The low-temperature device used was that described by Strouse (1976). For (II), intensity data were collected to θ = 50° in bisecting mode; the three standard reflections fluctuated by about 1%, with no significant decay. The remaining data were collected in parallel mode. The one standard reflection (15,0,1) fluctuated by about 5%, with only a very gradual decay (about 4% in 100 h), until the very end, when it began to drop significantly, falling about 10% in the last 20 h (out of some 270 h total). No effort was made to correct for the decay of this standard. The refinement of (I) went smoothly; there is twofold disorder in the position of one of the flanking methoxy methyl groups (C27), the occupancies being 0.64 and 0.36. Atoms C27*A* and C27*B* were refined with a common isotropic displacement parameter. The two largest shift/error values in the final least-squares cycle, 0.67 and 0.36, were for methyl torsions (on C22 and C27). No others were above 0.10. Except for the longer cryptand bridge, the structure of (II) conforms well to the space group *Pnma*, with the molecule lying on a mirror plane. The longer bridge, C30—C31—O32—C33—C34—O35—C36—C37, would have a mirror plane between C33 and C34 if the space-group symmetry was strictly obeyed. In the final model, the distances of atoms C34 to C37 from the mirror images of atoms (C33 to C30) that would be their equivalents vary from 0.17 (for C37 to C30′) to 1.14 Å (for C36 to C31′). The atoms in this disordered bridge were refined isotropically, with the *PART* and *DFIX* options of *SHELXL*93 (Sheldrick, 1993); each atom in a disordered pair was assigned an occupancy factor of 0.5. The largest shift/error value in the final least-squares cycle (2.04) was for the torsion angle about the C3—C4 bond, which depends upon the (imprecise) positions of the H atoms on C4. The next largest shift/error value (0.28) was for a displacement parameter. The largest shifts in atomic positions in the final cycle were of the order of 0.001 Å. Because this structure is disordered, no further refinement seemed warranted.

For both compounds, data collection: Syntex *P*$\bar{1}$ diffractometer software; cell refinement: Syntex *P*$\bar{1}$ diffractometer software; data reduction: *CARESS* (*UCLA Crystallographic Package*, 1984); program(s) used to solve structures: *MULTAN*80 (Declercq, Germain & Woolfson, 1979); molecular graphics: *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: local programs.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1281). Services for accessing these data are described at the back of the journal.

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(±)-2,3-Dihydro-3-oxo-1*H*-indenecarboxylic Acid: Hydrogen-Bonding Patterns in a γ-Keto Acid and its Monohydrate

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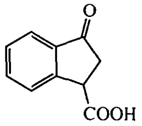
Abstract

Crystal structures have been determined for the title compound in both its anhydrous, (I), $C_{10}H_8O_3$, and monohydrate, (II), $C_{10}H_8O_3.H_2O$, forms. In (I), helical monoenantiomeric hydrogen-bonding (carboxyl-to-ketone) catemers, counteraligned with chains of the opposite chirality, pass through the cell in the **b** direction; a close contact of 2.57 Å is found between the sp^2 carboxyl O atom and aromatic H6 atom on a neighboring molecule of the same chirality. The hydrate (II) displays a complex hydrogen-bonding pattern in which each water molecule participates in three hydrogen bonds to three different keto acid molecules. A 2.54 Å close contact is found between the ketone and aromatic H4 atom on a neighboring centrosymmetrically-related molecule, as well as a 2.54 Å close contact between H1 and the ketone of a molecule of identical chirality translated one cell in the **a** direction.

Comment

Keto-carboxylic acids offer opportunities for variation on the standard pattern of dimeric hydrogen bonding observed in functionally unelaborated acids. In most cases, however, the ketone does not participate and mutually hydrogen-bonded dimers result. Less frequently, intermolecular carboxyl-to-ketone hydrogen bonds are seen, usually repeated helically along a cell axis, yielding a catemer. A third rare arrangement has an internal hydrogen bond and one example is known of acid-to-ketone dimerization. In addition, several instances are known of hydrates with more complex hydrogen-bonding modes. We have previously referenced and discussed numerous examples of these hydrogen-bonding modes (Thompson, Lalancette & Vanderhoff, 1992; Coté, Thompson & Lalancette, 1996).

We report here the structure and hydrogen-bonding behavior of the title compound, a γ-keto acid, in both its anhydrous, (I), and monohydrate, (II), forms. The category of γ-keto acids is especially rich in hydrogen-bonding types, embracing internal hydrogen bonds and catemers of both the helical and translational type, as well as dimers and hydrated patterns.



(I)

The labeled asymmetric unit for the anhydrous species (I), is shown in Fig. 1. The molecule is skeletally rigid except for rotation about the C1—C8 bond, projecting from the planar indane portion, and producing a C8—C1—C7a—C7 torsion angle of −50.8 (4)°. The carboxyl group is turned, with its C═O bond toward the aromatic ring, so that the carboxyl and the bicyclic ring system (excluding C2) have a 45.1 (1)° dihedral angle and the C7a—C1—C8—O2 torsion angle is 8.5 (5)°. A slight deviation of C2 from the general bicyclic plane produces a shallow dihedral angle of 7.2 (3)° between the bicyclic ring plane (excluding C2) and C1—C2—C3.

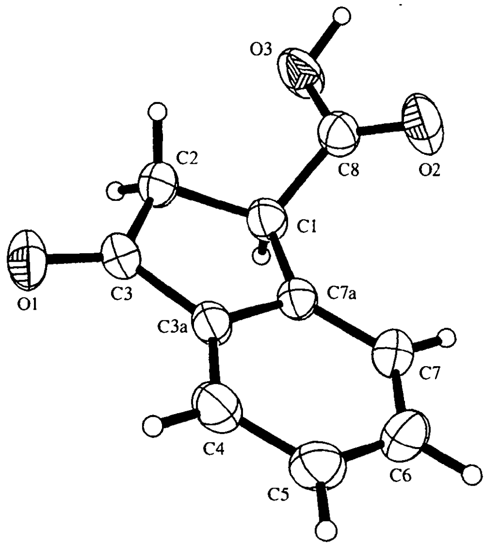


Fig. 1. The asymmetric unit of (I), with its numbering. Ellipsoids are set at the 40% probability level.

Averaging of the C—O bond lengths and C—C—O angles by disorder, although common in carboxyl dimers (Leiserowitz, 1976), is not observed in catemers, including (I), whose bond lengths are 1.192 (3) and 1.315 (3) Å, with angles of 126.2 (3) and 110.7 (3)°. Our own survey of 28 catemeric keto acid structures gives average values of 1.20 (1), 1.32 (1) Å and 124.5 (10), 112.8 (13)° for these lengths and angles. Values cited as typical for highly ordered dimeric carboxyls are 1.21, 1.31 Å and 123, 112° (Borthwick, 1980).

The packing for the anhydrous form, (I), is illustrated in Fig. 2. For both (I) and (II), graph-set analysis is useful in describing the hydrogen-bonding patterns (Etter, MacDonald & Bernstein, 1990; Etter, 1990; Bernstein *et al.*, 1995). For (I), the hydrogen-bonding pattern is a chain described as a simple first-order motif: $N_1 = C(7)$. The packing involved is of a type common for catemeric racemates, similar to that which we have recently reported for the C1—C7-trimethylene-bridged version of this compound (Brunskill, Thompson & Lalancette, 1997). Helices consisting exclusively of one enantiomer are counteraligned with helices of opposite chirality, both passing though the cell in the **b** direction. Fig. 2 also shows a 2.57 Å close contact found between O3 and the H6 atom of a neighboring molecule of the same chirality. This probably represents a polar

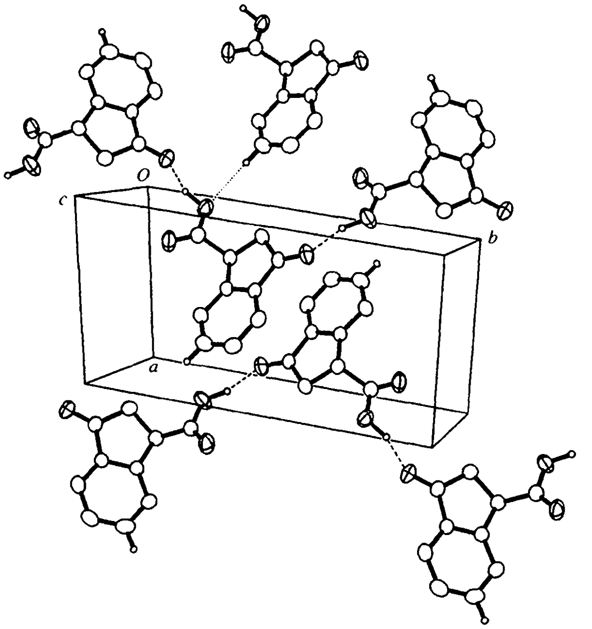


Fig. 2. A partial packing diagram for (I), with extracellular molecules included, illustrating two of the four helical monoenantiomeric carboxyl-to-ketone hydrogen-bonding catemers that pass through the cell in the **b** direction; the two shown are opposite in chirality and counteraligned. The 2.57 Å H6···O3 close contact is shown. For clarity, only the H atoms involved in bonding or in close contacts are shown. Ellipsoids are set at the 40% probability level.

attraction contributing materially to the packing forces (Jönsson, 1972; Leiserowitz, 1976; Berkovitch-Yellin & Leiserowitz, 1982).

The asymmetric unit for the hydrate, (II), is illustrated in Fig. 3. Here the C8—C1—C7a—C7 torsion angle is −57.2 (4)° [*versus* −50.8 (4)° in (I)] and the bicyclic ring plane/C1—C2—C3 dihedral angle is 2.3 (2)°, as opposed to 7.2 (3)° in (I). The organic portion of the asymmetric unit of (II) differs most from (I) in the rotation of the carboxyl group about C1—C8. In (II), the carboxyl group is turned approximately 110° relative to what is seen in (I), with the carbonyl group toward the ketone, so that the torsion angle C7a—C1—C8—O2 is −103.5 (3)°. The carboxyl (C1, C8, O2, O3) and bicyclic ring system in (II) have a 64.4 (1)° dihedral angle. The choice of specific relationship of the water molecule to the organic portion of the structure is arbitrary, since each water molecule is also hydrogen bonded to the carboxyl C═O of another molecule and to the ketone of a third. Equally valid asymmetric units could have been shown for any of these three relationships.

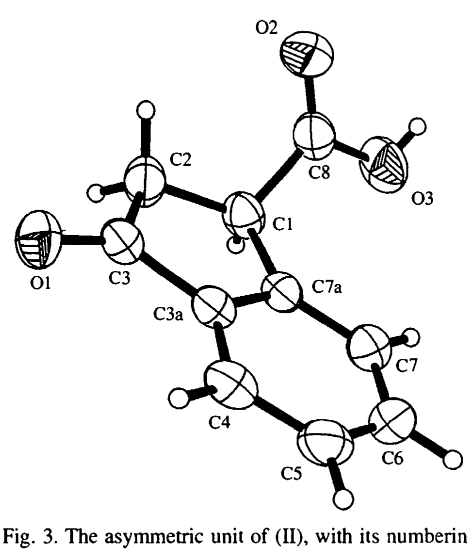


Fig. 3. The asymmetric unit of (II), with its numbering. Ellipsoids are set at the 40% probability level.

A partial packing diagram for the hydrate (II), with extracellular molecules, is shown in Fig. 4. The complex hydrogen-bonding pattern, in which each water molecule participates in three hydrogen bonds to as many different keto acid molecules, provides three distinct types of intermolecular hydrogen bonds (using graph-set analysis nomenclature, $N_1 = DDD$): H(carboxyl) to O(water), H(water) to O(carboxyl) and H(water) to O(ketone). There are three higher-order networks containing two distinct types of hydrogen bonds: two hydrated ring systems and an infinite hydrated chain. A 12-membered hydrogen-bonding ring, which may be seen as a hydrated carboxyl dimer, is centered at the origin: $N_2 = R^4_4(12)$. The two molecules centered across the inversion center in the *ab* face, plus the similarly centered pair of water molecules, are arranged in an 18-membered hydrogen-bonding ring: $N_2 = R^4_4(18)$; this network may be viewed as a hydrated carboxyl-to-ketone dimer. Finally, the carboxyl-to-water-to-ketone arrangement, $N_2 = C^2_2(9)$, represents a hydrated catemer, reminiscent of the helical one observed by Winkler, Hey & Williard (1986). Unlike that case, the chain here is translational and follows no crystallographic axis. Another higher-order network is present, $N_3 = R^6_6(24)$, and corresponds to a fusion of the adjacent 12- and 18-membered hydrate rings. This overall pattern is identical to that previously found for the hydrate of 2-benzoylbenzoic acid, also a γ-keto acid, but a dimer in its anhydrous form (Lalancette, Vanderhoff & Thompson, 1990).

A close contact of 2.54 Å between the ketone O atom and H4 in molecules located centrosymmetrically across the *c* cell edge is also shown in Fig. 4. A second 2.54 Å close contact (not shown) is found between H1 and the ketone of a molecule of identical chirality translated one cell in the **a** direction. These probably represent polar attractions contributing materially to the packing forces (Jönsson, 1972; Leiserowitz, 1976; Berkovitch-Yellin & Leiserowitz, 1982).

The displacement ellipsoid described by the water O atom has its principal axis approximately perpendicular to the plane of the three hydrogen bonds in which

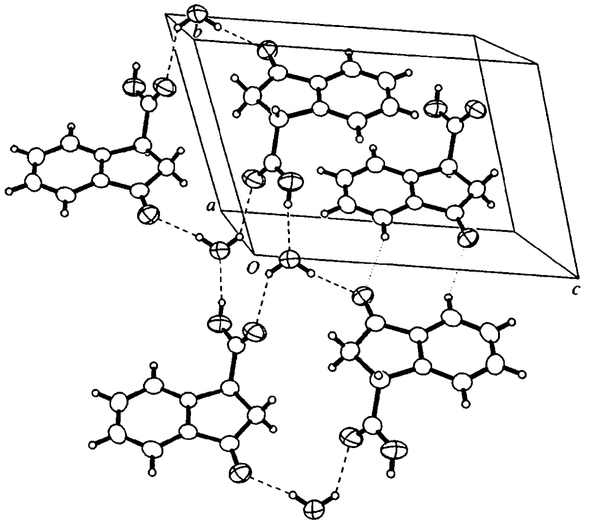


Fig. 4. A packing diagram for (II), with extracellular molecules, showing the basic repeating unit for the hydrogen-bonding scheme. Two translationally related molecules and a third enantiomerically related molecule are arranged with three water molecules in adjacent attached hydrogen-bonding rings having 12 and 18 members. A carboxyl-to-water-to-ketone chain system is also apparent. A 2.54 Å H4···O1 close contact is shown; a second 2.54 Å close contact between H1 and O1 in a translationally related molecule is not shown. Ellipsoids are set at the 40% probability level.

the water is involved [U_{11} = 0.206 (3) Å^2]. This is again similar to that seen in the hydrate of 2-benzoylbenzoic acid (Lalancette *et al.*, 1990), which also shows the principal axis of the water O-atom displacement ellipsoid in the same orientation and demonstrates that the O atom is relatively free to move along this axis due to the weak nature of the hydrogen bonds.

The disorder often observed in carboxyl dimers, and detected as averaging of the bond lengths and angles, might in principle be due to rotation of the entire dimer subunit, or, more plausibly, to static positional disorder in the crystal or to rapid tautomeric exchange within the dimer (Meier, Graf & Ernst, 1982; Nagaoka, Terao, Imashiro, Hirota & Hayashi, 1983). In (II), the more elaborate geometry present precludes all these mechanisms, and the observed bond lengths and angles are 1.196 (3) and 1.317 (3) Å, and 124.0 (3) and 112.1 (3)°, respectively.

The solid-state (KBr) IR spectrum of (I) has a peak for the carboxyl C═O at 1736 cm^{-1} and for the ketone at 1691 cm^{-1}, with satellites at 1702 and 1679 cm^{-1}. These C═O positions conform to the shifts seen in catemers, due to removal of hydrogen bonding from the carboxyl group and addition of hydrogen bonding to the ketone. The KBr spectrum of (II), where both carbonyl groups are hydrogen-bonded, has peaks at 1720 and 1691 cm^{-1}, for the carboxyl group and ketone, respectively. In $CHCl_3$ solution, where dimers predominate, the absorptions for (I) coalesce to a single broadened peak centered at 1715 cm^{-1}.

Experimental

The title compound was purchased from Aldrich Chemical Company. Crystals of (I), m.p. 386 K, were produced by slow evaporation of anhydrous 1:1 Et_2O–toluene only in a dry box; the compound was extremely hygroscopic and picked up water from either the air or trace water from supposedly dry solvents while it was crystallizing, to form (II); however, once (I) was crystallized in the dry box, it remained anhydrous. Crystals of (II), m.p. 340 K, were obtained from 50% aqueous ethanol by evaporation.

Compound (I)

Crystal data

$C_{10}H_8O_3$
M_r = 176.16
Monoclinic
$P2_1/c$
a = 8.151 (1) Å
b = 13.426 (2) Å
c = 8.344 (2) Å
β = 116.04 (1)°
V = 820.4 (3) Å^3
Z = 4
D_x = 1.426 Mg m^{-3}
D_m = 1.42 (1) Mg m^{-3}
D_m measured by flotation in cyclohexane/CCl_4

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 39 reflections
θ = 6.02–14.56°
μ = 0.11 mm^{-1}
T = 293 (2) K
Triangular prism
0.40 × 0.35 × 0.30 mm
Colorless

Data collection

Siemens $P4$ diffractometer
$2\theta/\theta$ scans
Absorption correction: none
2891 measured reflections
1432 independent reflections
893 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.062

$\theta_{\rm max}$ = 25.00°
$h = -9 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -9 \rightarrow 9$
3 standard reflections every 97 reflections intensity decay: 0.19%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.147
S = 1.03
1432 reflections
125 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$

$\Delta\rho_{\rm max}$ = 0.203 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.205 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1994)
Extinction coefficient: 0.011 (6)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °) for (I)*

O1—C3	1.222 (3)	O3—C8	1.315 (3)
O2—C8	1.192 (3)		
O1—C3—C3a	126.1 (3)	O2—C8—C1	126.2 (3)
O1—C3—C2	125.2 (3)	O3—C8—C1	110.7 (2)
C8—C1—C7a—C7	−50.8 (4)	C7a—C1—C8—O2	8.5 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1$^{\rm i}$	1.03 (4)	1.65 (4)	2.635 (3)	159 (3)
C6—H6···O3$^{\rm ii}$	0.93	2.57	3.464 (4)	162

Symmetry codes: (i) $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $x - 1, y, z - 1$.

Compound (II)

Crystal data

$C_{10}H_8O_3.H_2O$
M_r = 194.18
Triclinic
$P\bar{1}$
a = 5.984 (1) Å
b = 7.763 (1) Å
c = 11.086 (1) Å
α = 107.29 (1)°
β = 105.32 (1)°
γ = 93.12 (1)°
V = 469.27 (11) Å^3
Z = 2
D_x = 1.374 Mg m^{-3}
D_m = 1.37 (1) Mg m^{-3}
D_m measured by flotation in cyclohexane/CCl_4

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 19 reflections
θ = 5.56–17.41°
μ = 0.107 mm^{-1}
T = 293 (2) K
Plate
0.60 × 0.30 × 0.12 mm
Pale yellow

Data collection

Siemens $P4$ diffractometer
$2\theta/\theta$ scans
Absorption correction: face-indexed numerical
$T_{\rm min}$ = 0.958, $T_{\rm max}$ = 0.988

$R_{\rm int}$ = 0.032
$\theta_{\rm max}$ = 27.51°
$h = -1 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 14$

2717 measured reflections
2113 independent reflections
1132 reflections with $I > 2\sigma(I)$

3 standard reflections every 97 reflections
intensity decay: 1.84%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.150$
$S = 1.03$
2111 reflections
143 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.0808P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.001$
$\Delta\rho_{\max} = 0.210$ e Å^{-3}
$\Delta\rho_{\min} = -0.150$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.084 (14)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 3. *Selected geometric parameters (Å, °) for (II)*

O1—C3	1.219 (3)	O3—C8	1.317 (3)
O2—C8	1.196 (3)		
O2—C8—C1	124.0 (3)	O3—C8—C1	112.1 (3)
C8—C1—C7a—C7	−57.2 (4)	C7a—C1—C8—O2	−103.5 (3)

Table 4. *Hydrogen-bonding geometry (Å, °) for (II)*

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.75 (3)	1.87 (3)	2.615 (3)	170 (4)
O4—H4A···O2$^{\text{i}}$	0.77 (3)	2.18 (3)	2.845 (3)	144 (3)
O4—H4B···O1$^{\text{ii}}$	0.90 (3)	1.86 (3)	2.754 (3)	172 (3)
C4—H4···O1$^{\text{iii}}$	0.93	2.54	3.402 (3)	155
C1—H1···O1$^{\text{iv}}$	0.95	2.54	3.387 (3)	149

Symmetry codes: (i) $-x, -y, -z$; (ii) $x-1, y-1, z$; (iii) $2-x, 2-y, 1-z$; (iv) $x-1, y, z$.

For both (I) and (II), the H-atom treatment for the organic portion is the same. All non-carboxyl H atoms were found in electron-density difference maps but replaced in calculated positions and allowed to refine as riding models on their appropriate C atoms. The carboxyl H atom was found in an electron-density difference map and was allowed to refine with its displacement parameter fixed at 0.08 Å^2. The displacement parameter of the single methylene H atom on C1 was allowed to refine alone and the pair of H atoms on C2 as a group. The displacement parameters for the four aromatic H atoms were allowed to refine as a group. For the hydrate (II), the water H atoms were found in an electron-density difference map; they were allowed to refine with their displacement parameters fixed at 0.08 Å^2.

For both compounds, data collection: *XSCANS* (Fait, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structures: *SHELXTL* (Sheldrick, 1994); program(s) used to refine structures: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1331). Services for accessing these data are described at the back of the journal.

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2,4,5-Trimethylbenzoic Acid

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Abstract

The X-ray structure of the title compound, $C_{10}H_{12}O_2$, has been determined. The carboxyl and its *o*-methyl group display typical evasive in-plane splaying away from each other. The carboxyl is coplanar with the benzene ring and displays some minor disordering; the *para*-methyl group shows rotational disorder. Pairs of molecules form centrosymmetric carboxyl dimers [O···O 2.640 (2) Å].

Comment

Our continuing study of hydrogen bonding in keto-carboxylic acids, where four different basic hydrogen-bonding modes have been documented (Coté, Thompson & Lalancette, 1996), is currently being extended to include several simple unelaborated acids (Lalancette, Stringer & Coté, 1996). In the absence of other functional groups, carboxylic acids normally aggregate in the solid state as dimers (Leiserowitz, 1976). Rare instances

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