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7-Methoxy-3-(salicylideneamino)-coumarin

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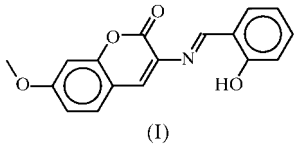
The title compound, $C_{17}H_{13}NO_4$, exists as a planar molecule; adjacent molecules are linked by electrostatic C—H···O [C···O = 3.318 (4) and 3.455 (4) Å] interactions into a linear chain.

Comment

Our observation that the fluorescence quantum yield (relative to quinine sulfate) of 7-methoxy-3-(salicylideneamino)-coumarin, (I), in methanol is twice that of unsubstituted 3-(salicylideneamino)coumarin in methanol prompted us to carry out an X-ray analysis of (I). Compound (I) exists as discrete molecules; however, adjacent molecules are linked by a pair of C—H···O interactions into chains. These interactions are not van der Waals contacts; these are electrostatic attractions, as the distances and angles compare well with values accepted for conventional C—H···*X* hydrogen bonding (Iyere *et al.*, 1998; Ng, 1999). Such interactions are not present in, for example, coumarin-3-carboxylic acid (Dobson & Gerkin, 1996) and 3-(2-benzothiazolyl)-7-(diethylamino)-coumarin (Jasinski & Paight, 1995); in these two compounds, the 4- and 5-positions of the coumarin unit are not substituted.



(I)

Experimental

7-Methoxy-3-aminocoumarin (Khoo, 1999) was condensed with salicylaldehyde in chloroform to yield the Schiff base (m.p. 410–411 K) in 60% yield. CNH elemental analysis: found (calculated) for $C_{17}H_{13}NO_4$: C 68.50 (69.15), H 3.56 (4.41), N 4.87% (4.75%). Yellow–orange plates were obtained upon recrystallization with benzene.

Crystal data

$C_{17}H_{13}NO_4$
M_r = 295.28
Monoclinic, $P2_1/n$
a = 6.660 (1) Å
b = 31.984 (8) Å
c = 7.123 (2) Å
β = 114.93 (2)°
V = 1375.9 (6) Å^3
Z = 4
D_x = 1.425 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 3.5–12.5°
μ = 0.103 mm^{-1}
T = 298 (2) K
Plate, yellow
0.60 × 0.40 × 0.14 mm

Data collection

Siemens *P*4 four-circle diffractometer
ω scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.875, T_{max} = 0.966
3194 measured reflections
2416 independent reflections
1449 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 24.99°
$h = -1 \rightarrow 7$
$k = -1 \rightarrow 38$
$l = -8 \rightarrow 8$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.172
S = 1.054
2416 reflections
202 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.6431P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.002 (1)

Table 1
Selected geometric parameters (Å, °).

O1—C12	1.375 (4)	C3—C4	1.368 (6)
O1—C8	1.374 (4)	C4—C5	1.381 (6)
O2—C8	1.201 (4)	C5—C6	1.375 (5)
O3—C14	1.354 (4)	C8—C9	1.462 (4)
O3—C17	1.420 (4)	C9—C10	1.355 (4)
O4—C2	1.348 (4)	C10—C11	1.426 (4)
N1—C7	1.292 (4)	C11—C12	1.385 (4)
N1—C9	1.390 (4)	C11—C16	1.401 (4)
C1—C6	1.395 (5)	C12—C13	1.373 (5)
C1—C2	1.403 (5)	C13—C14	1.373 (5)
C1—C7	1.438 (5)	C14—C15	1.406 (5)
C2—C3	1.375 (5)	C15—C16	1.357 (5)
C12—O1—C8	123.3 (2)	C10—C9—N1	118.0 (3)
C14—O3—C17	117.0 (3)	C10—C9—C8	119.1 (3)
C7—N1—C9	124.9 (3)	N1—C9—C8	122.9 (3)
C6—C1—C2	118.1 (3)	C9—C10—C11	122.0 (3)
C6—C1—C7	119.2 (3)	C12—C11—C16	116.8 (3)
C2—C1—C7	122.7 (3)	C12—C11—C10	118.3 (3)
O4—C2—C3	119.0 (3)	C16—C11—C10	124.9 (3)
O4—C2—C1	121.3 (3)	C13—C12—O1	116.6 (3)
C3—C2—C1	119.7 (3)	C13—C12—C11	123.4 (3)
C4—C3—C2	121.1 (4)	O1—C12—C11	120.0 (3)
C3—C4—C5	120.4 (4)	C12—C13—C14	118.4 (3)
C6—C5—C4	119.1 (4)	O3—C14—C13	124.8 (3)
C5—C6—C1	121.6 (4)	O3—C14—C15	115.2 (3)
N1—C7—C1	121.4 (3)	C13—C14—C15	120.0 (3)
O2—C8—O1	116.1 (3)	C16—C15—C14	120.2 (3)
O2—C8—C9	126.7 (3)	C15—C16—C11	121.2 (3)
O1—C8—C9	117.1 (3)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···N1	0.82	1.89	2.620 (3)	147
C16—H16···O1^{i}	0.93	2.54	3.455 (4)	168
C10—H10···O2^{i}	0.93	2.41	3.318 (4)	165

Symmetry code: (i) $x-1, y, z$.

Data collection: *XSCANS* (Siemens, 1998); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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References

Dobson, A. J. & Gerkin, R. E. (1996). *Acta Cryst.* C**52**, 3081–3083.
Iyere, P. A., Kayren, L. J., Cordes, A. W., Eagle, C. T., Nile, T. A., Schimek, G. L. & Pennington, W. T. (1998). *Cryst. Eng.* **1**, 159–167.
Jasinski, J. P. & Paight, E. S. (1995). *Acta Cryst.* C**51**, 533–535.
Khoo, L. E. (1999). *Synth. Commun.* **29**, 2533–2538.
Ng, S. W. (1999). *Acta Cryst.* C**55**, 2105–2107.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1998). *XSCANS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.