^{iv}	1.517(8)	C1^{vi}-N2-C1^{v}	112.3(5)
N2-C1^{vi}	1.484(7)	C1^{vi}-N2-C1''	109.8(5)
N2-C1^{v}	1.493(7)	C1^{v}-N2-C1''	112.3(5)
N2-C1''	1.530(7)	C6'-C1'-C2'	116.9(4)
C1-C1'	1.478(6)	C6'-C1'-C1	119.5(4)
C1'-C6'	1.385(7)	C2'-C1'-C1	123.5(4)
C1'-C2'	1.434(6)	C5'-C6'-C1'	122.7(5)
C6'-C5'	1.371(8)	C1'-C1-N1	112.5(4)
C5'-C4'	1.395(8)	C6'-C5'-C4'	119.6(5)
C4'-C3'	1.320(8)	C4'-C5'-C6'	119.8(5)
C3'-C2'	1.409(6)	C4'-C3'-C2'	122.8(5)
C2'-C1''	1.493(6)	C3'-C2'-C1'	118.3(4)
		C3'-C2'-C1''	117.8(4)
		C1'-C2'-C1''	123.9(4)
		C2'-C1''-N2	112.5(4)

Taula I. 4.- *Distàncies i angles d'enllaç del compost **9**.*

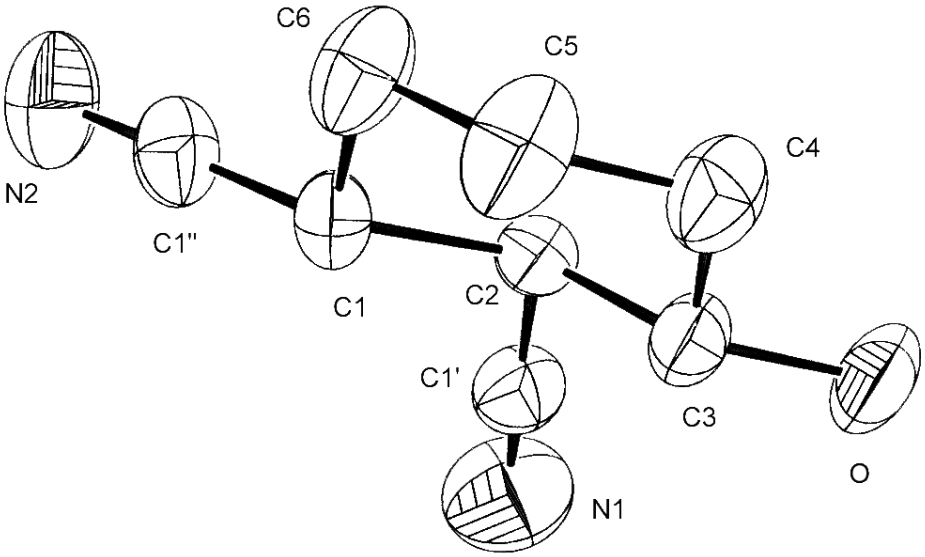

Figura I. 4.- *Estructura molecular del compost* ***40b****.*

Compost 40b			
Distàncies d'enllaç (Å)		**Angles d'enllaç (º)**	
		O-C1-C6	112.00
		O-C1-C2	109.22
O-C1	1.422	C6-C1-C2	109.83
N1-C1'	1.140	C1'-C2-C1	110.66
N2-C1''	1.139	C1'-C2-C3	112.91
C1-C6	1.499	C1-C2-C3	109.76
C1-C2	1.533	C1''-C3-C4	111.21
C2-C1'	1.470	C1''-C3-C2	112.19
C2-C3	1.536	C4-C3-C2	109.52
C3-C1''	1.465	C5-C4-C3	110.52
C3-C4	1.524	C6-C5-C4	111.78
C4-C5	1.514	C1-C6-C5	111.99
C5-C6	1.510	N1-C1'-C2	178.9
		N2-C1''-C3	178.6

Taula I. 5.- *Distàncies i angles d'enllaç del compost **40b**.*