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Isoquinoline-1-carboxylic acid

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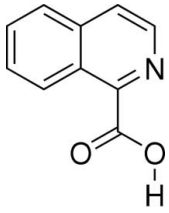
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.134; data-to-parameter ratio = 14.3.

The title compound, $C_{10}H_7NO_2$, crystallizes with three molecules in the asymmetric unit; these are linked by O—H···N hydrogen bonds.

Related literature

For related literature, see: Carlton & Molapisi (2000); Casnati *et al.* (2003); Ghosh & Bharadwaj (2004); Glidewell *et al.* (2005); Jennings *et al.* (2001); Kwon *et al.* (2005); Padbury & Lindwall (1945); Smith *et al.* (1995); You & Park (2005).



Experimental

Crystal data

$C_{10}H_7NO_2$
M_r = 173.17
Triclinic, $P\overline{1}$
a = 8.3707 (6) Å
b = 11.4278 (7) Å
c = 13.2044 (10) Å
α = 108.957 (2)°
β = 100.674 (2)°
γ = 91.447 (2)°
V = 1168.97 (14) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 153 (2) K
0.58 × 0.52 × 0.34 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
11161 measured reflections
5223 independent reflections
4016 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
S = 1.02
5223 reflections
365 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N1A	0.91 (3)	1.76 (3)	2.6673 (16)	177 (3)
O1A—H1OA···N1B	0.97 (3)	1.68 (3)	2.6407 (16)	172 (2)
O1B—H1OB···N1	0.99 (3)	1.69 (3)	2.6715 (17)	171 (3)

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2386).

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supplementary materials

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Comment

Non-covalent interactions, such as hydrogen bonding, π-π stacking and C—H···π interactions, play a dominant role in supramolecular self-assembly (Casnati *et al.*, 2003; Ghosh & Bharadwaj, 2004; Glidewell *et al.*, 2005; Jennings *et al.*, 2001). In order to further understand supramolecular self-assembly through non-covalent interactions, we have synthesized the title compound following a published procedure (Padbury and Lindwall, 1945). It is used as a material in the synthesis of organic metal compounds (You & Park, 2005; Kwon *et al.*, 2005; Carlton & Molapisi, 2000; Smith *et al.*, 1995).

Bond lengths and angles in (I) are normal. Compound (I) crystallizes in the triclinic space group P-1 with *Z*'=3. In (I), the three isoquinoline rings in the asymmetric unit are approximately planar, with maximum deviations of −0.014 (7)Å for atom C1 in N1/C1—C9 ring, 0.017 (6)Å for atom C2A in N1A/C1A—C9A ring and 0.022 (6)Å for atom C6B in N1B/C1B—C9B ring (Fig. 1). The torsion angles between the pyridine rings and carboxyl groups of three molecules in asymmetric unit are different. The N1—C1—C10—O1 torsion angle is −13.3 (2)°. However, the N1A—C1A—C10A—O1A and N1B—C1B—C10B—O1B are 36.17 (19) and −34.1 (2)°, respectively. The crystal packing is stabilized by O—H···N hydrogen bonds (Table 1).

Experimental

The title compound was prepared following a published procedure (Padbury and Lindwall, 1945). Colorless single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethylsulfoxide.

Refinement

O-bound H atoms were located in a difference Fourier map and refined isotropically. The C-bound H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, and with U_{iso}(H) value of 1.2U_{eq}(C).

Figures

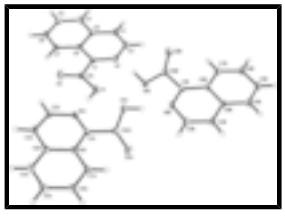


Fig. 1. The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Isoquinoline-1-carboxylic acid

Crystal data

$C_{10}H_7NO_2$	$Z = 6$
$M_r = 173.17$	$F_{000} = 540$
Triclinic, $P\overline{1}$	$D_x = 1.476$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.3707$ (6) Å	Cell parameters from 9042 reflections
$b = 11.4278$ (7) Å	$\theta = 3.1$–$27.6°$
$c = 13.2044$ (10) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 108.957$ (2)°	$T = 153$ (2) K
$\beta = 100.674$ (2)°	Block, colorless
$\gamma = 91.447$ (2)°	0.58 × 0.52 × 0.34 mm
$V = 1168.97$ (14) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4016 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	$R_{int} = 0.037$
Monochromator: graphite	$\theta_{max} = 27.5°$
$T = 153(2)$ K	$\theta_{min} = 3.2°$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -14 \rightarrow 14$
11161 measured reflections	$l = -17 \rightarrow 17$
5223 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 0.33P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.135$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.52$ e Å^{-3}
5223 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}
365 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.018 (3)
Secondary atom site location: difference Fourier map	

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}
O1	0.55014 (15)	0.22987 (10)	0.47803 (9)	0.0308 (3)
O2	0.44813 (17)	0.08212 (11)	0.31984 (9)	0.0403 (3)
N1	0.32740 (16)	0.37701 (11)	0.44770 (10)	0.0228 (3)
C1	0.33565 (18)	0.27907 (13)	0.36107 (11)	0.0197 (3)
C2	0.2212 (2)	0.46223 (14)	0.43699 (13)	0.0279 (4)
H2	0.2178	0.5322	0.4995	0.034*
C3	0.1195 (2)	0.45160 (14)	0.34056 (13)	0.0272 (3)
H3	0.0460	0.5127	0.3366	0.033*
C4	0.0189 (2)	0.33229 (15)	0.14450 (13)	0.0278 (3)
H4	−0.0574	0.3910	0.1385	0.033*
C5	0.0266 (2)	0.23220 (15)	0.05484 (12)	0.0297 (4)
H5	−0.0442	0.2218	−0.0132	0.036*
C6	0.1387 (2)	0.14449 (14)	0.06288 (12)	0.0271 (3)
H6	0.1433	0.0757	−0.0003	0.033*
C7	0.24126 (19)	0.15637 (14)	0.15988 (12)	0.0236 (3)
H7	0.3161	0.0960	0.1636	0.028*
C8	0.23623 (18)	0.25916 (13)	0.25556 (11)	0.0195 (3)
C9	0.12432 (19)	0.34902 (14)	0.24652 (12)	0.0224 (3)
C10	0.45201 (18)	0.18691 (13)	0.38325 (11)	0.0206 (3)
O1A	0.67121 (14)	0.22924 (10)	0.70186 (9)	0.0300 (3)
O2A	0.93960 (16)	0.25229 (11)	0.76675 (11)	0.0482 (4)
C1A	0.82048 (18)	0.06951 (13)	0.61722 (11)	0.0205 (3)
N1A	0.71612 (15)	0.05087 (11)	0.52356 (10)	0.0208 (3)
C2A	0.70952 (19)	−0.05813 (14)	0.43994 (12)	0.0238 (3)
H2A	0.6328	−0.0714	0.3736	0.029*
C3A	0.80874 (19)	−0.14899 (13)	0.44770 (12)	0.0240 (3)
H3A	0.8011	−0.2236	0.3874	0.029*
C4A	1.0295 (2)	−0.22249 (14)	0.55853 (12)	0.0264 (3)
H4A	1.0271	−0.2972	0.4991	0.032*
C5A	1.1356 (2)	−0.20353 (15)	0.65542 (13)	0.0285 (4)
H5A	1.2068	−0.2648	0.6632	0.034*
C6A	1.1395 (2)	−0.09298 (15)	0.74413 (13)	0.0280 (3)
H6A	1.2132	−0.0810	0.8114	0.034*

C7A	1.03937 (19)	−0.00292 (14)	0.73495 (12)	0.0249 (3)
H7A	1.0435	0.0707	0.7957	0.030*
C8A	0.92890 (18)	−0.01916 (13)	0.63473 (11)	0.0198 (3)
C9A	0.92297 (18)	−0.13159 (13)	0.54586 (12)	0.0213 (3)
C10A	0.81768 (19)	0.19380 (14)	0.70422 (12)	0.0237 (3)
O1B	0.50385 (15)	0.43664 (11)	0.65072 (9)	0.0333 (3)
O2B	0.28869 (16)	0.51262 (15)	0.71761 (10)	0.0535 (4)
N1B	0.65308 (16)	0.44696 (11)	0.84876 (10)	0.0223 (3)
C1B	0.54342 (18)	0.52634 (13)	0.83991 (11)	0.0207 (3)
C2B	0.75794 (19)	0.46784 (14)	0.94605 (12)	0.0244 (3)
H2B	0.8360	0.4101	0.9513	0.029*
C3B	0.75569 (19)	0.56808 (14)	1.03629 (12)	0.0245 (3)
H3B	0.8303	0.5790	1.1030	0.029*
C4B	0.6351 (2)	0.76283 (14)	1.12033 (12)	0.0278 (3)
H4B	0.7078	0.7764	1.1883	0.033*
C5B	0.5253 (2)	0.84668 (14)	1.11053 (13)	0.0322 (4)
H5B	0.5205	0.9176	1.1719	0.039*
C6B	0.4187 (2)	0.82810 (15)	1.00929 (14)	0.0320 (4)
H6B	0.3443	0.8880	1.0029	0.038*
C7B	0.4205 (2)	0.72551 (14)	0.92027 (13)	0.0268 (3)
H7B	0.3474	0.7145	0.8530	0.032*
C8B	0.53150 (18)	0.63544 (13)	0.92817 (11)	0.0203 (3)
C9B	0.64159 (19)	0.65562 (13)	1.02982 (12)	0.0217 (3)
C10B	0.43012 (19)	0.49211 (13)	0.72890 (12)	0.0244 (3)
H1O	0.608 (4)	0.170 (3)	0.493 (2)	0.086 (9)*
H1OA	0.674 (3)	0.312 (3)	0.755 (2)	0.074 (8)*
H1OB	0.431 (3)	0.413 (3)	0.580 (2)	0.080 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0374 (7)	0.0281 (6)	0.0188 (5)	0.0141 (5)	−0.0048 (5)	0.0020 (4)
O2	0.0531 (8)	0.0296 (6)	0.0243 (6)	0.0214 (6)	−0.0087 (5)	−0.0019 (5)
N1	0.0252 (7)	0.0221 (6)	0.0172 (6)	0.0071 (5)	0.0017 (5)	0.0026 (5)
C1	0.0207 (7)	0.0207 (6)	0.0165 (7)	0.0039 (6)	0.0032 (5)	0.0046 (5)
C2	0.0332 (9)	0.0239 (7)	0.0210 (7)	0.0095 (6)	0.0025 (6)	0.0011 (6)
C3	0.0293 (8)	0.0235 (7)	0.0266 (8)	0.0115 (6)	0.0026 (6)	0.0066 (6)
C4	0.0298 (8)	0.0303 (8)	0.0236 (8)	0.0086 (7)	0.0006 (6)	0.0117 (6)
C5	0.0326 (9)	0.0376 (9)	0.0163 (7)	0.0038 (7)	−0.0023 (6)	0.0096 (6)
C6	0.0343 (9)	0.0281 (7)	0.0158 (7)	0.0039 (7)	0.0040 (6)	0.0036 (6)
C7	0.0282 (8)	0.0241 (7)	0.0173 (7)	0.0063 (6)	0.0043 (6)	0.0051 (6)
C8	0.0210 (7)	0.0202 (7)	0.0165 (7)	0.0026 (6)	0.0037 (5)	0.0053 (5)
C9	0.0233 (7)	0.0242 (7)	0.0188 (7)	0.0038 (6)	0.0025 (6)	0.0068 (6)
C10	0.0231 (7)	0.0224 (7)	0.0153 (7)	0.0058 (6)	0.0028 (5)	0.0055 (5)
O1A	0.0294 (6)	0.0263 (6)	0.0252 (6)	0.0099 (5)	0.0014 (5)	−0.0019 (4)
O2A	0.0341 (7)	0.0336 (6)	0.0495 (8)	0.0101 (6)	−0.0102 (6)	−0.0128 (6)
C1A	0.0216 (7)	0.0222 (7)	0.0163 (7)	0.0033 (6)	0.0031 (5)	0.0050 (5)
N1A	0.0230 (6)	0.0218 (6)	0.0163 (6)	0.0056 (5)	0.0028 (5)	0.0051 (5)

C2A	0.0265 (8)	0.0263 (7)	0.0152 (7)	0.0041 (6)	0.0020 (6)	0.0035 (6)
C3A	0.0302 (8)	0.0220 (7)	0.0157 (7)	0.0042 (6)	0.0046 (6)	0.0007 (5)
C4A	0.0338 (9)	0.0240 (7)	0.0221 (7)	0.0092 (7)	0.0093 (6)	0.0063 (6)
C5A	0.0298 (8)	0.0318 (8)	0.0300 (8)	0.0133 (7)	0.0088 (6)	0.0162 (7)
C6A	0.0286 (8)	0.0347 (8)	0.0214 (8)	0.0059 (7)	0.0011 (6)	0.0124 (6)
C7A	0.0280 (8)	0.0275 (7)	0.0174 (7)	0.0045 (6)	0.0021 (6)	0.0063 (6)
C8A	0.0220 (7)	0.0208 (6)	0.0167 (7)	0.0044 (6)	0.0050 (5)	0.0058 (5)
C9A	0.0241 (8)	0.0224 (7)	0.0190 (7)	0.0060 (6)	0.0075 (6)	0.0072 (6)
C10A	0.0264 (8)	0.0230 (7)	0.0188 (7)	0.0079 (6)	0.0007 (6)	0.0047 (6)
O1B	0.0325 (6)	0.0445 (7)	0.0147 (5)	0.0103 (5)	0.0023 (5)	−0.0003 (5)
O2B	0.0323 (7)	0.0808 (11)	0.0255 (7)	0.0235 (7)	−0.0029 (5)	−0.0080 (7)
N1B	0.0263 (7)	0.0217 (6)	0.0162 (6)	0.0054 (5)	0.0040 (5)	0.0028 (5)
C1B	0.0230 (7)	0.0216 (7)	0.0150 (7)	0.0032 (6)	0.0041 (5)	0.0027 (5)
C2B	0.0270 (8)	0.0245 (7)	0.0205 (7)	0.0075 (6)	0.0021 (6)	0.0072 (6)
C3B	0.0290 (8)	0.0256 (7)	0.0154 (7)	0.0032 (6)	−0.0006 (6)	0.0052 (6)
C4B	0.0342 (9)	0.0270 (7)	0.0161 (7)	0.0028 (7)	0.0022 (6)	0.0005 (6)
C5B	0.0414 (10)	0.0245 (7)	0.0227 (8)	0.0064 (7)	0.0080 (7)	−0.0040 (6)
C6B	0.0356 (9)	0.0265 (8)	0.0305 (9)	0.0134 (7)	0.0072 (7)	0.0038 (6)
C7B	0.0289 (8)	0.0264 (7)	0.0214 (7)	0.0082 (6)	0.0031 (6)	0.0036 (6)
C8B	0.0231 (7)	0.0204 (6)	0.0151 (7)	0.0037 (6)	0.0038 (5)	0.0027 (5)
C9B	0.0250 (8)	0.0216 (7)	0.0161 (7)	0.0019 (6)	0.0041 (6)	0.0032 (5)
C10B	0.0286 (8)	0.0231 (7)	0.0159 (7)	0.0059 (6)	0.0014 (6)	0.0003 (5)

Geometric parameters (Å, °)

O1—C10	1.2967 (17)	C4A—C5A	1.364 (2)
O1—H1O	0.90 (3)	C4A—C9A	1.417 (2)
O2—C10	1.2136 (17)	C4A—H4A	0.9500
N1—C1	1.3293 (18)	C5A—C6A	1.411 (2)
N1—C2	1.3583 (19)	C5A—H5A	0.9500
C1—C8	1.4284 (19)	C6A—C7A	1.365 (2)
C1—C10	1.5133 (19)	C6A—H6A	0.9500
C2—C3	1.361 (2)	C7A—C8A	1.4210 (19)
C2—H2	0.9500	C7A—H7A	0.9500
C3—C9	1.412 (2)	C8A—C9A	1.4233 (19)
C3—H3	0.9500	O1B—C10B	1.2957 (18)
C4—C5	1.366 (2)	O1B—H1OB	0.97 (3)
C4—C9	1.419 (2)	O2B—C10B	1.204 (2)
C4—H4	0.9500	N1B—C1B	1.3230 (19)
C5—C6	1.406 (2)	N1B—C2B	1.3602 (18)
C5—H5	0.9500	C1B—C8B	1.4241 (18)
C6—C7	1.367 (2)	C1B—C10B	1.5149 (19)
C6—H6	0.9500	C2B—C3B	1.362 (2)
C7—C8	1.4268 (19)	C2B—H2B	0.9500
C7—H7	0.9500	C3B—C9B	1.412 (2)
C8—C9	1.426 (2)	C3B—H3B	0.9500
O1A—C10A	1.2990 (18)	C4B—C5B	1.364 (2)
O1A—H1OA	0.97 (3)	C4B—C9B	1.4171 (19)
O2A—C10A	1.2103 (19)	C4B—H4B	0.9500

C1A—N1A	1.3256 (18)	C5B—C6B	1.411 (2)
C1A—C8A	1.423 (2)	C5B—H5B	0.9500
C1A—C10A	1.5131 (19)	C6B—C7B	1.367 (2)
N1A—C2A	1.3617 (18)	C6B—H6B	0.9500
C2A—C3A	1.364 (2)	C7B—C8B	1.420 (2)
C2A—H2A	0.9500	C7B—H7B	0.9500
C3A—C9A	1.413 (2)	C8B—C9B	1.4261 (19)
C3A—H3A	0.9500		
C10—O1—H1O	111.1 (19)	C6A—C5A—H5A	119.9
C1—N1—C2	119.62 (12)	C7A—C6A—C5A	121.17 (14)
N1—C1—C8	122.42 (13)	C7A—C6A—H6A	119.4
N1—C1—C10	115.25 (12)	C5A—C6A—H6A	119.4
C8—C1—C10	122.27 (12)	C6A—C7A—C8A	120.13 (14)
N1—C2—C3	122.81 (13)	C6A—C7A—H7A	119.9
N1—C2—H2	118.6	C8A—C7A—H7A	119.9
C3—C2—H2	118.6	C7A—C8A—C1A	124.19 (13)
C2—C3—C9	119.41 (13)	C7A—C8A—C9A	118.68 (13)
C2—C3—H3	120.3	C1A—C8A—C9A	117.12 (13)
C9—C3—H3	120.3	C3A—C9A—C4A	122.19 (13)
C5—C4—C9	120.37 (14)	C3A—C9A—C8A	118.37 (13)
C5—C4—H4	119.8	C4A—C9A—C8A	119.43 (13)
C9—C4—H4	119.8	O2A—C10A—O1A	125.12 (13)
C4—C5—C6	120.28 (14)	O2A—C10A—C1A	122.87 (13)
C4—C5—H5	119.9	O1A—C10A—C1A	112.00 (13)
C6—C5—H5	119.9	C10B—O1B—H1OB	111.6 (16)
C7—C6—C5	121.24 (14)	C1B—N1B—C2B	119.50 (12)
C7—C6—H6	119.4	N1B—C1B—C8B	122.68 (13)
C5—C6—H6	119.4	N1B—C1B—C10B	115.00 (12)
C6—C7—C8	120.18 (14)	C8B—C1B—C10B	122.31 (12)
C6—C7—H7	119.9	N1B—C2B—C3B	122.76 (13)
C8—C7—H7	119.9	N1B—C2B—H2B	118.6
C9—C8—C7	118.35 (13)	C3B—C2B—H2B	118.6
C9—C8—C1	116.99 (12)	C2B—C3B—C9B	119.44 (13)
C7—C8—C1	124.66 (13)	C2B—C3B—H3B	120.3
C3—C9—C4	121.69 (13)	C9B—C3B—H3B	120.3
C3—C9—C8	118.74 (13)	C5B—C4B—C9B	120.47 (14)
C4—C9—C8	119.56 (13)	C5B—C4B—H4B	119.8
O2—C10—O1	124.09 (13)	C9B—C4B—H4B	119.8
O2—C10—C1	122.74 (13)	C4B—C5B—C6B	120.07 (14)
O1—C10—C1	113.12 (12)	C4B—C5B—H5B	120.0
C10A—O1A—H1OA	110.1 (16)	C6B—C5B—H5B	120.0
N1A—C1A—C8A	122.96 (13)	C7B—C6B—C5B	121.20 (14)
N1A—C1A—C10A	114.79 (12)	C7B—C6B—H6B	119.4
C8A—C1A—C10A	122.25 (12)	C5B—C6B—H6B	119.4
C1A—N1A—C2A	119.29 (12)	C6B—C7B—C8B	120.16 (14)
C3A—C2A—N1A	122.55 (13)	C6B—C7B—H7B	119.9
C3A—C2A—H2A	118.7	C8B—C7B—H7B	119.9
N1A—C2A—H2A	118.7	C7B—C8B—C1B	124.23 (13)
C2A—C3A—C9A	119.68 (13)	C7B—C8B—C9B	118.61 (13)

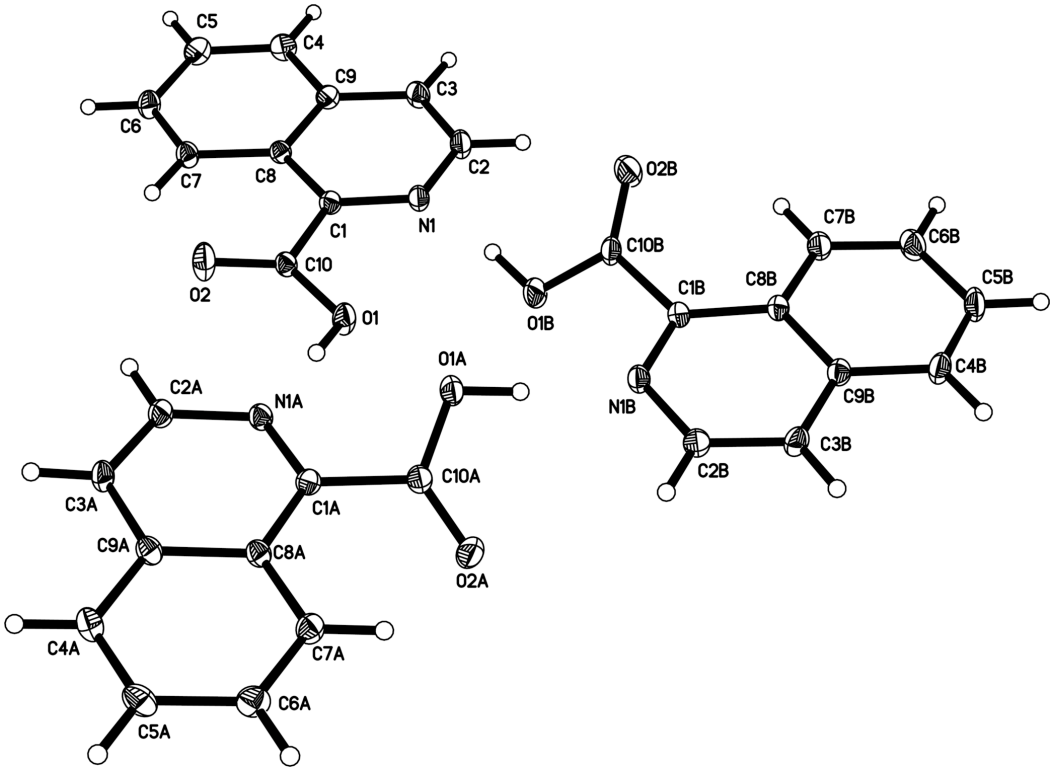
C2A—C3A—H3A	120.2	C1B—C8B—C9B	117.14 (12)
C9A—C3A—H3A	120.2	C3B—C9B—C4B	122.06 (14)
C5A—C4A—C9A	120.47 (14)	C3B—C9B—C8B	118.46 (13)
C5A—C4A—H4A	119.8	C4B—C9B—C8B	119.47 (13)
C9A—C4A—H4A	119.8	O2B—C10B—O1B	125.65 (14)
C4A—C5A—C6A	120.10 (14)	O2B—C10B—C1B	122.81 (14)
C4A—C5A—H5A	119.9	O1B—C10B—C1B	111.52 (13)
C2—N1—C1—C8	0.0 (2)	C2A—C3A—C9A—C4A	−179.77 (14)
C2—N1—C1—C10	−177.20 (14)	C2A—C3A—C9A—C8A	0.9 (2)
C1—N1—C2—C3	0.8 (3)	C5A—C4A—C9A—C3A	−178.48 (15)
N1—C2—C3—C9	−0.8 (3)	C5A—C4A—C9A—C8A	0.9 (2)
C9—C4—C5—C6	0.2 (3)	C7A—C8A—C9A—C3A	177.78 (14)
C4—C5—C6—C7	0.5 (3)	C1A—C8A—C9A—C3A	−1.3 (2)
C5—C6—C7—C8	−0.1 (2)	C7A—C8A—C9A—C4A	−1.6 (2)
C6—C7—C8—C9	−1.0 (2)	C1A—C8A—C9A—C4A	179.34 (14)
C6—C7—C8—C1	178.80 (15)	N1A—C1A—C10A—O2A	−142.98 (17)
N1—C1—C8—C9	−0.7 (2)	C8A—C1A—C10A—O2A	36.1 (2)
C10—C1—C8—C9	176.28 (13)	N1A—C1A—C10A—O1A	36.12 (19)
N1—C1—C8—C7	179.43 (14)	C8A—C1A—C10A—O1A	−144.80 (15)
C10—C1—C8—C7	−3.6 (2)	C2B—N1B—C1B—C8B	1.1 (2)
C2—C3—C9—C4	178.82 (16)	C2B—N1B—C1B—C10B	−178.41 (13)
C2—C3—C9—C8	0.0 (2)	C1B—N1B—C2B—C3B	0.0 (2)
C5—C4—C9—C3	179.88 (16)	N1B—C2B—C3B—C9B	−0.6 (2)
C5—C4—C9—C8	−1.3 (2)	C9B—C4B—C5B—C6B	−1.0 (3)
C7—C8—C9—C3	−179.45 (14)	C4B—C5B—C6B—C7B	1.4 (3)
C1—C8—C9—C3	0.7 (2)	C5B—C6B—C7B—C8B	−0.4 (3)
C7—C8—C9—C4	1.7 (2)	C6B—C7B—C8B—C1B	−179.46 (15)
C1—C8—C9—C4	−178.14 (14)	C6B—C7B—C8B—C9B	−1.0 (2)
N1—C1—C10—O2	163.91 (15)	N1B—C1B—C8B—C7B	176.98 (15)
C8—C1—C10—O2	−13.3 (2)	C10B—C1B—C8B—C7B	−3.5 (2)
N1—C1—C10—O1	−13.4 (2)	N1B—C1B—C8B—C9B	−1.5 (2)
C8—C1—C10—O1	169.42 (14)	C10B—C1B—C8B—C9B	178.01 (14)
C8A—C1A—N1A—C2A	0.8 (2)	C2B—C3B—C9B—C4B	−178.90 (15)
C10A—C1A—N1A—C2A	179.85 (13)	C2B—C3B—C9B—C8B	0.2 (2)
C1A—N1A—C2A—C3A	−1.3 (2)	C5B—C4B—C9B—C3B	178.75 (16)
N1A—C2A—C3A—C9A	0.4 (2)	C5B—C4B—C9B—C8B	−0.3 (2)
C9A—C4A—C5A—C6A	0.2 (3)	C7B—C8B—C9B—C3B	−177.78 (14)
C4A—C5A—C6A—C7A	−0.5 (3)	C1B—C8B—C9B—C3B	0.8 (2)
C5A—C6A—C7A—C8A	−0.2 (3)	C7B—C8B—C9B—C4B	1.3 (2)
C6A—C7A—C8A—C1A	−179.72 (15)	C1B—C8B—C9B—C4B	179.92 (14)
C6A—C7A—C8A—C9A	1.3 (2)	N1B—C1B—C10B—O2B	144.38 (17)
N1A—C1A—C8A—C7A	−178.52 (14)	C8B—C1B—C10B—O2B	−35.2 (2)
C10A—C1A—C8A—C7A	2.5 (2)	N1B—C1B—C10B—O1B	−34.05 (19)
N1A—C1A—C8A—C9A	0.5 (2)	C8B—C1B—C10B—O1B	146.41 (15)
C10A—C1A—C8A—C9A	−178.52 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O1—H1O···N1A	0.91 (3)	1.76 (3)	2.6673 (16)	177 (3)
O1A—H1OA···N1B	0.97 (3)	1.68 (3)	2.6407 (16)	172 (2)
O1B—H1OB···N1	0.99 (3)	1.69 (3)	2.6715 (17)	171 (3)

Fig. 1


C5
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N1A
C10A
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