Short Communications

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Comments on the paper *The determination of cyclicity hexagonality and other properties of polytypes* by Dornberger-Schiff, Schmittler and Farkas-Jahnke.

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Dornberger-Schiff *et al.* [*Acta Cryst.* (1971), A**27**, 216] derived some relations between the Zhdanov symbol and their $\pi(m,p)$ which is derived from the Fourier transform of the unitary intensities. It is pointed out that the same and other relations had previously been derived by the present authors. The most general forms of these relations are given.

Recently, Dornberger-Schiff, Schmittler & Farkas-Jahnke (1971) derived some relations between the Zhdanov symbol (Zhdanov, 1945) for the close-packed structures and the Patterson function $\pi(m,p)$, in their definition obtained from the cosine and sine transformations of the unitary intensities. However, the same and other relations had previously been derived by us (Kakinoki, Kodera & Aikami, 1969). The correspondence between their notation and ours is as follows:

Dornberger-Schiff *et al.*						
A	B	C	αN	CN	$\pi(0,p)$	$\pi(1,p)$
Kakinoki *et al.** †						
A	C	B	$2K$	$-(a-b)$	N_m^0	N_m^-
Dornberger-Schiff *et al.*						
$\pi(-1,p)$		[101]		[010]	[1010]	
Kakinoki *et al.*						
N_m^+		n_1		$n_{\bar{1}}$	$n_{1\bar{1}}$	...

where N_m^0 is the number of pairs of two layers of the same kind separated by m layers, N_m^+ is the number of positive pairs ($A\ldots B$, $B\ldots C$ or $C\ldots A$) and N_m^- is the number of negative pairs ($A\ldots C$, $C\ldots B$ or $B\ldots A$). n_1, $n_{\bar{1}}$, n_2, $n_{\bar{2}}$, ... are the frequencies of letters 1, $\bar{1}$, 2, $\bar{2}$, ... contained in the Zhdanov symbol and $n_{1\bar{1}}$, $n_{\bar{2}1}$, $n_{1\bar{2}1}$, ... are the frequencies of sequences $1\bar{1}$, $\bar{2}1$, $1\bar{2}1$, ... in this symbol, which is expressed as $(a_1\bar{b}_1a_2\bar{b}_2\ldots a_k\bar{b}_k)$ with conditions $a=\sum_{i=1}^{k}a_i$, $b=\sum_{i=1}^{k}b_i$ and $a+b=P$, where P is the period and a and b are the total numbers of positive and negative vectors in a period respectively; $2k$ is the number of partitions in the Zhdanov symbol. The other correspondence is as follows: $N\leftrightarrow P$, $p\leftrightarrow m$, and m in $\pi(m,p)$ stands for 0, 1 and -1, which correspond to our superscripts 0, $-$ and $+$ respectively. α and C are the hexagonality and the cyclicity defined by them.

Some relations between the Zhdanov symbol and N_m^0 and $D_m^*=D_m/3=(N_m^+-N_m^-)/3$ were given in Table 1 in our previous communication, including all the relations obtained by Dornberger-Schiff *et al.* (1971). We can now give a complete set of the relations as shown below.

In deriving general forms of N_m^0 and D_m^* for any m, it is convenient to use a quantity, ${}_TM_S$, defined as $\sum_{(ZS)}(\pm)n_{(ZS)}$, where (ZS) means a Zhdanov sequence corresponding to one of ${}_TC_S=T!/\{S!(T-S)!\}$ routes in a $(S,T-S)$-net as shown in Fig. 1, and $(\pm)$ means $+$ or $-$ according as the number of letters in the (ZS) is odd or even. In Fig. 1, a net with $T=5$ and $S=3$ is shown, where ↖ and ↗ correspond to a positive and negative vectors respectively. Some examples of ${}_TM_S$ are shown as follows:

$$
\begin{aligned}
&{}_TM_T=n_T,\ {}_TM_0=n_{\bar{T}},\ {}_2M_1=-(n_{1\bar{1}}+n_{\bar{1}1})\\
&{}_5M_3=-(n_{3\bar{2}}+n_{\bar{2}3})+(n_{2\bar{2}1}+n_{1\bar{2}2}+n_{\bar{1}3\bar{1}})\\
&\quad-(n_{2\bar{1}1\bar{1}}+n_{1\bar{1}2\bar{1}}+n_{\bar{1}2\bar{1}1}+n_{\bar{1}1\bar{1}2})+n_{1\bar{1}1\bar{1}1}\,.
\end{aligned}
$$

Using ${}_TM_S$, we can derive general forms of N_m^0 and D_m^* as follows:

$\boxed{m=3r}$ (r: integer)

$$
\begin{aligned}
N_m^0 &= P-4rk+r(n_1+n_{\bar{1}})\\
&\quad+\sum_{t=1}^{r-1}(r-t)\Big(4\sum_{s=0}^{t}{}_{3t}M_{3s}-2\sum_{s=1}^{t}{}_{3t}M_{3s-1}-2\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}\\
&\quad-2\sum_{s=1}^{t}{}_{3t+1}M_{3s-1}+\sum_{s=0}^{t}{}_{3t+1}M_{3s+1}+\sum_{s=0}^{t}{}_{3t+1}M_{3s}\\
&\quad-2\sum_{s=0}^{t-1}{}_{3t-1}M_{3s+1}+\sum_{s=0}^{t-1}{}_{3t-1}M_{3s}+\sum_{s=1}^{t}{}_{3t-1}M_{3s-1}\Big)\\
D_m^* &= -r(n_1-n_{\bar{1}})+\sum_{t=1}^{r-1}(r-t)\Big(2\sum_{s=1}^{t}{}_{3t}M_{3s-1}-2\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}\\
&\quad+\sum_{s=0}^{t}{}_{3t+1}M_{3s}-\sum_{s=0}^{t}{}_{3t+1}M_{3s+1}+\sum_{s=1}^{t}{}_{3t-1}M_{3s-1}\\
&\quad-\sum_{s=0}^{t-1}{}_{3t-1}M_{3s}\Big)
\end{aligned}
$$

* According to the notation in *International Tables for X-ray Crystallography* (Patterson & Kasper, 1959), coordinates for our A, B and C are taken as (0,0), $(\frac{2}{3},\frac{1}{3})$ and $(\frac{1}{3},\frac{2}{3})$ respectively, in the hexagonal lattice.

† In order to avoid confusion, m in m_1, $m_{\bar{1}}$, $m_{1\bar{1}}$, ... in our short communication is replaced by n in the present comments.

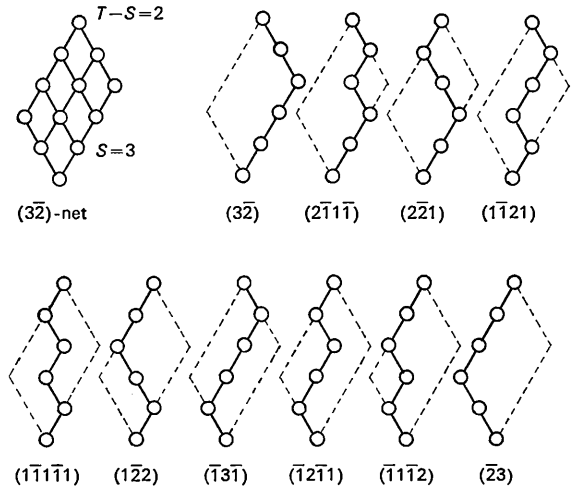

Fig. 1. Examples of Zhdanov sequences, (ZS), belonging to the (3,$\bar{2}$)-net.

$\boxed{m=3r+1}$

$$N_m^0=2rk-2r(n_1+n_{\bar{1}})+r(n_2+n_{\bar{2}})+2r(n_{1\bar{1}}+n_{\bar{1}1})$$
$$+\sum_{t=1}^{r-1}(r-t)\left(4\sum_{s=1}^{t}{}_{3t+1}M_{3s-1}-2\sum_{s=0}^{t}{}_{3t+1}M_{3s+1}\right.$$
$$-2\sum_{s=0}^{t}{}_{3t+1}M_{3s}-2\sum_{s=0}^{t}{}_{3t+2}M_{3s+1}+\sum_{s=0}^{t}{}_{3t+2}M_{3s}$$
$$+\sum_{s=1}^{t+1}{}_{3t+2}M_{3s-1}-2\sum_{s=0}^{t}{}_{3t}M_{3s}+\sum_{s=1}^{t}{}_{3t}M_{3s-1}$$
$$\left.+\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}\right)$$
$$D_m^*=(a-b)/3+2r(n_1-n_{\bar{1}})+r(n_2-n_{\bar{2}})$$
$$+\sum_{t=1}^{r-1}(r-t)\left(2\sum_{s=0}^{t}{}_{3t+1}M_{3s+1}-2\sum_{s=0}^{t}{}_{3t+1}M_{3s}\right.$$
$$+\sum_{s=1}^{t+1}{}_{3t+2}M_{3s-1}-\sum_{s=0}^{t}{}_{3t+2}M_{3s}+\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}$$
$$\left.-\sum_{s=1}^{t}{}_{3t}M_{3s-1}\right)$$

$\boxed{m=3r-1}$

$$N_m^0=2rk$$
$$+\sum_{t=1}^{r-1}(r-t)\left(4\sum_{s=0}^{t-1}{}_{3t-1}M_{3s+1}-2\sum_{s=0}^{t-1}{}_{3t-1}M_{3s}\right.$$
$$-2\sum_{s=1}^{t}{}_{3t-1}M_{3s-1}-2\sum_{s=0}^{t}{}_{3t}M_{3s}+\sum_{s=1}^{t}{}_{3t}M_{3s-1}$$
$$+\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}-2\sum_{s=1}^{t-1}{}_{3t-2}M_{3s-1}+\sum_{s=0}^{t-1}{}_{3t-2}M_{3s+1}$$
$$\left.+\sum_{s=0}^{t-1}{}_{3t-2}M_{3s}\right)$$
$$D_m^*=-(a-b)/3+\sum_{t=1}^{r-1}(r-t)\left(2\sum_{s=2}^{t-1}{}_{3t-1}M_{3s}-2\sum_{s=1}^{t}{}_{3t-1}M_{3s-1}\right.$$
$$+\sum_{s=0}^{t-1}{}_{3t}M_{3s+1}-\sum_{s=1}^{t}{}_{3t}M_{3s-1}+\sum_{s=0}^{t-1}{}_{3t-2}M_{3s}$$
$$\left.-\sum_{s=0}^{t-1}{}_{3t-2}M_{3s+1}\right).$$

Even when the structure is rhombohedral, these general forms are also valid with some modifications in the definitions of quantities used.

The details will be reported in the near future.

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A statistical evaluation of absorption.

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This paper reports an empirical method for evaluating the three-dimensional transmission by the statistical treatment of the intensity differences among equivalent reflexions, and the accuracy of the method is discussed.

In the course of a crystal structure analysis, small crystals are usually used for collecting intensity data without any correction for absorption. However, it is essential to give proper treatment of absorption effects when great accuracy is required. Numerical or analytical methods for absorption correction are very accurate, as is well known, but they are not always practical because they require an exact knowledge of the crystal shape and much computer-time.

In the study of protein crystal structure, it is necessary to take account not only the crystal but also its mounting, which usually comprises a glass capillary in which it is enclosed in contact with some mother liquor. North,