

different ribbons, $O(1)\cdots H(3)A$ (at $-x, -y, 2-z$), $2\cdot27$ (2) Å. The geometry of the hydrogen bonds is as follows: $N(3)\cdots O(2)$, $2\cdot831$ (2), $H(N3)\cdots O(2)$, $2\cdot04$ (2) Å, $N(3)-H(N3)\cdots O(2)$, 164 (2)°; $N(4)\cdots O(3)$, $2\cdot923$ (2), $H(N4)\cdots O(3)$, $2\cdot09$ (2) Å, $N(4)-H(N4)\cdots O(3)$, 161 (2)°.

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Structures of 1,4-Bis(trichloromethyl)benzene (I) and 6-Nitro-2,4-bis(trichloromethyl)benzo-1,3-dioxin (II)

BY KENSAKU HAMADA

Division of Science of Materials, The Graduate School of Science and Technology, Kobe University, Nada, Kobe 657, Japan

AND HIDEKO KIRIYAMA, HIROKO TSUJI AND MASAO HASHIMOTO

Department of Chemistry, Faculty of Science, Kobe University, Nada, Kobe 657, Japan

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Abstract. (I): $C_8H_4Cl_6$, $M_r = 312\cdot8$, triclinic, $P\bar{1}$, $a = 10\cdot402$ (5), $b = 14\cdot790$ (4), $c = 5\cdot944$ (1) Å, $\alpha = 98\cdot72$ (2), $\beta = 82\cdot69$ (2), $\gamma = 102\cdot25$ (2)°, $V = 879\cdot0$ (5) Å³, $Z = 3$, $D_m = 1\cdot778$ (9), $D_x = 1\cdot773$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0\cdot71073$ Å, $\mu = 1\cdot40$ mm⁻¹, $F(000) = 462$, $T = 298$ K, $R = 0\cdot065$ for 3247 observed reflections. (II): $C_{10}H_5Cl_6NO_4$, $M_r = 415\cdot9$, triclinic, $P\bar{1}$, $a = 7\cdot694$ (2), $b = 15\cdot231$ (3), $c = 6\cdot620$ (1) Å, $\alpha = 99\cdot42$ (2), $\beta = 90\cdot50$ (1), $\gamma = 91\cdot58$ (2)°, $V = 765\cdot0$ (3) Å³, $Z = 2$, $D_m = 1\cdot769$ (8), $D_x = 1\cdot806$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0\cdot71073$ Å, $\mu = 1\cdot11$ mm⁻¹, $F(000) = 412$, $T = 298$ K, $R = 0\cdot062$ for 3870 reflections. The Cl–C–Cl and C–C–Cl angles of the CCl₃ groups in (I) deviate significantly from the tetrahedral angle, while those in (II) are close to it. In (I), the intermolecular distance of $3\cdot407$ (3) Å for

Cl(15)⋯Cl(23) is shorter than twice the van der Waals radius. In (II), the C(11)Cl₃ and C(12)Cl₃ groups are respectively equatorial and axial to the dioxin ring, which has a distorted half-boat conformation.

Introduction. Both title compounds are characterized by their unique polymorphism. The stable phase of (I) (m.p. 383 K) and that of (II) (m.p. 375 K) show nine and six ³⁵Cl NQR signals at 77 K respectively (Hashimoto, 1977; Hashimoto, Adachi & Mano, 1986). These results indicate that the asymmetric unit of crystal (I) contains three crystallographically independent CCl₃ groups and that of (II) two.

Interestingly these signals show the so-called fade-out phenomenon: NQR signals become broader and broader with increasing temperature and above a

Table 1. *Experimental conditions and refinement details*

	(I)	(II)
Crystal shape	Transparent plate-like	
size (mm)	0.20 × 0.30 × 0.40	0.25 × 0.45 × 0.30
Number of reflections and 2θ range (°) used for measuring cell parameters	30 16 < 2θ < 31	30 20 < 2θ < 27
Max. 2θ (°)	55	60
Ranges of h	-14; 14	-11; 11
k	-20; 20	-23; 23
l	-8; 8	-9; 9
Number of reflections measured	8922	9601
Number of independent reflections	4084	4479
R _{int} (F)	0.06	0.11
Number of observed reflections	3247	3870
Criterion for observed reflections	F _o > 3σ(F _o)	
R(ωR)	0.065 (0.080)	0.062 (0.074)
S	0.82	0.66
Weighting scheme	w=1 for F _o < 21.5 w=[1+0.25(F _o -21.5)] ⁻¹ for F _o > 21.5	w=1 for F _o < 10.4 w=[1+0.20(F _o -10.4)] ⁻¹ for F _o > 10.4
(Δ/σ) _{max}	0.10	0.10
Final residual electron densities (e Å ⁻³)	< 0.70	< 0.68

certain temperature (T_f), which is often far below the melting point of the compound, the signals are too broad to be detected. It is well known that this phenomenon is caused by the reorientation of the CCl₃ group around its threefold axis in the crystal lattice. The magnitude of the potential barrier height hindering the reorientation varies from compound to compound, and the values reported so far are scattered in the range of approximately 15 to 50 kJ mol⁻¹ (Chihara & Nakamura, 1980). In general T_f tends to increase with increasing magnitude of V_0 . At T_f the number of jumps in unit time is known to be about 10³ to 10⁴ s⁻¹ (Ainbinder, Amirkanov, Izmet'ev, Osipenko & Soifer, 1971).

Of the nine NQR signals of (I), six were found to fade out at about 165 (5) K and the rest at 255 K. As a result no signals could be observed at room temperature. In the case of (II), three of the six NQR signals were observed to fade out at 305 K and the rest at 375 K. These observations indicate that the magnitudes of V_0 are considerably different even in a single compound. In order to get a definite structural base for further ³⁵Cl NQR studies, the crystal structures of these stable phases were determined by single-crystal X-ray diffractometry.

Experimental. Compound (I) recrystallized from *n*-hexane, and (II) prepared by the method of Chattaway (1926) and recrystallized from ethanol. Densities measured by pycnometry. Experimental conditions and refinement details are given in Table 1. Rigaku AFC-5 diffractometer, graphite-monochromated Mo Kα radiation; ω-2θ scan technique, Δω = 1.0 + 0.35 tanθ for (I) and Δω = 1.1 + 0.35 tanθ for (II), three standard reflections measured every 100 reflections,

variations <6% for (I) and <4% for (II); data for (I) corrected on the basis of the intensities of standard reflections, Lp effects corrected, but not absorption; structure solved by direct methods with *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and refined by block-diagonal least squares with anisotropic thermal parameters for non-H atoms and isotropic ones for H atoms; all H atoms found on difference electron density map, Σw(|F_o| - |F_c|)² minimized, atomic scattering factors from *International Tables for X-ray Crystallography* (1974). All calculations performed on an ACOS 1000 computer at the Information Processing Center of Kobe University with the *UNICS* (1979) system.

Discussion. Final atomic coordinates and thermal parameters for (I) and (II) are listed in Tables 2 and 3, respectively,* and selected bond distances and angles are given in Table 4. The molecular structures with the atom-numbering schemes are shown in Figs. 1 and 2 (*ORTEP*; Johnson, 1976).

(I): One of the two independent molecules is situated at a general position (molecule 1) and the other at a center of symmetry (molecule 2). The benzene ring of molecule 1 is planar with maximum deviation of 0.004 (6) Å for C(13); C(17), C(18) and C(24) of the CCl₃ groups deviate from each benzene plane by 0.095 (7), -0.076 (7) and 0.080 (15) Å, respectively. In both molecules, the C(17)-Cl(11), C(18)-Cl(14) and C(24)-Cl(22) directions of the CCl₃ groups are roughly perpendicular (*ca* 106°) to the benzene ring. The bond lengths and angles are within the normal range, except for some angles of the CCl₃ moieties. The average value of 109.2 (4)° for the C-C-Cl angles corresponding to the C-Cl bonds nearly perpendicular to the benzene rings is significantly smaller than that of 112.5 (5)° for the other C-C-Cl angles. This finding and also the presence of pseudo-mirror planes for both molecules are consistent with the NQR results as each set of the resonance lines splits into one at a lower frequency and two at higher frequencies. The average Cl-C-Cl angle of 107.5 (4)° is slightly less than the tetrahedral angle. The dihedral angle between each benzene ring of two independent molecules is 33.4 (2)°. The packing of the molecules is mainly governed by van der Waals forces. Only the intermolecular distance of 3.407 (3) Å for Cl(15)⋯Cl(23) is a little shorter than the van der Waals contact [3.5 Å (Bondi, 1964)].

(II): The geometries of the two CCl₃ groups in (II) are more regular than those in (I). In detail, the geometry of the C(11)Cl₃ group deviates slightly,

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43646 (32 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

but significantly, from the pseudo-threefold symmetry, as compared with the other C(12)Cl₃ group. The means of the C—Cl distances, C—C—Cl and Cl—C—Cl angles are 1.765 (8) Å, 109.6 (15) and 109.3 (4)°, respectively, which are comparable with those found in α - and β -parachloral (Hay & Mackay, 1980). In the dioxin moiety, the C(2)—O(3) bond length of 1.396 (4) Å is shorter than the O(3)—C(4) bond length of 1.425 (3) Å, and the C(2)—O(3)—C(4) bond angle of 115.7 (2)° is larger than 110.5 (4) and 112.6 (4)° for

Table 2. Final atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters (\AA^2) for compound (I) with e.s.d.'s in parentheses

$$B_{\text{eq}} = \frac{4}{3} \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
Cl(11)	7510 (1)	4402 (1)	6946 (2)	5.40 (2)
Cl(12)	8940 (2)	3697 (1)	2819 (3)	6.23 (3)
Cl(13)	6117 (2)	3252 (1)	3328 (3)	6.21 (3)
Cl(14)	7574 (2)	7393 (1)	-2560 (2)	6.89 (2)
Cl(15)	8748 (2)	8519 (1)	1279 (3)	7.55 (4)
Cl(16)	5947 (2)	8024 (1)	1352 (3)	7.11 (3)
C(11)	7475 (4)	5028 (3)	2945 (6)	3.56 (5)
C(12)	6296 (4)	5235 (3)	2495 (8)	4.23 (7)
C(13)	6281 (4)	6069 (3)	1733 (8)	4.41 (7)
C(14)	7446 (4)	6723 (3)	1419 (6)	3.55 (5)
C(15)	8613 (4)	6515 (3)	1866 (8)	4.36 (7)
C(16)	8631 (4)	5679 (3)	2612 (8)	4.53 (8)
C(17)	7499 (4)	4151 (3)	3916 (7)	4.07 (6)
C(18)	7435 (4)	7609 (3)	472 (7)	3.98 (6)
Cl(21)	1207 (1)	8870 (1)	6037 (3)	6.19 (2)
Cl(22)	2461 (1)	8162 (1)	1757 (3)	5.77 (2)
Cl(23)	1706 (1)	9941 (1)	2308 (3)	6.52 (4)
C(21)	3721 (4)	9633 (3)	4415 (6)	3.32 (5)
C(22)	4557 (4)	10288 (3)	3190 (7)	4.21 (6)
C(23)	4179 (4)	9345 (3)	6236 (8)	4.13 (7)
C(24)	2364 (4)	9196 (3)	3700 (7)	3.85 (6)

Table 3. Final atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters (\AA^2) for compound (II) with e.s.d.'s in parentheses

$$B_{\text{eq}} = \frac{4}{3} \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
Cl(1)	1591 (1)	6187 (1)	-12 (1)	4.36 (1)
Cl(2)	3287 (1)	7907 (1)	1074 (1)	4.75 (1)
Cl(3)	-453 (1)	7769 (1)	759 (1)	4.05 (1)
Cl(4)	-4442 (1)	6577 (1)	6995 (2)	4.77 (1)
Cl(5)	-3813 (1)	6164 (1)	2670 (2)	5.23 (1)
Cl(6)	-2226 (1)	5136 (1)	5430 (2)	5.30 (2)
O(1)	-1857 (3)	7708 (1)	5412 (3)	3.01 (3)
C(2)	-1295 (4)	6838 (2)	5456 (4)	2.66 (3)
O(3)	-109 (3)	6561 (1)	3912 (3)	2.95 (3)
C(4)	1338 (3)	7154 (2)	3793 (4)	2.48 (3)
C(5)	2582 (4)	8614 (2)	5793 (5)	2.80 (3)
C(6)	2262 (4)	9447 (2)	6893 (5)	2.90 (4)
C(7)	609 (4)	9730 (2)	7398 (5)	2.99 (4)
C(8)	-785 (4)	9150 (2)	6879 (5)	2.94 (4)
C(9)	-483 (3)	8305 (2)	5807 (4)	2.52 (3)
C(10)	1169 (3)	8037 (2)	5171 (4)	2.35 (3)
C(11)	-2888 (4)	6202 (2)	5112 (5)	3.23 (4)
C(12)	1436 (4)	7257 (2)	1500 (4)	3.12 (3)
N	3746 (4)	10050 (2)	7551 (5)	3.92 (4)
O(4)	3451 (4)	10798 (2)	8428 (7)	6.81 (9)
O(5)	5197 (4)	9796 (2)	7210 (7)	6.60 (8)

Table 4. Selected bond distances (\AA) and angles ($^\circ$)

Compound (I)			
Cl(11)—C(17)	1.784 (5)	Cl(12)—C(17)	1.780 (5)
Cl(13)—C(17)	1.771 (5)	Cl(14)—C(18)	1.775 (5)
Cl(15)—C(18)	1.760 (5)	Cl(16)—C(18)	1.773 (5)
Cl(21)—C(24)	1.773 (5)	Cl(22)—C(24)	1.784 (5)
Cl(23)—C(24)	1.764 (5)		
Cl(11)—C(17)—Cl(12)	107.6 (2)	Cl(11)—C(17)—Cl(13)	107.9 (2)
Cl(12)—C(17)—Cl(13)	107.1 (2)	Cl(11)—C(17)—C(11)	109.4 (3)
Cl(12)—C(17)—C(11)	111.6 (3)	Cl(13)—C(17)—C(11)	113.0 (3)
Cl(14)—C(18)—Cl(15)	107.9 (2)	Cl(14)—C(18)—Cl(16)	107.2 (2)
Cl(15)—C(18)—Cl(16)	107.3 (2)	Cl(14)—C(18)—C(14)	109.1 (3)
Cl(15)—C(18)—C(14)	112.7 (3)	Cl(16)—C(18)—C(14)	112.4 (3)
Cl(21)—C(24)—Cl(22)	107.2 (2)	Cl(21)—C(24)—Cl(23)	107.3 (2)
Cl(22)—C(24)—Cl(23)	107.6 (2)	Cl(21)—C(24)—C(21)	112.7 (3)
Cl(22)—C(24)—C(21)	109.2 (3)	Cl(23)—C(24)—C(21)	112.5 (3)
Compound (II)			
Cl(1)—C(12)	1.774 (3)	Cl(2)—C(12)	1.763 (3)
Cl(3)—C(12)	1.771 (3)	Cl(4)—C(11)	1.771 (4)
Cl(5)—C(11)	1.752 (4)	Cl(6)—C(11)	1.760 (4)
Cl(1)—C(12)—Cl(2)	108.6 (2)	Cl(1)—C(12)—Cl(3)	109.2 (2)
Cl(2)—C(12)—Cl(3)	109.3 (2)	Cl(1)—C(12)—C(4)	109.0 (2)
Cl(2)—C(12)—C(4)	110.4 (2)	Cl(3)—C(12)—C(4)	110.2 (2)
Cl(4)—C(11)—Cl(5)	109.5 (2)	Cl(4)—C(11)—Cl(6)	109.3 (2)
Cl(5)—C(11)—Cl(6)	110.0 (2)	Cl(4)—C(11)—C(2)	108.2 (2)
Cl(5)—C(11)—C(2)	111.8 (2)	Cl(6)—C(11)—C(2)	108.0 (2)

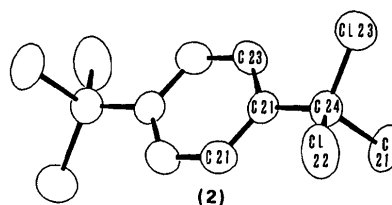
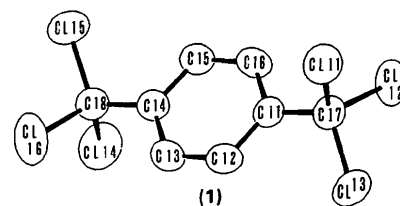


Fig. 1. Perspective views of molecules (1) and (2) for compound (I).

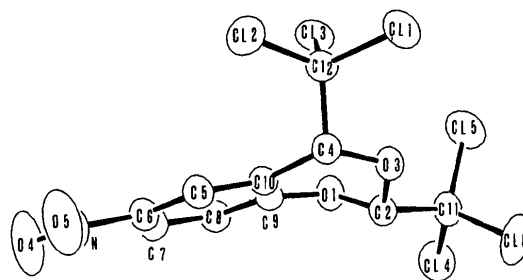


Fig. 2. Perspective view of compound (II).

the dioxane ring in *trans*-2-isopropyl-*N,N*-dimethyl-1,3-dioxane-5-carbothioamide (Shoja & Kaloustian, 1983). The C(4)–C(12) bond length [1.554 (4) Å] is longer than C(2)–C(11) [1.533 (3) Å], the latter being close to the corresponding mean value of 1.526 (16) Å for α - and β -parachloral. The dioxin ring has a distorted half-boat conformation with its 'flap' at C(2). C(2) and O(3) are displaced by 0.846 (4) and 0.331 (5) Å respectively from the best plane through O(1), C(4), C(9) and C(10). The torsion angles are -64.0 (3)° for C(9)–O(1)–C(2)–O(3), 51.8 (3)° for O(1)–C(2)–O(3)–C(4) and -8.6 (3)° for C(2)–O(3)–C(4)–C(10). It is noticeable that the C(11)Cl₃ group takes the equatorial position and C(12)Cl₃ the axial one. In each group, the Cl atoms are in staggered form with respect to the dioxin ring. The benzene ring is planar, the largest deviations from the best plane being -0.028 (3) Å for C(10) and 0.015 (4) Å for C(6). The N, O(1) and C(4) atoms deviate by 0.066 (5), 0.140 (4) and -0.172 (4) Å respectively from this plane. The plane of the nitro group makes an angle of 4.9 (2)° with the benzene ring. The crystal is composed of molecules held together by van der Waals interactions. The shortest intermolecular distance between Cl atoms is 3.597 (2) Å for Cl(2)⋯Cl(4); Cl(3)⋯H(1) [2.72 (4) Å] is slightly less than the van der Waals contact, 3.0 Å.

The ³⁵Cl NQR studies showed that the numbers of crystallographically independent chlorine atoms in (I) and (II) are nine and six, respectively, in accord with the present X-ray results. In (II) the thermal parameters of the Cl atoms of the C(11)Cl₃ group are somewhat larger than those of C(12)Cl₃. This observation may be

associated with the difference in V_0 which is proposed from the ³⁵Cl NQR results. However, no similar correlation was found for (I), possibly owing to its smaller V_0 magnitude suggested by the lower T_f 's as compared with those of (II). The expected correlation would be observed if the X-ray work were done at lower temperatures, for instance at 150 K.

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2,3-Epoxy-2,3-dihydro-1,4-naphthoquinone

BY K. ANN KERR

Departments of Chemistry and Physics, The University of Calgary, Calgary, Alberta, Canada T2N 1N4

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Abstract. C₁₀H₆O₃, $M_r = 174.16$, monoclinic, $P2_1$, $a = 12.9845$ (19), $b = 4.2866$ (3), $c = 7.0192$ (9) Å, $\beta = 97.182$ (6)°, $V = 387.62$ (8) Å³, $Z = 2$, $D_x = 1.492$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.7093$ Å, $\mu = 0.1207$ mm⁻¹, $F(000) = 180$, $T = 294$ K, $R = 0.033$ for 757 contributing reflections. The molecule adopts a shallow boat conformation with carbonyl groups bowed away from the oxirane ring. This conformation maximizes the conjugation between the carbonyl group and the oxirane ring with consequent shortening of the

oxirane C–O bond distance. Packing forces cause significant distortion as shown by the torsional angles about bonds C(4)–C(10) and C(9)–C(1).

Introduction. Epoxy compounds are powerful alkylating agents, thought to exert their biological activity by forming covalent bonds with information-carrying molecules like DNA and proteins. Chemicals of this class are antibiotics, mutagens, phytotoxins and carcinogens.