

Table IV. Least-Squares Planes and Deviations (Å)<sup>a</sup>

Atom	I	II	I'	II'
S	-0.044	-0.062	0.813	0.465
O(1)	0.111	0.108	0.000*	0.000*
O(2)	-1.894	-1.888	0.000*	0.000*
N	-0.492	-0.543	0.000*	0.000*
C(1)	0.006*	0.007*	0.189	0.119
C(2)	-0.002	-0.004*	1.344	1.241
C(3)	-0.001*	0.004*	1.560	1.349
C(4)	0.000*	-0.003*	0.561	0.328
C(5)	0.003*	0.003*	-0.621	-0.806
C(6)	-0.006*	-0.007*	-0.796	-0.906
C(7)	-0.866	-0.879	0.013	0.003
C(8)	-1.361	-1.440	-0.019	-0.042
C(9)	-0.036	-0.035	2.835	2.590
C(10)	1.671	1.662	1.303	1.098
C(11)	-0.010	0.008	-1.718	-1.929

<sup>a</sup> I,  $-0.195X - 0.038Y + 0.980Z = 0.790$ ; II,  $0.191X + 0.029Y + 0.981Z = 8.873$ ; I',  $-0.569X + 0.743Y + 0.353Z = 3.157$ ; II',  $0.101X + 0.907Y + 0.408Z = 11.474$ . The planes are defined by the atoms with an asterisk.

be found at the molecular level.

#### ACKNOWLEDGMENT

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**Supplementary Material Available:** A listing of the observed and calculated structure factor amplitudes, torsional angles around the bonds, and distances and angles involving hydrogen atoms (13 pages). Ordering information is given on any current masthead page.

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## Crystal and Molecular Structure of Carbamate Insecticides. 2. Aldicarb

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The crystal and molecular structure of aldicarb (2-methyl-2-(methylthio)propionaldehyde *O*-(methylcarbamoyl)oxime, C<sub>7</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>S) has been determined by single-crystal x-ray diffraction techniques. It crystallizes in an orthorhombic unit cell, *Pcab*, with unit cell dimensions  $a = 10.204$  (7),  $b = 21.155$  (9), and  $c = 10.003$  (7) Å and eight molecules per cell. The structure was refined to a final crystallographic discrepancy factor of 9.3% for 532 observed reflections ( $|F_o| > 3\sigma_{F_o}$ ). Large thermal parameters resulted from the refinement due to the close proximity to a phase transition (at  $13 \pm 3$  °C). The low-temperature phase was found to be monoclinic, *P2<sub>1</sub>/a*, with  $a = 10.25$ ,  $b = 20.99$ , and  $c = 10.07$  Å and  $\beta = 91.97^\circ$ . The C-O single bond distance in the carbamate group was found to be significantly lengthened (1.414 Å) relative to equivalent distances found in carboxylic acid esters. Such a lengthening would correlate well with any theory involving disruption of this bond in a reaction of this molecule with acetylcholinesterase enzyme.

In recent years the chlorinated hydrocarbon insecticides have largely been replaced by the carbamate and organophosphorus insecticides. The mode of action of the carbamate and/or organophosphorus insecticides is ac-

cepted to be via the inhibition of the enzyme acetylcholinesterase. In order to better understand the stereochemical requirements necessary for efficient carbamoylation or phosphorylation of the enzyme, we have undertaken a series of structural studies of various insecticides in this laboratory (Baughman and Jacobson, 1975; Gifkins and Jacobson, 1976; Rohrbaugh et al., 1976; Takusagawa and Jacobson, 1977). It is hoped that such

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Table I. Final Atomic Positional and Thermal<sup>a</sup> Parameters ( $\times 10^4$ )

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
C(1)	6840 (23) <sup>b</sup>	4232 (8)	47 (24)	471 (41)	42 (7)	444 (38)	-22 (12)	152 (37)	39 (13)
S(2)	7595 (4)	3506 (3)	729 (5)	211 (6)	81 (2)	263 (7)	-38 (3)	18 (6)	5 (4)
C(3)	6166 (16)	3011 (8)	951 (15)	235 (23)	52 (6)	205 (22)	-7 (10)	32 (22)	3 (11)
C(4)	6608 (19)	2377 (9)	1326 (18)	320 (33)	55 (6)	358 (39)	70 (12)	20 (27)	18 (12)
C(5)	5298 (15)	2988 (9)	-330 (15)	209 (23)	87 (8)	194 (25)	-6 (11)	-5 (19)	-43 (11)
C(6)	5448 (15)	3327 (8)	2153 (15)	150 (20)	51 (6)	262 (28)	6 (9)	10 (20)	8 (10)
N(7)	4354 (13)	3615 (5)	1938 (11)	218 (18)	49 (4)	118 (12)	-1 (7)	10 (15)	-6 (6)
O(8)	3823 (10)	3834 (4)	3198 (9)	214 (14)	51 (3)	103 (11)	14 (6)	1 (11)	3 (5)
C(9)	2586 (16)	4128 (6)	3064 (17)	209 (21)	37 (5)	153 (20)	-5 (9)	33 (25)	-11 (9)
O(10)	2060 (10)	4237 (5)	4144 (9)	268 (17)	67 (4)	115 (10)	25 (6)	27 (12)	2 (6)
N(11)	2141 (11)	4245 (5)	1851 (11)	209 (18)	51 (4)	94 (14)	4 (6)	-24 (14)	18 (6)
C(12)	846 (15)	4533 (7)	1699 (14)	176 (25)	68 (6)	218 (21)	33 (10)	1 (18)	13 (9)

<sup>a</sup> The anisotropic thermal parameters are defined by  $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ . <sup>b</sup> In this and succeeding tables, figures in parentheses correspond to standard deviations for the least significant figures.

a program will help determine the structural dependence of an insecticide's toxicity/activity and lead to a better understanding of the mechanism(s) involved. We wish to report here the structural study of aldicarb, the second of a series of carbamate insecticides to be studied in this laboratory.

#### EXPERIMENTAL SECTION

**Crystal data:**  $C_7H_{14}N_2O_2S$ , mol wt 190.3, orthorhombic, *Pcab*,  $a = 10.204$  (7),  $b = 21.155$  (9), and  $c = 10.003$  (7) Å,  $\rho_c = 1.17$  g/cm<sup>3</sup>,  $Z = 8$ ,  $\mu = 2.83$  cm<sup>-1</sup> for Mo  $K\alpha$  ( $\lambda = 0.70954$  Å), mp 98 to ~100 °C.

Crystals suitable for x-ray diffraction analysis were obtained in the form of colorless plates by recrystallization from a benzene solution. A crystal of approximate dimensions  $0.2 \times 0.15 \times 0.2$  mm was selected and mounted on a glass fiber. The crystal was then placed on a four-circle diffractometer and initial  $\omega$ -oscillation photographs were taken using a Polaroid cassette. The photographs verified that the crystal selected was indeed single and, from these photographs, the coordinates of 15 reflections were then input into our automatic indexing program (Jacobson, 1976). The reduced cell and reduced cell scalars that resulted from this program indicated orthorhombic symmetry. Subsequent Polaroid oscillation pictures around each of the three axes in turn verified the presence of *mmm* Laue symmetry. Observed layer line spacings agreed, within experimental error, with those predicted for this cell by the indexing program.

Data were collected at room temperature using an automated four-circle diffractometer designed and built in the Ames Laboratory and equipped with a graphite reflective-beam monochromator and scintillation counter. Using Mo  $K\alpha$  radiation ( $\lambda = 0.70954$  Å), all data in the *hkl*, *hk $\bar{l}$* , and *h $\bar{k}l$* , and partial data of the *h $\bar{k}l$*  octants in a sphere defined by  $2\theta \leq 50^\circ$  were collected using a modified peak-height data collection technique. Each peak was maximized in  $\omega$ , and two measurements were then taken bracketing the peak center and differing by  $0.01^\circ$  in  $\omega$ , followed by background measurements on each side of the peak. All counting times were 2.5 s. If the measurement at the peak center did not exceed the background by 7 counts or more, which corresponds to approximately 1 to 2 standard deviations in the background at larger values of  $\theta$ , no further measurement was made on the reflection; this procedure yielded 2633 reflections.

As a general check on electronic and crystal stability, three reflections were selected as standards and were remeasured every 50 reflections. These three standards showed no significant change over the entire period of data collection.

The unit cell parameters and their standard deviations were determined by a least-squares fit (Williams, 1964) to

the  $\pm 2\theta$  values of 15 independent high  $\theta$  angle reflections whose centers were accurately determined by half-height counting techniques on the previously aligned four-circle diffractometer.

Intensity data were corrected for Lorentz and polarization effects, but absorption and extinction corrections were not deemed necessary. The maximum and minimum transmission factors were estimated to be 0.958 and 0.945, respectively. The estimated variance in each intensity was calculated by:

$$\sigma_I^2 = C_T + 2C_B + (0.03C_T)^2 + (0.03C_B)^2 \quad (1)$$

where  $C_T$  and  $C_B$  are the total and background count, respectively. The factor 0.03 represents an estimate of nonstatistical errors. The 532 independent observed reflections ( $|F_o| > 3\sigma_{F_o}$ ) were obtained after averaging values for equivalent reflections. The discrepancy factor between equivalent reflections was 0.043.

**Structural Determination and Refinement.** The position of the sulfur atom was obtained from analysis of a sharpened three-dimensional Patterson map. The remaining nonhydrogen atoms were found by successive structure factor and electron density map calculations (Hubbard et al., 1971). The atomic positions and isotropic thermal parameters were first refined by a block-diagonal matrix least-squares procedure (Sakurai, 1967) to a conventional discrepancy factor,  $R = \sum||F_o| - |F_c|| / \sum|F_o|$ , of 17.3%. The isotropic thermal parameters of most atoms were found to be quite large, exceeding  $10 \text{ \AA}^2$  in many cases.

Anisotropic refinement of all nonhydrogen atoms was then carried out utilizing a full-matrix least-squares procedure (Busing et al., 1962) to a final conventional discrepancy factor,  $R_w = (\sum w(|F_o| - |F_c|)^2) / \sum w|F_o|^2$ , of 0.112, where  $w = 1/\sigma_{F_o}^2$ . The atomic scattering factors were those of Hanson et al. (1960). The final positional and thermal parameters are listed in Table I.

Due to the large thermal parameters encountered in this analysis, no attempt was made to determine the positions of the hydrogen atoms. However, in order to try to explain the presence of such large thermal parameters, a crystal was cooled down below room temperature using a cold nitrogen gas stream. We found that shortly below room temperature ( $13 \pm 3$  °C) a phase transition took place in which the crystal changed from orthorhombic (*Pcab*) to monoclinic (*P2<sub>1</sub>/a*). The unit cell changes were as follows:  $a = 10.204 \rightarrow 10.245$  Å,  $b = 21.155 \rightarrow 20.991$  Å,  $c = 10.003 \rightarrow 10.065$  Å,  $\beta = 90.00 \rightarrow 91.97^\circ$ . No further analysis of the low-temperature form was carried out.

#### RESULTS AND DISCUSSION

Figures 1 and 2 provide illustrations (Johnson, 1971) of the molecule and the crystal structure, respectively. The

Table II. Selected Bond Lengths and Angles

Å		Deg	
C(1)-S(2)	1.849 (24)	C(1)-S(2)-C(3)	101.0 (9)
S(2)-C(3)	1.809 (16)	S(2)-C(3)-C(4)	108.3 (12)
C(3)-C(4)	1.464 (24)	S(2)-C(3)-C(5)	112.0 (11)
C(3)-C(5)	1.558 (24)	S(2)-C(3)-C(6)	103.1 (10)
C(3)-C(6)	1.559 (22)	C(4)-C(3)-C(5)	110.9 (14)
C(6)-N(7)	1.289 (20)	C(4)-C(3)-C(6)	109.9 (13)
N(7)-O(8)	1.448 (15)	C(5)-C(3)-C(6)	112.3 (13)
O(8)-C(9)	1.414 (19)	C(3)-C(6)-N(7)	118.7 (14)
C(9)-O(10)	1.228 (19)	C(6)-N(7)-O(8)	109.2 (12)
C(9)-N(11)	1.319 (19)	N(7)-O(8)-C(9)	113.1 (10)
N(11)-C(12)	1.463 (19)	O(8)-C(9)-O(10)	112.9 (13)
N(11)-O(10)	2.828 (15)	O(8)-C(9)-N(11)	118.5 (13)
		O(10)-C(9)-N(11)	128.6 (15)
		C(9)-N(11)-C(12)	119.0 (12)

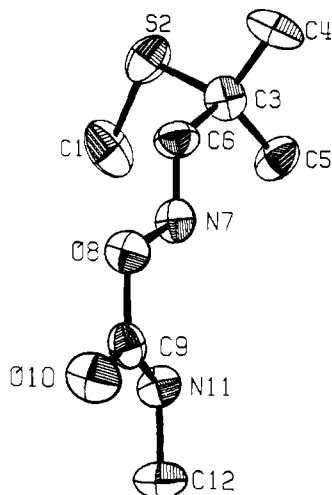


Figure 1. The aldicarb molecule. The thermal ellipsoids are drawn at the 20% probability level.

bond lengths and angles are listed in Table II while Table III presents least-squares plane information for several sections of the molecule, along with deviations from these planes. The angle between the planes formed by [C(3), C(6), N(7), and O(8)] and by [O(8), C(9), O(10), and N(11)] was found to be 9.2°.

As mentioned above, thermal motions of the atoms are large due to the fact that data collection was carried out at a temperature very close to a phase transition point. Although the estimated standard deviations in bond

Table III. Least-Squares Planes and Deviations (Å)

(1) Least-Squares Planes (Determined by Asterisked Atoms)		
(I)	$0.5066X + 0.8544Y - 0.1158Z = 8.5454$	
(II)	$0.4375X + 0.8989Y + 0.0226Z = 9.0709$	
X, Y, and Z are coordinates in Å along the a, b, and c axes, respectively		
(2) Deviations from the Least-Squares Planes (Å)		
Atom	I	II
C(1)	2.634	2.032
S(2)	1.634	1.004
C(3)	-0.026**	-0.571
C(4)	-0.987	-1.561
C(5)	-0.369	-1.032
C(6)	0.035**	-0.263
N(7)	0.014**	-0.210
O(8)	-0.009**	0.0**
C(9)	-0.102	0.003**
O(10)	-0.303	-0.001**
N(11)	0.020	-0.001**
C(12)	-0.112	-0.035

lengths and angles reflect the large thermal motion, some relevant conclusions concerning the dimensions of the carbamate group can still be drawn. As can be seen from Table III, this group is essentially planar. The C(9)-O(8) bond distance (1.414 (19)) appears to be significantly lengthened relative to those found in carboxylic acid esters, 1.358 (5) Å (Sutton, 1965), and also somewhat longer than that found for Mesurool (1.370 (4) Å) (Takusagawa and Jacobson, 1976), while the C(9)-O(10) and C(9)-N(11) bonds are approximately equal in length to those found in carboxylic acids, amides (Sutton, 1965), and urea (Carson and Donohue, 1969), respectively. Such distances along with bond angles O(8)-C(9)-O(10) (112.9°), O(8)-C(9)-N(11) (118.5°), and O(10)-C(9)-N(11) (128.6°) all suggest delocalization of the double bond from O(10) to C(9) to N(11), with the O(8) atom experiencing a slight reduction in electron density, thus weakening the C(9)-O(8) bond. Such a model would correlate quite well with any theory which proposes ready disruption of the C(9)-O(8) bond, as is usually assumed in a discussion of the interaction of carbamate insecticides with acetylcholinesterase (Kolbezen et al., 1954).

Distances and angles found in the remaining part of the aldicarb molecule appear normal. The N(11)···N(7) distance of 2.624 Å suggests the presence of a weak N-H···N intramolecular interaction (N(7)-H distance  $\approx$  2.2 Å,

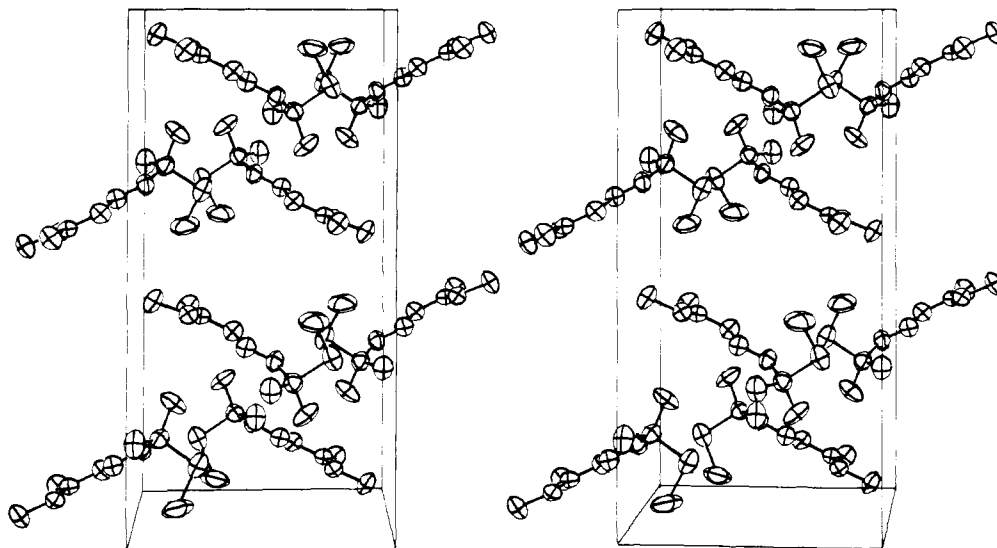


Figure 2. The crystal structure of aldicarb as viewed down the c axis. The a axis is horizontal.

$\angle(\text{N-H-N}) \approx 101^\circ$ ). Since the O(10) of a neighboring molecule is also close to N(11), 2.828 Å, a weak bifurcated hydrogen bond may be involved, as was found in the structure determination of Mesurol. No other significant short contacts are present; therefore, intermolecular interactions should have minimal effect on the molecular configuration found for the aldicarb molecule.

A crystal-structure investigation of methomyl is also underway as it has an LD<sub>50</sub> value intermediate between aldicarb and Mesurol. A comparison of the three structures will be given when the molecular structure of methomyl is reported.

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## Toxaphene and 1,1,1-Trichloro-2,2-bis(*p*-chlorophenyl)ethane (DDT) Losses from Cotton in an Agroecosystem Chamber

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Toxaphene at the rate of 200 to 267 mg/m<sup>2</sup> (2 to 2.7 kg/ha) and DDT at 100 to 133 mg/m<sup>2</sup> (1 to 1.3 kg/ha) were applied to cotton plants at weekly intervals for 6 weeks in an enclosed chamber (agroecosystem) and the residues monitored for 90 days. Twenty-four percent of the toxaphene and 15% of the DDTR (*p,p'*-DDE, *p,p'*-DDD, *p,p'*-DDT, and *o,p'*-DDT) volatilized and 20 and 24%, respectively, was found in the surface 1-cm soil. Most of the insecticide residues volatilized within 24 h from 18.9, 7.3, and 0.4 mg/m<sup>2</sup> per day (189, 73, and 4 g/ha per day) on days 1, 3, and 56 for toxaphene and 6.5, 1.8, and 0.2 mg/m<sup>2</sup> per day (65, 18, and 2 g/ha per day) for DDTR. Volatilization losses were insignificant, <0.1 mg/m<sup>2</sup> per day (<1 g/ha per day), for both toxaphene and DDTR after 90 days. Volatilization losses for both insecticides seemed to follow log concentration with log time the first week and then log concentration with linear time thereafter. Calculated first-order equation half-lives for volatilization of toxaphene, *p,p'*-DDT, *o,p'*-DDT, and *p,p'*-DDE were 15.1, 18.8, 14.3, and 15.1 days, respectively. On dry cotton leaves, toxaphene residues ranged from about 4000 to 700 ppm (100 to 18 mg/m<sup>2</sup>) from application to 56 days, and DDTR residues ranged from about 2000 to 380 ppm (50 to 10 mg/m<sup>2</sup>), respectively, for the same period.

Toxaphene (chlorinated camphene, 67–69% chlorine) has been used commercially for over 25 years and is the most widely used insecticide in the United States; about  $25.86 \times 10^6$  kg ( $57 \times 10^6$  lb) was used in agriculture in 1974 (von Rümker et al., 1974). Nearly 90% of the toxaphene produced is applied to cotton (*Gossypium hirsutum* L.) (von Rümker et al., 1974), and, before the 1973 restrictions

were placed upon using DDT, about half as much DDT was also used on cotton (a commonly used toxaphene/DDT mixture was 2/1). Although rarely have the adverse effects of these compounds on the environment been demonstrated, their fate, especially that of toxaphene, in a cotton field should be known. Environmental research has been limited on toxaphene, presumably because of its complexity, since toxaphene is a complex mixture of at least 175 compounds (Holmstead et al., 1974).

Recently, model systems have been used to trace the fate and movement of pesticides in the environment, i.e. the small aquatic/terrestrial ecosystem models of Metcalf et

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