Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-(Piperazine-1,4-diyl)diacetonitrile

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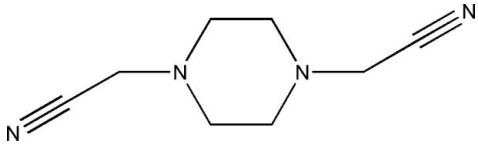
Received 11 May 2012; accepted 14 May 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.150; data-to-parameter ratio = 19.6.

The complete molecule of the title compound, $C_8H_{12}N_4$, is generated by a crystallographic inversion centre. The piperazine ring adopts a chair conformation with the N-bonded substituents in equatorial positions. In the crystal, molecules are linked by C—H$\cdots$N$_c$ (c = cyanide) hydrogen bonds.

Related literature

For related structures, see: Ma *et al.* (2007); Liu & Liu (2011); Luo & Weng (2011).



Experimental

Crystal data

$C_8H_{12}N_4$
M_r = 164.22
Monoclinic, $P2_1/c$
a = 6.3452 (13) Å
b = 6.6731 (13) Å
c = 11.077 (2) Å
β = 95.61 (3)°
V = 466.78 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.985, T_{max} = 0.992
3739 measured reflections
1076 independent reflections
835 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.150
S = 1.05
1076 reflections
55 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$A\cdots$N2^{i}	0.97	2.57	3.427 (2)	147

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

Data collection: *CrystalClear* (Rigaku/MSC, 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: *SHELXL97*.

We gratefully acknowledge financial support from the Doctoral Research Fund of Henan University of Traditional Chinese Medicine.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6795).

References

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supporting information

Acta Cryst. (2012). E**68**, o1798 [doi:10.1107/S1600536812021733]

2,2′-(Piperazine-1,4-diyl)diacetonitrile

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S1. Experimental

Piperazine (25 mmol) and triethylamine (50 mmol), dissolved in 20 ml 95% of ethanol, was added dropwise to the stirred solution of chloroacetonitrile (50 mmol) at reflux. The mixture was stirred for 8 h at reflux. The mixture was stirred overnight at room temperature, evaporated in vacuum and the residue was purified by recrystallization from ethanol to give the title compound. Colourless blocks were grown from dichloromethane/ethanol solution.

S2. Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

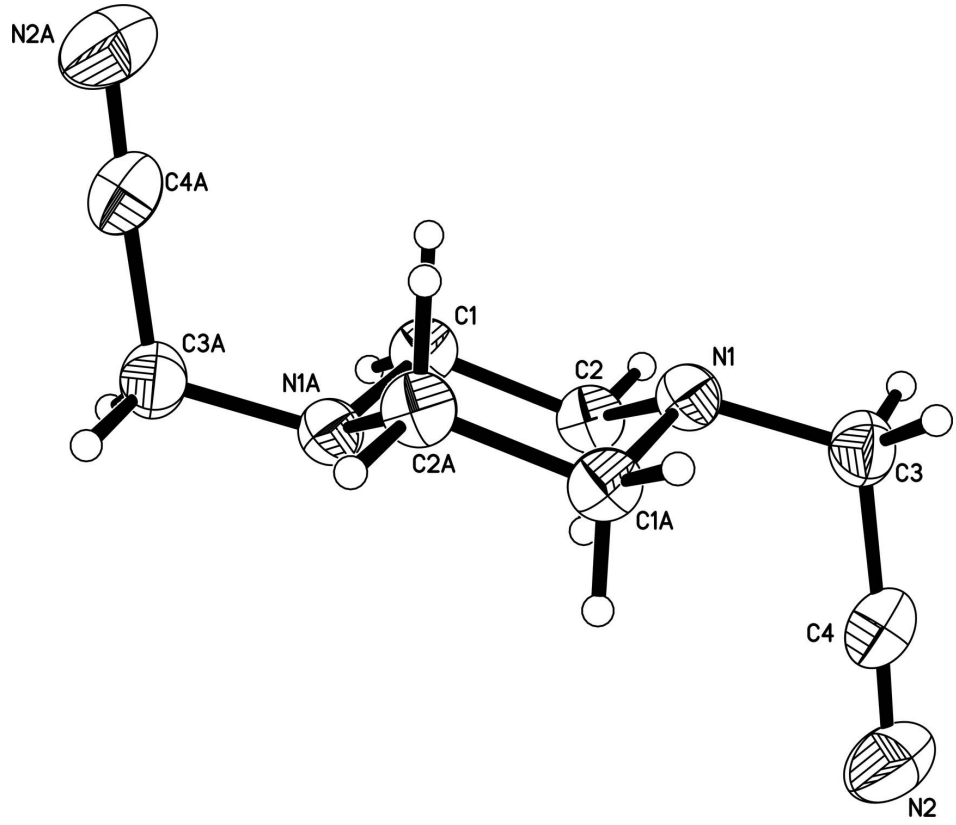

Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

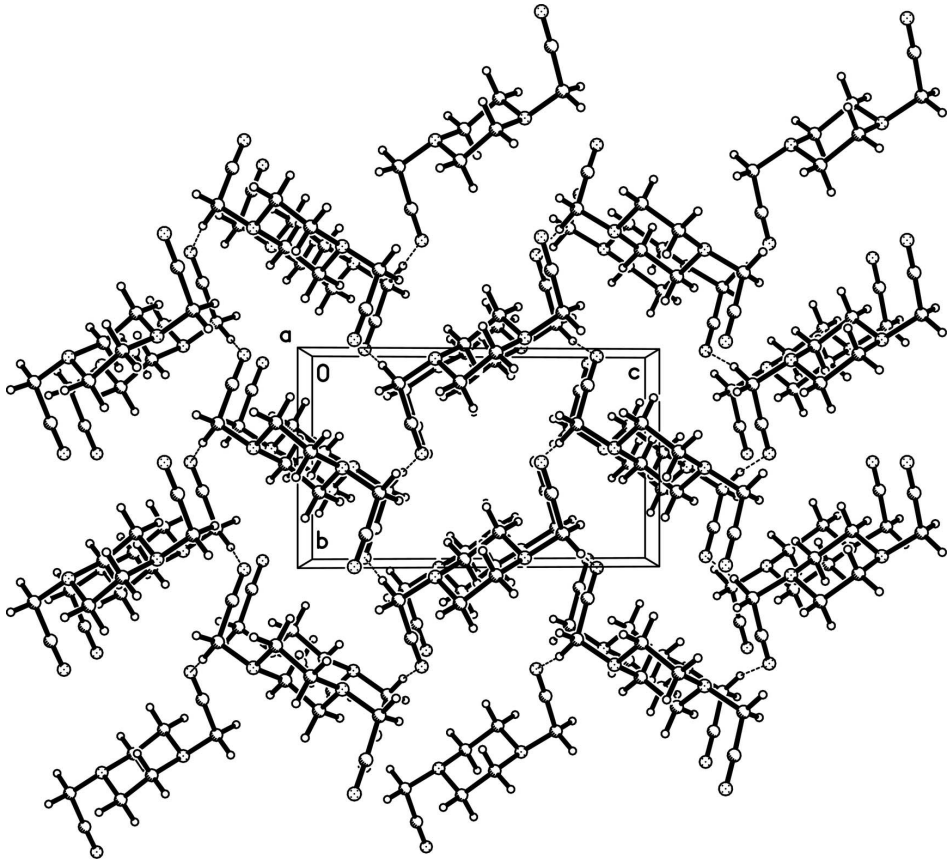

Figure 2

The crystal packing for (I).

2,2′-(Piperazine-1,4-diyl)diacetonitrile

Crystal data

$C_8H_{12}N_4$
M_r = 164.22
Monoclinic, $P2_1/c$
a = 6.3452 (13) Å
b = 6.6731 (13) Å
c = 11.077 (2) Å
β = 95.61 (3)°
V = 466.78 (16) Å^3
Z = 2
$F(000)$ = 176
D_x = 1.168 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1156 reflections
θ = 3.1–27.8°
μ = 0.08 mm^{-1}
T = 293 K
Block, colorless
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.985, T_{max} = 0.992
3739 measured reflections
1076 independent reflections
835 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.9°, θ_{min} = 6.4°
h = −8→5
k = −8→8
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.150$
$S = 1.05$
1076 reflections
55 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
$w = 1/[\sigma^2(F_o^2) + (0.0937P)^2 + 0.0176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.10$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ 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	0.06045 (14)	0.54542 (14)	0.12377 (8)	0.0464 (4)
N2	0.3536 (2)	0.9796 (2)	0.16532 (15)	0.0904 (6)
C1	−0.21559 (17)	0.52728 (19)	−0.04400 (11)	0.0497 (4)
H1A	−0.2823	0.4143	−0.0078	0.060*
H1B	−0.3249	0.6036	−0.0910	0.060*
C2	−0.10710 (17)	0.65762 (18)	0.05439 (11)	0.0499 (4)
H2A	−0.0474	0.7746	0.0184	0.060*
H2B	−0.2095	0.7030	0.1079	0.060*
C3	0.1569 (2)	0.6568 (2)	0.22683 (12)	0.0584 (4)
H3A	0.2562	0.5701	0.2741	0.070*
H3B	0.0476	0.6945	0.2779	0.070*
C4	0.2700 (2)	0.8402 (2)	0.19376 (13)	0.0647 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0471 (6)	0.0463 (6)	0.0461 (5)	0.0023 (4)	0.0062 (4)	−0.0010 (4)
N2	0.0816 (10)	0.0743 (10)	0.1129 (13)	−0.0215 (7)	−0.0029 (9)	−0.0028 (8)
C1	0.0410 (6)	0.0516 (7)	0.0570 (7)	0.0054 (4)	0.0062 (5)	−0.0018 (5)
C2	0.0465 (6)	0.0479 (7)	0.0561 (7)	0.0087 (4)	0.0092 (5)	−0.0032 (5)
C3	0.0657 (8)	0.0575 (8)	0.0512 (7)	−0.0009 (6)	0.0013 (5)	−0.0049 (5)
C4	0.0592 (8)	0.0618 (9)	0.0707 (9)	−0.0035 (6)	−0.0057 (6)	−0.0112 (7)

Geometric parameters (Å, º)

N1—C3	1.4471 (16)	C1—H1B	0.9700
N1—C2	1.4567 (15)	C2—H2A	0.9700
N1—C1^{i}	1.4680 (14)	C2—H2B	0.9700
N2—C4	1.1305 (19)	C3—C4	1.4824 (19)
C1—N1^{i}	1.4681 (14)	C3—H3A	0.9700
C1—C2	1.5071 (17)	C3—H3B	0.9700
C1—H1A	0.9700		
C3—N1—C2	112.51 (10)	C1—C2—H2A	109.6
C3—N1—C1^{i}	112.82 (9)	N1—C2—H2B	109.6
C2—N1—C1^{i}	110.49 (9)	C1—C2—H2B	109.6
N1^{i}—C1—C2	109.89 (9)	H2A—C2—H2B	108.2
N1^{i}—C1—H1A	109.7	N1—C3—C4	114.00 (10)
C2—C1—H1A	109.7	N1—C3—H3A	108.8
N1^{i}—C1—H1B	109.7	C4—C3—H3A	108.8
C2—C1—H1B	109.7	N1—C3—H3B	108.8
H1A—C1—H1B	108.2	C4—C3—H3B	108.8
N1—C2—C1	110.06 (9)	H3A—C3—H3B	107.6
N1—C2—H2A	109.6	N2—C4—C3	178.07 (16)
C3—N1—C2—C1	−174.46 (8)	C2—N1—C3—C4	−64.42 (14)
C1^{i}—N1—C2—C1	58.45 (13)	C1^{i}—N1—C3—C4	61.41 (14)
N1^{i}—C1—C2—N1	−58.10 (13)	N1—C3—C4—N2	13 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···N2^{ii}	0.97	2.57	3.427 (2)	147

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