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2-Benzoyl-1*H*-benzimidazole

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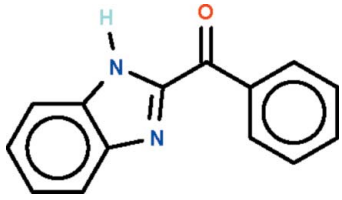
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.115; data-to-parameter ratio = 16.7.

In the title compound, $C_{14}H_{10}N_2O$, the benzoyl ring and benzimidazole ring system are aligned at a dihedral angle of 50.2 (2)°. In the crystal, intermolecular N—H···N hydrogen bonds between adjacent imidazole groups generate supramolecular $C(4)$ chains running along the b axis.

Related literature

For phototropism of 2-acetylbenzimidazole and 2-benzoylbenzimidazole, see: Chowdhury *et al.* (2005). For the crystal structure of 2-acetylbenzimidazole, see: Yang *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Orthorhombic, *Pbca*
a = 14.7356 (8) Å
b = 9.9530 (12) Å
c = 15.7981 (12) Å
V = 2317.0 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.40 × 0.40 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
10324 measured reflections
2658 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.115
S = 1.01
2658 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.90 (2)	1.95 (2)	2.829 (2)	164 (1)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Beijing Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5084).

References

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supplementary materials

Acta Cryst. (2010). E**66**, o3164 [**doi:10.1107/S1600536810045666**]

2-Benzoyl-1*H*-benzimidazole

L. Ai, X.-M. Shen and S. W. Ng

Comment

Acetyl-2-benzimidazole and benzoyl-2-benzimidazole are reported to exhibit excited-state prototropism in solvents at different pH levels (Chowdhury *et al.*, 2005). Acetyl-2-benzimidazole exists in the solid state as an N–H···O hydrogen bonded dimer; the molecule is essentially planar (Yang *et al.*, 2006). With the larger phenyl ring in place of the methyl group, the aromatic analog (Scheme I) requires rotation of the aromatic ring in order to reduce strain; this is reflected in the 50.2 (2) ° dihedral angle between the phenyl and benzimidazolyl rings (Fig. 1). Adjacent molecules are linked into a chan by N–H···O hydrogen bonds (Fig. 2).

Experimental

The compound was synthesized by using a literature procedure (Chowdhury *et al.*, 2005), and crystals were grown from a methanol solution of the compound.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C).

The amino H-atom was located in a difference Fourier map and was refined isotropically.

Figures

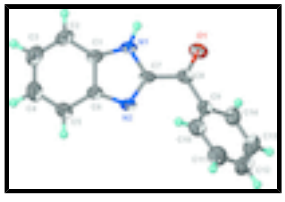

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{14}H_{11}N_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

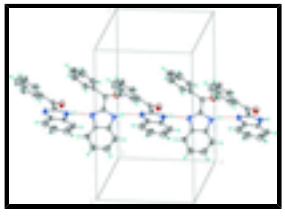

Fig. 2. Hydrogen-bonded chain structure.

2-Benzoyl-1*H*-benzimidazole

Crystal data

$C_{14}H_{10}N_2O$	$F(000) = 928$
$M_r = 222.24$	$D_x = 1.274$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2496 reflections
$a = 14.7356$ (8) Å	θ = 2.8–26.7°
$b = 9.9530$ (12) Å	μ = 0.08 mm^{-1}
$c = 15.7981$ (12) Å	$T = 293$ K
$V = 2317.0$ (4) Å^3	Block, colorless
$Z = 8$	0.40 × 0.40 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer	1885 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.030$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
ω scans	$h = -10 \rightarrow 19$
10324 measured reflections	$k = -12 \rightarrow 11$
2658 independent reflections	$l = -15 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.2609P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
2658 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
159 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0093 (12)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38338 (7)	0.51103 (10)	0.45822 (7)	0.0647 (3)
N1	0.23286 (7)	0.52044 (10)	0.35142 (7)	0.0456 (3)

H1	0.2500 (10)	0.6048 (17)	0.3643 (9)	0.066 (4)*
N2	0.22405 (7)	0.29711 (9)	0.35955 (7)	0.0450 (3)
C1	0.16927 (9)	0.48272 (12)	0.29302 (8)	0.0446 (3)
C2	0.11547 (10)	0.55500 (15)	0.23652 (9)	0.0609 (4)
H2	0.1189	0.6481	0.2328	0.073*
C3	0.05747 (12)	0.48239 (18)	0.18687 (10)	0.0733 (5)
H3	0.0207	0.5274	0.1483	0.088*
C4	0.05192 (13)	0.34275 (18)	0.19233 (10)	0.0767 (5)
H4	0.0111	0.2972	0.1577	0.092*
C5	0.10482 (11)	0.27110 (15)	0.24714 (10)	0.0647 (4)
H5	0.1011	0.1779	0.2501	0.078*
C6	0.16460 (9)	0.34273 (12)	0.29846 (8)	0.0453 (3)
C7	0.26312 (9)	0.40660 (11)	0.38936 (7)	0.0411 (3)
C8	0.33717 (9)	0.41037 (12)	0.45261 (8)	0.0444 (3)
C9	0.35378 (9)	0.28972 (13)	0.50523 (8)	0.0471 (3)
C10	0.28375 (11)	0.21174 (15)	0.53695 (9)	0.0613 (4)
H10	0.2238	0.2326	0.5240	0.074*
C11	0.30339 (17)	0.10285 (19)	0.58787 (11)	0.0904 (7)
H11	0.2566	0.0520	0.6110	0.108*
C12	0.3922 (2)	0.0697 (2)	0.60441 (13)	0.1081 (8)
H12	0.4052	−0.0053	0.6373	0.130*
C13	0.46157 (16)	0.1462 (2)	0.57286 (13)	0.0942 (7)
H13	0.5214	0.1224	0.5840	0.113*
C14	0.44330 (11)	0.25789 (16)	0.52484 (9)	0.0632 (4)
H14	0.4904	0.3119	0.5055	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0593 (6)	0.0444 (6)	0.0904 (8)	−0.0143 (5)	−0.0074 (5)	0.0005 (5)
N1	0.0576 (7)	0.0243 (5)	0.0551 (6)	−0.0016 (5)	0.0001 (5)	0.0018 (5)
N2	0.0574 (7)	0.0269 (5)	0.0506 (6)	−0.0008 (4)	−0.0037 (5)	0.0015 (4)
C1	0.0526 (7)	0.0335 (6)	0.0477 (7)	0.0013 (5)	0.0040 (6)	0.0032 (5)
C2	0.0731 (10)	0.0441 (8)	0.0656 (9)	0.0079 (7)	−0.0038 (8)	0.0136 (7)
C3	0.0784 (11)	0.0751 (11)	0.0663 (9)	0.0043 (9)	−0.0174 (9)	0.0174 (9)
C4	0.0894 (13)	0.0752 (12)	0.0656 (9)	−0.0134 (10)	−0.0262 (9)	0.0048 (9)
C5	0.0858 (11)	0.0455 (8)	0.0630 (8)	−0.0114 (7)	−0.0168 (8)	0.0004 (7)
C6	0.0561 (8)	0.0329 (6)	0.0469 (6)	−0.0008 (5)	−0.0013 (6)	0.0019 (5)
C7	0.0486 (7)	0.0273 (6)	0.0475 (6)	−0.0014 (5)	0.0044 (5)	0.0009 (5)
C8	0.0437 (7)	0.0354 (6)	0.0543 (7)	−0.0020 (5)	0.0046 (6)	−0.0045 (6)
C9	0.0559 (8)	0.0403 (7)	0.0450 (6)	−0.0009 (6)	−0.0049 (6)	−0.0037 (6)
C10	0.0725 (10)	0.0583 (9)	0.0531 (8)	−0.0141 (7)	−0.0062 (7)	0.0077 (7)
C11	0.1331 (19)	0.0743 (12)	0.0637 (10)	−0.0338 (12)	−0.0211 (11)	0.0238 (9)
C12	0.160 (2)	0.0778 (14)	0.0864 (13)	−0.0021 (15)	−0.0520 (15)	0.0288 (11)
C13	0.1035 (16)	0.0826 (14)	0.0967 (14)	0.0211 (12)	−0.0447 (12)	0.0051 (12)
C14	0.0632 (9)	0.0625 (9)	0.0641 (9)	0.0056 (7)	−0.0151 (7)	−0.0065 (7)

Geometric parameters (Å, °)

O1—C8	1.2146 (14)	C5—H5	0.9300
N1—C7	1.3571 (15)	C7—C8	1.4800 (18)
N1—C1	1.3677 (17)	C8—C9	1.4809 (18)
N1—H1	0.900 (17)	C9—C10	1.3851 (19)
N2—C7	1.3195 (15)	C9—C14	1.392 (2)
N2—C6	1.3802 (16)	C10—C11	1.380 (2)
C1—C2	1.3938 (19)	C10—H10	0.9300
C1—C6	1.3977 (17)	C11—C12	1.375 (3)
C2—C3	1.367 (2)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.369 (3)
C3—C4	1.395 (2)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.372 (2)
C4—C5	1.366 (2)	C13—H13	0.9300
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.3933 (19)		
C7—N1—C1	107.09 (10)	N2—C7—C8	125.70 (11)
C7—N1—H1	125.9 (10)	N1—C7—C8	121.28 (10)
C1—N1—H1	127.0 (10)	O1—C8—C7	118.92 (12)
C7—N2—C6	104.76 (10)	O1—C8—C9	122.35 (12)
N1—C1—C2	132.85 (12)	C7—C8—C9	118.71 (10)
N1—C1—C6	105.42 (11)	C10—C9—C14	119.88 (13)
C2—C1—C6	121.73 (13)	C10—C9—C8	122.30 (13)
C3—C2—C1	116.76 (14)	C14—C9—C8	117.79 (13)
C3—C2—H2	121.6	C11—C10—C9	119.64 (17)
C1—C2—H2	121.6	C11—C10—H10	120.2
C2—C3—C4	121.88 (15)	C9—C10—H10	120.2
C2—C3—H3	119.1	C12—C11—C10	119.92 (19)
C4—C3—H3	119.1	C12—C11—H11	120.0
C5—C4—C3	121.72 (15)	C10—C11—H11	120.0
C5—C4—H4	119.1	C13—C12—C11	120.55 (18)
C3—C4—H4	119.1	C13—C12—H12	119.7
C4—C5—C6	117.55 (14)	C11—C12—H12	119.7
C4—C5—H5	121.2	C12—C13—C14	120.36 (19)
C6—C5—H5	121.2	C12—C13—H13	119.8
N2—C6—C5	129.77 (12)	C14—C13—H13	119.8
N2—C6—C1	109.86 (11)	C13—C14—C9	119.56 (17)
C5—C6—C1	120.36 (12)	C13—C14—H14	120.2
N2—C7—N1	112.86 (11)	C9—C14—H14	120.2
C7—N1—C1—C2	179.42 (14)	C1—N1—C7—C8	176.10 (11)
C7—N1—C1—C6	−0.39 (14)	N2—C7—C8—O1	160.44 (13)
N1—C1—C2—C3	−179.47 (15)	N1—C7—C8—O1	−14.80 (19)
C6—C1—C2—C3	0.3 (2)	N2—C7—C8—C9	−17.95 (19)
C1—C2—C3—C4	0.2 (2)	N1—C7—C8—C9	166.81 (11)
C2—C3—C4—C5	−0.6 (3)	O1—C8—C9—C10	142.64 (14)
C3—C4—C5—C6	0.5 (3)	C7—C8—C9—C10	−39.03 (18)
C7—N2—C6—C5	−179.18 (15)	O1—C8—C9—C14	−35.36 (19)

C7—N2—C6—C1	−0.19 (14)	C7—C8—C9—C14	142.97 (12)
C4—C5—C6—N2	178.85 (14)	C14—C9—C10—C11	0.0 (2)
C4—C5—C6—C1	0.0 (2)	C8—C9—C10—C11	−177.95 (14)
N1—C1—C6—N2	0.37 (14)	C9—C10—C11—C12	−2.2 (3)
C2—C1—C6—N2	−179.47 (12)	C10—C11—C12—C13	2.0 (3)
N1—C1—C6—C5	179.46 (13)	C11—C12—C13—C14	0.6 (3)
C2—C1—C6—C5	−0.4 (2)	C12—C13—C14—C9	−2.8 (3)
C6—N2—C7—N1	−0.06 (14)	C10—C9—C14—C13	2.5 (2)
C6—N2—C7—C8	−175.65 (11)	C8—C9—C14—C13	−179.45 (14)
C1—N1—C7—N2	0.29 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.90 (2)	1.95 (2)	2.829 (2)	164 (1)

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

Fig. 1

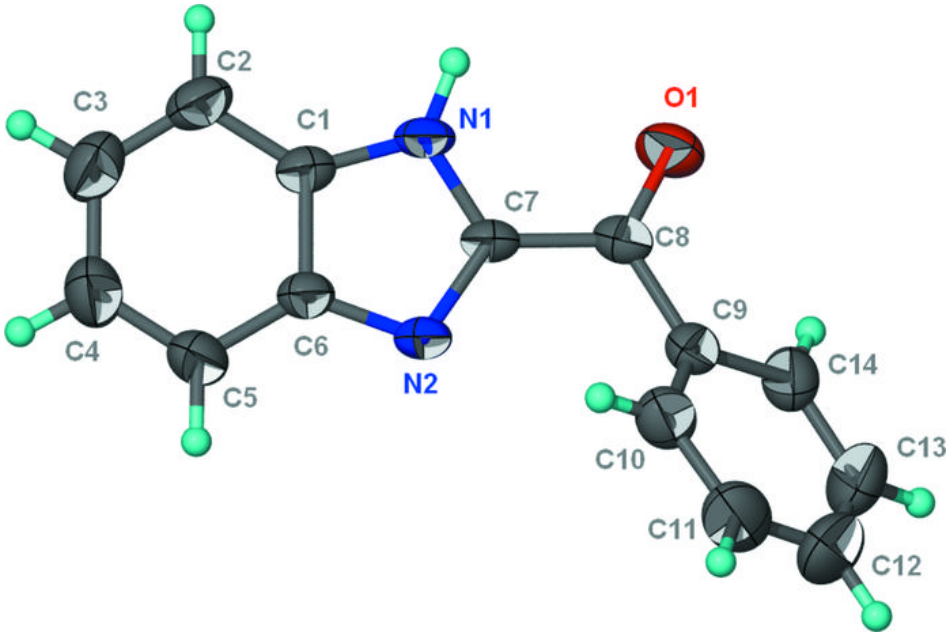

Fig. 2