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

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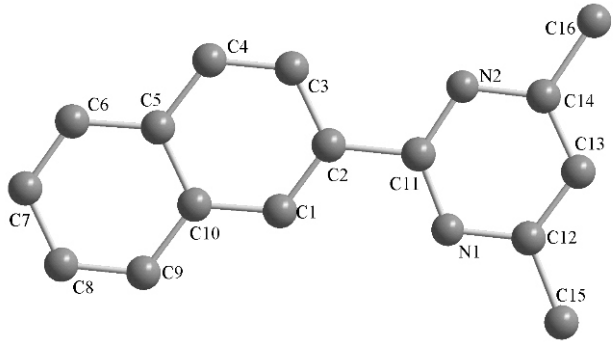


**Abstract**

$C_{16}H_{14}N_2$, monoclinic, $P12_1/c1$ (no. 14), $a$ = 8.387(1) Å, $b$ = 17.453(3) Å, $c$ = 8.694(1) Å, $\beta$ = 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 $\pi$-$\pi$ stacking interactions. One $\pi$-$\pi$ stacking interaction is between the pyrimidine rings (the inter-plane distance is 3.400 Å). The other $\pi$-$\pi$ 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 $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.73 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 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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