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Crystallographic data for aldrin, $C_{12}H_8Cl_6$.

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Aldrin is a well-known insecticide. The Shell product was crystallized in the Departamento de Farmacología de la Escuela de Medicina de la Universidad Católica, Santiago, Chile.

Chemical data (*The Merck Index*, 1960).

Crystalline aldrin contains not less than 95% of the *endo-exo* isomer of 1,2,3,4,10,10-hexachloro-1,4,4*a*,5,8,8*a*-hexahydro-1,4,5,8-dimethanonaphthalene. It crystallizes at 100–102 °C when the composition approaches the ideal formula to the extent of at least 90%. It does not dissolve in water but is easily soluble in organic solvents. It is stable in the presence of organic and inorganic bases and to the action of hydrated metal chlorides.

The proposed chemical structure (Bird, Cookson & Crundwell, 1961) can be schematized as in Fig. 1.

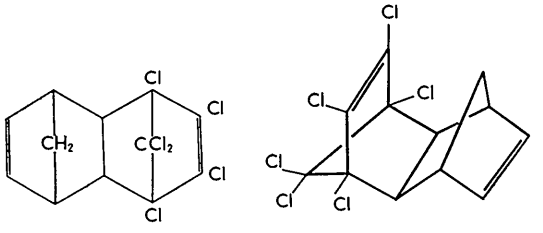

Fig. 1. Molecular structure of aldrin.

Physical properties.

Aldrin forms transparent white striated crystals. It shows a conchoidal fracture. It cleaves easily on (101) and the face just exfoliated presents a brilliant white colour. When exposed to X-rays the surface changes to a milky white. On exposure for over 24 hours, crystals as big as 0·5 × 0·5 × 0·8 mm change their habit and become cryptocrystalline. The density measured by the pycnometer method is 1·70 ± 0·01 g.cm^{-3}.

Crystallographic data.

Under the polarizing microscope, aldrin presents a biaxial character. The angle $2V$ measured by means of the extinction curves (Joel, 1963) is 23° ± 2°. The measurements were made on a two-axis goniometer (Villarroel & Joel, 1965) with the use of a red filter and an immersion liquid of refractive index 1·515.

Space group and cell constants were determined by oscillation, precession and Weissenberg photographs. Aldrin crystallizes in the monoclinic system with

$$a = 10{\cdot}76,\ b = 14{\cdot}70,\ c = 8{\cdot}98\ \text{Å},\ \beta = 93°.$$

The cell volume is 1420·93 Å^3, and for a cell content of 4 molecules the calculated density is 1·705 g.cm^{-3} which closely approaches the measured value.

The extinction rules, verified on all photographs, were as follows: $h0l$ reflexions present only if $h+l$ is even; $0k0$ reflexions present only if k is even. The space group compatible these conditions is $P2_1/n$ which is also found in compounds of the same type, such as γ-benzene hexachloride and 1,3-dichloronaphthalene.

The cell parameters given above were used to index the ASTM powder diagram:

hkl	d_o	d_c	*I*
011	7·7	7·650	5
101	7·2	7·077	25
10$\bar{1}$	6·7	6·720	40
111	6·4	6·380	100
120	6·1	6·078	80
11$\bar{1}$		6·111	
021	5·7	5·688	15
200	5·4	5·383	35
121	5·1	5·089	10
130	5·0	4·993	20
211	4·50	4·498	20
220	4·32	4·344	35
10$\bar{2}$	4·07	4·064	5
221	3·96	3·978	5
22$\bar{1}$	3·85	3·849	50
12$\bar{2}$	3·57	3·557	35
140	3·48	3·483	40
041	3·40	3·405	10
032	3·31	3·312	80
320	3·21	3·225	15
13$\bar{2}$	3·12	3·131	15
240	3·02	3·037	10
330	2·90	2·897	25
150	2·84	2·840	15
10$\bar{3}$		2·844	
051		2·841	
023	2·77	2·772	50
400	2·72	2·695	5
213	2·64	2·629	40
033	2·56	2·555	20
223	2·51	2·513	10
060	2·46	2·454	5
160	2·39	2·392	5
043	2·32	2·322	15
350	2·27	2·275	15
260	2·23	2·231	15
104		2·218	
024	2·15	2·147	10

No further work on this compound is contemplated at present.

References

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