Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-Dimethyl-4,4′-bipyridine

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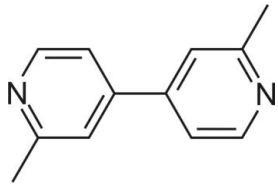
Received 7 May 2008; accepted 12 June 2008

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.001 Å; R factor = 0.045; wR factor = 0.140; data-to-parameter ratio = 25.1.

In the crystal structure of the title compound, $C_{12}H_{12}N_2$, the molecule is twisted around the central C—C bond, with a dihedral angle of 8.32 (5)° between the mean planes of the pyridyl rings. The crystal structure is stabilized by arene stacking interactions, with a distance of 3.81 (1) Å between the ring centroids.

Related literature

For related literature, see: Boag *et al.* (1999); Kraft *et al.* (2005); Leighton & Sanders (1987); Alcade *et al.* (2007); Boghala *et al.* (2005); Braunschweig *et al.* (2006); Diskin-Posner *et al.* (2005); Kryschenko *et al.* (2003); Lynch *et al.* (1999); Yaghi *et al.* (1995).



Experimental

Crystal data

$C_{12}H_{12}N_2$
M_r = 184.24
Orthorhombic, *Pbca*
a = 11.7961 (3) Å
b = 7.6130 (2) Å
c = 21.2977 (5) Å
V = 1912.61 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 (2) K
0.54 × 0.24 × 0.14 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.923, T_{max} = 0.989
26242 measured reflections
3233 independent reflections
2262 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 0.91
3233 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6*C*···N1^{i}	0.98	2.73	3.6728 (16)	161

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-NT* (Bruker, 2004); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Financial support from the German Research Foundation (DFG) under grant No. We 1016-9/1 is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2078).

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supporting information

Acta Cryst. (2008). E**64**, o1287 [doi:10.1107/S1600536808017807]

2,2′-Dimethyl-4,4′-bipyridine

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S1. Comment

The preparation of I was carried out according to the literature procedure (Leighton & Sanders, 1987). The title compound represents a derivative of 4,4′-bipyridine, which is widely used as a bifunctional bridging element for the synthesis of supramolecular assemblies which may be based on hydrogen bond interactions (Lynch *et al.*, 1999, Boghala *et al.*, 2005) or metal coordination complexes (Diskin-Posner *et al.*, 2005, Kryschenko *et al.*, 2003), involving catenanes (Alcade *et al.*, 2007), rotaxanes (Braunschweig *et al.*, 2006) and metal-organic frameworks (Yaghi *et al.*, 1995). In the crystal the title molecule adopts a slightly twisted conformation (see Figure 1), the mean planes of the hetero - aromatic rings make 8.32 (5)° dihedral angle. As there are no good hydrogen bond donors, the N1 nitrogen atom is only involved in the formation of a weak C-H···N hydrogen bond [C6-H6C···N1 distance ca. 2.73 Å]. The packing (Figure 2) is characterized by a columnar arrangement of molecules extending in the direction of the crystallographic *b*-axis. Within the molecular columns only one of the aromatic rings (designated as A in Fig. 1) of related molecules are involved in "face-to-face" interactions with a centroid···centroid distance of 3.81 (1) Å between such rings.

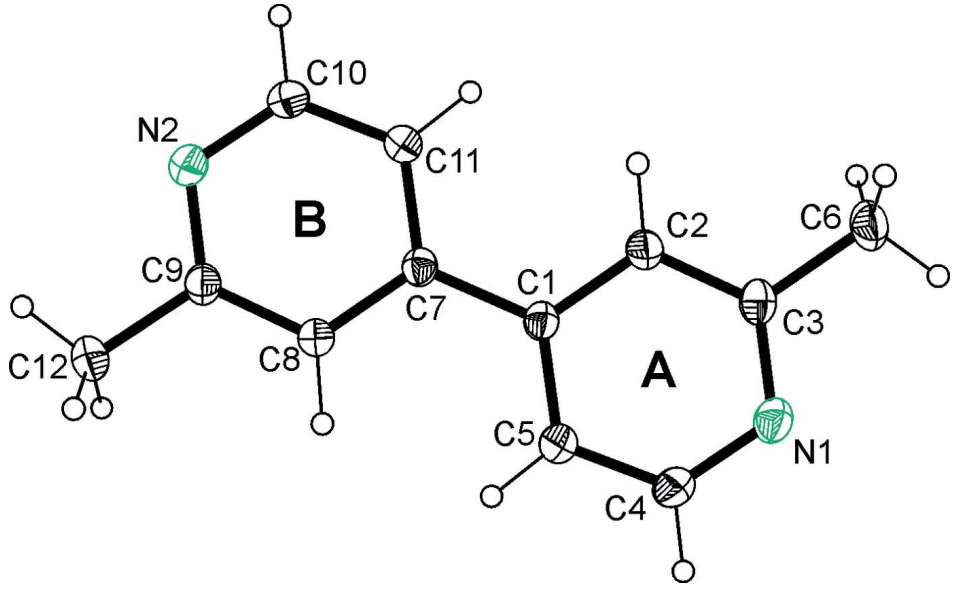

Figure 1

Molecular presentation of the title compound with atomic labels and 50% probability displacement ellipsoids for non H-atoms.

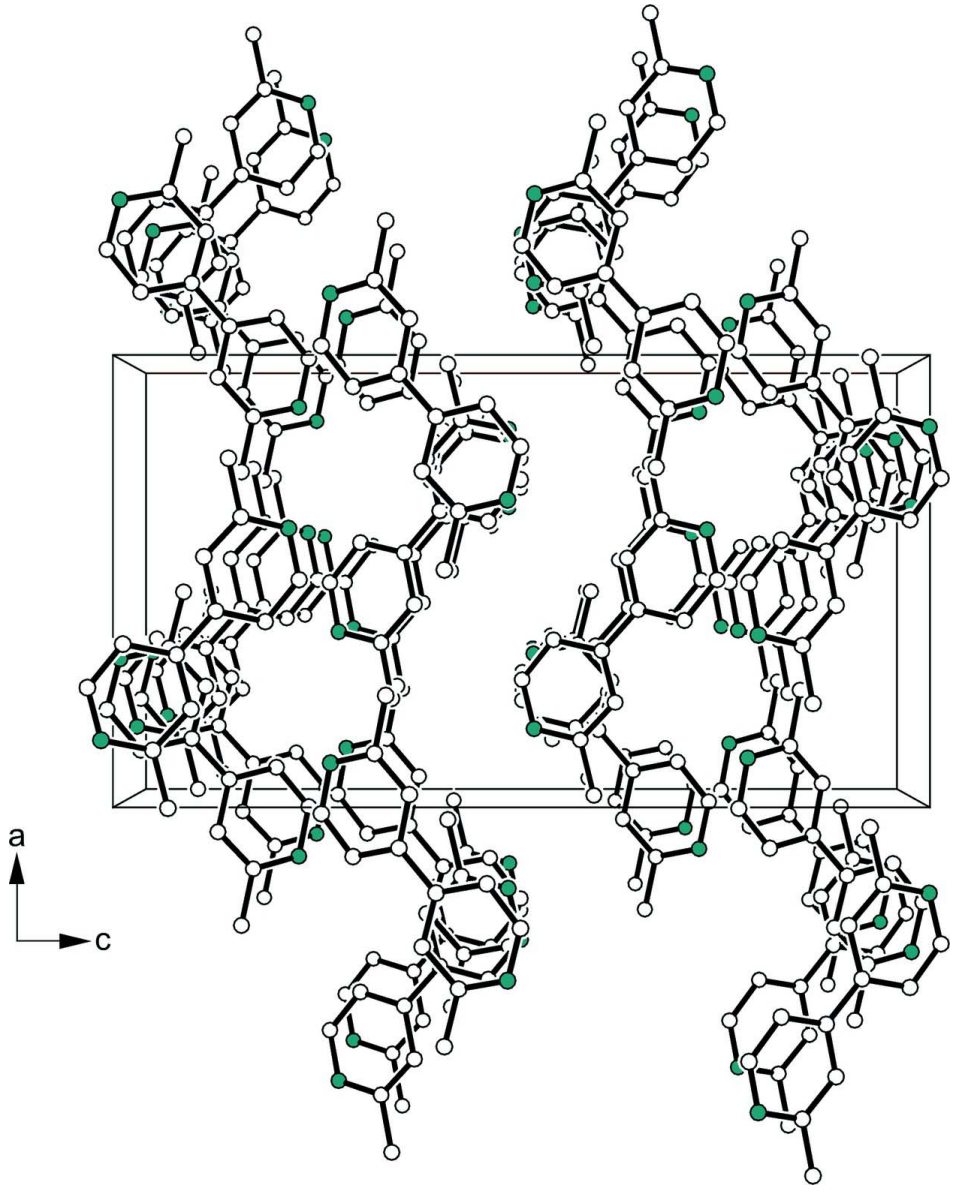

Figure 2

Packing diagram as viewed down the crystallographic *b* axis.

2,2′-Dimethyl-4,4′-bipyridine

Crystal data

$C_{12}H_{12}N_2$
M_r = 184.24
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.7961 (3) Å
b = 7.6130 (2) Å
c = 21.2977 (5) Å
V = 1912.61 (8) Å^3
Z = 8

F(000) = 784
D_x = 1.280 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 5227 reflections
θ = 2.6–31.2°
μ = 0.08 mm^{-1}
T = 153 K
Needle, colourless
0.54 × 0.24 × 0.14 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.924, T_{max} = 0.989
26242 measured reflections
3233 independent reflections
2262 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 31.7°, θ_{min} = 2.6°
h = −17→17
k = −10→11
l = −31→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 0.91
3233 reflections
129 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
$w = 1/[\sigma^2(F_o^2) + (0.0856P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.83087 (7)	0.16449 (12)	0.48415 (4)	0.0253 (2)
N2	0.38746 (7)	−0.09210 (12)	0.27478 (4)	0.0235 (2)
C1	0.65454 (8)	0.06887 (12)	0.40087 (5)	0.0179 (2)
C2	0.76889 (8)	0.05080 (13)	0.38471 (5)	0.0206 (2)
H2	0.7889	0.0062	0.3446	0.025*
C3	0.85371 (8)	0.09788 (13)	0.42717 (5)	0.0215 (2)
C4	0.72102 (9)	0.18301 (15)	0.49892 (5)	0.0269 (2)
H4	0.7034	0.2310	0.5389	0.032*
C5	0.63117 (8)	0.13748 (14)	0.46021 (5)	0.0230 (2)
H5	0.5551	0.1527	0.4738	0.028*
C6	0.97634 (9)	0.07391 (15)	0.41063 (6)	0.0278 (2)
H6A	1.0152	0.1875	0.4127	0.042*
H6B	0.9825	0.0265	0.3680	0.042*
H6C	1.0115	−0.0079	0.4404	0.042*
C7	0.56279 (8)	0.01492 (12)	0.35706 (5)	0.0175 (2)
C8	0.44859 (8)	0.05087 (13)	0.36967 (5)	0.0194 (2)
H8	0.4285	0.1139	0.4065	0.023*
C9	0.36413 (8)	−0.00544 (13)	0.32832 (5)	0.0206 (2)
C10	0.49692 (8)	−0.12586 (15)	0.26316 (5)	0.0247 (2)
H10	0.5148	−0.1876	0.2257	0.030*
C11	0.58594 (8)	−0.07721 (13)	0.30182 (5)	0.0220 (2)
H11	0.6618	−0.1061	0.2909	0.026*
C12	0.24104 (9)	0.02673 (16)	0.34184 (6)	0.0288 (3)
H12A	0.2111	0.1128	0.3119	0.043*
H12B	0.2327	0.0721	0.3847	0.043*

H12C	0.1990	−0.0837	0.3378	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0222 (4)	0.0285 (5)	0.0252 (5)	0.0012 (3)	−0.0059 (4)	−0.0026 (3)
N2	0.0210 (4)	0.0277 (5)	0.0218 (5)	−0.0023 (3)	−0.0015 (3)	−0.0032 (3)
C1	0.0165 (4)	0.0192 (4)	0.0179 (5)	−0.0005 (3)	−0.0014 (3)	0.0009 (3)
C2	0.0178 (4)	0.0245 (5)	0.0196 (5)	−0.0002 (3)	−0.0006 (4)	−0.0001 (3)
C3	0.0185 (4)	0.0220 (5)	0.0241 (5)	−0.0006 (3)	−0.0034 (4)	0.0030 (4)
C4	0.0250 (5)	0.0343 (6)	0.0214 (5)	0.0027 (4)	−0.0038 (4)	−0.0068 (4)
C5	0.0198 (4)	0.0290 (5)	0.0201 (5)	0.0010 (4)	−0.0012 (4)	−0.0027 (4)
C6	0.0173 (5)	0.0353 (6)	0.0310 (6)	0.0003 (4)	−0.0031 (4)	0.0008 (4)
C7	0.0164 (4)	0.0191 (4)	0.0170 (5)	−0.0013 (3)	−0.0009 (3)	0.0021 (3)
C8	0.0172 (4)	0.0221 (5)	0.0189 (5)	0.0002 (3)	−0.0005 (3)	−0.0017 (3)
C9	0.0173 (4)	0.0230 (5)	0.0214 (5)	−0.0002 (3)	−0.0018 (4)	0.0001 (4)
C10	0.0230 (5)	0.0313 (5)	0.0197 (5)	−0.0019 (4)	0.0011 (4)	−0.0053 (4)
C11	0.0182 (4)	0.0281 (5)	0.0196 (5)	−0.0006 (3)	0.0012 (4)	−0.0025 (4)
C12	0.0176 (5)	0.0371 (6)	0.0316 (6)	0.0027 (4)	−0.0023 (4)	−0.0076 (5)

Geometric parameters (Å, º)

N1—C4	1.3408 (13)	C6—H6B	0.9800
N1—C3	1.3426 (14)	C6—H6C	0.9800
N2—C10	1.3395 (13)	C7—C11	1.3967 (14)
N2—C9	1.3459 (13)	C7—C8	1.4006 (13)
C1—C5	1.3949 (14)	C8—C9	1.3971 (14)
C1—C2	1.3989 (13)	C8—H8	0.9500
C1—C7	1.4868 (13)	C9—C12	1.5004 (13)
C2—C3	1.3955 (14)	C10—C11	1.3848 (14)
C2—H2	0.9500	C10—H10	0.9500
C3—C6	1.5000 (14)	C11—H11	0.9500
C4—C5	1.3869 (14)	C12—H12A	0.9800
C4—H4	0.9500	C12—H12B	0.9800
C5—H5	0.9500	C12—H12C	0.9800
C6—H6A	0.9800		
C4—N1—C3	116.47 (9)	H6B—C6—H6C	109.5
C10—N2—C9	116.59 (9)	C11—C7—C8	116.59 (9)
C5—C1—C2	116.77 (9)	C11—C7—C1	121.67 (9)
C5—C1—C7	121.88 (9)	C8—C7—C1	121.73 (9)
C2—C1—C7	121.35 (9)	C9—C8—C7	120.34 (9)
C3—C2—C1	120.44 (10)	C9—C8—H8	119.8
C3—C2—H2	119.8	C7—C8—H8	119.8
C1—C2—H2	119.8	N2—C9—C8	122.59 (9)
N1—C3—C2	122.61 (9)	N2—C9—C12	116.14 (9)
N1—C3—C6	116.85 (9)	C8—C9—C12	121.27 (9)
C2—C3—C6	120.53 (10)	N2—C10—C11	124.74 (10)

N1—C4—C5	124.94 (10)	N2—C10—H10	117.6
N1—C4—H4	117.5	C11—C10—H10	117.6
C5—C4—H4	117.5	C10—C11—C7	119.13 (9)
C4—C5—C1	118.76 (10)	C10—C11—H11	120.4
C4—C5—H5	120.6	C7—C11—H11	120.4
C1—C5—H5	120.6	C9—C12—H12A	109.5
C3—C6—H6A	109.5	C9—C12—H12B	109.5
C3—C6—H6B	109.5	H12A—C12—H12B	109.5
H6A—C6—H6B	109.5	C9—C12—H12C	109.5
C3—C6—H6C	109.5	H12A—C12—H12C	109.5
H6A—C6—H6C	109.5	H12B—C12—H12C	109.5

C5—C1—C2—C3	0.87 (14)	C5—C1—C7—C8	8.36 (15)
C7—C1—C2—C3	−178.28 (9)	C2—C1—C7—C8	−172.52 (9)
C4—N1—C3—C2	0.45 (15)	C11—C7—C8—C9	0.41 (14)
C4—N1—C3—C6	−179.03 (9)	C1—C7—C8—C9	−178.39 (9)
C1—C2—C3—N1	−1.18 (15)	C10—N2—C9—C8	1.31 (15)
C1—C2—C3—C6	178.28 (9)	C10—N2—C9—C12	−178.16 (9)
C3—N1—C4—C5	0.55 (16)	C7—C8—C9—N2	−1.35 (15)
N1—C4—C5—C1	−0.80 (17)	C7—C8—C9—C12	178.10 (9)
C2—C1—C5—C4	0.05 (15)	C9—N2—C10—C11	−0.42 (17)
C7—C1—C5—C4	179.20 (9)	N2—C10—C11—C7	−0.46 (17)
C5—C1—C7—C11	−170.38 (9)	C8—C7—C11—C10	0.43 (14)
C2—C1—C7—C11	8.74 (14)	C1—C7—C11—C10	179.24 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*C*···N1^{i}	0.98	2.73	3.6728 (16)	161

Symmetry code: (i) −*x*+2, −*y*, −*z*+1.