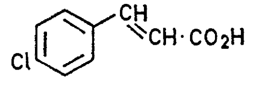
Structure Refinement and Molecular Packing of *p*-Chloro-*trans*-cinnamic Acid and β-(*p*-Chlorophenyl)propionic Acid

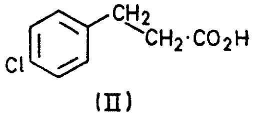
By **Jenny Pickworth Glusker,* David E. Zacharias,** and **Horace L. Carrell,** Institute for Cancer Research, Fox Chase Center for Cancer and Medical Sciences, Philadelphia, Pennsylvania 19111, U.S.A.

The crystal structures of *p*-chloro-*trans*-cinnamic acid (I) and β-(*p*-chlorophenyl)propionic acid (II) have been determined from *X*-ray diffractometer data. Both molecules are approximately planar and the crystal packing is similar when viewed down the *b* axis. Crystals of both compounds are monoclinic, space group $P2_1/a$, with $Z = 4$ in a unit cell of dimensions: for (I): $a = 32{\cdot}813(9)$, $b = 3{\cdot}890(1)$, $c = 6{\cdot}538(1)$ Å, $\beta = 95{\cdot}94(2)°$; and for (II): $a = 30{\cdot}024(6)$, $b = 5{\cdot}071(1)$, $c = 5{\cdot}728(1)$ Å, $\beta = 98{\cdot}70(1)°$. The structures were refined by full-matrix least-squares to R 0·059 [(I), 1160 observed reflections] and 0·052 [(II), 1372 observed reflections]. The cinnamic acid crystallizes in the β-form with head-to-head packing so that the ethylenic bonds lie near each other, thus explaining why a photo-dimerization to a β-truxinic acid can occur. There is disorder of the carboxy hydrogen atom in (I) but it is localized in (II).

THE structures of a cinnamic acid (I) and its hydrogenated derivative (II) were originally studied in this laboratory

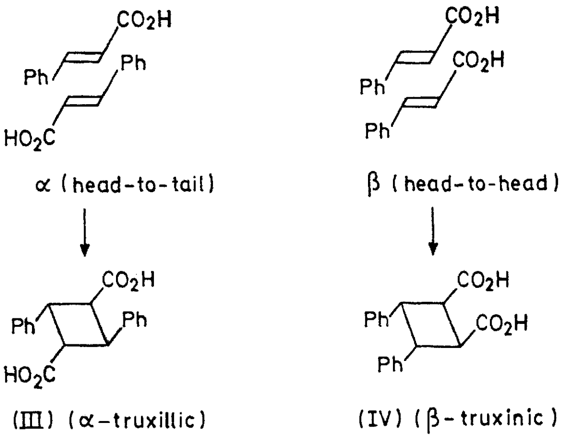


(I)



(II)

by Patterson and Clark[1] but atomic parameters were never published,[2] only Fourier maps in projection. The cinnamic acids are of great interest because a solid-state photoreaction is possible in the crystal, and a cyclobutanedicarboxylic acid results.[3,4] The *trans*-cinnamic acids with ring substituents crystallize in one or more of three possible types: α, β, or γ. They may be distinguished by the product of their photoreactions (see Scheme).



SCHEME

The α-form gives an α-truxillic acid derivative (III) (with a centre of symmetry $\bar{1}$) and the β-form a β-truxinic acid derivative (IV) (with a mirror plane of symmetry *m*), while the γ-form is light-stable. In addition the forms may be characterized by the lengths of their shortest axes, the least stable β-form crystallizing with one axis of 3·7—4·1 Å, while the α- and γ-forms have shortest axes >5·1 and *ca.* 4·9 Å, respectively. The β-form of *trans*-cinnamic acid does not give crystals suitable for an *X*-ray analysis, but the reported cell dimensions[2] are $a = 31{\cdot}3$, $b = 4{\cdot}04$, $c = 6{\cdot}05$ Å, $\beta = 90{\cdot}3°$, space group $P2_1/a$, very similar to those found[5] for *p*-chloro-*trans*-cinnamic acid. Thus, in view of the fact that this latter compound is an example of the β-form, and since it has been possible to relate the stereochemistry of the photoproduct to the crystalline form, a new structure determination was done.

The study had originally been initiated by Patterson in order to compare the configurations of *p*-chloro-*trans*-cinnamic acid (I) and its saturated derivative β-(*p*-chlorophenyl)propionic acid (II). This was of interest because neither *cis*- nor *trans*-cinnamic acids (β-phenylacrylic acids) inhibit the enzyme carboxypeptidase while β-phenylpropionic acid does.

EXPERIMENTAL

Crystal Data.—(i) p-*Chloro*-trans-*cinnamic acid* [trans-β (p-*chlorophenyl*)*acrylic acid*] (I). $C_9H_7ClO_2$. Monoclinic, $M = 182{\cdot}61$, $a = 32{\cdot}813(9)$, $b = 3{\cdot}890(1)$, $c = 6{\cdot}538(1)$ Å, $\beta = 95{\cdot}94(2)°$, $U = 829{\cdot}9(3)$ Å^3, $D_c = 1{\cdot}461$, $Z = 4$, D_o[5] $= 1{\cdot}458$ g cm^{-1}. $F(000) = 376$. λ(Cu-K_α) radiation = 1·5418 Å; μ(Cu-K_α) = 35·47 cm^{-1}. Space group $P2_1/a$. Crystals of (I) were grown by evaporation of an acetone solution. The crystal used for data collection was 0·20 × 0·15 × 0·11 mm.

(ii) β-(p-*Chlorophenyl*)*propionic acid* (II). $C_9H_9ClO_2$, Monoclinic. $M = 184{\cdot}62$, $a = 30{\cdot}024(6)$, $b = 5{\cdot}071(1)$, $c = 5{\cdot}728(1)$ Å, $\beta = 98{\cdot}70(1)°$, $U = 861{\cdot}9(3)$ Å^3, $D_c = 1{\cdot}423$, $Z = 4$, D_o[5] $= 1{\cdot}420$ g cm^{-1}, $F(000) = 384$. μ(Cu-K_α) = 35·6 cm^{-1}. Space group $P2_1/a$. Crystals of (II) were grown from solution in light petroleum (b.p. 90—120 °C) containing a small amount of benzene. The crystal used for data collection was 0·22 × 0·22 × 0·18 mm.

Data Collection.—Three-dimensional *X*-ray diffraction data were obtained with Cu-K_α monochromatized radiation in an automated four-circle diffractometer (Syntex P$\bar{1}$). The θ—2θ scan technique was used to a maximum value of sin θ/λ 0·61 Å^{-1}. The threshold for observation was considered to be $2{\cdot}33\,\sigma(I) = I_0$ for (I) and $3\sigma(I)$ for (II), where $\sigma(I)$ was derived from counting statistics. Values of $\sigma(F)$ were determined as $\sigma(F) = (F/2)\{[\sigma^2(I)/I^2] + \delta^2\}^{\frac{1}{2}}$ where δ is a measured instrumental uncertainty [0·015 for (I) and 0·022 for (II)]. The data were corrected for Lorentz and polarization factors and for absorption.[6] They were then placed

---

[1] A. L. Patterson and J. R. Clark, *Nature*, 1952, **169**, 1008.

[2] G. M. J. Schmidt, *J. Chem. Soc.*, 1964, 2014.

[3] M. D. Cohen, G. M. J. Schmidt, and F. J. Sonntag, *J. Chem. Soc.*, 1964, 2000.

[4] G. M. J. Schmidt, *Photochem. and Photobiol.*, 1967, **6**, 227.

[5] A. L. Patterson and J. R. Clark, unpublished observations.

[6] C. K. Johnson, 1620 Programs from I.C.R., I.C.R. No. 10 'Absorption Factors for a Crystal Ground as an Ellipsoid of Revolution,' 1963.

on an absolute scale by a Wilson plot. For (I) 1555 independent data were measured of which 395 were considered unobserved, and for (II) 1605 of which 233 were unobserved.

Structure Refinement.—The structure of (I), projected down the b axis, was determined by Patterson and Clark.[5] The x- and z-co-ordinates they determined were used with an $|F|^2$ map to derive a three-dimensional trial structure with an initial residual of R 0·207. This was refined by two electron-density maps to R 0·177. After anisotropic refinement by full-matrix least-squares methods all hydrogen atoms, except the one on the carboxy-group, were located in a difference map and were refined isotropically (with the heavier atoms anisotropic) to R 0·062. The hydrogen atom of the carboxy-group was placed, as two half hydrogen atoms, at the positions of two peaks of similar height on a difference map. Subsequent refinement gave R 0·059 for the 1160 observed data (R' 0·057).

TABLE 1

Final atomic parameters. Positional parameters are given as fractions of cell edges × 10^4 (× 10^3 for hydrogen). Anisotropic temperature factors are expressed as: $\exp[-\frac{1}{4}(h^2a^{*2}B_{11} + k^2b^{*2}B_{22} + l^2c^{*2}B_{33} + 2hka^*b^*B_{12} + 2hla^*c^*B_{13} + 2klb^*c^*B_{23})]$ and isotropic temperature factors as $\exp(-B \sin^2 \theta/\lambda^2)$ with all B and B_{ij} values given in Å^2. Standard deviations are determined from the inverted full-matrix, and are in parentheses

(*a*) Parameters for *p*-chloro-*trans*-cinnamic acid (I)

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cl	2860(1)	9370(3)	8746(1)	4·67(3)	5·88(5)	4·78(3)	0·57(4)	1·36(2)	−0·08(4)
O(1)	4496(1)	816(8)	269(4)	3·89(9)	8·14(16)	4·60(11)	0·24(11)	0·15(8)	−2·11(13)
O(2)	5050(1)	1809(9)	2397(4)	3·25(9)	10·81(22)	5·57(13)	0·45(12)	0·40(8)	−3·12(15)
C(1)	3200(1)	7677(10)	7130(5)	3·58(12)	4·28(16)	3·97(14)	−0·03(12)	0·91(11)	0·16(13)
C(2)	3054(1)	6694(10)	5147(5)	3·37(12)	5·17(20)	4·46(16)	0·14(13)	0·19(11)	−0·48(14)
C(3)	3326(1)	5330(10)	3908(5)	3·82(12)	5·20(19)	3·57(13)	−0·15(13)	0·16(10)	−0·36(14)
C(4)	3743(1)	5014(8)	4568(5)	3·49(12)	3·38(17)	3·76(13)	−0·14(11)	0·30(10)	−0·19(11)
C(5)	3872(1)	6046(11)	6562(5)	3·13(12)	5·48(19)	4·16(14)	0·15(13)	−0·06(10)	−0·35(15)
C(6)	3606(1)	7366(10)	7828(5)	4·10(12)	4·98(19)	3·67(15)	−0·01(14)	0·40(12)	−0·57(14)
C(7)	4018(1)	3600(10)	3180(5)	3·95(12)	4·49(18)	3·63(14)	−0·12(13)	0·32(11)	−0·39(13)
C(8)	4419(1)	3332(11)	3490(5)	3·79(12)	5·85(22)	3·79(15)	0·05(14)	0·39(11)	−0·94(15)
C(9)	4667(1)	1904(10)	1967(5)	3·55(12)	5·04(19)	4·15(15)	−0·05(13)	0·54(11)	−0·63(14)

	x	y	z	B		x	y	z	B
H(C2)	273(1)	707(8)	462(4)	3·4(7)	H(C7)	388(1)	287(11)	206(6)	6·1(11)
H(C3)	323(1)	455(9)	251(5)	5·4(8)	H(C8)	456(1)	402(10)	481(6)	5·9(9)
H(C5)	414(1)	583(9)	701(5)	3·9(8)	H(a)	470(3)	−22(23)	−17(14)	7·5(28)
H(C6)	370(1)	852(10)	920(5)	5·9(9)	H(b)	526(3)	96(24)	177(14)	6·8(23)

(*b*) Parameters for β-(*p*-chlorophenyl)propionic acid (II)

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cl	2866(2)	1376(1)	1215(1)	4·33(3)	4·45(3)	4·78(3)	−0·67(2)	0·10(2)	−1·03(2)
O(1)	4530(1)	13261(5)	9867(4)	5·36(7)	8·24(13)	6·80(11)	−2·90(9)	2·71(9)	−3·93(11)
O(2)	5023(1)	13067(5)	7460(5)	5·53(7)	9·58(14)	8·53(11)	−3·81(9)	3·68(9)	−5·36(13)
C(1)	3184(1)	3732(5)	2957(4)	3·31(10)	3·46(10)	3·73(10)	0·06(9)	0·02(8)	−0·07(9)
C(2)	3023(1)	4788(5)	4896(5)	3·35(10)	4·69(13)	4·69(12)	−0·38(9)	1·11(9)	−0·46(11)
C(3)	3278(1)	6629(6)	6243(5)	3·73(10)	4·50(13)	4·02(11)	−0·06(9)	1·27(9)	−1·19(10)
C(4)	3694(1)	7461(6)	5748(4)	3·42(10)	3·84(11)	3·65(11)	0·00(9)	0·51(8)	−0·25(9)
C(5)	3844(1)	6352(6)	3795(5)	3·49(10)	5·28(13)	4·13(11)	−0·80(10)	1·00(9)	−0·77(11)
C(6)	3593(1)	4483(6)	2399(5)	3·95(10)	5·09(14)	3·68(11)	−0·12(10)	0·88(9)	−0·78(10)
C(7)	3955(1)	9539(6)	7274(5)	4·09(10)	4·83(13)	4·08(12)	−0·67(10)	0·73(9)	−0·92(10)
C(8)	4401(1)	10295(6)	6583(5)	3·95(10)	4·46(13)	4·69(13)	−0·19(10)	0·52(10)	−1·16(11)
C(9)	4654(1)	12335(6)	8130(5)	3·49(10)	4·11(12)	5·08(13)	−0·26(10)	0·40(10)	−0·67(11)

	x	y	z	B		x	y	z	B
H(02)	517(1)	1440(8)	839(6)	7·2(10)	H(71)	402(1)	884(8)	871(7)	8·1(11)
H(2)	275(1)	425(5)	516(5)	4·1(6)	H(72)	377(1)	1117(8)	729(7)	8·4(11)
H(3)	318(1)	751(7)	725(6)	5·9(8)	H(81)	461(1)	887(7)	665(6)	7·5(10)
H(5)	415(1)	685(6)	340(5)	5·6(7)	H(82)	440(1)	1079(7)	489(6)	6·7(9)
H(6)	374(1)	369(6)	94(5)	5·7(7)					

The structure of (II) was determined by Patterson and Clark.[1,5] Their co-ordinates resulted in R 0·184. Anisotropic refinement gave R 0·099 and all hydrogen atoms were located and included, with isotropic temperature factors, in the full-matrix least-squares refinement to R 0·052 for the 1372 observed data (R' 0·061). An extinction coefficient,[7] $\alpha = 2·66 \times 10^{-6}$ was applied to the data for (II).

The '*X*-Ray '72' System of Programs[8] was used to calculate maps and a full-matrix least-squares method[9] was used for the refinement. The weights of the reflections during refinement were $1/[\sigma^2(F)]$ with zero weight for those reflections below the threshold value. The quantity minimized in the least-squares calculations was $\Sigma\omega\{||F_o| - |F_c||\}^2$. Atomic scattering factors for chlorine, oxygen, and carbon were taken from ref. 10 and for hydrogen from ref. 11, with corrections for the real component ($\Delta f'$) of the anomalous corrections for the chlorine atom from ref. 12.

Positional and thermal parameters for both compounds are listed in Table 1, and observed and calculated structure factors in Supplementary Publication No. SUP 21118 (7 pp.).*

---

* See Notice to Authors No. 7 in *J.C.S., Perkin II*, 1973, Index issue.

[7] W. H. Zachariasen, *Acta Cryst.*, 1963, **16**, 1139.

[8] J. M. Stewart, '*X*-Ray' System, Version of 1972, Technical Report TR 192 of the Computer Science Centre, University of Maryland, June 1972.

[9] P. K. Gantzel, R. A. Sparks, R. E. Long, and K. N. Trueblood, UCLALS4, Program in Fortran IV.

[10] 'International Tables for *X*-Ray Crystallography,' 1962, vol. III, Kynoch Press, Birmingham, pp. 201—207.

[11] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 1965, **42**, 3175.

[12] D. T. Cromer and D. Liberman, *J. Chem. Phys.*, 1970, **53**, 1891.

DISCUSSION

Distances and angles in molecules of (I) and (II) are given in Figure 1, and the temperature motion is represented by thermal ellipsoids [13] in Figure 2. A comparison of distances and angles in three cinnamic acids,[14] with those in (I) and (II) is given in Table 2.

In general the bond lengths in *p*-chlorocinnamic acid (I) are slightly shorter for the sequence C(4), C(7), C(8), C(9) than for the other cinnamic acids. The lengthening of some bonds in the saturated acid (II) is shown in Table 2. Torsion angles are given in Table 3. Both molecules (I) and (II) are approximately planar. The

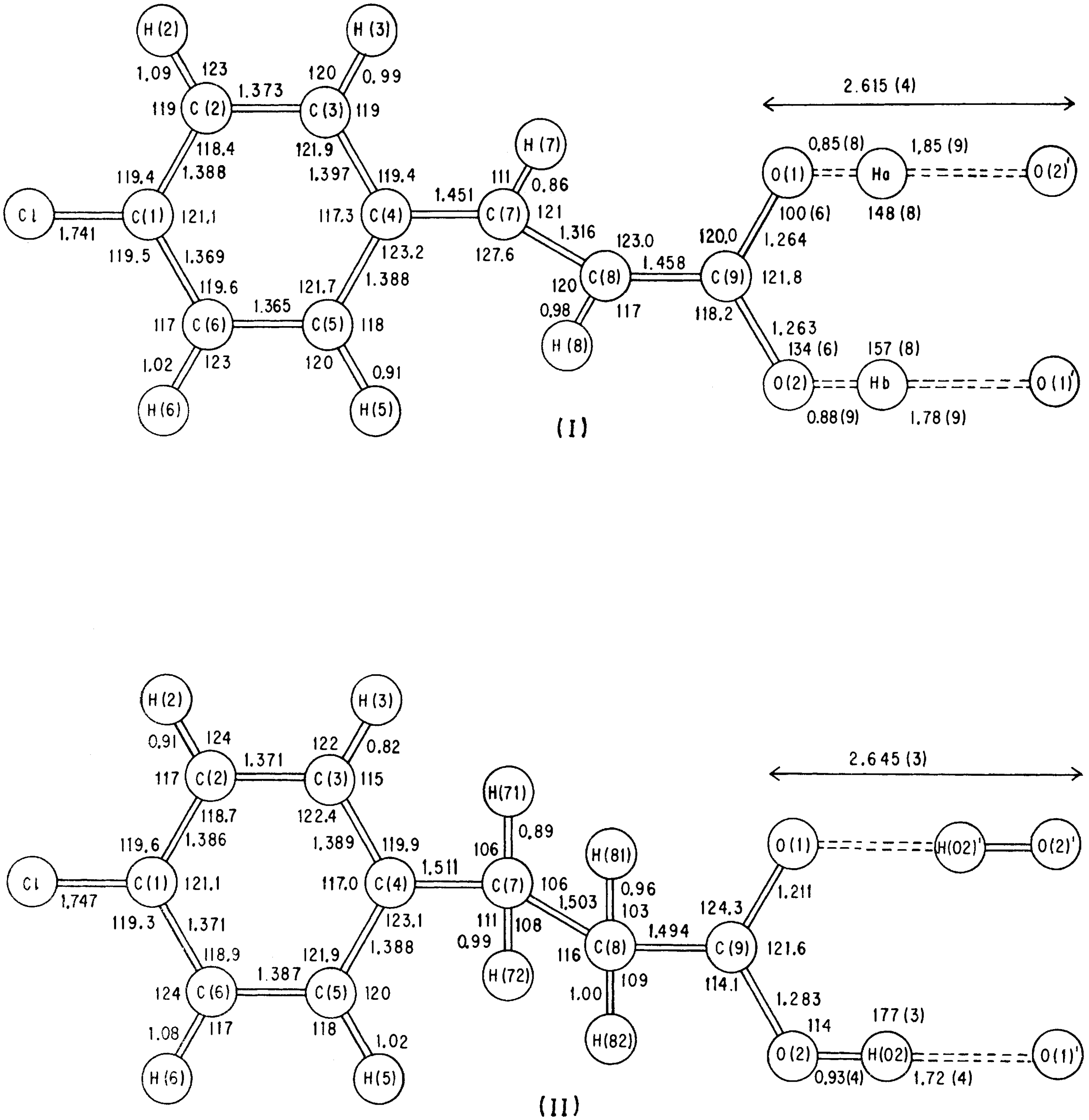


FIGURE 1 Angles and distances for (I) and (II). Estimated standard deviations are for (I): 0·002—0·004 Å for bonds (0·03—0·06 Å if H involved), and 0·2° for angles (1—2° if H involved); and for (II) 0·004—0·005 Å for bonds (0·07—0·14 Å if H involved), and 0·3° for angles (2—3° if H involved). Additional angles are: H(81)–C(8)–C(7) 114, C(4)–C(7)–C(8) 115·5(2), C(7)–C(8)–C(9) 114·5(2), H(71)–C(6)–H(72) 111(3), and H(81)–C(8)–H(82) 98(3)

---

[13] C. K. Johnson, ORTEP, a Fortran Thermal-ellipsoid Plot Program for Crystal Structure Illustrations, 1965.

[14] S. E. Filippakis, L. Leiserowitz, D. Rabinovich, and G. M. J. Schmidt, *J.C.S. Perkin II*, 1972, 1750.

least-squares planes through parts of the molecules (I) and (II) and deviations from them are listed in Table 4. The planarity of (II) results from a staggered conformation of hydrogen atoms of the two methylene groups on C(7) and C(8).

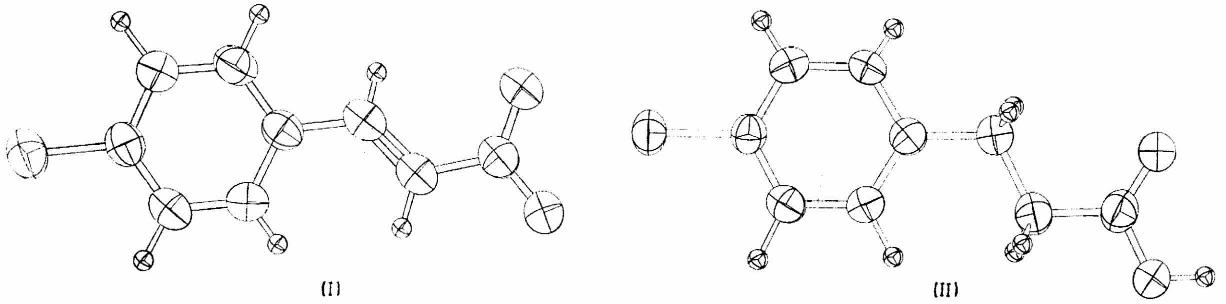


FIGURE 2 Thermal ellipsoids for (I) and (II): disordered hydrogen atoms are omitted

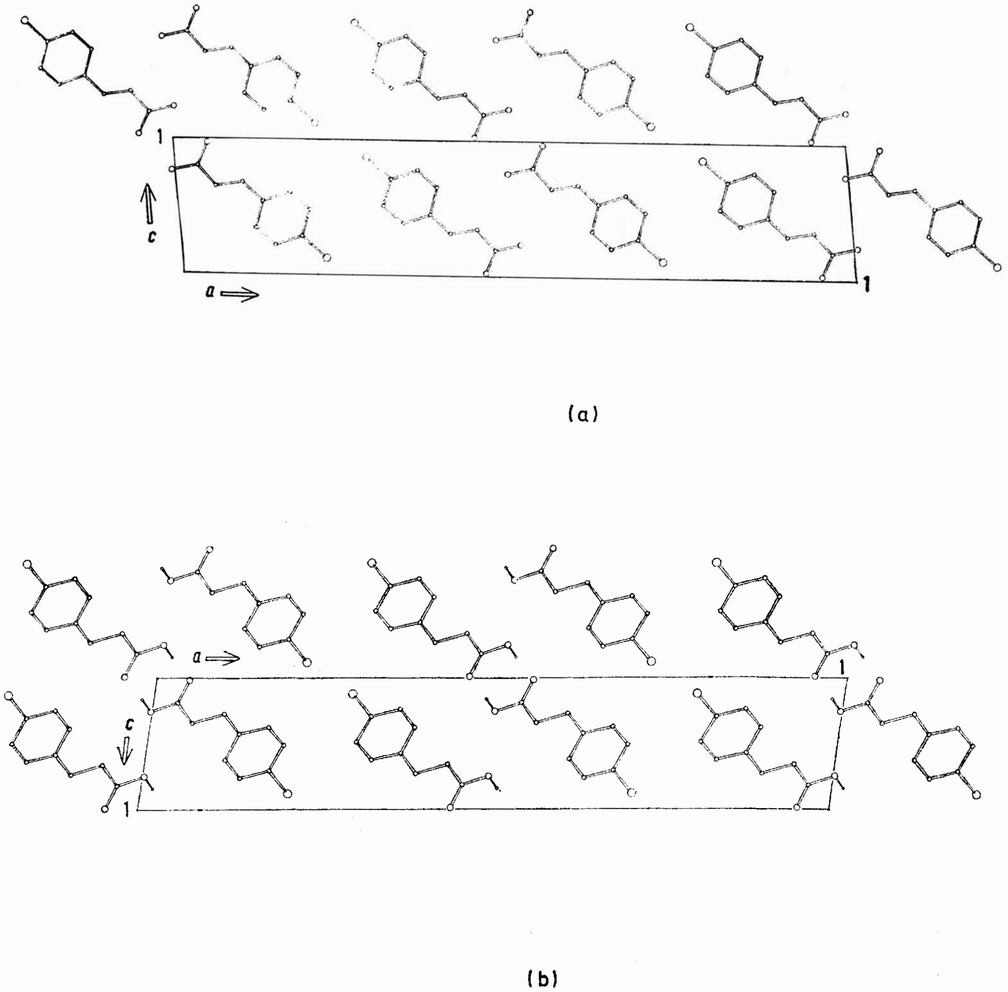


FIGURE 3 Packing in the unit cells of (a) (I), and (b) (II), both viewed down *b*

The packing in crystals of both compounds is similar when viewed down the *b* axis [Figure 3(a) and (b)]. The crystal structure is determined, at least in part, by the formation of hydrogen bonds between carboxy-groups to give dimers. The packing is also determined by the surroundings of the chlorine atom. There is a nearly linear C–Cl · · · Cl interaction (Figure 4) as found in 4-chlorobenzoic acid [15] with C–Cl · · · Cl angles of 167·3 for (I) and 168·2° for (II). In addition, in these three cases, hydrogen atoms on C(2) and C(3) interact with chlorine atoms in a similar, but not identical, manner. The ethylenic

---

[15] R. S. Miller, I. C. Paul, and D. Y. Curtin, *J. Amer. Chem. Soc.*, 1974, **96**, 6334.

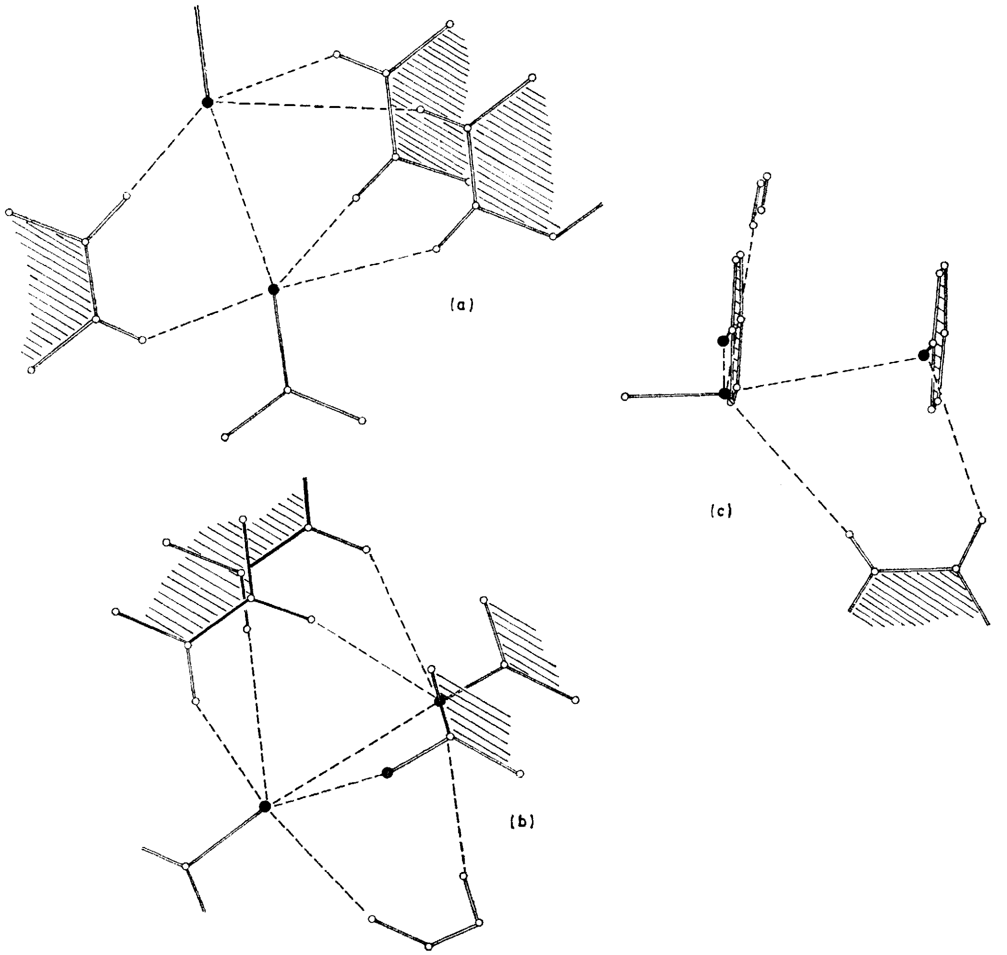


FIGURE 4 Surroundings of chlorine in (a) *p*-chlorobenzoic acid, (b) (I), and (c) (II). Cl atoms black, benzene rings shaded

double bonds in the cinnamic acid (I) can stack approximately 3·5 Å apart but this is not possible for the methylene groups in the phenylpropionic acid (II). As a result, the *b* axis is elongated in crystals of the latter and the molecule is more sharply inclined to this axis.

TABLE 2

Comparison of bond lengths (Å) and angles (deg.) in some cinnamic acids

	(V)	(VI)	(VII)	(I)	(II)
(*a*) Distances					
Bond adj. to benzene ring	1·486	1·469	1·484	1·451	1·511
Double bond	1·326	1·336	1·331	1·316	1·503
Bond adj. to carboxy	1·470	1·466	1·461	1·458	1·494
C–O (carboxy)	1·211	1·259	1·253	1·264	1·211
	1·322	1·264	1·275	1·263	1·283
H (carboxy)	H	2($\frac{1}{2}$H)	2($\frac{1}{2}$H)	2($\frac{1}{2}$H)	H
C–Cl	1·717	1·749		1·741	1·747
(*b*) Angles					
Ph—// angle	124·7	130·0	125·2	127·6	115·5
//—CO_2H angle	128·0	125·3	126·7	123·0	114·5
Carboxy angles	111·5	115·7	115·7	118·2	114·1
	125·9	121·2	122·4	120·0	124·3
	122·6	123·1	121·9	121·8	121·6

(V) β-Chloro-*trans*-, (VI) β-chloro-*cis*-, and (VII) β-methyl-*cis*-cinnamic acid; values from ref. 14.

The ethylenic double bonds in the cinnamic acid stack in the crystal (Figure 5) not precisely on top of each other.

TABLE 3

Torsion angles (deg.)

	(I)	(II)
C(3)–C(4)–C(7)–C(8)	175·0(4)	180·0(3)
C(5)–C(4)–C(7)–C(8)	−5·9(7)	−1·7(5)
C(4)–C(7)–C(8)–C(9)	−179·1(4)	−179·5(3)
C(7)–C(8)–C(9)–O(1)	−0·9(7)	3·0(5)
C(7)–C(8)–C(9)–O(2)	178·9(4)	−176·7(3)
H(7)–C(7)–C(8)–C(9)	2(4)	
H(71)–C(7)–C(8)–C(9)		−63(3)
H(72)–C(7)–C(8)–C(9)		56(3)
C(4)–C(7)–C(8)–H(8)	3(3)	
C(4)–C(7)–C(8)–H(81)		−61(3)
C(4)–C(7)–C(8)–H(82)		52(3)

This situation is compared with that for potassium *trans*-aconitate.[16] The effect of the double bond on the packing is seen by a comparison of the stacking of phenyl rings in the two compounds (I) and (II) (Figure 6). In the cinnamic acid (I) the benzene rings stack vertically, whereas in the phenylpropionic acid (II), with the more bulky methylene groups, the chlorine lies over the benzene ring of a neighbouring molecule. The bulkiness of the methylene groups cause the increase in the *b* axis for (II). In the packing of double bonds in (I) the distance

[16] H. L. Carrell, *Acta Cryst.*, 1973, **B29**, 2082.

apart of the two bond centres is 4·05 Å and the closest approach of carbon atoms is C(7) · · · C(7′) and C(8) · · · C(8′) both at 3·89 Å.

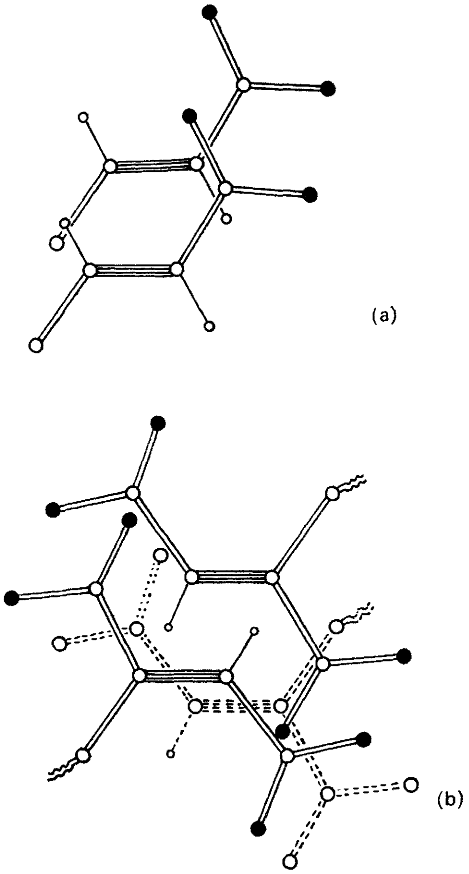


FIGURE 5 Vertical stacking of ethylenic double bonds; (a) *p*-chlorocinnamic acid; (b) potassium *trans*-aconitate

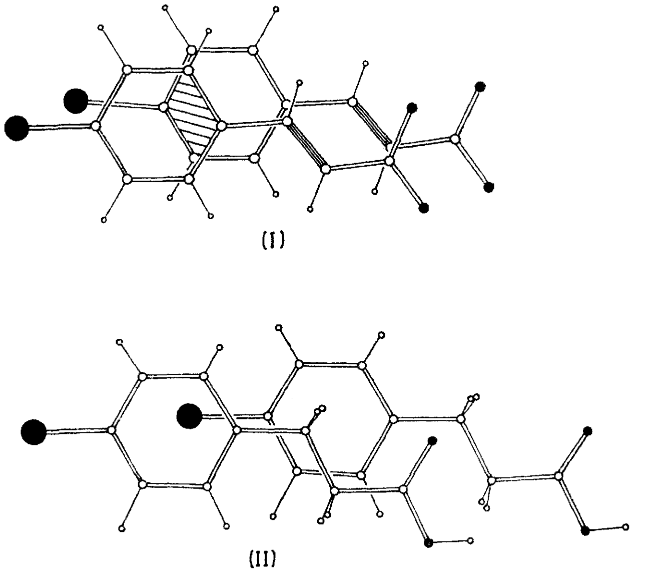


FIGURE 6 Vertical stacking of phenyl rings

TABLE 4

Least squares planes through portions of the molecules

(*a*) Equations with respect to crystal axes

(I)	C(1)–C(6)	$6{\cdot}74515x + 3{\cdot}57680y - 2{\cdot}31817z = 3{\cdot}25354$
	C(4), C(7), C(8), C(9)	$4{\cdot}43791x + 3{\cdot}53682y - 2{\cdot}65211z = 2{\cdot}21805$
	C(8), C(9), O(1), O(2),	$3{\cdot}91353x + 3{\cdot}53771y - 2{\cdot}67125z = 1{\cdot}97552$
(II)	C(1)–(6)	$-10{\cdot}97377x + 3{\cdot}70265y - 2{\cdot}94508z = -2{\cdot}98965$
	C(4), C(7), C(8), C(9)	$-10{\cdot}91779x + 3{\cdot}64051y - 3{\cdot}04981z = -3{\cdot}06730$
	C(8), C(9), O(1), O(2)	$-12{\cdot}30428x + 3{\cdot}65362y - 2{\cdot}81657z = -3{\cdot}50809$

(*b*) Deviations (Å) from these planes

	(I)			(II)		
Cl	0·000	0·046	0·123	0·004	0·069	0·143
C(1)	−0·002	0·026	0·088	0·003	0·047	0·121
C(2)	0·008	0·140	0·213	−0·002	0·017	0·159
C(3)	−0·009	0·107	0·168	0·001	−0·003	0·138
C(4)	0·006	0·000	0·043	−0·001	−0·003	0·070
C(5)	0·000	−0·102	−0·074	0·002	0·026	0·031
C(6)	−0·001	−0·089	−0·049	−0·003	0·045	0·049
C(7)	0·007	−0·005	0·021	0·031	0·003	0·078
C(8)	0·110	−0·004	0·000	0·026	0·003	0·001
C(9)	0·119	0·005	−0·001	0·046	−0·003	−0·002
O(1)	0·008	−0·006	0·000	0·012	−0·069	0·001
O(2)	0·244	0·027	0·000	0·110	0·065	0·001
H(2)	0·05	0·27	0·36	0·02	0·04	0·23
H(3)	−0·03	0·16	0·23	0·14	0·12	0·30
H(5)	0·00	−0·18	−0·16	−0·04	−0·01	−0·06
H(6)	0·16	0·00	0·03	−0·03	0·04	−0·09
H(7) [a]	−0·08	−0·03	0·01	−0·72	−0·76	−0·66
H(8) [b]	0·15	−0·05	−0·05	0·83	0·79	0·89
H(a) [c]	−0·13	−0·17	−0·17	−0·75	−0·77	−0·80
H(b) [d]	0·01	0·01	0·01	0·72	0·71	0·66
[e]				0·17	0·11	0·04

For (II) these atoms are numbered.

[a] H(71), [b] H(72), [c] H(81), [d] H(82), and [e] H(02).

In (I) there is disorder of the hydrogen in the carboxy dimers so that it is on O(1) in some unit cells and O(2) in others. In (II) the hydrogen atom is on O(2) and hydrogen bonds to O(1) (Figure 7). As seen in Table 2 both situations occur in other cinnamic acids.

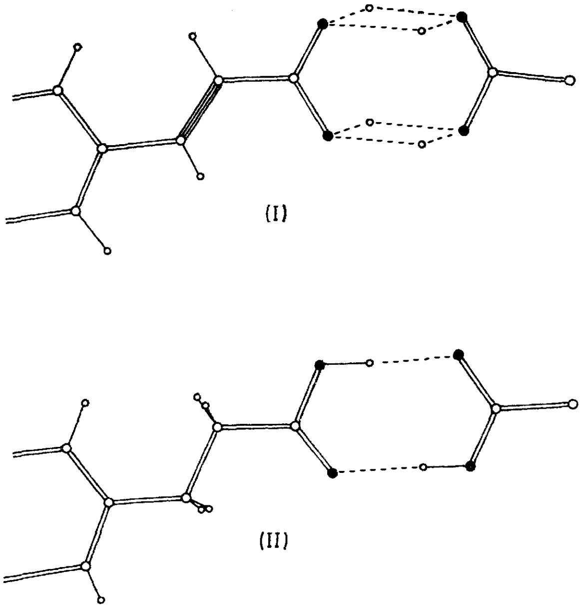


FIGURE 7 Hydrogen bonding

We have shown that a cinnamic acid and its hydrogenated derivative have similar crystal structures. In the packing in the former the ethylenic double bonds lie near each other. As stated by Cohen and Schmidt:[17] 'Reaction in the solid state occurs with a minimum amount of atomic or molecular movement.' Thus the head-to-head packing found in these crystals of the β-form of *p*-chlorocinnamic acid explains why only β-truxinic acid can result. In the *p*-chlorophenylpropionic acid, where no such interaction between ethylenic double bonds is possible, the packing is similar but not identical. Both molecules are approximately planar, as a result of the ethylenic double bond for (I) and of staggering of the hydrogen atoms of the $-CH_2-CH_2-$ group for (II).

We thank Dr. Iain C. Paul who suggested that we refine new data for (I) and Dr. Joan R. Clark for helpful discussions. This research was supported by grants from the National Institutes of Health, U.S. Public Health Service, and by an appropriation from the Commonwealth of Pennsylvania.

[4/1035 *Received, 29th May*, 1974]

---

[17] M. D. Cohen and G. M. J. Schmidt, *J. Chem. Soc.*, 1964, 1996.