in a hydrogen bond to the O atom of a glide-plane related molecule to form chains of molecules. The bond lengths are: N(1)···O(2) at $x, -y, \frac{1}{2}+z$ 2·888 (2) Å (I), N(1)···O(2) at $x, \frac{1}{2}-y, \frac{1}{2}+z$ 2·914 (3) Å (II).

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Structure of 2-Isopropylcrotonic Acid, $C_7H_{12}O_2$

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Abstract. $M_r = 128{\cdot}172$, monoclinic, $P2_1/c$, $a = 5{\cdot}507\,(1)$, $b = 10{\cdot}206\,(1)$, $c = 13{\cdot}717\,(1)$ Å, $\beta = 97{\cdot}15\,(1)^\circ$, $V = 764{\cdot}96$ Å^3, $Z = 4$, $D_x = 1{\cdot}113$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}861$ cm^{-1}, $F(000) = 280$, $T = 295$ K, $R = 0{\cdot}045$ for 884 observed reflections. The molecules are hydrogen-bonded in pairs to form centrosymmetric dimers. The molecules are inclined with respect to the *c*-glide planes, so that stereochemical control of reactions on the (010) planes is expected to be more difficult than if the molecules were parallel to the glide planes.

Introduction. The stereochemistry of addition to alkenes can be controlled by forcing the reaction to occur on one surface of a single crystal (Holland & Richardson, 1980; Chenchaiah, Holland & Richardson, 1982). 2-Isopropylcrotonic acid is a precursor to a number of biochemically interesting compounds, but its structure has not been previously determined. We have solved its structure to determine which way the alkene portion of the molecule is aligned with respect to the crystallographic symmetry elements, as this knowledge is essential in order to choose the appropriate surface for asymmetric reaction.

Experimental. White needles from slow evaporation of a 20% aqueous acetone solution, $0{\cdot}1 \times 0{\cdot}1 \times 0{\cdot}5$ mm, sealed in a thin-walled capillary, Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$, lattice parameters from 25 reflections with $8 < \theta < 15^\circ$, one standard reflection measured every hour – max. variation 2·8%, 1672 reflections (h $-6 \rightarrow 6$, k $0 \rightarrow 12$, l 0–16) with $\theta < 25^\circ$, 1344 independent, 884 with $I > 3\sigma(I)$, Lp correction, no absorption correction, direct methods, refinement by full-matrix least squares on F's, all non-H atoms anisotropic, all H atoms located on a difference map. Six peaks about the C(7) methyl group indicated twofold disorder. H-atom positions refined, C(7)—H distances and H—C(7)—H angles constrained to be 1·08 Å and 109·5°, isotropic temperature factors refined for methyl H atoms as a group and for other H atoms as a group, 130 parameters less 12 constraints, max. shift/$\sigma = 0{\cdot}51$ on final cycle, $w = [\sigma^2(F) + 0{\cdot}0011\,F^2]^{-1}$, $R = 0{\cdot}045$, $R_w = 0{\cdot}051$, final difference map with no features greater than $0{\cdot}15$ e Å^{-3} or less than $-0{\cdot}20$ e Å^{-3}, scattering factors from *International Tables for X-ray Crystallography* (1974), computer programs *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1976).

Discussion. The atomic coordinates are listed in Table 1, and bond distances and angles are given in Table 2.

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Table 1. *Fractional coordinates and equivalent isotropic thermal parameters for 2-isopropylcrotonic acid, with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} a^*_i a^*_j \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	$U_{\rm eq}$(Å^2)
O(1)	0·3477 (3)	0·0668 (2)	0·3995 (1)	0·0611
O(2)	0·2732 (4)	0·0925 (2)	0·5527 (1)	0·0683
C(1)	0·2292 (4)	0·1180 (2)	0·4595 (2)	0·0431
C(2)	0·0283 (4)	0·2129 (2)	0·4299 (2)	0·0437
C(3)	−0·0779 (5)	0·2690 (2)	0·5010 (2)	0·0533
C(4)	−0·0356 (5)	0·2420 (3)	0·3213 (2)	0·0542
C(5)	−0·1247 (6)	0·1232 (3)	0·2610 (2)	0·0715
C(6)	0·1732 (7)	0·3114 (4)	0·2785 (3)	0·0892
C(7)	−0·2748 (5)	0·3709 (3)	0·4907 (2)	0·0753

Table 2. *Bond distances* (Å) *and angles* (°) *in 2-isopropylcrotonic acid, with e.s.d.'s in parentheses*

C(1)—O(1)	1·229 (3)	C(3)—C(7)	1·496 (4)
C(1)—O(2)	1·298 (3)	C(2)—C(4)	1·517 (3)
C(1)—C(2)	1·488 (3)	C(4)—C(5)	1·515 (4)
C(2)—C(3)	1·328 (3)	C(4)—C(6)	1·528 (4)
O(1)—C(1)—O(2)	121·7 (2)	C(3)—C(2)—C(4)	124·6 (2)
O(1)—C(1)—C(2)	122·2 (2)	C(2)—C(3)—C(7)	127·6 (2)
O(2)—C(1)—C(2)	116·1 (2)	C(2)—C(4)—C(5)	113·5 (2)
C(1)—C(2)—C(4)	118·0 (2)	C(2)—C(4)—C(6)	112·0 (2)
C(1)—C(2)—C(3)	117·4 (2)	C(5)—C(4)—C(6)	111·7 (2)

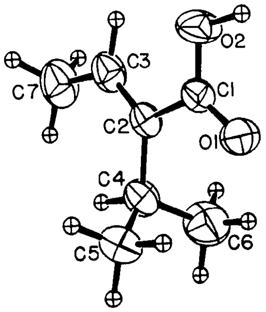

Fig. 1. *ORTEP* plot (Johnson, 1976) and numbering scheme for 2-isopropylcrotonic acid. Thermal ellipsoids are shown at the 50% probability level.

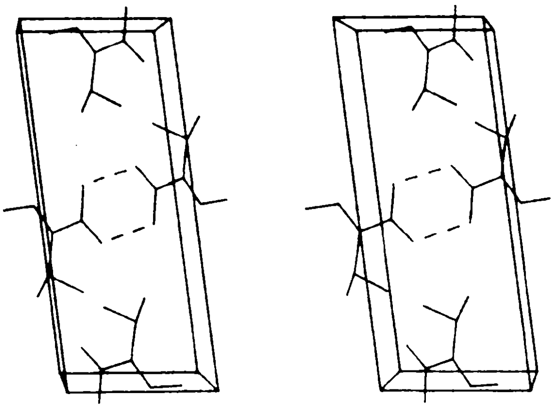

Fig. 2. Packing diagram for 2-isopropylcrotonic acid. Dotted lines indicate hydrogen bonds. The x axis is horizontal, z is vertical.

A view of the molecule and the numbering scheme are shown in Fig. 1. The packing diagram is presented in Fig. 2.*

Bond distances and angles are normal. The alkene part of the molecule is planar but the carboxylate group lies somewhat out of this plane, the deviations of C(1), O(1), and O(2) being 0·060 (2), 0·147 (2), and 0·019 (2) Å, respectively. The dihedral angle between the alkene plane and the (010) planes of the unit cell is 43·9°. Thus, the molecules are aligned at an angle to the c-glide planes. An essential prerequisite for asymmetric syntheses on the (010) planes of space group $P2_1/c$ is that the alkene planes should not be perpendicular to the glide plane; the chances for a successful asymmetric synthesis should increase as the alkene planes become more nearly parallel to the glide planes in $P2_1/c$ (Holland & Richardson, 1980).

The packing unit in 2-isopropylcrotonic acid is a pair of molecules, hydrogen-bonded to each other to form centrosymmetric dimers, which are common structural motifs in carboxylic acid structures. The O(2)—H(O2), H(O2)···O(1)′ and O(2)···O(1)′ distances are 0·87 (3), 1·81 (3) and 2·663 (3) Å, respectively, and the O(2)—H(O2)···O(1)′ angle is 168 (2)°. These values are within the range found by Ceccarelli, Jeffrey & Taylor (1981) for 100 O—H···O bonds whose geometries are known from neutron diffraction studies.

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* Lists of structure factors, anisotropic thermal parameters, H-atom positions and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39715 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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