

2-Coumaric Acid

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Abstract. C₉H₈O₃, monoclinic, $P2_1/c$, $a = 8.750(4)$, $b = 5.529(3)$, $c = 16.235(9)$ Å, $\beta = 94.24(3)^\circ$, $V = 782.9$ Å³, $Z = 4$, $D_m = 1.380$, $D_c = 1.387$ Mg m⁻³, $M_r = 164.2$. The structure was refined to $R = 0.069$. O—H...O hydrogen bonds link the molecules to form a dimer. The interplanar angle between the carboxyl group and the benzene ring is 4.8° .

Introduction. The crystal structure of 2-coumaric acid, a synthetic auxin, was investigated as part of a project on the structure and function of plant growth hormones.

Crystals of the compound were obtained by evaporation from ethanol. Intensities of 1224 reflections were measured on a Picker four-circle diffractometer with the $\theta/2\theta$ scan, Ni-filtered Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å) and a 2°min^{-1} scan speed. The scan range was 2° and background was measured on either side of the peak for 10 s. The data were corrected for Lorentz and polarization factors but not for absorption. The cell constants were obtained by a least-squares fit of 24 reflections.

The structure was solved by symbolic addition (Karle & Karle, 1963). 143 reflections with $E \geq 1.5$ were chosen and phase propagation was carried out by hand with the Σ_2 formula (Hauptman & Karle, 1953).

An E map revealed six atoms and a subsequent difference map the remainder ($R = 0.55$). Refinement of this model (model 1) terminated at $R = 0.47$. A difference map computed with model 1 resulted in another set of atoms (model 2, $R = 0.55$). An average of these two models ($R = 0.40$) was used for refinement.

Block-diagonal least-squares refinement, first with isotropic then with anisotropic temperature factors, reduced R to 0.095. The eight H atoms were located from a difference map. The H atoms were given the isotropic temperature factors of the atoms to which they are bonded. Full-matrix least-squares refinement was carried out (Gantzel, Sparks & Trueblood, 1961) with isotropic temperature factors for the H atoms,

Table 2. Positional ($\times 10^3$) and thermal parameters of the H atoms with e.s.d.'s in parentheses

	Bonded to	x	y	z	B (Å ²)
H(1)	C(6)	111 (5)	450 (8)	134 (2)	2.956
H(2)	C(7)	45 (5)	167 (8)	233 (3)	6.093
H(3)	C(8)	238 (5)	-139 (9)	268 (3)	4.468
H(4)	C(9)	467 (5)	-172 (8)	212 (2)	3.231
H(5)	C(3)	581 (5)	268 (8)	612 (2)	3.457
H(6)	C(2)	661 (5)	-196 (8)	134 (2)	4.478
H(7)	O(2)	998 (7)	-179 (11)	38 (3)	7.195
H(8)	O(3)	290 (5)	587 (9)	47 (3)	5.590

* Contribution No. 496.

Table 1. Positional parameters ($\times 10^4$) of the non-hydrogen atoms with e.s.d.'s in parentheses

	x	y	z
O(1)	8416 (3)	1556 (5)	96 (2)
O(2)	9070 (3)	-1958 (5)	700 (2)
C(1)	8107 (4)	-126 (7)	550 (2)
C(2)	6712 (4)	-372 (7)	984 (2)
C(3)	5655 (4)	1378 (6)	933 (2)
C(4)	4215 (3)	1394 (6)	1341 (2)
C(5)	3157 (4)	3249 (6)	1149 (2)
C(6)	1774 (4)	3326 (7)	1517 (2)
C(7)	1445 (4)	1593 (8)	2079 (2)
C(8)	2476 (4)	-237 (8)	2281 (2)
C(9)	3848 (4)	-345 (7)	1916 (2)
O(3)	3550 (3)	-4915 (5)	592 (2)

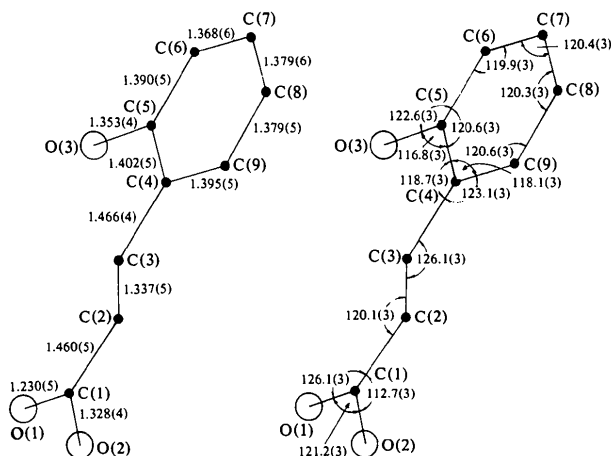


Fig. 1. Bond lengths (Å) and angles ($^\circ$). The e.s.d.'s of the last digits are given in parentheses.

anisotropic for the non-hydrogen atoms and unit weight for all observed reflections, giving a final R of 0.069. Scattering factors for C, O and H were taken from *International Tables for X-ray Crystallography* (1962). The final positional parameters are listed in Tables 1 and 2.*

Discussion. The bond lengths and angles are shown in Fig. 1. The average bond length in the ring is 1.385 (5) Å. The equations of the least-squares planes through C(4) to C(9) and through O(1), O(2), C(1) and C(2) are given in Table 3. The angle between the two planes is 4.8°; this is comparable to the angle between the ring and carboxyl-group planes in other growth hormones such as *p*-coumaric acid (5°) (Utsumi, Fujii, Irie, Furusaki & Nitta, 1970), β -naphthyloxyacetic acid (4.2°) (Pattabhi, Raghunathan & Chacko, 1978), 2-chlorophenoxyacetic acid (7.0, 6.6°) (Chandrasekhar & Pattabhi, 1977) and *trans*- β -2-furylacrylic acid (5.7°) (Filippakis & Schmidt, 1967). Fig. 2 shows the packing of the molecules viewed down *b*. The molecules are linked in dimers around a centre of symmetry by O—H...O hydrogen bonds (2.64 Å) and the dimers are joined by O—H...O hydrogen bonds (2.78 Å)

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33921 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

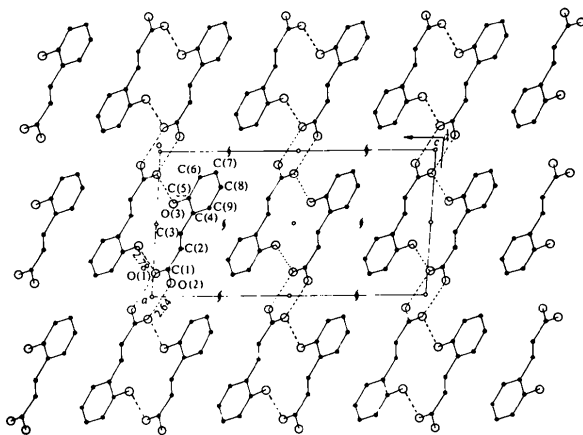


Fig. 2. The crystal structure of 2-coumaric acid viewed down *b*. Hydrogen bonds are shown by broken lines.

Table 3. *Least-squares planes and deviations (Å) of atoms from them*

Plane 1: through the benzene ring			
$0.3752X + 0.5603Y + 0.7383Z = 3.3611$			
C(4)	0.003	C(7)	0.001
C(5)	-0.004	C(8)	-0.002
C(6)	0.002	C(9)	0.000
*O(3)	-0.009	*C(3)	0.004
Plane 2: through the carboxyl group			
$0.3793X + 0.4900Y + 0.7847Z = 3.3324$			
O(1)	0.000	C(1)	0.002
O(2)	0.000	C(2)	0.000
*C(3)	-0.061		

* Not included in least-squares plane calculations.

Table 4. *Hydrogen-bond lengths (Å) and angles (°)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	<i>D</i> — <i>A</i>	H— <i>A</i>	<i>D</i> —H... <i>A</i>
O(2)—H(7)...O(1) ⁱ	0.97	2.64	1.66	176.5
O(3)—H(8)...O(1) ⁱⁱ	0.79	2.78	2.01	164.9
Symmetry code				
(i)	1 - <i>x</i> ,	- <i>y</i> ,	- <i>z</i>	
(ii)	1 - <i>x</i> ,	1 - <i>y</i> ,	- <i>z</i>	

involving the phenolic O atoms. The hydrogen-bonding scheme is given in Table 4.

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