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7*H*-Chromeno[3,2-*h*]quinolin-7-one methanol monosolvate

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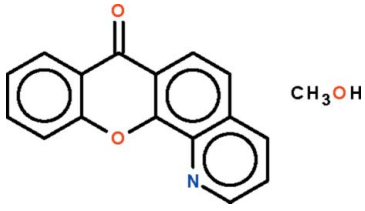
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.147; data-to-parameter ratio = 13.8.

The four-ring system in the title compound, $C_{16}H_9NO_2\cdot CH_3OH$, is planar (r.m.s deviation = 0.03 Å); the methanol solvent molecule forms a hydrogen bond to the quinoline N atom.

Related literature

The compound in this study was synthesized from the cyclization of 2-(quinolin-8-yloxy)benzoic acid; for the synthesis of this acid, see: Chen *et al.* (2007). For the synthesis by the Skraup reaction of amino-9*H*-xanthene-9-one, see: Fujiwara & Okabayashi (1994).



Experimental

Crystal data

$C_{16}H_9NO_2\cdot CH_4O$
M_r = 279.28
Triclinic, $P\overline{1}$
a = 8.102 (2) Å
b = 8.791 (3) Å
c = 10.150 (3) Å
α = 102.172 (3)°
β = 108.760 (3)°
γ = 93.532 (3)°
V = 662.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 K
0.41 × 0.30 × 0.18 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: none
3838 measured reflections
2655 independent reflections
1456 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.147
S = 1.02
2655 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···N1	0.82	2.07	2.852 (2)	160

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2605).

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supporting information

Acta Cryst. (2009). E**65**, o2368 [doi:10.1107/S160053680903534X]

7*H*-Chromeno[3,2-*h*]quinolin-7-one methanol monosolvate

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S1. Experimental

2-(Quinolin-8-yloxy)benzoic acid was synthesized by using a literature procedure (Chen *et al.*, 2007). The carboxylic acid (0.5 g) and polyphosphoric acid (3.5 g) were heated at 413 K for two hours; the reaction was monitored by thin layer chromatography. The hot mixture was poured into ice water (200 ml); the pH value of the solution was adjusted to 7–8 by concentrated ammonium hydroxide. The crude product that precipitated was collected and recrystallized from methanol (in 0.39 g yield). The formulation was established by ^{1}H NMR spectral integral analysis.

S2. Refinement

Carbon- and oxygen-bound hydrogen atoms were generated geometrically and were constrained to ride on their parent atoms [C–H = 0.93–0.96, O–H 0.82 Å; U_{iso}(H) =1.2–1.5U_{eq}(C,O)].

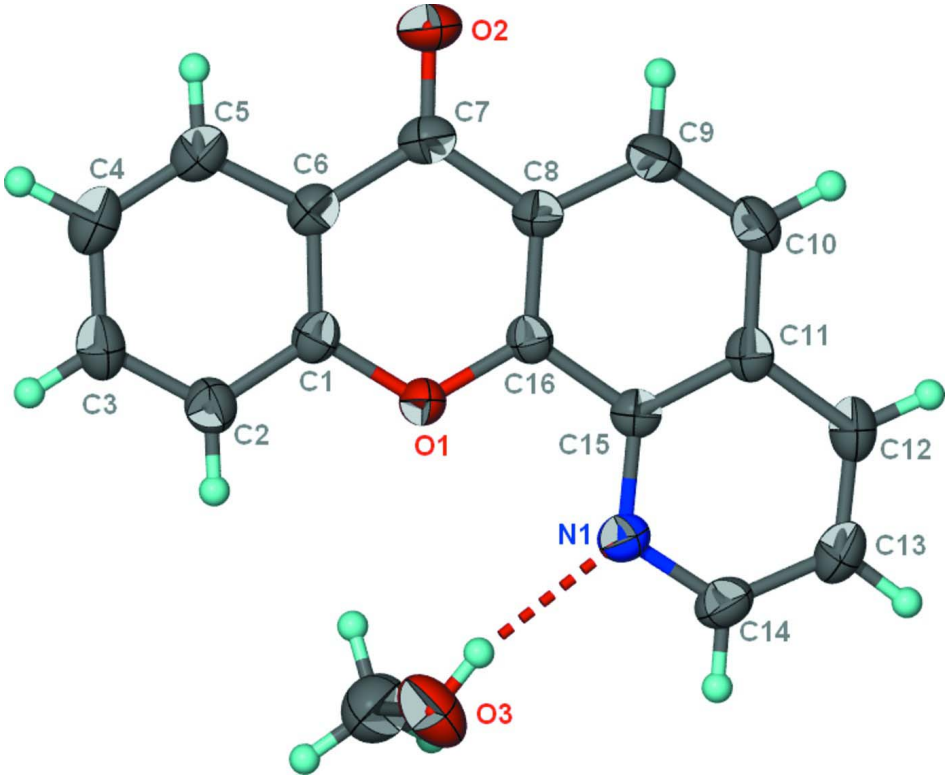

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{16}H_9NO_2{\cdot}CH_4O$ at the 50% probability level; hydrogen atoms are drawn as sphere of arbitrary radius. The dashed line denotes a hydrogen bond.

7*H*-Chromeno[3,2-*h*]quinolin-7-one methanol monosolvate

Crystal data

$C_{16}H_9NO_2{\cdot}CH_4O$
$M_r = 279.28$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.102\ (2)$ Å
$b = 8.791\ (3)$ Å
$c = 10.150\ (3)$ Å
$\alpha = 102.172\ (3)°$
$\beta = 108.760\ (3)°$
$\gamma = 93.532\ (3)°$
$V = 662.6\ (3)$ Å^3
$Z = 2$
$F(000) = 292$
$D_x = 1.400$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1000 reflections
$\theta = 2.2–26.5°$
$\mu = 0.10$ mm^{-1}
$T = 295$ K
Block, yellow
0.41 × 0.30 × 0.18 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
3838 measured reflections
2655 independent reflections
1456 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.2°$
$h = -10\rightarrow10$
$k = -9\rightarrow11$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.147$
$S = 1.02$
2655 reflections
192 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.0458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25297 (18)	0.41753 (15)	0.57244 (14)	0.0387 (4)
O2	0.2583 (2)	0.64419 (19)	0.25985 (17)	0.0601 (5)
O3	0.2226 (2)	0.2382 (2)	0.8300 (2)	0.0735 (6)
H3	0.1946	0.3170	0.8021	0.110*
N1	0.1800 (2)	0.5518 (2)	0.80538 (18)	0.0402 (5)
C1	0.2905 (3)	0.3418 (2)	0.4545 (2)	0.0359 (5)
C2	0.3238 (3)	0.1887 (3)	0.4504 (2)	0.0449 (6)
H2	0.3204	0.1427	0.5242	0.054*
C3	0.3619 (3)	0.1058 (3)	0.3359 (3)	0.0506 (6)
H3a	0.3839	0.0027	0.3318	0.061*
C4	0.3680 (3)	0.1741 (3)	0.2259 (3)	0.0535 (6)
H4	0.3943	0.1169	0.1489	0.064*
C5	0.3353 (3)	0.3254 (3)	0.2310 (2)	0.0475 (6)

H5	0.3398	0.3706	0.1570	0.057*
C6	0.2950 (3)	0.4136 (2)	0.3461 (2)	0.0374 (5)
C7	0.2553 (3)	0.5754 (2)	0.3526 (2)	0.0401 (5)
C8	0.2134 (2)	0.6488 (2)	0.4794 (2)	0.0341 (5)
C9	0.1720 (3)	0.8044 (2)	0.4991 (2)	0.0429 (6)
H9	0.1653	0.8579	0.4280	0.052*
C10	0.1423 (3)	0.8764 (3)	0.6186 (3)	0.0445 (6)
H10	0.1182	0.9795	0.6301	0.053*
C11	0.1473 (3)	0.7963 (2)	0.7271 (2)	0.0372 (5)
C12	0.1185 (3)	0.8653 (3)	0.8556 (3)	0.0487 (6)
H12	0.0984	0.9694	0.8738	0.058*
C13	0.1204 (3)	0.7792 (3)	0.9517 (3)	0.0521 (6)
H13	0.1023	0.8237	1.0367	0.063*
C14	0.1498 (3)	0.6225 (3)	0.9221 (2)	0.0476 (6)
H14	0.1481	0.5646	0.9886	0.057*
C15	0.1802 (2)	0.6383 (2)	0.7082 (2)	0.0341 (5)
C16	0.2159 (3)	0.5678 (2)	0.5817 (2)	0.0326 (5)
C17	0.4047 (4)	0.2427 (3)	0.8712 (3)	0.0733 (8)
H17A	0.4457	0.2784	0.8026	0.110*
H17B	0.4345	0.1394	0.8754	0.110*
H17C	0.4594	0.3135	0.9641	0.110*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0529 (10)	0.0317 (8)	0.0361 (9)	0.0084 (7)	0.0207 (7)	0.0087 (6)
O2	0.0888 (13)	0.0568 (11)	0.0475 (10)	0.0125 (9)	0.0329 (10)	0.0240 (8)
O3	0.0733 (14)	0.0473 (11)	0.1034 (17)	0.0123 (9)	0.0283 (12)	0.0276 (10)
N1	0.0469 (11)	0.0408 (11)	0.0351 (11)	0.0057 (8)	0.0163 (9)	0.0102 (8)
C1	0.0344 (12)	0.0363 (12)	0.0334 (12)	0.0019 (9)	0.0112 (10)	0.0025 (9)
C2	0.0480 (14)	0.0386 (13)	0.0490 (14)	0.0068 (10)	0.0187 (12)	0.0094 (11)
C3	0.0538 (15)	0.0383 (13)	0.0572 (16)	0.0093 (11)	0.0207 (13)	0.0025 (11)
C4	0.0523 (16)	0.0563 (16)	0.0487 (16)	0.0073 (12)	0.0223 (13)	−0.0019 (12)
C5	0.0496 (15)	0.0523 (15)	0.0401 (14)	0.0034 (11)	0.0183 (11)	0.0067 (11)
C6	0.0344 (12)	0.0396 (12)	0.0352 (13)	−0.0005 (9)	0.0116 (10)	0.0048 (10)
C7	0.0407 (13)	0.0429 (13)	0.0345 (13)	−0.0020 (10)	0.0108 (10)	0.0103 (10)
C8	0.0324 (12)	0.0331 (11)	0.0343 (12)	−0.0001 (9)	0.0092 (10)	0.0077 (9)
C9	0.0492 (14)	0.0376 (12)	0.0457 (14)	0.0065 (10)	0.0169 (11)	0.0168 (10)
C10	0.0478 (14)	0.0315 (12)	0.0561 (15)	0.0088 (10)	0.0190 (12)	0.0119 (11)
C11	0.0330 (12)	0.0337 (12)	0.0412 (13)	0.0023 (9)	0.0113 (10)	0.0039 (9)
C12	0.0506 (15)	0.0396 (13)	0.0528 (15)	0.0104 (11)	0.0195 (12)	0.0009 (11)
C13	0.0600 (16)	0.0543 (15)	0.0422 (14)	0.0091 (12)	0.0243 (13)	0.0010 (12)
C14	0.0549 (15)	0.0543 (15)	0.0368 (13)	0.0071 (12)	0.0193 (12)	0.0122 (11)
C15	0.0305 (12)	0.0351 (12)	0.0342 (12)	0.0012 (9)	0.0087 (9)	0.0081 (9)
C16	0.0323 (12)	0.0285 (11)	0.0349 (12)	0.0017 (9)	0.0105 (9)	0.0056 (9)
C17	0.077 (2)	0.080 (2)	0.069 (2)	0.0168 (16)	0.0302 (17)	0.0195 (16)

Geometric parameters (Å, º)

O1—C16	1.363 (2)	C7—C8	1.466 (3)
O1—C1	1.375 (2)	C8—C16	1.373 (3)
O2—C7	1.227 (2)	C8—C9	1.417 (3)
O3—C17	1.394 (3)	C9—C10	1.347 (3)
O3—H3	0.8200	C9—H9	0.9300
N1—C14	1.321 (3)	C10—C11	1.419 (3)
N1—C15	1.367 (2)	C10—H10	0.9300
C1—C2	1.384 (3)	C11—C15	1.415 (3)
C1—C6	1.388 (3)	C11—C12	1.415 (3)
C2—C3	1.371 (3)	C12—C13	1.352 (3)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.386 (3)	C13—C14	1.399 (3)
C3—H3a	0.9300	C13—H13	0.9300
C4—C5	1.366 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.429 (3)
C5—C6	1.403 (3)	C17—H17A	0.9600
C5—H5	0.9300	C17—H17B	0.9600
C6—C7	1.470 (3)	C17—H17C	0.9600
C16—O1—C1	118.65 (15)	C8—C9—H9	119.3
C17—O3—H3	109.5	C9—C10—C11	120.6 (2)
C14—N1—C15	117.14 (18)	C9—C10—H10	119.7
O1—C1—C2	115.76 (18)	C11—C10—H10	119.7
O1—C1—C6	122.41 (18)	C15—C11—C12	116.89 (19)
C2—C1—C6	121.82 (19)	C15—C11—C10	119.7 (2)
C3—C2—C1	119.0 (2)	C12—C11—C10	123.4 (2)
C3—C2—H2	120.5	C13—C12—C11	119.7 (2)
C1—C2—H2	120.5	C13—C12—H12	120.2
C2—C3—C4	120.7 (2)	C11—C12—H12	120.2
C2—C3—H3a	119.6	C12—C13—C14	119.4 (2)
C4—C3—H3a	119.6	C12—C13—H13	120.3
C5—C4—C3	119.9 (2)	C14—C13—H13	120.3
C5—C4—H4	120.0	N1—C14—C13	123.9 (2)
C3—C4—H4	120.0	N1—C14—H14	118.0
C4—C5—C6	121.0 (2)	C13—C14—H14	118.0
C4—C5—H5	119.5	N1—C15—C11	122.95 (19)
C6—C5—H5	119.5	N1—C15—C16	119.13 (18)
C1—C6—C5	117.6 (2)	C11—C15—C16	117.92 (18)
C1—C6—C7	120.34 (19)	O1—C16—C8	123.74 (18)
C5—C6—C7	122.08 (19)	O1—C16—C15	115.04 (16)
O2—C7—C8	122.5 (2)	C8—C16—C15	121.22 (18)
O2—C7—C6	122.8 (2)	O3—C17—H17A	109.5
C8—C7—C6	114.67 (18)	O3—C17—H17B	109.5
C16—C8—C9	119.21 (19)	H17A—C17—H17B	109.5
C16—C8—C7	120.17 (18)	O3—C17—H17C	109.5
C9—C8—C7	120.62 (18)	H17A—C17—H17C	109.5

C10—C9—C8	121.3 (2)	H17B—C17—H17C	109.5
C10—C9—H9	119.3		
C16—O1—C1—C2	−178.86 (17)	C9—C10—C11—C15	−1.3 (3)
C16—O1—C1—C6	1.1 (3)	C9—C10—C11—C12	179.5 (2)
O1—C1—C2—C3	179.87 (19)	C15—C11—C12—C13	−1.1 (3)
C6—C1—C2—C3	−0.1 (3)	C10—C11—C12—C13	178.0 (2)
C1—C2—C3—C4	0.3 (3)	C11—C12—C13—C14	−0.4 (4)
C2—C3—C4—C5	−0.2 (4)	C15—N1—C14—C13	−0.6 (3)
C3—C4—C5—C6	−0.1 (4)	C12—C13—C14—N1	1.4 (4)
O1—C1—C6—C5	179.83 (19)	C14—N1—C15—C11	−1.0 (3)
C2—C1—C6—C5	−0.2 (3)	C14—N1—C15—C16	178.70 (19)
O1—C1—C6—C7	−1.3 (3)	C12—C11—C15—N1	1.9 (3)
C2—C1—C6—C7	178.69 (19)	C10—C11—C15—N1	−177.29 (19)
C4—C5—C6—C1	0.3 (3)	C12—C11—C15—C16	−177.82 (18)
C4—C5—C6—C7	−178.6 (2)	C10—C11—C15—C16	3.0 (3)
C1—C6—C7—O2	179.7 (2)	C1—O1—C16—C8	0.2 (3)
C5—C6—C7—O2	−1.5 (3)	C1—O1—C16—C15	−179.36 (16)
C1—C6—C7—C8	0.2 (3)	C9—C8—C16—O1	179.58 (18)
C5—C6—C7—C8	179.03 (19)	C7—C8—C16—O1	−1.2 (3)
O2—C7—C8—C16	−178.4 (2)	C9—C8—C16—C15	−0.9 (3)
C6—C7—C8—C16	1.0 (3)	C7—C8—C16—C15	178.25 (19)
O2—C7—C8—C9	0.7 (3)	N1—C15—C16—O1	−2.1 (3)
C6—C7—C8—C9	−179.84 (18)	C11—C15—C16—O1	177.68 (17)
C16—C8—C9—C10	2.7 (3)	N1—C15—C16—C8	178.38 (18)
C7—C8—C9—C10	−176.5 (2)	C11—C15—C16—C8	−1.9 (3)
C8—C9—C10—C11	−1.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N1	0.82	2.07	2.852 (2)	160