1,1-cyclopropanedicarboxylic acid, one of the carbonyl O atoms and the hydroxy group of the other acid substituent form an intramolecular hydrogen bond. The second proton and carbonyl O atom are involved in intermolecular hydrogen bonding. The bond lengths and angles of the two acid groups are somewhat different from those of the title molecule, but the geometry of the one forming the intermolecular hydrogen bond is closer to that of the cyano acid, although their conformations are different. Thus, it appears that it is the type of hydrogen bonding which determines the similarity of geometries of the acid groups and not their conformation.

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Substituted Cyclopropanes. 6.* *trans*-Triethyl 1,2,3-Tricyano-1,2,3-cyclopropanetricarboxylate

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Abstract. $C_{15}H_{15}N_3O_6$, $M_r = 333\cdot31$, monoclinic, $P2_1/c$, $a = 9\cdot185\ (2)$, $b = 21\cdot797\ (5)$, $c = 8\cdot306\ (2)$ Å, $\beta = 91\cdot30\ (2)^\circ$, $V = 1663\ (1)$ Å^3, $Z = 4$, $D_x = 1\cdot33$ g cm^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0\cdot71069$ Å, $\mu = 1\cdot0$ cm^{-1}, $F(000) = 696$, $T = 293$ K, $R = 0\cdot071$ for 1535 unique observed reflections. The ring bond lengths show a marked asymmetry. The molecular symmetry is lower than ideal because of conformational differences in the ester groups. The C—C bonds from the ring to the ester groups are long.

Introduction. Polysubstituted cyclopropanes, particularly those with three mutually *cis* vicinal substituents, are excellent models for studying steric crowding. The rigid three-membered ring often forces upon substituents non-bonded contacts well below the sum of the respective van der Waals radii. In previous

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* Part 5: Jones & Schrumpf (1987*b*).

Table 1. *Atom coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2 × 10^3)

	x	y	z	U_{eq}*
C(1)	3813 (4)	5905 (2)	4259 (4)	38 (1)
C(2)	2265 (4)	6130 (2)	3936 (5)	40 (1)
C(3)	2713 (4)	5462 (2)	3536 (4)	39 (1)
C(11)	4956 (4)	6157 (2)	3260 (4)	44 (1)
C(12)	4378 (4)	5838 (2)	6004 (4)	41 (1)
C(13)	5075 (5)	6449 (2)	8249 (5)	66 (2)
C(14)	4732 (6)	7073 (2)	8804 (6)	85 (2)
C(21)	2015 (4)	6558 (2)	2620 (5)	45 (1)
C(22)	1345 (4)	6232 (2)	5418 (5)	42 (1)
C(23)	−575 (5)	6811 (2)	6474 (5)	69 (2)
C(24)	−1647 (5)	7268 (2)	5860 (7)	93 (2)
C(31)	2147 (4)	4973 (2)	4536 (4)	46 (1)
C(32)	2813 (4)	5312 (2)	1741 (4)	49 (2)
C(33)	2077 (5)	4662 (2)	−357 (4)	62 (2)
C(34)	1127 (5)	4118 (2)	−592 (5)	72 (2)
N(1)	5892 (3)	6387 (1)	2625 (4)	62 (1)
N(2)	1798 (4)	6907 (2)	1629 (4)	73 (2)
N(3)	1675 (4)	4575 (2)	5235 (4)	68 (2)
O(11)	4655 (3)	5364 (1)	6640 (3)	53 (1)
O(12)	4554 (3)	6398 (1)	6571 (3)	53 (1)
O(21)	1533 (3)	5947 (1)	6633 (3)	59 (1)
O(22)	372 (3)	6665 (1)	5128 (3)	52 (1)
O(31)	3465 (3)	5628 (1)	862 (3)	77 (1)
O(32)	2074 (3)	4816 (1)	1377 (3)	51 (1)

* Equivalent isotropic U calculated from anisotropic U:

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

investigations of several *cis*-1,2,3-trisubstituted cyclopropanes, we have shown that the steric repulsion between the substituents is relieved by an increase of bond angles (Schrumpf & Jones, 1987*a,c*; Jones & Schrumpf, 1987*a*). This is no longer feasible in hexasubstituted cyclopropanes, which instead relax by increasing ring bond lengths. This effect is however not always detectable, since it is superimposed on the electronic effects of the substituents; in hexachlorocyclopropane (Schrumpf & Jones, 1987*b*), the electronic and steric effects on the bond lengths nearly cancel each other out.

Substituents such as organic carbonyl functions, which have conformational degrees of freedom about the bonds adjacent to the ring, respond to steric crowding by torsion-angle relaxation, which tends to be much more marked than bond-length and -angle changes. Allen (1980), in a thorough review of crystal structures of substituted cyclopropanes, gives only one example of a structure containing two *cis* carbonyl groups, and only one of these is conformationally mobile. In order to study the distribution of steric crowding effects over bond lengths, bond angles and torsion angles, more structural data are needed for cyclopropanes substituted by *cis* carbonyl functions.

Here we present results for *trans*-triethyl 1,2,3-tricyano-1,2,3-cyclopropanetricarboxylate.

Experimental. The title compound was synthesized according to the literature (Griffin & Peterson, 1963). Single crystals in the form of colourless prisms were grown by the liquid–liquid diffusion method using acetic acid–water.

Crystal 0·35 × 0·2 × 0·15 mm. 8832 profile-fitted intensities (Clegg, 1981) recorded on a Stoe-Siemens four-circle diffractometer. Monochromated Mo *Kα* radiation, $2\theta_{max}$ 50°. Three check reflections, no significant intensity change. R_{int} 0·034 for 2911 unique reflections, 1535 with $F > 4\sigma(F)$ used for all calculations [program system *SHELXTL* (Sheldrick, 1978)]. Index ranges after merging $-10 \le h \le 10$, $0 \le k \le 25$, $0 \le l \le 9$. Cell constants refined from 2θ values of 40 reflections in the range 20–23°.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°)

C(1)—C(2)	1·522 (6)	C(1)—C(3)	1·513 (6)
C(1)—C(11)	1·460 (6)	C(1)—C(12)	1·535 (6)
C(2)—C(3)	1·552 (6)	C(2)—C(21)	1·451 (6)
C(2)—C(22)	1·526 (6)	C(3)—C(31)	1·455 (6)
C(3)—C(32)	1·530 (6)	C(11)—N(1)	1·135 (6)
C(12)—O(11)	1·187 (5)	C(12)—O(12)	1·317 (6)
C(13)—C(14)	1·473 (7)	C(13)—O(12)	1·467 (6)
C(21)—N(2)	1·135 (6)	C(22)—O(21)	1·194 (5)
C(22)—O(22)	1·318 (5)	C(23)—C(24)	1·484 (8)
C(23)—O(22)	1·466 (6)	C(31)—N(3)	1·136 (6)
C(32)—O(31)	1·178 (6)	C(32)—O(32)	1·309 (6)
C(33)—C(34)	1·482 (7)	C(33)—O(32)	1·480 (5)

C(2)—C(1)—C(3)	61·5 (3)	C(2)—C(1)—C(11)	117·4 (4)
C(3)—C(1)—C(11)	119·8 (4)	C(2)—C(1)—C(12)	119·4 (4)
C(3)—C(1)—C(12)	121·5 (4)	C(11)—C(1)—C(12)	109·9 (4)
C(1)—C(2)—C(3)	58·9 (3)	C(1)—C(2)—C(21)	118·1 (4)
C(3)—C(2)—C(21)	118·7 (4)	C(1)—C(2)—C(22)	115·9 (4)
C(3)—C(2)—C(22)	117·6 (4)	C(21)—C(2)—C(22)	115·7 (4)
C(1)—C(3)—C(2)	59·5 (3)	C(1)—C(3)—C(31)	119·0 (4)
C(2)—C(3)—C(31)	117·7 (4)	C(1)—C(3)—C(32)	117·9 (4)
C(2)—C(3)—C(32)	115·5 (4)	C(31)—C(3)—C(32)	115·5 (4)
C(1)—C(11)—N(1)	172·7 (5)	C(1)—C(12)—O(11)	124·6 (4)
C(1)—C(12)—O(12)	106·6 (4)	O(11)—C(12)—O(12)	128·7 (4)
C(14)—C(13)—O(12)	107·4 (4)	C(2)—C(21)—N(2)	177·6 (5)
C(2)—C(22)—O(21)	122·3 (4)	C(2)—C(22)—O(22)	110·0 (4)
O(21)—C(22)—O(22)	127·7 (5)	C(24)—C(23)—O(22)	106·5 (5)
C(3)—C(31)—N(3)	175·9 (5)	C(3)—C(32)—O(31)	121·4 (4)
C(3)—C(32)—O(32)	111·0 (4)	O(31)—C(32)—O(32)	127·5 (5)
C(34)—C(33)—O(32)	107·2 (4)	C(12)—O(12)—C(13)	116·3 (4)
C(22)—O(22)—C(23)	115·3 (4)	C(32)—O(32)—C(33)	113·6 (4)

C(3)—C(1)—C(2)—C(22)	108·0 (4)	C(3)—C(1)—C(2)—C(21)	−108·3 (5)
C(11)—C(1)—C(2)—C(21)	2·6 (6)	C(11)—C(1)—C(2)—C(3)	110·9 (5)
C(12)—C(1)—C(2)—C(3)	−112·1 (5)	C(11)—C(1)—C(2)—C(22)	−141·1 (4)
C(12)—C(1)—C(2)—C(22)	−4·1 (6)	C(12)—C(1)—C(2)—C(21)	139·6 (4)
C(2)—C(1)—C(3)—C(32)	104·7 (5)	C(2)—C(1)—C(3)—C(31)	−106·9 (5)
C(11)—C(1)—C(3)—C(31)	146·2 (4)	C(11)—C(1)—C(3)—C(2)	−107·0 (5)
C(12)—C(1)—C(3)—C(2)	108·8 (5)	C(11)—C(1)—C(3)—C(32)	−2·3 (6)
C(12)—C(1)—C(3)—C(32)	−146·5 (4)	C(12)—C(1)—C(3)—C(31)	1·9 (6)
C(2)—C(1)—C(12)—O(11)	112·2 (5)	C(2)—C(1)—C(12)—O(12)	−71·1 (5)
C(3)—C(1)—C(12)—O(11)	39·4 (6)	C(3)—C(1)—C(12)—O(12)	−143·9 (4)
C(11)—C(1)—C(12)—O(11)	−107·9 (5)	C(11)—C(1)—C(12)—O(12)	68·7 (5)
C(1)—C(2)—C(3)—C(31)	109·1 (5)	C(1)—C(2)—C(3)—C(32)	−108·8 (4)
C(21)—C(2)—C(3)—C(1)	107·3 (5)	C(21)—C(2)—C(3)—C(31)	−143·6 (4)
C(21)—C(2)—C(3)—C(32)	−1·5 (6)	C(22)—C(2)—C(3)—C(1)	−105·1 (5)
C(22)—C(2)—C(3)—C(31)	4·0 (6)	C(22)—C(2)—C(3)—C(32)	146·1 (4)
C(1)—C(2)—C(22)—O(22)	151·1 (4)	C(1)—C(2)—C(22)—O(21)	−28·7 (6)
C(3)—C(2)—C(22)—O(22)	−142·0 (4)	C(3)—C(2)—C(22)—O(21)	38·1 (6)
C(21)—C(2)—C(22)—O(22)	6·6 (5)	C(21)—C(2)—C(22)—O(21)	−173·3 (4)
C(1)—C(3)—C(32)—O(31)	−18·0 (6)	C(1)—C(3)—C(32)—O(32)	163·3 (4)
C(2)—C(3)—C(32)—O(31)	49·5 (6)	C(2)—C(3)—C(32)—O(32)	−129·2 (4)
C(31)—C(3)—C(32)—O(31)	−167·5 (5)	C(31)—C(3)—C(32)—O(32)	13·8 (6)
C(1)—C(12)—O(12)—C(13)	179·2 (4)	O(11)—C(12)—O(12)—C(13)	−4·3 (7)
C(14)—C(13)—O(12)—C(12)	−161·3 (4)	C(2)—C(22)—O(22)—C(23)	−179·4 (4)
O(21)—C(22)—O(22)—C(23)	0·5 (6)	C(24)—C(23)—O(22)—C(22)	−175·8 (4)
C(3)—C(32)—O(32)—C(33)	177·5 (4)	O(31)—C(32)—O(32)—C(33)	−1·0 (7)
C(34)—C(33)—O(32)—C(32)	−176·4 (4)		

Structure solution by routine direct methods. Refinement on F to R 0·071, wR 0·049 {226 parameters, weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}00015F^2$, H atoms with riding model [C—H 0·96 Å, H—C—H 109·5°, $U(\mathrm{H}) = 1{\cdot}2U_{\mathrm{eq}}(\mathrm{C})$], $S = 1{\cdot}54$, slope of normal probability plot 1·25}. Max. Δ/σ 0·02. Max. and min. features in final $\Delta\rho$ map $\pm 0{\cdot}3$ e Å^{-3}. Atomic scattering factors as incorporated in *SHELXTL*.

Discussion. Final atomic coordinates and derived structural parameters are presented in Tables 1 and 2.* A rigid-body libration correction was not feasible because of the ethoxycarbonyl groups; all bond lengths quoted here are thus uncorrected. The molecule is shown in Fig. 1 and a packing diagram is given in Fig. 2.

There are three unexpected observations. (1) The molecule adopts a symmetry lower than ideal because of a major conformational change. (2) The ring bond lengths show a marked asymmetry. (3) The CC bonds connecting the ring and the ester groups are much longer than usual. In the following, we will discuss these points and their interdependence.

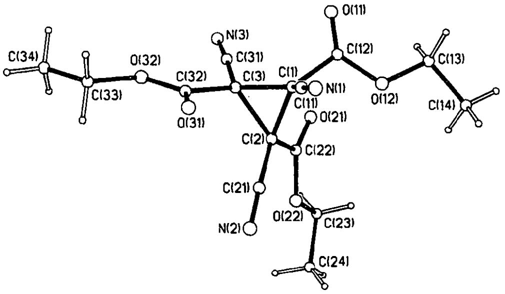

Fig. 1. The molecule of the title compound, showing the atom-numbering scheme; radii arbitrary.

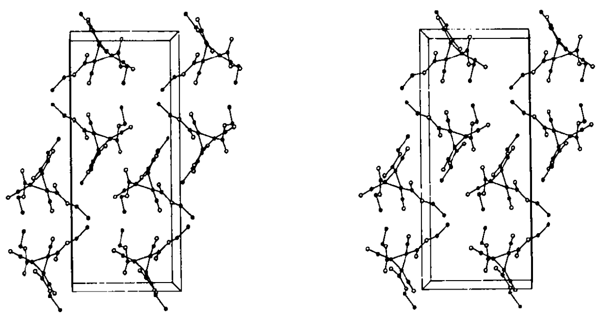

Fig. 2. Stereographic packing plot viewed along the c axis. Open circles, O; black dots, C. H atoms omitted.

The *cis* ester groups are chemically equivalent. In the solid state, however, the molecule is unsymmetric mainly in that the conformation of all three ester groups is different. The unique ester group at C(3), which opposes two cyano groups on the same side of the ring, is rotated by 17° from the *cis* bisected (*cb*) form as defined by the torsion angle [midpoint C(1) and C(2)]—C(3)—C(32)—C(31) (Allen, 1980). Of the two ester groups, the one at C(2) deviates from the *cb* conformation by 5°, but the group at C(1) adopts a nearly perpendicular (*p*, torsion angle 76°) conformation. It appears as if the carbonyl O(21) atom of the C(2) ester group 'pushes' the carbonyl O atom at C(1) away from the ring centre. The ethoxycarbonyl groups are planar except for the perpendicular ester group, where the terminal methyl C(14) is rotated from the antiperiplanar position by 19°.

The lengths of the CN triple bonds and the CC bonds joining the cyano groups to the ring are normal. This also holds for bond lengths involving oxygen. However, the CC bonds joining the ester groups to the cyclopropane ring (1·530 Å, av.) are unusual in that they are lengthened by about 0·05 Å compared with 1·46–1·49 Å in other cyclopropanecarboxylic acids and their derivatives. This seems to be independent of the degree of substitution at the ring C atom. We recognize a slight trend in the three values observed here with a shorter bond at C(2) (*cb* conformation) than at C(1) (*p* conformation). This parallels the expected extent of conjugation of the ester groups with the cyclopropane ring. Although the difference involved is barely significant, we have independent support of the conjugative consequences of the conformational differences.

The ring bond distances are markedly different, with an extremely long C(2)—C(3) bond (1·552 Å). The C(1)—C(2) and C(1)—C(3) bond lengths are similar (1·522 and 1·513 Å) and resemble the analogous bond lengths in 1,1,2,2-cyclopropanetetracarbonitrile (1·516 and 1·512 Å; Lemley, Skarstad & Hughes, 1976). The ring asymmetry pattern with a long bond between C(2) and C(3), which bear two groups each in conjugation with the ring [while C(1) has only one], is in accord with the additivity scheme outlined by Allen (1980). Similar long bonds in highly but unsymmetrically substituted cyclopropane rings have been observed in 1,1,2,2-cyclopropanetetracarbonitrile (1·559 Å, Lemley *et al.*, 1976) and in two substituted 1,2,2-tricyanocyclopropanecarboxylic esters (1·542 Å; Ramasubbu, Rajaram & Venkatesan, 1982; 1·557 Å; Ramasubbu & Venkatesan, 1982). The average ring bond length in many cyclopropane derivatives is less than 1·520 Å and for most carbonyl-substituted structures as low as 1·505 Å or less (Allen, 1980). In several cyano-substituted cyclopropanes, an average ring bond length of 1·515 Å has been given by Allen. Since these values are close to that in cyclopropane (1·510 Å;

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43896 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Bastiansen, Fritsch & Hedberg, 1964), Allen states that substituent influence on net ring bonding is absent in carbonyl- and cyano-substituted cyclopropanes. However, there appears to be a tendency to increase the ring bond length at high degrees of substitution, as seen in the present study, where we find 1·529 Å. The two 1,2,2-tricyanocyclopropanecarboxylic esters mentioned above display average ring bond lengths of 1·529 and 1·531 Å, and 1,1,2,2-cyclopropanetetracarbonitrile 1·529 Å. The most plausible interpretation for such an increase is bond-length relaxation of steric strain between the substituents. This has been observed in hexachloro- and in hexabromocyclopropane (1·529 and 1·544 Å; Schrumpf & Jones, 1987*b,c*).

The various steric interactions in the title molecule can be demonstrated by the angle deformations. The bond angle between the substituents in the 1-cyano-acid (117·2°; Jones & Schrumpf, 1987*b*) is a little smaller than in the 1,1-diacid (118·3°; Meester, Schenk & MacGillavry, 1971); we consider these as 'normal' bond angles between geminal CN and carboxyl groups without steric interference. The bond angle between the geminal substituents in the tricyanotriester studied here at C(2) is 115·7° and at C(3) 115·5°, *i.e.* somewhat smaller than in the cyano-acid. The bond angle at C(1), however, is drastically reduced (109·9°), obviously on account of substantial steric strain. The origin of the repulsion can be traced by analysing the angles between the individual exocyclic CC bonds and the adjacent ring CC bonds. In the cyano-acid model, these angles are practically the same for the cyano (117·2°) and the ester C atoms (117·5°). In the title molecule, the angles to the cyano C atoms have a narrower range (117·4–119·8°) than those to the ester C atoms (115·5–121·5°). Within each group, however, the angles between the two substituents at C(1) and the C(1)—C(3) bond are substantially larger than the average of each group with the ester C atom responding by an increase of 4°, the cyano carbon by 2° to the steric pressure of the substituents at C(3).

Since there are so few X-ray studies of highly cyano- and carboxyl-substituted cyclopropanes, several such compounds are currently being studied in our laboratories.

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Structure of 1,2,3,4-Tetraphenylbenzene

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Abstract. $C_{30}H_{22}$, $M_r = 382\cdot51$, orthorhombic, *Pbcn*, $a = 23\cdot577$ (4), $b = 9\cdot013$ (2), $c = 9\cdot950$ (2) Å, $V = 2114\cdot4$ (1·3) Å^3, $Z = 4$, $D_x = 1\cdot20$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0\cdot632$ cm^{-1}, $F(000) = 808$, $T = 213$ (1) K, $R = 0\cdot043$ for 1726 unique observed reflections [$I > 3\sigma(I)$]. The title compound adopts a propeller configuration. The peripheral rings are not perpendicular to the central ring but twisted about 40·2 and 22·2° from this position. The observed interplanar angles indicate absence of electronic interactions between the phenyl rings. The bond distances in the benzene rings range from 1·373 (3) to 1·415 (2) Å.

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