Supporting Information

Impact of the Linker Groups in Bis(7-azaindol-1-yl) Chelate Ligands on Structures and Stability of Pt(*N*,*N*-L)R_2 Complexes

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S1 X-ray structure data for BAHE.

Diagrams showing the structure of compound **BAHE** with labeling schemes:

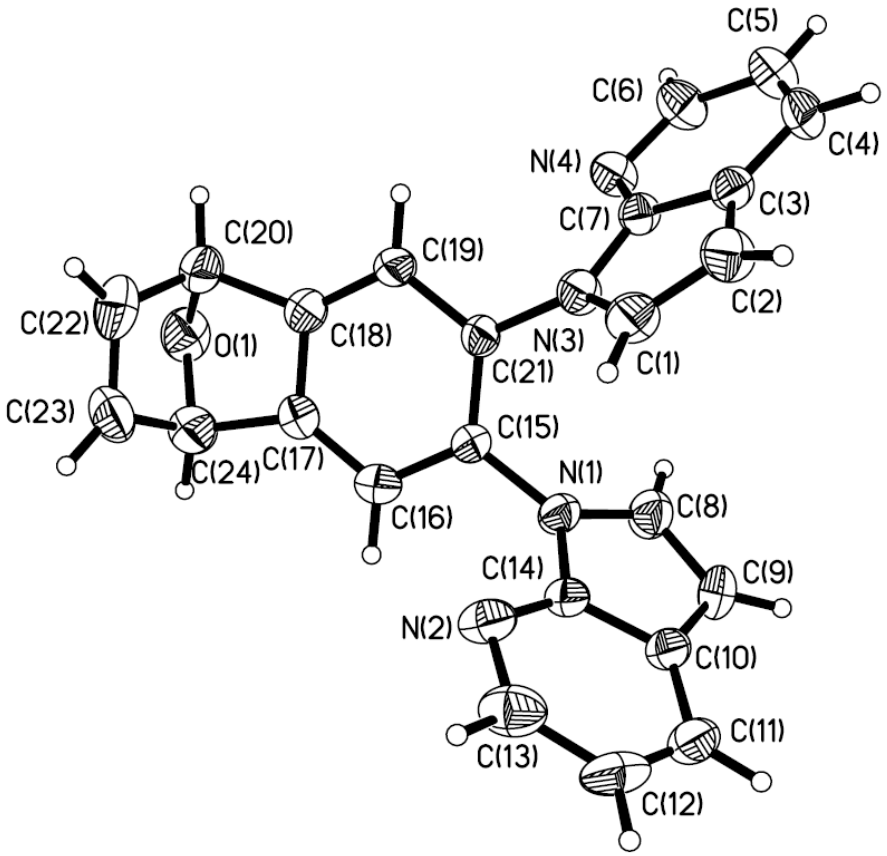

Table 1. Crystal data and structure refinement for **BAHE**.

Identification code	BAHE	
Empirical formula	C24 H18 N4 O	
Formula weight	378.42	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P4(3)2(1)2	
Unit cell dimensions	a = 10.721(5) Å	α= 90°.
	b = 10.721(5) Å	β= 90°.
	c = 32.66(3) Å	γ = 90°.
Volume	3753(5) $Å^3$	
Z	8	
Density (calculated)	1.339 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	1584	
Crystal size	0.2 x 0.2 x 0.1 mm^3	
Theta range for data collection	2.00 to 28.46°.	
Index ranges	-12<=h<=14, -14<=k<=13, -43<=l<=39	
Reflections collected	21383	
Independent reflections	4544 [R(int) = 0.1091]	
Completeness to theta = 28.46°	96.8 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4544 / 0 / 263	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1099	
R indices (all data)	R1 = 0.2214, wR2 = 0.1572	
Absolute structure parameter	-2(4)	
Extinction coefficient	0.0016(5)	
Largest diff. peak and hole	0.200 and -0.193 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for BAHE. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5245(3)	2723(3)	734(1)	79(1)
N(1)	7808(3)	7269(3)	1265(1)	52(1)
N(2)	8989(4)	7695(3)	665(1)	65(1)
N(3)	8929(3)	5367(3)	1736(1)	54(1)
N(4)	7860(3)	4422(3)	2302(1)	57(1)
C(1)	10043(5)	5993(4)	1694(1)	67(1)
C(2)	10637(4)	6079(4)	2056(2)	71(1)
C(3)	9863(4)	5489(4)	2354(1)	55(1)
C(4)	9903(5)	5284(5)	2771(1)	70(1)
C(5)	8943(5)	4639(5)	2945(1)	74(2)
C(6)	7951(5)	4230(5)	2708(1)	70(1)
C(7)	8814(4)	5045(4)	2145(1)	47(1)
C(8)	7459(5)	7942(4)	1603(1)	66(1)
C(9)	7877(5)	9125(5)	1575(1)	73(2)
C(10)	8550(5)	9221(4)	1202(1)	58(1)
C(11)	9230(5)	10125(5)	989(2)	74(2)
C(12)	9769(5)	9791(5)	627(2)	83(2)
C(13)	9640(5)	8593(6)	479(2)	80(2)
C(14)	8475(4)	8054(4)	1016(1)	49(1)
C(15)	7535(4)	5986(4)	1183(1)	50(1)
C(16)	6735(5)	5693(4)	862(1)	65(1)
C(17)	6470(4)	4465(5)	794(1)	62(1)
C(18)	7006(4)	3529(4)	1028(1)	59(1)
C(19)	7814(4)	3796(4)	1340(1)	55(1)
C(20)	6487(5)	2334(4)	839(1)	69(1)
C(21)	8091(4)	5060(4)	1415(1)	49(1)
C(22)	7082(5)	2218(5)	422(2)	86(2)
C(23)	6535(6)	3150(6)	196(2)	95(2)
C(24)	5627(5)	3777(5)	487(1)	79(2)

Table 3. Bond lengths [Å] and angles [°] for BAHE.

O(1)-C(20)	1.437(6)	C(23)-C(24)	1.517(7)
O(1)-C(24)	1.448(5)		
N(1)-C(14)	1.370(5)	C(20)-O(1)-C(24)	95.6(4)
N(1)-C(8)	1.372(5)	C(14)-N(1)-C(8)	107.2(3)
N(1)-C(15)	1.432(5)	C(14)-N(1)-C(15)	125.9(3)
N(2)-C(14)	1.329(5)	C(8)-N(1)-C(15)	126.9(4)
N(2)-C(13)	1.335(6)	C(14)-N(2)-C(13)	113.6(4)
N(3)-C(1)	1.377(5)	C(1)-N(3)-C(7)	107.1(3)
N(3)-C(7)	1.386(5)	C(1)-N(3)-C(21)	126.1(4)
N(3)-C(21)	1.419(5)	C(7)-N(3)-C(21)	126.7(3)
N(4)-C(7)	1.324(5)	C(7)-N(4)-C(6)	113.7(4)
N(4)-C(6)	1.347(5)	C(2)-C(1)-N(3)	110.9(4)
C(1)-C(2)	1.346(6)	C(1)-C(2)-C(3)	107.0(4)
C(2)-C(3)	1.426(6)	C(4)-C(3)-C(7)	116.8(4)
C(3)-C(4)	1.381(5)	C(4)-C(3)-C(2)	136.5(4)
C(3)-C(7)	1.398(5)	C(7)-C(3)-C(2)	106.7(4)
C(4)-C(5)	1.364(6)	C(5)-C(4)-C(3)	117.9(4)
C(5)-C(6)	1.386(6)	C(4)-C(5)-C(6)	120.4(4)
C(8)-C(9)	1.349(6)	N(4)-C(6)-C(5)	123.9(4)
C(9)-C(10)	1.422(6)	N(4)-C(7)-N(3)	124.5(4)
C(10)-C(14)	1.392(5)	N(4)-C(7)-C(3)	127.2(4)
C(10)-C(11)	1.397(6)	N(3)-C(7)-C(3)	108.3(4)
C(11)-C(12)	1.364(6)	C(9)-C(8)-N(1)	110.5(4)
C(12)-C(13)	1.380(7)	C(8)-C(9)-C(10)	107.1(4)
C(15)-C(21)	1.384(5)	C(14)-C(10)-C(11)	116.0(4)
C(15)-C(16)	1.390(6)	C(14)-C(10)-C(9)	106.2(4)
C(16)-C(17)	1.365(6)	C(11)-C(10)-C(9)	137.8(5)
C(17)-C(18)	1.386(6)	C(12)-C(11)-C(10)	118.0(5)
C(17)-C(24)	1.538(6)	C(11)-C(12)-C(13)	120.4(5)
C(18)-C(19)	1.368(5)	N(2)-C(13)-C(12)	124.3(5)
C(18)-C(20)	1.526(6)	N(2)-C(14)-N(1)	123.3(4)
C(19)-C(21)	1.408(5)	N(2)-C(14)-C(10)	127.7(4)
C(20)-C(22)	1.511(6)	N(1)-C(14)-C(10)	109.0(4)
C(22)-C(23)	1.374(7)	C(21)-C(15)-C(16)	121.1(4)

C(21)-C(15)-N(1)	119.9(4)	O(1)-C(20)-C(18)	101.0(4)
C(16)-C(15)-N(1)	119.0(4)	C(22)-C(20)-C(18)	106.2(4)
C(17)-C(16)-C(15)	118.0(4)	C(15)-C(21)-C(19)	120.3(4)
C(16)-C(17)-C(18)	121.5(4)	C(15)-C(21)-N(3)	120.7(4)
C(16)-C(17)-C(24)	133.7(4)	C(19)-C(21)-N(3)	119.0(4)
C(18)-C(17)-C(24)	104.8(4)	C(23)-C(22)-C(20)	104.1(5)
C(19)-C(18)-C(17)	121.4(4)	C(22)-C(23)-C(24)	105.1(4)
C(19)-C(18)-C(20)	135.0(4)	O(1)-C(24)-C(23)	100.7(4)
C(17)-C(18)-C(20)	103.6(4)	O(1)-C(24)-C(17)	100.2(4)
C(18)-C(19)-C(21)	117.7(4)	C(23)-C(24)-C(17)	104.1(5)
O(1)-C(20)-C(22)	101.5(4)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for BAHE. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	72(2)	81(2)	84(2)	-3(2)	-5(2)	-24(2)
N(1)	66(2)	41(2)	49(2)	2(2)	5(2)	-5(2)
N(2)	72(3)	52(2)	69(2)	12(2)	19(2)	12(2)
N(3)	50(2)	53(2)	57(2)	3(2)	-4(2)	-11(2)
N(4)	46(2)	67(2)	58(2)	10(2)	-2(2)	-11(2)
C(1)	66(3)	63(3)	71(3)	13(3)	3(3)	-22(3)
C(2)	54(3)	76(4)	84(3)	8(3)	-12(3)	-16(3)
C(3)	46(3)	46(3)	71(3)	-2(2)	-15(2)	-1(2)
C(4)	66(3)	76(4)	68(3)	-8(3)	-27(3)	0(3)
C(5)	70(4)	95(4)	55(3)	3(3)	-10(3)	-1(3)
C(6)	59(3)	89(4)	61(3)	8(3)	-2(3)	-4(3)
C(7)	42(3)	46(2)	54(2)	1(2)	-3(2)	-4(2)
C(8)	81(4)	60(3)	58(3)	-7(2)	7(3)	-3(3)
C(9)	98(4)	57(3)	64(3)	-22(3)	-8(3)	-3(3)
C(10)	65(3)	45(3)	65(3)	5(2)	-17(3)	-3(2)
C(11)	85(4)	49(3)	88(4)	10(3)	-24(3)	-10(3)
C(12)	84(4)	61(4)	104(4)	36(3)	2(3)	-7(3)
C(13)	80(4)	82(4)	78(3)	20(3)	21(3)	13(3)

C(14)	52(3)	43(3)	50(2)	5(2)	-3(2)	4(2)
C(15)	63(3)	40(3)	46(2)	1(2)	-3(2)	-3(2)
C(16)	79(3)	54(3)	61(3)	9(2)	-12(3)	5(3)
C(17)	73(3)	59(3)	53(2)	-3(2)	-13(2)	0(3)
C(18)	66(3)	50(3)	60(3)	-1(2)	-5(3)	-9(3)
C(19)	66(3)	43(3)	57(2)	5(2)	-15(2)	-7(2)
C(20)	77(4)	55(3)	74(3)	-7(3)	-12(3)	-5(3)
C(21)	57(3)	44(3)	46(2)	0(2)	-6(2)	-12(2)
C(22)	86(4)	83(4)	89(4)	-35(3)	9(3)	4(3)
C(23)	145(6)	92(5)	49(3)	-3(3)	-6(3)	-19(4)
C(24)	91(4)	72(4)	73(3)	3(3)	-12(3)	-6(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for BAHE.

	x	y	z	U(eq)
H(1A)	10345	6314	1448	80
H(2B)	11407	6452	2103	86
H(4B)	10564	5576	2928	84
H(5A)	8953	4473	3225	88
H(6A)	7311	3797	2837	84
H(8A)	6997	7626	1821	80
H(9A)	7749	9760	1765	88
H(11A)	9313	10930	1092	89
H(12A)	10227	10374	479	100
H(13A)	10031	8398	233	96
H(16A)	6391	6315	699	78
H(19A)	8168	3166	1497	66
H(20A)	6541	1590	1013	83
H(22A)	7682	1647	337	103
H(23A)	6687	3354	-76	114
H(24A)	4958	4268	361	94

S2 X-ray structure data for compound 1.

Diagrams showing the structure of compound **1** with labeling schemes:

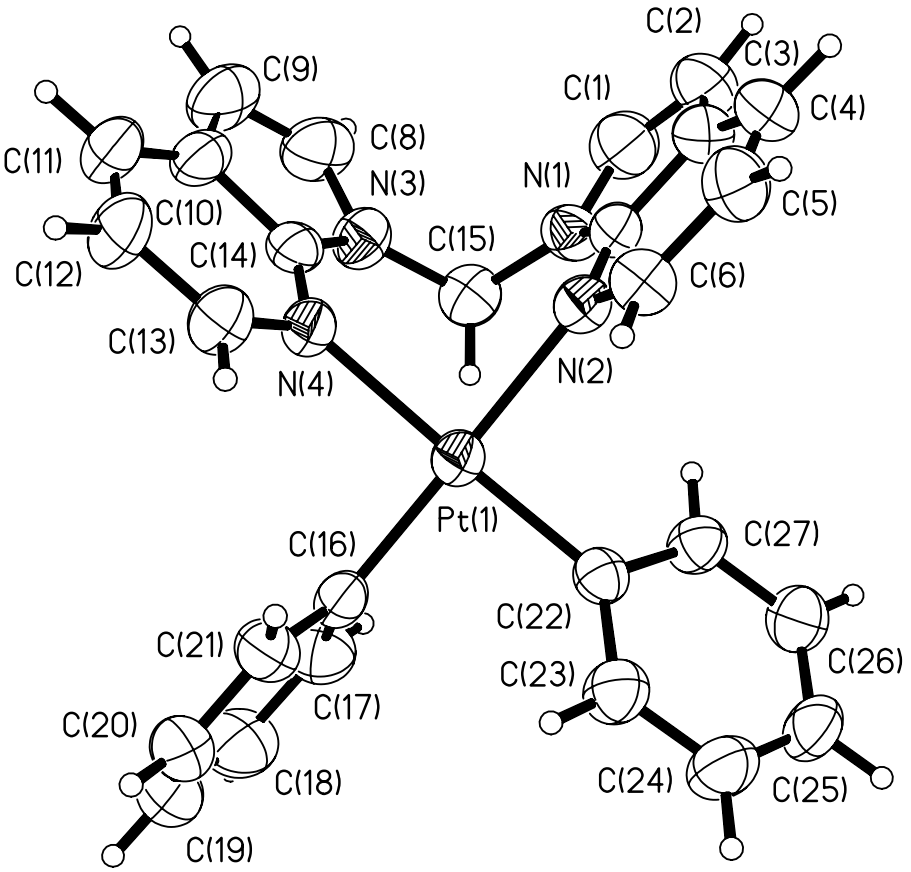

Table 1. Crystal data and structure refinement for compound **1**.

Identification code	**1**/THF	
Empirical formula	C27 H22 N4 Pt	
Formula weight	597.58	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.238(3) Å	α= 90°.
	b = 11.930(3) Å	β= 93.953(6)°.
	c = 18.202(4) Å	γ = 90°.
Volume	2651.0(10) $Å^3$	
Z	4	
Density (calculated)	1.497 Mg/m^3	
Absorption coefficient	5.312 mm^{-1}	
F(000)	1160	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.94 to 27.00°.	
Index ranges	-13<=h<=15, -15<=k<=15, -23<=l<=23	
Reflections collected	17999	
Independent reflections	5766 [R(int) = 0.0332]	
Completeness to theta = 27.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4164 and 0.4164	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5766 / 0 / 289	
Goodness-of-fit on F^2	0.723	
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0382	
R indices (all data)	R1 = 0.0468, wR2 = 0.0401	
Largest diff. peak and hole	1.031 and -0.526 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	6825(1)	8317(1)	668(1)	39(1)
N(1)	6144(2)	7979(3)	-1201(2)	49(1)
N(2)	6509(2)	6961(3)	-74(2)	42(1)
N(3)	7727(2)	9159(3)	-1010(2)	48(1)
N(4)	8370(2)	8510(3)	211(2)	42(1)
C(1)	5852(3)	7676(4)	-1921(3)	67(1)
C(2)	5709(3)	6557(5)	-1970(3)	67(1)
C(3)	5949(3)	6112(4)	-1261(3)	55(1)
C(4)	5988(3)	5055(4)	-944(3)	66(1)
C(5)	6299(3)	4966(4)	-211(3)	62(1)
C(6)	6543(3)	5913(4)	204(2)	52(1)
C(7)	6222(3)	7022(3)	-785(3)	42(1)
C(8)	8241(4)	9396(3)	-1645(3)	67(1)
C(9)	9337(4)	9238(3)	-1537(3)	72(2)
C(10)	9551(3)	8893(3)	-791(3)	53(1)
C(11)	10466(3)	8621(4)	-342(3)	66(2)
C(12)	10333(3)	8300(4)	359(3)	66(1)
C(13)	9294(3)	8253(3)	621(2)	55(1)
C(14)	8511(3)	8833(3)	-480(2)	44(1)
C(15)	6549(3)	9086(3)	-985(2)	51(1)
C(16)	7167(3)	9533(3)	1390(2)	41(1)
C(17)	6789(3)	10614(4)	1299(2)	59(1)
C(18)	7060(4)	11471(4)	1791(3)	72(1)
C(19)	7730(4)	11251(4)	2405(3)	77(2)
C(20)	8118(3)	10196(4)	2523(2)	66(1)
C(21)	7854(3)	9362(3)	2027(2)	50(1)
C(22)	5341(3)	8152(3)	1044(2)	38(1)
C(23)	5089(3)	8123(3)	1771(2)	52(1)
C(24)	4029(3)	7975(3)	1984(2)	59(1)
C(25)	3168(3)	7879(3)	1470(3)	55(1)
C(26)	3365(3)	7929(3)	749(3)	57(1)

C(27)	4432(3)	8047(3)	539(2)	44(1)

Table 3. Bond lengths [Å] and angles [°] for compound **1**.

Pt(1)-C(16)	1.983(4)	C(19)-C(20)	1.358(6)
Pt(1)-C(22)	1.994(3)	C(20)-C(21)	1.366(5)
Pt(1)-N(2)	2.125(3)	C(22)-C(23)	1.380(5)
Pt(1)-N(4)	2.130(3)	C(22)-C(27)	1.399(4)
N(1)-C(7)	1.369(4)	C(23)-C(24)	1.390(4)
N(1)-C(1)	1.382(5)	C(24)-C(25)	1.365(5)
N(1)-C(15)	1.455(4)	C(25)-C(26)	1.352(5)
N(2)-C(7)	1.319(5)	C(26)-C(27)	1.393(4)
N(2)-C(6)	1.349(5)		
N(3)-C(14)	1.369(4)	C(16)-Pt(1)-C(22)	90.01(14)
N(3)-C(8)	1.383(5)	C(16)-Pt(1)-N(2)	177.20(15)
N(3)-C(15)	1.448(4)	C(22)-Pt(1)-N(2)	90.72(13)
N(4)-C(14)	1.337(4)	C(16)-Pt(1)-N(4)	91.57(12)
N(4)-C(13)	1.346(4)	C(22)-Pt(1)-N(4)	177.04(14)
C(1)-C(2)	1.348(6)	N(2)-Pt(1)-N(4)	87.82(11)
C(2)-C(3)	1.409(6)	C(7)-N(1)-C(1)	108.0(4)
C(3)-C(4)	1.386(6)	C(7)-N(1)-C(15)	126.7(4)
C(3)-C(7)	1.414(5)	C(1)-N(1)-C(15)	123.7(4)
C(4)-C(5)	1.365(5)	C(7)-N(2)-C(6)	114.7(3)
C(5)-C(6)	1.381(5)	C(7)-N(2)-Pt(1)	127.3(3)
C(8)-C(9)	1.355(5)	C(6)-N(2)-Pt(1)	117.9(3)
C(9)-C(10)	1.426(6)	C(14)-N(3)-C(8)	108.0(3)
C(10)-C(11)	1.378(5)	C(14)-N(3)-C(15)	127.7(3)
C(10)-C(14)	1.431(5)	C(8)-N(3)-C(15)	123.4(4)
C(11)-C(12)	1.352(5)	C(14)-N(4)-C(13)	115.4(3)
C(12)-C(13)	1.390(5)	C(14)-N(4)-Pt(1)	125.0(2)
C(16)-C(17)	1.376(5)	C(13)-N(4)-Pt(1)	119.6(3)
C(16)-C(21)	1.400(5)	C(2)-C(1)-N(1)	110.3(4)
C(17)-C(18)	1.384(5)	C(1)-C(2)-C(3)	107.1(4)
C(18)-C(19)	1.365(6)	C(4)-C(3)-C(2)	136.3(5)

C(4)-C(3)-C(7)	116.3(4)	N(3)-C(14)-C(10)	107.9(4)
C(2)-C(3)-C(7)	107.3(4)	N(3)-C(15)-N(1)	111.6(3)
C(5)-C(4)-C(3)	118.5(5)	C(17)-C(16)-C(21)	114.4(4)
C(4)-C(5)-C(6)	120.4(5)	C(17)-C(16)-Pt(1)	123.5(3)
N(2)-C(6)-C(5)	123.7(4)	C(21)-C(16)-Pt(1)	122.0(3)
N(2)-C(7)-N(1)	126.3(4)	C(16)-C(17)-C(18)	123.5(4)
N(2)-C(7)-C(3)	126.5(4)	C(19)-C(18)-C(17)	119.4(5)
N(1)-C(7)-C(3)	107.2(4)	C(20)-C(19)-C(18)	119.5(5)
C(9)-C(8)-N(3)	110.7(4)	C(19)-C(20)-C(21)	120.4(5)
C(8)-C(9)-C(10)	107.0(4)	C(20)-C(21)-C(16)	122.8(4)
C(11)-C(10)-C(9)	136.2(4)	C(23)-C(22)-C(27)	114.0(3)
C(11)-C(10)-C(14)	117.5(4)	C(23)-C(22)-Pt(1)	127.0(3)
C(9)-C(10)-C(14)	106.3(4)	C(27)-C(22)-Pt(1)	119.0(3)
C(12)-C(11)-C(10)	118.8(4)	C(22)-C(23)-C(24)	123.1(4)
C(11)-C(12)-C(13)	120.5(4)	C(25)-C(24)-C(23)	120.7(4)
N(4)-C(13)-C(12)	123.6(4)	C(26)-C(25)-C(24)	118.7(4)
N(4)-C(14)-N(3)	128.0(3)	C(25)-C(26)-C(27)	120.2(4)
N(4)-C(14)-C(10)	124.2(4)	C(26)-C(27)-C(22)	123.2(4)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	33(1)	41(1)	43(1)	-3(1)	3(1)	-1(1)
N(1)	48(2)	58(3)	40(2)	-8(2)	-2(2)	2(2)
N(2)	37(2)	43(2)	45(2)	-2(2)	5(2)	1(2)
N(3)	47(2)	46(2)	52(2)	7(2)	8(2)	-1(2)
N(4)	35(2)	43(2)	49(2)	-4(2)	4(2)	-1(2)
C(1)	61(3)	83(4)	55(4)	-2(3)	0(3)	1(3)
C(2)	60(3)	86(4)	55(3)	-23(3)	-2(2)	-6(3)
C(3)	47(2)	55(3)	62(4)	-15(3)	9(2)	-1(2)
C(4)	57(3)	58(3)	85(4)	-31(3)	16(3)	-9(3)
C(5)	64(3)	47(3)	76(4)	-4(3)	12(3)	-9(2)
C(6)	52(2)	53(3)	52(3)	-6(3)	5(2)	-3(2)

C(7)	34(2)	42(3)	51(3)	-7(2)	8(2)	-2(2)
C(8)	83(3)	62(3)	59(4)	6(3)	26(3)	-7(3)
C(9)	75(3)	58(3)	88(4)	6(3)	39(3)	-9(3)
C(10)	49(2)	40(3)	72(4)	-7(2)	26(3)	-5(2)
C(11)	43(2)	70(4)	88(4)	-16(3)	22(3)	-7(2)
C(12)	34(2)	75(3)	88(4)	-10(3)	2(2)	6(2)
C(13)	43(2)	61(3)	62(3)	-2(3)	4(2)	3(2)
C(14)	49(2)	33(2)	50(3)	-9(2)	13(2)	-5(2)
C(15)	50(2)	49(3)	54(3)	4(2)	2(2)	5(2)
C(16)	33(2)	46(3)	43(3)	2(2)	8(2)	-3(2)
C(17)	61(3)	56(3)	59(3)	-1(3)	4(2)	7(2)
C(18)	85(3)	44(3)	90(4)	-11(3)	22(3)	4(3)
C(19)	67(3)	72(4)	92(5)	-36(3)	19(3)	-15(3)
C(20)	48(2)	91(4)	58(3)	-24(3)	2(2)	-7(3)
C(21)	50(2)	50(3)	49(3)	-8(2)	2(2)	0(2)
C(22)	40(2)	33(2)	41(2)	-1(2)	2(2)	1(2)
C(23)	43(2)	65(3)	47(3)	-1(2)	2(2)	1(2)
C(24)	57(3)	73(4)	48(3)	3(2)	14(2)	-2(2)
C(25)	37(2)	59(3)	70(4)	-3(3)	15(2)	-1(2)
C(26)	37(2)	70(3)	63(3)	-9(3)	-3(2)	3(2)
C(27)	40(2)	52(3)	41(3)	2(2)	3(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **1**.

	x	y	z	U(eq)
H(1A)	5767	8172	-2314	80
H(2A)	5492	6155	-2393	81
H(4A)	5808	4422	-1224	79
H(5A)	6346	4263	9	75
H(6A)	6741	5823	703	63
H(8A)	7884	9631	-2086	81
H(9A)	9853	9336	-1884	86

H(11A)	11160	8657	-518	79
H(12A)	10942	8110	668	79
H(13A)	9233	8031	1106	66
H(15A)	6205	9643	-1313	61
H(15B)	6351	9249	-489	61
H(17A)	6328	10777	886	70
H(18A)	6788	12190	1704	87
H(19A)	7919	11819	2739	92
H(20A)	8567	10039	2943	79
H(21A)	8143	8650	2117	60
H(23A)	5654	8206	2135	63
H(24A)	3906	7941	2482	71
H(25A)	2459	7780	1613	66
H(26A)	2785	7885	392	68
H(27A)	4546	8056	39	53

S3 X-ray structure data for compound 2.

Diagrams showing the structure of compound **2** with labeling schemes:

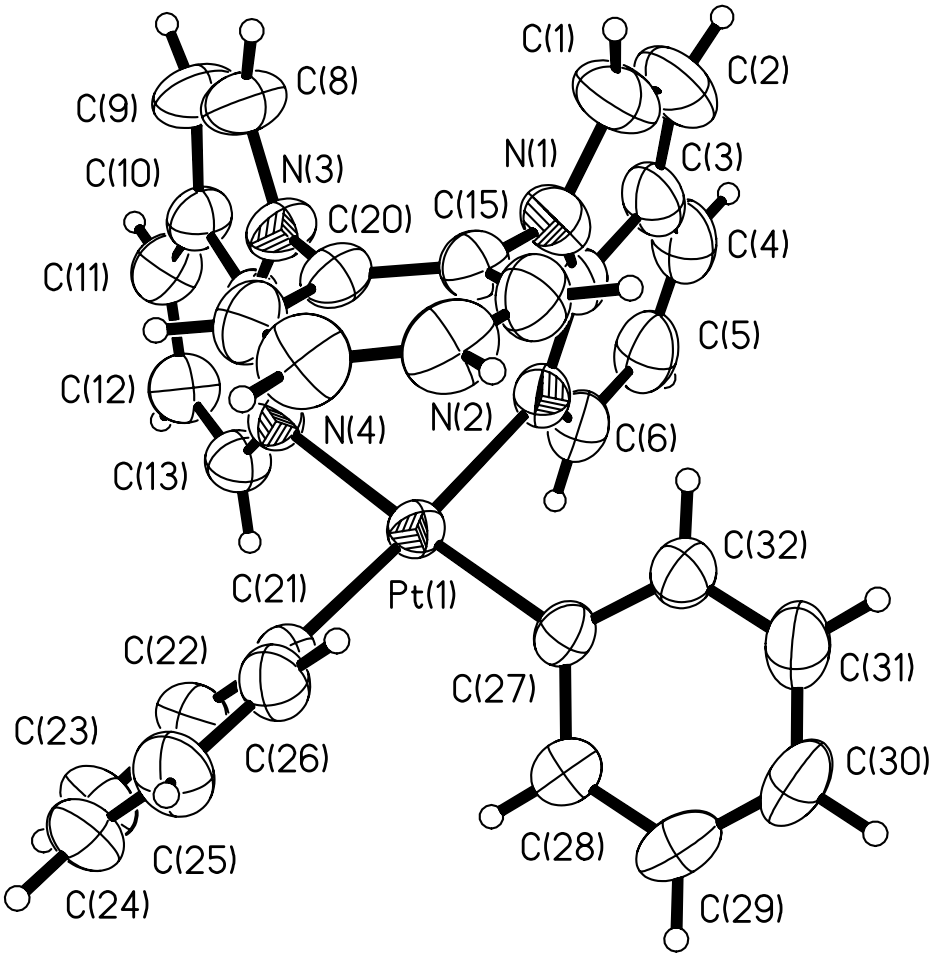

Table 1. Crystal data and structure refinement for compound **2**.

Identification code	**2**	
Empirical formula	C32 H24 N4 Pt	
Formula weight	659.64	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.404(3) Å	α= 90°.
	b = 11.527(2) Å	β= 112.390(4)°.
	c = 15.536(3) Å	γ = 90°.
Volume	2550.7(8) $Å^3$	
Z	4	
Density (calculated)	1.718 Mg/m^3	
Absorption coefficient	5.530 mm^{-1}	
F(000)	1288	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.27 to 27.00°.	
Index ranges	-17<=h<=19, -14<=k<=14, -17<=l<=19	
Reflections collected	17073	
Independent reflections	5546 [R(int) = 0.0174]	
Completeness to theta = 27.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6078 and 0.4043	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5546 / 0 / 334	
Goodness-of-fit on F^2	0.925	
Final R indices [I>2sigma(I)]	R1 = 0.0188, wR2 = 0.0340	
R indices (all data)	R1 = 0.0316, wR2 = 0.0363	
Largest diff. peak and hole	0.821 and -0.576 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	2895(1)	1149(1)	1800(1)	40(1)
N(1)	1840(2)	3927(2)	1426(2)	55(1)
N(2)	2999(2)	2723(2)	2584(1)	45(1)
N(3)	2941(2)	3378(2)	388(2)	48(1)
N(4)	3958(2)	1966(2)	1439(1)	40(1)
C(1)	1558(2)	5075(3)	1427(3)	76(1)
C(2)	2040(3)	5572(3)	2251(3)	84(1)
C(3)	2677(2)	4749(3)	2819(2)	61(1)
C(4)	3354(3)	4727(3)	3714(2)	73(1)
C(5)	3837(2)	3723(3)	4029(2)	68(1)
C(6)	3647(2)	2748(3)	3459(2)	57(1)
C(7)	2539(2)	3718(2)	2283(2)	47(1)
C(8)	3087(2)	4419(3)	22(2)	67(1)
C(9)	4012(2)	4663(3)	339(2)	70(1)
C(10)	4497(2)	3726(2)	926(2)	50(1)
C(11)	5422(2)	3438(3)	1439(2)	60(1)
C(12)	5601(2)	2413(3)	1919(2)	58(1)
C(13)	4867(2)	1712(3)	1913(2)	52(1)
C(14)	3802(2)	2940(2)	940(2)	41(1)
C(15)	1483(2)	3170(2)	643(2)	48(1)
C(16)	571(2)	2768(3)	349(2)	63(1)
C(17)	223(2)	2039(3)	-404(2)	71(1)
C(18)	785(2)	1701(3)	-870(2)	70(1)
C(19)	1690(2)	2123(3)	-595(2)	58(1)
C(20)	2035(2)	2858(2)	154(2)	45(1)
C(21)	2852(2)	-272(2)	1048(2)	42(1)
C(22)	3655(2)	-909(2)	1122(2)	53(1)
C(23)	3613(2)	-1879(3)	593(2)	63(1)
C(24)	2783(3)	-2252(3)	-48(2)	64(1)
C(25)	1981(2)	-1647(3)	-162(2)	65(1)
C(26)	2015(2)	-676(3)	379(2)	55(1)

C(27)	1973(2)	444(2)	2273(2)	43(1)
C(28)	1963(2)	-728(3)	2497(2)	50(1)
C(29)	1344(2)	-1171(3)	2873(2)	61(1)
C(30)	702(2)	-464(3)	3033(2)	66(1)
C(31)	675(2)	673(3)	2809(2)	66(1)
C(32)	1299(2)	1124(3)	2440(2)	55(1)

Table 3. Bond lengths [Å] and angles [°] for compound **2**.

Pt(1)-C(21)	1.998(3)	C(15)-C(16)	1.381(4)
Pt(1)-C(27)	2.003(3)	C(15)-C(20)	1.386(3)
Pt(1)-N(4)	2.141(2)	C(16)-C(17)	1.372(4)
Pt(1)-N(2)	2.157(2)	C(17)-C(18)	1.379(4)
N(1)-C(7)	1.378(4)	C(18)-C(19)	1.382(4)
N(1)-C(1)	1.394(4)	C(19)-C(20)	1.373(4)
N(1)-C(15)	1.426(3)	C(21)-C(26)	1.393(4)
N(2)-C(7)	1.335(3)	C(21)-C(22)	1.405(4)
N(2)-C(6)	1.346(3)	C(22)-C(23)	1.374(4)
N(3)-C(14)	1.373(3)	C(23)-C(24)	1.356(4)
N(3)-C(8)	1.381(3)	C(24)-C(25)	1.370(4)
N(3)-C(20)	1.432(3)	C(25)-C(26)	1.390(4)
N(4)-C(14)	1.333(3)	C(27)-C(28)	1.396(4)
N(4)-C(13)	1.343(3)	C(27)-C(32)	1.403(4)
C(1)-C(2)	1.340(4)	C(28)-C(29)	1.393(4)
C(2)-C(3)	1.407(5)	C(29)-C(30)	1.374(4)
C(3)-C(4)	1.385(4)	C(30)-C(31)	1.353(4)
C(3)-C(7)	1.420(4)	C(31)-C(32)	1.392(4)
C(4)-C(5)	1.362(4)		
C(5)-C(6)	1.390(4)	C(21)-Pt(1)-C(27)	90.66(10)
C(8)-C(9)	1.349(4)	C(21)-Pt(1)-N(4)	93.81(9)
C(9)-C(10)	1.428(4)	C(27)-Pt(1)-N(4)	174.03(8)
C(10)-C(11)	1.382(4)	C(21)-Pt(1)-N(2)	176.82(9)
C(10)-C(14)	1.409(3)	C(27)-Pt(1)-N(2)	92.52(9)
C(11)-C(12)	1.369(4)	N(4)-Pt(1)-N(2)	83.01(7)
C(12)-C(13)	1.387(4)	C(7)-N(1)-C(1)	107.1(3)

C(7)-N(1)-C(15)	128.6(2)	N(4)-C(14)-N(3)	126.2(2)
C(1)-N(1)-C(15)	124.2(3)	N(4)-C(14)-C(10)	125.4(3)
C(7)-N(2)-C(6)	115.1(2)	N(3)-C(14)-C(10)	108.3(2)
C(7)-N(2)-Pt(1)	127.55(18)	C(16)-C(15)-C(20)	119.4(3)
C(6)-N(2)-Pt(1)	117.1(2)	C(16)-C(15)-N(1)	120.1(3)
C(14)-N(3)-C(8)	107.8(2)	C(20)-C(15)-N(1)	120.5(2)
C(14)-N(3)-C(20)	128.3(2)	C(17)-C(16)-C(15)	120.4(3)
C(8)-N(3)-C(20)	123.7(2)	C(16)-C(17)-C(18)	120.1(3)
C(14)-N(4)-C(13)	115.0(2)	C(17)-C(18)-C(19)	120.0(3)
C(14)-N(4)-Pt(1)	122.40(18)	C(20)-C(19)-C(18)	119.9(3)
C(13)-N(4)-Pt(1)	120.11(18)	C(19)-C(20)-C(15)	120.3(3)
C(2)-C(1)-N(1)	110.4(3)	C(19)-C(20)-N(3)	119.9(2)
C(1)-C(2)-C(3)	108.1(3)	C(15)-C(20)-N(3)	119.7(2)
C(4)-C(3)-C(2)	136.0(3)	C(26)-C(21)-C(22)	115.0(2)
C(4)-C(3)-C(7)	117.4(3)	C(26)-C(21)-Pt(1)	121.7(2)
C(2)-C(3)-C(7)	106.6(3)	C(22)-C(21)-Pt(1)	123.3(2)
C(5)-C(4)-C(3)	118.4(3)	C(23)-C(22)-C(21)	122.5(3)
C(4)-C(5)-C(6)	120.3(3)	C(24)-C(23)-C(22)	120.9(3)
N(2)-C(6)-C(5)	123.8(3)	C(23)-C(24)-C(25)	118.9(3)
N(2)-C(7)-N(1)	127.1(2)	C(24)-C(25)-C(26)	120.5(3)
N(2)-C(7)-C(3)	125.0(3)	C(25)-C(26)-C(21)	122.1(3)
N(1)-C(7)-C(3)	107.9(3)	C(28)-C(27)-C(32)	114.5(2)
C(9)-C(8)-N(3)	110.3(3)	C(28)-C(27)-Pt(1)	124.1(2)
C(8)-C(9)-C(10)	107.4(3)	C(32)-C(27)-Pt(1)	121.4(2)
C(11)-C(10)-C(14)	117.4(3)	C(29)-C(28)-C(27)	122.2(3)
C(11)-C(10)-C(9)	136.4(3)	C(30)-C(29)-C(28)	120.9(3)
C(14)-C(10)-C(9)	106.3(3)	C(31)-C(30)-C(29)	118.8(3)
C(12)-C(11)-C(10)	118.1(3)	C(30)-C(31)-C(32)	120.6(3)
C(11)-C(12)-C(13)	120.4(3)	C(31)-C(32)-C(27)	123.0(3)
N(4)-C(13)-C(12)	123.6(3)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Pt(1)	43(1)	38(1)	41(1)	-2(1)	18(1)	-4(1)
N(1)	54(2)	47(2)	68(2)	-6(1)	26(1)	3(1)
N(2)	48(2)	44(1)	49(1)	-9(1)	25(1)	-9(1)
N(3)	40(1)	50(1)	55(1)	12(1)	19(1)	-2(1)
N(4)	39(1)	40(1)	45(1)	-2(1)	20(1)	-2(1)
C(1)	67(2)	54(2)	109(3)	4(2)	34(2)	16(2)
C(2)	91(3)	50(2)	119(3)	-26(2)	49(3)	0(2)
C(3)	66(2)	49(2)	79(2)	-21(2)	41(2)	-12(2)
C(4)	83(3)	71(2)	80(2)	-35(2)	46(2)	-27(2)
C(5)	74(2)	80(3)	55(2)	-22(2)	31(2)	-24(2)
C(6)	58(2)	64(2)	52(2)	-6(2)	26(2)	-9(2)
C(7)	48(2)	45(2)	58(2)	-10(2)	31(2)	-11(2)
C(8)	59(2)	61(2)	84(2)	28(2)	30(2)	4(2)
C(9)	58(2)	60(2)	96(2)	24(2)	33(2)	-9(2)
C(10)	44(2)	52(2)	58(2)	3(2)	23(1)	-7(2)
C(11)	44(2)	66(2)	69(2)	-2(2)	22(2)	-17(2)
C(12)	38(2)	65(2)	66(2)	2(2)	14(2)	-2(2)
C(13)	50(2)	51(2)	54(2)	4(1)	18(2)	3(2)
C(14)	40(2)	45(2)	40(1)	-1(1)	19(1)	-3(1)
C(15)	43(2)	50(2)	50(2)	2(1)	17(1)	-1(2)
C(16)	46(2)	74(2)	72(2)	1(2)	27(2)	1(2)
C(17)	44(2)	83(3)	76(2)	2(2)	13(2)	-16(2)
C(18)	62(2)	80(2)	53(2)	-10(2)	6(2)	-14(2)
C(19)	55(2)	72(2)	47(2)	1(2)	18(2)	-2(2)
C(20)	37(2)	51(2)	44(2)	11(1)	11(1)	0(1)
C(21)	47(2)	38(2)	42(1)	1(1)	20(1)	-4(1)
C(22)	56(2)	47(2)	50(2)	-1(1)	14(2)	2(2)
C(23)	68(2)	51(2)	67(2)	-7(2)	22(2)	11(2)
C(24)	82(3)	45(2)	68(2)	-13(2)	32(2)	-1(2)
C(25)	64(2)	61(2)	68(2)	-23(2)	24(2)	-18(2)
C(26)	53(2)	54(2)	62(2)	-11(2)	26(2)	-7(2)
C(27)	43(2)	48(2)	37(1)	-2(1)	16(1)	-7(1)
C(28)	49(2)	52(2)	47(2)	4(1)	17(1)	-5(2)
C(29)	66(2)	63(2)	48(2)	13(2)	16(2)	-17(2)
C(30)	68(2)	83(3)	57(2)	-4(2)	35(2)	-27(2)

C(31)	63(2)	75(2)	73(2)	-15(2)	41(2)	-11(2)
C(32)	61(2)	51(2)	63(2)	-5(2)	34(2)	-7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2**.

	x	y	z	U(eq)
H(1A)	1100	5444	927	92
H(2A)	1967	6329	2419	101
H(4A)	3476	5382	4091	88
H(5A)	4296	3689	4627	81
H(6A)	3987	2075	3697	68
H(8A)	2614	4885	-383	81
H(9A)	4284	5320	200	84
H(11A)	5909	3927	1457	71
H(12A)	6218	2185	2251	70
H(13A)	5012	1028	2256	63
H(16A)	191	2991	663	75
H(17A)	-392	1774	-600	85
H(18A)	555	1189	-1368	84
H(19A)	2064	1910	-918	70
H(22A)	4237	-665	1544	63
H(23A)	4160	-2285	676	76
H(24A)	2760	-2908	-405	77
H(25A)	1410	-1889	-606	78
H(26A)	1460	-282	292	66
H(28A)	2385	-1229	2391	60
H(29A)	1364	-1955	3018	73
H(30A)	294	-762	3290	79
H(31A)	236	1159	2902	79
H(32A)	1266	1911	2299	66

S4 X-ray structure data for compound 3.

Diagrams showing the structure of compound **3** with labeling schemes:

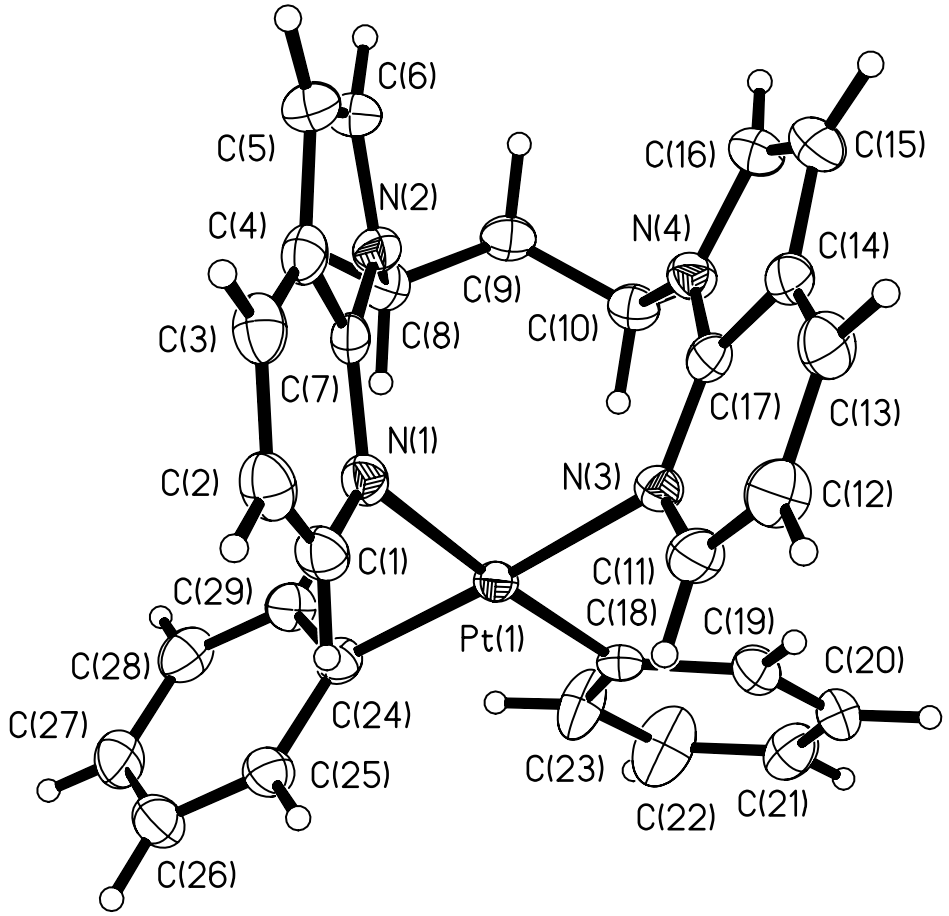

Table 1. Crystal data and structure refinement for compound **3**.

Identification code	**3**	
Empirical formula	C29 H26 N4 Pt	
Formula weight	625.63	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.27880(10) Å	α= 73.3860(10)°.
	b = 10.28780(10) Å	β= 89.3110(10)°.
	c = 15.4456(3) Å	γ = 69.1100(10)°.
Volume	1171.77(3) $Å^3$	
Z	2	
Density (calculated)	1.773 Mg/m^3	
Absorption coefficient	6.013 mm^{-1}	
F(000)	612	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.22 to 26.00°.	
Index ranges	-10<=h<=10, -12<=k<=12, -9<=l<=19	
Reflections collected	10077	
Independent reflections	4573 [R(int) = 0.0209]	
Completeness to theta = 26.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3793 and 0.3793	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4573 / 0 / 307	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0200, wR2 = 0.0449	
R indices (all data)	R1 = 0.0226, wR2 = 0.0461	
Largest diff. peak and hole	1.314 and -0.662 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1751(1)	1278(1)	7498(1)	20(1)
N(1)	3619(4)	118(3)	8669(2)	23(1)
N(2)	6078(3)	680(3)	8038(2)	23(1)
N(3)	3180(3)	-650(3)	7109(2)	23(1)
N(4)	5349(4)	65(3)	6232(2)	25(1)
C(1)	3205(5)	-780(4)	9382(2)	27(1)
C(2)	4423(5)	-1916(4)	10044(2)	31(1)
C(3)	6181(5)	-2200(4)	9998(2)	30(1)
C(4)	6660(4)	-1290(4)	9284(2)	26(1)
C(5)	8258(4)	-1165(4)	8993(2)	30(1)
C(6)	7853(4)	23(4)	8257(2)	28(1)
C(7)	5329(4)	-128(4)	8658(2)	22(1)
C(8)	5237(4)	2170(4)	7431(2)	25(1)
C(9)	5551(4)	2319(4)	6441(2)	26(1)
C(10)	4629(4)	1653(4)	5958(2)	25(1)
C(11)	2797(5)	-1839(4)	7511(2)	29(1)
C(12)	3826(5)	-3245(4)	7558(3)	34(1)
C(13)	5399(5)	-3529(4)	7173(2)	33(1)
C(14)	5830(4)	-2347(4)	6732(2)	26(1)
C(15)	7243(5)	-2156(4)	6249(2)	32(1)
C(16)	6905(5)	-706(4)	5957(2)	31(1)
C(17)	4664(4)	-928(4)	6705(2)	23(1)
C(18)	96(4)	2255(4)	6357(2)	22(1)
C(19)	-4(4)	1483(4)	5759(2)	30(1)
C(20)	-1051(5)	2147(4)	4930(2)	35(1)
C(21)	-2042(5)	3598(4)	4664(2)	36(1)
C(22)	-1986(6)	4399(5)	5242(3)	51(1)
C(23)	-947(5)	3742(4)	6060(3)	39(1)
C(24)	552(4)	2891(4)	8030(2)	23(1)
C(25)	-535(4)	2733(4)	8719(2)	28(1)
C(26)	-1306(5)	3808(4)	9134(2)	33(1)

C(27)	-1003(5)	5095(4)	8871(3)	36(1)
C(28)	56(5)	5298(4)	8187(3)	34(1)
C(29)	809(4)	4224(4)	7777(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for compound **3**.

Pt(1)-C(24)	2.000(3)	C(9)-H(9A)	0.9900
Pt(1)-C(18)	2.014(3)	C(9)-H(9B)	0.9900
Pt(1)-N(1)	2.146(3)	C(10)-H(10A)	0.9900
Pt(1)-N(3)	2.164(3)	C(10)-H(10B)	0.9900
N(1)-C(7)	1.347(4)	C(11)-C(12)	1.374(5)
N(1)-C(1)	1.349(4)	C(11)-H(11A)	0.9500
N(2)-C(7)	1.375(4)	C(12)-C(13)	1.394(5)
N(2)-C(6)	1.380(4)	C(12)-H(12A)	0.9500
N(2)-C(8)	1.464(4)	C(13)-C(14)	1.379(5)
N(3)-C(17)	1.346(4)	C(13)-H(13A)	0.9500
N(3)-C(11)	1.349(4)	C(14)-C(15)	1.422(5)
N(4)-C(17)	1.370(4)	C(14)-C(17)	1.423(5)
N(4)-C(16)	1.385(4)	C(15)-C(16)	1.352(5)
N(4)-C(10)	1.455(4)	C(15)-H(15A)	0.9500
C(1)-C(2)	1.389(5)	C(16)-H(16A)	0.9500
C(1)-H(1A)	0.9500	C(18)-C(19)	1.400(5)
C(2)-C(3)	1.384(5)	C(18)-C(23)	1.401(5)
C(2)-H(2A)	0.9500	C(19)-C(20)	1.401(5)
C(3)-C(4)	1.384(5)	C(19)-H(19A)	0.9500
C(3)-H(3A)	0.9500	C(20)-C(21)	1.362(5)
C(4)-C(7)	1.415(4)	C(20)-H(20A)	0.9500
C(4)-C(5)	1.429(5)	C(21)-C(22)	1.388(6)
C(5)-C(6)	1.350(5)	C(21)-H(21A)	0.9500
C(5)-H(5A)	0.9500	C(22)-C(23)	1.385(5)
C(6)-H(6A)	0.9500	C(22)-H(22A)	0.9500
C(8)-C(9)	1.522(5)	C(23)-H(23A)	0.9500
C(8)-H(8A)	0.9900	C(24)-C(25)	1.396(5)
C(8)-H(8B)	0.9900	C(24)-C(29)	1.406(5)
C(9)-C(10)	1.513(5)	C(25)-C(26)	1.391(5)

C(25)-H(25A)	0.9500	C(3)-C(4)-C(7)	118.2(3)
C(26)-C(27)	1.381(5)	C(3)-C(4)-C(5)	135.8(3)
C(26)-H(26A)	0.9500	C(7)-C(4)-C(5)	106.0(3)
C(27)-C(28)	1.382(5)	C(6)-C(5)-C(4)	107.2(3)
C(27)-H(27A)	0.9500	C(6)-C(5)-H(5A)	126.4
C(28)-C(29)	1.382(5)	C(4)-C(5)-H(5A)	126.4
C(28)-H(28A)	0.9500	C(5)-C(6)-N(2)	110.9(3)
C(29)-H(29A)	0.9500	C(5)-C(6)-H(6A)	124.5
		N(2)-C(6)-H(6A)	124.5
C(24)-Pt(1)-C(18)	92.56(13)	N(1)-C(7)-N(2)	126.3(3)
C(24)-Pt(1)-N(1)	91.61(11)	N(1)-C(7)-C(4)	125.1(3)
C(18)-Pt(1)-N(1)	175.82(11)	N(2)-C(7)-C(4)	108.6(3)
C(24)-Pt(1)-N(3)	172.24(11)	N(2)-C(8)-C(9)	113.5(3)
C(18)-Pt(1)-N(3)	94.62(12)	N(2)-C(8)-H(8A)	108.9
N(1)-Pt(1)-N(3)	81.24(10)	C(9)-C(8)-H(8A)	108.9
C(7)-N(1)-C(1)	114.8(3)	N(2)-C(8)-H(8B)	108.9
C(7)-N(1)-Pt(1)	124.2(2)	C(9)-C(8)-H(8B)	108.9
C(1)-N(1)-Pt(1)	118.0(2)	H(8A)-C(8)-H(8B)	107.7
C(7)-N(2)-C(6)	107.3(3)	C(10)-C(9)-C(8)	116.1(3)
C(7)-N(2)-C(8)	127.7(3)	C(10)-C(9)-H(9A)	108.3
C(6)-N(2)-C(8)	122.8(3)	C(8)-C(9)-H(9A)	108.3
C(17)-N(3)-C(11)	114.4(3)	C(10)-C(9)-H(9B)	108.3
C(17)-N(3)-Pt(1)	127.9(2)	C(8)-C(9)-H(9B)	108.3
C(11)-N(3)-Pt(1)	115.5(2)	H(9A)-C(9)-H(9B)	107.4
C(17)-N(4)-C(16)	107.4(3)	N(4)-C(10)-C(9)	114.2(3)
C(17)-N(4)-C(10)	130.3(3)	N(4)-C(10)-H(10A)	108.7
C(16)-N(4)-C(10)	122.1(3)	C(9)-C(10)-H(10A)	108.7
N(1)-C(1)-C(2)	123.8(3)	N(4)-C(10)-H(10B)	108.7
N(1)-C(1)-H(1A)	118.1	C(9)-C(10)-H(10B)	108.7
C(2)-C(1)-H(1A)	118.1	H(10A)-C(10)-H(10B)	107.6
C(3)-C(2)-C(1)	120.7(3)	N(3)-C(11)-C(12)	124.9(3)
C(3)-C(2)-H(2A)	119.7	N(3)-C(11)-H(11A)	117.6
C(1)-C(2)-H(2A)	119.7	C(12)-C(11)-H(11A)	117.6
C(2)-C(3)-C(4)	117.3(3)	C(11)-C(12)-C(13)	120.2(3)
C(2)-C(3)-H(3A)	121.3	C(11)-C(12)-H(12A)	119.9
C(4)-C(3)-H(3A)	121.3	C(13)-C(12)-H(12A)	119.9

C(14)-C(13)-C(12)	117.2(3)	C(22)-C(21)-H(21A)	121.1
C(14)-C(13)-H(13A)	121.4	C(23)-C(22)-C(21)	121.0(4)
C(12)-C(13)-H(13A)	121.4	C(23)-C(22)-H(22A)	119.5
C(13)-C(14)-C(15)	135.0(3)	C(21)-C(22)-H(22A)	119.5
C(13)-C(14)-C(17)	118.5(3)	C(22)-C(23)-C(18)	122.9(4)
C(15)-C(14)-C(17)	106.6(3)	C(22)-C(23)-H(23A)	118.5
C(16)-C(15)-C(14)	106.8(3)	C(18)-C(23)-H(23A)	118.5
C(16)-C(15)-H(15A)	126.6	C(25)-C(24)-C(29)	115.4(3)
C(14)-C(15)-H(15A)	126.6	C(25)-C(24)-Pt(1)	121.7(2)
C(15)-C(16)-N(4)	111.1(3)	C(29)-C(24)-Pt(1)	122.9(2)
C(15)-C(16)-H(16A)	124.5	C(26)-C(25)-C(24)	122.7(3)
N(4)-C(16)-H(16A)	124.5	C(26)-C(25)-H(25A)	118.6
N(3)-C(17)-N(4)	127.1(3)	C(24)-C(25)-H(25A)	118.6
N(3)-C(17)-C(14)	124.7(3)	C(27)-C(26)-C(25)	120.0(3)
N(4)-C(17)-C(14)	108.2(3)	C(27)-C(26)-H(26A)	120.0
C(19)-C(18)-C(23)	114.4(3)	C(25)-C(26)-H(26A)	120.0
C(19)-C(18)-Pt(1)	121.1(3)	C(26)-C(27)-C(28)	119.1(3)
C(23)-C(18)-Pt(1)	124.4(3)	C(26)-C(27)-H(27A)	120.5
C(18)-C(19)-C(20)	122.7(3)	C(28)-C(27)-H(27A)	120.5
C(18)-C(19)-H(19A)	118.7	C(29)-C(28)-C(27)	120.4(3)
C(20)-C(19)-H(19A)	118.7	C(29)-C(28)-H(28A)	119.8
C(21)-C(20)-C(19)	121.2(3)	C(27)-C(28)-H(28A)	119.8
C(21)-C(20)-H(20A)	119.4	C(28)-C(29)-C(24)	122.4(3)
C(19)-C(20)-H(20A)	119.4	C(28)-C(29)-H(29A)	118.8
C(20)-C(21)-C(22)	117.9(3)	C(24)-C(29)-H(29A)	118.8
C(20)-C(21)-H(21A)	121.1		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	18(1)	20(1)	23(1)	-8(1)	4(1)	-8(1)
N(1)	25(1)	23(2)	24(1)	-10(1)	4(1)	-9(1)
N(2)	22(1)	26(2)	24(1)	-8(1)	3(1)	-12(1)

N(3)	20(1)	22(2)	26(1)	-9(1)	4(1)	-7(1)
N(4)	24(1)	22(2)	29(2)	-10(1)	6(1)	-9(1)
C(1)	31(2)	30(2)	26(2)	-10(1)	9(1)	-16(2)
C(2)	43(2)	29(2)	24(2)	-8(1)	9(2)	-18(2)
C(3)	38(2)	24(2)	25(2)	-9(1)	-1(2)	-7(2)
C(4)	30(2)	23(2)	26(2)	-12(1)	-1(1)	-7(2)
C(5)	21(2)	33(2)	33(2)	-11(2)	-1(1)	-7(2)
C(6)	19(2)	34(2)	33(2)	-13(2)	6(1)	-10(2)
C(7)	24(2)	24(2)	20(2)	-12(1)	2(1)	-9(1)
C(8)	27(2)	23(2)	29(2)	-8(1)	4(1)	-11(2)
C(9)	24(2)	23(2)	31(2)	-4(1)	5(1)	-10(1)
C(10)	24(2)	25(2)	24(2)	-4(1)	4(1)	-9(1)
C(11)	30(2)	26(2)	38(2)	-13(2)	8(2)	-16(2)
C(12)	41(2)	23(2)	43(2)	-9(2)	6(2)	-16(2)
C(13)	37(2)	22(2)	40(2)	-14(2)	4(2)	-9(2)
C(14)	23(2)	26(2)	29(2)	-13(1)	0(1)	-6(1)
C(15)	27(2)	32(2)	39(2)	-17(2)	8(2)	-7(2)
C(16)	26(2)	38(2)	33(2)	-15(2)	11(2)	-13(2)
C(17)	21(2)	26(2)	21(2)	-7(1)	-2(1)	-8(1)
C(18)	17(2)	27(2)	25(2)	-9(1)	6(1)	-11(1)
C(19)	24(2)	32(2)	34(2)	-16(2)	4(1)	-5(2)
C(20)	34(2)	48(2)	32(2)	-24(2)	11(2)	-19(2)
C(21)	42(2)	44(2)	25(2)	-3(2)	-2(2)	-24(2)
C(22)	68(3)	27(2)	48(3)	2(2)	-22(2)	-14(2)
C(23)	50(2)	28(2)	39(2)	-11(2)	-14(2)	-13(2)
C(24)	21(2)	21(2)	27(2)	-8(1)	0(1)	-6(1)
C(25)	26(2)	27(2)	32(2)	-12(2)	5(1)	-9(2)
C(26)	30(2)	37(2)	30(2)	-14(2)	7(2)	-9(2)
C(27)	31(2)	33(2)	45(2)	-25(2)	1(2)	-1(2)
C(28)	32(2)	26(2)	44(2)	-11(2)	-3(2)	-9(2)
C(29)	27(2)	22(2)	31(2)	-8(1)	4(1)	-10(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **3**.

	x	y	z	U(eq)
H(1A)	2011	-627	9434	32
H(2A)	4046	-2504	10534	37
H(3A)	7026	-2989	10440	36
H(5A)	9393	-1800	9267	36
H(6A)	8680	362	7932	34
H(8A)	5672	2826	7634	30
H(8B)	3970	2494	7481	30
H(9A)	5190	3370	6106	32
H(9B)	6815	1863	6410	32
H(10A)	3390	1979	6073	30
H(10B)	4679	2027	5296	30
H(11A)	1736	-1692	7782	35
H(12A)	3465	-4026	7853	41
H(13A)	6143	-4497	7213	39
H(15A)	8235	-2904	6150	39
H(16A)	7637	-273	5609	37
H(19A)	665	467	5921	36
H(20A)	-1070	1576	4546	42
H(21A)	-2749	4048	4100	43
H(22A)	-2669	5412	5073	62
H(23A)	-942	4325	6438	47
H(25A)	-757	1854	8912	33
H(26A)	-2041	3657	9599	39
H(27A)	-1516	5830	9156	44
H(28A)	268	6181	7998	41
H(29A)	1528	4392	7307	32

S5 X-ray structure data for compound 4.

Diagrams showing the structure of compound **4** with labeling schemes:

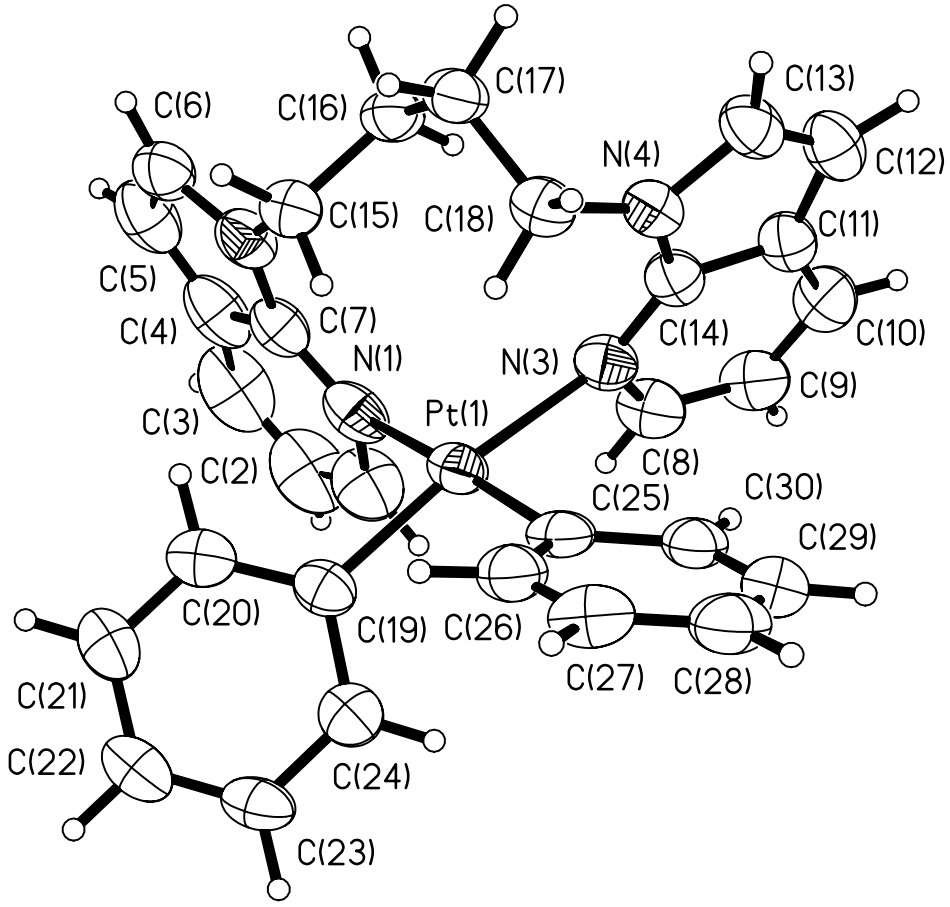

Table 1. Crystal data and structure refinement for compound **4**.

Identification code	**4**	
Empirical formula	C30 H28 N4 Pt	
Formula weight	639.65	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.0677(16) Å	α= 90°.
	b = 10.5124(12) Å	β= 109.140(2)°.
	c = 19.077(2) Å	γ = 90°.
Volume	2475.8(5) $Å^3$	
Z	4	
Density (calculated)	1.716 Mg/m^3	
Absorption coefficient	5.694 mm^{-1}	
F(000)	1256	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.26 to 27.00°.	
Index ranges	-16<=h<=16, -12<=k<=13, -24<=l<=23	
Reflections collected	16791	
Independent reflections	5408 [R(int) = 0.0396]	
Completeness to theta = 27.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5998 and 0.3955	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5408 / 0 / 316	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0835	
R indices (all data)	R1 = 0.0642, wR2 = 0.0946	
Largest diff. peak and hole	2.784 and -1.456 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	52(1)	4517(1)	2319(1)	42(1)
N(1)	1188(4)	5553(5)	3249(3)	52(1)
N(2)	59(5)	6479(5)	3911(3)	50(1)
N(3)	325(4)	2796(5)	2977(3)	46(1)
N(4)	-1443(4)	2211(4)	3050(3)	42(1)
C(1)	2211(6)	5554(7)	3228(5)	70(2)
C(2)	3045(6)	6242(8)	3724(6)	86(3)
C(3)	2848(7)	6973(8)	4257(5)	85(3)
C(4)	1825(6)	7012(7)	4312(4)	64(2)
C(5)	1310(7)	7644(7)	4755(4)	68(2)
C(6)	255(6)	7308(6)	4509(4)	57(2)
C(7)	1021(5)	6279(5)	3780(3)	45(2)
C(8)	1333(5)	2316(6)	3105(4)	54(2)
C(9)	1650(6)	1099(6)	3343(4)	56(2)
C(10)	923(6)	278(6)	3481(4)	55(2)
C(11)	-121(5)	728(5)	3383(3)	44(1)
C(12)	-1061(6)	219(6)	3485(4)	53(2)
C(13)	-1834(5)	1132(5)	3274(3)	49(2)
C(14)	-377(5)	1999(5)	3124(3)	42(1)
C(15)	-994(5)	5909(5)	3543(3)	45(1)
C(16)	-1188(5)	4737(5)	3942(3)	45(1)
C(17)	-2231(5)	4077(6)	3477(3)	47(2)
C(18)	-2103(5)	3350(5)	2821(3)	44(1)
C(19)	35(5)	6042(5)	1693(3)	43(1)
C(20)	-55(5)	7280(6)	1925(4)	52(2)
C(21)	74(6)	8339(6)	1534(4)	58(2)
C(22)	309(5)	8187(6)	881(4)	57(2)
C(23)	405(5)	6987(6)	627(3)	51(2)
C(24)	262(5)	5928(6)	1021(4)	48(2)
C(25)	-922(5)	3563(6)	1440(3)	43(1)
C(26)	-1802(5)	4116(6)	890(3)	50(2)

C(27)	-2503(6)	3435(7)	316(4)	57(2)
C(28)	-2361(6)	2142(7)	242(4)	59(2)
C(29)	-1492(6)	1570(6)	758(4)	57(2)
C(30)	-810(5)	2231(5)	1339(3)	46(2)

Table 3. Bond lengths [Å] and angles [°] for compound **4**.

Pt(1)-C(19)	1.995(6)	C(17)-C(18)	1.522(8)
Pt(1)-C(25)	2.010(6)	C(19)-C(20)	1.392(8)
Pt(1)-N(3)	2.163(5)	C(19)-C(24)	1.414(8)
Pt(1)-N(1)	2.193(5)	C(20)-C(21)	1.381(8)
N(1)-C(7)	1.341(8)	C(21)-C(22)	1.388(9)
N(1)-C(1)	1.350(9)	C(22)-C(23)	1.371(9)
N(2)-C(7)	1.377(8)	C(23)-C(24)	1.390(8)
N(2)-C(6)	1.393(8)	C(25)-C(26)	1.403(8)
N(2)-C(15)	1.452(8)	C(25)-C(30)	1.428(8)
N(3)-C(14)	1.338(7)	C(26)-C(27)	1.375(9)
N(3)-C(8)	1.356(8)	C(27)-C(28)	1.386(10)
N(4)-C(13)	1.370(7)	C(28)-C(29)	1.374(9)
N(4)-C(14)	1.371(7)	C(29)-C(30)	1.363(9)
N(4)-C(18)	1.457(7)		
C(1)-C(2)	1.389(11)	C(19)-Pt(1)-C(25)	91.3(2)
C(2)-C(3)	1.366(12)	C(19)-Pt(1)-N(3)	170.6(2)
C(3)-C(4)	1.375(11)	C(25)-Pt(1)-N(3)	90.3(2)
C(4)-C(5)	1.408(11)	C(19)-Pt(1)-N(1)	87.5(2)
C(4)-C(7)	1.424(9)	C(25)-Pt(1)-N(1)	176.7(2)
C(5)-C(6)	1.349(10)	N(3)-Pt(1)-N(1)	90.40(18)
C(8)-C(9)	1.375(8)	C(7)-N(1)-C(1)	115.4(6)
C(9)-C(10)	1.371(9)	C(7)-N(1)-Pt(1)	131.2(4)
C(10)-C(11)	1.398(9)	C(1)-N(1)-Pt(1)	113.0(5)
C(11)-C(12)	1.410(9)	C(7)-N(2)-C(6)	108.1(5)
C(11)-C(14)	1.426(7)	C(7)-N(2)-C(15)	128.8(5)
C(12)-C(13)	1.356(9)	C(6)-N(2)-C(15)	123.0(6)
C(15)-C(16)	1.513(8)	C(14)-N(3)-C(8)	114.9(5)
C(16)-C(17)	1.528(8)	C(14)-N(3)-Pt(1)	130.7(4)

C(8)-N(3)-Pt(1)	112.4(4)	N(3)-C(14)-N(4)	128.3(5)
C(13)-N(4)-C(14)	107.7(5)	N(3)-C(14)-C(11)	124.1(6)
C(13)-N(4)-C(18)	122.0(5)	N(4)-C(14)-C(11)	107.6(5)
C(14)-N(4)-C(18)	130.2(5)	N(2)-C(15)-C(16)	112.4(5)
N(1)-C(1)-C(2)	122.9(8)	C(15)-C(16)-C(17)	110.0(5)
C(3)-C(2)-C(1)	120.2(8)	C(18)-C(17)-C(16)	112.8(5)
C(2)-C(3)-C(4)	119.9(8)	N(4)-C(18)-C(17)	112.3(5)
C(3)-C(4)-C(5)	136.6(8)	C(20)-C(19)-C(24)	115.6(5)
C(3)-C(4)-C(7)	116.0(8)	C(20)-C(19)-Pt(1)	123.2(5)
C(5)-C(4)-C(7)	107.4(7)	C(24)-C(19)-Pt(1)	120.7(4)
C(6)-C(5)-C(4)	107.6(7)	C(21)-C(20)-C(19)	123.0(6)
C(5)-C(6)-N(2)	110.0(7)	C(20)-C(21)-C(22)	119.6(6)
N(1)-C(7)-N(2)	127.5(5)	C(23)-C(22)-C(21)	119.7(6)
N(1)-C(7)-C(4)	125.6(7)	C(22)-C(23)-C(24)	120.2(6)
N(2)-C(7)-C(4)	107.0(6)	C(23)-C(24)-C(19)	121.8(6)
N(3)-C(8)-C(9)	125.1(7)	C(26)-C(25)-C(30)	113.6(6)
C(10)-C(9)-C(8)	119.8(6)	C(26)-C(25)-Pt(1)	123.9(5)
C(9)-C(10)-C(11)	117.9(6)	C(30)-C(25)-Pt(1)	122.4(5)
C(10)-C(11)-C(12)	135.2(6)	C(27)-C(26)-C(25)	123.2(6)
C(10)-C(11)-C(14)	118.1(6)	C(26)-C(27)-C(28)	121.0(7)
C(12)-C(11)-C(14)	106.7(6)	C(29)-C(28)-C(27)	117.6(7)
C(13)-C(12)-C(11)	106.8(5)	C(30)-C(29)-C(28)	121.7(6)
C(12)-C(13)-N(4)	111.1(6)	C(29)-C(30)-C(25)	122.7(6)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	41(1)	46(1)	43(1)	9(1)	19(1)	2(1)
N(1)	39(3)	56(3)	59(3)	18(3)	12(3)	-5(3)
N(2)	58(4)	48(3)	40(3)	6(2)	12(3)	-8(3)
N(3)	43(3)	53(3)	41(3)	5(2)	13(2)	1(2)
N(4)	41(3)	44(2)	40(3)	4(2)	12(2)	-4(2)
C(1)	43(4)	76(5)	93(6)	10(4)	23(4)	-1(4)

C(2)	37(4)	92(6)	121(8)	20(6)	14(5)	-9(4)
C(3)	63(6)	84(5)	81(6)	13(5)	-14(5)	-23(5)
C(4)	56(5)	62(4)	59(5)	25(4)	-4(4)	-6(4)
C(5)	82(6)	59(4)	47(4)	12(3)	0(4)	-16(4)
C(6)	77(5)	53(4)	43(4)	3(3)	21(4)	-6(4)
C(7)	40(4)	47(3)	41(3)	10(3)	4(3)	-6(3)
C(8)	45(4)	65(4)	52(4)	12(3)	15(3)	7(3)
C(9)	48(4)	69(4)	50(4)	12(3)	14(3)	18(3)
C(10)	59(4)	54(4)	46(4)	11(3)	8(3)	16(3)
C(11)	47(4)	44(3)	37(3)	4(2)	8(3)	0(3)
C(12)	56(4)	48(3)	48(4)	7(3)	8(3)	-5(3)
C(13)	49(4)	50(3)	47(4)	-1(3)	14(3)	-15(3)
C(14)	47(4)	45(3)	30(3)	2(2)	7(3)	-2(3)
C(15)	42(4)	49(3)	43(3)	4(3)	14(3)	1(3)
C(16)	50(4)	52(3)	37(3)	4(3)	19(3)	2(3)
C(17)	48(4)	50(3)	47(4)	7(3)	24(3)	0(3)
C(18)	40(3)	49(3)	43(3)	6(3)	13(3)	1(3)
C(19)	37(3)	48(3)	43(4)	7(3)	13(3)	0(3)
C(20)	51(4)	61(4)	45(4)	5(3)	18(3)	0(3)
C(21)	59(4)	47(3)	66(5)	13(3)	18(4)	3(3)
C(22)	52(4)	58(4)	59(4)	20(3)	17(3)	-4(3)
C(23)	44(4)	68(4)	48(4)	15(3)	23(3)	3(3)
C(24)	36(3)	53(3)	55(4)	4(3)	16(3)	3(3)
C(25)	44(4)	56(3)	38(3)	8(3)	23(3)	7(3)
C(26)	53(4)	56(3)	45(4)	7(3)	25(3)	9(3)
C(27)	50(4)	79(4)	44(4)	5(3)	19(3)	6(4)
C(28)	62(5)	74(4)	49(4)	-5(4)	27(4)	-18(4)
C(29)	75(5)	50(3)	53(4)	3(3)	33(4)	-2(3)
C(30)	49(4)	51(3)	46(4)	6(3)	28(3)	3(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **4**.

	x	y	z	U(eq)

H(1A)	2367	5062	2857	84
H(2A)	3754	6203	3692	104
H(3A)	3417	7454	4591	102
H(5A)	1645	8206	5154	81
H(6A)	-275	7595	4715	68
H(8A)	1862	2863	3024	65
H(9A)	2370	828	3412	67
H(10A)	1123	-571	3638	66
H(12A)	-1137	-605	3667	64
H(13A)	-2554	1036	3282	59
H(15A)	-1047	5676	3030	54
H(15B)	-1566	6543	3515	54
H(16A)	-1245	4983	4429	54
H(16B)	-570	4145	4031	54
H(17A)	-2463	3478	3797	56
H(17B)	-2808	4723	3291	56
H(18A)	-2828	3106	2482	53
H(18B)	-1764	3914	2544	53
H(20A)	-213	7402	2372	62
H(21A)	2	9168	1712	70
H(22A)	404	8911	610	68
H(23A)	571	6880	182	61
H(24A)	317	5104	832	57
H(26A)	-1919	5004	914	59
H(27A)	-3094	3857	-34	68
H(28A)	-2847	1667	-151	71
H(29A)	-1362	690	709	68
H(30A)	-237	1786	1692	55

S6 X-ray structure data for compound 5.

Diagrams showing the structure of compound **5** with labeling schemes:

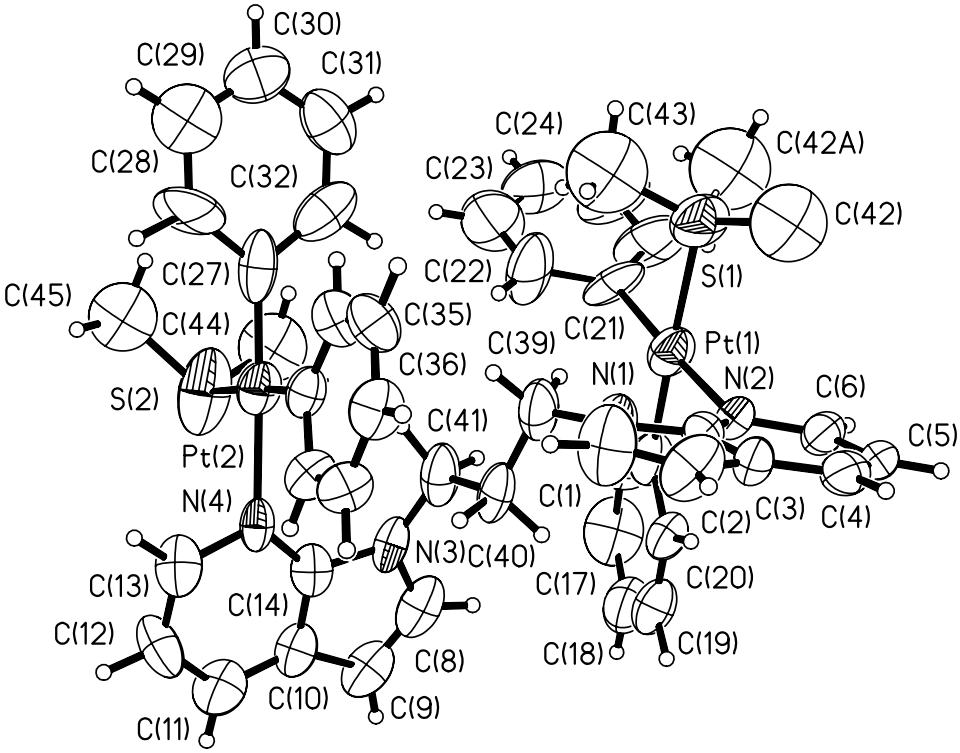

Table 1. Crystal data and structure refinement for compound **5**.

Identification code	5	
Empirical formula	C45 H48 N4 Pt2 S2	
Formula weight	1099.17	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7088(15) Å	α= 80.192(2)°.
	b = 12.9165(17) Å	β= 83.251(3)°.
	c = 14.9862(19) Å	γ = 63.096(2)°.
Volume	1989.5(4) $Å^3$	
Z	2	
Density (calculated)	1.835 Mg/m^3	
Absorption coefficient	7.167 mm^{-1}	
F(000)	1068	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.95 to 28.00°.	
Index ranges	-15<=h<=15, -14<=k<=16, -19<=l<=18	
Reflections collected	14309	
Independent reflections	9042 [R(int) = 0.0444]	
Completeness to theta = 28.00°	94.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5343 and 0.3282	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9042 / 7 / 470	
Goodness-of-fit on F^2	0.804	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.0639	
R indices (all data)	R1 = 0.1638, wR2 = 0.0758	
Largest diff. peak and hole	1.188 and -1.375 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	-51(1)	2221(1)	7608(1)	62(1)
Pt(2)	5064(1)	3186(1)	7584(1)	55(1)
S(1)	882(3)	300(3)	8374(2)	84(1)
S(2)	5492(4)	3591(4)	6021(2)	114(2)
N(1)	792(8)	2903(7)	9473(5)	62(3)
N(2)	-963(7)	2810(7)	8859(5)	41(2)
N(3)	1976(9)	5312(9)	7004(5)	52(3)
N(4)	3992(8)	5036(7)	7463(5)	42(2)
C(1)	1040(12)	2964(11)	10345(7)	89(4)
C(2)	17(11)	3075(10)	10901(7)	76(4)
C(3)	-887(10)	3021(9)	10417(7)	46(3)
C(4)	-2054(10)	3044(8)	10630(7)	54(3)
C(5)	-2706(9)	2989(8)	9948(7)	47(3)
C(6)	-2150(9)	2864(8)	9101(6)	47(3)
C(7)	-410(10)	2907(9)	9505(7)	43(3)
C(8)	990(12)	6245(14)	6638(7)	67(4)
C(9)	1150(11)	7201(11)	6489(6)	65(4)
C(10)	2337(11)	6880(12)	6796(7)	52(3)
C(11)	3056(12)	7451(10)	6822(7)	72(4)
C(12)	4230(12)	6830(11)	7176(7)	69(4)
C(13)	4673(10)	5652(11)	7500(6)	61(3)
C(14)	2854(12)	5689(12)	7123(6)	47(3)
C(15)	-895(9)	3866(10)	6940(7)	52(3)
C(16)	-873(13)	4153(13)	6007(9)	103(5)
C(17)	-1505(13)	5309(15)	5603(8)	93(5)
C(18)	-2124(11)	6229(12)	6052(9)	83(4)
C(19)	-2183(10)	5970(12)	6927(8)	65(4)
C(20)	-1611(10)	4848(11)	7342(7)	59(3)
C(21)	929(10)	1509(10)	6480(6)	78(4)
C(22)	2159(12)	1448(12)	6303(8)	109(5)
C(23)	2945(15)	885(13)	5639(10)	134(7)

C(24)	2487(16)	411(13)	5120(9)	107(5)
C(25)	1327(14)	384(12)	5296(10)	110(5)
C(26)	632(13)	913(12)	5997(9)	121(6)
C(27)	6106(11)	1495(7)	7581(7)	71(5)
C(28)	7340(15)	920(12)	7698(9)	108(5)
C(29)	8046(15)	-298(15)	7643(9)	122(5)
C(30)	7503(15)	-955(12)	7450(9)	101(5)
C(31)	6264(16)	-444(14)	7285(8)	82(4)
C(32)	5585(11)	791(16)	7371(7)	101(6)
C(33)	4703(9)	2910(10)	8927(6)	43(3)
C(34)	4949(10)	1870(10)	9444(7)	58(3)
C(35)	4687(10)	1728(10)	10359(7)	59(3)
C(36)	4154(9)	2667(11)	10805(7)	56(3)
C(37)	3862(9)	3737(10)	10375(7)	53(3)
C(38)	4135(8)	3854(9)	9410(6)	47(3)
C(39)	1627(9)	2921(9)	8683(6)	68(3)
C(40)	1394(8)	4178(10)	8288(6)	60(3)
C(41)	1983(9)	4196(10)	7343(6)	68(4)
C(42A)	690(30)	-510(30)	7634(18)	166(15)
C(42)	120(30)	100(30)	9469(13)	163(12)
C(43)	2506(11)	-263(11)	8392(9)	158(6)
C(44)	4811(13)	3016(14)	5431(7)	163(8)
C(45)	7130(10)	2727(12)	5760(7)	144(7)

Table 3. Bond lengths [Å] and angles [°] for 5.

Pt(1)-C(15)	2.026(11)	C(12)-C(13)	1.383(13)
Pt(1)-C(21)	2.035(7)	C(15)-C(20)	1.362(12)
Pt(1)-N(2)	2.125(7)	C(15)-C(16)	1.385(14)
Pt(1)-S(1)	2.353(3)	C(16)-C(17)	1.394(15)
Pt(2)-C(27)	1.962(8)	C(17)-C(18)	1.329(15)
Pt(2)-C(33)	2.013(9)	C(18)-C(19)	1.299(13)
Pt(2)-N(4)	2.124(8)	C(19)-C(20)	1.358(13)
Pt(2)-S(2)	2.357(3)	C(21)-C(26)	1.314(13)
S(1)-C(43)	1.702(11)	C(21)-C(22)	1.402(13)
S(1)-C(42A)	1.746(17)	C(22)-C(23)	1.338(13)
S(1)-C(42)	1.809(15)	C(23)-C(24)	1.351(17)
S(2)-C(44)	1.700(9)	C(24)-C(25)	1.368(16)
S(2)-C(45)	1.765(10)	C(25)-C(26)	1.331(14)
N(1)-C(1)	1.394(11)	C(27)-C(28)	1.309(14)
N(1)-C(7)	1.400(11)	C(27)-C(32)	1.393(16)
N(1)-C(39)	1.449(10)	C(28)-C(29)	1.420(16)
N(2)-C(7)	1.278(10)	C(29)-C(30)	1.350(15)
N(2)-C(6)	1.369(9)	C(30)-C(31)	1.328(15)
N(3)-C(8)	1.323(12)	C(31)-C(32)	1.447(16)
N(3)-C(14)	1.361(11)	C(33)-C(34)	1.355(12)
N(3)-C(41)	1.441(12)	C(33)-C(38)	1.380(11)
N(4)-C(14)	1.320(12)	C(34)-C(35)	1.369(11)
N(4)-C(13)	1.368(11)	C(35)-C(36)	1.341(11)
C(1)-C(2)	1.343(12)	C(36)-C(37)	1.327(12)
C(2)-C(3)	1.384(12)	C(37)-C(38)	1.441(11)
C(3)-C(4)	1.354(11)	C(39)-C(40)	1.539(12)
C(3)-C(7)	1.420(11)	C(40)-C(41)	1.502(11)
C(4)-C(5)	1.375(11)		
C(5)-C(6)	1.357(10)	C(15)-Pt(1)-C(21)	93.8(4)
C(8)-C(9)	1.310(13)	C(15)-Pt(1)-N(2)	91.5(4)
C(9)-C(10)	1.371(13)	C(21)-Pt(1)-N(2)	174.5(4)
C(10)-C(11)	1.354(13)	C(15)-Pt(1)-S(1)	178.4(3)
C(10)-C(14)	1.394(13)	C(21)-Pt(1)-S(1)	86.1(3)
C(11)-C(12)	1.358(13)	N(2)-Pt(1)-S(1)	88.5(2)

C(27)-Pt(2)-C(33)	89.8(4)	N(2)-C(7)-C(3)	126.8(10)
C(27)-Pt(2)-N(4)	174.8(3)	N(1)-C(7)-C(3)	105.5(9)
C(33)-Pt(2)-N(4)	95.3(4)	C(9)-C(8)-N(3)	114.1(12)
C(27)-Pt(2)-S(2)	92.4(3)	C(8)-C(9)-C(10)	105.2(12)
C(33)-Pt(2)-S(2)	177.3(3)	C(11)-C(10)-C(9)	134.2(15)
N(4)-Pt(2)-S(2)	82.5(2)	C(11)-C(10)-C(14)	118.1(12)
C(43)-S(1)-C(42A)	102.4(11)	C(9)-C(10)-C(14)	107.7(11)
C(43)-S(1)-C(42)	113.6(11)	C(10)-C(11)-C(12)	117.9(12)
C(42A)-S(1)-C(42)	109.7(13)	C(11)-C(12)-C(13)	120.8(11)
C(43)-S(1)-Pt(1)	112.4(5)	N(4)-C(13)-C(12)	123.1(10)
C(42A)-S(1)-Pt(1)	102.7(11)	N(4)-C(14)-N(3)	126.1(12)
C(42)-S(1)-Pt(1)	114.7(10)	N(4)-C(14)-C(10)	126.9(11)
C(44)-S(2)-C(45)	100.4(6)	N(3)-C(14)-C(10)	107.0(11)
C(44)-S(2)-Pt(2)	109.1(4)	C(20)-C(15)-C(16)	110.0(11)
C(45)-S(2)-Pt(2)	109.0(4)	C(20)-C(15)-Pt(1)	124.9(9)
C(1)-N(1)-C(7)	108.2(8)	C(16)-C(15)-Pt(1)	125.0(10)
C(1)-N(1)-C(39)	123.8(9)	C(15)-C(16)-C(17)	121.2(12)
C(7)-N(1)-C(39)	127.9(9)	C(18)-C(17)-C(16)	124.8(12)
C(7)-N(2)-C(6)	113.9(8)	C(19)-C(18)-C(17)	114.6(13)
C(7)-N(2)-Pt(1)	125.3(7)	C(18)-C(19)-C(20)	122.1(12)
C(6)-N(2)-Pt(1)	119.3(6)	C(19)-C(20)-C(15)	127.2(11)
C(8)-N(3)-C(14)	105.9(11)	C(26)-C(21)-C(22)	115.9(10)
C(8)-N(3)-C(41)	125.2(11)	C(26)-C(21)-Pt(1)	126.3(10)
C(14)-N(3)-C(41)	128.1(11)	C(22)-C(21)-Pt(1)	116.5(9)
C(14)-N(4)-C(13)	113.2(10)	C(23)-C(22)-C(21)	121.8(12)
C(14)-N(4)-Pt(2)	128.1(8)	C(22)-C(23)-C(24)	117.2(15)
C(13)-N(4)-Pt(2)	116.0(8)	C(23)-C(24)-C(25)	123.3(13)
C(2)-C(1)-N(1)	109.2(10)	C(26)-C(25)-C(24)	115.5(14)
C(1)-C(2)-C(3)	108.6(10)	C(21)-C(26)-C(25)	125.7(15)
C(4)-C(3)-C(2)	134.3(10)	C(28)-C(27)-C(32)	112.7(10)
C(4)-C(3)-C(7)	117.2(10)	C(28)-C(27)-Pt(2)	125.9(9)
C(2)-C(3)-C(7)	108.4(9)	C(32)-C(27)-Pt(2)	121.2(10)
C(3)-C(4)-C(5)	118.0(9)	C(27)-C(28)-C(29)	122.9(12)
C(6)-C(5)-C(4)	119.8(9)	C(30)-C(29)-C(28)	122.7(15)
C(5)-C(6)-N(2)	124.2(9)	C(31)-C(30)-C(29)	119.1(15)
N(2)-C(7)-N(1)	127.7(9)	C(30)-C(31)-C(32)	115.9(13)

C(27)-C(32)-C(31)	126.7(12)	C(37)-C(36)-C(35)	121.4(10)
C(34)-C(33)-C(38)	113.5(8)	C(36)-C(37)-C(38)	117.5(10)
C(34)-C(33)-Pt(2)	127.2(8)	C(33)-C(38)-C(37)	123.1(9)
C(38)-C(33)-Pt(2)	119.3(8)	N(1)-C(39)-C(40)	111.8(8)
C(33)-C(34)-C(35)	125.0(10)	C(41)-C(40)-C(39)	110.1(9)
C(36)-C(35)-C(34)	119.5(10)	N(3)-C(41)-C(40)	111.9(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	54(1)	72(1)	59(1)	-25(1)	8(1)	-24(1)
Pt(2)	51(1)	75(1)	42(1)	-18(1)	8(1)	-30(1)
S(1)	85(3)	72(2)	72(2)	-13(2)	24(2)	-21(2)
S(2)	98(3)	217(5)	46(2)	-36(3)	19(2)	-87(3)
N(1)	54(7)	81(7)	48(6)	-11(6)	7(5)	-29(6)
N(2)	31(5)	46(6)	36(5)	-3(5)	-2(4)	-10(5)
N(3)	32(6)	79(8)	37(5)	-4(6)	5(4)	-21(6)
N(4)	38(6)	70(7)	27(5)	-8(5)	4(4)	-34(6)
C(1)	93(11)	147(13)	58(8)	-27(9)	-16(8)	-73(10)
C(2)	68(10)	106(11)	43(7)	-10(8)	0(7)	-29(9)
C(3)	38(7)	51(8)	47(7)	-8(6)	1(6)	-18(6)
C(4)	56(8)	43(8)	48(7)	6(6)	14(6)	-18(7)
C(5)	37(7)	39(7)	65(7)	-20(6)	16(6)	-16(6)
C(6)	44(7)	45(7)	51(7)	-14(6)	1(5)	-17(6)
C(7)	45(8)	39(7)	40(7)	6(6)	0(6)	-17(6)
C(8)	47(9)	119(13)	31(7)	-27(8)	1(6)	-28(10)
C(9)	52(9)	85(11)	36(7)	15(7)	-10(6)	-17(8)
C(10)	41(8)	74(11)	39(7)	3(7)	-12(6)	-27(8)
C(11)	63(10)	68(10)	53(8)	27(7)	-17(7)	-11(8)
C(12)	90(11)	68(10)	69(8)	21(8)	-22(7)	-58(9)
C(13)	59(8)	83(10)	39(6)	12(7)	-19(6)	-32(8)

C(14)	49(9)	66(10)	32(6)	-4(7)	-2(6)	-32(8)
C(15)	50(7)	68(9)	37(6)	-13(7)	10(6)	-27(7)
C(16)	138(14)	105(13)	76(11)	-36(10)	-9(10)	-55(12)
C(17)	104(13)	133(15)	30(7)	29(10)	-21(7)	-52(12)
C(18)	67(10)	94(12)	78(11)	-17(10)	16(8)	-29(9)
C(19)	53(9)	77(11)	54(8)	-16(8)	14(7)	-21(8)
C(20)	45(8)	67(9)	60(8)	-15(8)	10(7)	-22(8)
C(21)	46(8)	81(10)	75(9)	-48(8)	5(7)	10(7)
C(22)	89(11)	174(15)	89(10)	-71(10)	54(9)	-76(11)
C(23)	177(17)	140(15)	121(13)	-91(12)	85(12)	-97(13)
C(24)	126(14)	94(12)	57(9)	-24(8)	40(9)	-15(11)
C(25)	88(12)	114(13)	93(11)	-62(10)	-28(9)	8(11)
C(26)	108(12)	130(14)	118(12)	-100(11)	-12(10)	-16(10)
C(27)	62(10)	147(15)	42(7)	-21(8)	-2(6)	-75(11)
C(28)	102(12)	80(11)	173(14)	-58(10)	-31(11)	-47(10)
C(30)	77(11)	78(11)	136(13)	-36(10)	8(10)	-19(10)
C(31)	96(13)	99(13)	69(9)	-22(9)	9(9)	-57(11)
C(32)	37(9)	150(15)	39(7)	24(10)	-4(6)	13(10)
C(33)	35(7)	63(8)	35(6)	-10(6)	0(5)	-24(6)
C(34)	76(9)	63(9)	44(7)	-7(7)	-4(6)	-39(8)
C(35)	76(9)	62(9)	50(7)	-1(7)	-3(7)	-43(8)
C(36)	62(8)	73(10)	31(6)	-3(7)	2(6)	-30(8)
C(37)	50(8)	62(9)	43(7)	-10(7)	-2(6)	-20(7)
C(38)	42(7)	58(8)	32(6)	-3(6)	-12(5)	-14(6)
C(39)	53(8)	94(10)	69(8)	-23(8)	22(6)	-45(8)
C(40)	26(6)	107(10)	56(7)	-18(7)	-4(5)	-33(7)
C(41)	49(8)	125(12)	50(7)	-39(8)	17(6)	-51(8)
C(44)	160(16)	350(20)	65(9)	-75(12)	38(9)	-175(17)
C(45)	94(12)	300(20)	77(9)	-85(12)	34(8)	-106(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5.

	x	y	z	U(eq)
H(1A)	1811	2933	10517	107
H(2A)	-72	3173	11524	92
H(4A)	-2411	3098	11233	65
H(5A)	-3543	3039	10069	56
H(6A)	-2615	2809	8647	56
H(8A)	233	6223	6495	81
H(9A)	568	7956	6224	78
H(11A)	2748	8260	6600	86
H(12A)	4754	7210	7201	83
H(13A)	5488	5253	7761	73
H(16A)	-418	3550	5635	123
H(17A)	-1493	5451	4959	111
H(18A)	-2494	7012	5756	100
H(19A)	-2640	6583	7289	78
H(20A)	-1724	4737	7983	70
H(22A)	2442	1816	6665	131
H(23A)	3789	822	5537	161
H(24A)	2996	80	4607	129
H(25A)	1038	12	4943	132
H(26A)	-147	854	6163	145
H(28A)	7782	1335	7826	130
H(29A)	8937	-665	7745	146
H(30A)	8001	-1772	7433	121
H(31A)	5850	-864	7120	99
H(32A)	4692	1161	7276	121
H(34A)	5332	1187	9149	69
H(35A)	4882	970	10677	71
H(36A)	3982	2565	11441	67
H(37A)	3487	4401	10692	64
H(38A)	3915	4616	9091	56
H(39A)	1480	2545	8214	81

H(39B)	2531	2463	8852	81
H(40A)	460	4695	8277	72
H(40B)	1774	4477	8676	72
H(41A)	2878	3576	7341	82
H(41B)	1503	4023	6936	82
H(42A)	737	-1250	7970	249
H(42B)	1372	-680	7156	249
H(42C)	-146	-62	7362	249
H(43A)	2876	-1119	8523	237
H(43B)	2730	46	8863	237
H(43C)	2847	-42	7801	237
H(44A)	5030	3140	4783	245
H(44B)	3878	3402	5535	245
H(44C)	5134	2175	5637	245
H(45A)	7321	2904	5114	216
H(45B)	7327	1896	5902	216
H(45C)	7654	2900	6120	216

S7 X-ray structure data for compound 6.

Diagrams showing the structure of compound **6** with labeling schemes:

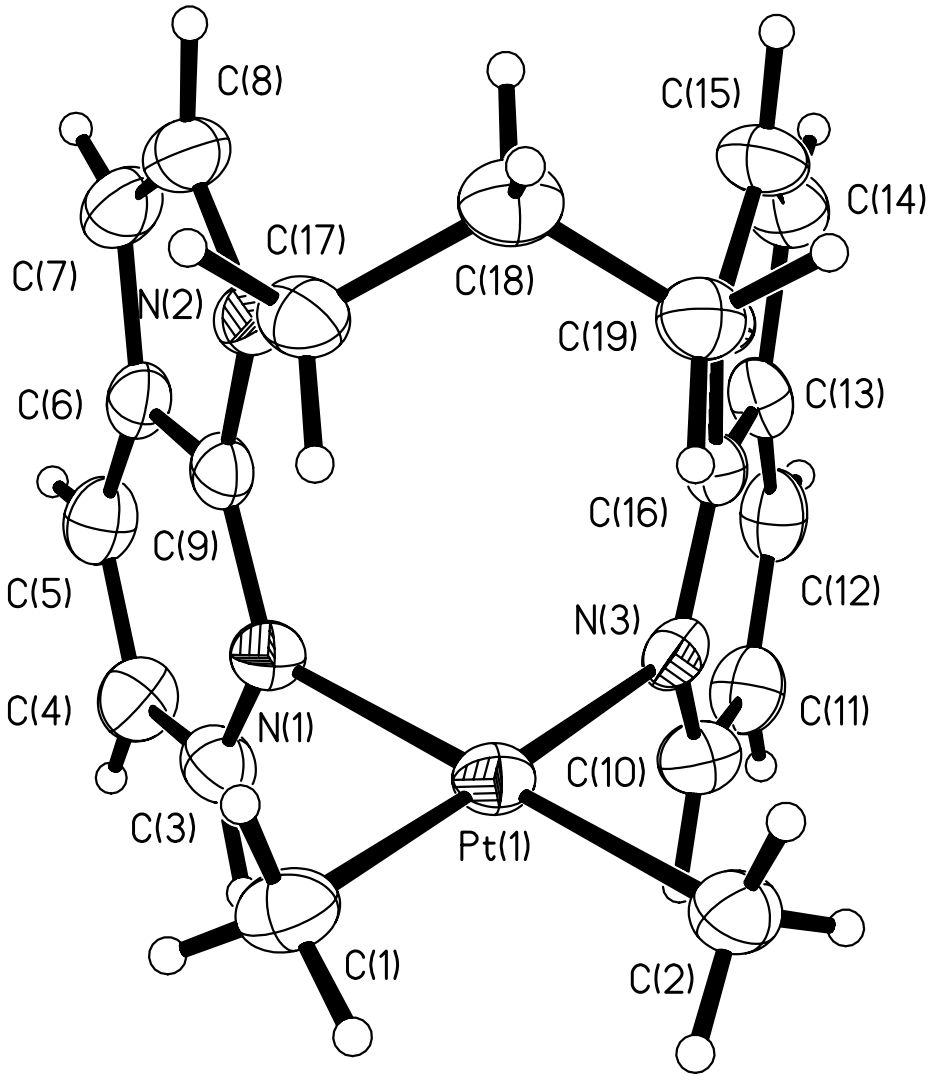

Table 1. Crystal data and structure refinement for compound **6**.

Identification code	**6**	
Empirical formula	C38 H44 N8 Pt2	
Formula weight	1002.99	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.9960(11) Å	α= 84.184(2)°.
	b = 9.6192(13) Å	β= 72.328(2)°.
	c = 11.9856(16) Å	γ = 87.362(2)°.
Volume	873.7(2) $Å^3$	
Z	1	
Density (calculated)	1.906 Mg/m^3	
Absorption coefficient	8.037 mm^{-1}	
F(000)	484	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.79 to 27.00°.	
Index ranges	-10<=h<=10, -12<=k<=12, -15<=l<=14	
Reflections collected	6093	
Independent reflections	3768 [R(int) = 0.0251]	
Completeness to theta = 27.00°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5004 and 0.2963	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3768 / 0 / 219	
Goodness-of-fit on F^2	0.924	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0621	
R indices (all data)	R1 = 0.0420, wR2 = 0.0645	
Largest diff. peak and hole	1.738 and -1.085 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	2545(1)	8396(1)	2648(1)	27(1)
C(1)	2749(7)	8789(7)	4229(5)	37(2)
C(2)	3682(7)	10245(6)	1930(6)	38(2)
C(3)	2619(8)	5285(7)	3178(5)	33(1)
C(4)	2194(8)	3900(6)	3208(5)	37(2)
C(5)	462(8)	3533(7)	3378(5)	37(2)
C(6)	-793(7)	4595(6)	3537(5)	29(1)
C(7)	-2636(8)	4685(7)	3734(5)	40(2)
C(8)	-3121(7)	6042(7)	3835(5)	36(2)
C(9)	-225(7)	5988(6)	3507(4)	27(1)
C(10)	3671(7)	7088(7)	346(5)	36(1)
C(11)	3557(8)	6299(7)	-519(5)	37(2)
C(12)	1997(8)	6213(7)	-762(5)	37(2)
C(13)	580(7)	6991(6)	-146(5)	31(1)
C(14)	-1178(8)	7246(7)	-168(5)	39(2)
C(15)	-1878(8)	8189(7)	613(6)	40(2)
C(16)	826(7)	7820(6)	705(5)	27(1)
C(17)	-1823(7)	8292(7)	3990(5)	34(1)
C(18)	-2414(7)	9317(6)	3107(5)	36(2)
C(19)	-1038(7)	9669(6)	1941(5)	32(1)
N(1)	1448(6)	6358(5)	3307(4)	29(1)
N(2)	-1664(6)	6851(5)	3691(4)	29(1)
N(3)	2326(6)	7845(5)	1004(4)	27(1)
N(4)	-695(6)	8538(5)	1170(4)	30(1)

Table 3. Bond lengths [Å] and angles [°] for compound **6**.

Pt(1)-C(2)	2.023(6)	N(3)-Pt(1)-N(1)	83.75(17)
Pt(1)-C(1)	2.025(5)	N(1)-C(3)-C(4)	124.3(5)
Pt(1)-N(3)	2.150(4)	C(3)-C(4)-C(5)	120.3(6)
Pt(1)-N(1)	2.159(5)	C(6)-C(5)-C(4)	117.5(6)
C(3)-N(1)	1.349(7)	C(5)-C(6)-C(7)	135.7(6)
C(3)-C(4)	1.384(8)	C(5)-C(6)-C(9)	117.9(5)
C(4)-C(5)	1.394(8)	C(7)-C(6)-C(9)	106.3(5)
C(5)-C(6)	1.384(8)	C(8)-C(7)-C(6)	107.4(5)
C(6)-C(7)	1.420(8)	C(7)-C(8)-N(2)	110.2(5)
C(6)-C(9)	1.427(8)	N(1)-C(9)-N(2)	127.0(5)
C(7)-C(8)	1.352(9)	N(1)-C(9)-C(6)	125.0(5)
C(8)-N(2)	1.388(7)	N(2)-C(9)-C(6)	107.9(5)
C(9)-N(1)	1.344(6)	N(3)-C(10)-C(11)	124.7(5)
C(9)-N(2)	1.362(7)	C(10)-C(11)-C(12)	120.4(6)
C(10)-N(3)	1.356(7)	C(11)-C(12)-C(13)	118.0(6)
C(10)-C(11)	1.371(8)	C(12)-C(13)-C(16)	118.0(5)
C(11)-C(12)	1.372(8)	C(12)-C(13)-C(14)	135.6(5)
C(12)-C(13)	1.384(8)	C(16)-C(13)-C(14)	106.4(5)
C(13)-C(16)	1.420(8)	C(15)-C(14)-C(13)	106.5(5)
C(13)-C(14)	1.423(8)	C(14)-C(15)-N(4)	111.4(5)
C(14)-C(15)	1.349(9)	N(3)-C(16)-N(4)	126.9(5)
C(15)-N(4)	1.383(6)	N(3)-C(16)-C(13)	124.5(5)
C(16)-N(3)	1.354(6)	N(4)-C(16)-C(13)	108.5(4)
C(16)-N(4)	1.363(7)	N(2)-C(17)-C(18)	113.4(5)
C(17)-N(2)	1.457(7)	C(19)-C(18)-C(17)	115.7(5)
C(17)-C(18)	1.538(8)	N(4)-C(19)-C(18)	113.3(5)
C(18)-C(19)	1.510(8)	C(9)-N(1)-C(3)	114.9(5)
C(19)-N(4)	1.460(7)	C(9)-N(1)-Pt(1)	126.7(4)
		C(3)-N(1)-Pt(1)	115.4(4)
C(2)-Pt(1)-C(1)	89.9(3)	C(9)-N(2)-C(8)	108.1(5)
C(2)-Pt(1)-N(3)	93.3(2)	C(9)-N(2)-C(17)	128.1(4)
C(1)-Pt(1)-N(3)	176.5(2)	C(8)-N(2)-C(17)	122.1(5)
C(2)-Pt(1)-N(1)	176.0(2)	C(16)-N(3)-C(10)	114.2(5)
C(1)-Pt(1)-N(1)	93.0(2)	C(16)-N(3)-Pt(1)	126.2(4)

C(10)-N(3)-Pt(1)	116.9(3)	C(16)-N(4)-C(19)	129.6(4)
C(16)-N(4)-C(15)	107.1(5)	C(15)-N(4)-C(19)	122.3(5)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	25(1)	26(1)	32(1)	-5(1)	-9(1)	0(1)
C(1)	28(3)	46(4)	38(4)	-12(3)	-6(3)	-2(3)
C(2)	32(3)	32(4)	50(4)	3(3)	-16(3)	0(3)
C(3)	33(3)	36(4)	31(3)	-3(3)	-10(3)	6(3)
C(4)	39(3)	25(4)	44(4)	-2(3)	-8(3)	5(3)
C(5)	46(4)	31(4)	34(4)	-3(3)	-9(3)	-6(3)
C(6)	33(3)	32(4)	23(3)	-1(3)	-7(2)	-6(3)
C(7)	35(3)	49(5)	36(4)	-2(3)	-8(3)	-15(3)
C(8)	27(3)	45(4)	36(4)	-5(3)	-7(3)	-5(3)
C(9)	30(3)	31(4)	19(3)	-1(2)	-6(2)	1(3)
C(10)	30(3)	36(4)	40(4)	-4(3)	-9(3)	-1(3)
C(11)	42(4)	36(4)	29(3)	-7(3)	-3(3)	2(3)
C(12)	54(4)	30(4)	27(3)	-3(3)	-12(3)	-7(3)
C(13)	40(3)	26(3)	29(3)	1(3)	-14(3)	0(3)
C(14)	42(4)	41(4)	42(4)	-4(3)	-22(3)	-7(3)
C(15)	31(3)	47(5)	48(4)	-1(3)	-21(3)	-3(3)
C(16)	28(3)	23(3)	29(3)	5(2)	-8(2)	-1(2)
C(17)	29(3)	44(4)	30(3)	-9(3)	-8(3)	7(3)
C(18)	32(3)	30(4)	46(4)	-11(3)	-11(3)	5(3)
C(19)	31(3)	27(4)	40(4)	-4(3)	-12(3)	1(3)
N(1)	25(2)	33(3)	30(3)	-2(2)	-8(2)	1(2)
N(2)	26(2)	33(3)	28(3)	-3(2)	-6(2)	-1(2)
N(3)	25(2)	26(3)	27(3)	2(2)	-3(2)	-5(2)
N(4)	27(2)	34(3)	32(3)	-4(2)	-13(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **6**.

	x	y	z	U(eq)
H(1A)	3656	9487	4114	56
H(1B)	3069	7925	4628	56
H(1C)	1621	9147	4711	56
H(2A)	2783	10989	2045	57
H(2B)	4254	10195	1086	57
H(2C)	4558	10445	2310	57
H(3A)	3814	5494	3059	40
H(4A)	3087	3197	3113	44
H(5A)	155	2590	3383	45
H(7A)	-3389	3930	3786	48
H(8A)	-4291	6393	3982	44
H(10A)	4771	7105	494	43
H(11A)	4565	5808	-952	45
H(12A)	1893	5637	-1335	44
H(14A)	-1747	6833	-639	47
H(15A)	-3036	8566	761	48
H(17A)	-674	8589	4028	41
H(17B)	-2680	8338	4780	41
H(18A)	-3433	8915	2954	43
H(18B)	-2819	10196	3476	43
H(19A)	-1428	10512	1536	39
H(19B)	69	9894	2087	39

S8 X-ray structure data for compound 7.

Diagrams showing the structure of compound **7** with labeling schemes:

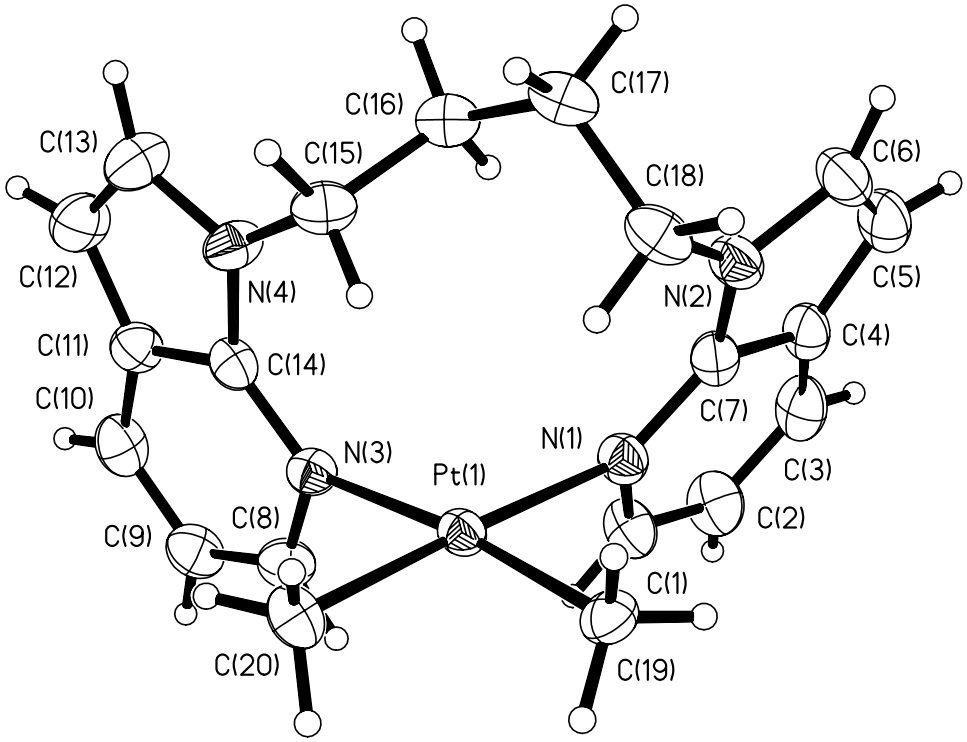

Table 1. Crystal data and structure refinement for **7.**

Identification code	7	
Empirical formula	C20 H24 N4 Pt	
Formula weight	515.52	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0310(7) Å	α= 82.4630(10)°.
	b = 10.7070(8) Å	β= 85.1300(10)°.
	c = 13.8631(11) Å	γ = 83.6180(10)°.
Volume	1171.44(16) $Å^3$	
Z	2	
Density (calculated)	1.462 Mg/m^3	
Absorption coefficient	5.997 mm^{-1}	
F(000)	500	
Crystal size	0.30 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.49 to 26.00°.	
Index ranges	-9<=h<=9, -12<=k<=13, -17<=l<=15	
Reflections collected	7432	
Independent reflections	4542 [R(int) = 0.0171]	
Completeness to theta = 26.00°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3801 and 0.2663	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4542 / 0 / 228	
Goodness-of-fit on F^2	0.979	
Final R indices [I>2sigma(I)]	R1 = 0.0190, wR2 = 0.0405	
R indices (all data)	R1 = 0.0213, wR2 = 0.0407	
Largest diff. peak and hole	1.229 and -0.682 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	313(1)	1393(1)	2923(1)	22(1)
N(1)	181(3)	3413(2)	2956(2)	27(1)
N(2)	-1693(4)	3816(2)	4397(2)	30(1)
N(3)	-904(3)	1648(2)	1567(2)	24(1)
N(4)	-3853(4)	1430(3)	2087(2)	30(1)
C(1)	1132(5)	4011(3)	2237(2)	33(1)
C(2)	1274(5)	5312(3)	2110(3)	39(1)
C(3)	413(5)	6064(3)	2756(3)	39(1)
C(4)	-569(5)	5497(3)	3516(3)	32(1)
C(5)	-1602(5)	5928(3)	4312(3)	40(1)
C(6)	-2254(5)	4908(3)	4820(3)	38(1)
C(7)	-647(4)	4165(3)	3592(2)	27(1)
C(8)	135(5)	1760(3)	748(2)	32(1)
C(9)	-354(5)	1787(3)	-188(2)	36(1)
C(10)	-2013(5)	1705(3)	-337(3)	37(1)
C(11)	-3143(4)	1592(3)	466(2)	30(1)
C(12)	-4892(5)	1487(3)	624(3)	40(1)
C(13)	-5263(5)	1390(3)	1596(3)	42(1)
C(14)	-2506(4)	1559(3)	1405(2)	27(1)
C(15)	-3838(5)	1349(3)	3151(2)	31(1)
C(16)	-4400(5)	2611(3)	3520(2)	33(1)
C(17)	-4093(4)	2533(3)	4603(2)	36(1)
C(18)	-2262(4)	2589(3)	4783(2)	33(1)
C(19)	1650(4)	1040(3)	4128(2)	28(1)
C(20)	535(5)	-505(3)	2859(2)	32(1)

Table 3. Bond lengths [Å] and angles [°] for **7.**

Pt(1)-C(19)	2.033(3)	C(20)-Pt(1)-N(3)	88.13(11)
Pt(1)-C(20)	2.034(3)	N(1)-Pt(1)-N(3)	91.82(9)
Pt(1)-N(1)	2.160(2)	C(1)-N(1)-C(7)	115.0(3)
Pt(1)-N(3)	2.165(3)	C(1)-N(1)-Pt(1)	113.8(2)
N(1)-C(1)	1.341(4)	C(7)-N(1)-Pt(1)	131.2(2)
N(1)-C(7)	1.354(4)	C(7)-N(2)-C(6)	107.1(3)
N(2)-C(7)	1.376(4)	C(7)-N(2)-C(18)	130.8(2)
N(2)-C(6)	1.389(4)	C(6)-N(2)-C(18)	122.0(3)
N(2)-C(18)	1.459(4)	C(14)-N(3)-C(8)	114.0(3)
N(3)-C(14)	1.340(4)	C(14)-N(3)-Pt(1)	130.0(2)
N(3)-C(8)	1.351(4)	C(8)-N(3)-Pt(1)	115.4(2)
N(4)-C(13)	1.377(4)	C(13)-N(4)-C(14)	108.0(3)
N(4)-C(14)	1.382(4)	C(13)-N(4)-C(15)	124.6(3)
N(4)-C(15)	1.467(4)	C(14)-N(4)-C(15)	127.4(3)
C(1)-C(2)	1.397(4)	N(1)-C(1)-C(2)	124.6(3)
C(2)-C(3)	1.374(5)	C(3)-C(2)-C(1)	119.7(3)
C(3)-C(4)	1.378(5)	C(2)-C(3)-C(4)	118.2(3)
C(4)-C(5)	1.418(5)	C(3)-C(4)-C(5)	134.9(3)
C(4)-C(7)	1.424(4)	C(3)-C(4)-C(7)	118.5(3)
C(5)-C(6)	1.351(5)	C(5)-C(4)-C(7)	106.6(3)
C(8)-C(9)	1.384(5)	C(6)-C(5)-C(4)	107.2(3)
C(9)-C(10)	1.380(5)	C(5)-C(6)-N(2)	110.9(3)
C(10)-C(11)	1.377(5)	N(1)-C(7)-N(2)	127.8(3)
C(11)-C(12)	1.417(5)	N(1)-C(7)-C(4)	124.0(3)
C(11)-C(14)	1.433(4)	N(2)-C(7)-C(4)	108.2(3)
C(12)-C(13)	1.349(5)	N(3)-C(8)-C(9)	124.8(3)
C(15)-C(16)	1.516(4)	C(10)-C(9)-C(8)	120.1(3)
C(16)-C(17)	1.531(5)	C(11)-C(10)-C(9)	118.2(3)
C(17)-C(18)	1.521(5)	C(10)-C(11)-C(12)	135.5(3)
		C(10)-C(11)-C(14)	117.4(3)
C(19)-Pt(1)-C(20)	88.13(13)	C(12)-C(11)-C(14)	107.1(3)
C(19)-Pt(1)-N(1)	91.72(11)	C(13)-C(12)-C(11)	106.9(3)
C(20)-Pt(1)-N(1)	177.54(12)	C(12)-C(13)-N(4)	111.2(3)
C(19)-Pt(1)-N(3)	174.07(11)	N(3)-C(14)-N(4)	127.7(3)

N(3)-C(14)-C(11)	125.5(3)	C(15)-C(16)-C(17)	110.1(3)
N(4)-C(14)-C(11)	106.8(3)	C(18)-C(17)-C(16)	113.3(3)
N(4)-C(15)-C(16)	112.2(3)	N(2)-C(18)-C(17)	111.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	23(1)	19(1)	24(1)	-3(1)	1(1)	-2(1)
N(1)	29(2)	23(1)	29(2)	-4(1)	-2(1)	-1(1)
N(2)	31(2)	27(1)	32(2)	-8(1)	-3(1)	4(1)
N(3)	24(2)	23(1)	23(2)	-1(1)	2(1)	-3(1)
N(4)	23(2)	41(2)	26(2)	-1(1)	-1(1)	-5(1)
C(1)	43(2)	27(2)	30(2)	-4(2)	4(2)	-8(2)
C(2)	50(3)	26(2)	41(2)	1(2)	-1(2)	-11(2)
C(3)	49(3)	22(2)	46(2)	-3(2)	-13(2)	-6(2)
C(4)	36(2)	22(2)	39(2)	-8(2)	-14(2)	4(2)
C(5)	44(2)	30(2)	48(2)	-15(2)	-15(2)	9(2)
C(6)	38(2)	42(2)	35(2)	-18(2)	-6(2)	10(2)
C(7)	31(2)	23(2)	28(2)	-3(1)	-9(2)	2(2)
C(8)	30(2)	35(2)	30(2)	-3(2)	2(2)	-1(2)
C(9)	39(2)	42(2)	25(2)	-6(2)	5(2)	-2(2)
C(10)	49(3)	33(2)	28(2)	-4(2)	-9(2)	0(2)
C(11)	29(2)	31(2)	29(2)	-4(1)	-4(2)	1(2)
C(12)	34(2)	51(2)	37(2)	-7(2)	-11(2)	-1(2)
C(13)	29(2)	50(2)	47(2)	-5(2)	-6(2)	-7(2)
C(14)	32(2)	23(2)	26(2)	-5(1)	0(2)	-2(2)
C(15)	27(2)	35(2)	30(2)	0(2)	2(2)	-2(2)
C(16)	28(2)	35(2)	36(2)	-3(2)	1(2)	0(2)
C(17)	32(2)	40(2)	34(2)	-7(2)	7(2)	2(2)
C(18)	39(2)	32(2)	25(2)	-2(1)	5(2)	3(2)
C(19)	22(2)	30(2)	33(2)	-3(1)	-1(2)	-7(2)

C(20)	39(2)	24(2)	34(2)	-7(1)	-1(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(1A)	1752	3516	1782	40
H(2A)	1963	5676	1580	47
H(3A)	493	6950	2681	46
H(5A)	-1799	6776	4460	48
H(6A)	-2996	4934	5390	46
H(8A)	1287	1826	821	39
H(9A)	454	1863	-729	43
H(10A)	-2366	1725	-976	44
H(12A)	-5656	1486	137	48
H(13A)	-6355	1305	1902	50
H(15A)	-2687	1056	3344	38
H(15B)	-4590	716	3460	38
H(16A)	-5610	2841	3430	40
H(16B)	-3768	3279	3141	40
H(17A)	-4783	3241	4883	43
H(17B)	-4468	1732	4947	43
H(18A)	-2124	2430	5493	40
H(18B)	-1556	1915	4469	40
H(19A)	933	701	4687	42
H(19B)	2043	1829	4266	42
H(19C)	2618	422	4013	42
H(20A)	-16	-929	3450	48
H(20B)	1727	-825	2809	48
H(20C)	2	-676	2286	48

S9 X-ray structure data for compound 8.

Diagrams showing the structure of compound **8** with labeling schemes:

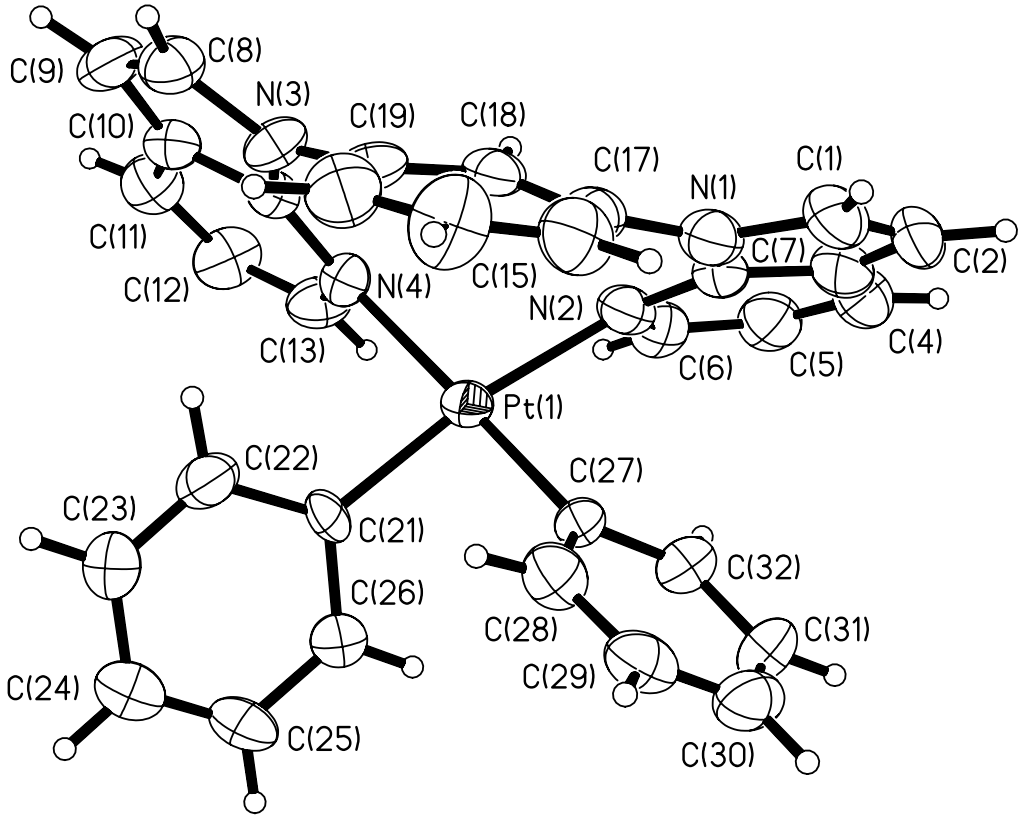

Table 1. Crys tal data and structure refinement for compound **8**.

Identification code	**8**	
Empirical formula	C32 H24 N4 Pt	
Formula weight	659.64	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.778(2) Å	α= 103.297(4)°.
	b = 9.984(2) Å	β= 96.241(4)°.
	c = 13.777(3) Å	γ = 115.883(3)°.
Volume	1260.4(4) $Å^3$	
Z	2	
Density (calculated)	1.738 Mg/m^3	
Absorption coefficient	5.595 mm^{-1}	
F(000)	644	
Crystal size	0.40 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.56 to 26.00°.	
Index ranges	-13<=h<=12, -12<=k<=12, -16<=l<=16	
Reflections collected	8109	
Independent reflections	4909 [R(int) = 0.0977]	
Completeness to theta = 26.00°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2846 and 0.2131	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4909 / 0 / 334	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0775, wR2 = 0.2071	
R indices (all data)	R1 = 0.0791, wR2 = 0.2089	
Largest diff. peak and hole	3.384 and -2.846 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	5302(1)	7241(1)	1973(1)	34(1)
N(1)	8842(10)	10063(10)	3186(7)	47(2)
N(2)	7331(10)	8064(11)	1571(7)	41(2)
N(3)	4761(9)	10610(9)	2146(6)	42(2)
N(4)	4393(9)	8114(11)	957(6)	36(2)
C(1)	10233(12)	10634(13)	3727(10)	57(3)
C(2)	10898(11)	9958(15)	3136(10)	61(3)
C(3)	9884(12)	8936(14)	2201(10)	56(3)
C(4)	9869(13)	7942(16)	1309(10)	60(3)
C(5)	8626(14)	7092(15)	527(9)	57(3)
C(6)	7404(13)	7159(14)	702(8)	45(2)
C(7)	8620(11)	8990(12)	2271(8)	44(2)
C(8)	4132(12)	11551(12)	2101(8)	48(2)
C(9)	3227(13)	11037(13)	1199(9)	53(3)
C(10)	3213(12)	9651(13)	606(9)	44(2)
C(11)	2445(13)	8535(14)	-346(8)	52(2)
C(12)	2728(13)	7326(14)	-640(8)	55(3)
C(13)	3690(12)	7148(12)	-3(8)	47(2)
C(14)	4188(10)	9402(11)	1224(7)	37(2)
C(15)	6769(15)	11383(17)	4742(9)	68(3)
C(16)	7800(14)	11036(16)	4522(10)	58(3)
C(17)	7851(12)	10570(12)	3491(8)	46(2)
C(18)	6929(10)	10599(10)	2734(7)	41(2)
C(19)	5815(12)	10838(10)	2955(7)	43(2)
C(20)	5731(14)	11252(14)	3984(9)	59(3)
C(21)	3410(9)	6131(11)	2266(7)	32(2)
C(22)	2483(12)	6781(12)	2459(8)	47(2)
C(23)	1193(13)	5947(17)	2652(12)	62(3)
C(24)	715(14)	4414(15)	2676(11)	62(3)
C(25)	1543(12)	3720(13)	2450(10)	59(3)
C(26)	2867(11)	4565(12)	2275(8)	47(2)

C(27)	6116(11)	6519(11)	2985(8)	35(2)
C(28)	5879(12)	6709(13)	3971(8)	50(2)
C(29)	6493(12)	6300(13)	4711(8)	52(2)
C(30)	7261(13)	5555(13)	4465(9)	55(3)
C(31)	7468(15)	5270(16)	3483(12)	58(3)
C(32)	6913(13)	5749(13)	2767(9)	50(2)

Table 3. Bond lengths [Å] and angles [°] for compound **8**.

Pt(1)-C(21)	1.990(9)	C(15)-C(16)	1.34(2)
Pt(1)-C(27)	1.996(10)	C(15)-C(20)	1.384(18)
Pt(1)-N(2)	2.161(9)	C(16)-C(17)	1.404(17)
Pt(1)-N(4)	2.165(8)	C(17)-C(18)	1.375(14)
N(1)-C(7)	1.373(15)	C(18)-C(19)	1.374(15)
N(1)-C(1)	1.394(14)	C(19)-C(20)	1.407(15)
N(1)-C(17)	1.429(15)	C(21)-C(26)	1.413(14)
N(2)-C(6)	1.358(15)	C(21)-C(22)	1.427(14)
N(2)-C(7)	1.375(14)	C(22)-C(23)	1.367(17)
N(3)-C(8)	1.385(13)	C(23)-C(24)	1.396(18)
N(3)-C(14)	1.387(12)	C(24)-C(25)	1.369(19)
N(3)-C(19)	1.402(13)	C(25)-C(26)	1.386(15)
N(4)-C(13)	1.345(13)	C(27)-C(32)	1.394(15)
N(4)-C(14)	1.374(13)	C(27)-C(28)	1.395(15)
C(1)-C(2)	1.39(2)	C(28)-C(29)	1.387(16)
C(2)-C(3)	1.418(18)	C(29)-C(30)	1.355(18)
C(3)-C(4)	1.384(19)	C(30)-C(31)	1.380(19)
C(3)-C(7)	1.400(16)	C(31)-C(32)	1.378(17)
C(4)-C(5)	1.397(18)		
C(5)-C(6)	1.391(17)	C(21)-Pt(1)-C(27)	89.3(4)
C(8)-C(9)	1.329(17)	C(21)-Pt(1)-N(2)	170.4(4)
C(9)-C(10)	1.429(15)	C(27)-Pt(1)-N(2)	86.1(4)
C(10)-C(11)	1.391(17)	C(21)-Pt(1)-N(4)	89.2(4)
C(10)-C(14)	1.422(15)	C(27)-Pt(1)-N(4)	176.3(3)
C(11)-C(12)	1.356(17)	N(2)-Pt(1)-N(4)	95.9(3)
C(12)-C(13)	1.382(16)	C(7)-N(1)-C(1)	107.5(10)

C(7)-N(1)-C(17)	125.8(9)	C(18)-C(17)-N(1)	117.7(9)
C(1)-N(1)-C(17)	126.6(10)	C(16)-C(17)-N(1)	122.5(10)
C(6)-N(2)-C(7)	113.2(10)	C(19)-C(18)-C(17)	120.3(9)
C(6)-N(2)-Pt(1)	116.9(7)	C(18)-C(19)-N(3)	119.2(8)
C(7)-N(2)-Pt(1)	124.3(7)	C(18)-C(19)-C(20)	119.3(10)
C(8)-N(3)-C(14)	107.6(8)	N(3)-C(19)-C(20)	121.5(10)
C(8)-N(3)-C(19)	127.1(8)	C(15)-C(20)-C(19)	118.7(12)
C(14)-N(3)-C(19)	125.3(8)	C(26)-C(21)-C(22)	114.3(8)
C(13)-N(4)-C(14)	114.1(9)	C(26)-C(21)-Pt(1)	120.7(7)
C(13)-N(4)-Pt(1)	117.1(7)	C(22)-C(21)-Pt(1)	125.0(8)
C(14)-N(4)-Pt(1)	127.3(7)	C(23)-C(22)-C(21)	121.9(10)
C(2)-C(1)-N(1)	109.4(11)	C(22)-C(23)-C(24)	121.7(12)
C(1)-C(2)-C(3)	106.7(10)	C(25)-C(24)-C(23)	118.4(12)
C(4)-C(3)-C(7)	117.2(11)	C(24)-C(25)-C(26)	120.4(11)
C(4)-C(3)-C(2)	135.6(12)	C(25)-C(26)-C(21)	123.3(10)
C(7)-C(3)-C(2)	107.2(11)	C(32)-C(27)-C(28)	114.7(10)
C(3)-C(4)-C(5)	118.9(12)	C(32)-C(27)-Pt(1)	123.8(8)
C(6)-C(5)-C(4)	119.1(11)	C(28)-C(27)-Pt(1)	121.5(8)
N(2)-C(6)-C(5)	124.9(11)	C(29)-C(28)-C(27)	122.9(11)
N(1)-C(7)-N(2)	124.5(10)	C(30)-C(29)-C(28)	120.1(11)
N(1)-C(7)-C(3)	109.1(10)	C(29)-C(30)-C(31)	119.0(10)
N(2)-C(7)-C(3)	126.2(11)	C(32)-C(31)-C(30)	120.4(12)
C(9)-C(8)-N(3)	111.3(9)	C(31)-C(32)-C(27)	122.5(12)
C(8)-C(9)-C(10)	107.3(10)		
C(11)-C(10)-C(14)	117.7(10)		
C(11)-C(10)-C(9)	135.4(11)		
C(14)-C(10)-C(9)	106.7(10)		
C(12)-C(11)-C(10)	117.7(10)		
C(11)-C(12)-C(13)	121.8(10)		
N(4)-C(13)-C(12)	123.8(10)		
N(4)-C(14)-N(3)	128.3(9)		
N(4)-C(14)-C(10)	124.4(9)		
N(3)-C(14)-C(10)	107.1(9)		
C(16)-C(15)-C(20)	122.1(12)		
C(15)-C(16)-C(17)	119.0(11)		
C(18)-C(17)-C(16)	119.8(11)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	33(1)	27(1)	38(1)	10(1)	7(1)	12(1)
N(1)	44(5)	39(4)	51(5)	16(4)	8(4)	14(4)
N(2)	38(4)	34(4)	44(4)	14(3)	8(3)	10(3)
N(3)	56(5)	31(4)	43(4)	8(3)	11(3)	27(4)
N(4)	37(4)	39(4)	36(4)	12(3)	8(3)	20(4)
C(1)	39(5)	46(6)	66(7)	19(5)	-6(5)	6(5)
C(2)	30(5)	63(7)	83(8)	41(6)	2(5)	11(5)
C(3)	47(6)	59(7)	68(7)	39(6)	21(5)	21(5)
C(4)	52(7)	69(8)	78(8)	39(6)	35(6)	32(6)
C(5)	62(7)	65(7)	59(6)	33(6)	30(5)	34(6)
C(6)	53(6)	54(6)	36(5)	22(4)	13(4)	28(5)
C(7)	38(5)	41(5)	56(5)	26(4)	10(4)	16(4)
C(8)	52(6)	36(5)	53(6)	10(4)	13(5)	20(5)
C(9)	69(7)	45(5)	64(6)	27(5)	23(5)	36(5)
C(10)	42(5)	39(5)	53(6)	22(4)	13(4)	17(4)
C(11)	55(7)	58(6)	45(5)	21(5)	13(5)	26(6)
C(12)	66(7)	51(6)	38(5)	6(4)	-4(5)	25(5)
C(13)	57(6)	35(5)	42(5)	9(4)	5(4)	18(5)
C(14)	34(5)	32(4)	44(5)	14(4)	12(4)	13(4)
C(15)	78(9)	86(9)	40(6)	12(6)	6(5)	46(8)
C(16)	50(7)	63(8)	46(6)	16(5)	-4(5)	18(6)
C(17)	44(5)	35(5)	51(5)	14(4)	6(4)	13(4)
C(18)	40(5)	26(4)	49(5)	13(4)	13(4)	9(4)
C(19)	62(6)	25(4)	39(4)	8(3)	11(4)	21(4)
C(20)	62(7)	47(6)	60(7)	5(5)	12(5)	25(5)
C(21)	16(4)	32(4)	35(4)	7(3)	1(3)	4(3)
C(22)	57(6)	43(5)	53(5)	21(4)	16(5)	31(5)

C(23)	44(6)	63(8)	89(9)	34(7)	16(6)	29(6)
C(24)	52(7)	49(6)	82(8)	29(6)	21(6)	16(5)
C(25)	42(6)	38(5)	82(8)	25(5)	15(5)	4(5)
C(26)	43(5)	40(5)	62(6)	21(4)	16(5)	21(4)
C(27)	34(5)	27(4)	46(5)	11(4)	10(4)	17(4)
C(28)	44(6)	52(6)	47(5)	15(4)	10(4)	18(5)
C(29)	45(6)	45(5)	49(5)	16(4)	8(4)	8(5)
C(30)	53(6)	49(6)	55(6)	23(5)	-3(5)	15(5)
C(31)	57(7)	56(7)	79(8)	31(6)	15(6)	38(6)
C(32)	52(6)	45(6)	63(6)	24(5)	15(5)	28(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **8**

	x	y	z	U(eq)
H(1A)	10651	11356	4381	69
H(2A)	11827	10140	3318	73
H(4A)	10674	7841	1232	72
H(5A)	8614	6489	-103	68
H(6A)	6575	6538	184	54
H(8A)	4320	12430	2633	58
H(9A)	2700	11495	991	64
H(11A)	1762	8616	-767	63
H(12A)	2262	6596	-1289	66
H(13A)	3861	6312	-252	57
H(15A)	6753	11722	5427	81
H(16A)	8469	11104	5044	70
H(18A)	7060	10457	2069	49
H(20A)	4993	11433	4151	71
H(22A)	2764	7802	2453	56
H(23A)	618	6413	2770	74
H(24A)	-144	3877	2841	74
H(25A)	1216	2676	2414	71
H(26A)	3424	4078	2158	56
H(28A)	5283	7129	4140	60

H(29A)	6377	6537	5378	62
H(30A)	7643	5240	4950	67
H(31A)	7986	4752	3303	69
H(32A)	7075	5551	2112	60

S10 X-ray structure data for compound 9a.

Diagrams showing the structure of compound **9a** with labeling schemes:

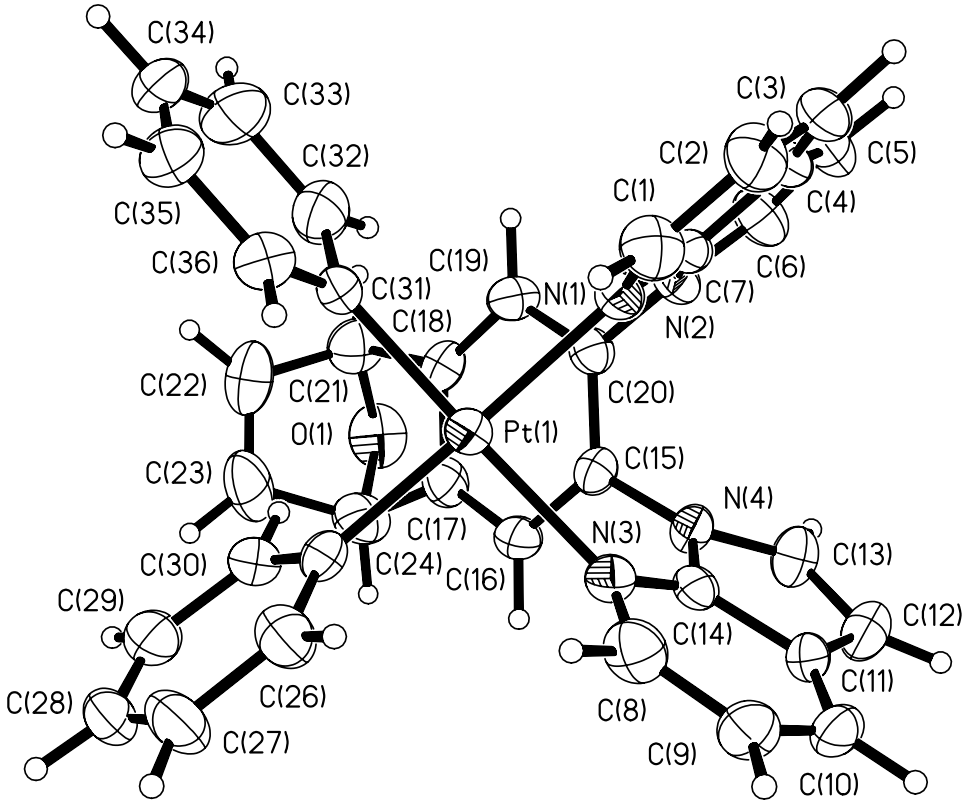

Table 1. Crystal data and structure refinement for compound **9a**.

Identification code	**9a**	
Empirical formula	C36 H26 N4 O Pt	
Formula weight	725.70	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.6466(3) Å	α= 90°.
	b = 9.7584(2) Å	β= 104.8460(10)°.
	c = 17.6630(3) Å	γ = 90°.
Volume	2773.47(9) $Å^3$	
Z	4	
Density (calculated)	1.738 Mg/m^3	
Absorption coefficient	5.097 mm^{-1}	
F(000)	1424	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.39 to 27.18°.	
Index ranges	-17<=h<=21, -9<=k<=12, -22<=l<=22	
Reflections collected	16310	
Independent reflections	6130 [R(int) = 0.0343]	
Completeness to theta = 27.18°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6297 and 0.4288	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6130 / 0 / 379	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0321, wR2 = 0.0736	
R indices (all data)	R1 = 0.0469, wR2 = 0.0794	
Largest diff. peak and hole	2.297 and -0.751 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **9a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3251(2)	8280(4)	-2591(2)	53(1)
Pt(1)	2909(1)	9415(1)	963(1)	28(1)
N(1)	1737(2)	10424(3)	757(2)	31(1)
N(2)	1424(2)	11029(4)	-620(2)	32(1)
N(3)	3484(2)	11394(4)	1138(2)	30(1)
N(4)	3021(2)	12195(4)	-185(2)	30(1)
C(1)	1426(3)	10533(5)	1392(3)	42(1)
C(2)	691(3)	11192(5)	1386(3)	45(1)
C(3)	218(3)	11762(5)	715(3)	40(1)
C(4)	504(3)	11681(5)	51(3)	33(1)
C(5)	214(3)	12136(5)	-736(3)	42(1)
C(6)	778(3)	11730(5)	-1126(3)	43(1)
C(7)	1269(3)	10999(4)	106(2)	28(1)
C(8)	3824(3)	11832(5)	1872(3)	42(1)
C(9)	4027(3)	13182(5)	2066(3)	40(1)
C(10)	3878(3)	14172(5)	1506(3)	37(1)
C(11)	3537(3)	13776(5)	739(3)	32(1)
C(12)	3264(3)	14445(5)	6(3)	42(1)
C(13)	2960(3)	13485(5)	-538(3)	40(1)
C(14)	3367(2)	12368(4)	595(2)	28(1)
C(15)	2884(3)	10960(4)	-632(2)	29(1)
C(16)	3542(3)	10394(4)	-890(3)	34(1)
C(17)	3364(3)	9333(5)	-1404(3)	36(1)
C(18)	2561(3)	8806(5)	-1663(3)	36(1)
C(19)	1915(3)	9334(5)	-1394(3)	36(1)
C(20)	2090(2)	10424(4)	-870(2)	29(1)
C(21)	2645(3)	7652(6)	-2241(3)	47(1)
C(22)	3155(4)	6578(6)	-1761(3)	58(2)
C(23)	3918(4)	7053(6)	-1514(3)	59(2)
C(24)	3874(3)	8487(6)	-1848(3)	50(1)
C(25)	4002(3)	8419(4)	1211(3)	32(1)

C(26)	4512(3)	8384(5)	1953(3)	43(1)
C(27)	5254(3)	7641(6)	2132(3)	52(1)
C(28)	5471(3)	6869(6)	1571(3)	50(1)
C(29)	4975(3)	6904(5)	817(3)	51(1)
C(30)	4249(3)	7675(5)	647(3)	42(1)
C(31)	2337(3)	7589(5)	901(3)	32(1)
C(32)	1883(3)	7029(5)	208(3)	49(1)
C(33)	1467(4)	5768(6)	167(4)	60(2)
C(34)	1507(3)	5065(6)	844(4)	57(2)
C(35)	1932(3)	5586(5)	1537(4)	53(1)
C(36)	2342(3)	6842(5)	1562(3)	45(1)

Table 3. Bond lengths [Å] and angles [°] for compound **9a**.

O(1)-C(21)	1.446(6)	C(4)-C(5)	1.420(6)
O(1)-C(24)	1.463(6)	C(5)-C(6)	1.358(7)
Pt(1)-C(25)	2.009(4)	C(5)-H(5A)	0.9500
Pt(1)-C(31)	2.011(4)	C(6)-H(6A)	0.9500
Pt(1)-N(1)	2.132(3)	C(8)-C(9)	1.382(7)
Pt(1)-N(3)	2.143(4)	C(8)-H(8A)	0.9500
N(1)-C(7)	1.337(5)	C(9)-C(10)	1.359(7)
N(1)-C(1)	1.355(6)	C(9)-H(9A)	0.9500
N(2)-C(7)	1.372(5)	C(10)-C(11)	1.384(6)
N(2)-C(6)	1.390(5)	C(10)-H(10A)	0.9500
N(2)-C(20)	1.422(5)	C(11)-C(14)	1.413(6)
N(3)-C(14)	1.328(5)	C(11)-C(12)	1.416(6)
N(3)-C(8)	1.344(5)	C(12)-C(13)	1.344(6)
N(4)-C(14)	1.360(5)	C(12)-H(12A)	0.9500
N(4)-C(13)	1.398(6)	C(13)-H(13A)	0.9500
N(4)-C(15)	1.427(5)	C(15)-C(20)	1.383(6)
C(1)-C(2)	1.380(7)	C(15)-C(16)	1.403(6)
C(1)-H(1A)	0.9500	C(16)-C(17)	1.359(6)
C(2)-C(3)	1.363(7)	C(16)-H(16A)	0.9500
C(2)-H(2A)	0.9500	C(17)-C(18)	1.396(6)
C(3)-C(4)	1.377(6)	C(17)-C(24)	1.536(7)
C(3)-H(3A)	0.9500	C(18)-C(19)	1.381(7)
C(4)-C(7)	1.417(6)	C(18)-C(21)	1.551(7)

C(19)-C(20)	1.390(6)	C(25)-Pt(1)-N(3)	93.35(15)
C(19)-H(19A)	0.9500	C(31)-Pt(1)-N(3)	174.14(16)
C(21)-C(22)	1.473(7)	N(1)-Pt(1)-N(3)	87.90(13)
C(21)-H(21A)	1.0000	C(7)-N(1)-C(1)	114.7(4)
C(22)-C(23)	1.317(8)	C(7)-N(1)-Pt(1)	130.3(3)
C(22)-H(22A)	0.9500	C(1)-N(1)-Pt(1)	115.0(3)
C(23)-C(24)	1.513(8)	C(7)-N(2)-C(6)	108.2(4)
C(23)-H(23A)	0.9500	C(7)-N(2)-C(20)	129.0(4)
C(24)-H(24A)	1.0000	C(6)-N(2)-C(20)	122.7(4)
C(25)-C(26)	1.367(6)	C(14)-N(3)-C(8)	114.6(4)
C(25)-C(30)	1.378(7)	C(14)-N(3)-Pt(1)	124.3(3)
C(26)-C(27)	1.396(7)	C(8)-N(3)-Pt(1)	119.2(3)
C(26)-H(26A)	0.9500	C(14)-N(4)-C(13)	107.7(3)
C(27)-C(28)	1.366(8)	C(14)-N(4)-C(15)	129.2(4)
C(27)-H(27A)	0.9500	C(13)-N(4)-C(15)	122.0(3)
C(28)-C(29)	1.376(7)	N(1)-C(1)-C(2)	123.8(5)
C(28)-H(28A)	0.9500	N(1)-C(1)-H(1A)	118.1
C(29)-C(30)	1.390(6)	C(2)-C(1)-H(1A)	118.1
C(29)-H(29A)	0.9500	C(3)-C(2)-C(1)	120.7(5)
C(30)-H(30A)	0.9500	C(3)-C(2)-H(2A)	119.6
C(31)-C(36)	1.374(7)	C(1)-C(2)-H(2A)	119.6
C(31)-C(32)	1.377(6)	C(2)-C(3)-C(4)	117.9(4)
C(32)-C(33)	1.404(7)	C(2)-C(3)-H(3A)	121.0
C(32)-H(32A)	0.9500	C(4)-C(3)-H(3A)	121.0
C(33)-C(34)	1.366(9)	C(3)-C(4)-C(7)	118.0(4)
C(33)-H(33A)	0.9500	C(3)-C(4)-C(5)	135.3(4)
C(34)-C(35)	1.346(8)	C(7)-C(4)-C(5)	106.8(4)
C(34)-H(34A)	0.9500	C(6)-C(5)-C(4)	107.4(4)
C(35)-C(36)	1.398(7)	C(6)-C(5)-H(5A)	126.3
C(35)-H(35A)	0.9500	C(4)-C(5)-H(5A)	126.3
C(36)-H(36A)	0.9500	C(5)-C(6)-N(2)	109.8(4)
		C(5)-C(6)-H(6A)	125.1
C(21)-O(1)-C(24)	95.0(3)	N(2)-C(6)-H(6A)	125.1
C(25)-Pt(1)-C(31)	88.49(16)	N(1)-C(7)-N(2)	127.3(4)
C(25)-Pt(1)-N(1)	176.82(15)	N(1)-C(7)-C(4)	124.9(4)
C(31)-Pt(1)-N(1)	89.98(15)	N(2)-C(7)-C(4)	107.9(4)

N(3)-C(8)-C(9)	123.9(4)	C(15)-C(20)-C(19)	120.8(4)
N(3)-C(8)-H(8A)	118.0	C(15)-C(20)-N(2)	120.5(4)
C(9)-C(8)-H(8A)	118.0	C(19)-C(20)-N(2)	118.6(4)
C(10)-C(9)-C(8)	120.6(4)	O(1)-C(21)-C(22)	100.7(4)
C(10)-C(9)-H(9A)	119.7	O(1)-C(21)-C(18)	99.4(4)
C(8)-C(9)-H(9A)	119.7	C(22)-C(21)-C(18)	105.9(4)
C(9)-C(10)-C(11)	117.9(4)	O(1)-C(21)-H(21A)	116.1
C(9)-C(10)-H(10A)	121.1	C(22)-C(21)-H(21A)	116.1
C(11)-C(10)-H(10A)	121.1	C(18)-C(21)-H(21A)	116.1
C(10)-C(11)-C(14)	117.4(4)	C(23)-C(22)-C(21)	107.7(5)
C(10)-C(11)-C(12)	136.2(4)	C(23)-C(22)-H(22A)	126.1
C(14)-C(11)-C(12)	106.4(4)	C(21)-C(22)-H(22A)	126.1
C(13)-C(12)-C(11)	107.8(4)	C(22)-C(23)-C(24)	104.5(5)
C(13)-C(12)-H(12A)	126.1	C(22)-C(23)-H(23A)	127.8
C(11)-C(12)-H(12A)	126.1	C(24)-C(23)-H(23A)	127.8
C(12)-C(13)-N(4)	109.7(4)	O(1)-C(24)-C(23)	100.0(4)
C(12)-C(13)-H(13A)	125.1	O(1)-C(24)-C(17)	100.1(4)
N(4)-C(13)-H(13A)	125.1	C(23)-C(24)-C(17)	106.0(4)
N(3)-C(14)-N(4)	126.0(4)	O(1)-C(24)-H(24A)	116.1
N(3)-C(14)-C(11)	125.5(4)	C(23)-C(24)-H(24A)	116.1
N(4)-C(14)-C(11)	108.4(4)	C(17)-C(24)-H(24A)	116.1
C(20)-C(15)-C(16)	121.1(4)	C(26)-C(25)-C(30)	117.0(4)
C(20)-C(15)-N(4)	119.5(4)	C(26)-C(25)-Pt(1)	121.7(4)
C(16)-C(15)-N(4)	119.0(4)	C(30)-C(25)-Pt(1)	121.2(3)
C(17)-C(16)-C(15)	117.6(4)	C(25)-C(26)-C(27)	121.7(5)
C(17)-C(16)-H(16A)	121.2	C(25)-C(26)-H(26A)	119.2
C(15)-C(16)-H(16A)	121.2	C(27)-C(26)-H(26A)	119.2
C(16)-C(17)-C(18)	121.8(4)	C(28)-C(27)-C(26)	120.4(5)
C(16)-C(17)-C(24)	134.2(4)	C(28)-C(27)-H(27A)	119.8
C(18)-C(17)-C(24)	104.0(4)	C(26)-C(27)-H(27A)	119.8
C(19)-C(18)-C(17)	120.9(4)	C(27)-C(28)-C(29)	118.9(5)
C(19)-C(18)-C(21)	135.0(4)	C(27)-C(28)-H(28A)	120.6
C(17)-C(18)-C(21)	104.1(4)	C(29)-C(28)-H(28A)	120.6
C(18)-C(19)-C(20)	117.8(4)	C(28)-C(29)-C(30)	119.7(5)
C(18)-C(19)-H(19A)	121.1	C(28)-C(29)-H(29A)	120.1
C(20)-C(19)-H(19A)	121.1	C(30)-C(29)-H(29A)	120.1

C(25)-C(30)-C(29)	122.2(5)	C(32)-C(33)-H(33A)	120.6
C(25)-C(30)-H(30A)	118.9	C(35)-C(34)-C(33)	120.2(5)
C(29)-C(30)-H(30A)	118.9	C(35)-C(34)-H(34A)	119.9
C(36)-C(31)-C(32)	115.3(4)	C(33)-C(34)-H(34A)	119.9
C(36)-C(31)-Pt(1)	121.6(3)	C(34)-C(35)-C(36)	119.9(6)
C(32)-C(31)-Pt(1)	123.0(4)	C(34)-C(35)-H(35A)	120.1
C(31)-C(32)-C(33)	123.0(5)	C(36)-C(35)-H(35A)	120.1
C(31)-C(32)-H(32A)	118.5	C(31)-C(36)-C(35)	122.8(5)
C(33)-C(32)-H(32A)	118.5	C(31)-C(36)-H(36A)	118.6
C(34)-C(33)-C(32)	118.8(5)	C(35)-C(36)-H(36A)	118.6
C(34)-C(33)-H(33A)	120.6		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **9a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	67(2)	59(2)	38(2)	-5(2)	22(2)	6(2)
Pt(1)	24(1)	27(1)	33(1)	2(1)	6(1)	1(1)
N(1)	27(2)	29(2)	38(2)	-4(2)	12(2)	0(2)
N(2)	29(2)	37(2)	33(2)	-4(2)	12(2)	6(2)
N(3)	27(2)	30(2)	35(2)	1(2)	9(2)	-1(2)
N(4)	33(2)	23(2)	36(2)	-1(2)	10(2)	-1(2)
C(1)	45(3)	46(3)	40(3)	-1(2)	17(2)	1(2)
C(2)	50(3)	45(3)	48(3)	-3(2)	28(2)	4(2)
C(3)	31(2)	38(3)	55(3)	-7(2)	20(2)	1(2)
C(4)	24(2)	31(3)	44(3)	-6(2)	10(2)	0(2)
C(5)	33(2)	46(3)	47(3)	-3(2)	9(2)	12(2)
C(6)	37(3)	53(3)	38(2)	4(2)	4(2)	12(2)
C(7)	24(2)	27(2)	34(2)	-6(2)	9(2)	-2(2)
C(8)	43(3)	48(3)	33(2)	3(2)	3(2)	4(2)
C(9)	39(3)	45(3)	33(2)	-13(2)	3(2)	-1(2)
C(10)	35(2)	32(3)	48(3)	-14(2)	14(2)	-6(2)
C(11)	28(2)	26(2)	42(2)	-6(2)	11(2)	2(2)
C(12)	51(3)	29(3)	47(3)	-4(2)	17(2)	-4(2)
C(13)	52(3)	29(3)	40(3)	3(2)	13(2)	2(2)

C(14)	21(2)	30(2)	35(2)	-5(2)	11(2)	2(2)
C(15)	34(2)	25(2)	30(2)	-2(2)	11(2)	-1(2)
C(16)	27(2)	34(3)	41(2)	-2(2)	11(2)	-2(2)
C(17)	36(2)	36(3)	40(2)	-3(2)	16(2)	5(2)
C(18)	44(3)	27(2)	38(2)	-4(2)	11(2)	-3(2)
C(19)	32(2)	38(3)	38(2)	-3(2)	8(2)	-6(2)
C(20)	30(2)	30(3)	30(2)	-1(2)	10(2)	2(2)
C(21)	53(3)	49(3)	39(3)	-12(2)	10(2)	-5(3)
C(22)	86(5)	36(3)	53(3)	-2(3)	20(3)	10(3)
C(23)	66(4)	50(4)	57(3)	-14(3)	7(3)	25(3)
C(24)	38(3)	55(4)	64(3)	-17(3)	24(2)	2(3)
C(25)	33(2)	24(2)	40(2)	8(2)	10(2)	-4(2)
C(26)	38(3)	46(3)	47(3)	7(2)	13(2)	6(2)
C(27)	34(3)	59(4)	58(3)	14(3)	4(2)	10(3)
C(28)	30(3)	42(3)	77(4)	16(3)	12(2)	6(2)
C(29)	36(3)	40(3)	77(4)	-6(3)	18(3)	0(2)
C(30)	29(2)	36(3)	59(3)	3(2)	7(2)	-1(2)
C(31)	26(2)	26(2)	44(3)	3(2)	11(2)	4(2)
C(32)	50(3)	39(3)	55(3)	-3(3)	7(2)	1(2)
C(33)	53(4)	51(4)	71(4)	-17(3)	6(3)	-13(3)
C(34)	40(3)	28(3)	105(5)	-4(3)	25(3)	-6(2)
C(35)	46(3)	43(3)	76(4)	11(3)	26(3)	-3(3)
C(36)	37(3)	39(3)	57(3)	2(3)	8(2)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound 9a.

	x	y	z	U(eq)
H(1A)	1732	10131	1869	51
H(2A)	513	11250	1855	53
H(3A)	-294	12202	705	48
H(5A)	-283	12634	-949	51
H(6A)	736	11899	-1665	52
H(8A)	3930	11173	2282	51

H(9A)	4274	13421	2596	48
H(10A)	4004	15105	1637	45
H(12A)	3290	15402	-84	50
H(13A)	2739	13658	-1080	48
H(16A)	4091	10740	-711	40
H(19A)	1370	8966	-1562	43
H(21A)	2118	7340	-2613	57
H(22A)	2967	5699	-1650	70
H(23A)	4390	6598	-1197	71
H(24A)	4413	8897	-1884	60
H(26A)	4357	8877	2357	52
H(27A)	5609	7674	2646	62
H(28A)	5958	6317	1699	60
H(29A)	5128	6402	415	61
H(30A)	3912	7690	124	50
H(32A)	1849	7518	-264	59
H(33A)	1164	5410	-324	72
H(34A)	1233	4207	827	68
H(35A)	1954	5100	2008	63
H(36A)	2637	7194	2057	54