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2-(4,5-Dihydro-1,3-oxazol-2-yl)quinoline

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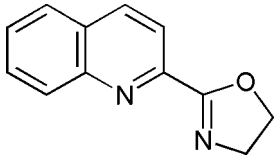
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.048; wR factor = 0.142; data-to-parameter ratio = 15.9.

The title compound, $C_{12}H_{10}N_2O$, is approximately planar. The angle between the quinoline and 4,5-dihydrooxazole ring systems is 11.91 (12)°. The molecules pack into a herringbone array with no significant π–π interactions. The dihydrooxazole N and O atoms are disordered over two positions, with almost equal site occupancy factors.

Related literature

For related 2-substituted quinoline compounds, see: Mague *et al.* (1997); Yang *et al.* (2001); Qi *et al.* (2003); Xu *et al.* (2006). For the synthesis, see: Ishihara & Togo (2007). For related literature, see: Allen (2002); Cunico *et al.* (2006); Hartline *et al.* (2005).



Experimental

Crystal data

$C_{12}H_{10}N_2O$
M_r = 198.22
Monoclinic, $P2_1/c$
a = 6.2240 (3) Å
b = 13.6649 (6) Å
c = 11.8186 (6) Å
β = 102.097 (3)°
V = 982.86 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.24 × 0.21 × 0.13 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.705, T_{max} = 1
(expected range = 0.697–0.989)
9874 measured reflections
2183 independent reflections
1128 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.00
2183 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *APEX2*/*COSMO*/*BIS* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* and *SADABS* (Bruker, 2006); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2491).

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supplementary materials

Acta Cryst. (2008). E**64**, o154 [**doi:10.1107/S1600536807045023**]

2-(4,5-Dihydro-1,3-oxazol-2-yl)quinoline

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Comment

Quinoline derivatives are known to possess a variety of biological properties such as antimalarial and antiviral activity (Cunico *et al.*, 2006; Hartline *et al.*, 2005). In addition, oxazoline-derived complexes of Pd(II) and other metals have attracted a great deal of attention due to their high efficiency in enantioselective catalysis. In this context, we were interested in detailed knowledge of the molecular structure of the above derivatives. In this communication we report the crystal structure of the title compound, 2-(4,5-dihydrooxazol-2-yl)quinoline. The analysis was focused on the planarity of the molecule. Both the quinoline and the 4,5-dihydrooxazole rings are planar, with r.m.s. deviations from planarity of 0.0136 Å for the first and 0.0176 ° for the last. The entire molecule is almost planar; the angle between the two rings is 11.91 (12) °. Quinoline and dihydrooxazole rings are essentially planar, with an average r.m.s. deviation from planarity of 0.06 (3) Å for 552 observations for the first and 0.05 (3) Å for 31 observations for the last in the Cambridge Structural Database [CSD, Version 5.28, update of May 2007; Allen, 2002)]. The molecules pack into a herringbone array with no significant π-π interactions.

Experimental

The title compound was synthesized from quinoline-2-carbaldehyde and aminoethanol according to the general procedure of Ishihara & Togo (2007). The crystal used for the data collection was obtained by recrystallization from hexane followed by slow evaporation at room temperature.

Refinement

All H atoms were refined using a riding model, with C—H = 0.97%A and U_{iso}(H) = 1.2Ueq(C) for the methylene C atoms and C—H = 0.93 Å and U_{iso} = 1.2Ueq(C) for the quinoline C atoms.

Figures

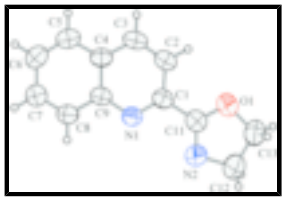

Fig. 1. View of the asymmetric unit of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

2-(4,5-Dihydro-1,3-oxazol-2-yl)quinoline

Crystal data

$C_{12}H_{10}N_2O$ F_{000} = 416

M_r = 198.22	D_x = 1.34 Mg m^{-3}
Monoclinic, $P2(1)/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1185 reflections
a = 6.2240 (3) Å	θ = 6.9–40.4º
b = 13.6649 (6) Å	μ = 0.09 mm^{-1}
c = 11.8186 (6) Å	T = 273 (2) K
β = 102.097 (3)º	Block, colourless
V = 982.86 (8) Å^3	0.24 × 0.21 × 0.13 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	1128 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 296(2) K	θ_{max} = 27.5º
phi and ω scans	θ_{min} = 3.4º
Absorption correction: multi-scan (SADABS; Bruker, 2006) was used to perform the multi-scan semi-empirical (using intensity measurements) absorption correction and to scale the data.	$h = -7 \rightarrow 8$
T_{min} = 0.705, T_{max} = 1	$k = -16 \rightarrow 16$
9874 measured reflections	$l = -15 \rightarrow 15$
2183 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.143	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
2183 reflections	Extinction correction: none
137 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
C1	0.0592 (3)	0.64386 (12)	0.61057 (14)	0.0526 (5)	
C2	−0.0108 (3)	0.68102 (15)	0.49740 (15)	0.0664 (5)	
H2	−0.1414	0.6592	0.4508	0.080*	
C3	0.1126 (3)	0.74813 (14)	0.45761 (15)	0.0671 (6)	
H3	0.0666	0.7738	0.3836	0.080*	
C4	0.3119 (3)	0.77950 (12)	0.52818 (13)	0.0531 (5)	
C5	0.4498 (3)	0.85086 (13)	0.49471 (15)	0.0644 (5)	
H5	0.4114	0.8792	0.4217	0.077*	
C6	0.6375 (4)	0.87843 (14)	0.56788 (18)	0.0701 (6)	
H6	0.7272	0.9256	0.5448	0.084*	
C7	0.6978 (3)	0.83631 (15)	0.67849 (17)	0.0729 (6)	
H7	0.8267	0.8561	0.7283	0.087*	
C8	0.5700 (3)	0.76724 (14)	0.71306 (15)	0.0644 (5)	
H8	0.6128	0.7392	0.7860	0.077*	
C9	0.3723 (3)	0.73727 (12)	0.63946 (13)	0.0514 (5)	
C11	−0.0822 (3)	0.57463 (13)	0.65666 (15)	0.0591 (5)	
C12	−0.2299 (4)	0.48788 (16)	0.77775 (19)	0.0812 (7)	
H12A	−0.3146	0.5189	0.8280	0.097*	
H12B	−0.1788	0.4247	0.8099	0.097*	
C13	−0.3652 (4)	0.47695 (17)	0.65699 (18)	0.0815 (7)	
H13A	−0.3657	0.4096	0.6312	0.098*	
H13B	−0.5156	0.4977	0.6533	0.098*	
N1	0.2441 (2)	0.67018 (10)	0.67998 (11)	0.0538 (4)	
N2	−0.2574 (3)	0.54003 (12)	0.58733 (13)	0.0854 (7)	0.473 (17)
O1	−0.0448 (2)	0.54973 (11)	0.76424 (12)	0.0751 (7)	0.473 (17)
O1A	−0.2574 (3)	0.54003 (12)	0.58733 (13)	0.0854 (7)	0.527 (17)
N2A	−0.0448 (2)	0.54973 (11)	0.76424 (12)	0.0751 (7)	0.527 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0561 (11)	0.0528 (10)	0.0477 (10)	0.0063 (9)	0.0085 (9)	−0.0031 (8)
C2	0.0650 (13)	0.0777 (13)	0.0509 (11)	−0.0018 (11)	−0.0007 (9)	0.0018 (9)
C3	0.0771 (14)	0.0744 (14)	0.0450 (10)	0.0102 (11)	0.0019 (10)	0.0063 (8)
C4	0.0640 (12)	0.0516 (10)	0.0448 (9)	0.0099 (9)	0.0141 (9)	0.0004 (7)
C5	0.0796 (14)	0.0627 (12)	0.0534 (11)	0.0080 (11)	0.0194 (11)	0.0074 (9)
C6	0.0747 (14)	0.0647 (13)	0.0751 (13)	−0.0037 (11)	0.0253 (11)	0.0090 (10)
C7	0.0706 (14)	0.0771 (14)	0.0676 (13)	−0.0116 (11)	0.0071 (11)	0.0052 (10)
C8	0.0699 (14)	0.0682 (13)	0.0515 (10)	−0.0032 (10)	0.0047 (10)	0.0087 (8)

C9	0.0583 (11)	0.0506 (10)	0.0439 (9)	0.0083 (9)	0.0075 (8)	−0.0007 (7)
C11	0.0600 (12)	0.0562 (11)	0.0604 (12)	0.0043 (9)	0.0112 (10)	−0.0050 (9)
C12	0.0734 (15)	0.0889 (15)	0.0850 (15)	−0.0119 (12)	0.0249 (12)	0.0050 (11)
C13	0.0698 (14)	0.0826 (15)	0.0923 (16)	−0.0137 (11)	0.0178 (13)	0.0012 (11)
N1	0.0580 (9)	0.0536 (9)	0.0481 (8)	0.0009 (7)	0.0075 (7)	0.0019 (6)
N2	0.0765 (12)	0.1034 (13)	0.0690 (11)	−0.0272 (9)	−0.0013 (9)	0.0046 (8)
O1	0.0772 (12)	0.0848 (12)	0.0607 (10)	−0.0168 (8)	0.0083 (8)	0.0091 (7)
O1A	0.0765 (12)	0.1034 (13)	0.0690 (11)	−0.0272 (9)	−0.0013 (9)	0.0046 (8)
N2A	0.0772 (12)	0.0848 (12)	0.0607 (10)	−0.0168 (8)	0.0083 (8)	0.0091 (7)

Geometric parameters (Å, °)

C1—N1	1.315 (2)	C7—H7	0.9300
C1—C2	1.412 (2)	C8—C9	1.411 (2)
C1—C11	1.472 (3)	C8—H8	0.9300
C2—C3	1.343 (3)	C9—N1	1.366 (2)
C2—H2	0.9300	C11—O1	1.289 (2)
C3—C4	1.409 (2)	C11—N2	1.307 (2)
C3—H3	0.9300	C12—O1	1.464 (2)
C4—C5	1.409 (2)	C12—C13	1.505 (3)
C4—C9	1.413 (2)	C12—H12A	0.9700
C5—C6	1.353 (2)	C12—H12B	0.9700
C5—H5	0.9300	C13—N2	1.450 (2)
C6—C7	1.405 (2)	C13—H13A	0.9700
C6—H6	0.9300	C13—H13B	0.9700
C7—C8	1.352 (3)		
N1—C1—C2	123.27 (18)	C9—C8—H8	119.7
N1—C1—C11	117.23 (15)	N1—C9—C8	118.48 (15)
C2—C1—C11	119.46 (16)	N1—C9—C4	122.63 (16)
C3—C2—C1	119.45 (17)	C8—C9—C4	118.87 (18)
C3—C2—H2	120.3	O1—C11—N2	118.51 (18)
C1—C2—H2	120.3	O1—C11—C1	122.40 (16)
C2—C3—C4	119.85 (16)	N2—C11—C1	119.03 (16)
C2—C3—H3	120.1	O1—C12—C13	104.53 (16)
C4—C3—H3	120.1	O1—C12—H12A	110.8
C3—C4—C5	123.84 (16)	C13—C12—H12A	110.8
C3—C4—C9	117.14 (18)	O1—C12—H12B	110.8
C5—C4—C9	119.01 (17)	C13—C12—H12B	110.8
C6—C5—C4	120.54 (17)	H12A—C12—H12B	108.9
C6—C5—H5	119.7	N2—C13—C12	104.22 (15)
C4—C5—H5	119.7	N2—C13—H13A	110.9
C5—C6—C7	120.47 (19)	C12—C13—H13A	110.9
C5—C6—H6	119.8	N2—C13—H13B	110.9
C7—C6—H6	119.8	C12—C13—H13B	110.9
C8—C7—C6	120.50 (18)	H13A—C13—H13B	108.9
C8—C7—H7	119.7	C1—N1—C9	117.63 (14)
C6—C7—H7	119.7	C11—N2—C13	106.47 (15)
C7—C8—C9	120.60 (17)	C11—O1—C12	106.02 (16)
C7—C8—H8	119.7		

N1—C1—C2—C3	−1.4 (3)	N1—C1—C11—O1	8.9 (3)
C11—C1—C2—C3	176.45 (16)	C2—C1—C11—O1	−169.11 (17)
C1—C2—C3—C4	1.1 (3)	N1—C1—C11—N2	−173.99 (16)
C2—C3—C4—C5	−178.70 (17)	C2—C1—C11—N2	8.0 (3)
C2—C3—C4—C9	0.2 (3)	O1—C12—C13—N2	−4.9 (2)
C3—C4—C5—C6	179.00 (17)	C2—C1—N1—C9	0.3 (2)
C9—C4—C5—C6	0.2 (3)	C11—C1—N1—C9	−177.55 (14)
C4—C5—C6—C7	0.0 (3)	C8—C9—N1—C1	179.31 (15)
C5—C6—C7—C8	0.4 (3)	C4—C9—N1—C1	1.0 (2)
C6—C7—C8—C9	−0.9 (3)	O1—C11—N2—C13	−1.2 (2)
C7—C8—C9—N1	−177.34 (17)	C1—C11—N2—C13	−178.42 (15)
C7—C8—C9—C4	1.1 (3)	C12—C13—N2—C11	3.8 (2)
C3—C4—C9—N1	−1.3 (2)	N2—C11—O1—C12	−2.2 (2)
C5—C4—C9—N1	177.67 (14)	C1—C11—O1—C12	174.98 (16)
C3—C4—C9—C8	−179.57 (15)	C13—C12—O1—C11	4.4 (2)
C5—C4—C9—C8	−0.6 (2)		

Fig. 1