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1-Benzyl-2,3-dihydroquinolin-4(1*H*)-one

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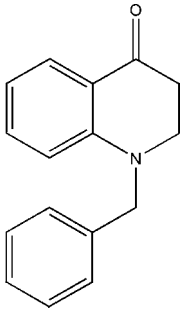
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.068; wR factor = 0.182; data-to-parameter ratio = 13.7.

In the title compound, $C_{16}H_{15}NO$, the two aromatic rings are approximately perpendicular; the carbonyl group is twisted out of the adjacent benzene ring by 14.8 (2)°. In the heterocyclic ring, the C atom linked to the carbonyl group and the C atom linked to the N atom have opposite deviations of 0.467 (5) and 0.184 (4) Å, respectively, from the plane of the benzene ring. The N atom lies approximately in the plane of the phenyl ring. There are no conventional hydrogen bonds; the packing of molecules in the crystal structure is stabilized by van der Waals forces.

Related literature

For related literature, see: Johnson *et al.* (1949); Anilkumar *et al.* (2005); Kazak *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{15}NO$
M_r = 237.29
Monoclinic, $P2_1/n$
a = 5.5992 (11) Å
b = 9.786 (2) Å
c = 23.313 (5) Å
β = 96.79 (3)°
V = 1268.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.25 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.898, T_{max} = 1.00
(expected range = 0.894–0.996)
9867 measured reflections
2242 independent reflections
1252 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.182
S = 1.05
2242 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2078).

References

Anilkumar, H. G., Yathirajan, H. S., Nagaraja, P. & Bolte, M. (2005). *Acta Cryst.* E**61**, o2551–o2552.
Kazak, C., Aygün, M., Kuş, C., Özbey, S. & Büyükgüngör, O. (2002). *Acta Cryst.* E**58**, o612–o614.
Rigaku (2005). *CrystalClear*. Version 1.4.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Johnson, W. S.,Woroch, E. L. & Buell, B. G. (1949). *J. Am. Chem. Soc.* **71**, 1901–1905.

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supplementary materials

Acta Cryst. (2008). E**64**, o447 [**doi:10.1107/S1600536808000792**]

1-Benzyl-2,3-dihydroquinolin-4(1*H*)-one

M.-L. Wang, W.-B. Wu, H.-Y. Ye and Y.-M. Sun

Comment

The title compound, belongs to the class of 4-dihydroquinolinone derivatives (Johnson *et al.*, 1949), which have hitherto received relatively little attention. We have recently found that it has two-photon absorption and two-photon excited fluorescence. So it is of interest for non-linear optics. An X-ray crystal structure determination was undertaken in order to elucidate the conformation, and the results are presented here.

The two aromatic rings in the molecule are approximately perpendicular, with an angle between the two planes of 88.3 (1) °. The plane through atom O1, C2 and C3 is twisted out of the plane of the ring through atoms C4 to C9 by 14.8 (2) °, while in acetophenone (Kazak *et al.*, 2002; Anilkumar *et al.*, 2005) the acetyl is nearly coplanar with phenyl ring. The twist is probably due to the sp^3-hybridization of C1 and C2. The N atom lies approximately in the plane of the adjacent aromatic ring plane with a tiny deviation of 0.013 (3) Å, as would be expected for maximum conjugation and as is normally found for N attached to benzene rings. There are no conventional hydrogen bonds.

Experimental

Melting points were determined with a Yanagimoto MP-35 melting-point apparatus and were uncorrected. The ^{1}H NMR spectra were measured with a Bruker DRX (300 MHz) (relative to TMS) spectrometer. The solid state IR spectra were recorded from KBr discs on a Nicolet-170.

2, 3-Dihydroquinolin-4-one (5.7 g,), benzyl iodide (6.54 g), tetrabutylammonium bromide (TBAB, 0.5 g) and 20 ml 50% aqueous sodium hydroxide in 25 ml toluene were vigorously stirred and heated to reflux for 3 h. After cooling, the mixture was washed with 20 ml water three times, and evaporated under reduced pressure to remove toluene. The residue was recrystallized from ethanol to afford a yellow solid. Yield: 7.8 g (85%); m.p.391–392 K. IR (KBr): ν= 1672 cm^{-1} (C═O). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.77 (*t*, 2H, CH_2, J = 6.9 Hz), 3.61 (*t*, 2H, CH_2, J = 6.9 Hz), 4.58 (*s*, 2H, CH_2), 6.73 (*m*, 2H, ArH), 7.27–7.39 (*m*, 6H, ArH), 7.94 (*d*, 1H, ArH, J = 7.5 Hz,). Single crystals suitable for crystallographic analysis were obtained by slow evaporation of a methanol/water (4:1 *v*/*v*) solution.

Refinement

Positional parameters of all the H atoms bonded to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with d(C—H) = 0.93 Å for sp^2 C or d(C—H) = 0.97 Å for sp^3 C and U_{iso}(H) = 1.2Ueq(C).

Figures

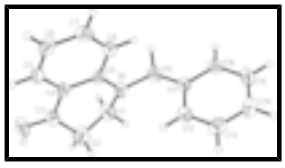

Fig. 1. The molecular structure with displacement ellipsoids were drawn at the 30% probability level

1-Benzyl-2,3-dihydroquinolin-4(1*H*)-one

Crystal data

$C_{16}H_{15}NO$	F_{000} = 504
M_r = 237.29	D_x = 1.243 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7530 reflections
a = 5.5992 (11) Å	θ = 3.7–27.5º
b = 9.786 (2) Å	μ = 0.08 mm^{-1}
c = 23.313 (5) Å	T = 293 (2) K
β = 96.79 (3)º	Block, colourless
V = 1268.5 (5) Å^3	0.25 × 0.05 × 0.05 mm
Z = 4	

Data collection

Rigaku Mercury2 CCD diffractometer	2242 independent reflections
Radiation source: fine-focus sealed tube	1252 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.081
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 25.0º
T = 293(2) K	θ_{min} = 3.4º
ω scans	h = −6→6
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −11→11
T_{min} = 0.898, T_{max} = 1	l = −27→27
9867 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.068	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.1531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.182	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.38 e Å^{-3}

2242 reflections

164 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.20$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.010 (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 $F^2 > 2\sigma(F^2)$ 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}
C11	0.6399 (5)	0.3558 (3)	0.11589 (12)	0.0427 (8)
C4	1.0812 (5)	0.7455 (3)	0.15820 (13)	0.0432 (8)
N1	0.7645 (4)	0.5798 (3)	0.16157 (11)	0.0513 (7)
O1	1.2200 (4)	0.8547 (3)	0.24606 (10)	0.0790 (8)
C9	0.9179 (5)	0.6500 (3)	0.13068 (13)	0.0431 (8)
C3	1.1014 (5)	0.7645 (3)	0.22089 (14)	0.0515 (9)
C8	0.9186 (6)	0.6306 (3)	0.07149 (13)	0.0550 (9)
H8A	0.8132	0.5679	0.0522	0.066*
C6	1.2320 (6)	0.7970 (4)	0.06840 (16)	0.0644 (10)
H6A	1.3355	0.8455	0.0475	0.077*
C5	1.2345 (5)	0.8172 (3)	0.12615 (15)	0.0540 (9)
H5A	1.3411	0.8805	0.1447	0.065*
C10	0.5711 (5)	0.4967 (3)	0.13269 (15)	0.0571 (9)
H10A	0.5028	0.5445	0.0981	0.068*
H10B	0.4459	0.4891	0.1579	0.068*
C7	1.0728 (6)	0.7029 (4)	0.04123 (14)	0.0621 (10)
H7A	1.0700	0.6883	0.0017	0.074*
C16	0.4733 (6)	0.2784 (4)	0.08129 (13)	0.0548 (9)
H16A	0.3272	0.3171	0.0666	0.066*
C13	0.9027 (6)	0.1602 (4)	0.12313 (15)	0.0626 (10)
H13A	1.0492	0.1209	0.1372	0.075*
C12	0.8556 (5)	0.2948 (4)	0.13631 (13)	0.0527 (9)
H12A	0.9712	0.3450	0.1593	0.063*
C15	0.5218 (7)	0.1445 (4)	0.06844 (15)	0.0657 (10)
H15A	0.4079	0.0940	0.0451	0.079*
C2	0.9820 (7)	0.6579 (4)	0.25256 (15)	0.0730 (11)
H2A	1.0860	0.5785	0.2581	0.088*

H2B	0.9568	0.6924	0.2904	0.088*
C14	0.7342 (7)	0.0850 (4)	0.08949 (16)	0.0669 (11)
H14A	0.7643	−0.0059	0.0811	0.080*
C1	0.7489 (6)	0.6170 (4)	0.22115 (15)	0.0685 (11)
H1A	0.6863	0.5399	0.2408	0.082*
H1B	0.6360	0.6919	0.2221	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0380 (18)	0.046 (2)	0.0451 (18)	−0.0061 (14)	0.0103 (13)	0.0013 (14)
C4	0.0414 (18)	0.0368 (19)	0.051 (2)	0.0025 (14)	0.0037 (14)	−0.0018 (13)
N1	0.0495 (16)	0.0503 (18)	0.0558 (17)	−0.0120 (13)	0.0127 (12)	−0.0106 (13)
O1	0.0837 (18)	0.080 (2)	0.0707 (17)	−0.0265 (15)	−0.0011 (13)	−0.0288 (13)
C9	0.0432 (19)	0.0362 (19)	0.050 (2)	0.0026 (14)	0.0044 (14)	−0.0004 (14)
C3	0.049 (2)	0.050 (2)	0.056 (2)	−0.0029 (16)	0.0075 (15)	−0.0085 (16)
C8	0.062 (2)	0.052 (2)	0.049 (2)	−0.0099 (16)	−0.0028 (16)	−0.0046 (15)
C6	0.080 (3)	0.054 (2)	0.062 (2)	−0.0076 (19)	0.0185 (18)	0.0112 (18)
C5	0.054 (2)	0.042 (2)	0.066 (2)	−0.0093 (16)	0.0050 (16)	−0.0012 (16)
C10	0.042 (2)	0.051 (2)	0.078 (2)	−0.0071 (15)	0.0055 (16)	−0.0056 (17)
C7	0.077 (3)	0.065 (3)	0.044 (2)	0.000 (2)	0.0057 (17)	0.0029 (17)
C16	0.048 (2)	0.062 (3)	0.054 (2)	−0.0091 (16)	0.0002 (15)	0.0012 (17)
C13	0.050 (2)	0.058 (3)	0.082 (3)	0.0065 (18)	0.0159 (18)	0.0066 (19)
C12	0.043 (2)	0.059 (3)	0.057 (2)	−0.0051 (16)	0.0078 (15)	−0.0019 (17)
C15	0.073 (3)	0.059 (3)	0.066 (2)	−0.023 (2)	0.0113 (19)	−0.0126 (18)
C2	0.088 (3)	0.076 (3)	0.057 (2)	−0.002 (2)	0.018 (2)	−0.0104 (19)
C14	0.073 (3)	0.047 (2)	0.085 (3)	−0.007 (2)	0.027 (2)	−0.0069 (19)
C1	0.058 (2)	0.085 (3)	0.065 (2)	−0.0107 (19)	0.0169 (18)	−0.0036 (19)

Geometric parameters (Å, °)

C11—C12	1.380 (4)	C10—H10A	0.9700
C11—C16	1.384 (4)	C10—H10B	0.9700
C11—C10	1.497 (4)	C7—H7A	0.9300
C4—C5	1.392 (4)	C16—C15	1.378 (5)
C4—C9	1.408 (4)	C16—H16A	0.9300
C4—C3	1.464 (4)	C13—C14	1.368 (4)
N1—C9	1.369 (4)	C13—C12	1.385 (4)
N1—C1	1.448 (4)	C13—H13A	0.9300
N1—C10	1.454 (4)	C12—H12A	0.9300
O1—C3	1.214 (3)	C15—C14	1.362 (5)
C9—C8	1.393 (4)	C15—H15A	0.9300
C3—C2	1.482 (5)	C2—C1	1.474 (4)
C8—C7	1.374 (4)	C2—H2A	0.9700
C8—H8A	0.9300	C2—H2B	0.9700
C6—C5	1.359 (5)	C14—H14A	0.9300
C6—C7	1.382 (4)	C1—H1A	0.9700
C6—H6A	0.9300	C1—H1B	0.9700
C5—H5A	0.9300		

C12—C11—C16	117.8 (3)	C8—C7—C6	121.2 (3)
C12—C11—C10	123.4 (3)	C8—C7—H7A	119.4
C16—C11—C10	118.7 (3)	C6—C7—H7A	119.4
C5—C4—C9	119.9 (3)	C15—C16—C11	120.7 (3)
C5—C4—C3	119.5 (3)	C15—C16—H16A	119.7
C9—C4—C3	120.5 (3)	C11—C16—H16A	119.7
C9—N1—C1	119.4 (3)	C14—C13—C12	120.2 (3)
C9—N1—C10	121.1 (3)	C14—C13—H13A	119.9
C1—N1—C10	117.3 (3)	C12—C13—H13A	119.9
N1—C9—C8	121.9 (3)	C11—C12—C13	121.1 (3)
N1—C9—C4	120.5 (3)	C11—C12—H12A	119.5
C8—C9—C4	117.6 (3)	C13—C12—H12A	119.5
O1—C3—C4	123.2 (3)	C14—C15—C16	121.0 (3)
O1—C3—C2	121.6 (3)	C14—C15—H15A	119.5
C4—C3—C2	115.0 (3)	C16—C15—H15A	119.5
C7—C8—C9	120.9 (3)	C1—C2—C3	111.6 (3)
C7—C8—H8A	119.5	C1—C2—H2A	109.3
C9—C8—H8A	119.5	C3—C2—H2A	109.3
C5—C6—C7	118.8 (3)	C1—C2—H2B	109.3
C5—C6—H6A	120.6	C3—C2—H2B	109.3
C7—C6—H6A	120.6	H2A—C2—H2B	108.0
C6—C5—C4	121.5 (3)	C15—C14—C13	119.3 (4)
C6—C5—H5A	119.2	C15—C14—H14A	120.3
C4—C5—H5A	119.2	C13—C14—H14A	120.3
N1—C10—C11	115.8 (2)	N1—C1—C2	113.2 (3)
N1—C10—H10A	108.3	N1—C1—H1A	108.9
C11—C10—H10A	108.3	C2—C1—H1A	108.9
N1—C10—H10B	108.3	N1—C1—H1B	108.9
C11—C10—H10B	108.3	C2—C1—H1B	108.9
H10A—C10—H10B	107.4	H1A—C1—H1B	107.7
C1—N1—C9—C8	−171.7 (3)	C1—N1—C10—C11	−114.3 (3)
C10—N1—C9—C8	−9.2 (4)	C12—C11—C10—N1	13.5 (4)
C1—N1—C9—C4	8.0 (4)	C16—C11—C10—N1	−171.1 (3)
C10—N1—C9—C4	170.6 (3)	C9—C8—C7—C6	0.0 (5)
C5—C4—C9—N1	−179.3 (3)	C5—C6—C7—C8	0.1 (5)
C3—C4—C9—N1	4.3 (4)	C12—C11—C16—C15	0.7 (4)
C5—C4—C9—C8	0.4 (4)	C10—C11—C16—C15	−174.9 (3)
C3—C4—C9—C8	−175.9 (3)	C16—C11—C12—C13	−0.7 (4)
C5—C4—C3—O1	11.5 (5)	C10—C11—C12—C13	174.7 (3)
C9—C4—C3—O1	−172.1 (3)	C14—C13—C12—C11	−0.2 (5)
C5—C4—C3—C2	−163.6 (3)	C11—C16—C15—C14	0.1 (5)
C9—C4—C3—C2	12.8 (4)	O1—C3—C2—C1	144.7 (3)
N1—C9—C8—C7	179.5 (3)	C4—C3—C2—C1	−40.1 (4)
C4—C9—C8—C7	−0.3 (5)	C16—C15—C14—C13	−1.0 (5)
C7—C6—C5—C4	0.1 (5)	C12—C13—C14—C15	1.0 (5)
C9—C4—C5—C6	−0.3 (5)	C9—N1—C1—C2	−36.7 (4)
C3—C4—C5—C6	176.1 (3)	C10—N1—C1—C2	160.1 (3)
C9—N1—C10—C11	82.8 (4)	C3—C2—C1—N1	51.8 (4)

Fig. 1