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Bisphenol Flukicides. I. Crystal Structures of 2,2'-Ethylidenebis(4-chloro-6-nitrophenol) and 2,2'-Isopropylidenebis(4-chloro-6-nitrophenol)

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Abstract

2,2'-Ethylidenebis(4-chloro-6-nitrophenol), $C_{14}H_{10}Cl_2N_2O_6$, is monoclinic, space group $P2_1/c$, with $a = 9.859$ (13), $b = 12.557$ (10), $c = 12.451$ (6) Å, $\beta = 94.46$ (7)°, $Z = 4$. 2,2'-Isopropylidenebis(4-chloro-6-nitrophenol), $C_{15}H_{12}Cl_2N_2O_6$, is monoclinic space group $C2/c$, with $a = 13.785$ (2), $b = 13.077$ (5), $c = 9.291$ (3) Å, $\beta = 97.81$ (3)°, $Z = 4$. Both structures were deduced from Mo $K\alpha$ intensities measured on a diffractometer. The ethane structure was determined by direct methods and refined to an R of 0.065 for 1218 observed terms. The heavy-atom method was used to solve the isopropane structure, which was refined to an R of 0.049 for 1051 observed terms. In the ethane structure, the Cl atoms lie on the same side of the molecular skeleton and the dihedral angle between the phenyl rings is 92.4°. In the isopropane structure, however, the phenyl rings are mutually inclined at 77.4° and the Cl atoms lie on opposite sides of the molecular skeleton which has twofold symmetry.

Introduction

5,5'-Dichloro-3,3'-dinitro-2,2'-biphenyldiol (I), otherwise known as menichlopholan, is an effective curative for *Fasciola hepatica* (liver-fluke) infection in sheep and cattle (Burrows, 1973). Menichlopholan uncouples oxidative phosphorylation in warm-blooded animals (van Miert & Groeneveld, 1969) and it is probable that the effectiveness of the compound against liver-flukes is due to the same effect. The related compound, 2,2'-methylenebis(4-chloro-6-nitrophenol) (II), has been shown to be an effective fasciolicide; similarly, 2,2'-ethylidenebis(4-chloro-6-nitrophenol) (III) exhibits

(I)

(II) $R = R' = H$
(III) $R = CH_3, R' = H$
(IV) $R = R' = CH_3$
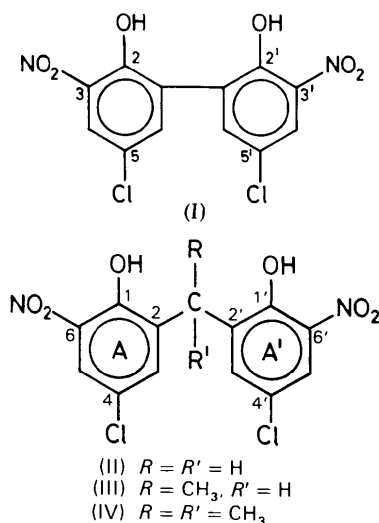
even stronger activity than (II) against mature *F. hepatica*, but 2,2'-isopropylidenebis(4-chloro-6-nitrophenol) (IV) possesses no effective fasciolicidal properties (information supplied by ICI Australia Ltd).

It has been suggested that the variation of anthelmintic (worm-killing) properties of bisphenol analogues may be attributed to differing conformations in the molecules (ICI Australia Ltd). We are currently carrying out crystallographic studies of a number of bisphenols in an attempt to derive a possible relationship between their conformations and biological activity.The first two crystal structures determined in this series, (III) and (IV), are reported here and subsequently referred to as the ethane and isopropane respectively.

Experimental

Weissenberg photographs showed that yellow plate-like crystals of (III), grown from ethanol in a desiccator over sulphuric acid, were monoclinic, space group $P2_1/c$. Yellow needles of (IV), similarly grown from ethyl acetate, were also shown to be monoclinic, space group Cc or $C2/c$, subsequently confirmed as $C2/c$. Cell parameters were determined by least squares from 2θ values for ten strong reflections for the ethane and 25 for the isopropane structure, measured on a diffractometer with Mo $K\alpha$ radiation. The densities were determined by flotation in a mixture of o-xylene and bromoform and indicated $Z = 4$ for both structures. Crystal data are given in Table 1.

For both compounds, intensities were recorded with Mo $K\alpha$ radiation on a Rigaku-AFC four-circle diffractometer, with the X-ray beam monochromatized by a graphite crystal. The crystal dimensions were $0.18 \times 0.12 \times 0.11$ mm and $0.30 \times 0.21 \times 0.20$ mm for the ethane and isopropane derivatives respectively. The crystal of the ethane compound was aligned with c approximately parallel to the diffractometer φ axis whilst that of the isopropane compound had c approximately perpendicular to the φ axis. Intensities were recorded

by the ω–2θ scan technique, with a scan rate of 2° min^{-1} and 10s stationary background counts. Three reference reflections were monitored every 50 reflections, and showed no significant variation in intensity for either crystal. Intensities were recorded to a 2θ limit of 45° for the ethane crystal. Of the 1583 non-equivalent terms measured, 1218 had $|F_o| > 3\sigma|F_o|$ and were considered observed. For the isopropane, of the 1154 non-equivalent terms recorded to a 2θ limit of 50°, 1051 which had $|F_o| > 3\sigma|F_o|$ were considered observed. The intensities were corrected for Lorentz and polarization factors but not for absorption or extinction. Scattering factors were from Cromer & Mann (1968) for C, Cl, N and O and from Stewart, Davidson & Simpson (1965) for H.

Structure analysis

The ethane compound was solved with *MULTAN* (Main, Woolfson & Germain, 1971). Phases for 199 $|E|$ values >1.6 were derived by application of a weighted tangent formula (Germain, Main & Woolfson, 1971) and yielded a value of R_K (Karle & Karle, 1966) of 0.23. The non-hydrogen atoms were located on an E map and all 25 atoms could be differentiated as C, Cl, N or O from the known chemical formula. The analysis was continued with the 1218 diffractometer data. Full-matrix least-squares refinement with anisotropic temperature factors for the Cl atoms, and individual isotropic temperature factors for C, N and O, yielded $R = \sum ||F_o| - |F_c||/\sum |F_o| = 0.19$. Refinement in which anisotropic temperature factors were assigned to all the non-hydrogen atoms reduced R to 0.09. Calculated positions for all the H atoms except those of the hydroxyl groups were included in the final refinement cycles, but their parameters were not refined. This yielded an R of 0.065.

For the isopropane compound, the Cl atoms were located from the vector map. The sites of all the other non-hydrogen atoms were located from a Fourier synthesis. Refinement in which individual isotropic temperature factors were given to all the non-hydrogen atoms yielded an R of 0.20. Further full-matrix least-squares refinement with anisotropic temperature factors for the non-hydrogen atoms reduced R to 0.07. Final cycles, in which the calculated coordinates for all but the hydroxyl H atoms were included but not refined, yielded an R of 0.049.

For both structures, the H atoms were given the same isotropic thermal parameters as the atom to which they were bonded. From the subsequent difference maps, the calculated sites of the H atoms were verified and the hydroxyl H atoms located. All least-squares refinements were carried out with *ORFLS* (Busing, Martin & Levy, 1962); the function minimized

Table 1. *Crystal data*

	Compound (III)	Compound (IV)
Molecular formula	$C_{14}H_{10}Cl_2N_2O_6$	$C_{15}H_{12}Cl_2N_2O_6$
M_r	373·15	387·18
$F(000)$	760	792
Space group	$P2_1/c$	$C2/c$
a	9·859 (13) Å	13·785 (2) Å
b	12·557 (10)	13·077 (5)
c	12·451 (6)	9·291 (3)
β	94·46 (7)°	97·81 (3)°
V_c	1537 (3) Å^3	1659 (2) Å^3
Z	4	4
D_m	1·64 (2) Mg m^{-3}	1·59 (2) Mg m^{-3}
D_c	1·61	1·55
λ	0·7107 Å	0·7107 Å
μ(Mo $K\alpha$)	0·462 mm^{-1}	0·431 mm^{-1}

Table 2. *Final atomic parameters for the non-hydrogen atoms* ($\times 10^4$) *with e.s.d.'s in parentheses*

(a) Ethane structure

	x	y	z
Cl	4192 (2)	6270 (2)	6994 (2)
Cl'	6265 (4)	11091 (2)	4138 (2)
N	7475 (8)	3458 (6)	5793 (5)
N'	9896 (10)	9784 (9)	6982 (7)
O(1)	8458 (7)	3171 (5)	5293 (6)
O(2')	9995 (10)	10696 (7)	7269 (7)
O(2)	6874 (8)	2845 (6)	6352 (6)
O(1')	10570 (8)	9047 (7)	7404 (6)
O(3)	8666 (6)	5015 (5)	4426 (4)
O(3')	9558 (6)	7633 (5)	6098 (5)
C(1)	7210 (8)	6340 (7)	5037 (6)
C(1')	7952 (9)	8247 (7)	4773 (6)
C(2)	7665 (8)	5279 (7)	5056 (6)
C(2')	8848 (9)	8463 (8)	5679 (6)
C(3)	7038 (8)	4559 (6)	5717 (6)
C(3')	8942 (9)	9509 (8)	6074 (7)
C(4)	5981 (8)	4849 (7)	6329 (6)
C(4')	8144 (11)	10316 (8)	5612 (8)
C(5)	5535 (8)	5878 (7)	6263 (6)
C(5')	7263 (10)	10084 (7)	4739 (6)
C(6)	6152 (8)	6622 (7)	5637 (7)
C(6')	7164 (9)	9069 (7)	4324 (7)
C(7)	7884 (9)	7130 (7)	4314 (7)
C(8)	7190 (10)	7064 (7)	3164 (7)

(b) Isopropane structure

	x	y	z
Cl	1371 (1)	7445 (2)	3284 (2)
N	3132 (4)	9566 (4)	−166 (6)
O(2)	2378 (3)	10063 (3)	−388 (6)
O(1)	3852 (3)	9757 (3)	−781 (6)
O(3)	4845 (2)	8291 (2)	475 (4)
C(1)	4074 (3)	7336 (3)	2150 (5)
C(2)	4044 (3)	8130 (3)	1128 (5)
C(3)	3188 (3)	8717 (4)	838 (5)
C(4)	2355 (3)	8522 (4)	1489 (6)
C(5)	2395 (3)	7730 (4)	2433 (5)
C(6)	3238 (3)	7141 (4)	2797 (5)
C(7)	5000	6672 (5)	2500
C(8)	4949 (3)	5974 (4)	3823 (6)

Table 3. *Calculated* H *atom coordinates* ($\times 10^3$)

The atoms are given the same numbers as the heavier atoms to which they are bonded.

(a) Ethane structure

	x	y	z
H(4)	558	430	685
H(6)	585	743	563
H(7)	888	686	422
H(8')	792	685	263
H(8")	642	649	314
H(8‴)	678	781	294
H(4')	821	1110	592
H(6')	646	891	365
H(O3)*	878	506	379
H(O3')*	996	700	616

(b) Isopropane structure

	x	y	z
H(4)	172	897	126
H(6)	324	655	356
H(8')	559	554	402
H(8")	488	642	474
H(8‴)	434	548	361
H(O3)*	477	887	−020

* Coordinates derived from the difference map.

was $\omega(|F_o| - |F_c|)^2$ with $\omega = 1\cdot0$. Fourier summations were calculated with *MUFR*-3 (White, 1966) and H atom coordinates were calculated with *HYDROGEN* (Davies, 1973). The final atomic parameters for the two compounds are given in Tables 2 and 3.* Bond lengths and angles were calculated with *BNDANG* (Satzke, 1971) and are given in Table 4. No corrections for thermal effects have been applied. Perspective views of the molecules prepared with *ORTEP* (Johnson, 1965) are given in Fig. 1. Projections of the crystal structures down a for the ethane
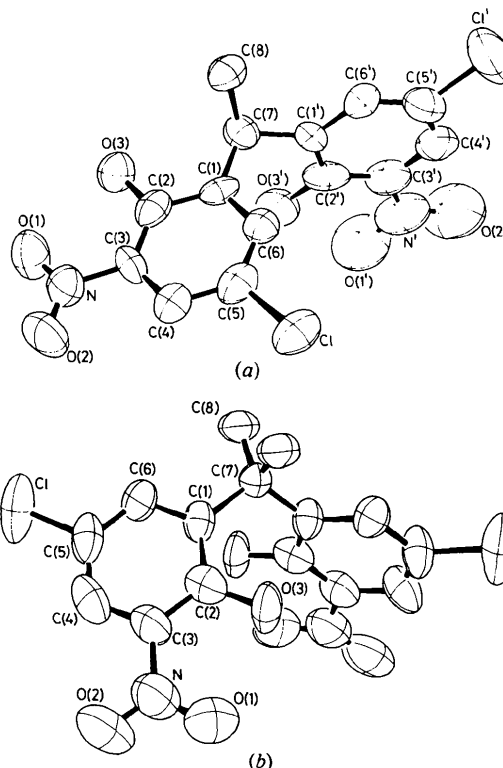
Fig. 1. Perspective views of the molecules with thermal ellipsoids scaled to 75% probability; (a) ethane, (b) isopropane. Note that the atomic numbering given here, in the text and tables differs from that used to name the compounds.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34690 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. *Bond lengths* (Å) *and angles* (°) *involving the non-hydrogen atoms with e.s.d.'s in parentheses*

	Ethane structure		Isopropane structure
	Ring *A*	Ring *B*	
Cl–C(5)	1·735 (8)	1·736 (9)	1·749 (5)
N–O(1)	1·25 (1)	1·23 (1)	1·236 (7)
N–O(2)	1·22 (1)	1·20 (1)	1·219 (7)
N–C(3)	1·45 (1)	1·45 (1)	1·445 (7)
O(3)–C(2)	1·35 (1)	1·34 (1)	1·347 (5)
C(1)–C(2)	1·41 (1)	1·40 (1)	1·404 (6)
C(2)–C(3)	1·40 (1)	1·40 (1)	1·403 (6)
C(3)–C(4)	1·39 (1)	1·38 (1)	1·392 (6)
C(4)–C(5)	1·37 (1)	1·37 (1)	1·353 (7)
C(5)–C(6)	1·39 (1)	1·38 (1)	1·397 (6)
C(6)–C(1)	1·38 (1)	1·38 (1)	1·394 (6)
C(7)–C(1)	1·53 (1)	1·51 (1)	1·541 (6)
C(7)–C(8)	1·54 (1)		1·540 (7)
C(4)–C(3)–N	116·5 (7)	117·5 (9)	116·5 (4)
C(2)–C(3)–N	120·8 (7)	121·0 (8)	120·9 (4)
O(1)–N–O(2)	122·2 (8)	124·1 (7)	122·2 (5)
O(1)–N–C(3)	118·9 (7)	116·6 (7)	118·5 (5)
O(2)–N–C(3)	118·9 (7)	119·3 (7)	119·2 (5)
C(4)–C(5)–Cl	119·5 (6)	119·4 (7)	119·5 (4)
C(6)–C(5)–Cl	119·3 (6)	119·4 (7)	118·0 (4)
C(3)–C(2)–O(3)	124·1 (7)	125·0 (8)	123·2 (4)
C(1)–C(2)–O(3)	118·1 (7)	116·1 (8)	118·0 (4)
C(1)–C(2)–C(3)	117·9 (7)	118·9 (8)	118·8 (4)
C(2)–C(3)–C(4)	122·6 (7)	121·4 (9)	122·6 (4)
C(3)–C(4)–C(5)	117·9 (7)	118·7 (9)	117·3 (5)
C(4)–C(5)–C(6)	121·2 (8)	121·2 (8)	122·6 (5)
C(5)–C(6)–C(1)	121·1 (8)	121·2 (8)	120·3 (4)
C(2)–C(1)–C(7)	118·2 (7)	119·3 (8)	120·5 (4)
C(6)–C(1)–C(7)	122·4 (7)	122·1 (8)	121·0 (4)
C(1)–C(7)–C(8)	109·3 (7)	113·8 (7)	112·1 (3)
C(2)–C(1)–C(6)	119·3 (7)	118·6 (8)	118·5 (4)
C(1)–C(7)–C(1')	112·8 (7)		

Table 5. *Intermolecular approach distances* (Å) <3·7 Å

(a) Ethane structure

Symmetry code

(I)   1 − x, 1 − y, 1 − z   (III)   1 − x, −½ + y, 1½ − z.
(II)   x, 1½ − y, −½ + z

O(3)···Cl^{I}	3·59 (1)	O(3)···O(1')^{II}	3·46 (1)
C(2)···Cl^{I}	3·60 (1)	O(3)···O(2')^{II}	3·21 (1)
C(3)···Cl^{I}	3·65 (1)	C(8)···O(3')^{II}	3·63 (1)
C(3)···C(5)^{I}	3·44 (1)	C(8)···C(2')^{II}	3·67 (1)
C(4)···C(5)^{I}	3·57 (1)	C(8)···C(6)^{II}	3·63 (1)
C(4)···C(6)^{I}	3·61 (1)	O(2)···Cl^{III}	3·10 (1)
O(3)···N'^{III}	3·37 (1)		

(b) Isopropane structure

Symmetry code

(I)   ½ − x, 1½ − y,   −z   (IV)   1 − x,   1 − y,   1 − z
(II)   ½ − x, 1½ − y, 1 − z   (V)   ½ + x, 1½ − y, ½ + z
(III) 1 − x,   2 − y,   −z   (VI) −½ + x, 1½ − y, ½ + z.

Cl···O(I)^{I}	3·688 (5)	C(6)···Cl^{II}	3·648 (5)
C(4)···C(2)^{I}	3·609 (7)	O(1)···O(3)^{III}	3·112 (7)
C(5)···N^{I}	3·683 (7)	C(8)···C(8)^{IV}	3·348 (7)
C(5)···C(3)^{I}	3·578 (7)	C(8)···O(2)^{V}	3·594 (6)
C(6)···N^{I}	3·643 (7)	Cl···O(3)^{VI}	3·265 (4)
C(6)···O(2)^{I}	3·677 (7)		

Fig. 2. Projections of the structure showing some intermolecular distances (Å). (a) Ethane viewed down a, (b) isopropane viewed down c.

and down c for the isopropane compound are shown in Fig. 2. Some short intermolecular approach distances are given in Table 5 and Fig. 2.

Discussion

Perspective views of the two compounds, Fig. 1, provide a comparison of their conformations. In the ethane structure, the phenyl-ring planes, A and A', are mutually inclined at 92·4° and their equivalent substituents lie on the same side of plane B, formed by C(1), C(7) and C(1'). As implied by the space-group symmetry, the isopropane molecules have twofold symmetry with the bridging C(7) lying on the crystallographic twofold axis. As a consequence, the equivalent substituents of the phenyl rings lie on opposite sides of plane B. The phenyl rings are mutually inclined at 77·4°. The phenyl C atoms and associated Cl, N and hydroxyl O atoms in both compounds are planar to within 0·05 Å. The angles between planes A and B and

Table 6. *Dihedral angles* (°)

	Ethane structure	Isopropane structure
Planes A and A'	92.4 (5)	77.4 (3)
Planes A and B	93.6 (3)	48.7 (2)
Planes A' and B	59.5 (3)	
Planes A and C	1.5 (3)	0.5 (2)
Planes A' and C'	3.6 (3)	

Table 7. *Equations of least-squares planes and distances* (Å) *of atoms from these planes*

X, Y and Z are expressed in Å and referred to orthogonal axes parallel to a, b and c^*

(a) Ethane structure

Plane A	$-0.5991X$	$-0.2326Y$	$-0.7661Z$	$+10.5842 = 0$
Plane A'	$0.7660X$	$+0.2082Y$	$-0.6083Z$	$-4.2001 = 0$
Plane B	$0.6719X$	$-0.7044Y$	$-0.2287Z$	$+2.5898 = 0$
Plane C	$-0.5657X$	$-0.2391Y$	$-0.7899Z$	$+10.5605 = 0$
Plane C'	$0.7578X$	$+0.1513Y$	$-0.6347Z$	$-3.2392 = 0$

Plane A			Plane A'	
C(1) -0.024 (8)	C(6) -0.017 (8)	C(1') 0.003 (8)	C(6') -0.005 (9)	
C(2) 0.000 (8)	C(7) -0.007 (9)	C(2') -0.016 (8)	C(7) 0.040 (9)	
C(3) -0.009 (8)	Cl 0.032 (2)	C(3') 0.001 (9)	Cl' -0.001 (3)	
C(4) -0.016 (8)	N -0.014 (8)	C(4') -0.008 (11)	N' 0.040 (10)	
C(5) 0.006 (8)	O(3) 0.049 (6)	C(5') -0.010 (9)	O(3') -0.044 (6)	

Plane B	Plane C	Plane C'
C(1)	N	N'
C(7)	O(1)	O(1')
C(1')	O(2)	O(2')

(b) Isopropane structure

Plane A	$-0.2348X$	$-0.6254Y$	$-0.7442Z$	$+8.7039 = 0$
Plane B	$0.2529X$	$+0.0000Y$	$-0.9675Z$	$+0.5629 = 0$
Plane C	$-0.2486X$	$-0.6206Y$	$-0.7437Z$	$+8.7281 = 0$

Plane A		Plane B	Plane C
C(1) -0.023 (4)	C(6) -0.017 (5)	C(1)	N
C(2) 0.007 (4)	C(7) -0.009 (4)	C(7)	O(1)
C(3) -0.006 (5)	Cl 0.020 (2)	C(1')	O(2)
C(4) -0.003 (5)	N -0.024 (5)		
C(5) 0.013 (5)	O(3) 0.044 (3)		

A' and B, Table 6, are 93.6 and 59.5° respectively for the ethane and 48.7° for the isopropane molecule. A similar conformation to that of the isopropane molecule was observed in 4,4'-methylenebis(2-chlorophenol) (Whittaker, 1953) where the comparable dihedral angle was 52°. Least-squares-planes equations are given in Table 7.

Bond lengths and angles for both structures are in good agreement, Table 4, so discussion of numerical values will refer to the mean values for the two compounds. The aromatic C—C length is 1.39 Å (mean e.s.d. 0.01 Å). The C—O and C—N lengths are 1.35 (1) and 1.45 (1) Å respectively and the C—Cl bond has a length of 1.74 (1) Å, typical of values reported for this bond (Rudman, 1971). The exocylic angles at positions of substitution by the nitro and hydroxyl groups are distorted from regular trigonal geometry; the angles enclosed by the groups are 120.9 (6) and 124.1 (6)° respectively and the external angles are 116.8 (6) and 117.4 (6)°. Similar distortion for aromatic *ortho* substitution of hydroxyl and nitro

groups has been noted previously (Kawai, Kashino & Haisa, 1976; Iwasaki, Sato & Aihara, 1976). The nitro groups are almost coplanar with the bonded phenyl ring, the interplanar angles ranging from 0.5 to 3.6°. The O—N—O angle is 122.8 (7)° whilst the N—O length is 1.23 (1) Å; these values do not differ significantly from those of nitro groups in comparable structures (Hanson, 1975; Pattahbi, 1975).

The molecules of the ethane compound are orientated in the crystal with their long molecular axes approximately parallel to the (100) planes, whilst in the isopropane crystal, the long molecular axes are approximately parallel to the (001) planes, Fig. 2. In the isopropane structure, the hydroxyl H(O3) atom forms an intramolecular hydrogen bond in which the hydroxyl O acts as a donor to an adjacent nitro group O atom, the O(1)⋯O(3) distance being 2.54 Å; the H(O3)—O(3) length is 0.99 Å, the H(O3)⋯O(1) distance 1.74 Å and the angle O(3)—H(O3)⋯O(1) 135.8°. A similar indication of hydrogen bonding was noted in the X-ray structure of methyl 4-hydroxy-3-nitro-*trans*-cinnamate (Hanson, 1975), where the comparable O⋯O distance is 2.59 Å, and the O—H⋯O angle 110.5°. In the ethane molecule, the derived hydroxyl H atom coordinates indicate that no comparable hydrogen bonding occurs. There is, however, indication of a weak intermolecular interaction between the hydroxyl O and an adjacent nitro group O atom of the molecule related by the crystallographic glide plane, the O(2')⋯O(3) distance being 3.21 Å. No other unusually short intermolecular approaches were noted in either structure; approach distances <3.7 Å are given in Table 5 and Fig. 2. In the ethane structure, most of the short intermolecular distances are between molecules related by the translation along *b*; the molecules are arranged in layers parallel to (001). In the isopropane structure the molecules are arranged in layers parallel to (010). The presence of glide planes in both structures requires the molecules to adopt two geometric isomeric configurations in the crystal.

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Crystal Structure of 1-Cyanoadamantane, $C_{10}H_{15}CN$, in Its Plastic Phase

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Abstract

Single-crystal X-ray diffraction data were collected and interpreted for the plastic phase of 1-cyano-adamantane, $C_{11}H_{15}N$, at 293 K. The unit cell is face-centred cubic with $a = 9.813$ (3) Å, space group $Fm3m$, $Z = 4$. On the assumption of a rigid molecular skeleton, several types of orientational disorder were investigated: isotropic rotation of the molecules about their centre of mass, hindered re-orientations between equally weighted orientations and free uniaxial rotations of the molecule about the C—C≡N axis. For the second and third model, fair agreement is found between observed and calculated structure factors (residual $R_w = 8\%$), but the third is thought to be the best. The C—C≡N axis has six possible orientations along the fourfold axes of the crystal. The molecule performs free uniaxial rotations around these six equilibrium positions of the cyano group.

I. Introduction

1-Cyanoadamantane or adamantanecarbonitrile, $C_{10}H_{15}CN$, formally known as tricyclo[3.3.1.1^{3,7}]-decane-1-carbonitrile, is a globular molecule of C_{3v} symmetry, obtained from adamantane ($C_{10}H_{16}$) by substitution of one methyl H by a —C≡N radical.

Like adamantane, it is a plastic crystal. A specially interesting point is the existence of a very high dipolar momentum for this molecule. This compound is studied here as a test for determining plastic-crystal structures for molecules with a rigid skeleton when numerous independent Bragg reflexions are observed, allowing a Frenkel model to be used.

II. Structure of a plastic crystal made of rigid molecules

(1) The molecule

The molecule is defined in a set of orthonormal axes referred to the centre of mass of the four tertiary C atoms (Fig. 1). In the following, we will assume that the

Table 1. *Parameters defining the molecule*

R_j: distance between the atom j and the origin of the crystal lattice.
θ: angle between a secondary carbon and its two bonded hydrogen atoms.

Parameter	Atoms	Value
R_{CT}	4 tertiary C	1.52 Å
R_{CS}	6 secondary C	1.77
R_{HT}	3 tertiary H	2.60
R_{HS}	12 secondary H	2.55
R_{CNT}	C bonded to the N	2.98
R_{NT}	N	4.14
θ	12 secondary H	109.47°