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Crystal structure of 2,3-diphenyl-5,6-bis(4-methoxyphenyl)pyrazine, $C_{30}H_{24}N_2O_2$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.26 × 0.24 × 0.22 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	29.2°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	19331, 5674, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3798
$N(\text{param})_{\text{refined}}$:	309
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

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Abstract

$C_{30}H_{24}N_2O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 11.4545(6)$ Å, $b = 21.0333(10)$ Å, $c = 10.0604(5)$ Å, $\beta = 103.571(6)^\circ$, $V = 2356.1(2)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0652$, $wR_{\text{ref}}(F^2) = 0.1414$, $T = 289.3(7)$ K.

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Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was one-pot synthesized by heating a mixture of 4,4'-dimethoxybenzophenone and (1*R*,2*R*)-(+)-1,2-diphenylethylenediamine in acetic acid [4]. White needle crystal of the title compound was obtained through solvent evaporation method from a mixed solvent of trichloromethane and methanol 1:1 at room temperature.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.00507(14)	0.57509(8)	0.61802(18)	0.0632(5)
O2	0.51168(18)	0.70680(9)	1.06008(16)	0.0768(6)
N1	0.45629(15)	0.56612(8)	0.32044(17)	0.0385(4)
N2	0.30725(15)	0.63543(8)	0.44263(17)	0.0384(4)
C1	0.26886(18)	0.61532(9)	0.3139(2)	0.0384(5)
C2	0.34062(18)	0.57388(9)	0.2573(2)	0.0370(5)
C3	0.49996(18)	0.59313(9)	0.4428(2)	0.0356(4)
C4	0.41984(17)	0.62251(9)	0.5125(2)	0.0351(4)
C5	0.44834(17)	0.64224(9)	0.65868(19)	0.0350(4)
C6	0.53646(19)	0.61362(10)	0.7586(2)	0.0426(5)
H6	0.5796	0.5798	0.7347	0.051*
C7	0.5622(2)	0.63398(10)	0.8934(2)	0.0456(5)
H7	0.6231	0.6147	0.9584	0.055*
C8	0.4967(2)	0.68315(11)	0.9302(2)	0.0476(5)
C9	0.4051(2)	0.71098(11)	0.8330(2)	0.0528(6)
H9	0.3590	0.7432	0.8585	0.063*
C10	0.38188(19)	0.69124(10)	0.6991(2)	0.0441(5)
H10	0.3211	0.7108	0.6344	0.053*
C11	0.6031(2)	0.68205(14)	1.1656(2)	0.0676(7)
H11A	0.6793	0.6877	1.1430	0.101*
H11B	0.5891	0.6376	1.1765	0.101*
H11C	0.6032	0.7039	1.2494	0.101*
C12	0.63276(18)	0.59038(9)	0.49285(19)	0.0357(4)
C13	0.69941(19)	0.64107(10)	0.5585(2)	0.0435(5)
H13	0.6600	0.6781	0.5734	0.052*
C14	0.82324(19)	0.63804(10)	0.6024(2)	0.0467(5)
H14	0.8660	0.6725	0.6472	0.056*
C15	0.88311(19)	0.58338(10)	0.5793(2)	0.0432(5)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C16	0.81841(19)	0.53251(10)	0.5118(2)	0.0450(5)
H16	0.8582	0.4959	0.4951	0.054*
C17	0.69519(18)	0.53604(9)	0.4693(2)	0.0395(5)
H17	0.6527	0.5016	0.4241	0.047*
C18	1.0759(2)	0.62266(14)	0.6995(3)	0.0780(9)
H18A	1.0651	0.6624	0.6512	0.117*
H18B	1.1590	0.6106	0.7182	0.117*
H18C	1.0515	0.6271	0.7840	0.117*
C19	0.29538(18)	0.53887(9)	0.1265(2)	0.0378(5)
C20	0.3598(2)	0.53922(11)	0.0262(2)	0.0488(6)
H20	0.4332	0.5602	0.0422	0.059*
C21	0.3167(2)	0.50888(12)	−0.0972(2)	0.0558(6)
H21	0.3601	0.5104	−0.1645	0.067*
C22	0.2096(2)	0.47631(11)	−0.1207(2)	0.0560(6)
H22	0.1802	0.4561	−0.2040	0.067*
C23	0.1462(2)	0.47375(11)	−0.0204(2)	0.0552(6)
H23	0.0748	0.4509	−0.0353	0.066*
C24	0.18811(19)	0.50509(10)	0.1028(2)	0.0462(5)
H24	0.1444	0.5035	0.1698	0.055*
C25	0.1521(2)	0.64165(10)	0.2378(2)	0.0449(5)
C26	0.1397(2)	0.66663(11)	0.1075(3)	0.0599(7)
H26	0.2033	0.6646	0.0648	0.072*
C27	0.0315(3)	0.69472(13)	0.0411(3)	0.0785(9)
H27	0.0234	0.7120	−0.0457	0.094*
C28	−0.0632(3)	0.69690(14)	0.1033(4)	0.0811(9)
H28	−0.1359	0.7146	0.0572	0.097*
C29	−0.0513(2)	0.67334(14)	0.2320(3)	0.0752(8)
H29	−0.1152	0.6756	0.2743	0.090*
C30	0.0560(2)	0.64606(12)	0.2996(3)	0.0589(6)
H30	0.0639	0.6304	0.3878	0.071*

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C, aromatic ring})$, and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{C, methyl})$. The final refinement by using geometrical restraints, with C—H = 0.93 Å (aromatic ring), and C—H = 0.96 Å (methyl).

Comment

Since the aggregation induced emission (AIE) phenomenon was reported for the first time in 2001 [5], AIE molecules have been widely used in OLED, fluorescence sensors, biosensors and cell imaging and further applications [6–10]. Very recently, tetraphenylpyrazine (TPP), as a new AIE core, has attracted much interest due to its advantages of easy preparation, facile modification, excellent stability and tunable light emission [11–17].

Bartnik and co-workers reported the dimorphism of TPP in 1999, with crystallographically imposed symmetry of the

title molecules in both modifications [17]. In the title structure the molecules occupy a general position (*cf.* the figure). The dihedral angle between the planes defined by C5—C10 and C12—C17 is 50.9°, and two phenyl rings defined by C19—C24 and C25—C30 form a dihedral angle of 61.1°. In addition, bond angles of C15—O1—C18 and C8—O2—C11 are 118.72(19)° and 119.36(19)°, respectively. Bond lengths and angles are all in the expected ranges.

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