Crystal structure of 4-(4-(1*H*-imidazol-1-yl)phenyl)-2,6-diphenylpyridine, $C_{26}H_{19}N_3$

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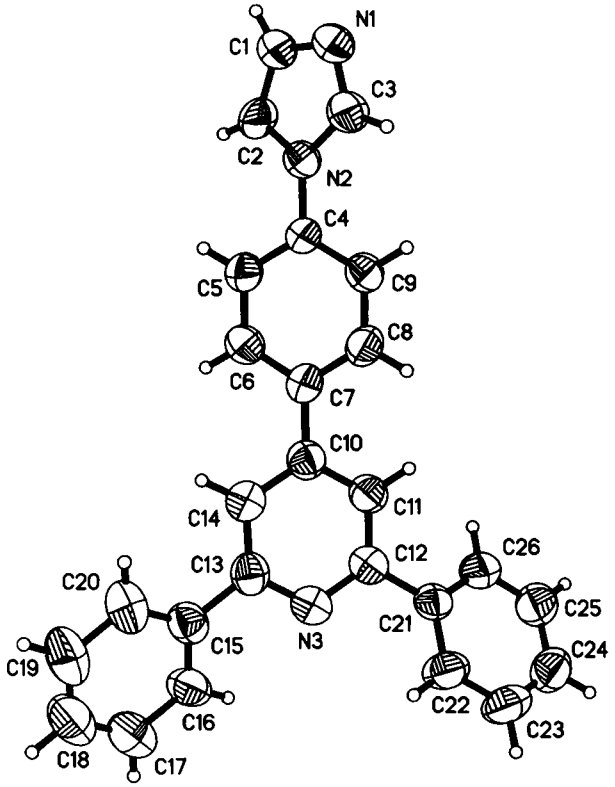

Abstract

$C_{26}H_{19}N_3$, monoclinic, $P12_1/c1$ (no. 14), $a = 12.885(1)$ Å, $b = 15.007(2)$ Å, $c = 10.863(2)$ Å, $\beta = 109.460(8)°$, $V = 1980.4$ Å^3, $Z = 4$, $R_{gt}(F) = 0.060$, $wR_{ref}(F^2) = 0.184$, $T = 293$ K.

Source of material

The title compound was readily accessible via sequential solventless aldol condensation and Michael addition involving NaOH, followed by treatment with ammonium acetate in ethanol [1-3]. Acetophenone (15 mmol) and 3-(4-imidazol-1-yl-phenyl)-1-phenylpro-2-en-1-one (15 mmol) and NaOH powder (60 mmol) were crashed together with a pestle and mortar 2 h. The yellow powder was added to a stirred solution of ammonium acetate (10 g, excess) in ethanol (100 mL). The reaction mixture was heated at reflux for 10 h. After cooling to room temperature a precipitate was filtered, washed with water three times and dried to afford the product. Recrystallization from ethanol afforded white needle-shaped crystals.

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Discussion

Light-emitting materials are the basis for the organic light-emitting diodes (OLEDs) for flat panel display applications. A challenge in this area is to achieve light-emitting materials with long-term stability and high efficiency [4,5]. Metal-chelate complexes are often used in the OLEDs because they have a good carrier transporting capability and strong fluorescence. It is essential to design organic ligands, which play an important role in the metal-chelate complex to tune the emission in a broad band [6,7]. As part of our studies on the synthesis and characterization of the ligand with two kind of aromatic heterocyclic center (DAHC) and its complexes, in the present work, we report the crystal structure of the newly designed and synthesized DAHC-type ligand, 4-(4-1*H*-imidazol-1-yl)phenyl-2,6-dipenylpyridine.

In the title structure, the C12—N3 and C13—N3 distances of 1.350 Å and 1.346 Å, respectively, agree well with the literature data (1.340 Å), being intermediate between the values of 1.47 Å for a C—N single bond and 1.30 Å for a C=N double bond. It is the same for C—C distance and the C–N–C, C–C–N and C–C–C angles in the pyridine group [8]. These data show that the pyridine group still retains aromatic character. The C4—N2, C7—C10, C12—C21, C13—C15 distances of 1.425 Å, 1.479 Å, 1.493 Å, 1.485 Å, respectively, are close to the C—N or C—C single bond lengths, which shows that the electrons are not delocalized in the molecule. The C9–C4–N2–C2, C6–C7–C10–C11, N3–C13–C15–C20, N3–C12–C21–C26 (158.3°, 149.7°, 154.3°, 149.8°, respectively) torsion angles show clearly that the five rings do not share a common plane probably as a result of the steric configuration of C, N atoms and the free rotation around C4—N2, C7—C10, C12—C21, C13—C15 single bonds. The molecules are linked to each other by C–H···N and van der Waals forces to form the 3D network. Because of the small polarity of this organic molecule and the weak intermolecular attraction, the tendency to get faulty single crystals is large and, therefore, the N_{gt}/N_{param} ratio is smaller and the wR_{ref} value somewhat larger than usual. These results were also observed for the structure determination of 4-(4-fluorophenyl)-2,6-diphenylpyridine [9].

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.20 × 0.28 × 0.38 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.75 cm^{-1}
Diffractometer, scan mode:	Bruker P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5655, 4552
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1266
$N(param)_{refined}$:	263
Program:	SHELXTL [10]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	–0.0523	0.8311	0.0255	0.082
H(2A)	4e	0.0047	0.7245	0.2050	0.076
H(3A)	4e	0.1064	0.6421	–0.0817	0.078
H(5A)	4e	0.1373	0.6263	0.3374	0.075
H(6A)	4e	0.2095	0.4996	0.4556	0.078
H(8A)	4e	0.2031	0.3777	0.1259	0.075
H(9A)	4e	0.1275	0.5023	0.0088	0.073
H(11A)	4e	0.1907	0.2534	0.2386	0.070
H(14A)	4e	0.3540	0.4019	0.5485	0.077
H(16A)	4e	0.4489	0.1436	0.7465	0.086
H(17A)	4e	0.5806	0.1414	0.9516	0.103
H(18A)	4e	0.6856	0.2653	1.0292	0.115
H(19A)	4e	0.6605	0.3921	0.9053	0.117
H(20A)	4e	0.5276	0.3959	0.7001	0.101
H(22A)	4e	0.4153	0.0427	0.4295	0.089
H(23A)	4e	0.3806	–0.0985	0.3394	0.100
H(24A)	4e	0.2104	–0.1332	0.1923	0.098
H(25A)	4e	0.0725	–0.0289	0.1391	0.096
H(26A)	4e	0.1058	0.1130	0.2228	0.081

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)	4e	–0.0125(3)	0.7793(3)	0.0264(4)	0.093(3)	0.062(3)	0.050(2)	0.006(3)	0.024(2)	0.002(2)
C(2)	4e	0.0186(3)	0.7206(3)	0.1265(4)	0.084(3)	0.056(3)	0.062(3)	0.013(2)	0.038(2)	–0.008(2)
C(3)	4e	0.0741(3)	0.6764(3)	–0.0330(4)	0.086(3)	0.066(3)	0.053(3)	0.007(3)	0.036(2)	0.005(2)
C(4)	4e	0.1225(3)	0.5763(2)	0.1613(4)	0.060(2)	0.045(2)	0.048(2)	0.004(2)	0.017(2)	–0.002(2)
C(5)	4e	0.1492(3)	0.5757(3)	0.2945(4)	0.081(3)	0.055(3)	0.052(2)	0.005(2)	0.025(2)	–0.002(2)
C(6)	4e	0.1938(3)	0.4998(3)	0.3656(4)	0.084(3)	0.065(3)	0.048(2)	0.003(2)	0.025(2)	0.006(2)
C(7)	4e	0.2154(3)	0.4238(3)	0.3043(4)	0.058(3)	0.052(3)	0.056(3)	0.000(2)	0.021(2)	–0.006(2)
C(8)	4e	0.1893(3)	0.4273(3)	0.1695(4)	0.089(3)	0.048(3)	0.057(3)	–0.001(2)	0.032(2)	–0.004(2)
C(9)	4e	0.1439(3)	0.5019(3)	0.0989(4)	0.084(3)	0.058(3)	0.045(2)	–0.001(2)	0.027(2)	0.003(2)
C(10)	4e	0.2639(3)	0.3430(3)	0.3792(4)	0.056(3)	0.060(3)	0.057(3)	0.000(2)	0.017(2)	–0.002(2)
C(11)	4e	0.2397(3)	0.2592(3)	0.3232(4)	0.060(3)	0.058(3)	0.054(2)	–0.003(2)	0.015(2)	0.002(2)
C(12)	4e	0.2882(3)	0.1843(3)	0.3930(4)	0.051(2)	0.056(3)	0.055(2)	–0.006(2)	0.017(2)	0.004(2)
C(13)	4e	0.3873(3)	0.2702(3)	0.5697(4)	0.061(3)	0.068(3)	0.056(3)	–0.002(3)	0.024(2)	–0.005(2)
C(14)	4e	0.3377(3)	0.3472(3)	0.5061(4)	0.067(3)	0.060(3)	0.063(3)	0.002(2)	0.018(2)	–0.004(2)
C(15)	4e	0.4726(3)	0.2705(3)	0.7014(4)	0.055(3)	0.082(3)	0.055(3)	0.009(3)	0.017(2)	–0.004(3)
C(16)	4e	0.4907(3)	0.1943(3)	0.7781(4)	0.065(3)	0.081(3)	0.061(3)	0.015(3)	0.011(2)	0.007(3)
C(17)	4e	0.5699(4)	0.1926(3)	0.9008(5)	0.074(3)	0.110(4)	0.069(3)	0.009(3)	0.015(3)	0.007(3)
C(18)	4e	0.6323(4)	0.2665(4)	0.9468(5)	0.076(4)	0.134(5)	0.066(3)	0.014(4)	0.008(3)	–0.008(4)
C(19)	4e	0.6173(4)	0.3421(4)	0.8732(5)	0.076(3)	0.126(5)	0.076(4)	–0.020(3)	0.005(3)	–0.019(4)
C(20)	4e	0.5375(4)	0.3443(3)	0.7501(4)	0.077(3)	0.100(4)	0.066(3)	–0.015(3)	0.013(3)	–0.011(3)
C(21)	4e	0.2643(3)	0.0929(3)	0.3361(4)	0.068(3)	0.049(3)	0.051(2)	–0.004(2)	0.018(2)	0.009(2)
C(22)	4e	0.3463(4)	0.0290(3)	0.3704(4)	0.076(3)	0.056(3)	0.086(3)	0.012(3)	0.023(3)	0.006(3)
C(23)	4e	0.3253(4)	–0.0556(3)	0.3164(5)	0.098(4)	0.059(3)	0.098(4)	0.022(3)	0.040(3)	0.010(3)
C(24)	4e	0.2236(5)	–0.0766(3)	0.2290(5)	0.111(4)	0.061(3)	0.077(3)	0.001(3)	0.036(3)	–0.006(3)
C(25)	4e	0.1419(4)	–0.0142(3)	0.1964(4)	0.096(4)	0.066(3)	0.074(3)	–0.006(3)	0.025(3)	0.000(3)
C(26)	4e	0.1615(4)	0.0705(3)	0.2475(4)	0.074(3)	0.055(3)	0.066(3)	0.003(2)	0.016(2)	0.004(2)
N(1)	4e	0.0227(3)	0.7520(2)	–0.0735(3)	0.084(3)	0.063(2)	0.051(2)	0.001(2)	0.027(2)	0.008(2)
N(2)	4e	0.0747(2)	0.6541(2)	0.0894(3)	0.064(2)	0.054(2)	0.046(2)	0.001(2)	0.022(2)	0.002(2)
N(3)	4e	0.3628(2)	0.1892(2)	0.5143(3)	0.055(2)	0.064(2)	0.058(2)	0.001(2)	0.018(2)	0.005(2)

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