show that the effect of the biphenyl group is approximately the same as that of a phenyl in bisected position *i.e.* δb −0·020 Å. The predicted bond lengths for C1–C2, C1–C3 and C2–C3 in the title compound would thus be respectively 1·532, 1·506 and 1·502 Å. They agree quite well with the observed values of 1·545, 1·497 and 1·498 Å. This demonstrates the validity of the additivity principle for π-acceptor substituents and confirms the simple model for charge transfer from cyclopropane to the π system (Hoffmann & Stohrer, 1971).

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Intermolecular Interactions in the Structure of Methyl 4-Iodobenzoate

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Abstract. $C_8H_7IO_2$, $M_r = 262{\cdot}05$, orthorhombic, *Pbca*, $a = 14{\cdot}378\ (2)$, $b = 5{\cdot}944\ (1)$, $c = 20{\cdot}361\ (6)$ Å, $V = 1740{\cdot}2\ (6)$ Å^3, $Z = 8$, $D_x = 2{\cdot}000$ g cm^{-3}, Mo $K\alpha$ (graphite monochromator), $\lambda = 0{\cdot}71073$ Å, $\mu = 35{\cdot}9$ cm^{-1}, $F(000) = 992$, $T = 295\ (1)$ K, $R = 0{\cdot}037$ for 1338 unique reflections with $(\sin\theta)/\lambda \leq 0{\cdot}65$ Å^{-1}. Bond lengths and angles are normal. The structure contains chains of molecules linked by short –I···O=C– [3·203 (4) Å] interactions.

Introduction. A structure determination undertaken to confirm the stereochemistry of a supposed intermediate in a long synthetic scheme revealed instead that decomposition had taken place to yield methyl 4-iodobenzoate. We were surprised to discover that the structure of this simple material had never been reported even though several groups have been interested in short intermolecular I···I and I···O interactions.

Experimental. A large, colorless prism grown from an ethanol solution was cut to give a chunk with approximate dimensions 0·42 × 0·38 × 0·48 mm. Data collected on an Enraf–Nonius CAD-4F diffractometer in the ω–2θ mode; 22 reflections with $10{\cdot}7 \leq \theta \leq 19{\cdot}2°$ used to determine lattice parameters; $2 \leq \theta \leq 27{\cdot}5°$; octant of data with $0 \leq h \leq 18$, $0 \leq k \leq 7$, $0 \leq l \leq 26$; average intensity loss for three control reflections of 21·5% overall (corrected) appeared to result from sublimation; no absorption correction ($\mu = 35{\cdot}9$ cm^{-1}) since size and shape of crystal changed substantially during data collection; 1989 unique reflections measured; 1338 data with $I > 3\sigma(I)$ used for refinement; coordinates of I atom determined from solution of Patterson function, remaining non-H atoms located using *DIRDIF* (Beurskens, *et al.*, 1984); H atoms located in difference Fourier maps, idealized at a late point in the refinement [r(C–H) = 1·00 Å, B 1·0 Å^2 larger than B_{eq} of attached C atom]; extinction correction [final value 2·29 (23) × 10^{-7}] (Zachariasen, 1967) included; 101 variables; refinement on F magnitudes; R, $wR = 0{\cdot}037$, 0·049; error in an observation of unit weight = 2·25 e$^-$; $w = 4I/[\sigma^2(I)]$ where $[\sigma^2(I)]$ includes a term $(0{\cdot}03I)^2$; maximum Δ/σ in last cycle of 0·01; largest features in final difference Fourier synthesis have heights +1·0 and −1·5 e Å^{-3} (top nine

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peaks and five deepest troughs are within 1·2 Å of the I atom); computer programs as described previously (Brock & Webster, 1976); scattering factors, including anomalous terms for the I atom, from Cromer & Waber (1974).

The molecular structure and the atom-numbering scheme are shown in Fig. 1; the crystal packing is displayed in Fig. 2. Atomic coordinates are listed in Table 1, and bond lengths and angles are given in Table 2.*

Discussion. The structure of 4-iodobenzoic acid (Baughman & Nelson, 1984) contains hydrogen-bonded carboxylic-acid dimers linked by short I···I interactions (4·00 and 4·16 Å). Replacement of the acidic H atom by a methyl group precludes the formation of hydrogen-bonded dimers and so changes the crystal packing. In the title compound the short interactions are between the I and the carbonyl O atoms [3·203 (4) Å]; the shortest I···I contact is 4·863 (1) Å. Chains of molecules are formed in both the acid and the ester, but the arrangement in the latter is 'head to tail' (see Fig. 2) while in the former it is 'head to head'.

Table 1. *Positional and displacement parameters for the atoms of methyl 4-iodobenzoate*

The equivalent displacement parameter is defined as $\frac{4}{3}\mathrm{Tr}(\beta.\mathbf{G})$, where $\beta_{ij} = 2\pi^2 a_i^* a_j^* U_{ij}$.

	x	y	z	B_{eq}(Å^2)
I	0·11613 (3)	0·20340 (9)	0·11177 (2)	3·97 (1)
O(1)	0·1074 (3)	0·3788 (9)	0·4564 (2)	4·6 (1)
O(2)	0·1502 (3)	0·7171 (7)	0·4191 (2)	4·0 (1)
C(1)	0·1271 (3)	0·4328 (9)	0·3407 (3)	2·6 (1)
C(2)	0·0907 (4)	0·2245 (9)	0·3243 (3)	3·1 (1)
C(3)	0·0872 (4)	0·1574 (9)	0·2587 (3)	3·1 (1)
C(4)	0·1212 (3)	0·3023 (10)	0·2107 (3)	2·7 (1)
C(5)	0·1570 (4)	0·5101 (9)	0·2268 (3)	3·0 (1)
C(6)	0·1601 (4)	0·5761 (9)	0·2918 (3)	3·0 (1)
C(7)	0·1275 (4)	0·5010 (11)	0·4114 (3)	3·1 (1)
C(8)	0·1444 (5)	0·8043 (13)	0·4844 (3)	5·0 (2)

Table 2. *Bond lengths* (Å) *and angles* (°) *for methyl 4-iodobenzoate*

I–C(4)	2·099 (6)	C(2)–C(3)	1·396 (8)
O(1)–C(7)	1·205 (7)	C(3)–C(4)	1·392 (8)
O(2)–C(7)	1·335 (7)	C(4)–C(5)	1·378 (8)
O(2)–C(8)	1·430 (8)	C(5)–C(6)	1·382 (7)
C(1)–C(2)	1·385 (8)	C(6)–C(1)	1·393 (7)
C(1)–C(7)	1·496 (8)		

C(7)–O(2)–C(8)	116·3 (5)	C(3)–C(4)–I	119·2 (4)
C(7)–C(1)–C(2)	118·3 (5)	C(5)–C(4)–I	119·5 (4)
C(7)–C(1)–C(6)	121·4 (5)	C(4)–C(5)–C(6)	119·6 (5)
C(2)–C(1)–C(6)	120·2 (5)	C(5)–C(6)–C(1)	120·0 (5)
C(1)–C(2)–C(3)	120·0 (5)	C(1)–C(7)–O(1)	124·6 (6)
C(2)–C(3)–C(4)	118·9 (5)	C(1)–C(7)–O(2)	112·0 (5)
C(3)–C(4)–C(5)	121·3 (5)	O(1)–C(7)–O(2)	123·4 (6)

Short I···I, I···O and I···N interactions are quite common, especially if the I-containing molecule is relatively simple and the O or N atom participates in a double or triple bond (Schlemper & Britton, 1965; Ahn, Soled & Carpenter, 1972; McPhail & Onan, 1975). A search of the May 1986 version of the Cambridge Structural Database (Allen *et al.*, 1979) for the 4-iodobenzoate fragment produced references to 23 compounds, most of which are esters of natural products. A search for the *para* I–Ph–C fragment gave 14 additional hits. Of the 31 different entries in the CSD containing the *para* I–Ph–C fragment and having archived coordinates, five have short I···I contacts, while nine others have short I···O or I···N distances. Intermolecular distances in the remaining 17 structures, most of which contain large and irregularly shaped molecules, are normal. For the purposes of this tabulation 'short' contact distances are defined as those at least 0·15 Å shorter than the sum of the van der Waals radii (4·30, 3·55 and 3·65 Å, respectively, for I···I, I···O and I···N contacts; Pauling, 1960). No allowance has been made for any 'polar flattening' of the I atom (Nyburg & Faerman, 1985).

Although short contacts involving I atoms are rather common, individual I atoms usually take part in only

* The refined atomic displacement parameters and the observed and calculated structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44004 (13 pp.). Some information obtained from the May 1986 version of the Cambridge Structural Database is also included. Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

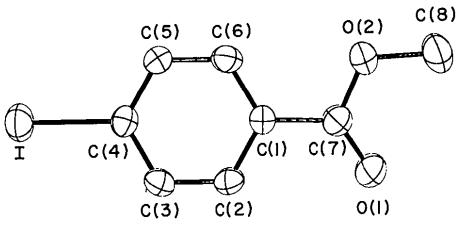

Fig. 1. Perspective drawing of the molecular structure of methyl 4-iodobenzoate. In this and the following drawing the shapes of the ellipsoids correspond to 50% probability contours of atomic displacement, and the H atoms have been omitted for the sake of clarity.

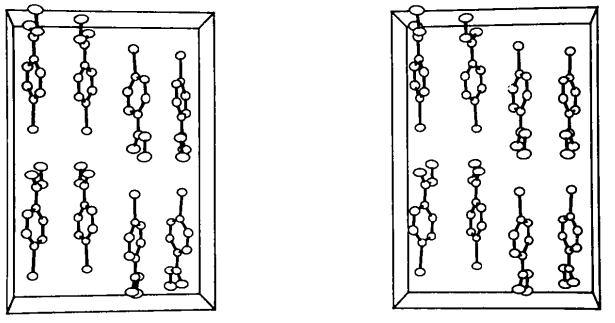

Fig. 2. Stereoscopic view of the unit cell of methyl 4-iodobenzoate. The *a* axis points from left to right, the *c* axis points upwards, and the *b* axis points into the plane of the paper.

one type of interaction. The same monovalent I atom rarely participates in both short I···I and short I···O or I···N contacts. In the CSD there are 1559 compounds containing both an I atom and either an O or an N atom. In many of these structures there are short intermolecular distances involving I atoms, but only 16 structures contain monovalent I atoms 'close' to *both* an I and an O or N atom. In all but two of these 16 structures the O or N atom is multiply bonded to a C atom.

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Structure of 4-Aminolactivinic Acid

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Abstract. 2-(4-Ammonio-3-oxo-1,2-oxazolidin-2-yl)-5-oxotetrahydrofuran-2-carboxylate, $C_8H_{10}N_2O_6$, M_r = 230·2, orthorhombic, $P2_12_12_1$, a = 7·833 (3), b = 21·577 (5), c = 5·565 (2) Å, V = 940·6 (5) Å^3, Z = 4, D_x = 1·63 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 1·5 cm^{-1}, $F(000)$ = 480, room temperature. Final R = 0·065 for 530 observed reflections. The title compound is a derivative of the new antibiotic lactivicin. The molecule consists of two five-membered rings (3-isoxazolidone and γ-lactone) directly connected by a C—N bond. The isoxazolidone ring exhibits a half-chair conformation and the γ-lactone ring is in an envelope form.

Introduction. Lactivicin (LTV) is a novel antibiotic isolated from culture filtrates of *Empedobacter lactamgenus* sp. nov. YK-258 and *Lysobacter albus* sp. nov. YK-422 (Nozaki, Katayama, Ono, Tsubotani, Harada, Okazaki & Nakao, 1987). An X-ray analysis as part of the structural study of this compound (Harada, Tsubotani, Hida, Ono & Okazaki, 1986) was undertaken for the determination in particular of the relative stereochemistry and the absolute configuration. Among various derivatives and salts of LTV examined in an attempt to obtain suitable crystals, 4-aminolactivinic acid gave tolerable crystals for X-ray analysis.

Table 1. *Positional parameters* (×10^4) *and* U_{eq}(Å^2×10^3) *for non-hydrogen atoms with e.s.d.'s in parentheses*

$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$

	x	y	z	U_{eq}
O(1)	8080 (11)	1383 (4)	1482 (18)	42 (5)
N(2)	6920 (13)	1037 (5)	3064 (18)	31 (6)
C(3)	7842 (16)	714 (5)	4682 (25)	30 (8)
O(3)	7278 (10)	435 (4)	6390 (16)	35 (5)
C(4)	9701 (15)	735 (5)	3932 (21)	21 (6)
C(5)	9567 (18)	988 (5)	1332 (24)	37 (7)
C(6)	5378 (16)	1350 (5)	3635 (22)	27 (6)
O(7)	5753 (12)	1841 (3)	5405 (14)	33 (5)
C(8)	5616 (19)	2395 (6)	4585 (25)	40 (9)
O(8)	5908 (15)	2853 (5)	5817 (20)	71 (8)
C(9)	5102 (20)	2406 (7)	1919 (24)	46 (9)
C(10)	4574 (18)	1729 (6)	1474 (25)	42 (8)
C(11)	4084 (17)	897 (6)	4605 (23)	35 (8)
O(11*A*)	3829 (11)	433 (4)	3365 (17)	39 (5)
O(11*B*)	3302 (11)	1026 (4)	6519 (16)	43 (5)
N(12)	10473 (13)	114 (5)	4006 (17)	31 (6)

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