Xin-Sheng Xiao, Guo-Kai Jia*, Wen-Yi Li and Xiu-Wen Chen

Crystal structure of (Z)-N-(4-nitrophenyl)-3-phenyl-3-(phenylamino)acrylamide, C₂₁H₁₇N₃O₃

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.25 × 0.18 × 0.18 mm
Wavelength:	Cu K α radiation (1.54178 Å)
μ :	7.3 cm ⁻¹
Diffractometer, scan mode:	Xcalibur Sapphire 3, ω scans
2 $\theta_{\max}$, completeness:	125.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10224, 2923, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2426
$N(\text{param})_{\text{refined}}$:	245
Programs:	Bruker programs [1], SHELX [2]

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Abstract

C₂₁H₁₇N₃O₃, orthorhombic, *Pbca* (no. 61), $a = 14.3606(4)$ Å, $b = 7.4250(2)$ Å, $c = 34.2840(9)$ Å, $V = 3655.62(17)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0399$, $wR_{\text{ref}}(F^2) = 0.1178$, $T = 571(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

To a screw capped vial with a spinvane triangular-shaped Teflon stir bar were added *N*-(1-phenylethylidene)aniline (0.2 mmol), 4-nitrobenzoyl azide (0.2 mmol) and

1,2-dichloroethane (1.0 mL) under argon atmosphere conditions. The reaction mixture was stirred at 373 K for 12 h, filtered through a pad of celite and then washed with ethyl acetate (10 mL 3 times). Organic solvents were removed under reduced pressure and the residue was purified by chromatography on silica gel with ethyl acetate/petroleum (3:1, v/v) as the eluent to give the title compound as a yellow solid.

Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The methyl groups were idealized and refined using rigid groups allowed to rotate about the C–C bond (AFIX 137 option of the SHELXL program). The U_{iso} values of all other hydrogen atoms were set to $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Discussion

(Z)-*N*-3-diphenyl-3-(phenylamino)acrylamide derivatives contain attractive structural motifs because of their wide distribution in bioactive molecules and pharmaceuticals [3–6]. Hence, there is considerable interest in the development of effective methods for the synthesis of (Z)-*N*-3-diphenyl-3-(phenylamino)acrylamide and its analogues [7, 8]. Herein the crystal structure of the title compound is described to enrich the related crystal structures of (Z)-*N*-(4-nitrophenyl)-3-phenyl-3-(phenylamino)acrylamide.

Similar to our previous study [9, 10], the title compound, built up by the C₂₁H₁₇N₃O₃ molecules, has been synthesized. The single crystal structure verifies that all bond lengths are

*Corresponding author: Guo-Kai Jia, Department of Biology and Chemistry, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China; and Hunan Key Laboratory of Comprehensive Utilization of Advantage Plants Resources of Hunan South, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China, e-mail: 609158809@qq.com

Xin-Sheng Xiao, Wen-Yi Li and Xiu-Wen Chen: Department of Biology and Chemistry, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China; and Hunan Key Laboratory of Comprehensive Utilization of Advantage Plants Resources of Hunan South, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.65345(9)	0.05732(18)	0.37001(4)	0.0796(4)
O2	0.31779(10)	−0.3752(3)	0.50822(5)	0.1158(6)
O3	0.25421(10)	−0.2581(3)	0.45739(4)	0.1117(6)
N1	0.81351(10)	0.1057(2)	0.32865(4)	0.0739(4)
H1A	0.7570	0.1424	0.3311	0.089*
N2	0.67252(9)	−0.0362(2)	0.43292(4)	0.0706(4)
H2B	0.7128	−0.0387	0.4515	0.085*
N3	0.32194(11)	−0.2859(3)	0.47814(5)	0.0828(5)
C1	0.84768(11)	0.1020(2)	0.29017(5)	0.0652(4)
C2	0.81285(14)	0.2236(3)	0.26350(7)	0.0854(6)
H2A	0.7682	0.3069	0.2713	0.102*
C3	0.84371(18)	0.2228(4)	0.22515(7)	0.1004(7)
H3A	0.8194	0.3047	0.2073	0.120*
C4	0.90962(18)	0.1019(4)	0.21363(7)	0.1044(8)
H4A	0.9316	0.1027	0.1881	0.125*
C5	0.94295(16)	−0.0200(4)	0.23976(7)	0.1012(8)
H5A	0.9876	−0.1031	0.2318	0.121*
C6	0.91179(13)	−0.0225(3)	0.27762(6)	0.0800(5)
H6A	0.9342	−0.1088	0.2949	0.096*
C7	0.85638(11)	0.0600(2)	0.36253(5)	0.0638(4)
C8	0.95999(11)	0.0530(2)	0.36397(5)	0.0641(4)
C9	1.01408(12)	0.1790(3)	0.34450(5)	0.0694(5)
H9A	0.9855	0.2702	0.3303	0.083*
C10	1.10992(13)	0.1699(3)	0.34612(6)	0.0841(6)
H10A	1.1456	0.2536	0.3326	0.101*
C11	1.15295(14)	0.0379(4)	0.36769(7)	0.0942(7)
H11A	1.2176	0.0320	0.3687	0.113*
C12	1.10006(15)	−0.0853(3)	0.38774(7)	0.0970(7)
H12A	1.1289	−0.1736	0.4027	0.116*
C13	1.00411(13)	−0.0782(3)	0.38563(6)	0.0833(6)
H13A	0.9688	−0.1631	0.3990	0.100*
C14	0.80657(12)	0.0283(2)	0.39545(5)	0.0683(5)
H14A	0.8394	0.0102	0.4185	0.082*
C15	0.70617(12)	0.0208(2)	0.39717(5)	0.0661(4)
C16	0.58295(11)	−0.0899(2)	0.44317(5)	0.0609(4)
C17	0.57356(11)	−0.1889(2)	0.47746(5)	0.0684(5)
H17A	0.6259	−0.2126	0.4926	0.082*
C18	0.48855(12)	−0.2517(2)	0.48914(5)	0.0690(5)
H18A	0.4827	−0.3184	0.5120	0.083*
C19	0.41173(11)	−0.2144(2)	0.46654(5)	0.0642(4)
C20	0.41844(11)	−0.1137(3)	0.43327(5)	0.0685(5)
H20A	0.3653	−0.0877	0.4188	0.082*
C21	0.50398(11)	−0.0507(2)	0.42120(5)	0.0665(4)
H21A	0.5089	0.0174	0.3985	0.080*

in normal ranges. The keto-tautomer is found in the solid state (*cf.* the figure).

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