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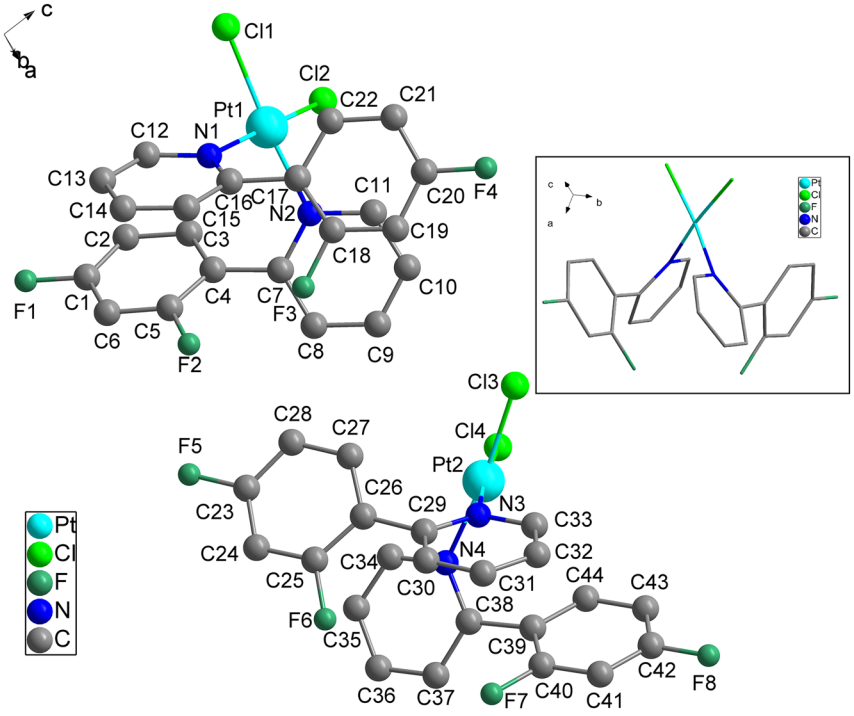
Crystal structure of dichlorido-bis[2-(2,4-difluorophenyl)pyridine-κ^1N]platinum(II), $C_{22}H_{14}Cl_2F_4N_2Pt$



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Abstract

$C_{22}H_{14}Cl_2F_4N_2Pt$, monoclinic, $P2_1/n$ (no. 14), a = 16.858(9) Å, b = 14.876(8) Å, c = 17.125(9) Å, β = 98.552(6)°, V = 4247(4) Å^3, Z = 8, $R_{gt}(F)$ = 0.0337, $wR_{ref}(F^2)$ = 0.0778, T = 296 K.

CCDC no.: 2280556

Table 1: Data collection and handling.

Crystal:	Yellow cube
Size:	0.08 × 0.06 × 0.06 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	6.91 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.9°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	31,284, 8484, 0.060
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 6411
$N(param)_{refined}$:	559
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

2-(2,4-Difluorophenyl)pyridine (0.2294 g, 0.0012 mol) and K_2PtCl_4 (1.6602 g, 0.0004 mol) were suspended in

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.67725 (2)	0.33224 (2)	0.83343 (2)	0.03549 (7)
Cl1	0.57814 (8)	0.23191 (10)	0.85281 (9)	0.0560 (4)
Cl2	0.63300 (9)	0.43984 (9)	0.91278 (9)	0.0539 (4)
F1	0.5717 (3)	0.4418 (3)	0.4792 (2)	0.1147 (17)
F2	0.8289 (3)	0.3955 (3)	0.6100 (2)	0.0968 (13)
F3	0.9427 (2)	0.2695 (3)	0.7658 (3)	0.0915 (12)
F4	1.0004 (2)	0.2177 (3)	1.0365 (2)	0.1103 (16)
N1	0.7098 (2)	0.2458 (3)	0.7512 (2)	0.0379 (10)
N2	0.7733 (2)	0.4132 (3)	0.8248 (2)	0.0397 (10)
C1	0.6242 (6)	0.4419 (4)	0.5466 (4)	0.073 (2)
C2	0.5974 (4)	0.4671 (4)	0.6149 (4)	0.0660 (19)
H2	0.543993	0.483036	0.614493	0.079*
C3	0.6506 (4)	0.4685 (3)	0.6848 (3)	0.0502 (15)
H3	0.632793	0.485306	0.731553	0.060*
C4	0.7314 (3)	0.4447 (3)	0.6856 (3)	0.0444 (13)
C5	0.7525 (4)	0.4193 (4)	0.6141 (4)	0.0620 (17)
C6	0.7010 (5)	0.4175 (4)	0.5443 (4)	0.074 (2)
H6	0.718091	0.400130	0.497387	0.089*
C7	0.7913 (3)	0.4509 (3)	0.7574 (3)	0.0441 (13)
C8	0.8632 (4)	0.4953 (4)	0.7577 (4)	0.0634 (18)
H8	0.875399	0.520853	0.711365	0.076*
C9	0.9169 (4)	0.5021 (5)	0.8264 (5)	0.075 (2)
H9	0.965680	0.531174	0.826467	0.090*
C10	0.8979 (4)	0.4658 (4)	0.8942 (4)	0.0655 (19)
H10	0.933861	0.469400	0.940843	0.079*
C11	0.8253 (3)	0.4240 (4)	0.8929 (3)	0.0504 (15)
H11	0.811146	0.402460	0.939865	0.060*
C12	0.6570 (4)	0.2347 (3)	0.6850 (3)	0.0502 (14)
H12	0.606050	0.259239	0.683155	0.060*
C13	0.6740 (4)	0.1894 (4)	0.6202 (4)	0.0618 (18)
H13	0.635675	0.183519	0.575513	0.074*
C14	0.7491 (4)	0.1526 (4)	0.6227 (4)	0.0616 (17)
H14	0.763348	0.122699	0.579135	0.074*
C15	0.8027 (4)	0.1611 (4)	0.6910 (3)	0.0557 (16)
H15	0.853240	0.135063	0.693992	0.067*
C16	0.7832 (3)	0.2075 (3)	0.7552 (3)	0.0410 (13)
C17	0.8397 (3)	0.2128 (3)	0.8295 (3)	0.0419 (13)
C18	0.9180 (4)	0.2402 (4)	0.8335 (4)	0.0568 (16)
C19	0.9728 (4)	0.2453 (5)	0.9016 (5)	0.072 (2)
H19	1.024490	0.266918	0.901321	0.086*
C20	0.9475 (4)	0.2173 (5)	0.9687 (4)	0.071 (2)
C21	0.8717 (4)	0.1868 (4)	0.9712 (4)	0.0620 (17)
H21	0.856711	0.166911	1.018399	0.074*
C22	0.8170 (3)	0.1859 (3)	0.9014 (3)	0.0490 (14)
H22	0.764576	0.167145	0.902669	0.059*
Pt2	1.18565 (2)	0.53581 (2)	0.83735 (2)	0.03959 (7)
Cl3	1.16205 (10)	0.43187 (11)	0.93062 (9)	0.0660 (4)
Cl4	1.09727 (9)	0.63671 (11)	0.87734 (10)	0.0659 (4)
F5	0.9815 (2)	0.4044 (3)	0.5253 (2)	0.0971 (14)
F6	1.2586 (2)	0.4461 (3)	0.5761 (2)	0.0874 (12)
F7	1.4176 (2)	0.5909 (3)	0.7083 (3)	0.1012 (14)
F8	1.5388 (3)	0.6492 (3)	0.9653 (3)	0.1240 (18)
N3	1.2720 (2)	0.4520 (3)	0.8076 (2)	0.0381 (10)
N4	1.1989 (2)	0.6194 (3)	0.7460 (2)	0.0401 (10)
C23	1.0498 (4)	0.4074 (4)	0.5775 (4)	0.0613 (17)
C24	1.1195 (4)	0.4262 (4)	0.5497 (3)	0.0638 (18)
H24	1.120301	0.438370	0.496496	0.077*
C25	1.1887 (4)	0.4266 (4)	0.6035 (4)	0.0525 (15)
C26	1.1912 (3)	0.4099 (3)	0.6833 (3)	0.0391 (12)
C27	1.1175 (3)	0.3914 (3)	0.7080 (3)	0.0411 (13)
H27	1.115796	0.379675	0.761045	0.049*
C28	1.0470 (3)	0.3903 (4)	0.6551 (4)	0.0516 (15)
H28	0.998324	0.378025	0.672323	0.062*
C29	1.2681 (3)	0.4081 (3)	0.7379 (3)	0.0398 (12)
C30	1.3329 (4)	0.3611 (4)	0.7202 (4)	0.0575 (16)
H30	1.329079	0.330641	0.672401	0.069*
C31	1.4036 (4)	0.3581 (4)	0.7719 (5)	0.0669 (19)
H31	1.448217	0.328131	0.758879	0.080*
C32	1.4060 (4)	0.4005 (4)	0.8427 (4)	0.0673 (19)
H32	1.452513	0.398332	0.879370	0.081*
C33	1.3412 (4)	0.4458 (4)	0.8602 (4)	0.0541 (16)
H33	1.343810	0.473470	0.909180	0.065*
C34	1.1327 (4)	0.6311 (4)	0.6910 (3)	0.0551 (15)
H34	1.084344	0.605974	0.700082	0.066*
C35	1.1346 (4)	0.6785 (4)	0.6226 (4)	0.0608 (18)
H35	1.088116	0.684974	0.586289	0.073*
C36	1.2049 (5)	0.7163 (4)	0.6079 (4)	0.0671 (19)
H36	1.207090	0.747173	0.561072	0.080*
C37	1.2724 (4)	0.7078 (4)	0.6639 (3)	0.0537 (15)
H37	1.320577	0.734071	0.655742	0.064*
C38	1.2677 (3)	0.6593 (3)	0.7330 (3)	0.0429 (13)
C39	1.3386 (3)	0.6534 (3)	0.7965 (3)	0.0435 (13)
C40	1.4110 (4)	0.6219 (4)	0.7810 (4)	0.0608 (17)
C41	1.4788 (4)	0.6180 (5)	0.8371 (5)	0.082 (2)
H41	1.526743	0.594307	0.825574	0.098*
C42	1.4719 (5)	0.6508 (5)	0.9107 (5)	0.083 (2)
C43	1.4030 (4)	0.6829 (4)	0.9297 (4)	0.0673 (19)
H43	1.400939	0.704430	0.980329	0.081*
C44	1.3344 (4)	0.6838 (3)	0.8730 (3)	0.0512 (15)
H44	1.286063	0.704526	0.886069	0.061*

2-ethoxyethanol (90 mL). Under nitrogen atmosphere, the suspension was stirred at 80 °C for 10 h. 2-Ethoxyethanol was removed by rotary evaporator, dichloromethane (20 mL) was added and stirred at 20 °C for 10 h. The title crystals were obtained by slow evaporation from dichloromethane at room temperature.

2 Experimental details

Absorption corrections were used by using multi-scan program [1]. The structure was solved with SHELX [3, 4]. Hydrogen atoms were placed in their geometrically idealized positions. Hydrogen atoms were constrained to ride on their parent atoms.

3 Comment

Platinum-based drugs are widely used for chemotherapeutic eradication of cancer [5]. Cisplatin, carboplatin, and oxaliplatin have excellent performance in the treatment of lung cancer, ovarian cancer and colon cancer respectively [6–8]. Platinum(II) complexes can also play an important role in detection of highly toxic pollutant perchlorate in the environment [9]. In addition, platinum(II) complexes also have significant applications in catalysis and optics [10, 11].

The title compound is a planar quadrilateral configuration with platinum(II) as the central metal. The coordination sites of the compound were occupied by two nitrogens atoms and two chlorine atoms respectively. The atoms are derived from the bidentate ligand 2-(2,4-difluorophenyl)pyridine, the chlorine atoms are derived from K_2PtCl_4. The distances of Pt1–Cl1 bonds are 2.3009(16) Å, the distances of Pt1–Cl2 bonds are 2.2951(16) Å, the distances of Pt1–N1 bonds are 2.041(4) Å, the distances of Pt1–N2 bonds are 2.041(4) Å. The distances of Pt2–Cl3 bonds are 2.2999(17) Å, the distances of Pt2–Cl4 bonds are 2.2903(17) Å, the distances of Pt2–N3 bonds are 2.039(4) Å, the distances of Pt2–N4 bonds are 2.037(4) Å. In addition, the Cl2–Pt1–Cl1 angle is 93.44(6)°, the N1–Pt1–Cl1 angle is 88.08(12)°, the N1–Pt1–Cl2 angle is 172.86(12)°, the N1–Pt1–N2 angle is 91.36(16)°, the N2–Pt1–Cl1 angle is 173.79(12)°, the N2–Pt1–Cl2 angle is 87.87(12)°, the Cl4–Pt2–Cl3 angle is 92.61(7)°, the N3–Pt2–Cl3 angle is 88.06(12)°, the N3–Pt2–Cl4 angle is 175.07(12)°, the N4–Pt2–Cl3 angle is 173.76(12)°, the N4–Pt2–Cl4 angle is 88.84(12)°, the N4–Pt2–N3 angle is 91.01(16)°, the Cl2–Pt1–Cl1 angle is 93.44(6)°, the Cl2–Pt1–Cl1 angle is 93.44(6)°, the Cl2–Pt1–Cl1 angle is 93.44(6)°, the Cl2–Pt1–Cl1 angle is 93.44(6)°, the Cl2–Pt1–Cl1 angle is 93.44(6)°. All bond lengths and bond angles fall within the normal ranges [12, 13].

In the columns, several p⋯p interactions between adjacent aromatic rings are present. All the p⋯p interactions are in the range of 3.624(4)–3.969(4) Å [14]. Also the crystal packing is consolidated by weak C–F⋯p interactions. The C–F⋯p (centroid) distance in these motifs were in the range of 3.474(5)–3.719(5) Å [15].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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