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2-(1-Naphthyl)propionic acid

Erik Riis* and Sine Larsen

Centre for Crystallographic Studies, Department of Chemistry, Universitetsparken 5, DK-2100 Copenhagen, Denmark

Correspondence e-mail: erik@ccs.ki.ku.dk

2-(1-Naphthyl)propionic acid, $C_{13}H_{12}O_2$, is one of the chiral compounds which exhibit the highest difference (80 K) in melting points between the racemic and enantiomeric crystals. We report here the structure of the racemic compound.

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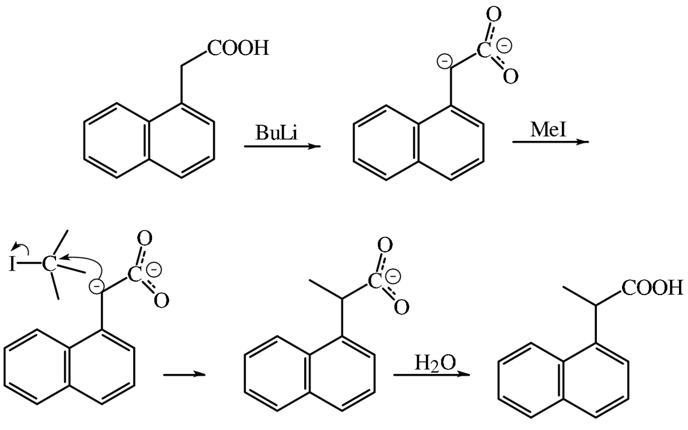
Key indicators

Single-crystal X-ray study
T = 122 K
Mean σ(C–C) = 0.002 Å
R factor = 0.055
wR factor = 0.161
Data-to-parameter ratio = 14.2

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

Comment

The structure determination of the title compound, (I), was undertaken as part of an investigation of racemic and enantiomeric crystals of chiral compounds, which focuses on the relations between differences in physicochemical properties (*e.g.* melting point) and crystal packing. The unit-cell parameters of (I) have been reported previously (Husebye, 1961), but no coordinates have been published or are available in the Cambridge Structural Database (Version of November 2004; Allen, 2002). The preparative route for racemic 2-(1-naphthyl)propionic acid is shown in the scheme below. It differs from the previously used procedure (Hecht *et al.*, 1978) by using butyllithium instead of sodium to deprotonate the starting material, 1-naphthylacetic acid.



(I)

The carboxylic acid group of 2-(1-naphthyl)propionic acid is hydrogen bonded to the carboxylic acid group of another molecule related by inversion symmetry, forming cyclic carboxylic acid dimers. This packing motif is common in other aromatic monofunctional carboxylic acids (Sørensen & Larsen, 2003). In addition, the carboxy group serves as an acceptor for two C—H hydrogen bonds (Table 1) from two other molecules related by the twofold screw axis and the glide plane, respectively. These interactions are presumably important for the arrangement of the naphthyl groups into a herring-bone pattern, in which the naphthyl groups have C═O$\cdots\pi$ interactions on one side and C—H$\cdots\pi$ on the opposite side. Since these interactions are between molecules of opposite chirality, they can not exist in the enantiomeric crystals, which could explain the higher melting point of the racemic acid.

Experimental

Butyllithium in hexane (20 mmol) was added dropwise to a stirred solution of 1-naphthylacetic acid (1.86 g, 10 mmol) in THF under a nitrogen atmosphere and cooled with solid carbon dioxide. The mixture turned red, indicating the formation of the highly conjugated dianion. MeI (10.5 mmol) was then added slowly and the mixture was allowed to reach room temperature. In order to protonate the anion, the solution was then extracted with water and 4 *M* HCl was added followed by evaporation. This yielded an orange oil (1.95 g, 9.75 mmol). The oil was recrystallized from *n*-heptane to yield a white powder (1.60 g, 80% yield). Further recrystallization was required to obtain small crystals.

Crystal data

$C_{13}H_{12}O_2$
$M_r = 200.24$
Monoclinic, $P2_1/c$
$a = 7.8089$ (4) Å
$b = 8.8904$ (5) Å
$c = 14.7466$ (12) Å
$\beta = 96.143$ (7)°
$V = 1017.89$ (11) Å^3
$Z = 4$

$D_x = 1.307$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11792 reflections
$\theta = 1.4$–37.0°
$\mu = 0.09$ mm^{-1}
$T = 122.0$ (10) K
Plate, colorless
$0.48 \times 0.36 \times 0.09$ mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: none
25823 measured reflections
2456 independent reflections
2071 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.046$
$\theta_{\rm max} = 28.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.161$
$S = 1.05$
2456 reflections
173 parameters
Only coordinates of H atoms refined

$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 0.705P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.005$
$\Delta\rho_{\rm max} = 0.54$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2$^{\rm i}$	0.91 (3)	1.74 (3)	2.6511 (17)	176 (2)
C9—H9···O1$^{\rm ii}$	1.06 (2)	2.54 (2)	3.4631 (19)	145 (2)
C8—H8···O2$^{\rm iii}$	0.96 (3)	2.64 (2)	3.4331 (18)	140 (2)

Symmetry codes: (i) $-x, -y, -z$; (ii) $1 - x, \frac{1}{2} + y+, \frac{1}{2} - z+$; (iii) $1 + x, \frac{1}{2} - y+, \frac{1}{2} + z+$.

The positions of H atoms were refined. For H atoms bound to carbon, $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(H), while $U_{\rm iso}$(H) was refined for the hydroxyl H atom, H1.

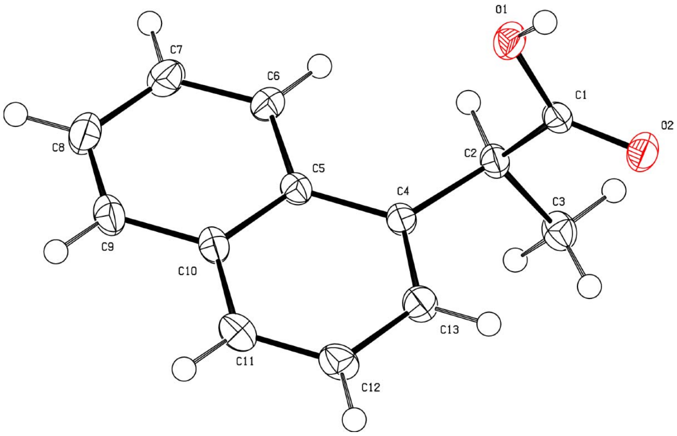


Figure 1
An *ORTEPII* (Johnson, 1976) drawing of the title molecule. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres with fixed radius.

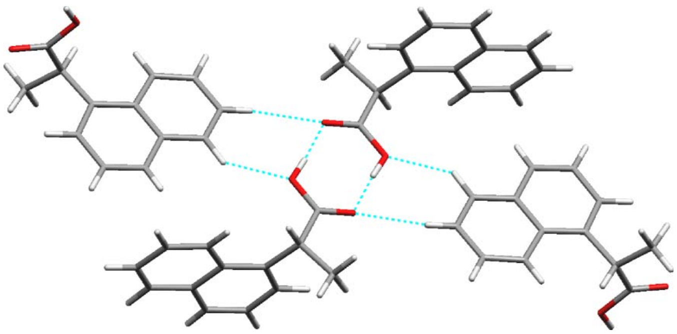


Figure 2
MERCURY plot (Bruno *et al.*, 2002) showing intermolecular interactions of four residues. Hydrogen bonds are highlighted in cyan.

Data collection: *KappaCCD Software* (Nonius, 1997); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2003); data reduction: *EvalCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR*97(Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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