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

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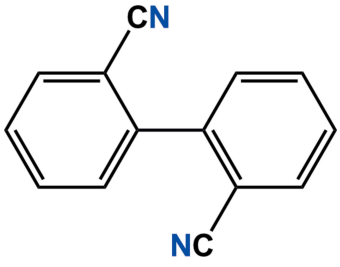
The complete molecule of the title compound, $C_{14}H_8N_2$, is generated by a twofold rotation axis located at the midpoint of the biphenyl C—C bond. The dihedral angle between the symmetry-related phenyl rings is 46.16 (3)°. In the crystal, molecules are linked by slipped parallel π–π interactions [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

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

2.2. Data collection

Bruker APEXII CCD diffractometer
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_{int} = 0.030

2.3. Refinement

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

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

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

Gihaeng Kang, Tae Ho Kim, Youngeun Jeon and Jineun Kim

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(C—H) = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C).

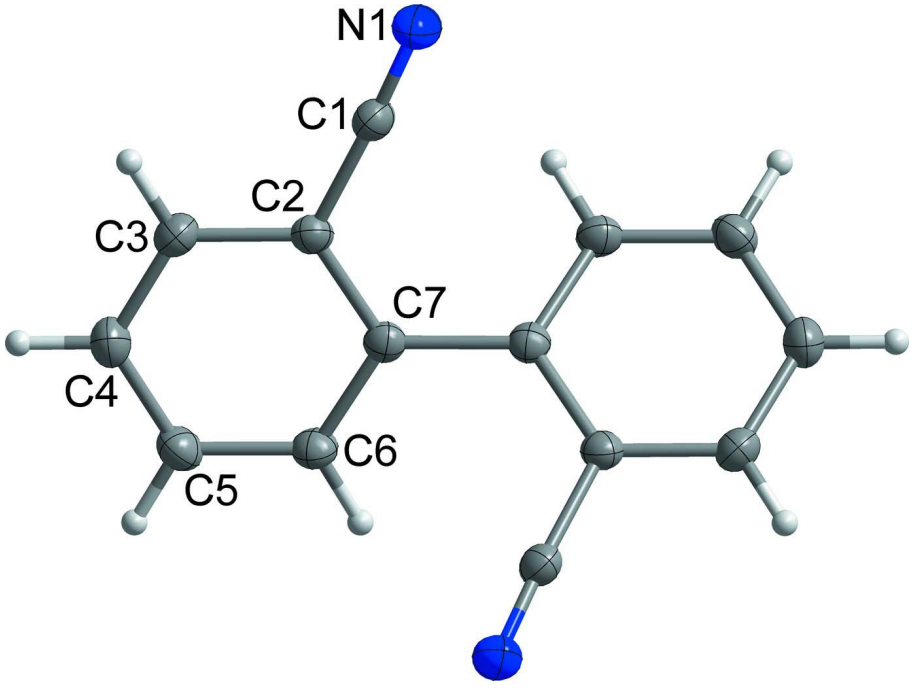

Figure 1

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.

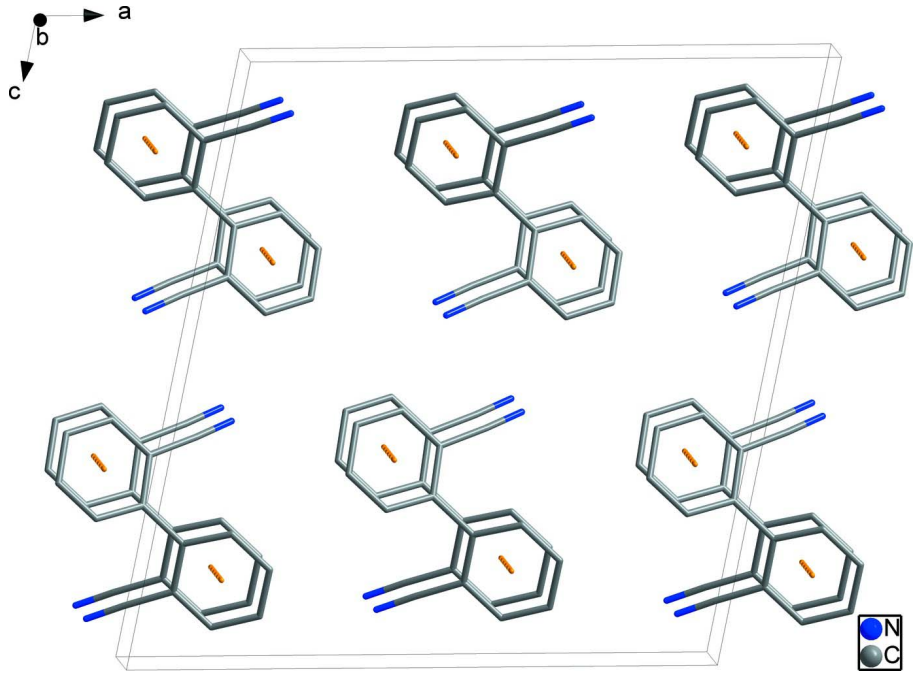

Figure 2

Crystal packing viewed along the *b* axis. The intermolecular π–π interactions between the phenyl ring systems [*Cg*1···*Cg*1^{i}, 3.9451 (7) Å; *Cg*1 is the centroid of the C2···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, *C*2/*c*
a = 15.7839 (9) Å
b = 3.9451 (2) Å
c = 16.6079 (9) Å
β = 101.630 (3)°
V = 1012.93 (9) Å^3
Z = 4
F(000) = 424
D_x = 1.339 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1375 reflections
θ = 3.3–27.5°
μ = 0.08 mm^{-1}
T = 173 K
Block, colourless
0.43 × 0.12 × 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_{int} = 0.030
θ_{max} = 27.6°, θ_{min} = 3.3°
h = −20→20
k = −5→1
l = −21→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 methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.5212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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, º)

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.