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Multiplicity of solutions of crystal-structure equations.

By H. HAUPTMAN and J. KARLE. *U.S. Naval Research Laboratory, Washington, D.C., U.S.A.*

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In a previous note (Hauptman & Karle, 1950), it was stated that $3(N-1)$ independent magnitudes were sufficient to determine the solution of the crystal-structure problem, and that for the case of three atoms in one dimension the solution is unique. The former statement is ambiguous and the latter incorrect. In general, $3(N-1)$ independent magnitudes are sufficient to determine a finite number of solutions of the crystal-structure problem (Karle & Hauptman, 1951). Since, as a general rule, many more than $3(N-1)$ magnitudes are available from experiment, a unique solution (except, of course, for ambiguities of the Patterson (1944) type) is determined by the data. The following example exhibits four solutions determined by the method described by Karle & Hauptman (1951) for the case of three atoms in one dimension when the minimum amount of algebraic data is used (two magnitudes).

	Co-ordinates of the atoms			
	Solution I	Solution II	Solution III	Solution IV
x_1	0·000 000	0·000 000	0·000 000	0·000 000
x_2	0·159 155	0·386 169	0·320 276	0·159 931
x_3	0·477 465	0·100 825	0·899 699	0·658 078
or, if $\phi_j = 2\pi x_j$				
ϕ_1 =	0·000°	0·000°	0·000°	0·000°
ϕ_2 =	57·296°	139·021°	115·299°	57·575°
ϕ_3 =	171·887°	36·297°	323·892°	236·908°

The atomic scattering factors are given by:

	Plane (100)	Plane (200)	Plane (300)
Atom 1	$f_{11}=0{\cdot}40$	$f_{21}=0{\cdot}30$	$f_{31}=0{\cdot}25$
Atom 2	$f_{12}=0{\cdot}30$	$f_{22}=0{\cdot}25$	$f_{32}=0{\cdot}23$
Atom 3	$f_{13}=0{\cdot}20$	$f_{23}=0{\cdot}16$	$f_{33}=0{\cdot}14$

If $$F_h = \sum_{j=1}^{3} f_{hj}\, e^{-2\pi i h x_j} \quad (h=1,2,3)$$

it is readily verified that

$$|F_1|^2 = 0{\cdot}211\,336 \quad |F_2|^2 = 0{\cdot}155\,563$$

for each of the four solutions. However,

$$|F_3|^2 = 0{\cdot}01921,\quad 0{\cdot}21466,\quad 0{\cdot}21978,\quad 0{\cdot}02565$$

for the respective solutions, so that the specification of $|F_3|^2$ (in addition to $|F_1|^2$ and $|F_2|^2$) would be sufficient to determine a unique solution.

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Notes and News

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Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing

The National Bureau of Standards announces the publication of *Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing*. The first six tables give the spacing values for the angles θ from 0 to 90° at intervals of 0·01°. These tables were calculated by using the $K\alpha_1$ wave-