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

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, α = 110.002(2)°, β = 98.837(2)°, γ = 94.263(2)°, V = 873.55(9) Å³, Z = 2, R_{gt} = 0.0471, wR_{ref} = 0.1376, T = 293 K.

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\textsubscript{2}CO\textsubscript{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 SADABBS-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...
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 field 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(H11···N2) = 2.47 Å, C20–H20···N3 hydrogen bond (d(H20···N3) = 2.60 Å.

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**References**


