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Crystal structure of 2-(2-naphthyl)-4,6-dimethylpyrimidine, $C_{16}H_{14}N_2$

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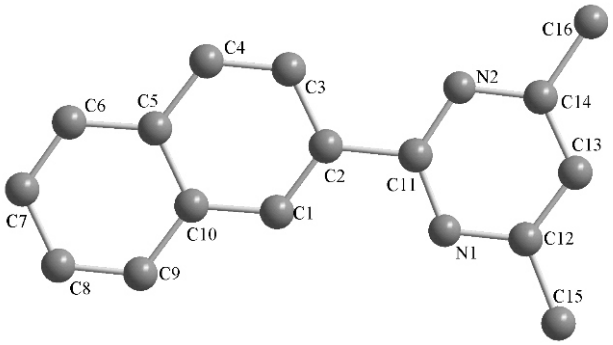

Abstract

$C_{16}H_{14}N_2$, monoclinic, $P12_1/c1$ (no. 14), a = 8.387(1) Å, b = 17.453(3) Å, c = 8.694(1) Å, β = 93.092(2)°, V = 1270.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.046, $wR_{ref}(F^2)$ = 0.129, T = 294 K.

Source of material

The title compound was obtained from the coupling reaction of 2-naphthaleneboronic acid and 2-iodo-4,6-dimethylpyrimidine as described in literature [1] and recrystallized from dichloromethane/petroleum ether solution at room temperature to give the desired crystals suitable for single crystal X-ray diffraction.

Experimental details

All the hydrogen atoms were positioned geometrically with d(C—H) = 0.93 Å, U_{iso}(H) = 1.2 U_{eq}(C) for the aromatic groups and d(C—H) = 0.96 Å, U_{iso}(H) = 1.5 U_{eq}(C) for the methyl groups. The H atoms of the methyl groups in the pyrimidine ring are disordered over two positions with occupation factors fixed at 0.5.

Discussion

Cyclometalated iridium complexes have attracted considerable attention in material research because of their outstanding performance in organic light-emitting diodes (OLED) [2,3]. In recent years, various types of cyclometalated Ir(III) complexes have been developed, such as homoleptic complexes, heteroleptic neutral complexes and cationic complexes [4-6]. In contrast to the most famous substituted phenylpyridine ligands, few examples of naphthalenylpyridine iridium complexes have been reported [7,8].

The pyrimidine ring and naphthalene ring in the crystal structure of the title compound are approximately coplanar with a dihedral angle of 2.4°. There exist two types of intermolecular π-π stacking interactions. One π-π stacking interaction is between the pyrimidine rings (the inter-plane distance is 3.400 Å). The other π-π stacking interaction is between pyrimidine ring and naphthalene ring (the inter-plane distance is 3.748 Å). Both are attributed to construct the layer structure.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.03 × 0.31 × 0.42 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.73 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7463, 2367
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1465
$N(param)_{refined}$:	164
Programs:	SHELXS-97, SHELXL-97, SHELXTL [9]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1)	4*e*		0.3477	0.5292	0.6776	0.058
H(3)	4*e*		0.0869	0.6172	0.5798	0.066
H(4)	4*e*		0.0189	0.7064	0.4241	0.069
H(6)	4*e*		0.2569	0.7642	0.3034	0.074
H(7)	4*e*		0.5251	0.7632	0.2707	0.081
H(8)	4*e*		0.6882	0.6728	0.3957	0.076
H(9)	4*e*		0.5846	0.5857	0.5581	0.066
H(13)	4*e*		0.1134	0.3600	0.9823	0.070
H(15A)	4*e*	0.50	0.3113	0.3528	0.9412	0.120
H(15B)	4*e*	0.50	0.1751	0.2913	0.9411	0.120
H(15C)	4*e*	0.50	0.2029	0.3466	1.0820	0.120
H(15D)	4*e*	0.50	0.1482	0.3076	1.0350	0.120
H(15E)	4*e*	0.50	0.2844	0.3692	1.0351	0.120
H(15F)	4*e*	0.50	0.2566	0.3138	0.8942	0.120
H(16A)	4*e*	0.50	0.3891	0.4981	0.8181	0.109
H(16B)	4*e*	0.50	0.3589	0.4632	0.9832	0.109
H(16C)	4*e*	0.50	0.3923	0.4091	0.8411	0.109
H(16D)	4*e*	0.50	0.3711	0.4154	0.9435	0.109
H(16E)	4*e*	0.50	0.4013	0.4504	0.7784	0.109
H(16F)	4*e*	0.50	0.3679	0.5045	0.9204	0.109

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.2820(2)	0.5648(1)	0.6258(2)	0.045(1)	0.051(1)	0.049(1)	0.0058(8)	0.0011(9)	0.0031(9)
C(2)	4*e*	0.1210(2)	0.5624(1)	0.6445(2)	0.042(1)	0.051(1)	0.045(1)	0.0045(8)	0.0020(8)	0.0076(9)
C(3)	4*e*	0.0225(2)	0.6175(1)	0.5672(2)	0.042(1)	0.061(1)	0.062(1)	0.0081(9)	0.0025(9)	0.004(1)
C(4)	4*e*	0.0861(2)	0.6710(1)	0.4744(2)	0.052(1)	0.057(1)	0.063(1)	0.0140(9)	0.002(1)	0.001(1)
C(5)	4*e*	0.2516(2)	0.6742(1)	0.4527(2)	0.054(1)	0.046(1)	0.050(1)	0.0043(9)	0.0003(9)	0.0070(9)
C(6)	4*e*	0.3211(3)	0.7280(1)	0.3549(2)	0.070(1)	0.052(1)	0.062(1)	0.004(1)	0.003(1)	0.005(1)
C(7)	4*e*	0.4810(3)	0.7274(1)	0.3351(3)	0.073(2)	0.062(1)	0.068(2)	0.009(1)	0.010(1)	0.007(1)
C(8)	4*e*	0.5793(2)	0.6732(1)	0.4111(2)	0.052(1)	0.069(1)	0.070(1)	0.009(1)	0.009(1)	0.003(1)
C(9)	4*e*	0.5174(2)	0.6209(1)	0.5071(2)	0.047(1)	0.059(1)	0.059(1)	0.0001(9)	0.0013(9)	0.002(1)
C(10)	4*e*	0.3515(2)	0.6195(1)	0.5306(2)	0.047(1)	0.048(1)	0.046(1)	0.0014(8)	0.0020(9)	0.0068(9)
C(11)	4*e*	0.0512(2)	0.5032(1)	0.7431(2)	0.043(1)	0.054(1)	0.044(1)	0.0009(9)	0.0017(8)	0.0110(9)
C(12)	4*e*	0.0910(2)	0.3986(1)	0.8973(2)	0.054(1)	0.056(1)	0.056(1)	0.0023(9)	0.007(1)	0.003(1)
C(13)	4*e*	0.0706(2)	0.3975(1)	0.9207(2)	0.057(1)	0.061(1)	0.058(1)	0.010(1)	0.009(1)	0.003(1)
C(14)	4*e*	0.1669(2)	0.4524(1)	0.8516(2)	0.045(1)	0.069(1)	0.051(1)	0.008(1)	0.0056(9)	0.014(1)
C(15)	4*e*	0.2053(3)	0.3423(1)	0.9721(3)	0.070(2)	0.071(1)	0.100(2)	0.008(1)	0.011(1)	0.024(1)
C(16)	4*e*	0.3426(2)	0.4560(1)	0.8756(3)	0.045(1)	0.095(2)	0.078(2)	0.007(1)	0.010(1)	0.007(1)
N(1)	4*e*	0.1527(2)	0.45174(8)	0.8067(2)	0.0465(9)	0.0518(9)	0.056(1)	0.0018(7)	0.0069(8)	0.0002(8)
N(2)	4*e*	0.1066(2)	0.50631(9)	0.7609(2)	0.0422(9)	0.065(1)	0.051(1)	0.0008(7)	0.0038(7)	0.0089(8)

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