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The crystal structure of 1-benzyl-4-(2-(phenylethynyl)phenyl)-1*H*-1,2,3-triazole, C₂₃H₁₇N₃

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Abstract

C₂₃H₁₇N₃, monoclinic, *P*2₁ (no. 4), *a* = 11.7817(14) Å, *b* = 5.3165(6) Å, *c* = 14.1747(16) Å, β = 95.731(2)°, *V* = 883.43(18) Å³, *Z* = 2, *R*_{gt}(*F*) = 0.0663, *wR*_{ref}(*F*²) = 1567, *T* = 298(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

CuI (0.019 g; 0.1 mmol) was added to a solution of 1-ethynyl-2-(phenylethynyl)benzene (0.202 g; 1 mmol) and benzyl azide (0.133 g; 1 mmol) in 5 mL DMF. The mixture was stirred at room temperature under argon atmosphere. After completion of the reaction, the residue was diluted with water and

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.13 × 0.12 × 0.10 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.08 mm ^{−1}
Diffractometer, scan mode:	Bruker SMART APEX-II, φ and ω
θ _{max} , completeness:	27.5°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	6342, 3896, 0.086
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2690
<i>N</i> (<i>param</i>) _{refined} :	235
Programs:	Bruker [1], SHELX [2–5], Olex2 [6], PLATON [7]

extracted with ethyl acetate. The organic layer was combined and washed with brine, dried over MgSO₄, then filtered off and evaporated under reduced pressure to give a crude oil, which was further purified by flash chromatography (ethyl acetate/petroleum ether, *V/V* = 1:10) to obtain 1-benzyl-4-(2-(phenylethynyl)phenyl)-1*H*-1,2,3-triazole as a white solid. Crystals of the title compound were grown through slow evaporation of a dichloromethane/methanol solution (*V/V* = 1:5) at 25 °C for five days.

Experimental details

Hydrogen atoms bonded to carbon atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms with C–H = 0.93 Å (aromatic), 0.97 Å (methylene) and *U*_{iso}(H) = 1.2*U*_{eq}(all the carbon atoms). In cases where the anomalous scattering power is too low, its Flack parameter is meaningless. In the absence of significant anomalous scattering, the value of the refined Flack parameter is meaningless.

Comment

1,2,3-Triazoles have received considerable attention because they exhibit a wide range of applications in medicinal chemistry [8], materials chemistry [9] and other fields [10]. Cu(I)-catalyzed alkyne azide cycloaddition is the most classic method for synthesis of 1,4-disubstituted 1,2,3-triazoles. The structures of 1,2,3-triazoles and their assemblies are important for their diverse properties, especially for metal-coordination [11] and biological activity [8]. In continuation of our investigations on 1,2,3-triazole and related heterocycles chemistry [12], we synthesized the title compound (I) and obtained its crystal structure.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	0.3291(3)	0.6785(7)	0.7662(3)	0.0460(9)
C2	0.3617(3)	0.8472(8)	0.6976(3)	0.0478(9)
C3	0.2846(3)	1.0328(8)	0.6602(3)	0.0570(11)
H3	0.3067	1.1450	0.6151	0.068*
C4	0.1769(3)	1.0501(9)	0.6895(3)	0.0651(12)
H4	0.1264	1.1733	0.6647	0.078*
C5	0.1449(3)	0.8831(9)	0.7560(3)	0.0667(13)
H5	0.0720	0.8932	0.7756	0.080*
C6	0.2187(3)	0.7015(9)	0.7939(3)	0.0593(11)
H6	0.1950	0.5914	0.8390	0.071*
C7	0.4726(3)	0.8410(8)	0.6632(3)	0.0507(10)
C8	0.5636(3)	0.8481(8)	0.6338(3)	0.0512(10)
C9	0.6760(3)	0.8587(8)	0.6024(3)	0.0479(9)
C10	0.7604(4)	0.6921(9)	0.6379(3)	0.0667(12)
H10	0.7436	0.5679	0.6806	0.080*
C11	0.8687(4)	0.7099(11)	0.6102(4)	0.0746(13)
H11	0.9246	0.5970	0.6343	0.090*
C12	0.8950(4)	0.8899(10)	0.5483(3)	0.0686(13)
H12	0.9688	0.9026	0.5309	0.082*
C13	0.8126(4)	1.0517(10)	0.5119(3)	0.0752(14)
H13	0.8300	1.1722	0.4680	0.090*
C14	0.7032(4)	1.0398(9)	0.5392(3)	0.0635(12)
H14	0.6482	1.1541	0.5147	0.076*
C15	0.4042(3)	0.4856(7)	0.8118(3)	0.0448(9)
C16	0.5104(3)	0.4014(8)	0.7972(3)	0.0524(10)
H16	0.5557	0.4587	0.7516	0.063*
C17	0.6416(3)	0.0723(8)	0.8775(3)	0.0545(10)
H17A	0.6485	−0.0375	0.8237	0.065*
H17B	0.6378	−0.0319	0.9332	0.065*
C18	0.7446(3)	0.2417(7)	0.8916(3)	0.0451(9)
C19	0.7519(3)	0.4251(8)	0.9598(3)	0.0566(11)
H19	0.6926	0.4451	0.9978	0.068*
C20	0.8456(3)	0.5799(9)	0.9727(3)	0.0668(13)
H20	0.8491	0.7044	1.0190	0.080*
C21	0.9341(3)	0.5508(9)	0.9173(4)	0.0662(13)
H21	0.9976	0.6553	0.9259	0.079*
C22	0.9282(3)	0.3688(10)	0.8500(3)	0.0651(12)
H22	0.9882	0.3484	0.8127	0.078*
C23	0.8338(3)	0.2129(9)	0.8360(3)	0.0582(11)
H23	0.8304	0.0893	0.7894	0.070*
N1	0.3703(3)	0.3483(8)	0.8846(2)	0.0630(10)
N2	0.4501(3)	0.1879(8)	0.9149(2)	0.0645(10)
N3	0.5365(3)	0.2219(6)	0.8607(2)	0.0510(8)

Compound (I) was crystallized in the noncentrosymmetric *P*2₁ space group with one complete molecule in its asymmetric unit. All bond lengths in (I) are in normal ranges and similar to some known analogs [13]. The C1–C6 and C9–C14 benzene rings are nearly coplanar with a dihedral angle of 5.54(1)° between them. The C18–C23 benzene ring on the benzyl group is approximately perpendicular to the other two benzene rings with the dihedral angles of 79.74° and 80.42° between them. The 1,2,3-triazole ring and the corresponding linked benzene ring are approximately, the dihedral angle is

6.67°, and the nitrogen atoms in the 1,2,3-triazole ring are not facing the alkyne moiety because of electron repulsion.

In the crystal packing, the molecules are linked by weak intermolecular interactions. For instance, a $\pi \cdots \pi$ stacking interaction is observed between the triazole and C1–C6 benzene ring (symmetry code: *x*, 1 + *y*, *z*, centroid-to-centroid = 3.753(2) Å [7]. In addition, weak intermolecular C19–H19 $\cdots$ N2 (1 − *x*, −1/2 + *y*, −*z*) and C17–H17 $\cdots$ N1 (1 − *x*, −1/2 + *y*, −*z*) hydrogen bonds form hydrogen-bonded helices that extend along the *a*-axis.

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