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2-[4-(Azidomethyl)phenyl]benzonitrile

Bo Peng

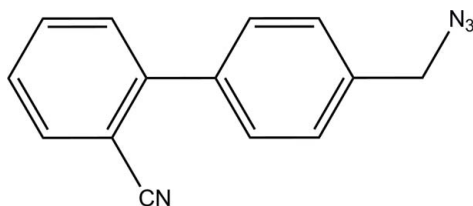
 Department of Applied Chemistry, Nanjing College of Chemical Technology,
 Nanjing 210048, People's Republic of China
 Correspondence e-mail: pengbnjcc@126.com

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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.058; wR factor = 0.146; data-to-parameter ratio = 16.9.

The title compound, $\text{C}_{14}\text{H}_{10}\text{N}_4$, was obtained by a reaction of 4'-(bromomethyl)biphenyl-2-carbonitrile and sodium azide. The dihedral angle between the benzene rings is $46.41(7)^\circ$. Weak intermolecular $\text{C}-\text{H}\cdots\pi$ interactions occur in the crystal.

Related literature

 For background literature, see: Haertling (1999); Homes *et al.* (2001).


Experimental

Crystal data

 $\text{C}_{14}\text{H}_{10}\text{N}_4$
 $M_r = 234.26$

 Triclinic, $P\bar{1}$
 $a = 8.0763(16)$ Å

 $b = 8.2183(16)$ Å
 $c = 10.116(2)$ Å
 $\alpha = 76.22(3)^\circ$
 $\beta = 69.36(3)^\circ$
 $\gamma = 85.94(3)^\circ$
 $V = 610.2(2)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

 Rigaku Mercury2 diffractometer
 6204 measured reflections
 2748 independent reflections

 1559 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.146$
 $S = 1.02$
 2748 reflections

 163 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 C_g is the centroid of the C7–C12 benzene ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C14}-\text{H14B}\cdots\text{Cg}^i$	0.97	2.75	3.642 (3)	154

 Symmetry code: (i) $-x + 1, -y + 1, -z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5575).

References

- Haertling, G. H. (1999). *J. Am. Ceram. Soc.* **82**, 797–810.
 Homes, C. C., Vogt, T., Shapiro, S. M., Wakimoto, S. & Ramirez, A. P. (2001). *Science*, **293**, 673–676.
 Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

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2-[4-(Azidomethyl)phenyl]benzotrile

Bo Peng

Comment

At present, much attention in ferroelectric material field is focused on developing ferroelectric pure organic or inorganic compounds (Haertling *et al.* 1999; Homes *et al.* 2001). In order to find more dielectric ferroelectric materials, we investigate the physical properties of the title compound (Fig. 1). The dielectric constant of the title compound as a function of temperature indicates that the permittivity is basically temperature-independent (dielectric constant equaling to 3.5 to 4.8), suggesting that this compound should be not a real ferroelectrics or there may be no distinct phase transition occurred within the measured temperature range. Similarly, below the melting point (373 K) of the compound, the dielectric constant as a function of temperature also goes smoothly, and there is no dielectric anomaly observed (dielectric constant equaling to 3.5 to 4.8). Herein, we report the synthesis and crystal structure of the title compound, 2-[4-(azidomethyl)phenyl]benzotrile.

Molecules of the title compound have normal geometric parameters. The bond lengths and angles are within their normal ranges. All benzene rings are planar and the azide group is linear. The dihedral angle between the benzene rings in the molecule is 46.41 (7). Dipole–dipole and van der Waals interactions are effective in the molecular packing.

Experimental

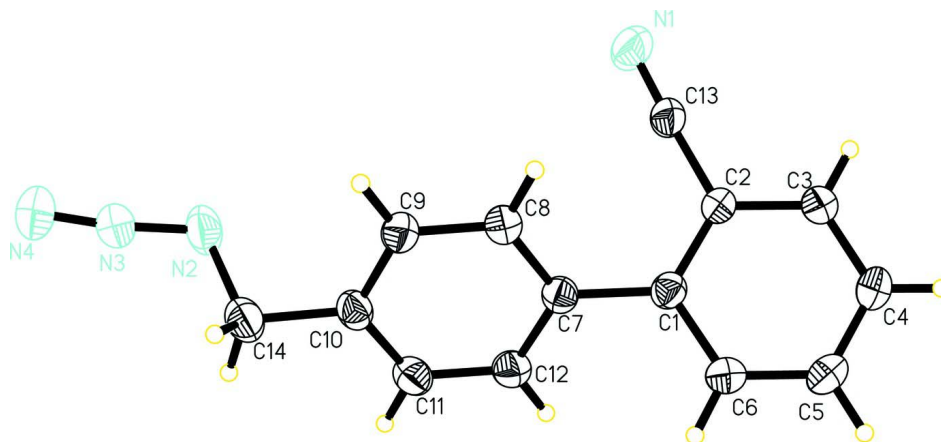
To a stirred solution of 4'-(bromomethyl)biphenyl-2-carbonitrile (5.42 g, 0.02 mol) in 30 mL of methanol, sodium azide (1.3 g, 0.02 mol) was added at the room temperature. The temperature was raised to 50°C in half an hour gradually and the mixture was stirred at this temperature for 12 h. The precipitate was filtered and washed with a small amount of water. The title compound was isolated using column chromatography (Petroleum ether: ethyl acetate-4:1). Single crystals suitable for X-ray diffraction analysis were obtained

Refinement

The H-atoms bonded to the C-atom were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).


Figure 1

Perspective structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

2-[4-(Azidomethyl)phenyl]benzonitrile

Crystal data

$C_{14}H_{10}N_4$

$M_r = 234.26$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.0763\ (16)\ \text{\AA}$

$b = 8.2183\ (16)\ \text{\AA}$

$c = 10.116\ (2)\ \text{\AA}$

$\alpha = 76.22\ (3)^\circ$

$\beta = 69.36\ (3)^\circ$

$\gamma = 85.94\ (3)^\circ$

$V = 610.2\ (2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 244$

$D_x = 1.275\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2748 reflections

$\theta = 2.6\text{--}27.4^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, colorless

$0.20 \times 0.20 \times 0.20\ \text{mm}$

Data collection

Rigaku Mercury2
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $13.6612\ \text{pixels mm}^{-1}$

CCD_Profile_fitting scans

6204 measured reflections

2748 independent reflections

1559 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\text{max}} = 27.4^\circ$, $\theta_{\text{min}} = 3.5^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.058$

$wR(F^2) = 0.146$

$S = 1.02$

2748 reflections

163 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.0517P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.14\ \text{e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.21\ \text{e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C7	0.0733 (2)	0.6414 (2)	0.1795 (2)	0.0441 (5)
C1	-0.0353 (2)	0.7492 (2)	0.2778 (2)	0.0444 (5)
C9	0.2358 (3)	0.3876 (2)	0.1389 (2)	0.0519 (5)
H9A	0.2727	0.2827	0.1769	0.062*
C11	0.2308 (3)	0.6036 (3)	-0.0645 (2)	0.0565 (5)
H11A	0.2629	0.6449	-0.1643	0.068*
C8	0.1297 (2)	0.4830 (2)	0.2324 (2)	0.0482 (5)
H8A	0.0957	0.4404	0.3321	0.058*
C3	-0.2866 (3)	0.7958 (2)	0.4875 (2)	0.0545 (5)
H3A	-0.3858	0.7539	0.5675	0.065*
C12	0.1262 (3)	0.7001 (2)	0.0292 (2)	0.0538 (5)
H12A	0.0908	0.8055	-0.0091	0.065*
C6	0.0093 (3)	0.9192 (2)	0.2491 (2)	0.0579 (6)
H6A	0.1082	0.9631	0.1695	0.070*
C2	-0.1865 (2)	0.6899 (2)	0.3994 (2)	0.0446 (5)
C14	0.4070 (3)	0.3449 (3)	-0.1131 (2)	0.0662 (6)
H14A	0.4233	0.4016	-0.2127	0.079*
H14B	0.5220	0.3337	-0.1020	0.079*
C10	0.2877 (2)	0.4470 (2)	-0.0112 (2)	0.0499 (5)
C13	-0.2470 (3)	0.5166 (3)	0.4378 (2)	0.0555 (5)
C5	-0.0900 (3)	1.0228 (3)	0.3361 (2)	0.0655 (6)
H5A	-0.0571	1.1349	0.3142	0.079*
C4	-0.2381 (3)	0.9620 (2)	0.4556 (2)	0.0612 (6)
H4A	-0.3041	1.0327	0.5137	0.073*
N1	-0.2994 (3)	0.3814 (2)	0.4726 (2)	0.0849 (7)
N3	0.4183 (2)	0.0789 (2)	-0.14723 (19)	0.0640 (5)
N2	0.3271 (3)	0.1777 (2)	-0.0802 (2)	0.0799 (6)
N4	0.4870 (3)	-0.0238 (3)	-0.2027 (3)	0.1025 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.0391 (10)	0.0458 (11)	0.0475 (11)	0.0000 (8)	-0.0138 (9)	-0.0123 (9)
C1	0.0476 (11)	0.0399 (10)	0.0465 (11)	0.0041 (9)	-0.0176 (9)	-0.0100 (9)
C9	0.0494 (11)	0.0464 (11)	0.0566 (13)	0.0062 (9)	-0.0146 (10)	-0.0128 (10)
C11	0.0573 (12)	0.0613 (13)	0.0447 (11)	-0.0030 (11)	-0.0098 (10)	-0.0113 (10)
C8	0.0487 (11)	0.0478 (11)	0.0465 (11)	0.0024 (9)	-0.0139 (10)	-0.0123 (9)

C3	0.0575 (12)	0.0490 (12)	0.0486 (12)	0.0016 (10)	-0.0079 (10)	-0.0120 (10)
C12	0.0551 (12)	0.0487 (11)	0.0511 (12)	0.0022 (10)	-0.0140 (10)	-0.0062 (10)
C6	0.0596 (13)	0.0462 (11)	0.0567 (13)	-0.0065 (10)	-0.0073 (11)	-0.0084 (10)
C2	0.0479 (11)	0.0382 (10)	0.0467 (11)	0.0005 (9)	-0.0140 (9)	-0.0114 (9)
C14	0.0547 (13)	0.0708 (15)	0.0653 (15)	-0.0037 (12)	-0.0034 (11)	-0.0266 (12)
C10	0.0395 (10)	0.0560 (12)	0.0525 (12)	-0.0037 (9)	-0.0080 (9)	-0.0202 (10)
C13	0.0507 (12)	0.0486 (12)	0.0593 (13)	0.0009 (10)	-0.0055 (10)	-0.0185 (11)
C5	0.0763 (16)	0.0402 (11)	0.0744 (16)	-0.0047 (11)	-0.0167 (13)	-0.0153 (11)
C4	0.0704 (14)	0.0466 (12)	0.0632 (14)	0.0088 (11)	-0.0148 (12)	-0.0212 (11)
N1	0.0769 (14)	0.0530 (12)	0.1028 (17)	-0.0111 (11)	0.0031 (12)	-0.0261 (12)
N3	0.0634 (12)	0.0643 (12)	0.0597 (12)	0.0051 (10)	-0.0131 (10)	-0.0197 (10)
N2	0.0686 (12)	0.0743 (13)	0.0863 (14)	-0.0054 (11)	0.0052 (11)	-0.0461 (12)
N4	0.1053 (18)	0.0736 (15)	0.1081 (19)	0.0189 (14)	-0.0048 (15)	-0.0375 (14)

Geometric parameters (Å, °)

C7—C8	1.395 (2)	C12—H12A	0.9300
C7—C12	1.397 (3)	C6—C5	1.381 (3)
C7—C1	1.496 (2)	C6—H6A	0.9300
C1—C6	1.403 (2)	C2—C13	1.456 (3)
C1—C2	1.408 (3)	C14—N2	1.474 (3)
C9—C8	1.389 (2)	C14—C10	1.514 (3)
C9—C10	1.395 (3)	C14—H14A	0.9700
C9—H9A	0.9300	C14—H14B	0.9700
C11—C10	1.386 (3)	C13—N1	1.146 (2)
C11—C12	1.393 (3)	C5—C4	1.385 (3)
C11—H11A	0.9300	C5—H5A	0.9300
C8—H8A	0.9300	C4—H4A	0.9300
C3—C4	1.378 (3)	N3—N4	1.128 (2)
C3—C2	1.403 (2)	N3—N2	1.220 (2)
C3—H3A	0.9300		
C8—C7—C12	117.61 (17)	C1—C6—H6A	119.2
C8—C7—C1	122.25 (17)	C3—C2—C1	121.39 (17)
C12—C7—C1	120.11 (17)	C3—C2—C13	117.21 (17)
C6—C1—C2	116.68 (17)	C1—C2—C13	121.39 (16)
C6—C1—C7	120.17 (17)	N2—C14—C10	109.67 (17)
C2—C1—C7	123.13 (16)	N2—C14—H14A	109.7
C8—C9—C10	120.86 (18)	C10—C14—H14A	109.7
C8—C9—H9A	119.6	N2—C14—H14B	109.7
C10—C9—H9A	119.6	C10—C14—H14B	109.7
C10—C11—C12	120.88 (19)	H14A—C14—H14B	108.2
C10—C11—H11A	119.6	C11—C10—C9	118.27 (17)
C12—C11—H11A	119.6	C11—C10—C14	120.86 (19)
C9—C8—C7	121.18 (18)	C9—C10—C14	120.84 (19)
C9—C8—H8A	119.4	N1—C13—C2	177.4 (2)
C7—C8—H8A	119.4	C6—C5—C4	120.90 (19)
C4—C3—C2	120.07 (19)	C6—C5—H5A	119.6
C4—C3—H3A	120.0	C4—C5—H5A	119.6
C2—C3—H3A	120.0	C3—C4—C5	119.36 (19)

C11—C12—C7	121.20 (19)	C3—C4—H4A	120.3
C11—C12—H12A	119.4	C5—C4—H4A	120.3
C7—C12—H12A	119.4	N4—N3—N2	172.5 (2)
C5—C6—C1	121.59 (19)	N3—N2—C14	115.65 (18)
C5—C6—H6A	119.2		

Hydrogen-bond geometry (Å, °)

C_g is the centroid of the C7–C12 benzene ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C14—H14B \cdots Cg ⁱ	0.97	2.75	3.642 (3)	154

Symmetry code: (i) $-x+1, -y+1, -z$.