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A 1:1 cocrystal of 2,8-bis(trifluoromethyl)quinolin-4-ol and 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one

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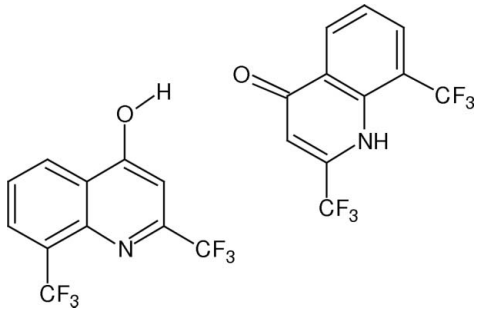
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.055; wR factor = 0.144; data-to-parameter ratio = 13.9.

In the title compound, $C_{11}H_5F_6NO\cdot C_{11}H_5F_6NO$, both molecules (except F and H atoms) are essentially planar (the r.m.s. deviations for all non-H atoms are 0.008 and 0.034 Å for the alcohol and ketone, respectively). The two molecules are connected by an O—H···O hydrogen bond. The protonated N atom is shielded and therefore does not form a hydrogen bond. The F atoms of one trifluoromethyl group are disordered over two positions; the site occupancy factors are 0.88 and 0.12.

Related literature

For related literature, see: Bourne *et al.* (2006); Butcher *et al.* (2007); Egan *et al.* (1994); El-Masry *et al.* (2000); Fahlquist *et al.* (2006); Maguire *et al.* (1994); Roma *et al.* (2000); Tilley *et al.* (2001); Yathirajan, Sarojini *et al.* (2007); Yathirajan, Sreevidya *et al.* (2007); Zhang & Jenekhe (2000).



Experimental

Crystal data

$C_{11}H_5F_6NO\cdot C_{11}H_5F_6NO$
M_r = 562.32
Monoclinic, $P2_1/n$
a = 9.1868 (4) Å
b = 13.9634 (8) Å
c = 17.1928 (8) Å
β = 94.687 (4)°
V = 2198.10 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 173 (2) K
0.34 × 0.29 × 0.21 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
32900 measured reflections
5055 independent reflections
3976 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.144
S = 1.14
5055 reflections
364 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1A···O1	0.87 (4)	1.78 (4)	2.656 (3)	174 (4)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

ANM thank SeQuent Scientific Ltd, Mangalore, for the gift sample of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2454).

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supplementary materials

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A 1:1 cocrystal of 2,8-bis(trifluoromethyl)quinolin-4-ol and 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one

B. K. Sarojini, B. Narayana, A. N. Mayekar, H. S. Yathirajan and M. Bolte

Comment

It is well known that the quinoline ring system is an important structural unit widely existing in alkaloids, therapeutics and synthetic analogues with interesting biological activities. A large variety of quinoline derivatives have been used as antimalarial, anti-inflammatory agents, antiasthmatic, antibacterial, antihypertensive and tyrokinase PDGF-RTK inhibiting agents (El-Masry *et al.*, 2000; Roma *et al.*, 2000; Zhang & Jenekhe, 2000; Maguire *et al.*, 1994). Furthermore, poly-substituted quinolines have been found to undergo hierarchical self-assembly into a variety of nano- and mesostructures with enhanced electronic and photonic functions. Quinoline antimalarial drugs, such as chloroquine, quinine and amodiaquine have been used as effective treatments for malaria (Tilley *et al.*, 2001). Until the onset of parasite resistance, chloroquine was especially valuable, owing to its affordability, limited toxicity and potency. It is believed to accumulate in its diprotonated state in the acidic environment of the Plasmodium food vacuole in an infected red blood cell, unable to re-cross the lipid membrane. The drug activity is understood to arise from complex formation between the 4-aminoquinoline drug and its target, haematin, thus preventing the haematin from aggregating to crystalline haemozoin (Egan *et al.*, 1994). This class of compounds form complexes with haematin and prevents its aggregation to crystalline haemozoin, complexes between the drug molecule and haematin are notoriously diffcult to crystallize. The structures of 4-chloro-8-(trifluoromethyl)quinoline (Yathirajan, Sreevidya, Prathap *et al.*, 2007), bis{4-[(2-hydroxybenzylidine)hydrazino]-8-(trifluoromethyl)quinolinium} sulfate tetrahydrate (Yathirajan, Sarojini, Narayana *et al.*, 2007), 1-(quinolin-2-yl)ethanone (Butcher *et al.*, 2007), 2-phenylquinoline 1-oxide (Fahlquist *et al.*, 2006). Three 4-aminoquinolines (Bourne *et al.*, 2006) have been published. In view of the importance of quinoline derivatives, we report the crystal structure of a new quinoline derivative, (I) which actually a mixture of hydrogen bonded 2,8-bis(trifluoromethyl)quinolin-4-ol and 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one.

The title co-crystal contains 2,8-bis(trifluoromethyl)quinolin-4-ol [$C_{11}H_5F_6NO$], and 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one [$C_{11}H_5F_6NO$]. Both molecules (except F and H atoms) are essentially planar [r.m.s. deviation for all non-H atoms 0.008Å and 0.034Å for 2,8-bis(trifluoromethyl)quinolin-4-ol and 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one, respectively]. The two molecules are connected by a O—H···O hydrogen bond. The protonated N atom is shielded and therefore does not form a hydrogen bond.

Experimental

The title compound was obtained from SeQuent Scientific Ltd, Mangalore, as a gift sample and was crystallized from acetone [m.p.: 391–395 K].

Refinement

All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.95 Å. The amino and hydroxyl

H atoms were freely refined. One of the CF_3 groups is disordered over two sites with a site occupation factor of 0.884 (4) for the major occupied site. The atoms (F1', F2' and, F3') of the minor occupied site were refined isotropically.

Figures

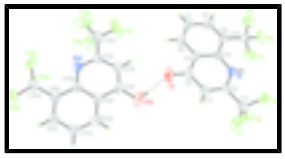


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. For clarity, the major component with atoms F1, F2 and F3, of the disordered CF_3 group is shown.

2,8-bis(trifluoromethyl)quinolin-4-ol– 2,8-bis(trifluoromethyl)quinolin-4(1*H*)-one (1/1)

Crystal data

$C_{11}H_5F_6NO{\cdot}C_{11}H_5F_6NO$	F_{000} = 1120
M_r = 562.32	D_x = 1.699 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25632 reflections
a = 9.1868 (4) Å	θ = 3.4–27.6º
b = 13.9634 (8) Å	μ = 0.18 mm^{-1}
c = 17.1928 (8) Å	T = 173 (2) K
β = 94.687 (4)º	Block, colourless
V = 2198.10 (19) Å^3	0.34 × 0.29 × 0.21 mm
Z = 4	

Data collection

Stoe IPDSII two-circle diffractometer	3976 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.046
Monochromator: graphite	θ_{max} = 27.6º
T = 173(2) K	θ_{min} = 3.5º
ω scans	h = −11→11
Absorption correction: none	k = −18→18
32900 measured reflections	l = −22→22
5055 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 1.036P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.14	$(\Delta/\sigma)_{max} < 0.001$
5055 reflections	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
364 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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)
F1	0.6119 (4)	0.10065 (17)	0.66836 (11)	0.1030 (13)	0.884 (4)
F2	0.5877 (3)	−0.01257 (14)	0.58753 (12)	0.0726 (7)	0.884 (4)
F3	0.7957 (2)	0.04131 (19)	0.61350 (14)	0.0849 (9)	0.884 (4)
F1'	0.7539 (16)	0.1174 (10)	0.6622 (8)	0.057 (4)*	0.116 (4)
F2'	0.5544 (18)	0.0447 (13)	0.6319 (10)	0.068 (5)*	0.116 (4)
F3'	0.707 (2)	−0.0044 (13)	0.5915 (10)	0.071 (5)*	0.116 (4)
F4	0.74374 (17)	−0.02462 (10)	0.34336 (10)	0.0573 (4)	
F5	0.8738 (2)	0.04206 (13)	0.26057 (9)	0.0688 (5)	
F6	0.93313 (16)	0.05552 (11)	0.38408 (9)	0.0541 (4)	
O1	0.4403 (2)	0.35464 (12)	0.47983 (12)	0.0564 (5)	
N1	0.69448 (19)	0.11665 (12)	0.47114 (10)	0.0314 (4)	
H1	0.750 (3)	0.067 (2)	0.4707 (16)	0.049 (7)*	
C2	0.6335 (2)	0.14076 (14)	0.53776 (12)	0.0332 (4)	
C3	0.5485 (2)	0.21923 (16)	0.54371 (14)	0.0396 (5)	
H3	0.5089	0.2334	0.5917	0.047*	
C4	0.5180 (2)	0.28136 (15)	0.47720 (15)	0.0402 (5)	
C5	0.5811 (2)	0.25282 (14)	0.40537 (13)	0.0357 (4)	
C6	0.5528 (3)	0.30743 (16)	0.33642 (15)	0.0465 (6)	
H6	0.4943	0.3635	0.3373	0.056*	
C7	0.6091 (3)	0.28020 (18)	0.26844 (16)	0.0522 (6)	
H7	0.5885	0.3170	0.2224	0.063*	
C8	0.6970 (3)	0.19818 (18)	0.26646 (14)	0.0468 (5)	
H8	0.7355	0.1798	0.2190	0.056*	
C9	0.7281 (2)	0.14387 (15)	0.33295 (12)	0.0353 (4)	
C10	0.6693 (2)	0.17045 (13)	0.40361 (12)	0.0309 (4)	
C11	0.6610 (3)	0.07092 (16)	0.60443 (13)	0.0405 (5)	
C12	0.8194 (3)	0.05538 (16)	0.32928 (13)	0.0404 (5)	

F1A	0.3274 (3)	0.5647 (3)	0.29670 (13)	0.1443 (14)
F2A	0.2343 (2)	0.70616 (15)	0.29298 (10)	0.0827 (6)
F3A	0.1012 (2)	0.58500 (14)	0.26504 (9)	0.0748 (5)
F4A	−0.21334 (16)	0.85612 (10)	0.51026 (9)	0.0543 (4)
F5A	−0.02372 (15)	0.85788 (9)	0.44455 (9)	0.0512 (4)
F6A	−0.20327 (14)	0.76233 (9)	0.41182 (7)	0.0425 (3)
O1A	0.2846 (2)	0.46104 (12)	0.57062 (11)	0.0495 (4)
H1A	0.341 (4)	0.426 (3)	0.543 (2)	0.082 (12)*
N1A	0.08353 (19)	0.66696 (12)	0.42119 (10)	0.0338 (4)
C2A	0.1814 (2)	0.60571 (16)	0.39848 (13)	0.0379 (5)
C3A	0.2539 (2)	0.53454 (15)	0.44419 (14)	0.0394 (5)
H3A	0.3229	0.4934	0.4229	0.047*
C4A	0.2224 (2)	0.52599 (14)	0.52074 (13)	0.0367 (5)
C5A	0.1184 (2)	0.58982 (14)	0.54984 (12)	0.0330 (4)
C6A	0.0808 (3)	0.58667 (16)	0.62811 (13)	0.0435 (5)
H6A	0.1258	0.5408	0.6631	0.052*
C7A	−0.0192 (3)	0.64892 (19)	0.65348 (14)	0.0504 (6)
H7A	−0.0441	0.6458	0.7060	0.060*
C8A	−0.0864 (3)	0.71823 (17)	0.60235 (13)	0.0430 (5)
H8A	−0.1559	0.7612	0.6208	0.052*
C9A	−0.0521 (2)	0.72396 (14)	0.52660 (12)	0.0327 (4)
C10A	0.0518 (2)	0.65905 (13)	0.49738 (11)	0.0294 (4)
C11A	0.2134 (3)	0.6153 (2)	0.31353 (16)	0.0562 (7)
C12A	−0.1217 (2)	0.79917 (15)	0.47330 (13)	0.0375 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.208 (3)	0.0682 (14)	0.0386 (11)	0.0600 (18)	0.0466 (15)	0.0101 (10)
F2	0.0940 (17)	0.0544 (11)	0.0674 (13)	−0.0245 (10)	−0.0054 (11)	0.0189 (10)
F3	0.0376 (10)	0.119 (2)	0.0972 (17)	0.0134 (11)	0.0032 (10)	0.0760 (15)
F4	0.0614 (9)	0.0341 (7)	0.0777 (11)	−0.0009 (6)	0.0134 (8)	−0.0042 (7)
F5	0.0832 (12)	0.0799 (11)	0.0468 (9)	0.0208 (9)	0.0264 (8)	0.0021 (8)
F6	0.0453 (8)	0.0533 (8)	0.0618 (9)	0.0160 (6)	−0.0068 (7)	−0.0074 (7)
O1	0.0496 (10)	0.0402 (9)	0.0782 (13)	0.0213 (8)	−0.0013 (9)	−0.0024 (8)
N1	0.0308 (8)	0.0295 (8)	0.0338 (9)	0.0074 (7)	0.0017 (7)	0.0032 (6)
C2	0.0297 (9)	0.0340 (10)	0.0355 (10)	0.0036 (8)	0.0013 (8)	−0.0001 (8)
C3	0.0348 (11)	0.0392 (11)	0.0445 (12)	0.0089 (8)	0.0023 (9)	−0.0045 (9)
C4	0.0298 (10)	0.0310 (10)	0.0584 (14)	0.0059 (8)	−0.0052 (9)	−0.0023 (9)
C5	0.0304 (10)	0.0279 (9)	0.0472 (12)	0.0001 (7)	−0.0073 (8)	0.0036 (8)
C6	0.0448 (12)	0.0327 (10)	0.0594 (15)	0.0031 (9)	−0.0122 (11)	0.0118 (10)
C7	0.0594 (15)	0.0449 (13)	0.0500 (14)	−0.0024 (11)	−0.0106 (12)	0.0189 (11)
C8	0.0524 (14)	0.0484 (13)	0.0389 (12)	−0.0061 (11)	−0.0013 (10)	0.0117 (10)
C9	0.0353 (10)	0.0341 (10)	0.0360 (11)	−0.0034 (8)	−0.0001 (8)	0.0060 (8)
C10	0.0259 (9)	0.0285 (9)	0.0370 (10)	−0.0021 (7)	−0.0045 (7)	0.0041 (7)
C11	0.0432 (12)	0.0404 (11)	0.0391 (11)	0.0078 (9)	0.0108 (9)	0.0041 (9)
C12	0.0423 (12)	0.0435 (11)	0.0358 (11)	0.0010 (9)	0.0059 (9)	−0.0005 (9)
F1A	0.124 (2)	0.244 (3)	0.0723 (14)	0.132 (2)	0.0543 (14)	0.0448 (17)

F2A	0.1043 (15)	0.0947 (14)	0.0513 (10)	−0.0278 (12)	0.0199 (10)	0.0103 (9)
F3A	0.1025 (14)	0.0797 (12)	0.0410 (9)	0.0030 (10)	−0.0013 (9)	−0.0131 (8)
F4A	0.0539 (8)	0.0489 (8)	0.0596 (9)	0.0237 (7)	0.0024 (7)	−0.0143 (7)
F5A	0.0451 (7)	0.0335 (7)	0.0742 (10)	0.0015 (6)	0.0006 (7)	0.0149 (6)
F6A	0.0413 (7)	0.0430 (7)	0.0418 (7)	0.0081 (5)	−0.0045 (5)	−0.0041 (5)
O1A	0.0580 (11)	0.0344 (8)	0.0537 (10)	0.0143 (7)	−0.0101 (8)	0.0056 (7)
N1A	0.0320 (8)	0.0350 (8)	0.0345 (9)	0.0059 (7)	0.0024 (7)	0.0006 (7)
C2A	0.0359 (11)	0.0404 (11)	0.0372 (11)	0.0089 (9)	0.0018 (8)	−0.0013 (9)
C3A	0.0356 (11)	0.0344 (10)	0.0474 (13)	0.0099 (8)	−0.0007 (9)	−0.0047 (9)
C4A	0.0374 (10)	0.0255 (9)	0.0450 (12)	0.0022 (8)	−0.0094 (9)	−0.0002 (8)
C5A	0.0344 (10)	0.0274 (9)	0.0361 (10)	−0.0023 (7)	−0.0043 (8)	−0.0006 (7)
C6A	0.0543 (13)	0.0386 (11)	0.0362 (12)	−0.0035 (10)	−0.0042 (10)	0.0060 (9)
C7A	0.0638 (16)	0.0553 (14)	0.0326 (12)	−0.0005 (12)	0.0074 (11)	0.0004 (10)
C8A	0.0471 (12)	0.0435 (12)	0.0392 (12)	0.0021 (10)	0.0081 (10)	−0.0083 (9)
C9A	0.0328 (10)	0.0284 (9)	0.0365 (10)	0.0002 (7)	0.0012 (8)	−0.0044 (8)
C10A	0.0291 (9)	0.0260 (9)	0.0327 (10)	−0.0014 (7)	−0.0006 (7)	−0.0018 (7)
C11A	0.0525 (15)	0.0713 (17)	0.0462 (14)	0.0241 (13)	0.0118 (12)	0.0061 (12)
C12A	0.0343 (10)	0.0326 (10)	0.0453 (12)	0.0064 (8)	0.0019 (9)	−0.0060 (9)

Geometric parameters (Å, °)

F1—C11	1.290 (3)	C9—C10	1.419 (3)
F2—C11	1.366 (3)	C9—C12	1.498 (3)
F3—C11	1.302 (3)	F1A—C11A	1.316 (3)
F1'—C11	1.413 (14)	F2A—C11A	1.335 (4)
F2'—C11	1.180 (16)	F3A—C11A	1.340 (4)
F2'—F3'	1.76 (2)	F4A—C12A	1.354 (2)
F3'—C11	1.163 (17)	F5A—C12A	1.341 (3)
F4—C12	1.348 (3)	F6A—C12A	1.347 (2)
F5—C12	1.332 (3)	O1A—C4A	1.343 (3)
F6—C12	1.348 (3)	O1A—H1A	0.87 (4)
O1—C4	1.250 (3)	N1A—C2A	1.323 (3)
N1—C2	1.358 (3)	N1A—C10A	1.369 (3)
N1—C10	1.386 (3)	C2A—C3A	1.401 (3)
N1—H1	0.86 (3)	C2A—C11A	1.519 (3)
C2—C3	1.354 (3)	C3A—C4A	1.376 (3)
C2—C11	1.510 (3)	C3A—H3A	0.9500
C3—C4	1.444 (3)	C4A—C5A	1.427 (3)
C3—H3	0.9500	C5A—C6A	1.417 (3)
C4—C5	1.462 (3)	C5A—C10A	1.425 (3)
C5—C10	1.408 (3)	C6A—C7A	1.362 (4)
C5—C6	1.416 (3)	C6A—H6A	0.9500
C6—C7	1.370 (4)	C7A—C8A	1.415 (3)
C6—H6	0.9500	C7A—H7A	0.9500
C7—C8	1.403 (4)	C8A—C9A	1.367 (3)
C7—H7	0.9500	C8A—H8A	0.9500
C8—C9	1.382 (3)	C9A—C10A	1.436 (3)
C8—H8	0.9500	C9A—C12A	1.502 (3)
C11—F2'—F3'	41.1 (8)	F5—C12—C9	113.85 (19)

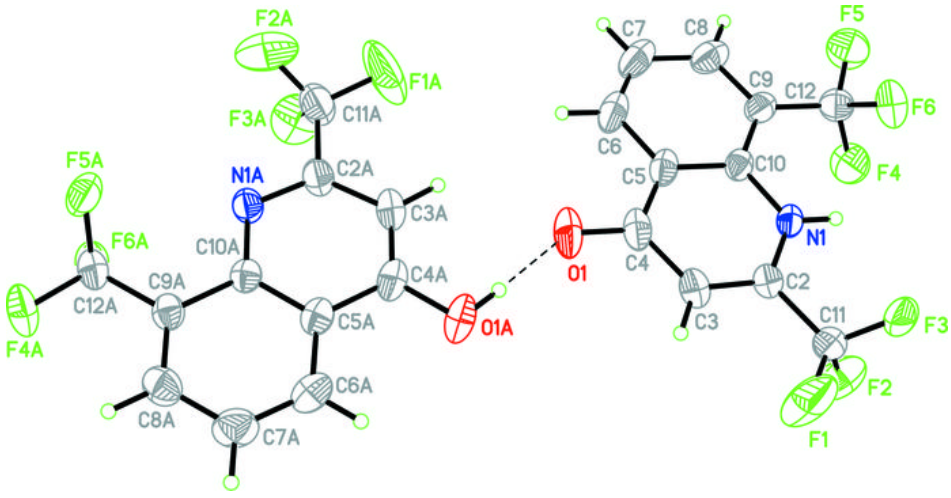
C11—F3'—F2'	41.8 (8)	F4—C12—C9	112.15 (18)
C2—N1—C10	121.32 (17)	F6—C12—C9	111.96 (18)
C2—N1—H1	119.5 (18)	C4A—O1A—H1A	106 (2)
C10—N1—H1	119.1 (18)	C2A—N1A—C10A	115.66 (17)
C3—C2—N1	123.0 (2)	N1A—C2A—C3A	126.6 (2)
C3—C2—C11	121.78 (19)	N1A—C2A—C11A	114.60 (19)
N1—C2—C11	115.16 (17)	C3A—C2A—C11A	118.78 (19)
C2—C3—C4	120.1 (2)	C4A—C3A—C2A	118.08 (19)
C2—C3—H3	119.9	C4A—C3A—H3A	121.0
C4—C3—H3	119.9	C2A—C3A—H3A	121.0
O1—C4—C3	122.5 (2)	O1A—C4A—C3A	123.9 (2)
O1—C4—C5	121.4 (2)	O1A—C4A—C5A	117.4 (2)
C3—C4—C5	116.11 (18)	C3A—C4A—C5A	118.71 (18)
C10—C5—C6	119.2 (2)	C6A—C5A—C10A	119.80 (19)
C10—C5—C4	120.62 (19)	C6A—C5A—C4A	122.38 (19)
C6—C5—C4	120.1 (2)	C10A—C5A—C4A	117.82 (19)
C7—C6—C5	120.6 (2)	C7A—C6A—C5A	120.5 (2)
C7—C6—H6	119.7	C7A—C6A—H6A	119.8
C5—C6—H6	119.7	C5A—C6A—H6A	119.8
C6—C7—C8	120.3 (2)	C6A—C7A—C8A	120.6 (2)
C6—C7—H7	119.8	C6A—C7A—H7A	119.7
C8—C7—H7	119.8	C8A—C7A—H7A	119.7
C9—C8—C7	120.5 (2)	C9A—C8A—C7A	120.6 (2)
C9—C8—H8	119.7	C9A—C8A—H8A	119.7
C7—C8—H8	119.7	C7A—C8A—H8A	119.7
C8—C9—C10	119.8 (2)	C8A—C9A—C10A	120.51 (19)
C8—C9—C12	119.8 (2)	C8A—C9A—C12A	120.16 (19)
C10—C9—C12	120.38 (18)	C10A—C9A—C12A	119.32 (18)
N1—C10—C5	118.78 (19)	N1A—C10A—C5A	123.11 (17)
N1—C10—C9	121.75 (18)	N1A—C10A—C9A	118.88 (17)
C5—C10—C9	119.46 (18)	C5A—C10A—C9A	118.00 (18)
F3'—C11—F2'	97.1 (13)	F1A—C11A—F2A	108.5 (3)
F1—C11—F3	113.3 (3)	F1A—C11A—F3A	106.2 (3)
F1—C11—F2	104.8 (2)	F2A—C11A—F3A	104.8 (2)
F3—C11—F2	101.6 (2)	F1A—C11A—C2A	112.6 (2)
F3'—C11—F1'	109.9 (11)	F2A—C11A—C2A	112.4 (2)
F2'—C11—F1'	109.6 (11)	F3A—C11A—C2A	111.8 (2)
F1—C11—C2	112.97 (19)	F5A—C12A—F6A	106.93 (18)
F3—C11—C2	113.21 (18)	F5A—C12A—F4A	106.00 (17)
F2—C11—C2	109.93 (19)	F6A—C12A—F4A	105.37 (16)
F1'—C11—C2	106.9 (6)	F5A—C12A—C9A	112.78 (17)
F5—C12—F4	106.24 (19)	F6A—C12A—C9A	113.19 (17)
F5—C12—F6	107.15 (19)	F4A—C12A—C9A	111.99 (18)
F4—C12—F6	104.91 (19)		
C10—N1—C2—C3	−1.9 (3)	C3—C2—C11—F1'	−71.5 (7)
C10—N1—C2—C11	175.22 (18)	N1—C2—C11—F1'	111.4 (7)
N1—C2—C3—C4	0.5 (3)	C8—C9—C12—F5	5.5 (3)
C11—C2—C3—C4	−176.4 (2)	C10—C9—C12—F5	−176.58 (19)
C2—C3—C4—O1	−179.9 (2)	C8—C9—C12—F4	−115.1 (2)

C2—C3—C4—C5	1.2 (3)	C10—C9—C12—F4	62.8 (3)
O1—C4—C5—C10	179.5 (2)	C8—C9—C12—F6	127.3 (2)
C3—C4—C5—C10	−1.6 (3)	C10—C9—C12—F6	−54.9 (3)
O1—C4—C5—C6	−1.1 (3)	C10A—N1A—C2A—C3A	0.3 (3)
C3—C4—C5—C6	177.8 (2)	C10A—N1A—C2A—C11A	179.4 (2)
C10—C5—C6—C7	0.7 (3)	N1A—C2A—C3A—C4A	−0.1 (4)
C4—C5—C6—C7	−178.7 (2)	C11A—C2A—C3A—C4A	−179.2 (2)
C5—C6—C7—C8	−0.7 (4)	C2A—C3A—C4A—O1A	−179.8 (2)
C6—C7—C8—C9	−0.1 (4)	C2A—C3A—C4A—C5A	−0.2 (3)
C7—C8—C9—C10	0.8 (3)	O1A—C4A—C5A—C6A	0.4 (3)
C7—C8—C9—C12	178.7 (2)	C3A—C4A—C5A—C6A	−179.3 (2)
C2—N1—C10—C5	1.4 (3)	O1A—C4A—C5A—C10A	179.95 (18)
C2—N1—C10—C9	−177.64 (19)	C3A—C4A—C5A—C10A	0.3 (3)
C6—C5—C10—N1	−179.02 (19)	C10A—C5A—C6A—C7A	0.5 (3)
C4—C5—C10—N1	0.3 (3)	C4A—C5A—C6A—C7A	−180.0 (2)
C6—C5—C10—C9	0.1 (3)	C5A—C6A—C7A—C8A	−0.5 (4)
C4—C5—C10—C9	179.42 (18)	C6A—C7A—C8A—C9A	0.0 (4)
C8—C9—C10—N1	178.3 (2)	C7A—C8A—C9A—C10A	0.6 (3)
C12—C9—C10—N1	0.4 (3)	C7A—C8A—C9A—C12A	−178.7 (2)
C8—C9—C10—C5	−0.8 (3)	C2A—N1A—C10A—C5A	−0.1 (3)
C12—C9—C10—C5	−178.66 (19)	C2A—N1A—C10A—C9A	179.19 (18)
F2'—F3'—C11—F1	48.0 (11)	C6A—C5A—C10A—N1A	179.41 (19)
F2'—F3'—C11—F3	139.3 (10)	C4A—C5A—C10A—N1A	−0.2 (3)
F2'—F3'—C11—F2	−29.6 (12)	C6A—C5A—C10A—C9A	0.1 (3)
F2'—F3'—C11—F1'	113.9 (11)	C4A—C5A—C10A—C9A	−179.48 (17)
F2'—F3'—C11—C2	−122.7 (11)	C8A—C9A—C10A—N1A	−180.0 (2)
F3'—F2'—C11—F1	−132.7 (10)	C12A—C9A—C10A—N1A	−0.7 (3)
F3'—F2'—C11—F3	−43.1 (12)	C8A—C9A—C10A—C5A	−0.6 (3)
F3'—F2'—C11—F2	28.4 (11)	C12A—C9A—C10A—C5A	178.67 (18)
F3'—F2'—C11—F1'	−114.1 (12)	N1A—C2A—C11A—F1A	169.4 (3)
F3'—F2'—C11—C2	126.0 (10)	C3A—C2A—C11A—F1A	−11.4 (4)
C3—C2—C11—F3'	163.7 (12)	N1A—C2A—C11A—F2A	46.5 (3)
N1—C2—C11—F3'	−13.5 (12)	C3A—C2A—C11A—F2A	−134.4 (2)
C3—C2—C11—F2'	50.0 (11)	N1A—C2A—C11A—F3A	−71.1 (3)
N1—C2—C11—F2'	−127.2 (11)	C3A—C2A—C11A—F3A	108.1 (3)
C3—C2—C11—F1	−8.4 (4)	C8A—C9A—C12A—F5A	120.6 (2)
N1—C2—C11—F1	174.4 (3)	C10A—C9A—C12A—F5A	−58.7 (2)
C3—C2—C11—F3	−138.9 (3)	C8A—C9A—C12A—F6A	−117.8 (2)
N1—C2—C11—F3	44.0 (3)	C10A—C9A—C12A—F6A	62.9 (2)
C3—C2—C11—F2	108.2 (2)	C8A—C9A—C12A—F4A	1.1 (3)
N1—C2—C11—F2	−68.9 (3)	C10A—C9A—C12A—F4A	−178.17 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1A—H1A···O1	0.87 (4)	1.78 (4)	2.656 (3)	174 (4)

Fig. 1


F2A
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C6
C5
C10
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N1
C2
C3
C11
F3
F2
F1