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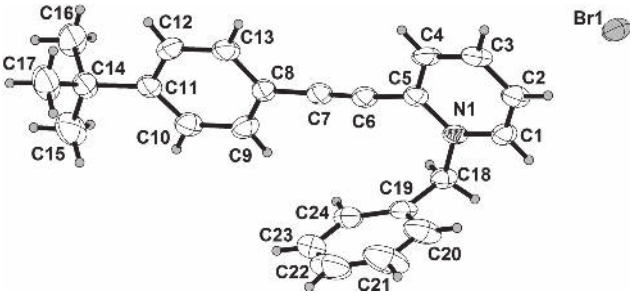
The crystal structure of 1-benzyl-2-((4-(tert-butyl) phenyl)ethynyl)pyridin-1-ium bromide, $C_{24}H_{24}BrN$



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Abstract

$C_{24}H_{24}BrN$, orthorhombic, $P2_1/n$ (no. 14), $a = 9.875(6)$ Å, $b = 10.415(6)$ Å, $c = 20.562(12)$ Å, $\beta = 98.130(7)°$, $V = 2094(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0367$, $wR_{ref}(F^2) = 0.1044$, $T = 273(2)$ 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

2-((4-(*tert*-Butyl)phenyl)ethynyl)pyridine [3] (1.0 mmol) and (bromomethyl)benzene (1.2 mmol) were dissolved in 25 mL acetone. The reaction mixture was stirred at room temperature for 12 h. Upon the reaction completion (monitored by TLC), the mixture was filtered and washed with acetone to obtain the 1-benzyl-2-((4-(*tert*-butyl)phenyl)ethynyl)pyridin-1-

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.26 × 0.22 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.97 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.5°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	20663, 4052, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3368
$N(param)_{refined}$:	238
Programs:	Bruker [1], SHELX [2]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Br1	0.21114(2)	1.25943(2)	0.51416(2)	0.05462(13)
N1	0.22566(19)	0.70650(18)	0.44933(9)	0.0380(4)
C1	0.1538(2)	0.8163(2)	0.46128(13)	0.0478(6)
H1	0.062214	0.810955	0.466980	0.057*
C2	0.2180(3)	0.9313(2)	0.46458(13)	0.0526(7)
H2	0.171166	1.006162	0.472030	0.063*
C3	0.3595(3)	0.9354(2)	0.45637(13)	0.0535(7)
H3	0.404246	1.014232	0.458974	0.064*
C4	0.4335(3)	0.8237(2)	0.44442(13)	0.0501(6)
H4	0.525395	0.828388	0.439128	0.060*
C5	0.3655(2)	0.7075(2)	0.44084(11)	0.0389(5)
C6	0.4386(2)	0.5909(2)	0.42822(11)	0.0436(6)
C7	0.5118(2)	0.5004(2)	0.41617(11)	0.0439(6)
C8	0.6019(2)	0.3950(2)	0.39733(11)	0.0417(5)
C9	0.5511(3)	0.2720(2)	0.38968(14)	0.0496(6)
H5	0.464283	0.251509	0.399157	0.059*
C10	0.6398(3)	0.1742(2)	0.36588(13)	0.0514(6)
H6	0.604788	0.091329	0.361271	0.062*
C11	0.7788(2)	0.1936(2)	0.34850(11)	0.0453(6)
C12	0.8281(3)	0.3163(3)	0.35956(14)	0.0550(7)
H7	0.916300	0.336202	0.351937	0.066*
C13	0.7424(3)	0.4155(3)	0.38328(13)	0.0534(7)
H8	0.779318	0.497431	0.389973	0.064*
C14	0.8759(3)	0.0897(3)	0.31638(13)	0.0566(7)
C15	0.8036(4)	−0.0383(3)	0.3088(2)	0.0890(12)
H9	0.784466	−0.067057	0.350943	0.134*
H10	0.860995	−0.099931	0.291243	0.134*

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
H11	0.719442	−0.029320	0.279507	0.134*
C16	0.9911(3)	0.0668(4)	0.35920(17)	0.0916(13)
H12	0.966574	0.037312	0.400200	0.137*
H13	1.043356	0.144543	0.366298	0.137*
H14	1.044894	0.002362	0.341388	0.137*
C17	0.9386(4)	0.1364(4)	0.24807(15)	0.0806(10)
H15	0.991523	0.067890	0.233124	0.121*
H16	0.995701	0.210482	0.257747	0.121*
H17	0.864293	0.157327	0.214402	0.121*
C18	0.1496(2)	0.5844(2)	0.44285(12)	0.0433(6)
H18	0.058919	0.594386	0.455147	0.052*
H19	0.198088	0.517801	0.469731	0.052*
C19	0.1424(2)	0.5543(2)	0.37125(13)	0.0470(6)
C20	0.0685(4)	0.6348(3)	0.33529(16)	0.0759(10)
H20	0.024044	0.703596	0.351891	0.091*
C21	0.0619(5)	0.6092(4)	0.27036(19)	0.1045(14)
H21	0.009321	0.664781	0.241722	0.125*
C22	0.1279(4)	0.5045(5)	0.24074(18)	0.0976(14)
H22	0.117551	0.497500	0.195217	0.117*
C23	0.1992(3)	0.4226(4)	0.2756(2)	0.0878(12)
H23	0.241931	0.353304	0.258474	0.105*
C24	0.2067(3)	0.4477(3)	0.34192(15)	0.0648(8)
H24	0.257627	0.390882	0.370513	0.078*

ium bromide as a yellow solid. Crystals of the title compound were obtained by slow evaporation of a water solution within 2 weeks.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. Some bad points were removed during the refinement.

Comment

Molecules and materials with phenylene ethynylene linkages have been widely used as (opto-)electronic materials [4], molecular wires [5–7], emissive devices and sensors [8, 9]. *N*-Heteroaromatic cations, species with quaternary pyridine-type nitrogen atoms, are of considerable interest due to their rich application potential [10–12]. Recently the synthesis of nitrogen heteroaromatic cations by [2+2+2] cycloaddition was reported. The product is comparable with the title compound [13]. Encouraged by the excellent photophysical properties of phenylene ethynylene molecules and rich application potential of nitrogen heteroaromatic cations, we synthesized the phenylene ethynylene linked pyridinium derivatives. The title compound, built up by the $C_{24}H_{24}BrN$ molecules, has been synthesized. The single crystal structure verifies that all bond lengths are in normal ranges [13].

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