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1-[(2-Carboxy-1-phenylethyl)iminiomethylene]-naphth-2-olate

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2-Hydroxy-1-naphthaldehyde condenses with *β*-phenylalanine to form the Schiff base *N*-(2-hydroxy-1-naphthalidene)-*β*-phenylalanine, which in the solid state exists in the zwitterionic form as (2-carboxy-1-phenylethyl)iminiomethylene-1-naphth-2-olate, $C_{20}H_{17}NO_3$. The zwitterions are linked by a hydrogen bond from the carboxylic acid group to the negatively charged naphtholate O atom of an adjacent molecule.

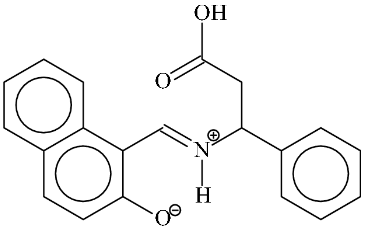
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.127
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Salicylaldehyde and other aromatic aldehydes having a hydroxy substituent in the *ortho* position condense with primary amines to furnish Schiff bases that are used as chelating ligands in a plethora of metal derivatives, as noted from a cursory examination of the Cambridge Structural Database (Version 5.25; Allen, 2002). Among the Schiff bases are some existing in the zwitterionic form (Aguiari *et al.*, 1992; Dubs *et al.*, 2000; Cottone *et al.*, 2002; Mondal *et al.*, 2002; Muthuraman *et al.*, 2001*a*,*b*; Zarza *et al.*, 1988); the reason for the preference for this form over the neutral form is not evident from these few examples. Nevertheless, for one (Mondal *et al.*, 2002), the strongly electron-withdrawing nitro substituent in the *para* position relative to the hydroxy group explains the ready transfer of its H atom to the imine N atom.



(I)

N-(2-Hydroxy-1-naphthalidene)phenylalanine represents another example of such a class of zwitterionic Schiff bases, the compound being (2-carboxy-1-phenylethyl)iminiomethylene-1-naphthol-2-ate, (I) (Fig. 1). The compound possesses a carboxylic acid –CO_2H unit; however, the acid H atom is retained and instead it interacts with the negatively charged naphtholate O atom of an adjacent molecule, at (x, $1 - y$, $z - \frac{1}{2}$), to give rise to a chain that runs along the c axis (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (0.17 g, 1 mmol) and D,L-phenyl-*β*-alanine (0.16 g, 1 mmol) were reacted in refluxing ethanol for 2 h. The solution was filtered and the solvent was allowed to evaporate to furnish yellow prismatic crystals after a week. Analysis calculated for

$C_{20}H_{16}NO_3$: C 75.46, H 5.07, N 4.40%; found: C 75.64, H 5.11 N 4.43%.

Crystal data

$C_{20}H_{17}NO_3$
$M_r = 319.35$
Monoclinic, $C2/c$
$a = 25.152$ (5) Å
$b = 9.760$ (2) Å
$c = 15.557$ (3) Å
$\beta = 123.01$ (3)°
$V = 3202$ (1) Å^3
$Z = 8$
$D_x = 1.325$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12 138 reflections
$\theta = 3.1$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.35 × 0.23 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.641$, $T_{\max} = 0.986$
14 977 measured reflections
3644 independent reflections
2488 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\max} = 27.5°$
$h = -32 \rightarrow 31$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.127$
$S = 1.05$
3644 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.5726P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.291 (2)	C7—C8	1.372 (2)
O2—C14	1.201 (2)	C8—C9	1.408 (2)
O3—C14	1.310 (2)	C9—C10	1.453 (2)
N1—C11	1.306 (2)	C10—C11	1.405 (2)
N1—C12	1.475 (2)	C12—C15	1.514 (2)
C1—C10	1.429 (2)	C12—C13	1.527 (2)
C1—C2	1.432 (2)	C13—C14	1.512 (2)
C2—C3	1.349 (2)	C15—C20	1.383 (2)
C3—C4	1.428 (2)	C15—C16	1.387 (2)
C4—C5	1.407 (2)	C16—C17	1.380 (2)
C4—C9	1.414 (2)	C17—C18	1.376 (3)
C5—C6	1.362 (3)	C18—C19	1.366 (3)
C6—C7	1.391 (3)	C19—C20	1.383 (2)
C11—N1—C12	124.3 (1)	C9—C10—C11	119.8 (1)
O1—C1—C10	121.4 (1)	N1—C11—C10	125.2 (1)
O1—C1—C2	120.7 (1)	N1—C12—C15	109.0 (1)
C2—C1—C10	117.9 (1)	N1—C12—C13	111.3 (1)
C1—C2—C3	121.4 (2)	C13—C12—C15	111.7 (1)
C2—C3—C4	122.5 (2)	C12—C13—C14	114.8 (1)
C5—C4—C9	119.9 (2)	O2—C14—O3	124.2 (2)
C3—C4—C5	121.4 (2)	O2—C14—C13	124.1 (2)
C3—C4—C9	118.7 (1)	O3—C14—C13	111.6 (1)
C4—C5—C6	121.2 (2)	C12—C15—C16	120.8 (2)
C5—C6—C7	119.4 (2)	C12—C15—C20	120.5 (1)
C6—C7—C8	120.7 (2)	C16—C15—C20	118.7 (2)
C7—C8—C9	121.5 (2)	C15—C16—C17	120.7 (2)
C4—C9—C8	117.3 (1)	C16—C17—C18	119.8 (2)
C4—C9—C10	119.1 (1)	C17—C18—C19	120.2 (2)
C8—C9—C10	123.6 (1)	C18—C19—C20	120.3 (2)
C1—C10—C11	119.9 (1)	C15—C20—C19	120.3 (2)
C1—C10—C9	120.3 (1)		

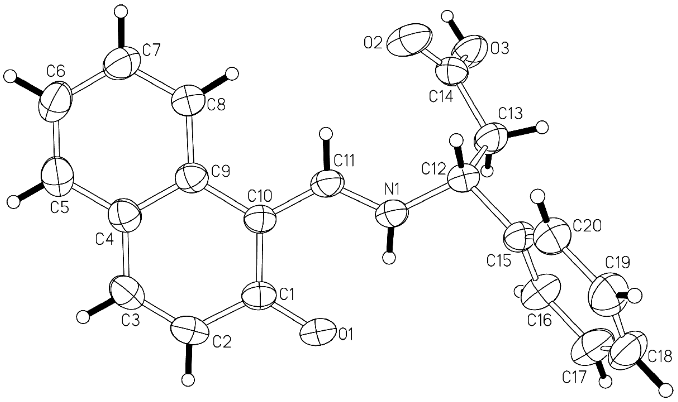


Figure 1
ORTEPII (Johnson, 1976) plot of $C_{20}H_{17}NO_3$; displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

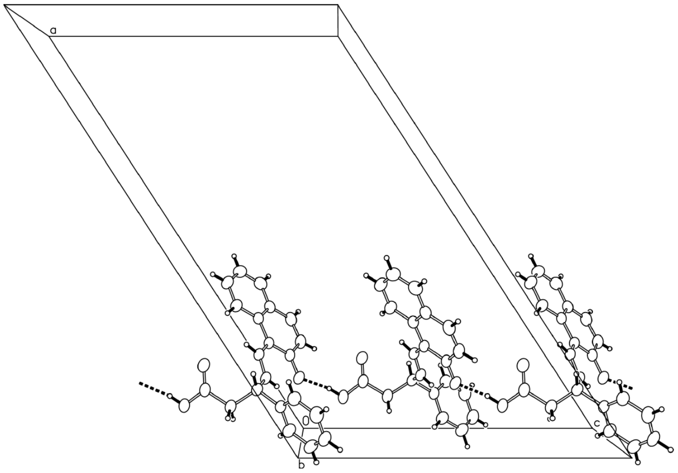


Figure 2
ORTEPII (Johnson, 1976) plot of the hydrogen-bonded chain (dashed lines).

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

D—H$\cdots A$	D—H	$D\cdots A$	D—H$\cdots A$
O3—H3O$\cdots$O1$^{\rm i}$	0.86 (1)	2.547 (2)	169 (2)
N1—H1N$\cdots$O1	0.86 (1)	2.609 (2)	138 (2)

Symmetry code: (i) $x, -y+1, z-\frac{1}{2}$.

The aromatic and methylene H atoms were positioned geometrically [Csp^2—H = 0.93 Å, C—$H_{\rm methine}$ = 0.98 Å and C—$H_{\rm methylene}$ = 0.97 Å, and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$], and they were included in the refinement in the riding-model approximation. The imine and carboxylic H atoms were located in a difference Fourier map and refined with a distance restraint of N—H = O—H = 0.85 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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