parameters of the Cl atoms were allowed to refine anisotropically. The H atoms were not included in the model. The coordinates of the H atoms involved in the hydrogen bonds (H4 and H19) were allowed to refine. Isotropic displacement parameters equal to $1.2U_{eq}$ of the atom covalently bonded to the H atom were used.

Data collection: *CAD-4 Operations Manual* (Enraf–Nonius, 1977). Cell refinement: *CAD-4 Operations Manual*. Data reduction: *PROCESS* in *MolEN* (Fair, 1990). Program(s) used to solve structure: direct methods (*MULTAN*80; Main *et al.*, 1980). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *CIF VAX* in *MolEN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SX1011). Services for accessing these data are described at the back of the journal.

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Phenylpyruvic Acid

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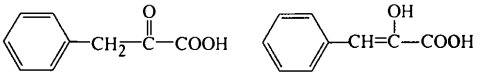
Abstract

The title compound, $C_9H_8O_3$, determined as the enolic form, 2-hydroxy-3-phenylpropenoic acid, has a fully extended pyruvic side chain. An intramolecular hydrogen bond is formed between the enol and the carboxyl O atoms. The molecules are held together by hydrogen bonds between the carboxyl groups. The O···O distances of the intra- and intermolecular hydrogen bonds are 2.639 (3) and 2.673 (3) Å, respectively.

Comment

The title compound is a well known metabolite of phenylalanine, which is a deaminated product of phenylalanine, the deamination catalysed by transaminase. The title compound is present in the urine and blood of a phenylketonuria patient (Martin, Mayes & Rodwell, 1983). To date, however, its crystal structure has not been determined. Accurate information on its structure and conformation is important for understanding its physicochemical role in the metabolic pathway.



(I) (II)

The molecular structure of the title compound is shown in Fig. 1, with the unit-cell packing shown in Fig. 2. The structural formula of the title compound has usually been given in its ketonic form, (I). However, our results show the molecule has the enolic form, (II), a tautomer of the ketonic one. As a result of tautomerism, the π electron in a double bond of the keto group is transferred to C7═C8 [1.339 (3) Å]. The phenyl and carboxyl groups are *trans* to each other about the C7═C8 double bond. The enolic O3 and the carboxyl O2 atoms form an intramolecular hydrogen bond [O3···O2 2.639 (3) Å]. Three torsion angles, O1—C9—C8—O3 −176.2 (3)°, C1—C7—C8—C9 175.5 (3)° and C8—C7—C1—C6 18.6 (4)°, indicate that the structure of this compound is characterized by an almost planar and fully extended conformation.

At present, no structural information is available on the enzymatic recognition mechanism of phenylpyruvic acid for producing further metabolites such as phenyllactic acid or phenylacetic acid. It may be important to consider the planar conformation of the enolic form

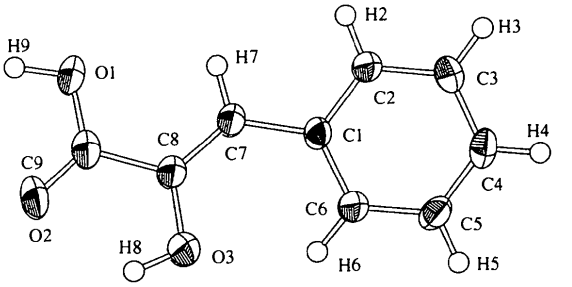


Fig. 1. An *ORTEP*II (Johnson, 1976) drawing of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

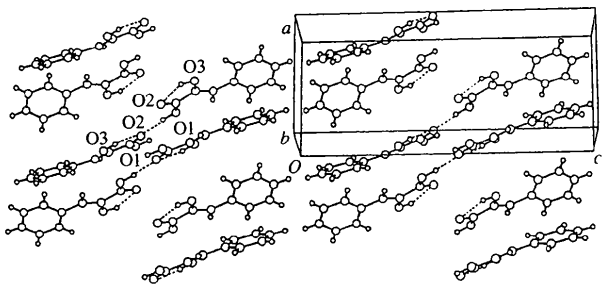


Fig. 2. A packing diagram of the title compound viewed approximately down the *b* axis.

of phenylpyruvic acid when studying the mechanism of the enzymatic action. No stacking interaction between phenolic groups is observed. The crystal structure is stabilized by van der Waals interactions between phenyl rings along the *a* axis and hydrogen bonds along the *c* axis between carboxyl groups [O1—H9···O2($-\frac{1}{2}-x$, $\frac{1}{2}+y$, $1-z$) 2.673 (3) Å].

Experimental

Crystals of the title compound were obtained by slow evaporation of a diethyl ether solution at room temperature.

Crystal data

$C_9H_8O_3$
M_r = 164.16
Monoclinic
$P2_1/a$
a = 7.489 (1) Å
b = 5.534 (4) Å
c = 18.722 (2) Å
β = 91.30 (3)°
V = 776 (1) Å^3
Z = 4
D_x = 1.405 Mg m^{-3}
D_m not determined

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 15.34–19.59°
μ = 0.099 mm^{-1}
T = 296 K
Plate
0.5 × 0.5 × 0.1 mm
Colourless

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: none
2110 measured reflections
1964 independent reflections
1301 reflections with $I > 1.5\sigma(I)$

R_{int} = 0.061
θ_{max} = 27.5°
h = 0 → 9
k = 0 → 7
l = −24 → 24
3 standard reflections
every 150 reflections
intensity decay: 2.76%

Refinement

Refinement on F
R = 0.057
wR = 0.070
S = 2.160
1301 reflections
141 parameters
H atoms refined isotropically
$w = 4F_o^2/\sigma^2(F_o^2)$

$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

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

O1—C9	1.311 (3)	C2—C3	1.391 (3)
O2—C9	1.222 (3)	C3—C4	1.373 (4)
O3—C8	1.355 (3)	C4—C5	1.382 (4)
C1—C2	1.395 (3)	C5—C6	1.388 (3)
C1—C6	1.395 (3)	C7—C8	1.339 (3)
C1—C7	1.467 (3)	C8—C9	1.479 (3)
C2—C1—C6	118.7 (2)	C1—C7—C8	128.6 (2)
C2—C1—C7	117.2 (2)	O3—C8—C7	123.5 (2)
C6—C1—C7	124.1 (2)	O3—C8—C9	114.1 (2)
C1—C2—C3	120.6 (2)	C7—C8—C9	122.3 (2)
C2—C3—C4	120.0 (2)	O1—C9—O2	124.4 (2)
C3—C4—C5	120.1 (2)	O1—C9—C8	116.2 (2)
C4—C5—C6	120.4 (2)	O2—C9—C8	119.4 (2)
C1—C6—C5	120.1 (2)		

All H atoms were located from difference Fourier maps and included in the refinement calculations isotropically. C—H distances ranged from 0.94 (2) to 1.03 (3) Å, O—H distances from 0.88 (5) to 0.97 (4) Å and B_{iso} values for H atoms from 2.5 (5) to 8 (1) Å^2.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1984) and *DIRDIF* (Beurskens, 1984). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEP*II (Johnson, 1976).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1047). Services for accessing these data are described at the back of the journal.

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