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Structural Studies of Polychlorinated Hydrocarbons.
IV. 2,2-Bis(*p*-chlorophenyl)acetic Acid

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$(C_6H_4Cl)_2CHCOOH$, 2,2-bis(*p*-chlorophenyl)acetic acid, *pp'*-DDA, monoclinic, $P2_1/c$, $a = 14{\cdot}11$ (2), $b = 6{\cdot}10$ (1), $c = 16{\cdot}00$ (2) Å, $\beta = 111{\cdot}5$ (1)°, $Z = 4$, $D_{calc} = 1{\cdot}46$ g cm^{-3}. The molecules crystallize as centrosymmetric dimers joined by hydrogen bonds between the carboxyl groups. The torsion angles of the two phenyl rings [+ 76 (1)° and −32 (1)°] relative to the central ethyl group differ significantly. The intramolecular Cl(Ph)–Cl(Ph) distance is 10·08 A.

Introduction

The structure of *pp'*-DDA was determined in order to learn more about the mode of action and biodegradation of DDT. More than one hundred DDT analogues with or without insecticidal activity have so far been synthesized (Rogers, Brown, Rasmussen & Heal, 1953; Frear, 1948; Gunther, Blinn, Carman & Metcalf, 1954; Holan, 1969). However, only four crystal structures of DDT analogues have been determined: *pp'*-DDT[1,1-bis(*p*-chlorophenyl)-2,2,2-trichloroethane (I)], *op'*-DDT [1-(*o*-chlorophenyl)-1-(*p*-chlorophenyl)-2,2,2-trichloroethane (II)] (DeLacy & Kennard, 1972*b*), 1,1-bis(*p*-chlorophenyl)-2,2-dichlorocyclopropane (III) and 1,1-bis(*p*-ethoxyphenyl)-2,2-dimethylpropane (IV) (DeLacy & Kennard, 1972*a*). *pp'*-DDA is known to be a common metabolite of *pp'*-DDT (O'Brien, 1967).

Table 1. *Fractional atomic coordinates* (×10⁴) *and anisotropic thermal parameters* (×10⁴)

Estimated standard deviations are given in parentheses. The expression for the thermal parameters is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl(1)	3449 (1)	12868 (2)	559 (1)	102 (1)	434 (4)	55 (1)	53 (3)	83 (1)	72 (3)
Cl(2)	−700 (1)	7644 (3)	4134 (1)	72 (1)	710 (7)	103 (1)	98 (4)	116 (2)	128 (4)
C(1)	3124 (3)	7783 (6)	2480 (2)	47 (2)	345 (12)	33 (2)	15 (8)	31 (3)	−26 (7)
C(2)	3765 (3)	9534 (7)	2787 (3)	68 (3)	367 (13)	38 (2)	−27 (9)	30 (4)	−29 (8)
C(3)	3880 (3)	11102 (8)	2202 (3)	69 (3)	389 (14)	44 (2)	−46 (11)	48 (4)	−39 (8)
C(4)	3336 (3)	10873 (7)	1298 (3)	61 (2)	391 (13)	40 (2)	60 (9)	55 (3)	20 (8)
C(5)	2705 (3)	9131 (8)	971 (3)	73 (3)	467 (16)	35 (2)	−27 (11)	30 (4)	−13 (9)
C(6)	2596 (3)	7597 (8)	1552 (3)	66 (3)	446 (16)	36 (2)	−73 (11)	25 (3)	−35 (8)
C(7)	1999 (3)	6529 (6)	3321 (2)	44 (2)	325 (11)	33 (2)	9 (7)	22 (3)	9 (6)
C(8)	1855 (3)	8532 (7)	3659 (3)	59 (3)	326 (13)	50 (2)	7 (9)	44 (4)	13 (8)
C(9)	1028 (3)	8902 (8)	3910 (3)	72 (3)	373 (14)	59 (2)	53 (11)	63 (4)	33 (9)
C(10)	348 (3)	7224 (9)	3819 (3)	50 (2)	485 (17)	51 (2)	51 (10)	43 (4)	66 (10)
C(11)	457 (3)	5246 (9)	3475 (3)	52 (3)	474 (17)	61 (2)	−42 (11)	39 (4)	39 (10)
C(12)	1294 (3)	4893 (8)	3231 (3)	61 (3)	327 (13)	51 (2)	−21 (10)	32 (4)	−15 (8)
C(13)	2935 (3)	6051 (7)	3084 (2)	49 (2)	315 (11)	36 (2)	13 (8)	24 (3)	−34 (7)
C(14)	3866 (3)	5667 (6)	3932 (2)	46 (2)	317 (11)	37 (2)	1 (8)	33 (3)	−10 (7)
O(1)	4425 (2)	4085 (5)	3932 (2)	60 (2)	415 (10)	44 (2)	77 (7)	21 (3)	−35 (6)
O(2)	4035 (2)	6944 (5)	4591 (2)	61 (2)	401 (10)	39 (1)	37 (6)	16 (2)	−55 (6)

	x	y	z	B(Å²)		x	y	z	B(Å²)
H(2)	4185 (42)	9792 (88)	3455 (41)	8·1 (1·4)	H(9)	964 (43)	10392 (100)	4219 (39)	8·8 (1·5)
H(3)	4368 (36)	12106 (76)	2420 (30)	5·9 (1·1)	H(11)	−26 (34)	4116 (82)	3396 (29)	6·0 (1·1)
H(5)	2297 (35)	8928 (78)	300 (31)	6·2 (1·0)	H(12)	1409 (29)	3619 (73)	3052 (26)	3·7 (0·8)
H(6)	2131 (33)	6450 (77)	1326 (28)	5·2 (1·0)	H(13)	2832 (26)	4577 (59)	2756 (24)	3·7 (0·7)
H(8)	2348 (38)	9737 (84)	3759 (33)	7·3 (1·3)	H(O1)	5092 (66)	3750 (147)	4583 (54)	14·2 (2·6)

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Transparent single-crystal needles of *pp'*-DDA were grown from an ethanol–water mixture. From a crystal of dimensions 0·13 × 0·36 × 0·30 mm, the 2458 independent reflexions, 1584 of which had $\sigma(I)/I < 0{\cdot}33$, were measured on a four-circle single-crystal diffractometer, with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å), ω–2θ scan (fixed scan width 2°) within $\theta = 70°$. Data were corrected for Lorentz and polarization effects, but not for absorption ($\mu = 45{\cdot}1$ cm^{-1}). Single-crystal X-ray photographs showed systematic absences corresponding to $P2_1/c$ ($0k0$: k odd, $h0l$: l odd). The unit-cell parameters were refined from a Guinier–Hägg powder photograph by the method of least squares. A difference electron density map, based on the two Cl positions found from a Patterson map, revealed all the non-hydrogen atoms. After anisotropic refinement, all hydrogens were found in a subsequent electron-density map. Full-matrix least-squares refinement yielded a linear R value ($R = \|F_o| - |F_c\|/|F_o|$) of 0·063 for all the 1584 reflexions. The scattering factors were those of *International Tables for X-ray Crystallography* (1974). In the final least-squares refinement, with only the non-hydrogen atoms allowed thermal anisotropy, Hughes's weighting scheme with $|F_o^{(\min)}| = 2{\cdot}0$ was used. The final positional and thermal parameters are listed in Table 1. The atomic labelling used is indicated in Fig. 1. Interatomic distances are given in Table 2 and angles in Table 3.*

Table 2. *Interatomic distances of pp'-DDA* (Å)

Estimated standard deviations are given in parentheses.

Cl(1)–C(4)	1·744 (4)	C(7)–C(13)	1·529 (5)
Cl(2)–C(10)	1·747 (4)	C(13)–C(14)	1·521 (5)
C(1)–C(2)	1·369 (6)	C(14)–O(1)	1·246 (5)
C(2)–C(3)	1·388 (6)	C(14)–O(2)	1·262 (4)
C(3)–C(4)	1·374 (5)	C(2)–H(2)	1·03 (6)
C(4)–C(5)	1·362 (6)	C(3)–H(3)	0·89 (5)
C(5)–C(6)	1·366 (6)	C(5)–H(5)	1·02 (5)
C(6)–C(1)	1·400 (5)	C(6)–H(6)	0·94 (5)
C(7)–C(8)	1·381 (6)	C(8)–H(8)	0·98 (5)
C(8)–C(9)	1·384 (6)	C(9)–H(9)	1·05 (6)
C(9)–C(10)	1·374 (6)	C(11)–H(11)	0·95 (5)
C(10)–C(11)	1·358 (7)	C(12)–H(12)	0·86 (5)
C(11)–C(12)	1·390 (6)	C(13)–H(13)	1·02 (4)
C(12)–C(7)	1·379 (6)	O(1)–H(O1)	1·14 (8)
C(1)–C(13)	1·520 (5)	O(2)–H(O1)	1·50 (8)

Table 3. *Interatomic angles* (°)

Estimated standard deviations are 0·3°, but are ~3° for angles involving H atoms.

C(2)–C(1)–C(6)	117·9	C(8)–C(7)–C(12)	118·5
C(2)–C(1)–C(13)	124·1	C(8)–C(7)–C(13)	122·0
C(6)–C(1)–C(13)	118·0	C(12)–C(7)–C(13)	119·4
C(1)–C(2)–C(3)	121·4	C(7)–C(8)–C(9)	121·2
C(1)–C(2)–H(2)	123	C(7)–C(8)–H(8)	122
C(3)–C(2)–H(2)	116	C(9)–C(8)–H(8)	117
C(2)–C(3)–C(4)	118·8	C(8)–C(9)–C(10)	118·6
C(2)–C(3)–H(3)	118	C(8)–C(9)–H(9)	120
C(4)–C(3)–H(3)	122	C(10)–C(9)–H(9)	121
C(3)–C(4)–C(5)	121·2	C(9)–C(10)–C(11)	121·8
C(3)–C(4)–Cl(1)	119·2	C(9)–C(10)–Cl(2)	119·5
C(5)–C(4)–Cl(1)	119·6	C(11)–C(10)–Cl(2)	118·7
C(4)–C(5)–C(6)	119·6	C(10)–C(11)–C(12)	119·0
C(4)–C(5)–H(5)	122	C(10)–C(11)–H(11)	121
C(6)–C(5)–H(5)	118	C(12)–C(11)–H(11)	120
C(5)–C(6)–C(1)	121·1	C(11)–C(12)–C(7)	120·9
C(5)–C(6)–H(6)	120	C(11)–C(12)–H(12)	121
C(1)–C(6)–H(6)	119	C(7)–C(12)–H(12)	118
C(1)–C(13)–C(7)	113·2	C(13)–C(14)–O(1)	117·4
C(1)–C(13)–C(14)	112·2	C(13)–C(14)–O(2)	119·1
C(1)–C(13)–H(13)	108	O(1)–C(14)–O(2)	123·5
C(7)–C(13)–C(14)	110·6	C(14)–O(1)–H(O1)	117
C(7)–C(13)–H(13)	109	C(14)–O(2)–H(O1')	114
C(14)–C(13)–H(13)	104	O(1)–H(O1)–O(2')	174

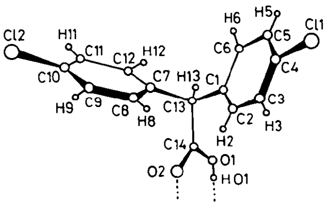

Fig. 1. Configuration of the *pp'*-DDA molecule.

The investigation is part of a research programme on the structural aspects of the action of chlorinated hydrocarbons.

Discussion

The mode of action of DDT, and whether it interacts with an enzyme, some other protein, a membrane or some combination of these, are not yet known (O'Brien, 1967; Holan, 1969; Metcalf, 1973). The conformation of the molecule has been discussed and hypothetically correlated with function (Rogers *et al.*, 1953; Holan, 1969; Metcalf, 1973). Relevant conformational parameters are suggested to be *inter alia* the distances between the chlorines at the phenyl rings [Cl(Ph)–Cl(Ph)], predicted to be 11·0 Å (Rogers *et al.*, 1953), and the rotation of the phenyl groups about their bonds with the central C atom. In Table 4 these two parameters are listed for the DDT analogues so far determined. The Cl(Ph)–Cl(Ph) distances for the three *pp'*-analogues (10·02–10·35 Å) and the O(Ph)–O(Ph) distance for the *pp'*-ethoxy analogue (IV) are all quite similar.

The space groups of all DDT-analogue crystal structures solved to date are centrosymmetric. Thus all the analogues exist in two mirror-image conformations, although only *op'*-DDT (II) has an asymmetric C

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* A list of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32021 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

atom. Both the *R* and *S* forms of *op*′-DDT exist in two different conformations in the crystal, with Cl(Ph)—Cl(Ph) distances of 6·56 and 7·07 Å respectively. Despite the difference in Cl(Ph)—Cl(Ph) distances between *pp*′-DDT and *op*′-DDT, *op*′-DDT is an active insecticide (Frear, 1948).

Free rotation of phenyl groups has been suggested as playing a role in the action of DDT (Rogers *et al.*, 1953; Riemschneider & Otto, 1954). The absolute configurations of the two centrosymmetrically related molecules of *pp*′-DDA in a dimer (Fig. 2) differ markedly. From Table 4 it can be seen that if a molecule of *pp*′-DDA is converted to its mirror image, the phenyl groups must undergo an apparent net rotation of 44° about their bonds to the central C atom. This indicates a considerable freedom of rotation for the phenyl groups of *pp*′-DDA. To compare the orientations of the phenyl groups in different DDT analogues, a common description of the rotation is needed. The deviation from an ideal butterfly conformation has been used, but it presents difficulties when the molecular symmetry breaks down. Moreover, two definitions of the symmetrical butterfly conformation have been proposed: either that configuration which when projected on to the plane perpendicular to C(13)—C(14) depicts the phenyl rings with maximum area (DeLacy & Kennard, 1972*b*), or in relation to structure III, that configuration in which the 'plane' of the butterfly wings is normal to the bisector of the cyclopropanyl C—C bonds meeting at C(13) (DeLacy & Kennard, 1972*a*). A more general nomenclature for bridged diphenyls has been proposed by van der Heijden, Griffith, Chandler & Robertson (1975).

Here we prefer to discuss these structures in terms of torsion angles. Table 4 compares the values found in the present study with those we have calculated for the

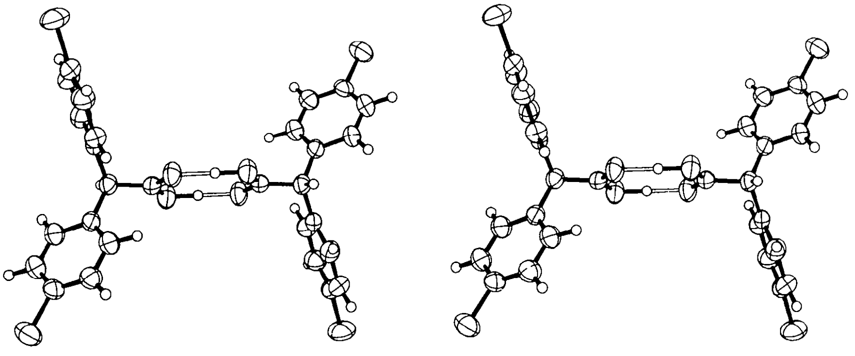
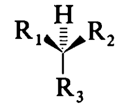
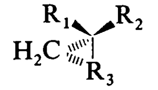


Fig. 2. Stereo view of a *pp*′-DDA dimer.

Table 4. *Torsion angles and* Cl(Ph)—Cl(Ph) *distances in DDT and its analogues*



(I), (II), (IV), (V)



(III)

	R_1	R_2	R_3
(I)	*p*ClPh	*p*ClPh	CCl_3
(II)	*p*ClPh	*o*ClPh	CCl_3
(III)	*p*ClPh	*p*ClPh	CCl_2
(IV)	*p*EtOPh	*p*EtOPh	CMe_3
(V)	*p*ClPh	*p*ClPh	COOH

The molecules designated 1 or 2 are the independent molecules listed in the earlier publications. To make valid comparisons it has been necessary in the calculations to adopt the conventions detailed in the text. The identity of each torsion angle is given for convenience in terms of the original atomic numbering: 2—1—13—14 for example denotes C(2)C(1)C(13)C(14). (*o*) and (*p*) denote *ortho* and *para*-substituted rings respectively. (O—O) denotes the oxygen–oxygen distance in the non-halogenated ethoxyphenyl derivative (IV).

		Torsion angles (°)				Cl(Ph)—Cl(Ph)
Compound		τ_1			τ_2	distance (Å)
pp′-DDA	(V)	8–7–13–14	+76	−32	2–1–13–14	10·08
pp′-DDT	(I)	6–1–14–13	+87	−47	8–7–14–13	10·35
op′-DDT	(II)1	2–1–13–14(*p*)	+96	−27(*o*)	8–7–13–14	6·56
op′-DDT	(II)2	2–1–13–14(*p*)	+87	−42(*o*)	8–7–13–14	7·07
Cyclo-	(III)1	12–7–13–15	+70	−69	2–1–13–15	10·02
Cyclo-	(III)2	12–7–13–15	+66	−62	6–1–13–15	10·12
Ethoxy-	(IV)	8–7–13–14	+82	−66	6–1–13–14	10·14(O—O)

analogous molecules previously reported. To achieve comparable results despite variations in atomic numbering, it became necessary to standardize on two torsion angles, τ_1 and τ_2, which are determined by re-expressing all the other molecules in a form analogous to Fig. 1. Thus, the bond C(13)–C(14) lies in the paper, C(14) below C(13), and the pseudosymmetry plane C(13)C(14)H(13) lies perpendicular to the paper with H(13) below the page. As both enantiomers occur in the cell, that one is chosen which has the left-hand ring the more steeply inclined to the page, and this is called ring 1. The numbering is standardized to match Fig. 1, *i.e.* ring 1 is attached at C(7) and ring 2 at C(1). The closest *ortho*-hydrogen atoms are designated H(8) on ring 1 and H(2) on ring 2. τ_1 is then defined as C(8)C(7)C(13)C(14) and is positive. τ_2 is C(2)C(1)C(13)C(14) and is negative. $|\tau_1|$ is by definition $> |\tau_2|$. This facilitates comparison of their values. To be precise and to facilitate recognition of these angles in earlier structures they are designated in Table 4 and Fig. 3 in terms of the relevant original atom numbering. [Readers are warned that some of the diagrams in the earlier papers depict enantiomorphs of the molecules listed, so that application of the torsion angles quoted in the adjacent text to the molecules shown will in those cases lead to erroneous values of τ_1 and τ_2. There is an inconsistency between Fig. 2 and its caption for structure (III). Also, for (III) only, we have defined the torsion angles with reference to C(15) which is chlorinated rather than to the methylene C(14), for in all the other structures it is C(14) that carries the chlorine atoms or the methyl groups.] The values of τ_1 and τ_2 for DeLacy & Kennard's (1972*b*) first definition are +90° and −90°, but for their second definition (1972*a*) they are +60° and −60°. It is clear that (III) is nearly symmetrical as a result of the constraints imposed by the cyclopropane ring. But in all other cases there is marked asymmetry, τ_1 being generally close to 90°, but τ_2 varying widely (from −27 to −66°). $\Delta\tau$ ($= |\tau_1| - |\tau_2|$) also varies considerably: it is largest for (II). Evidently a good deal of rotational freedom is possible: indeed it seems feasible that the inversion of any molecule that occurs in solution may involve rotations approaching 180° which, for example, interchange H(2) and H(6).

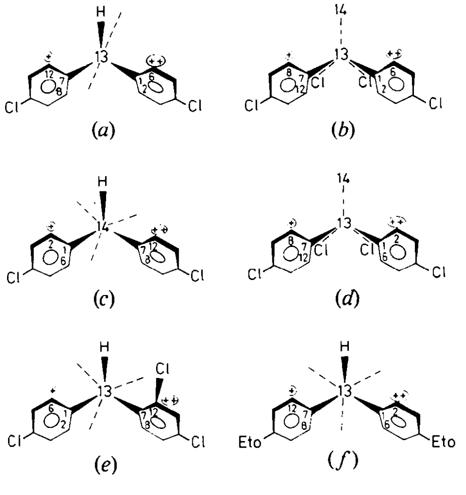


Fig. 3. Configuration and numbering of the DDT-analogues: (*a*) *pp*′-DDA (V), (*b*) (III)1, (*c*) *pp*′-DDT (I), (*d*) (III)2, (*e*) *op*′-DDT (II)1 and (II)2. (*f*) (IV). ⊕ and ⊕⊕ denote which way the phenyl group is turned: ⊕ above the paper, ⊕⊕ even higher above the paper. τ_1 is always the torsion angle to the left, τ_2 is to the right. The molecules (I), (II)2 and (III)2 are the enantiomorphs of those listed in the original papers.

The *pp*′-DDA molecules are held together in the crystals as dimers (Fig. 2) by short hydrogen bonds (O···O distance 2·63 Å) between the carboxyl groups, yielding an almost planar eight-membered ring with no atom more than 0·03 Å away from a least-squares plane through the atoms. The C–O bond distances are almost equal (1·246 and 1·262 Å with e.s.d. 0·005 Å) and the H atom is near the line joining the O atoms, as is usual for strong (short) hydrogen bonds (Brown, 1976). The plane of the two carboxyl groups deviates by 19° from the pseudosymmetry plane through H(13)–C(13)–C(14). This is probably in order to avoid close contact between the *ortho*-hydrogen atoms, attached to the benzene rings, and the O atoms of the carboxyl groups. As is indicated in Fig. 3, the CCl_3 groups of (I) and (II) are similarly rotated about 20° away from a perfect staggered conformation in order to avoid contact between Cl and the most inclined

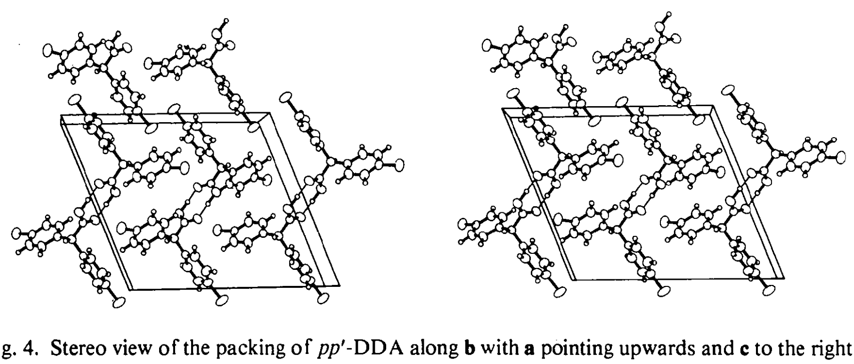


Fig. 4. Stereo view of the packing of *pp*′-DDA along **b** with **a** pointing upwards and **c** to the right.

phenyl group. The Cl—C distances (1·744 and 1·748 Å) are in agreement with those found for Cl—C (sp^2) bonds. The packing of the molecule is shown in Fig. 4. No intermolecular distances are less than 3·4 Å.

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References

Brown, I. D. (1976). *Acta Cryst.* A**32**, 24–31.

DeLacy, T. P. & Kennard, C. H. L. (1972*a*). *J. Chem. Soc. Perkin* II, pp. 2141–2147.

DeLacy, T. P. & Kennard, C. H. L. (1972*b*). *J. Chem. Soc. Perkin* II, pp. 2148–2153.

Frear, E. H. (1948). *Chemistry of Insecticides, Fungicides and Herbicides*, 2nd ed., pp. 57–88. New York: Van Nostrand.

Gunther, F. A., Blinn, R. C., Carman, G. E & Metcalf, R. L. (1954). *Arch. Biochem.* **50**, 504–505.

Heijden, S. P. N. van der, Griffith, E. A. H., Chandler, W. D. & Robertson, B. E. (1975). *Canad. J. Chem.* **53**, 2084–2092.

Holan, G. (1969). *Nature, Lond.* **221**, 1025–1029.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 72–102. Birmingham: Kynoch Press.

Metcalf, R. L. (1973). *J. Agric. Food Chem.* **21**, 511–519.

O'Brien, R. D. (1967). *Insecticides, Action and Metabolism*, pp. 108–132. New York: Academic Press.

Riemschneider, R. D. & Otto, H. D. (1954). *Z. Naturforsch.* **9b**, 95–110.

Rogers, E. F., Brown, H. D., Rasmussen, I. M. & Heal, R. E. (1953). *J. Amer. Chem. Soc.* **75**, 2991–2999.

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The Crystal Structure of $Rb_2Be_2Si_2O_7$

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The structure of the Rb beryllosilicate, $Rb_2Be_2Si_2O_7$, has been solved from three-dimensional single-crystal X-ray diffraction data obtained with a linear diffractometer. The orthorhombic unit cell, $a = 8·92\,(1)$, $b = 8·32\,(1)$, $c = 5·15\,(1)$ Å, contains two formula units of $Rb_2Be_2Si_2O_7$. The structure, refined in the space group $P2nn$ by block-diagonal least squares ($R = 5·4\%$), is that of an infinite beryllosilicate framework, with large cavities containing 13 and 14-coordinate Rb (Rb—O = 2·85–3·83 Å). The framework consists of Si_2O_7 units whose non-bridging O atoms form the corners of planar BeO_3 groups. Mean Be—O and Si—O bond distances are 1·55 and 1·59 Å. The occurrence of several related Rb and Cs beryllosilicate phases is reported.

Introduction

During a study of compound formation in A_2O—BeO—SiO_2 systems, a new orthosilicate phase, Rb_2BeSiO_4, was encountered. A single crystal picked from a bulk preparation of Rb_2BeSiO_4 had a geometrically hexagonal pseudocell which was similar in size to the hexagonal unit cell of tridymite. On the supposition that this phase might be a novel type of filled tridymite structure, a full crystallographic study was undertaken. During the analysis, it soon became clear that the composition of the crystal was different from that of the bulk preparation and instead, corresponded to the formula $Rb_2Be_2Si_2O_7$. This had been overlooked previously because Rb_2BeSiO_4 and $Rb_2Be_2Si_2O_7$ (a bulk preparation was subsequently made) have very similar powder patterns, both of which could be indexed on similar-sized orthorhombic, geometrically hexagonal cells. The crystal structure of $Rb_2Be_2Si_2O_7$ is reported here. It bears no relation to tridymite and instead, contains unusual, planar BeO_3 units [Howie & West (1976), preliminary note].

$Rb_2Be_2Si_2O_7$ appears to be a thermodynamically stable phase, although loss of rubidium oxide by volatilization occurs above 1000–1100 °C. Up to 850 °C, however, differential thermal analysis gives no indication of chemical or structural change.