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1-(Quinolin-2-yl)ethanone

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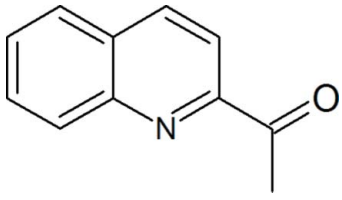
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.061; wR factor = 0.188; data-to-parameter ratio = 25.2.

The title compound, $C_{11}H_9NO$, crystallizes with four independent molecules in the asymmetric unit. The formyl group in each molecule is coplanar with the attached quinoline ring system. The independent molecules exist as two pseudo-inversion-related pairs. Each set of these molecules forms sheets parallel to the *ac* plane which are alternately stacked along the *b* axis. The crystal packing is stabilized by C—H···O intermolecular hydrogen-bonding interactions.

Related literature

For related structures, see: Lynch & McClenaghan (2001); Firley *et al.* (2005); Yathirajan *et al.* (2007). For related literature, see: Padwa *et al.* (1999); Robert & Meunier (1998); Franck *et al.* (2004).



Experimental

Crystal data

$C_{11}H_9NO$
M_r = 171.19
Monoclinic, $P2_1/c$
a = 10.3292 (4) Å
b = 24.1165 (9) Å
c = 15.0923 (5) Å
β = 109.782 (1)°
V = 3537.7 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 203 K
0.49 × 0.41 × 0.19 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlisPro*; Oxford Diffraction, 2007)
T_{min} = 0.914, T_{max} = 1.000 (expected range 0.896–0.980)
55457 measured reflections
11936 independent reflections
5086 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.188
S = 1.01
11936 reflections
473 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3B—H3BA···O1A^{i}	0.94	2.48	3.410 (2)	169
C6D—H6DA···O1D^{ii}	0.94	2.49	3.399 (2)	163

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

ANM thanks Sequent Scientific Ltd, Mangalore, India, for the gift of the sample of the title compound. RJB acknowledges the NSF–MRI program (grant No. CHE-0619278) for funds to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2423).

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supplementary materials

Acta Cryst. (2007). E**63**, o3603 [**doi:10.1107/S160053680703574X**]

1-(Quinolin-2-yl)ethanone

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Comment

Quinolines have been interesting to researchers for many years because a large number of natural products contain these heterocycles. They are found in numerous commercial products, including pharmaceuticals, fragrances and dyes. Quinoline alkaloids such as quinine, chloroquin, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria. Several quinoline derivatives have been evaluated *in vitro* against several parasites and HTLV-1 transformed cells. Prompted by the varied biological activities, the crystal structure of the title compound is reported.

The asymmetric unit of the title compound contains four independent molecules A, B, C and D; one of the independent molecules, A, is shown in Fig. 1. The N1—C1—C10—C11 torsion angles [(A) 1.7 (2)°, (B) 1.0 (2)°, (C) −1.0 (2)° and (D) 0.2 (2)°] indicate that the acetate group in each independent molecule is coplanar with the attached quinoline ring system.

The independent molecules exist as two pseudo inversion-related pairs (A/C and B/D). In the B/D pair the centroids of the pyridine rings are separated by a distance of 3.7181 (9) Å, indicating π-π stacking interaction. Crystal packing shows each set of these molecules form sheets parallel to the *ac* plane. One of the sheets is shown in Fig. 2. The sheets formed by the A/C and B/D pairs are alternately stacked along the *b* axis. The sheets are cross-linked by C—H···O intermolecular hydrogen-bonding interactions (Fig. 3).

Experimental

The title compound was obtained as a gift sample from Sequent Scientific Ltd, Mangalore, India. The sample was crystallized from ethyl acetate (m.p. 325–327 K).

Refinement

The H atoms were included in the riding model approximation with C—H = 0.94 or 0.97 Å, and with U_{iso}(H) = 1.18–1.50U_{eq}(C). A rotating group model was used for the methyl groups. Owing to the poor diffraction quality of the crystal, the ratio of observed to unique reflections is low (43%).

Figures

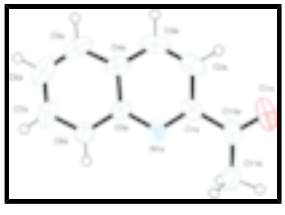

Fig. 1. Molecular structure of one of the independent molecules (A) in the title compound. Displacement ellipsoids are drawn at the 50% probability level.

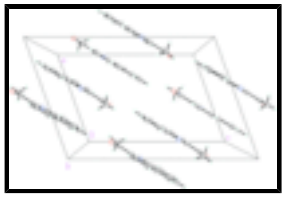

Fig. 2. A view of a sheet formed by two of the four independent molecules in the title compound, showing π-π stacking among inverted quinoline ring systems.

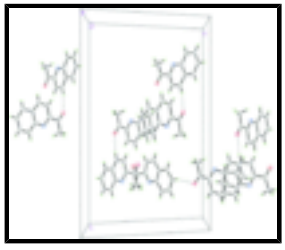

Fig. 3. Packing diagram of the title compound, viewed down the *a* axis. Dashed lines indicate C—H···O hydrogen bonds.

1-(Quinolin-2-yl)ethanone

Crystal data

$C_{11}H_9NO$	F_{000} = 1440
M_r = 171.19	D_x = 1.286 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11806 reflections
a = 10.3292 (4) Å	θ = 4.6–32.5º
b = 24.1165 (9) Å	μ = 0.08 mm^{-1}
c = 15.0923 (5) Å	T = 203 K
β = 109.782 (1)º	Prism, colourless
V = 3537.7 (2) Å^3	0.49 × 0.41 × 0.19 mm
Z = 16	

Data collection

Oxford Diffraction Gemini R diffractometer	R_{int} = 0.074
Radiation source: fine-focus sealed tube	θ_{max} = 32.5º
Monochromator: graphite	θ_{min} = 4.6º
T = 203 K	h = −15→15
φ and ω scans	k = −33→36
Absorption correction: multi-scan (CrysAlisPro; Oxford Diffraction, 2007)	l = −22→22
T_{min} = 0.914, T_{max} = 1.000	1 standard reflections
55457 measured reflections	every 50 reflections
11936 independent reflections	intensity decay: none
5086 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.188$

$S = 1.01$

11936 reflections

473 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.26$ e Å^{-3}

$\Delta\rho_{min} = -0.29$ e Å^{-3}

Extinction correction: none

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}
O1A	−0.07703 (15)	1.04971 (5)	0.28167 (9)	0.0632 (4)
O1B	0.61623 (16)	0.69661 (6)	0.42156 (10)	0.0748 (4)
O1C	0.56572 (15)	0.94486 (6)	0.22088 (10)	0.0671 (4)
O1D	−0.01689 (13)	0.78006 (5)	−0.12826 (9)	0.0606 (4)
N1A	0.09636 (13)	0.98762 (5)	0.14437 (8)	0.0355 (3)
N1B	0.34651 (13)	0.78162 (5)	0.28716 (8)	0.0373 (3)
N1C	0.40511 (13)	1.02002 (5)	0.35393 (8)	0.0360 (3)
N1D	0.27293 (13)	0.70810 (5)	0.01421 (8)	0.0357 (3)
C1A	0.05158 (15)	1.02859 (6)	0.18400 (10)	0.0353 (4)
C2A	0.07495 (16)	1.08525 (7)	0.17001 (11)	0.0406 (4)
H2AA	0.0408	1.1131	0.1998	0.049*
C3A	0.14743 (16)	1.09886 (7)	0.11289 (11)	0.0401 (4)
H3AA	0.1639	1.1363	0.1028	0.048*
C4A	0.19768 (15)	1.05654 (6)	0.06896 (10)	0.0334 (3)
C5A	0.27301 (16)	1.06655 (7)	0.00820 (10)	0.0404 (4)
H5AA	0.2923	1.1033	−0.0042	0.048*
C6A	0.31811 (18)	1.02406 (7)	−0.03262 (11)	0.0454 (4)
H6AA	0.3688	1.0314	−0.0726	0.054*
C7A	0.28899 (18)	0.96909 (7)	−0.01509 (11)	0.0477 (4)
H7AA	0.3201	0.9398	−0.0438	0.057*
C8A	0.21618 (17)	0.95771 (7)	0.04305 (11)	0.0425 (4)
H8AA	0.1976	0.9207	0.0542	0.051*

C9A	0.16879 (15)	1.00091 (6)	0.08646 (9)	0.0331 (3)
C10A	−0.03023 (17)	1.01341 (7)	0.24530 (11)	0.0410 (4)
C11A	−0.05311 (19)	0.95347 (7)	0.26026 (12)	0.0482 (4)
H11A	−0.1211	0.9500	0.2912	0.072*
H11B	0.0327	0.9368	0.2994	0.072*
H11C	−0.0858	0.9346	0.1999	0.072*
C1B	0.40895 (18)	0.73489 (7)	0.32194 (10)	0.0404 (4)
C2B	0.3457 (2)	0.68248 (7)	0.29934 (13)	0.0538 (5)
H2BA	0.3941	0.6500	0.3253	0.065*
C3B	0.2143 (2)	0.67967 (8)	0.23973 (14)	0.0576 (5)
H3BA	0.1708	0.6450	0.2245	0.069*
C4B	0.14213 (19)	0.72846 (7)	0.20026 (11)	0.0457 (4)
C5B	0.0050 (2)	0.72994 (10)	0.13782 (14)	0.0641 (6)
H5BA	−0.0446	0.6967	0.1206	0.077*
C6B	−0.0568 (2)	0.77907 (11)	0.10202 (14)	0.0671 (6)
H6BA	−0.1480	0.7793	0.0601	0.080*
C7B	0.01464 (19)	0.82881 (9)	0.12728 (12)	0.0579 (5)
H7BA	−0.0285	0.8624	0.1022	0.069*
C8B	0.14661 (18)	0.82904 (7)	0.18805 (11)	0.0467 (4)
H8BA	0.1936	0.8629	0.2047	0.056*
C9B	0.21395 (17)	0.77913 (6)	0.22641 (10)	0.0369 (4)
C10B	0.55432 (19)	0.73872 (8)	0.38828 (11)	0.0480 (4)
C11B	0.6186 (2)	0.79410 (9)	0.41227 (14)	0.0618 (5)
H11D	0.7146	0.7898	0.4508	0.093*
H11E	0.5711	0.8150	0.4469	0.093*
H11F	0.6123	0.8138	0.3549	0.093*
C1C	0.44322 (15)	0.97599 (6)	0.31720 (10)	0.0346 (3)
C2C	0.41114 (17)	0.92106 (7)	0.33494 (11)	0.0425 (4)
H2CA	0.4389	0.8910	0.3059	0.051*
C3C	0.34016 (17)	0.91224 (7)	0.39416 (11)	0.0431 (4)
H3CA	0.3187	0.8759	0.4070	0.052*
C4C	0.29849 (15)	0.95769 (7)	0.43651 (10)	0.0370 (4)
C5C	0.22541 (17)	0.95245 (8)	0.49916 (11)	0.0473 (4)
H5CA	0.2040	0.9169	0.5158	0.057*
C6C	0.18511 (18)	0.99770 (9)	0.53622 (12)	0.0534 (5)
H6CA	0.1352	0.9934	0.5776	0.064*
C7C	0.21778 (19)	1.05106 (9)	0.51296 (13)	0.0568 (5)
H7CA	0.1893	1.0823	0.5388	0.068*
C8C	0.29049 (18)	1.05791 (7)	0.45319 (12)	0.0487 (4)
H8CA	0.3127	1.0938	0.4387	0.058*
C9C	0.33226 (15)	1.01170 (7)	0.41326 (10)	0.0359 (4)
C10C	0.52527 (17)	0.98490 (7)	0.25350 (11)	0.0426 (4)
C11C	0.55773 (19)	1.04276 (7)	0.23343 (12)	0.0482 (4)
H11G	0.6110	1.0421	0.1914	0.072*
H11H	0.6105	1.0609	0.2919	0.072*
H11I	0.4728	1.0630	0.2039	0.072*
C1D	0.19891 (16)	0.75186 (6)	−0.02455 (9)	0.0345 (3)
C2D	0.24719 (18)	0.80692 (7)	−0.00719 (11)	0.0426 (4)
H2DA	0.1905	0.8368	−0.0366	0.051*

C3D	0.37661 (19)	0.81588 (7)	0.05259 (11)	0.0478 (4)
H3DA	0.4104	0.8523	0.0652	0.057*
C4D	0.46046 (17)	0.77089 (7)	0.09584 (10)	0.0395 (4)
C5D	0.59782 (19)	0.77644 (9)	0.15884 (12)	0.0535 (5)
H5DA	0.6376	0.8118	0.1732	0.064*
C6D	0.67187 (19)	0.73061 (9)	0.19843 (12)	0.0566 (5)
H6DA	0.7625	0.7347	0.2402	0.068*
C7D	0.61497 (19)	0.67772 (9)	0.17777 (12)	0.0551 (5)
H7DA	0.6676	0.6466	0.2061	0.066*
C8D	0.48436 (17)	0.67053 (7)	0.11711 (11)	0.0442 (4)
H8DA	0.4476	0.6346	0.1036	0.053*
C9D	0.40373 (16)	0.71704 (6)	0.07426 (10)	0.0365 (4)
C10D	0.05534 (17)	0.74153 (7)	−0.09018 (10)	0.0403 (4)
C11D	0.00576 (19)	0.68309 (8)	−0.10771 (14)	0.0571 (5)
H11J	−0.0888	0.6828	−0.1502	0.086*
H11K	0.0107	0.6659	−0.0486	0.086*
H11L	0.0631	0.6627	−0.1357	0.086*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0817 (10)	0.0495 (8)	0.0786 (9)	0.0120 (7)	0.0535 (8)	0.0025 (6)
O1B	0.0790 (10)	0.0721 (10)	0.0684 (9)	0.0381 (8)	0.0186 (8)	0.0202 (7)
O1C	0.0861 (10)	0.0576 (9)	0.0776 (9)	−0.0007 (7)	0.0538 (8)	−0.0101 (7)
O1D	0.0498 (8)	0.0568 (8)	0.0599 (8)	0.0169 (6)	−0.0014 (6)	−0.0007 (6)
N1A	0.0360 (7)	0.0342 (7)	0.0349 (6)	0.0040 (6)	0.0100 (6)	0.0010 (5)
N1B	0.0383 (8)	0.0360 (7)	0.0369 (7)	0.0031 (6)	0.0117 (6)	−0.0001 (5)
N1C	0.0356 (7)	0.0375 (7)	0.0352 (6)	−0.0034 (6)	0.0122 (6)	0.0005 (5)
N1D	0.0356 (7)	0.0386 (7)	0.0325 (6)	0.0060 (6)	0.0112 (6)	−0.0005 (5)
C1A	0.0325 (8)	0.0378 (9)	0.0332 (7)	0.0025 (7)	0.0080 (7)	−0.0007 (6)
C2A	0.0434 (9)	0.0357 (9)	0.0417 (8)	0.0046 (7)	0.0133 (8)	−0.0058 (7)
C3A	0.0424 (9)	0.0312 (8)	0.0445 (9)	−0.0023 (7)	0.0119 (8)	−0.0025 (7)
C4A	0.0289 (8)	0.0355 (8)	0.0316 (7)	−0.0007 (6)	0.0045 (6)	0.0000 (6)
C5A	0.0353 (9)	0.0428 (9)	0.0403 (8)	−0.0051 (7)	0.0092 (7)	0.0037 (7)
C6A	0.0427 (10)	0.0561 (11)	0.0388 (8)	0.0042 (8)	0.0157 (8)	0.0058 (8)
C7A	0.0542 (11)	0.0474 (10)	0.0461 (9)	0.0133 (9)	0.0229 (9)	−0.0018 (8)
C8A	0.0485 (10)	0.0355 (9)	0.0459 (9)	0.0075 (7)	0.0190 (8)	−0.0002 (7)
C9A	0.0322 (8)	0.0350 (8)	0.0284 (7)	0.0034 (6)	0.0057 (6)	0.0015 (6)
C10A	0.0401 (9)	0.0430 (10)	0.0406 (8)	0.0069 (7)	0.0144 (7)	0.0033 (7)
C11A	0.0561 (11)	0.0457 (10)	0.0482 (9)	0.0046 (8)	0.0248 (9)	0.0074 (8)
C1B	0.0524 (10)	0.0382 (9)	0.0368 (8)	0.0079 (8)	0.0232 (8)	0.0019 (7)
C2B	0.0767 (14)	0.0375 (10)	0.0551 (10)	0.0043 (9)	0.0326 (11)	0.0004 (8)
C3B	0.0812 (15)	0.0402 (10)	0.0643 (11)	−0.0196 (10)	0.0414 (11)	−0.0133 (9)
C4B	0.0524 (11)	0.0506 (11)	0.0424 (9)	−0.0134 (8)	0.0269 (9)	−0.0115 (8)
C5B	0.0569 (13)	0.0849 (16)	0.0556 (11)	−0.0321 (12)	0.0258 (11)	−0.0266 (11)
C6B	0.0388 (11)	0.1102 (19)	0.0487 (11)	−0.0032 (12)	0.0102 (9)	−0.0180 (11)
C7B	0.0441 (11)	0.0798 (15)	0.0437 (9)	0.0137 (10)	0.0069 (9)	−0.0084 (9)
C8B	0.0430 (10)	0.0488 (10)	0.0447 (9)	0.0045 (8)	0.0100 (8)	−0.0019 (8)

C9B	0.0392 (9)	0.0420 (9)	0.0332 (7)	−0.0016 (7)	0.0170 (7)	−0.0049 (6)
C10B	0.0516 (11)	0.0562 (11)	0.0388 (8)	0.0187 (9)	0.0186 (8)	0.0082 (8)
C11B	0.0444 (11)	0.0722 (14)	0.0578 (11)	0.0055 (10)	0.0028 (9)	0.0006 (10)
C1C	0.0301 (8)	0.0373 (9)	0.0345 (7)	−0.0012 (6)	0.0084 (7)	0.0014 (6)
C2C	0.0456 (10)	0.0379 (9)	0.0428 (8)	−0.0018 (7)	0.0133 (8)	−0.0004 (7)
C3C	0.0436 (9)	0.0360 (9)	0.0458 (9)	−0.0073 (7)	0.0100 (8)	0.0022 (7)
C4C	0.0290 (8)	0.0460 (9)	0.0328 (8)	−0.0061 (7)	0.0061 (7)	0.0033 (7)
C5C	0.0406 (9)	0.0557 (11)	0.0439 (9)	−0.0111 (8)	0.0120 (8)	0.0040 (8)
C6C	0.0397 (10)	0.0794 (14)	0.0435 (9)	−0.0074 (9)	0.0172 (8)	−0.0014 (9)
C7C	0.0541 (11)	0.0648 (13)	0.0555 (11)	0.0047 (10)	0.0237 (10)	−0.0120 (9)
C8C	0.0542 (11)	0.0469 (10)	0.0495 (9)	−0.0042 (8)	0.0235 (9)	−0.0036 (8)
C9C	0.0284 (8)	0.0426 (9)	0.0322 (7)	−0.0030 (7)	0.0043 (7)	0.0003 (6)
C10C	0.0420 (9)	0.0483 (10)	0.0385 (8)	−0.0011 (8)	0.0149 (8)	−0.0025 (7)
C11C	0.0487 (10)	0.0552 (11)	0.0438 (9)	−0.0046 (9)	0.0196 (8)	0.0072 (8)
C1D	0.0370 (8)	0.0398 (9)	0.0282 (7)	0.0071 (7)	0.0129 (7)	−0.0014 (6)
C2D	0.0503 (10)	0.0360 (9)	0.0406 (8)	0.0086 (8)	0.0142 (8)	−0.0001 (7)
C3D	0.0532 (11)	0.0402 (9)	0.0477 (9)	−0.0040 (8)	0.0138 (9)	−0.0057 (7)
C4D	0.0378 (9)	0.0488 (10)	0.0338 (8)	0.0004 (7)	0.0144 (7)	−0.0032 (7)
C5D	0.0424 (10)	0.0699 (13)	0.0458 (10)	−0.0072 (9)	0.0116 (9)	−0.0077 (9)
C6D	0.0329 (9)	0.0939 (16)	0.0384 (9)	0.0066 (10)	0.0062 (8)	−0.0008 (10)
C7D	0.0491 (11)	0.0734 (14)	0.0414 (9)	0.0198 (10)	0.0133 (9)	0.0068 (9)
C8D	0.0428 (10)	0.0514 (10)	0.0382 (8)	0.0123 (8)	0.0135 (8)	0.0036 (7)
C9D	0.0345 (8)	0.0452 (9)	0.0318 (7)	0.0062 (7)	0.0140 (7)	0.0011 (6)
C10D	0.0385 (9)	0.0466 (10)	0.0351 (8)	0.0067 (8)	0.0116 (7)	−0.0041 (7)
C11D	0.0453 (11)	0.0532 (11)	0.0646 (11)	−0.0002 (9)	0.0077 (9)	−0.0086 (9)

Geometric parameters (Å, °)

O1A—C10A	1.2170 (19)	C8B—C9B	1.412 (2)
O1B—C10B	1.214 (2)	C8B—H8BA	0.94
O1C—C10C	1.220 (2)	C10B—C11B	1.481 (3)
O1D—C10D	1.2084 (18)	C11B—H11D	0.97
N1A—C1A	1.3173 (19)	C11B—H11E	0.97
N1A—C9A	1.3671 (19)	C11B—H11F	0.97
N1B—C1B	1.3162 (19)	C1C—C2C	1.413 (2)
N1B—C9B	1.367 (2)	C1C—C10C	1.497 (2)
N1C—C1C	1.318 (2)	C2C—C3C	1.351 (2)
N1C—C9C	1.3653 (19)	C2C—H2CA	0.94
N1D—C1D	1.3183 (19)	C3C—C4C	1.408 (2)
N1D—C9D	1.3654 (19)	C3C—H3CA	0.94
C1A—C2A	1.416 (2)	C4C—C5C	1.401 (2)
C1A—C10A	1.494 (2)	C4C—C9C	1.423 (2)
C2A—C3A	1.360 (2)	C5C—C6C	1.354 (3)
C2A—H2AA	0.94	C5C—H5CA	0.94
C3A—C4A	1.408 (2)	C6C—C7C	1.405 (3)
C3A—H3AA	0.94	C6C—H6CA	0.94
C4A—C5A	1.410 (2)	C7C—C8C	1.365 (2)
C4A—C9A	1.419 (2)	C7C—H7CA	0.94
C5A—C6A	1.357 (2)	C8C—C9C	1.403 (2)

C5A—H5AA	0.94	C8C—H8CA	0.94
C6A—C7A	1.404 (2)	C10C—C11C	1.490 (2)
C6A—H6AA	0.94	C11C—H11G	0.97
C7A—C8A	1.363 (2)	C11C—H11H	0.97
C7A—H7AA	0.94	C11C—H11I	0.97
C8A—C9A	1.404 (2)	C1D—C2D	1.411 (2)
C8A—H8AA	0.94	C1D—C10D	1.499 (2)
C10A—C11A	1.494 (2)	C2D—C3D	1.353 (2)
C11A—H11A	0.97	C2D—H2DA	0.94
C11A—H11B	0.97	C3D—C4D	1.404 (2)
C11A—H11C	0.97	C3D—H3DA	0.94
C1B—C2B	1.411 (2)	C4D—C9D	1.417 (2)
C1B—C10B	1.499 (2)	C4D—C5D	1.422 (2)
C2B—C3B	1.352 (3)	C5D—C6D	1.362 (3)
C2B—H2BA	0.94	C5D—H5DA	0.94
C3B—C4B	1.413 (3)	C6D—C7D	1.395 (3)
C3B—H3BA	0.94	C6D—H6DA	0.94
C4B—C5B	1.411 (3)	C7D—C8D	1.361 (2)
C4B—C9B	1.415 (2)	C7D—H7DA	0.94
C5B—C6B	1.367 (3)	C8D—C9D	1.416 (2)
C5B—H5BA	0.94	C8D—H8DA	0.94
C6B—C7B	1.392 (3)	C10D—C11D	1.492 (2)
C6B—H6BA	0.94	C11D—H11J	0.97
C7B—C8B	1.361 (2)	C11D—H11K	0.97
C7B—H7BA	0.94	C11D—H11L	0.97
C1A—N1A—C9A	117.82 (13)	H11D—C11B—H11F	109.5
C1B—N1B—C9B	118.31 (14)	H11E—C11B—H11F	109.5
C1C—N1C—C9C	117.83 (13)	N1C—C1C—C2C	123.57 (15)
C1D—N1D—C9D	117.59 (14)	N1C—C1C—C10C	117.99 (14)
N1A—C1A—C2A	123.53 (15)	C2C—C1C—C10C	118.44 (15)
N1A—C1A—C10A	117.15 (14)	C3C—C2C—C1C	119.18 (16)
C2A—C1A—C10A	119.31 (14)	C3C—C2C—H2CA	120.4
C3A—C2A—C1A	119.06 (15)	C1C—C2C—H2CA	120.4
C3A—C2A—H2AA	120.5	C2C—C3C—C4C	119.70 (15)
C1A—C2A—H2AA	120.5	C2C—C3C—H3CA	120.1
C2A—C3A—C4A	119.57 (15)	C4C—C3C—H3CA	120.1
C2A—C3A—H3AA	120.2	C5C—C4C—C3C	123.61 (15)
C4A—C3A—H3AA	120.2	C5C—C4C—C9C	118.82 (15)
C3A—C4A—C5A	123.68 (14)	C3C—C4C—C9C	117.57 (14)
C3A—C4A—C9A	117.61 (14)	C6C—C5C—C4C	121.14 (17)
C5A—C4A—C9A	118.70 (14)	C6C—C5C—H5CA	119.4
C6A—C5A—C4A	121.06 (15)	C4C—C5C—H5CA	119.4
C6A—C5A—H5AA	119.5	C5C—C6C—C7C	120.09 (18)
C4A—C5A—H5AA	119.5	C5C—C6C—H6CA	120.0
C5A—C6A—C7A	119.94 (16)	C7C—C6C—H6CA	120.0
C5A—C6A—H6AA	120.0	C8C—C7C—C6C	120.56 (18)
C7A—C6A—H6AA	120.0	C8C—C7C—H7CA	119.7
C8A—C7A—C6A	120.76 (16)	C6C—C7C—H7CA	119.7
C8A—C7A—H7AA	119.6	C7C—C8C—C9C	120.39 (17)

C6A—C7A—H7AA	119.6	C7C—C8C—H8CA	119.8
C7A—C8A—C9A	120.43 (16)	C9C—C8C—H8CA	119.8
C7A—C8A—H8AA	119.8	N1C—C9C—C8C	118.89 (15)
C9A—C8A—H8AA	119.8	N1C—C9C—C4C	122.12 (14)
N1A—C9A—C8A	118.49 (14)	C8C—C9C—C4C	118.99 (15)
N1A—C9A—C4A	122.41 (13)	O1C—C10C—C11C	121.86 (16)
C8A—C9A—C4A	119.10 (14)	O1C—C10C—C1C	119.43 (16)
O1A—C10A—C11A	121.36 (16)	C11C—C10C—C1C	118.70 (15)
O1A—C10A—C1A	119.82 (15)	C10C—C11C—H11G	109.5
C11A—C10A—C1A	118.83 (14)	C10C—C11C—H11H	109.5
C10A—C11A—H11A	109.5	H11G—C11C—H11H	109.5
C10A—C11A—H11B	109.5	C10C—C11C—H11I	109.5
H11A—C11A—H11B	109.5	H11G—C11C—H11I	109.5
C10A—C11A—H11C	109.5	H11H—C11C—H11I	109.5
H11A—C11A—H11C	109.5	N1D—C1D—C2D	123.74 (14)
H11B—C11A—H11C	109.5	N1D—C1D—C10D	117.10 (14)
N1B—C1B—C2B	123.13 (17)	C2D—C1D—C10D	119.16 (14)
N1B—C1B—C10B	117.29 (15)	C3D—C2D—C1D	118.76 (15)
C2B—C1B—C10B	119.58 (16)	C3D—C2D—H2DA	120.6
C3B—C2B—C1B	118.95 (17)	C1D—C2D—H2DA	120.6
C3B—C2B—H2BA	120.5	C2D—C3D—C4D	120.10 (16)
C1B—C2B—H2BA	120.5	C2D—C3D—H3DA	120.0
C2B—C3B—C4B	120.43 (17)	C4D—C3D—H3DA	120.0
C2B—C3B—H3BA	119.8	C3D—C4D—C9D	117.36 (15)
C4B—C3B—H3BA	119.8	C3D—C4D—C5D	123.86 (16)
C5B—C4B—C3B	124.74 (18)	C9D—C4D—C5D	118.78 (16)
C5B—C4B—C9B	118.52 (18)	C6D—C5D—C4D	120.14 (18)
C3B—C4B—C9B	116.73 (17)	C6D—C5D—H5DA	119.9
C6B—C5B—C4B	120.96 (19)	C4D—C5D—H5DA	119.9
C6B—C5B—H5BA	119.5	C5D—C6D—C7D	120.83 (17)
C4B—C5B—H5BA	119.5	C5D—C6D—H6DA	119.6
C5B—C6B—C7B	120.34 (19)	C7D—C6D—H6DA	119.6
C5B—C6B—H6BA	119.8	C8D—C7D—C6D	120.91 (17)
C7B—C6B—H6BA	119.8	C8D—C7D—H7DA	119.5
C8B—C7B—C6B	120.33 (19)	C6D—C7D—H7DA	119.5
C8B—C7B—H7BA	119.8	C7D—C8D—C9D	120.14 (17)
C6B—C7B—H7BA	119.8	C7D—C8D—H8DA	119.9
C7B—C8B—C9B	120.97 (17)	C9D—C8D—H8DA	119.9
C7B—C8B—H8BA	119.5	N1D—C9D—C8D	118.36 (15)
C9B—C8B—H8BA	119.5	N1D—C9D—C4D	122.46 (14)
N1B—C9B—C8B	118.68 (14)	C8D—C9D—C4D	119.18 (15)
N1B—C9B—C4B	122.45 (15)	O1D—C10D—C11D	121.49 (15)
C8B—C9B—C4B	118.86 (16)	O1D—C10D—C1D	119.99 (15)
O1B—C10B—C11B	121.54 (18)	C11D—C10D—C1D	118.52 (14)
O1B—C10B—C1B	119.53 (18)	C10D—C11D—H11J	109.5
C11B—C10B—C1B	118.93 (15)	C10D—C11D—H11K	109.5
C10B—C11B—H11D	109.5	H11J—C11D—H11K	109.5
C10B—C11B—H11E	109.5	C10D—C11D—H11L	109.5
H11D—C11B—H11E	109.5	H11J—C11D—H11L	109.5

C10B—C11B—H11F	109.5	H11K—C11D—H11L	109.5
C9A—N1A—C1A—C2A	−0.2 (2)	C9C—N1C—C1C—C2C	0.9 (2)
C9A—N1A—C1A—C10A	178.60 (12)	C9C—N1C—C1C—C10C	−178.92 (13)
N1A—C1A—C2A—C3A	−0.1 (2)	N1C—C1C—C2C—C3C	−1.5 (2)
C10A—C1A—C2A—C3A	−178.89 (14)	C10C—C1C—C2C—C3C	178.34 (14)
C1A—C2A—C3A—C4A	0.0 (2)	C1C—C2C—C3C—C4C	0.5 (2)
C2A—C3A—C4A—C5A	179.59 (14)	C2C—C3C—C4C—C5C	−179.58 (15)
C2A—C3A—C4A—C9A	0.4 (2)	C2C—C3C—C4C—C9C	0.9 (2)
C3A—C4A—C5A—C6A	−179.58 (15)	C3C—C4C—C5C—C6C	−178.47 (15)
C9A—C4A—C5A—C6A	−0.4 (2)	C9C—C4C—C5C—C6C	1.1 (2)
C4A—C5A—C6A—C7A	0.5 (2)	C4C—C5C—C6C—C7C	−0.8 (3)
C5A—C6A—C7A—C8A	−0.3 (3)	C5C—C6C—C7C—C8C	−0.2 (3)
C6A—C7A—C8A—C9A	0.1 (2)	C6C—C7C—C8C—C9C	0.8 (3)
C1A—N1A—C9A—C8A	−179.46 (13)	C1C—N1C—C9C—C8C	−179.97 (14)
C1A—N1A—C9A—C4A	0.6 (2)	C1C—N1C—C9C—C4C	0.6 (2)
C7A—C8A—C9A—N1A	−179.89 (14)	C7C—C8C—C9C—N1C	−179.86 (15)
C7A—C8A—C9A—C4A	0.0 (2)	C7C—C8C—C9C—C4C	−0.4 (2)
C3A—C4A—C9A—N1A	−0.7 (2)	C5C—C4C—C9C—N1C	178.95 (13)
C5A—C4A—C9A—N1A	−179.96 (13)	C3C—C4C—C9C—N1C	−1.5 (2)
C3A—C4A—C9A—C8A	179.38 (13)	C5C—C4C—C9C—C8C	−0.5 (2)
C5A—C4A—C9A—C8A	0.1 (2)	C3C—C4C—C9C—C8C	179.09 (14)
N1A—C1A—C10A—O1A	−178.13 (15)	N1C—C1C—C10C—O1C	177.67 (15)
C2A—C1A—C10A—O1A	0.8 (2)	C2C—C1C—C10C—O1C	−2.2 (2)
N1A—C1A—C10A—C11A	1.7 (2)	N1C—C1C—C10C—C11C	−1.0 (2)
C2A—C1A—C10A—C11A	−179.44 (14)	C2C—C1C—C10C—C11C	179.15 (14)
C9B—N1B—C1B—C2B	0.2 (2)	C9D—N1D—C1D—C2D	−0.2 (2)
C9B—N1B—C1B—C10B	179.92 (13)	C9D—N1D—C1D—C10D	−179.85 (12)
N1B—C1B—C2B—C3B	−0.5 (3)	N1D—C1D—C2D—C3D	−0.1 (2)
C10B—C1B—C2B—C3B	179.72 (15)	C10D—C1D—C2D—C3D	179.60 (14)
C1B—C2B—C3B—C4B	0.5 (3)	C1D—C2D—C3D—C4D	0.2 (2)
C2B—C3B—C4B—C5B	−179.74 (17)	C2D—C3D—C4D—C9D	−0.1 (2)
C2B—C3B—C4B—C9B	−0.1 (3)	C2D—C3D—C4D—C5D	179.46 (16)
C3B—C4B—C5B—C6B	−179.29 (18)	C3D—C4D—C5D—C6D	179.45 (16)
C9B—C4B—C5B—C6B	1.0 (3)	C9D—C4D—C5D—C6D	−1.0 (2)
C4B—C5B—C6B—C7B	−0.5 (3)	C4D—C5D—C6D—C7D	0.3 (3)
C5B—C6B—C7B—C8B	−0.2 (3)	C5D—C6D—C7D—C8D	0.4 (3)
C6B—C7B—C8B—C9B	0.2 (3)	C6D—C7D—C8D—C9D	−0.3 (3)
C1B—N1B—C9B—C8B	−179.41 (14)	C1D—N1D—C9D—C8D	179.52 (13)
C1B—N1B—C9B—C4B	0.3 (2)	C1D—N1D—C9D—C4D	0.3 (2)
C7B—C8B—C9B—N1B	−179.98 (15)	C7D—C8D—C9D—N1D	−179.66 (14)
C7B—C8B—C9B—C4B	0.3 (2)	C7D—C8D—C9D—C4D	−0.4 (2)
C5B—C4B—C9B—N1B	179.38 (14)	C3D—C4D—C9D—N1D	−0.1 (2)
C3B—C4B—C9B—N1B	−0.3 (2)	C5D—C4D—C9D—N1D	−179.74 (14)
C5B—C4B—C9B—C8B	−0.9 (2)	C3D—C4D—C9D—C8D	−179.36 (14)
C3B—C4B—C9B—C8B	179.36 (15)	C5D—C4D—C9D—C8D	1.0 (2)
N1B—C1B—C10B—O1B	−179.49 (15)	N1D—C1D—C10D—O1D	−179.47 (14)
C2B—C1B—C10B—O1B	0.3 (2)	C2D—C1D—C10D—O1D	0.8 (2)
N1B—C1B—C10B—C11B	1.0 (2)	N1D—C1D—C10D—C11D	−0.2 (2)
C2B—C1B—C10B—C11B	−179.21 (16)	C2D—C1D—C10D—C11D	−179.92 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3B—H3BA···O1A^{i}	0.94	2.48	3.410 (2)	169
C6D—H6DA···O1D^{ii}	0.94	2.49	3.399 (2)	163

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*+1, −*y*+3/2, *z*+1/2.

Fig. 1

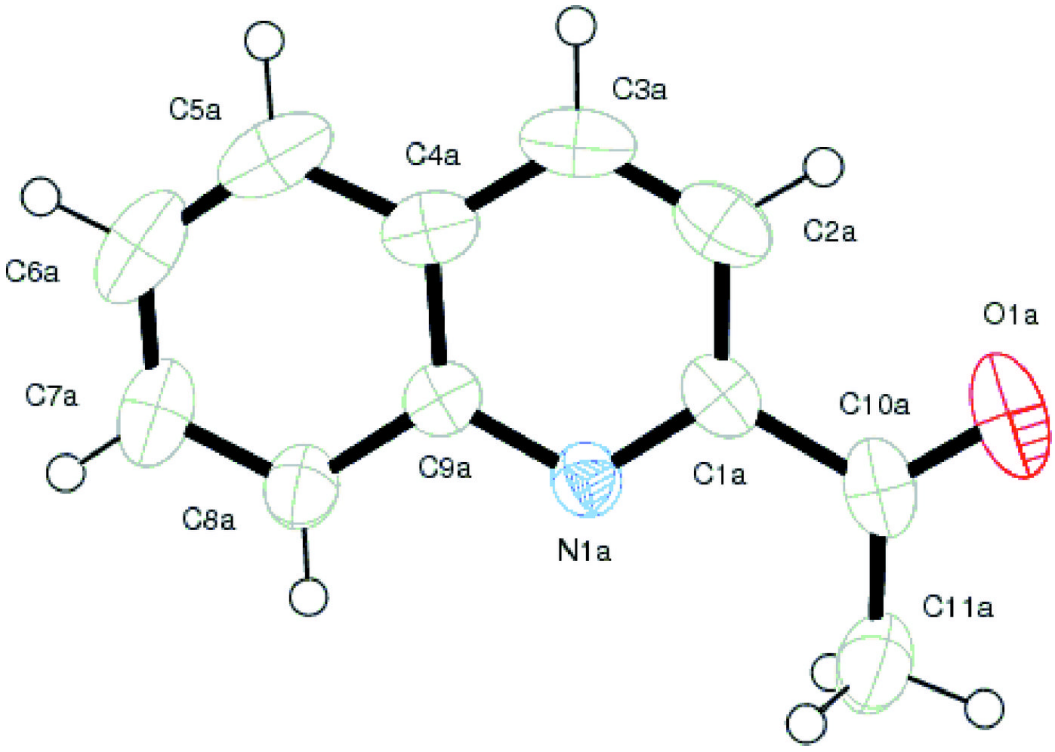

Fig. 2

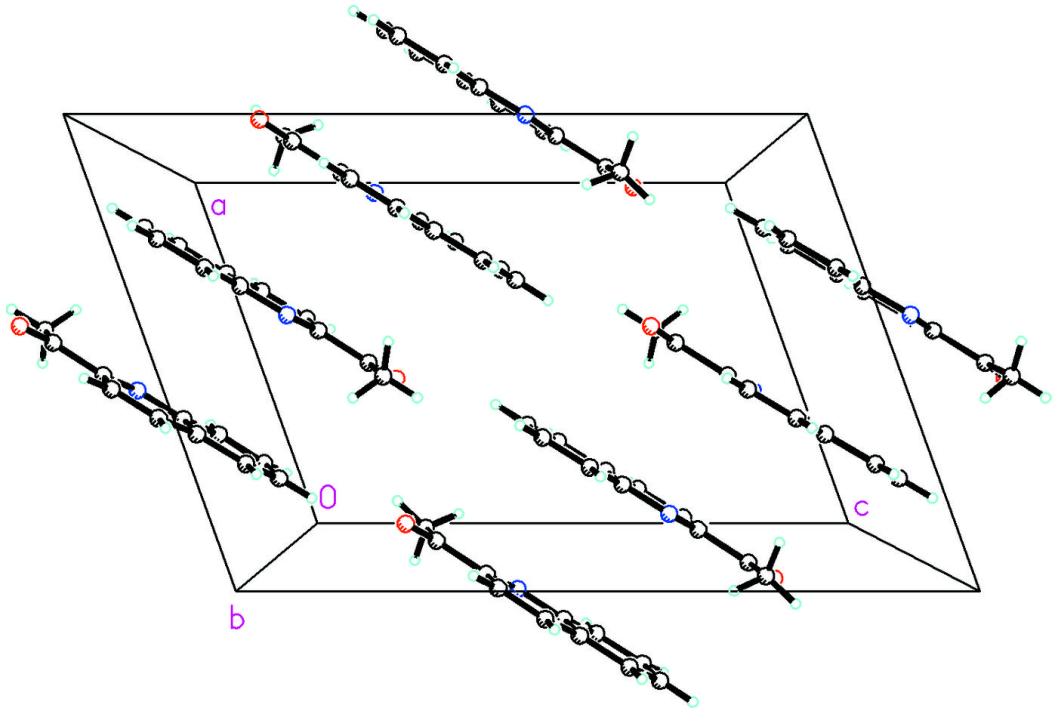

Fig. 3