

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

Identification code	JF139A	
Empirical formula	C ₁₆ H ₂₃ Cl N ₂ Pt	
Formula weight	473.90	
Temperature	160(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /a	
Unit cell dimensions	a = 14.299(8) Å	α = 90°.
	b = 11.748(4) Å	β = 110.66(8)°.
	c = 10.478(6) Å	γ = 90°.
	1646.9(14) Å ³	
Volume		
Z	4	
Density (calculated)	1.911 Mg/m ³	
Absorption coefficient	8.674 mm ⁻¹	
F(000)	912	
Crystal size	0.30 x 0.25 x 0.20 mm ³	
Theta range for data collection	2.31 to 25.05°.	
Index ranges	0 ≤ h ≤ 17, -5 ≤ k ≤ 13, -12 ≤ l ≤ 11	
Reflections collected	3085	
Independent reflections	2894 [R(int) = 0.0157]	
Completeness to theta = 25.05°	99.3 %	
Max. and min. transmission	0.2758 and 0.1806	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2894 / 0 / 188	
Goodness-of-fit on F ²	1.028	
Final R indices [I > 2σ(I)]	R1 = 0.0289, wR2 = 0.0693	
R indices (all data)	R1 = 0.0442, wR2 = 0.0740	
Extinction coefficient	0.0062(3)	
Largest diff. peak and hole	1.678 and -2.092 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	2404(1)	1039(1)	2545(1)	11(1)
Cl(2)	3802(1)	2315(2)	2901(2)	30(1)
N(3)	1771(4)	1690(4)	3915(5)	15(1)
N(4)	2566(4)	-57(4)	1057(5)	14(1)
C(5)	1832(5)	-755(5)	583(6)	13(1)
C(6)	1050(5)	-723(5)	1147(6)	12(1)
C(7)	186(4)	-1372(5)	839(6)	15(1)
C(8)	-468(5)	-1192(5)	1534(7)	18(1)
C(9)	-279(4)	-334(5)	2525(6)	16(1)
C(10)	581(4)	316(5)	2837(6)	16(1)
C(11)	1241(4)	102(5)	2164(6)	10(1)
C(12)	943(4)	1222(5)	3822(6)	14(1)
C(13)	3434(5)	-88(5)	558(7)	18(1)
C(14)	3334(5)	-1038(6)	-465(7)	25(2)
C(15)	4365(5)	-279(6)	1779(8)	25(2)
C(16)	3443(5)	1061(5)	-149(7)	24(2)
C(17)	2220(5)	2603(6)	4996(6)	21(2)
C(18)	3253(5)	2202(6)	5867(7)	26(2)
C(19)	2236(6)	3722(6)	4252(7)	26(2)
C(20)	1587(6)	2786(7)	5890(7)	32(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$].

Pt(1)-C(11)	1.915(6)
Pt(1)-N(3)	2.093(5)
Pt(1)-N(4)	2.097(5)
Pt(1)-Cl(2)	2.4192(19)
N(3)-C(12)	1.277(8)
N(3)-C(17)	1.528(8)
N(4)-C(5)	1.285(8)
N(4)-C(13)	1.508(7)
C(5)-C(6)	1.438(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.390(9)
C(6)-C(11)	1.394(8)
C(7)-C(8)	1.388(9)
C(7)-H(7)	0.9500
C(8)-C(9)	1.403(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.385(8)
C(9)-H(9)	0.9500
C(10)-C(11)	1.387(8)
C(10)-C(12)	1.445(9)
C(12)-H(12)	0.9500
C(13)-C(15)	1.502(9)
C(13)-C(14)	1.519(9)
C(13)-C(16)	1.543(8)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.512(9)
C(17)-C(20)	1.529(9)
C(17)-C(19)	1.533(10)

C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

C(11)-Pt(1)-N(3)	78.4(2)
C(11)-Pt(1)-N(4)	78.9(2)
N(3)-Pt(1)-N(4)	157.2(2)
C(11)-Pt(1)-Cl(2)	175.89(17)
N(3)-Pt(1)-Cl(2)	101.64(15)
N(4)-Pt(1)-Cl(2)	101.15(15)
C(12)-N(3)-C(17)	119.6(5)
C(12)-N(3)-Pt(1)	113.8(4)
C(17)-N(3)-Pt(1)	126.5(4)
C(5)-N(4)-C(13)	120.6(5)
C(5)-N(4)-Pt(1)	113.0(4)
C(13)-N(4)-Pt(1)	126.4(4)
N(4)-C(5)-C(6)	118.1(6)
N(4)-C(5)-H(5)	120.9
C(6)-C(5)-H(5)	120.9
C(7)-C(6)-C(11)	118.5(6)
C(7)-C(6)-C(5)	130.4(6)
C(11)-C(6)-C(5)	111.2(5)
C(8)-C(7)-C(6)	120.2(6)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	120.5(6)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(10)-C(9)-C(8)	119.6(6)
C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(9)-C(10)-C(11)	119.2(6)

C(9)-C(10)-C(12)	129.8(6)
C(11)-C(10)-C(12)	111.1(5)
C(10)-C(11)-C(6)	122.0(5)
C(10)-C(11)-Pt(1)	119.1(5)
C(6)-C(11)-Pt(1)	118.7(4)
N(3)-C(12)-C(10)	117.4(5)
N(3)-C(12)-H(12)	121.3
C(10)-C(12)-H(12)	121.3
C(15)-C(13)-N(4)	107.5(5)
C(15)-C(13)-C(14)	109.0(6)
N(4)-C(13)-C(14)	112.3(5)
C(15)-C(13)-C(16)	112.5(6)
N(4)-C(13)-C(16)	107.0(5)
C(14)-C(13)-C(16)	108.6(5)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-N(3)	107.1(5)
C(18)-C(17)-C(20)	109.7(6)
N(3)-C(17)-C(20)	111.6(5)
C(18)-C(17)-C(19)	112.8(6)
N(3)-C(17)-C(19)	107.6(5)
C(20)-C(17)-C(19)	108.0(6)

C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

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

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pt(1)	14(1)	11(1)	10(1)	-1(1)	5(1)	-1(1)
Cl(2)	28(1)	28(1)	40(1)	-15(1)	19(1)	-15(1)
N(3)	24(3)	14(3)	7(3)	-3(2)	4(2)	2(2)
N(4)	19(3)	15(3)	13(3)	6(2)	10(2)	7(2)
C(5)	20(3)	9(3)	10(3)	3(2)	5(3)	0(2)
C(6)	22(3)	5(3)	9(3)	3(2)	7(3)	5(2)
C(7)	20(3)	11(3)	13(3)	2(3)	4(3)	0(2)
C(8)	16(3)	17(3)	20(4)	4(3)	4(3)	-1(3)
C(9)	15(3)	21(4)	14(3)	4(3)	6(3)	-3(3)
C(10)	17(3)	18(3)	13(3)	7(3)	6(3)	2(3)
C(11)	11(3)	13(3)	4(3)	4(2)	-2(2)	1(2)
C(12)	17(3)	19(3)	7(3)	1(3)	4(3)	4(3)
C(13)	24(3)	14(3)	22(4)	-2(3)	18(3)	1(3)
C(14)	35(4)	25(4)	23(4)	-3(3)	22(3)	0(3)
C(15)	24(3)	22(4)	35(4)	3(3)	17(3)	6(3)
C(16)	36(4)	19(4)	28(4)	11(3)	25(3)	5(3)
C(17)	31(4)	20(4)	11(3)	-10(3)	8(3)	-3(3)
C(18)	33(4)	28(4)	11(3)	-4(3)	0(3)	-1(3)
C(19)	41(4)	14(4)	22(4)	-9(3)	9(4)	-6(3)
C(20)	43(4)	39(5)	18(4)	-17(3)	18(4)	-9(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(5)	1808	-1277	-121	16
H(7)	41	-1940	152	18
H(8)	-1048	-1654	1337	22
H(9)	-738	-200	2979	20
H(12)	580	1460	4379	17
H(14A)	3917	-1034	-751	37
H(14B)	2725	-921	-1263	37
H(14C)	3294	-1772	-42	37
H(15A)	4436	332	2443	38
H(15B)	4948	-280	1492	38
H(15C)	4320	-1013	2197	38
H(16A)	3501	1683	498	36
H(16B)	2822	1147	-933	36
H(16C)	4014	1083	-460	36
H(18A)	3199	1501	6343	39
H(18B)	3584	2791	6537	39
H(18C)	3647	2054	5285	39
H(19A)	2644	3627	3679	40
H(19B)	2522	4326	4922	40
H(19C)	1553	3929	3680	40
H(20A)	908	3006	5316	47
H(20B)	1885	3391	6554	47
H(20C)	1564	2079	6374	47

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

Identification code	JF139C	
Empirical formula	C ₂₀ H ₁₅ Cl N ₂ Pt	
Formula weight	513.88	
Temperature	160(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	I 2/a	
Unit cell dimensions	a = 11.251(4) Å	$\alpha = 90^\circ$.
	b = 15.329(8) Å	$\beta = 98.35(5)^\circ$.
	c = 18.937(10) Å	$\gamma = 90^\circ$.
	3231(3) Å ³	
Volume	8	
Z	2.113 Mg/m ³	
Density (calculated)	8.852 mm ⁻¹	
Absorption coefficient	1952	
F(000)	0.40 x 0.40 x 0.30 mm ³	
Crystal size	1.72 to 24.98°.	
Theta range for data collection	-13 ≤ h ≤ 13, -3 ≤ k ≤ 18, -10 ≤ l ≤ 22	
Index ranges	2989	
Reflections collected	2842 [R(int) = 0.0110]	
Independent reflections	99.7 %	
Completeness to theta = 24.98°	0.1765 and 0.1258	
Max. and min. transmission	Full-matrix least-squares on F ²	
Refinement method	2842 / 0 / 218	
Data / restraints / parameters	0.962	
Goodness-of-fit on F ²	R1 = 0.0290, wR2 = 0.0731	
Final R indices [I > 2σ(I)]	R1 = 0.0421, wR2 = 0.0784	
R indices (all data)	0.00090(6)	
Extinction coefficient	1.370 and -2.415 e.Å ⁻³	
Largest diff. peak and hole		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	6247(1)	859(1)	3387(1)	6(1)
Cl(2)	5482(1)	2293(1)	3106(1)	13(1)
N(3)	4936(4)	76(3)	2837(3)	9(1)
N(4)	7851(4)	1176(3)	4005(3)	8(1)
C(5)	8445(5)	503(4)	4282(3)	11(1)
C(6)	7915(5)	-349(4)	4140(3)	10(1)
C(7)	8336(6)	-1174(4)	4358(3)	13(1)
C(8)	7632(6)	-1904(4)	4127(4)	16(2)
C(9)	6540(6)	-1828(4)	3687(4)	12(1)
C(10)	6113(5)	-1006(4)	3473(3)	9(1)
C(11)	6819(6)	-270(4)	3693(3)	9(1)
C(12)	5095(6)	-754(4)	2977(3)	11(1)
C(13)	8392(5)	2023(4)	4149(3)	9(1)
C(14)	8882(5)	2247(4)	4846(3)	10(1)
C(15)	9431(5)	3043(4)	4973(4)	14(1)
C(16)	9490(6)	3625(5)	4414(4)	20(2)
C(17)	8985(6)	3398(4)	3723(4)	17(2)
C(18)	8419(5)	2610(4)	3593(3)	12(1)
C(19)	3998(5)	308(4)	2267(3)	8(1)
C(20)	3877(6)	-174(5)	1639(4)	14(1)
C(22)	2180(6)	710(5)	1184(4)	19(2)
C(23)	2311(6)	1185(4)	1818(4)	17(2)
C(24)	3231(5)	998(4)	2356(4)	11(1)
C(21)	2959(6)	34(5)	1094(4)	21(2)

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

Pt(1)-C(11)	1.908(6)
Pt(1)-N(4)	2.061(5)
Pt(1)-N(3)	2.064(5)
Pt(1)-Cl(2)	2.3914(18)
N(3)-C(12)	1.307(8)
N(3)-C(19)	1.440(8)
N(4)-C(5)	1.298(8)
N(4)-C(13)	1.442(8)
C(5)-C(6)	1.444(9)
C(5)-H(5)	0.9500
C(6)-C(7)	1.392(9)
C(6)-C(11)	1.396(9)
C(7)-C(8)	1.404(9)
C(7)-H(7)	0.9500
C(8)-C(9)	1.385(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.388(9)
C(9)-H(9)	0.9500
C(10)-C(11)	1.407(9)
C(10)-C(12)	1.425(9)
C(12)-H(12)	0.9500
C(13)-C(18)	1.388(9)
C(13)-C(14)	1.398(9)
C(14)-C(15)	1.373(9)
C(14)-H(14)	0.9500
C(15)-C(16)	1.394(10)
C(15)-H(15)	0.9500
C(16)-C(17)	1.393(10)
C(16)-H(16)	0.9500
C(17)-C(18)	1.372(9)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.390(9)
C(19)-C(20)	1.391(9)
C(20)-C(21)	1.387(9)
C(20)-H(20)	0.9500

C(22)-C(21)	1.383(10)
C(22)-C(23)	1.393(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.374(9)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(21)-H(21)	0.9500
C(11)-Pt(1)-N(4)	79.2(2)
C(11)-Pt(1)-N(3)	79.1(2)
N(4)-Pt(1)-N(3)	157.9(2)
C(11)-Pt(1)-Cl(2)	174.93(19)
N(4)-Pt(1)-Cl(2)	99.61(15)
N(3)-Pt(1)-Cl(2)	102.37(15)
C(12)-N(3)-C(19)	117.2(5)
C(12)-N(3)-Pt(1)	113.4(4)
C(19)-N(3)-Pt(1)	128.8(4)
C(5)-N(4)-C(13)	117.4(5)
C(5)-N(4)-Pt(1)	113.5(4)
C(13)-N(4)-Pt(1)	129.1(4)
N(4)-C(5)-C(6)	118.0(6)
N(4)-C(5)-H(5)	121.0
C(6)-C(5)-H(5)	121.0
C(7)-C(6)-C(11)	119.4(6)
C(7)-C(6)-C(5)	130.8(6)
C(11)-C(6)-C(5)	109.8(5)
C(6)-C(7)-C(8)	118.7(6)
C(6)-C(7)-H(7)	120.7
C(8)-C(7)-H(7)	120.7
C(9)-C(8)-C(7)	122.1(6)
C(9)-C(8)-H(8)	119.0
C(7)-C(8)-H(8)	119.0
C(8)-C(9)-C(10)	119.4(6)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3
C(9)-C(10)-C(11)	119.0(6)
C(9)-C(10)-C(12)	130.5(6)
C(11)-C(10)-C(12)	110.0(5)

C(6)-C(11)-C(10)	121.4(6)
C(6)-C(11)-Pt(1)	119.5(5)
C(10)-C(11)-Pt(1)	119.1(5)
N(3)-C(12)-C(10)	118.1(6)
N(3)-C(12)-H(12)	120.9
C(10)-C(12)-H(12)	120.9
C(18)-C(13)-C(14)	120.5(6)
C(18)-C(13)-N(4)	119.7(6)
C(14)-C(13)-N(4)	119.8(6)
C(15)-C(14)-C(13)	119.4(6)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(14)-C(15)-C(16)	120.4(6)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	119.7(6)
C(17)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2
C(18)-C(17)-C(16)	120.3(6)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(17)-C(18)-C(13)	119.8(6)
C(17)-C(18)-H(18)	120.1
C(13)-C(18)-H(18)	120.1
C(24)-C(19)-C(20)	121.5(6)
C(24)-C(19)-N(3)	119.8(6)
C(20)-C(19)-N(3)	118.7(5)
C(21)-C(20)-C(19)	118.9(6)
C(21)-C(20)-H(20)	120.5
C(19)-C(20)-H(20)	120.5
C(21)-C(22)-C(23)	120.5(6)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	120.3(6)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(23)-C(24)-C(19)	118.9(6)
C(23)-C(24)-H(24)	120.6

C(19)-C(24)-H(24)	120.6
C(22)-C(21)-C(20)	119.8(7)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1

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

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pt(1)	6(1)	6(1)	4(1)	0(1)	0(1)	1(1)
Cl(2)	14(1)	8(1)	17(1)	3(1)	0(1)	2(1)
N(3)	4(2)	14(3)	8(3)	1(2)	1(2)	3(2)
N(4)	10(3)	9(3)	5(3)	-5(2)	2(2)	-2(2)
C(5)	10(3)	17(3)	6(3)	-2(3)	2(2)	-2(3)
C(6)	9(3)	11(3)	9(3)	0(3)	3(2)	1(2)
C(7)	14(3)	17(3)	7(3)	6(3)	-3(3)	4(3)
C(8)	23(4)	10(3)	15(4)	7(3)	0(3)	6(3)
C(9)	16(3)	6(3)	17(4)	1(3)	10(3)	-5(2)
C(10)	15(3)	8(3)	5(3)	2(3)	3(3)	2(2)
C(11)	14(3)	6(3)	7(3)	2(3)	2(3)	5(2)
C(12)	8(3)	13(3)	12(3)	1(3)	3(2)	-3(2)
C(13)	3(3)	11(3)	11(3)	-4(3)	1(2)	-1(2)
C(14)	12(3)	9(3)	7(3)	1(3)	-2(2)	0(2)
C(15)	9(3)	17(3)	15(4)	-6(3)	0(3)	-3(3)
C(16)	20(3)	11(3)	27(4)	-3(3)	1(3)	-4(3)
C(17)	12(3)	18(4)	22(4)	8(3)	9(3)	4(3)
C(18)	12(3)	16(3)	6(3)	0(3)	1(2)	-2(3)
C(19)	5(3)	10(3)	10(3)	4(3)	1(2)	-3(2)
C(20)	14(3)	15(4)	14(4)	-2(3)	3(3)	0(3)
C(22)	15(3)	23(4)	15(4)	13(3)	-8(3)	-5(3)
C(23)	12(3)	14(3)	24(4)	8(3)	1(3)	-5(3)
C(24)	9(3)	13(3)	13(3)	-1(3)	6(3)	-1(2)
C(21)	27(4)	26(4)	8(4)	2(3)	-3(3)	-6(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(5)	9205	569	4569	13
H(7)	9084	-1242	4657	16
H(8)	7913	-2469	4276	19
H(9)	6088	-2334	3533	15
H(12)	4549	-1178	2754	13
H(14)	8836	1852	5228	12
H(15)	9772	3198	5445	17
H(16)	9874	4175	4504	23
H(17)	9033	3791	3340	20
H(18)	8047	2466	3125	14
H(20)	4415	-639	1583	17
H(22)	1551	852	811	22
H(23)	1762	1641	1878	20
H(24)	3341	1334	2782	14
H(21)	2864	-286	660	25

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

Identification code	JF153A	
Empirical formula	C ₁₇ H ₂₅ F ₃ N ₂ O ₄ Pt S	
Formula weight	605.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.528(7) Å	α = 90°.
	b = 20.812(7) Å	β = 117.50(4)°.
	c = 11.141(6) Å	γ = 90°.
Volume	2165(2) Å ³	
Z	4	
Density (calculated)	1.858 Mg/m ³	
Absorption coefficient	6.626 mm ⁻¹	
F(000)	1176	
Crystal size	0.60 x 0.40 x 0.20 mm ³	
Theta range for data collection	2.18 to 24.97°.	
Index ranges	0 ≤ h ≤ 12, 0 ≤ k ≤ 24, -13 ≤ l ≤ 11	
Reflections collected	4125	
Independent reflections	3803 [R(int) = 0.0159]	
Completeness to theta = 24.97°	99.9 %	
Max. and min. transmission	0.3508 and 0.1092	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3803 / 2 / 268	
Goodness-of-fit on F ²	1.059	
Final R indices [I > 2σ(I)]	R1 = 0.0278, wR2 = 0.0678	
R indices (all data)	R1 = 0.0428, wR2 = 0.0734	
Extinction coefficient	0.0030(2)	
Largest diff. peak and hole	1.715 and -0.813 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	8963(1)	8463(1)	395(1)	31(1)
O(2)	7551(5)	7885(2)	917(4)	51(1)
N(3)	10988(5)	8204(2)	1911(4)	37(1)
N(4)	7413(5)	8918(2)	-1323(4)	36(1)
C(5)	7963(6)	9306(3)	-1859(5)	40(1)
C(6)	9507(6)	9366(3)	-1230(5)	35(1)
C(7)	10376(6)	9733(3)	-1588(5)	42(1)
C(8)	11854(6)	9699(3)	-819(6)	48(2)
C(9)	12487(6)	9302(3)	304(6)	45(1)
C(10)	11612(5)	8940(3)	675(5)	36(1)
C(11)	10145(6)	8972(2)	-84(5)	32(1)
C(12)	12014(6)	8498(3)	1797(5)	36(1)
C(13)	5819(6)	8824(3)	-1981(6)	41(1)
C(14)	5018(7)	9233(4)	-3262(7)	61(2)
C(15)	5314(7)	8998(4)	-941(7)	62(2)
C(16)	5558(7)	8123(3)	-2373(6)	52(2)
C(17)	11325(6)	7731(3)	3035(5)	44(1)
C(18)	10628(8)	7983(4)	3863(7)	70(2)
C(19)	10732(8)	7093(3)	2395(7)	65(2)
C(20)	12941(7)	7667(4)	3970(7)	70(2)
C(21)	7881(8)	5648(4)	-658(7)	60(2)
S(22)	6678(2)	6324(1)	-1168(2)	51(1)
O(23)	7056(10)	6673(3)	-2029(8)	126(3)
O(24)	7015(7)	6648(2)	76(6)	83(2)
O(25)	5318(5)	6026(3)	-1721(7)	104(2)
F(26)	9220(5)	5832(3)	28(7)	129(2)
F(27)	7741(8)	5302(3)	-1675(6)	133(2)
F(28)	7672(5)	5249(2)	149(5)	85(1)

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

Pt(1)-C(11)	1.889(5)
Pt(1)-N(4)	2.083(4)
Pt(1)-N(3)	2.089(5)
Pt(1)-O(2)	2.188(4)
O(2)-H(2A)	0.90(2)
O(2)-H(2B)	0.88(2)
N(3)-C(12)	1.298(7)
N(3)-C(17)	1.500(7)
N(4)-C(5)	1.290(7)
N(4)-C(13)	1.501(7)
C(5)-C(6)	1.448(7)
C(5)-H(5)	0.9300
C(6)-C(7)	1.384(7)
C(6)-C(11)	1.401(7)
C(7)-C(8)	1.389(8)
C(7)-H(7)	0.9300
C(8)-C(9)	1.386(8)
C(8)-H(8)	0.9300
C(9)-C(10)	1.393(7)
C(9)-H(9)	0.9300
C(10)-C(11)	1.378(7)
C(10)-C(12)	1.448(7)
C(12)-H(12)	0.9300
C(13)-C(16)	1.511(9)
C(13)-C(15)	1.525(8)
C(13)-C(14)	1.537(9)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(19)	1.501(9)

C(17)-C(18)	1.513(8)
C(17)-C(20)	1.536(8)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-F(27)	1.292(8)
C(21)-F(26)	1.312(8)
C(21)-F(28)	1.316(8)
C(21)-S(22)	1.800(7)
S(22)-O(23)	1.400(6)
S(22)-O(25)	1.415(6)
S(22)-O(24)	1.430(5)

C(11)-Pt(1)-N(4)	79.9(2)
C(11)-Pt(1)-N(3)	79.2(2)
N(4)-Pt(1)-N(3)	159.11(18)
C(11)-Pt(1)-O(2)	178.7(2)
N(4)-Pt(1)-O(2)	98.84(18)
N(3)-Pt(1)-O(2)	102.04(18)
Pt(1)-O(2)-H(2A)	117(4)
Pt(1)-O(2)-H(2B)	121(5)
H(2A)-O(2)-H(2B)	116(6)
C(12)-N(3)-C(17)	120.3(5)
C(12)-N(3)-Pt(1)	112.6(4)
C(17)-N(3)-Pt(1)	127.1(4)
C(5)-N(4)-C(13)	119.7(4)
C(5)-N(4)-Pt(1)	112.4(4)
C(13)-N(4)-Pt(1)	127.9(4)
N(4)-C(5)-C(6)	118.3(5)
N(4)-C(5)-H(5)	120.9
C(6)-C(5)-H(5)	120.9
C(7)-C(6)-C(11)	118.9(5)

C(7)-C(6)-C(5)	130.7(5)
C(11)-C(6)-C(5)	110.4(5)
C(6)-C(7)-C(8)	119.7(5)
C(6)-C(7)-H(7)	120.2
C(8)-C(7)-H(7)	120.2
C(9)-C(8)-C(7)	121.5(5)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	118.8(5)
C(8)-C(9)-H(9)	120.6
C(10)-C(9)-H(9)	120.6
C(11)-C(10)-C(9)	120.0(5)
C(11)-C(10)-C(12)	111.0(5)
C(9)-C(10)-C(12)	129.0(5)
C(10)-C(11)-C(6)	121.2(5)
C(10)-C(11)-Pt(1)	119.8(4)
C(6)-C(11)-Pt(1)	119.0(4)
N(3)-C(12)-C(10)	117.3(5)
N(3)-C(12)-H(12)	121.3
C(10)-C(12)-H(12)	121.3
N(4)-C(13)-C(16)	106.3(4)
N(4)-C(13)-C(15)	107.5(5)
C(16)-C(13)-C(15)	111.6(5)
N(4)-C(13)-C(14)	113.1(5)
C(16)-C(13)-C(14)	108.6(5)
C(15)-C(13)-C(14)	109.8(5)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(3)-C(17)-C(19)	107.3(4)
N(3)-C(17)-C(18)	106.7(5)
C(19)-C(17)-C(18)	112.6(6)
N(3)-C(17)-C(20)	112.6(5)
C(19)-C(17)-C(20)	109.4(6)
C(18)-C(17)-C(20)	108.3(5)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
F(27)-C(21)-F(26)	109.3(7)
F(27)-C(21)-F(28)	105.0(7)
F(26)-C(21)-F(28)	105.0(6)
F(27)-C(21)-S(22)	112.4(5)
F(26)-C(21)-S(22)	111.5(6)
F(28)-C(21)-S(22)	113.2(5)
O(23)-S(22)-O(25)	118.7(5)
O(23)-S(22)-O(24)	113.5(5)

O(25)-S(22)-O(24)	112.1(4)
O(23)-S(22)-C(21)	103.9(4)
O(25)-S(22)-C(21)	102.6(4)
O(24)-S(22)-C(21)	103.8(4)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Pt(1)	35(1)	33(1)	29(1)	-2(1)	18(1)	-2(1)
O(2)	71(3)	49(3)	49(2)	-9(2)	42(2)	-19(2)
N(3)	42(3)	44(3)	26(2)	-1(2)	15(2)	1(2)
N(4)	34(2)	39(3)	35(2)	-2(2)	15(2)	3(2)
C(5)	42(3)	46(3)	32(3)	6(2)	16(2)	5(3)
C(6)	41(3)	35(3)	32(3)	1(2)	19(2)	0(2)
C(7)	54(3)	41(3)	33(3)	2(2)	21(3)	-7(3)
C(8)	54(3)	54(4)	45(3)	-1(3)	30(3)	-15(3)
C(9)	40(3)	53(4)	45(3)	-3(3)	21(3)	-8(3)
C(10)	35(3)	40(3)	35(3)	-1(2)	19(2)	-5(2)
C(11)	43(3)	27(3)	35(3)	-3(2)	25(2)	-4(2)
C(12)	33(3)	40(3)	35(3)	-1(2)	16(2)	1(2)
C(13)	33(3)	43(3)	46(3)	-4(3)	18(2)	2(2)
C(14)	36(3)	67(5)	65(4)	12(4)	11(3)	8(3)
C(15)	44(4)	73(5)	74(4)	-15(4)	32(3)	1(3)
C(16)	50(3)	51(4)	49(4)	-5(3)	17(3)	-4(3)
C(17)	49(3)	53(4)	28(3)	9(2)	17(2)	6(3)
C(18)	83(5)	96(6)	40(4)	6(4)	38(4)	15(4)
C(19)	90(5)	47(4)	51(4)	14(3)	27(4)	-3(4)
C(20)	65(4)	86(6)	47(4)	21(4)	15(3)	19(4)
C(21)	60(4)	65(5)	60(4)	2(4)	31(4)	2(4)
S(22)	51(1)	59(1)	44(1)	-2(1)	24(1)	1(1)
O(23)	197(8)	109(5)	144(6)	75(5)	140(7)	65(5)
O(24)	118(5)	63(3)	69(3)	-26(3)	45(3)	-11(3)
O(25)	47(3)	95(5)	128(5)	-19(4)	5(3)	-3(3)
F(26)	54(3)	121(5)	183(6)	39(4)	29(4)	3(3)
F(27)	211(7)	122(5)	94(4)	-3(3)	95(4)	71(5)
F(28)	107(4)	67(3)	73(3)	8(2)	34(3)	-4(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(5)	7384	9541	-2630	48
H(7)	9972	10001	-2340	51
H(8)	12432	9947	-1063	58
H(9)	13479	9278	801	54
H(12)	12969	8427	2410	43
H(14A)	5223	9679	-3037	91
H(14B)	4007	9161	-3627	91
H(14C)	5324	9115	-3920	91
H(15A)	5461	9449	-741	93
H(15B)	5848	8756	-128	93
H(15C)	4313	8900	-1300	93
H(16A)	6045	7861	-1580	78
H(16B)	5914	8026	-3005	78
H(16C)	4549	8036	-2782	78
H(18A)	11049	8388	4259	105
H(18B)	10771	7682	4566	105
H(18C)	9620	8040	3288	105
H(19A)	11259	6937	1945	98
H(19B)	9742	7141	1750	98
H(19C)	10816	6792	3082	98
H(20A)	13315	8072	4404	105
H(20B)	13413	7544	3446	105
H(20C)	13105	7346	4644	105
H(2A)	7420(70)	7473(13)	650(60)	60(20)
H(2B)	7440(70)	7970(40)	1640(40)	70(20)

Table 6. Hydrogen bonds for jf153a [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(2)-H(2A)...O(24)	0.90(2)	1.82(2)	2.709(7)	175(6)
O(2)-H(2B)...O(23)#1	0.88(2)	1.86(3)	2.730(7)	168(7)

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+3/2, z+1/2$