Table 1. *Refined atomic parameters*

Positional parameters and thermal parameters, B_i, where $T_i = \exp(-B_i \sin^2\theta/\lambda^2)$, from the final least-squares analysis

No.	Type	x	σ_x	y	σ_y	z	σ_z	B
1	C	0·071	(5)	−0·140	(6)	0·028	(2)	1·0
2	C	0·056	(7)	−0·024	(5)	0·093	(3)	1·0
3	C	−0·011	(6)	0·124	(5)	0·063	(3)	1·0
4	Cl	−0·024	(2)	0·260	(2)	0·142	(1)	5·5
5	Cl	0·141	(2)	−0·335	(2)	0·071	(1)	5·5
6	O	0·095	(4)	−0·058	(4)	0·181	(2)	3·4
7	C	0·576	(6)	−0·132	(6)	0·057	(3)	1·9
8	C	0·542	(8)	0·007	(5)	0·098	(3)	1·9
9	C	0·479	(6)	0·130	(6)	0·037	(3)	1·9
10	CH_3	0·446	(6)	0·302	(7)	0·086	(3)	6·0
11	CH_3	0·654	(6)	−0·265	(8)	0·116	(4)	6·0
12	CH_3	0·590	(7)	0·034	(8)	0·202	(4)	6·0

deviations are listed in Table 1; the standard deviations are about 0·06 Å for the positions of the light atoms and 0·02 Å for the chlorine atoms. (These values are in approximately the expected ratio whereas, as Donohue & Trueblood point out, the standard deviations given by HW are greater for the chlorine atoms than for the lighter atoms.) The standard deviations in the temperature factors B are about 2·0 for the light atoms and 0·7 for the chlorine atoms. In the last least-squares refinement cycle no coordinate shift was as much as 1/3 of its standard deviation. The final R factor was 0·14 compared with the value 0·27 we obtained with the parameters of HW.

Our results indicate that, within the large experimental errors, both the chloranil and the hexamethylbenzene molecules are planar. The maximum deviation from the least-squares plane of the chloranil molecule, calculated with weights proportional to the atomic numbers,* is 0·087 Å for two of the carbon atoms; the maximum deviation from the best plane of the hexamethylbenzene molecule is 0·045 Å. The two planes are closely parallel, the calculated dihedral angle being 2·1°. Similarly, the bond distances show no significant deviations from the expected values, the extreme value 1·71 Å calculated for a pair of C–CH_3 bonds being only two standard deviations from the normal distance of 1·54 Å.

Accordingly, we reach the conclusion that the experimental data are compatible with planar molecules having normal dimensions and that it is not necessary to postulate, as HW have done, a zigzag arrangement of polarization bonds to explain the structure.

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References

DONOHUE, J. & TRUEBLOOD, K. N. (1956). *Acta Cryst.* **9**, 965.

HARDING, T. T. & WALLWORK, S. C. (1955). *Acta Cryst.* **8**, 787.

NYBURG, S. C. (1961). *X-ray Analysis of Organic Structures*, p. 287. New York: Academic Press.

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* It is clearly more appropriate to include all twelve atoms of the chloranil molecule in the calculation of the best plane than (as HW did) to consider only the six carbon atoms.

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The crystal structure of the chloranil-hexamethylbenzene complex.

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The refinement of the crystal structure of the chloranil-hexamethylbenzene complex by Jones & Marsh (1962) confirms the suggestion already made (Wallwork, 1961) that the molecular distortions originally reported (Harding & Wallwork, 1955) are probably not significant. They were mistakenly interpreted as being significant in the original work because the standard deviations of atomic positions were incorrectly calculated. In spite of the improvements in R and molecular planarity brought about by the recent refinement it is clear that the present X-ray data are not sufficient to establish accurate atomic positions. New and more extensive data are now being obtained at about −100 °C. and these will be used in a further refinement of the structure.

References

HARDING, T. T. & WALLWORK, S. C. (1955). *Acta Cryst.* **8**, 787.

JONES, N. D. & MARSH, R. E. (1962). *Acta Cryst.* **15**, 809.

WALLWORK, S. C. (1961). *J. Chem. Soc.*, p. 494.

Acta Cryst. (1962). **15**, 810

Some observations on growing crystals of argon.

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There is considerable interest in the measurement of the properties of single crystals of the rare gases [Kyoto Conference on Magnetism and Crystallography (1961), Cook (1961), Jones (1958), and Dobbs & Jones (1957)].