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4-(4-Cyanobenzoylmethyl)benzonitrile

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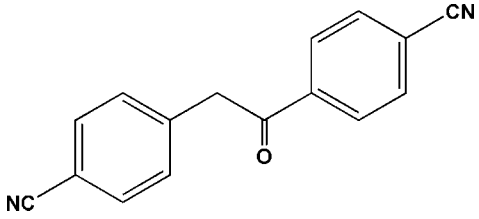
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.060; wR factor = 0.157; data-to-parameter ratio = 16.8.

In the title compound, $C_{16}H_{10}N_2O$, the dihedral angle formed by the benzene rings is 84.99 (7)°. The crystal structure is stabilized by intermolecular C—H···N and C—H···O hydrogen-bond interactions, forming chains running parallel to the b axis.

Related literature

For related literature, see: Arıcı *et al.* (2004); Radl *et al.* (2000); Bernstein *et al.* (1995); Zhao (2008).



Experimental

Crystal data

$C_{16}H_{10}N_2O$
M_r = 246.26
Triclinic, $P\overline{1}$
a = 7.5217 (15) Å
b = 7.9759 (16) Å
c = 10.881 (2) Å
α = 96.78 (3)°
β = 93.34 (3)°
γ = 102.10 (3)°
V = 631.5 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.16 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.964, T_{max} = 0.988
6576 measured reflections
2898 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.157
S = 1.04
2898 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.93	2.62	3.486 (3)	154
C12—H12···O1^{ii}	0.93	2.42	3.268 (2)	152

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, y-1, z$.

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: *SHELXTL*.

This work was supported by a Start-up Grant from SEU to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2215).

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supporting information

Acta Cryst. (2008). E**64**, o1148 [doi:10.1107/S1600536808015079]

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S1. Comment

Benzonitriles and their derivatives are important starting materials in the synthesis of some heterocyclic molecules (Radl *et al.*, 2000; Arıcı *et al.*, 2004). As part of our ongoing study on benzonitrile derivatives (Zhao, 2008), the crystal structure of one such derivatives is reported here.

The molecular structure of the title compound (Fig. 1) shows normal bond lengths and angles. The C≡N triple bond and C=O double bond lengths are 1.142 (2) and and 1.193 (2) Å, respectively. The benzene ring are oriented nearly perpendicular to each other, the dihedral angle they form being 84.99 (7)°. In the crystal structure, centrosymmetrically-related molecules are linked into dimeric units by intermolecular C—H···N hydrogen bonds (Table 1) forming ten-membered rings of graph-set $R^2_2(10)$ (Berstein *et al.*, 1995). These dimers are further connected by intermolecular C—H···O hydrogen interactions to form chains running parallel to the *b* axis.

S2. Experimental

To a solution of sodium cyanide (2 g) in water (18 ml) was added 4-formylbenzonitrile (2.62 g). The mixture was stirred for 15 min at room temperature, then a saturated sodium hydrosulfite solution (15 ml) was added dropwise. The resulting mixture was stirred at 293K until a yellow solid was obtained. The solid was filtered and recrystallized from a mixture of methanol (18 ml) and DMF (6 ml), to give crystals of the title compound suitable for X-ray diffraction analysis on slow evaporation of the solvents.

S3. Refinement

All hydrogen atoms were placed at calculated positions and refined using the riding model approximation, with C—H = 0.93-0.97 Å and with U_{iso}(H) = 1.2 U_{eq}(C).

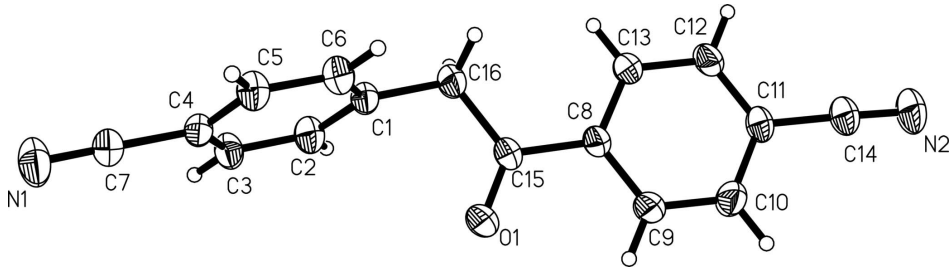

Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids were drawn at the 30% probability level

4-(4-Cyanobenzoylmethyl)benzonitrile

Crystal data

$C_{16}H_{10}N_2O$
M_r = 246.26
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.5217 (15) Å
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c = 10.881 (2) Å
α = 96.78 (3)°
β = 93.34 (3)°
γ = 102.10 (3)°
V = 631.5 (2) Å^3
Z = 2
F(000) = 256
D_x = 1.295 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2232 reflections
θ = 3.0–27.4°
μ = 0.08 mm^{-1}
T = 293 K
Block, yellow
0.20 × 0.20 × 0.16 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.964, T_{max} = 0.988
6576 measured reflections
2898 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.5°, θ_{min} = 3.0°
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.157
S = 1.04
2898 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.1009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.168 (18)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1774 (2)	0.4661 (2)	0.18751 (15)	0.0468 (4)

C2	0.0347 (3)	0.5506 (2)	0.18255 (17)	0.0546 (5)
H2	−0.0715	0.5081	0.2189	0.066*
C3	0.0475 (3)	0.6970 (2)	0.12455 (17)	0.0532 (5)
H3	−0.0493	0.7528	0.1218	0.064*
C4	0.2055 (2)	0.7599 (2)	0.07065 (15)	0.0468 (4)
C5	0.3487 (3)	0.6762 (2)	0.07410 (17)	0.0550 (5)
H5	0.4545	0.7181	0.0371	0.066*
C6	0.3339 (3)	0.5301 (2)	0.13273 (17)	0.0550 (5)
H6	0.4306	0.4742	0.1353	0.066*
C7	0.2217 (3)	0.9131 (2)	0.00999 (17)	0.0558 (5)
C8	0.2389 (2)	0.2017 (2)	0.46012 (15)	0.0457 (4)
C9	0.2979 (3)	0.2430 (2)	0.58529 (16)	0.0580 (5)
H9	0.3178	0.3571	0.6226	0.070*
C10	0.3274 (3)	0.1162 (2)	0.65476 (17)	0.0599 (5)
H10	0.3668	0.1447	0.7387	0.072*
C11	0.2980 (2)	−0.0536 (2)	0.59929 (16)	0.0476 (4)
C12	0.2369 (2)	−0.0974 (2)	0.47534 (17)	0.0521 (5)
H12	0.2158	−0.2118	0.4384	0.062*
C13	0.2074 (3)	0.0309 (2)	0.40669 (16)	0.0508 (5)
H13	0.1656	0.0018	0.3232	0.061*
C14	0.3367 (3)	−0.1839 (2)	0.67244 (18)	0.0560 (5)
C15	0.2138 (3)	0.3455 (2)	0.38867 (17)	0.0589 (5)
N1	0.2355 (3)	1.0349 (2)	−0.03745 (18)	0.0757 (5)
N2	0.3690 (3)	−0.2834 (2)	0.73238 (17)	0.0742 (6)
O1	0.2335 (4)	0.48933 (19)	0.44054 (14)	0.1312 (10)
C16	0.1648 (3)	0.3057 (2)	0.25106 (16)	0.0529 (5)
H16A	0.0413	0.2365	0.2358	0.063*
H16B	0.2458	0.2374	0.2147	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0585 (11)	0.0387 (8)	0.0433 (9)	0.0106 (8)	−0.0022 (8)	0.0092 (7)
C2	0.0563 (11)	0.0512 (10)	0.0595 (11)	0.0119 (9)	0.0080 (9)	0.0189 (9)
C3	0.0581 (11)	0.0491 (10)	0.0585 (11)	0.0204 (8)	0.0042 (9)	0.0166 (8)
C4	0.0600 (11)	0.0400 (8)	0.0405 (8)	0.0105 (8)	−0.0016 (8)	0.0090 (7)
C5	0.0575 (11)	0.0531 (10)	0.0572 (11)	0.0126 (9)	0.0064 (9)	0.0171 (9)
C6	0.0573 (11)	0.0531 (10)	0.0592 (11)	0.0196 (9)	0.0014 (9)	0.0142 (9)
C7	0.0694 (13)	0.0504 (10)	0.0516 (10)	0.0168 (9)	0.0060 (9)	0.0153 (8)
C8	0.0579 (10)	0.0367 (8)	0.0456 (9)	0.0140 (7)	0.0060 (8)	0.0104 (7)
C9	0.0864 (14)	0.0370 (9)	0.0500 (10)	0.0134 (9)	0.0019 (10)	0.0055 (8)
C10	0.0798 (14)	0.0507 (10)	0.0478 (10)	0.0099 (10)	−0.0036 (9)	0.0133 (8)
C11	0.0474 (9)	0.0431 (9)	0.0569 (10)	0.0109 (7)	0.0092 (8)	0.0212 (8)
C12	0.0656 (12)	0.0330 (8)	0.0596 (11)	0.0121 (8)	0.0076 (9)	0.0106 (8)
C13	0.0668 (11)	0.0378 (9)	0.0486 (10)	0.0132 (8)	0.0022 (8)	0.0073 (7)
C14	0.0566 (11)	0.0512 (10)	0.0661 (12)	0.0144 (9)	0.0103 (9)	0.0243 (9)
C15	0.0930 (15)	0.0367 (9)	0.0514 (10)	0.0225 (9)	0.0028 (10)	0.0108 (8)
N1	0.0880 (13)	0.0672 (11)	0.0853 (13)	0.0269 (10)	0.0212 (10)	0.0399 (10)

N2	0.0837 (13)	0.0672 (11)	0.0843 (13)	0.0263 (10)	0.0116 (10)	0.0410 (10)
O1	0.296 (3)	0.0429 (8)	0.0603 (10)	0.0630 (13)	−0.0189 (13)	0.0018 (7)
C16	0.0680 (12)	0.0387 (9)	0.0527 (10)	0.0126 (8)	−0.0010 (9)	0.0108 (8)

Geometric parameters (Å, º)

C1—C6	1.380 (3)	C8—C15	1.496 (2)
C1—C2	1.383 (2)	C9—C10	1.377 (2)
C1—C16	1.513 (2)	C9—H9	0.9300
C2—C3	1.381 (2)	C10—C11	1.384 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.381 (3)	C11—C12	1.379 (2)
C3—H3	0.9300	C11—C14	1.446 (2)
C4—C5	1.382 (3)	C12—C13	1.382 (2)
C4—C7	1.442 (2)	C12—H12	0.9300
C5—C6	1.381 (2)	C13—H13	0.9300
C5—H5	0.9300	C14—N2	1.140 (2)
C6—H6	0.9300	C15—O1	1.193 (2)
C7—N1	1.142 (2)	C15—C16	1.501 (3)
C8—C13	1.383 (2)	C16—H16A	0.9700
C8—C9	1.387 (2)	C16—H16B	0.9700
C6—C1—C2	118.89 (15)	C8—C9—H9	119.7
C6—C1—C16	119.65 (16)	C9—C10—C11	119.80 (17)
C2—C1—C16	121.46 (16)	C9—C10—H10	120.1
C3—C2—C1	121.07 (17)	C11—C10—H10	120.1
C3—C2—H2	119.5	C12—C11—C10	120.45 (15)
C1—C2—H2	119.5	C12—C11—C14	120.50 (16)
C2—C3—C4	119.32 (17)	C10—C11—C14	119.03 (17)
C2—C3—H3	120.3	C11—C12—C13	119.21 (16)
C4—C3—H3	120.3	C11—C12—H12	120.4
C3—C4—C5	120.28 (15)	C13—C12—H12	120.4
C3—C4—C7	120.13 (16)	C12—C13—C8	121.10 (17)
C5—C4—C7	119.59 (16)	C12—C13—H13	119.5
C6—C5—C4	119.70 (17)	C8—C13—H13	119.5
C6—C5—H5	120.2	N2—C14—C11	178.3 (2)
C4—C5—H5	120.2	O1—C15—C8	120.30 (17)
C1—C6—C5	120.74 (17)	O1—C15—C16	120.78 (16)
C1—C6—H6	119.6	C8—C15—C16	118.92 (15)
C5—C6—H6	119.6	C15—C16—C1	113.15 (14)
N1—C7—C4	179.5 (2)	C15—C16—H16A	108.9
C13—C8—C9	118.91 (15)	C1—C16—H16A	108.9
C13—C8—C15	122.97 (16)	C15—C16—H16B	108.9
C9—C8—C15	118.12 (15)	C1—C16—H16B	108.9
C10—C9—C8	120.52 (16)	H16A—C16—H16B	107.8
C10—C9—H9	119.7		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N1^{i}	0.93	2.62	3.486 (3)	154
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