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## Comments on Allegra's paper »A simplified formula for the calculation of the X-ray intensity diffracted by a monodimensionally disordered structure«.

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The intensity of X-rays diffracted by a one-dimensionally disordered crystal was given, in a matrix form, first by Hendricks & Teller (1942) and also by Kakinoki & Komura (1952) as follows:

$$I = N \text{ spur } \mathbf{VF} + \sum_{n=1}^{N-1} (N-n) \text{ spur } \mathbf{VFQ}^n + \text{conj.}, \quad (1)$$

where:

$N$ is the total number of layers;
$(\mathbf{VF})_{ts} = w_s V_s V_t^*$;
$(\mathbf{Q})_{st} = P_{st} \exp(-i\varphi_s)$;
$\varphi_s$ is the phase shift due to the layer of $s$th kind;
$V_s$ is the layer form factor of the layer of $s$th kind;
$w_s$ is the probability of finding the layer of $s$th kind;
$P_{st}$ is the probability of finding the layer of $t$th kind after that of $s$th kind;
conj. means the complex conjugate of the second term in (1).

Allegra (1961) recently reported a new method of carrying out the summation in (1) regardless of whether the matrix **Q** could be diagonalized by the similarity operation $\mathbf{OQO}^{-1}$ or not. His formula is rewritten by using our notation as

$$I_{\text{av.}} = \text{spur } \mathbf{VF}(\mathbf{1}-\mathbf{Q})^{-1} + \text{conj.} - \text{spur } \mathbf{VF}, \quad (2)$$

where $N$ in (1) is taken as infinite. The same result has already been given by us (Kakinoki & Komura, 1952) leaving $N$ as finite:

$$I = N\{\text{spur } \mathbf{VF} + \text{spur } \mathbf{VFQ}(\mathbf{1}-\mathbf{Q})^{-1} + \text{conj.}\} + \text{spur } \mathbf{VF}(\mathbf{Q}^{N+1}-\mathbf{Q})(\mathbf{1}-\mathbf{Q})^{-2} + \text{conj.} \quad (3)$$

The first three terms (called diffuse term) are found to be the same with (2) in which $I_{\text{av.}}$ means the average intensity per layer while $I$ in (1) is the average per crystallite with $N$ layers. The rest of (3) (called higher term) contributes to the intensity when $N$ is very small or when the structure tends to regular one.

In our study calculation of the intensity equation (1) has further progressed even when the matrix **Q** cannot be diagonalized. The idea is to use a Jordan's normal form reduced from any type of matrix **Q** by the similarity transformation. Let us take a simple example in which the eigenvalues of $3 \times 3\mathbf{Q}$ matrix are all equal and the normal form is expressed by

$$\mathbf{OQO}^{-1} = \mathbf{Q}_0 = \begin{pmatrix} x_1 & 1 & 0 \\ 0 & x_1 & 1 \\ 0 & 0 & x_1 \end{pmatrix} \quad (4)$$

In this case spur $\mathbf{VFQ}^n$ can be written in a form as

$$\text{spur } \mathbf{VFQ}^n = c_1^{(0)} x_1^n + c_1^{(1)} n x_1^{n-1} + c_1^{(2)} \tfrac{1}{2} n(n-1) x_1^{n-2}, \quad (5)$$

and then (1) (neglecting higher term) can be expressed by

$$I = N\left\{\frac{c_1^{(0)}}{(1-x_1)} + \frac{c_1^{(1)}}{(1-x_1)^2} + \frac{c_1^{(2)}}{(1-x_1)^3} + \text{conj.} - \text{spur } \mathbf{VF}\right\}. \quad (6)$$

$c_1^{(0)}, c_1^{(1)}, c_1^{(2)}$ in (6) are the solutions of simultaneous equations obtained from (5) by putting $n = 0$, 1 and 2. There is no need, in this calculation, to evaluate **O**, $\mathbf{O}^{-1}$ and $\mathbf{OVFO}^{-1}$.

Further simplification can be made without obtaining eigenvalues and $c_\nu$'s. If we use the relations between roots and coefficients in

$$\det(x\mathbf{1}-\mathbf{Q}) = \sum_{n=0}^{S} a_n x^{S-n}, \quad (7)$$

and other relations such as

$$J_n = \text{spur } \mathbf{VFQ}^n = \sum_{\nu} \sum_{p_\nu} c_\nu^{(p_\nu)} \frac{n(n-1)\ldots(n-p_\nu+1)}{p_\nu!} x_\nu^{n-p_\nu}. \quad (8)$$

$I$ in (1) can be expressed in a general form as

$$I = ND + H,$$
$$D = D' + \text{conj.} - J_0, \quad H \text{ is the higher term,}$$
$$D' = \sum_{n=1}^{S-1} \sum_{m=0}^{n} a_{n-m} J_m \Big/ \sum_{n=0}^{S} a_n. \quad (9)$$

This equation is found to be valid for any type of **Q**. The general derivation and discussion of this result will be given in this Journal in a near future.

### References

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## The molecular dimensions of 2:3-dihydro-2:3-methylene-1:4-naphthaquinone: a comparison of the results of two- and three-dimensional analysis.

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The compound, $C_{11}H_8O_2$, with the chemical constitution implied in Fig. 1, crystallizes in the space group $P2_1/m$ with two molecules in a cell of dimensions,

$$a = 6{\cdot}98,\ b = 10{\cdot}55,\ c = 5{\cdot}46 \text{ Å};\ \beta = 94{\cdot}5°.$$

For a non-planar molecule, it is remarkable in having