

are listed also in Table 1. The $_{\text{obs.}}N(z)$ results in Table 1 agree more closely with the centric $_{\bar{1}}N(z)$ distribution of Howells *et al.* than with the acentric $_{1}N(z)$ distribution.

Table 1. *The distribution of values of $|F|^2$ for azulene*

z	$_{\text{obs.}}N(z)$	σ	calc. $_{\bar{1}}N(z)$	σ	calc. $_{1}N(z)$	σ
0	0.000		0.000		0.000	
0.1	0.225	0.012	0.232	0.015	0.102	0.011
0.2	0.326	0.022	0.340	0.010	0.210	0.012
0.3	0.390	0.021	0.404	0.012	0.288	0.021
0.4	0.440	0.018	0.454	0.011	0.355	0.014
0.5	0.485	0.016	0.506	0.008	0.409	0.012
0.6	0.527	0.013	0.551	0.009	0.475	0.003
0.7	0.574	0.011	0.584	0.015	0.525	0.010
0.8	0.615	0.010	0.619	0.019	0.563	0.014
0.9	0.655	0.010	0.655	0.021	0.610	0.017
1.0	0.695	0.003	0.690	0.023	0.648	0.020
1.2	0.740	0.006	0.733	0.016	0.728	0.008
1.4	0.775	0.004	0.775	0.010	0.771	0.008
1.6	0.809	0.007	0.779	0.009	0.804	0.006
1.8	0.849	0.007	0.827	0.008	0.827	0.009
2.0	0.868	0.005	0.851	0.004	0.863	0.007

Although these results appeared fairly conclusive it was felt that a much more direct test of the two alternative structures was desirable and this was achieved by repeating the calculations detailed above but with values of $|F_c|$ for the two alternative structures replacing values of $|F_o|$. The results, denoted by $_{\text{calc.}}\bar{1}N(z)$ and $_{\text{calc.}}1N(z)$ for the disordered and ordered structures, respectively, are listed in Table 1 along with the appropriate standard deviations.

3. Discussion

An examination of the results listed in Table 1 shows that the differences between values of $_{\text{obs.}}N(z)$ and of $_{\text{calc.}}\bar{1}N(z)$, when compared with the appropriate standard deviations, can not be regarded as significant. On the

other hand the differences between values of $_{\text{obs.}}N(z)$ and of $_{\text{calc.}}1N(z)$ must be highly significant. These results provide strong evidence for the centrosymmetric disordered crystal structure attributed to azulene.

It is interesting that an examination of the statistical distribution of $|F_c|^2$ values should have provided a clear indication of which of the alternative structures is the more acceptable at a stage of refinement at which it was not possible to decide on the basis of the agreement between observed and calculated structure amplitudes that one structure was clearly correct and the other incorrect. If the problem of alternative structures should occur again it would seem worthwhile to repeat this type of analysis to distinguish the structure more likely to be correct.

An advantage possessed by this procedure for deciding between alternative space groups is that in the case of a molecule possessing one or more 'heavy' atoms and/or any appreciable degree of symmetry the necessity for deciding which of the many theoretical $N(z)$ distributions should be selected for comparison with the $_{\text{obs.}}N(z)$ distribution is avoided. Moreover sampling errors arising from the grouping adopted for the intensity data will be common to the $_{\text{calc.}}N(z)$ and $_{\text{obs.}}N(z)$ distributions and so will not normally cause trouble.

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Unit-cell dimensions and space groups of some optically active oxims. By H. A. J. OONK and J. B. HULSCHER, *Laboratorium v. Kristalchemie, Rijksuniversiteit, Catharijnesingel 51, Utrecht, the Netherlands*

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The oxims in question are camphoroxim, with its hydrochloride and hydrobromide, and carvoxim.

From systematic absences on Weissenberg photographs (Cu $K\alpha$ -radiation) the following space groups are found:

Carvoxim	$P2_1$	$Z=2$
Camphoroxim	$P2_1$	$Z=2$
Camphoroximhydrochloride	$P2_1^2 2_1$	$Z=4$
Camphoroximhydrobromide	$P2_1$	$Z=2$

The unit-cell dimensions of these compounds were determined from Weissenberg photographs, calibrated with NaCl-powder. The results are tabulated below and agree with the data given by Groth.

The structure analyses of carvoxim and camphoroxim are in progress.

	a	b	c	β
	in Å ± 0.02 Å			$\pm 0.1^\circ$
Carvoxim	10.17	11.64	8.54	100.8°
Camphoroxim	12.17	11.82	7.19	99.7
Camphoroxim HCl	21.15	6.96	7.44	—
Camphoroxim HBr	10.39	7.09	7.68	99.3
	a	b	c	β
	from X-rays			
Carvoxim	0.874	1	0.734	100.8°
Camphoroxim	1.021	1	0.608	99.7
Camphoroxim HCl	3.039	1	1.069	—
Camphoroxim HBr	1.465	1	1.083	99.3
	a	b	c	β
	Groth			
Carvoxim	0.8739	1	0.3667	100° 54'
Camphoroxim	1.0252	1	0.6073	99° 42'
Camphoroxim HCl				
Camphoroxim HBr	1.4699	1	1.0796	99° 19'