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The crystal structure of 2-(naphthalen-2-yloxy)-4-phenyl-6-(prop-2-yn-1-yloxy)-1,3,5-triazine, $C_{22}H_{15}N_3O_2$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.50 × 0.40 × 0.30 mm
Wavelength:	Cu K α radiation (1.54178 Å)
μ :	0.71 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	68.4°, 96%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7418, 3066, 0.040
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2651
$N(\text{param})_{\text{refined}}$:	244
Programs:	Bruker [1], SHELX [2], Olex2 [3]

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Abstract

$C_{22}H_{15}N_3O_2$, triclinic, $P\bar{1}$ (no. 2), $a = 5.7613(4)$ Å, $b = 12.3545(7)$ Å, $c = 13.3427(8)$ Å, $\alpha = 110.002(2)^\circ$, $\beta = 98.837(2)^\circ$, $\gamma = 94.263(2)^\circ$, $V = 873.55(9)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0471$, $wR_{\text{ref}}(F^2) = 0.1376$, $T = 293$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

To a suspension of 2-chloro-4-phenyl-6-(prop-2-yn-1-yloxy)-1,3,5-triazine (2.46 g, 0.01 mol) in 60 mL of tetrahydrofuran was added K_2CO_3 (2.76 g, 0.02 mol) and naphthalen-2-ol (1.44 g, 0.01 mol). The mixture was refluxed for 12 h and then filtered to get a yellow solution. The solvent was evaporated under reduced pressure to get a yellow solid, which was purified by chromatography on silica gel to afford 2-(naphthalen-2-yloxy)-4-phenyl-6-(prop-2-yn-1-yloxy)-1,3,5-triazine as a white solid (2.19 g, 62%). The crystal suitable for X-ray diffraction was obtained by recrystallization in petroleum ether.

Experimental details

The data were scaled and corrected for absorption using SADABS-2016/2 (Bruker, APEX-II CCD). The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

In the past years, 1,3,5-triazine derivatives have drawn more and more attentions of the scientists all over the world, for the reason that these compounds demonstrated promising

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

Atom	x	y	z	U _{iso} */U _{eq}
C1	0.6791 (3)	0.80235 (13)	0.49698 (11)	0.0340 (3)
C2	0.5614 (3)	0.68237 (12)	0.57501 (11)	0.0322 (3)
C3	0.9145 (2)	0.79381 (12)	0.64194 (10)	0.0325 (3)
C4	0.2665 (3)	0.70929 (13)	0.15173 (11)	0.0378 (4)
C5	1.1372 (3)	0.83424 (12)	0.72438 (11)	0.0340 (3)
C6	0.2154 (3)	0.47962 (13)	0.64986 (11)	0.0372 (3)
C7	0.4465 (3)	0.81493 (13)	0.33863 (11)	0.0369 (4)
C8	1.5257 (3)	0.94723 (14)	0.79300 (12)	0.0418 (4)
H8	1.6484	0.9989	0.7866	0.050*
C9	0.0689 (3)	0.76997 (14)	0.16714 (12)	0.0399 (4)
C10	0.2478 (3)	0.87277 (14)	0.35597 (12)	0.0413 (4)
H10	0.2422	0.9269	0.4258	0.050*
C11	1.1665 (3)	0.79735 (14)	0.81235 (12)	0.0406 (4)
H11	1.0441	0.7461	0.8194	0.049*
C12	1.3179 (3)	0.90983 (13)	0.71503 (11)	0.0371 (3)
H12	1.2991	0.9358	0.6553	0.045*
C13	0.4305 (3)	0.55656 (13)	0.66080 (11)	0.0366 (3)
H13A	0.4642	0.6201	0.7328	0.044*
H13B	0.5677	0.5126	0.6537	0.044*
C14	1.5539 (3)	0.90919 (15)	0.87986 (12)	0.0445 (4)
H14	1.6968	0.9340	0.9325	0.053*
C15	0.4586 (3)	0.73378 (13)	0.24121 (12)	0.0382 (3)
H15	0.5932	0.6939	0.2327	0.046*
C16	1.3748 (3)	0.83532 (15)	0.89021 (12)	0.0462 (4)
H16	1.3937	0.8104	0.9505	0.055*
C17	0.2738 (3)	0.62900 (15)	0.04751 (13)	0.0464 (4)
H17	0.4063	0.5880	0.0365	0.056*
C18	−0.1180 (3)	0.74880 (17)	0.07634 (14)	0.0499 (4)
H18	−0.2515	0.7894	0.0853	0.060*
C19	0.0620 (3)	0.85032 (15)	0.27122 (13)	0.0426 (4)
H19	−0.0732	0.8892	0.2825	0.051*
C20	0.0421 (3)	0.41615 (14)	0.63930 (13)	0.0438 (4)
H20	−0.0972	0.3651	0.6308	0.053*
C21	0.0894 (4)	0.61021 (17)	−0.03798 (13)	0.0551 (5)
H21	0.0944	0.5558	−0.1077	0.066*
C22	−0.1065 (3)	0.67124 (19)	−0.02254 (14)	0.0573 (5)
H22	−0.2324	0.6579	−0.0822	0.069*
N1	0.8839 (2)	0.84255 (11)	0.56690 (9)	0.0352 (3)
N2	0.7583 (2)	0.71178 (10)	0.64955 (9)	0.0336 (3)
N3	0.5076 (2)	0.72386 (10)	0.49517 (9)	0.0334 (3)
O1	0.65067 (19)	0.85193 (10)	0.42123 (8)	0.0420 (3)
O2	0.38915 (18)	0.60368 (9)	0.57509 (7)	0.0365 (3)

biological activities such as anticancer [4–5], antiviral [6], antibacterial [7–9], antifungal [10], anti-Alzheimer's [11] and anti-inflammatory [12] properties. Thus the synthesis and property studies of novel 1,3,5-triazine derivatives is an active fields in medicinal chemistry. The title 1,3,5-triazine derivative was synthesized by a nucleophilic substitution reaction using 2-chloro-4-phenyl-6-(prop-2-yn-1-yloxy)-1,3,5-triazine as the starting material.

Bond lengths and angles are in the expected ranges (see the Figure) [13, 14]. The torsion angle of C10–C7–O1–C1

is 91.3°, which demonstrated that naphthyl moiety and the 1,3,5-triazine ring are not coplanar. Meanwhile, the torsion angle of C12–C5–C3–N2 is 173.2°, which demonstrated that phenyl ring and the 1,3,5-triazine ring were almost in the same plane (cf. the figure). In molecular packing, non-classical hydrogen bonds were observed as following: C11–H11...N2 hydrogen bond ($d(\text{H11}\cdots\text{N2}) = 2.47 \text{ \AA}$, C20–H20...N3 hydrogen bond ($d(\text{H20}\cdots\text{N3}) = 2.60 \text{ \AA}$).

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