The crystal structure comprises molecules of SBG 107 and water linked by a complex system of intermolecular hydrogen bonds (see Table 3). There is one strong hydrogen bond [O(912)—H(912)···O(132)'] between the two carboxyl groups where the O—H [1·24 (7) Å] and H···O [1·31 (7) Å] distances are almost equal with respect to the standard deviations.

The above-mentioned hydrogen bond causes a connection along the **b** direction, all further bonds of that type contribute to a network in the *ac* plane (see Fig. 4). N(12) has intramolecular N···O contacts to O(101) and O(131) of 2·723 (5) and 2·618 (5) Å. The corresponding H···O contacts of the protons H(122) and H(121) are 2·50 (4) and 2·23 (5) Å. The H(122)···O(101) contact is rather large; however, at least the N(12)—H(121)···O(131) contact can be coded as an intramolecular hydrogen bond.

The high inhibitory potency of SBG 107 suggests that an additional hydrophobic pocket can be integrated in the postulated model of the ACE at the position of the thiophene ring found in this X-ray analysis.

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1,2,3,4-Tetrachlorodibenzo-*p*-dioxin*

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Abstract. $C_{12}H_4Cl_4O_2$, $M_r = 321{\cdot}98$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 4{\cdot}820$ (1), $b = 14{\cdot}666$ (2), $c = 16{\cdot}917$ (2) Å, $V = 1196{\cdot}0$ Å^3, $Z = 4$, $D_x = 1{\cdot}79$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}98$ mm^{-1}, $F(000) = 640$, $T = 296$ K, final $R = 0{\cdot}037$ for 543 unique observed reflections. The large size of the molecule does not allow it to fit into the dioxin receptor and therefore it does not have similar toxic effects to 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). Molecular dimensions are: maximum length 9·405 (3) Å [Cl(3)—H(10)], maximum height 6·182 (3) Å [Cl(1)—Cl(4)]. A small deviation from planarity occurs; the maximum distance from the least-squares plane is 0·081 (4) Å [Cl(2)].

Introduction. It has been suggested that the extreme toxicity of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) is related to its molecular structure. The dioxin receptor theory as proposed by Poland & Knutson (1982) and Gillner, Fernström, Gustafsson, Cambilleau & Bergman (1985) proposes that the dimensions of the TCDD molecule allow it to fit exactly into a particular liver cell receptor (now called the dioxin receptor) and cause cytochrome-488 induction. This induction is the manifestation of the extreme toxicity of TCDD. The purpose of our study was to solve the molecular

* 1,2,3,4-Tetrachlorodibenzo[*b*,*e*][1,4]dioxin.

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structure of 1,2,3,4-tetrachlorodibenzo-*p*-dioxin (an isomeric form of TCDD) and compare its dimensions to the dimensions of other chlorinated dibenzo-*p*-dioxins of known structure, especially TCDD (Boer, van Remoortere, North & Neuman, 1972; Boer & North, 1972; Neuman, North & Boer, 1972; Boer, Neuman & Aniline, 1972), with the knowledge that 1,2,3,4-tetrachlorodibenzo-*p*-dioxin is essentially non-toxic.

Table 1. *Fractional coordinates and equivalent isotropic thermal parameters for* 1,2,3,4-*tetrachlorodibenzo-p-dioxin, with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

	x	*y*	*z*	B_{eq}(Å^2)
Cl(1)	0·2919 (8)	0·5637 (2)	0·4000 (2)	4·62 (7)
Cl(2)	−0·0908 (8)	0·3934 (2)	0·4170 (2)	4·81 (7)
Cl(3)	−0·1075 (7)	0·2886 (2)	0·5770 (2)	4·30 (7)
Cl(4)	0·2915 (8)	0·3469 (2)	0·7134 (2)	4·38 (7)
O(1)	0·6407 (16)	0·4987 (5)	0·6769 (4)	3·7 (2)
O(2)	0·6337 (18)	0·6001 (5)	0·5337 (4)	3·7 (2)
C(1)	0·2896 (26)	0·5018 (8)	0·4856 (6)	3·0 (2)
C(2)	0·1187 (25)	0·4268 (8)	0·4952 (6)	2·9 (2)
C(3)	0·1106 (26)	0·3787 (7)	0·5647 (7)	3·3 (3)
C(4)	0·2929 (23)	0·4029 (7)	0·6256 (6)	2·8 (2)
C(5)	0·4630 (23)	0·4784 (8)	0·6153 (6)	2·8 (2)
C(6)	0·4631 (23)	0·5266 (7)	0·5465 (7)	2·7 (3)
C(7)	0·8075 (25)	0·6212 (7)	0·5967 (7)	3·1 (2)
C(8)	0·9745 (23)	0·6965 (8)	0·5879 (7)	3·5 (3)
C(9)	1·1528 (26)	0·7196 (8)	0·6484 (8)	4·7 (3)
C(10)	1·1614 (28)	0·6702 (9)	0·7169 (7)	4·9 (3)
C(11)	0·9859 (8)	0·5967 (2)	0·7259 (2)	4·0 (3)
C(12)	0·8076 (24)	0·5731 (8)	0·6651 (6)	2·9 (2)

Table 2. *Bond distances* (Å) *and angles* (°) *in* 1,2,3,4-*tetrachlorodibenzo-p-dioxin, with e.s.d.'s in parentheses*

Cl(1)–C(1)	1·710 (11)	C(8)–C(9)	1·379 (18)
Cl(2)–C(2)	1·736 (11)	C(9)–C(10)	1·367 (19)
Cl(3)–C(3)	1·701 (12)	C(10)–C(11)	1·379 (14)
Cl(4)–C(4)	1·697 (11)	C(11)–C(12)	1·385 (11)
O(1)–C(5)	1·381 (13)	C(5)–C(6)	1·362 (15)
O(1)–C(12)	1·370 (14)	C(7)–C(12)	1·355 (15)
O(2)–C(6)	1·373 (13)	C(3)–C(4)	1·400 (16)
C(1)–C(2)	1·384 (17)	C(4)–C(5)	1·389 (16)
C(1)–C(6)	1·376 (16)	C(7)–C(8)	1·375 (16)
C(2)–C(3)	1·371 (15)	O(2)–C(7)	1·391 (14)
C(5)–O(1)–C(12)	115·2 (8)	C(3)–C(4)–C(5)	119 (1)
C(6)–O(2)–C(7)	114·5 (8)	O(1)–C(5)–C(4)	116·3 (9)
Cl(1)–C(1)–C(2)	121·7 (8)	O(1)–C(5)–C(6)	122 (1)
Cl(1)–C(1)–C(6)	119·3 (9)	C(4)–C(5)–C(6)	121 (1)
C(2)–C(1)–C(6)	119 (1)	O(2)–C(6)–C(1)	117 (1)
Cl(2)–C(2)–C(1)	118·8 (8)	O(2)–C(6)–C(5)	123 (1)
Cl(2)–C(2)–C(3)	119·4 (9)	C(1)–C(6)–C(5)	120 (1)
C(1)–C(2)–C(3)	122 (1)	O(2)–C(7)–C(8)	117 (1)
Cl(3)–C(3)–C(2)	121·5 (9)	O(2)–C(7)–C(12)	123 (1)
Cl(3)–C(3)–C(4)	119·7 (8)	C(8)–C(7)–C(12)	121 (1)
C(2)–C(3)–C(4)	119 (1)	C(7)–C(8)–C(9)	119 (1)
Cl(4)–C(4)–C(3)	121·2 (8)	C(7)–C(12)–C(11)	120 (1)
Cl(4)–C(4)–C(5)	119·9 (8)	C(8)–C(9)–C(10)	121 (1)
C(9)–C(10)–C(11)	119 (1)	C(10)–C(11)–C(12)	119·6 (7)
O(1)–C(12)–C(7)	123 (1)	O(1)–C(12)–C(11)	117·1 (8)

Experimental. Colourless needles from a commercial source (Analabs, RCS-057), 0·6 × 0·1 × 0·05 mm, mounted on a glass fibre, Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo$K\alpha$, ω–2θ method, lattice parameters from 25 reflections with $5 < \theta < 12°$, two standard reflections measured every hour, no loss of intensity, 1281 reflections (h 0→8, k0→9, l0→12) with $\theta < 25°$, 1281 independent, 547 with $I > 3\sigma(I)$, four reflections with high F_c/F_o ratios (possibly due to extinction) removed, Lp correction, empirical absorption correction (Walker & Stuart, 1983), correction factors max. 1·152 and min. 0·781. Structure solved by direct methods, refinement by full-matrix least-squares method using unit weights and F's, all non-H atoms anisotropic, all H atoms calculated and used as riding atoms in final refinement (C—H distance fixed 0·95 Å), 179 parameters, max. shift/σ = 0·30 in final cycle, R = 0·037, wR = 0·041, S = 1·62, final difference map with no features greater than 0·236 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974), computer programs *MULTAN*11/82 (Main *et al.*, 1982), *SDP* (Frenz, 1978) and *ORTEP*II (Johnson, 1976).

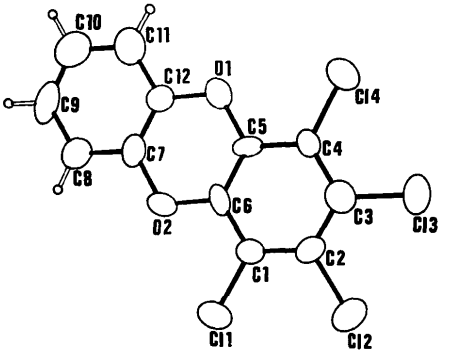

Fig. 1. *ORTEP*II plot (Johnson, 1976) and numbering scheme for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin. Thermal ellipsoids are shown at the 50% probability level.

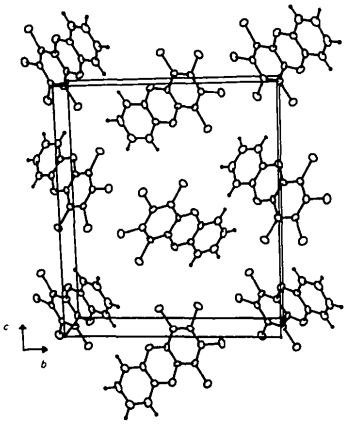

Fig. 2. Packing scheme for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin.

Discussion. The atomic coordinates are listed in Table 1, and bond distances and angles are given in Table 2.* A view of the molecule and the numbering scheme are shown in Fig. 1. The packing scheme is presented in Fig. 2.

Bond distances and angles are normal. Refinement of H atoms with isotropic thermal parameters and free coordinates was not successful. The H atoms had to be used as riding atoms with the C—H distance fixed until acceptable results were obtained. Earlier structural studies of chlorinated dibenzo-*p*-dioxins, *viz.* 2,3,7,8-tetrachloro- (TCDD) (Boer, van Remoortere, North & Neuman, 1972), 2,7-dichloro- (Boer & North, 1972), octachloro- (Neuman, North & Boer, 1972) and 2,8-dichlorodibenzo-*p*-dioxin (Boer, Neuman & Aniline, 1972), confirmed the assumed planarity of these molecules. The compound under study is less planar than the chlorinated dibenzo-*p*-dioxins just mentioned, but the deviations are so small that the molecule can be regarded as planar {largest deviation 0·081 (4) Å [Cl(2)] from least-squares plane}.

On the basis of the molecular dimensions of TCDD, Poland (Poland & Knutson, 1982) proposed that the TCDD molecule fits exactly into a particular receptor, disturbing its normal functioning and causing the toxic effects observed. The dimensions of this rectangular receptor would be 10 × 3 Å. Recently Gillner *et al.* (1985) improved Poland's theory by using instead molecular dimensions and van der Waals radii to evaluate the size of the dioxin receptor; namely, the receptor size proposed by Poland cannot explain the similar toxic effects observed for polycyclic aromatic hydrocarbons (PAH). The receptor size as expanded by the van der Waals radii is 13·7 × 6·8 Å. The van der Waals expanded dimensions of the title compound are length 10·905 Å and height 7·928 Å. The height of 1,2,3,4-tetrachlorodibenzo-*p*-dioxin is thus too great for the molecule to fit exactly into the dioxin receptor. The compound does not, therefore, have similar toxic effects to TCDD and other molecules that fit into the dioxin receptor.

* Lists of structure factors, anisotropic thermal parameters, least-squares planes and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43434 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (3*R*,6*S*)-3-Neopentyl-1,4-diazabicyclo[4.3.0]nonane-2,5-dione

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Abstract. $C_{12}H_{20}N_2O_2$, $M_r = 224{\cdot}30$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}006\ (2)$, $b = 19{\cdot}696\ (6)$, $c = 6{\cdot}365\ (1)$ Å, $V = 1254{\cdot}4\ (5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}19\ (1)$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 6{\cdot}19$ cm^{-1}, $F(000) = 488$, $T = 295$ K, final $R = 0{\cdot}067$ for 1178 unique observed reflections. The 2,5-piperazinedione

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