



Crystal structure of [1,1'-biphenyl]-2,2'-dicarbonitrile

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Received 12 May 2015; accepted 19 May 2015

Edited by M. Weil, Vienna University of Technology, Austria

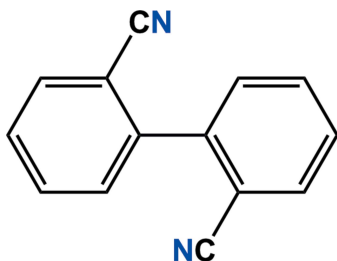
The complete molecule of the title compound, $C_{14}H_8N_2$, is generated by a twofold rotation axis located at the midpoint of the biphenyl C—C bond. The dihedral angle between the symmetry-related phenyl rings is $46.16(3)^\circ$. In the crystal, molecules are linked by slipped parallel π – π interactions [centroid–centroid distance = $3.9451(7)$ Å, normal distance = $3.6293(5)$ Å, slippage 1.547 Å], forming columns along the b -axis direction.

Keywords: crystal structure; biphenyl; π – π contacts.

CCDC reference: 1401615

1. Related literature

The title compound has been used as a reactant for phthalocyanine synthesis (Shimizu *et al.*, 2011, 2014). Related crystal structures were reported by Furukawa *et al.* (2008) and Paek *et al.* (1989). For synthetic details, see: Wu *et al.* (2007).



2. Experimental

2.1. Crystal data

$C_{14}H_8N_2$	$V = 1012.93(9)$ Å ³
$M_r = 204.22$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 15.7839(9)$ Å	$\mu = 0.08$ mm ^{−1}
$b = 3.9451(2)$ Å	$T = 173$ K
$c = 16.6079(9)$ Å	$0.43 \times 0.12 \times 0.06$ mm
$\beta = 101.630(3)^\circ$	

2.2. Data collection

Bruker APEXII CCD diffractometer	4708 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	1157 independent reflections
$T_{\min} = 0.966$, $T_{\max} = 0.995$	988 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	73 parameters
$wR(F^2) = 0.116$	H-atom parameters constrained
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.21$ e Å ^{−3}
1157 reflections	$\Delta\rho_{\text{min}} = -0.24$ e Å ^{−3}

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: DIAMOND (Brandenburg, 2010); software used to prepare material for publication: SHELXTL.

Acknowledgements

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2014R1A1A4A01009105).

Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5163).

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supporting information

Acta Cryst. (2015). E71, o430 [doi:10.1107/S2056989015009561]

Crystal structure of [1,1'-biphenyl]-2,2'-dicarbonitrile

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S1. Experimental

The title compound was prepared by Suzuki coupling reaction of 2-bromobenzonitrile and 2-cyanophenyl boronic acid in acetonitrile (Wu *et al.*, 2007). Slow evaporation of a solution in acetone/ethyl acetate gave single crystals suitable for X-ray analysis.

S2. Refinement

All H-atoms were positioned geometrically and refined using a riding model with $d(\text{C—H}) = 0.95 \text{ \AA}$, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

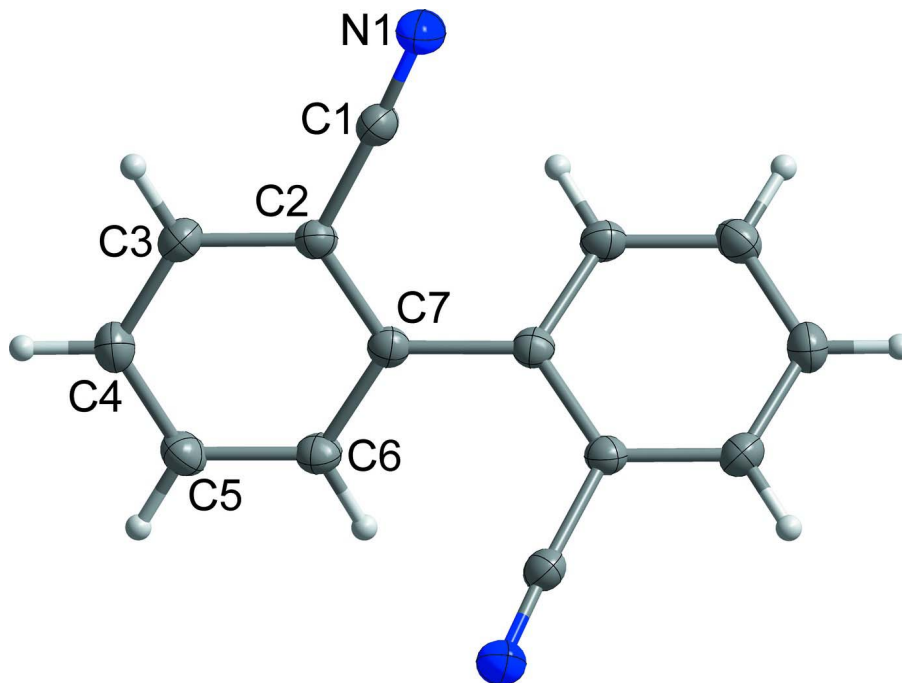
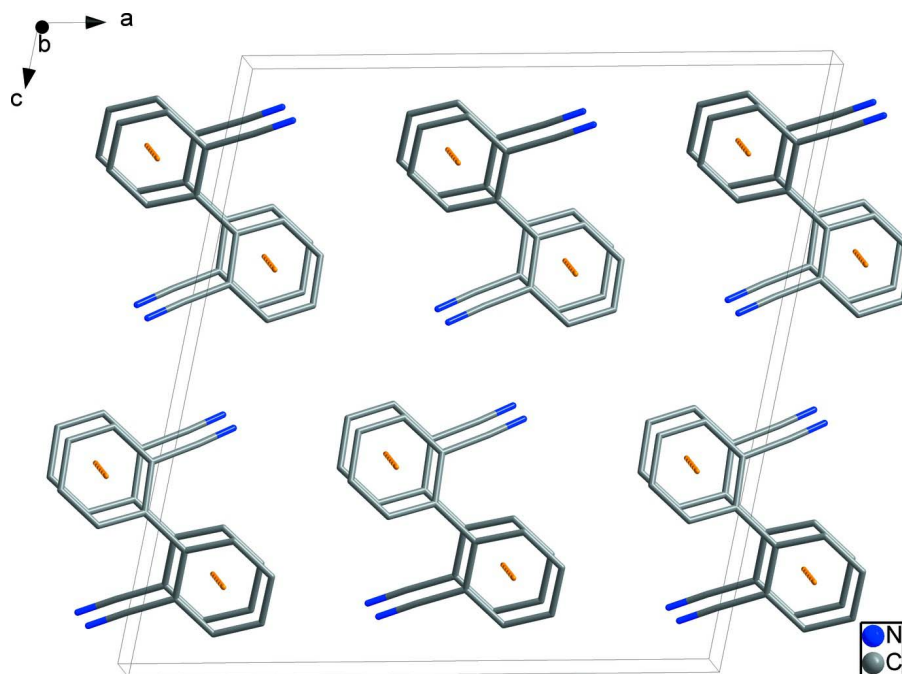


Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius. Symmetry-related atoms (not labelled) are generated by symmetry code $x+1, y, -z+1/2$.

**Figure 2**

Crystal packing viewed along the *b* axis. The intermolecular π - π interactions between the phenyl ring systems [$Cg1 \cdots Cg1^i$, 3.9451 (7) Å; *Cg1* is the centroid of the C2 \cdots C7 ring; symmetry code (i): $x, y - 1, z$] are shown as dashed lines. They link molecules into columns along [010].

[1,1'-Biphenyl]-2,2'-dicarbonitrile

Crystal data

$C_{14}H_8N_2$
 $M_r = 204.22$
 Monoclinic, $C2/c$
 $a = 15.7839$ (9) Å
 $b = 3.9451$ (2) Å
 $c = 16.6079$ (9) Å
 $\beta = 101.630$ (3)°
 $V = 1012.93$ (9) Å³
 $Z = 4$

$F(000) = 424$
 $D_x = 1.339$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 1375 reflections
 $\theta = 3.3$ – 27.5°
 $\mu = 0.08$ mm⁻¹
 $T = 173$ K
 Block, colourless
 $0.43 \times 0.12 \times 0.06$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.966$, $T_{\max} = 0.995$

4708 measured reflections
 1157 independent reflections
 988 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 3.3^\circ$
 $h = -20 \rightarrow 20$
 $k = -5 \rightarrow 1$
 $l = -21 \rightarrow 19$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$ $wR(F^2) = 0.116$ $S = 1.09$

1157 reflections

73 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.5212P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$ *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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.58879 (7)	0.3650 (3)	0.08819 (7)	0.0323 (3)
C1	0.53155 (8)	0.2522 (3)	0.11172 (7)	0.0233 (3)
C2	0.45640 (7)	0.1152 (3)	0.13725 (7)	0.0206 (3)
C3	0.37963 (8)	0.1099 (3)	0.07828 (7)	0.0244 (3)
H3	0.3791	0.1894	0.0242	0.029*
C4	0.30457 (8)	-0.0108 (3)	0.09854 (8)	0.0273 (3)
H4	0.2522	-0.0139	0.0586	0.033*
C5	0.30609 (8)	-0.1274 (3)	0.17741 (8)	0.0257 (3)
H5	0.2545	-0.2117	0.1914	0.031*
C6	0.38225 (8)	-0.1224 (3)	0.23640 (7)	0.0231 (3)
H6	0.3819	-0.2037	0.2902	0.028*
C7	0.45930 (7)	-0.0004 (3)	0.21832 (7)	0.0196 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0275 (6)	0.0450 (7)	0.0253 (6)	-0.0066 (5)	0.0075 (4)	0.0013 (5)
C1	0.0244 (6)	0.0277 (7)	0.0176 (6)	-0.0017 (5)	0.0034 (4)	-0.0014 (5)
C2	0.0208 (6)	0.0225 (6)	0.0194 (6)	-0.0003 (4)	0.0059 (4)	-0.0015 (4)
C3	0.0258 (6)	0.0290 (7)	0.0180 (6)	-0.0002 (5)	0.0037 (5)	0.0003 (4)
C4	0.0214 (6)	0.0331 (7)	0.0255 (7)	-0.0011 (5)	0.0000 (5)	-0.0016 (5)
C5	0.0206 (6)	0.0286 (6)	0.0286 (7)	-0.0028 (5)	0.0069 (5)	-0.0006 (5)
C6	0.0245 (6)	0.0239 (6)	0.0216 (6)	-0.0017 (5)	0.0068 (5)	0.0020 (4)
C7	0.0205 (6)	0.0187 (6)	0.0199 (6)	0.0012 (4)	0.0044 (5)	-0.0013 (4)

Geometric parameters (Å, °)

N1—C1	1.1443 (16)	C4—H4	0.9500
C1—C2	1.4427 (16)	C5—C6	1.3893 (17)
C2—C3	1.3963 (16)	C5—H5	0.9500
C2—C7	1.4135 (16)	C6—C7	1.3957 (16)
C3—C4	1.3800 (17)	C6—H6	0.9500
C3—H3	0.9500	C7—C7 ⁱ	1.488 (2)
C4—C5	1.3839 (18)		
N1—C1—C2	176.92 (12)	C4—C5—C6	120.68 (11)
C3—C2—C7	121.34 (11)	C4—C5—H5	119.7
C3—C2—C1	116.62 (10)	C6—C5—H5	119.7
C7—C2—C1	122.02 (10)	C5—C6—C7	121.38 (11)
C4—C3—C2	120.04 (11)	C5—C6—H6	119.3
C4—C3—H3	120.0	C7—C6—H6	119.3
C2—C3—H3	120.0	C6—C7—C2	116.99 (11)
C3—C4—C5	119.57 (11)	C6—C7—C7 ⁱ	120.90 (12)
C3—C4—H4	120.2	C2—C7—C7 ⁱ	122.09 (12)
C5—C4—H4	120.2		
C7—C2—C3—C4	−0.18 (18)	C5—C6—C7—C7 ⁱ	−179.21 (9)
C1—C2—C3—C4	−178.65 (11)	C3—C2—C7—C6	0.51 (17)
C2—C3—C4—C5	−0.26 (19)	C1—C2—C7—C6	178.91 (11)
C3—C4—C5—C6	0.34 (19)	C3—C2—C7—C7 ⁱ	179.27 (9)
C4—C5—C6—C7	0.02 (19)	C1—C2—C7—C7 ⁱ	−2.34 (15)
C5—C6—C7—C2	−0.44 (17)		

Symmetry code: (i) $-x+1, y, -z+1/2$.