(II) Consider the case when all n_i are equal to 3. It is readily seen from Fig. 2 that the interval becomes 3 for axis A, and 2 and 4 for axes B and C.

(III) If we take the case when all are equal to 2 and starting from A (say), it is seen that the interval becomes 4 for axes A and C while it is 2 for axis B. (Fig. 3).

(IV) If in the sequence n_1, n_2, n_3 ... 2's are sandwiched between 3's, then again the results of cases (II) and (III) become operative and thus any combination of 3's and 2's produces only intervals of 2, 3 and 4 and none greater than 4 (Fig. 4).

The case in which the interval can be greater than 4 can be realized only if 1's are involved in the Zhdanov symbol. Thus a sequence of complete 1's (polytype 2H) produces intervals of 2 in two of the axes while the third axis is completely unoccupied (it may be considered to be of infinite interval). This infinite interval can be brought down to a finite one of any desired value if an appropriate sequence of 1's is sandwiched by n_1 and n_2, with both n_1 and $n_2 \geq 2$. (Fig. 5). Thus, the interval sequence need not be restricted to 2, 3 and 4 provided 1's occur in the Zhdanov symbol. This is not the case in SiC polytypes, and the observed intervals of 2, 3 and 4 can thus be attributed to the absence of 1's in the Zhdanov symbol. These remarks can be readily extended to the rhombohedral lattice where the axes A, B and C become equivalent.

The non-occurrence of 1's in the Zhdanov symbol might itself find an explanation from a physical mechanism, such as for instance Mitchell's (1957) treatment based on screw dislocations, and the generation of certain family series of polytypes or from Schneer's (1955) treatment. These, however, need not concern us here.

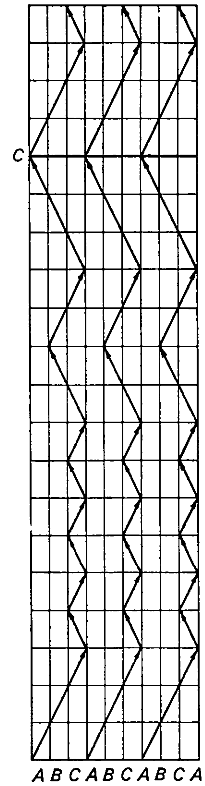

Fig. 5. Hypothetical polytype 16H with Zhdanov symbol 3(11)$_3$223. Note an interval of 10 occurring along B.

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A clarification of differences in site orientation in crystals.

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Tables are presented whereby physically relevant differences in the relationship of the elements of symmetry of a Wyckoff site to those of the crystal class can be distinguished.

In *International Tables for X-ray Crystallography*, (1969) the various sets of equivalent points (Wyckoff sites) are described by the point group of the elements of symmetry passing through a typical point (*i.e.* the site group), the number of points in the set, their coordinates, the Wyckoff label and some information of relevance to X-ray crystallographers. For those interested in spectroscopic and other tensorial properties of crystals, however, this is often insufficient and a detailed examination of the coordinates has hitherto been necessary in some cases where differences in site orientation within the unit cell can lead to different correlations of the representations of the crystal class and those of the site group.

The problem can be illustrated simply by means of the crystal class $D_2=222$. A site of symmetry $C_2=2$ can lie on the crystallographic x, y or z axes of the unit cell and accordingly the correlation between the representations of D_2 and C_2 is given on descent in symmetry by the subgroup table

D_2	C_2^x	C_2^y	C_2^z
A	A	A	A
B_1	B	B	A
B_2	B	A	B
B_3	A	B	B

and on ascent in symmetry by the supergroup tables

Table 1. *Orientation of C_2 sites in crystals*

Supergroup	Orientation	Wyckoff sites
	$C_2 \to C_2^z$	$D_2^1(q,r,s,t)$, $D_2^3(a,b)$, $D_2^6(i,j,k)$, $D_2^7(g,h)$, $D_2^8(i,j)$, $D_2^9(c)$.
D_2	$C_2 \to C_2^y$	$D_2^1(m,n,o,p)$, $D_2^2(c,d)$, $D_2^5(b)$, $D_2^6(g,h)$, $D_2^7(f,i)$, $D_2^8(g,h)$, $D_2^9(b)$.
	$C_2 \to C_2^x$	$D_2^1(i,j,k,l)$ $D_2^2(a,b)$, $D_2^5(a)$, $D_2^6(e,f)$, $D_2^7(e,j)$, $D_2^8(e,f)$, $D_2^9(a)$.
	$C_2 \to C_2$	$D_4^1(i)$, $D_4^2(d)$, $D_4^5(g,h,i)$, $D_4^6(c,d)$, $D_4^9(f)$, $D_4^{10}(c)$.
D_4	$C_2 \to C_2'$	$D_4^1(l,m,n,o)$, $D_4^3(a,b)$, $D_4^5(j,k,l,m)$, $D_4^7(a,b)$, $D_4^9(h,i)$, $D_4^{10}(f)$.
	$C_2 \to C_2''$	$D_4^1(j,k)$, $D_4^2(e,f)$, $D_4^3(c)$, $D_4^4(a)$, $D_4^5(n,o)$, $D_4^6(e,f)$, $D_4^7(c)$, $D_4^8(a)$, $D_4^9(g,j)$, $D_4^{10}(d,e)$
	$C_2 \to C_2$	$D_6^1(i)$, $D_6^4(e,f)$, $D_6^5(e,f)$.
D_6	$C_2 \to C_2'$	$D_6^1(j,k)$, $D_6^2(a)$, $D_6^3(a)$, $D_6^4(g,h)$, $D_6^5(g,h)$, $D_6^6(g)$.
	$C_2 \to C_2''$	$D_6^1(l,m)$, $D_6^2(b)$, $D_6^3(b)$, $D_6^4(i,j)$, $D_6^5(i,j)$, $D_6^6(h)$.
	$C_2 \to C_2$	$D_{2d}^1(m)$, $D_{2d}^2(k,l,m)$, $D_{2d}^3(d)$, $D_{2d}^4(c,d)$, $D_{2d}^6(g,h,i)$, $D_{2d}^7(e,f)$, $D_{2d}^8(e,h)$, $D_{2d}^{10}(f,g)$, $D_{2d}^{11}(h)$, $D_{2d}^{12}(c)$.
D_{2d}	$C_2 \to C_2'$	$D_{2d}^1(i,j,k,l)$, $D_{2d}^2(g,h,i,j)$, $D_{2d}^5(h,i)$, $D_{2d}^6(e,f)$, $D_{2d}^7(g,h)$, $D_{2d}^8(f,g)$, $D_{2d}^9(g,h)$, $D_{2d}^{10}(e,h)$, $D_{2d}^{11}(f,g)$, $D_{2d}^{12}(d)$.
	$C_2 \to C_2^z$	$D_{2h}^2(k,l)$, $D_{2h}^3(m,n,o,p)$, $D_{2h}^4(k,l)$, $D_{2h}^6(c)$, $D_{2h}^8(d,e)$, $D_{2h}^9(e,f)$, $D_{2h}^{10}(c,d)$, $D_{2h}^{12}(e,f)$, $D_{2h}^{19}(m)$, $D_{2h}^{20}(i,j,k)$, $D_{2h}^{21}(l)$, $D_{2h}^{22}(g,h)$, $D_{2h}^{23}(j)$, $D_{2h}^{24}(g)$, $D_{2h}^{26}(h,i)$, $D_{2h}^{27}(e)$.
D_{2h}	$C_2 \to C_2^y$	$D_{2h}^2(i,j)$, $D_{2h}^3(k,l)$, $D_{2h}^4(i,j)$, $D_{2h}^5(g,h)$, $D_{2h}^7(g)$, $D_{2h}^8(c)$, $D_{2h}^{14}(c)$, $D_{2h}^{18}(e)$, $D_{2h}^{20}(h)$, $D_{2h}^{21}(j,k)$, $D_{2h}^{22}(f)$, $D_{2h}^{23}(k)$, $D_{2h}^{24}(f)$, $D_{2h}^{26}(g)$, $D_{2h}^{27}(d)$, $D_{2h}^{28}(g)$.
	$C_2 \to C_2^x$	$D_{2h}^2(g,h)$, $D_{2h}^3(i,j)$, $D_{2h}^4(g,h)$, $D_{2h}^6(d)$, $D_{2h}^7(e,f)$, $D_{2h}^{11}(c)$, $D_{2h}^{17}(e)$, $D_{2h}^{18}(d)$, $D_{2h}^{20}(g)$, $D_{2h}^{21}(h,i)$, $D_{2h}^{22}(e)$, $D_{2h}^{23}(l)$, $D_{2h}^{24}(e)$, $D_{2h}^{26}(f)$, $D_{2h}^{27}(c)$, $D_{2h}^{28}(f)$.
	$C_2 \to C_2$	$D_{4h}^2(i)$, $D_{4h}^4(g)$, $D_{4h}^6(f)$, $D_{4h}^8(e)$, $D_{4h}^{10}(k)$, $D_{4h}^{11}(f,g)$, $D_{4h}^{12}(h)$, $D_{4h}^{13}(e,f)$, $D_{2h}^{14}(h)$, $D_{4h}^{16}(f)$, $D_{4h}^{20}(d)$.
D_{4h}	$C_2 \to C_2'$	$D_{4h}^2(k,l)$, $D_{4h}^3(k,l)$, $D_{4h}^4(i,j)$, $D_{4h}^{10}(l,m)$, $D_{4h}^{11}(h,i)$, $D_{4h}^{12}(i,j)$, $D_{4h}^{18}(j)$, $D_{4h}^{19}(f)$, $D_{4h}^{20}(e)$.
	$C_2 \to C_2''$	$D_{4h}^2(j)$, $D_{4h}^3(i,j)$, $D_{4h}^4(h)$, $D_{4h}^6(g)$, $D_{4h}^7(g,h)$, $D_{4h}^8(f)$, $D_{4h}^9(n)$, $D_{4h}^{11}(j)$, $D_{4h}^{12}(k,l)$, $D_{4h}^{13}(g)$, $D_{4h}^{15}(f)$, $D_{4h}^{16}(g,h)$, $D_{4h}^{17}(k)$, $D_{4h}^{18}(i)$, $D_{4h}^{19}(g)$, $D_{4h}^{20}(f)$.
	$C_2 \to C_2$	$D_{6h}^2(i)$.
D_{6h}	$C_2 \to C_2'$	$D_{6h}^2(j)$, $D_{6h}^4(i)$.
	$C_2 \to C_2''$	$D_{6h}^2(k)$, $D_{6h}^3(i)$.
O	$C_2 \to C_2$	$O^1(h)$, $O^2(h,i,j)$, $O^3(i)$, $O^4(f)$, $O^5(g)$, $O^8(f)$.
	$C_2 \to C_2'$	$O^1(i,j)$, $O^2(k,l)$, $O^3(g,h)$, $O^4(g)$, $O^5(h,i)$, $O^6(d)$, $O^7(d)$ $O^8(g,h)$.
O_h	$C_2 \to C_2'$	$O_h^2(g)$, $O_h^4(h)$, $O_h^8(f)$, $O_h^{10}(f)$.
	$C_2 \to C_2'$	$O_h^2(h)$, $O_h^3(j)$, $O_h^4((i,j)$, $O_h^6(h)$, $O_h^7(h)$, $O_h^8(g)$, $O_h^9(i)$, $O_h^{10}(g)$.

Table 2. *Orientation of $C_{1h}(=C_s)$ sites in crystals*

Supergroup	Orientation	Wyckoff sites
C_{2v}	$\sigma \to \sigma^{zx}$	$C_{2v}^1(e,f)$, $C_{2v}^{11}(d)$, $C_{2v}^{14}(c)$, $C_{2v}^{15}(c)$, $C_{2v}^{18}(d)$, $C_{2v}^{20}(c)$.
	$\sigma \to \sigma^{yz}$	$C_{2v}^1(g,h)$, $C_{2v}^2(a,b)$, $C_{2v}^4(c)$, $C_{2v}^7(a)$, $C_{2v}^{11}(e)$, $C_{2v}^{12}(a)$, $C_{2v}^{14}(d,e)$, $C_{2v}^{16}(b)$, $C_{2v}^{18}(c)$, $C_{2v}^{20}(d)$, $C_{2v}^{22}(b)$.
C_{4v}	$\sigma \to \sigma_v$	$C_{4v}^1(e,f)$, $C_{4v}^7(d,e)$, $C_{4v}^9(d)$, $C_{4v}^{11}(b)$.
	$\sigma \to \sigma_d$	$C_{4v}^1(d)$, $C_{4v}^2(c)$, $C_{4v}^3(d)$, $C_{4v}^4(c)$, $C_{4v}^9(c)$, $C_{4v}^{10}(c)$.
C_{6v}	$\sigma \to \sigma_v$	$C_{6v}^1(e)$, $C_{6v}^4(c)$.
	$\sigma \to \sigma_d$	$C_{6v}^1(d)$, $C_{6v}^3(c)$.
	$\sigma \to \sigma^{zx}$	$D_{2h}^1(w,x)$, $D_{2h}^5(i,j)$, $D_{2h}^{13}(f)$, $D_{2h}^{16}(c)$, $D_{2h}^{19}(o)$, $D_{2h}^{21}(n)$, $D_{2h}^{23}(n)$, $D_{2h}^{25}(m)$, $D_{2h}^{28}(i)$.
D_{2h}	$\sigma \to \sigma^{xy}$	$D_{2h}^1(y,z)$, $D_{2h}^3(q)$, $D_{2h}^9(g,h)$, $D_{2h}^{11}(d)$, $D_{2h}^{12}(g)$, $D_{2h}^{17}(g)$, $D_{2h}^{19}(p,q)$, $D_{2h}^{20}(l)$, $D_{2h}^{23}(o)$, $D_{2h}^{25}(n)$, $D_{2h}^{26}(j)$.
	$\sigma \to \sigma^{yz}$	$D_{2h}^1(u,v)$, $D_{2h}^5(k)$, $D_{2h}^7(h)$, $D_{2h}^{13}(e)$, $D_{2h}^{17}(f)$, $D_{2h}^{18}(f)$, $D_{2h}^{19}(n)$, $D_{2h}^{21}(m)$, $D_{2h}^{23}(m)$, $D_{2h}^{25}(l)$, $D_{2h}^{28}(h)$.
D_{3h}	$\sigma \to \sigma_h$	$D_{3h}^1(l,m)$, $D_{3h}^2(k)$, $D_{3h}^3(j,k)$, $D_{4h}^4(h)$.
	$\sigma \to \sigma_v$	$D_{3h}^1(n)$, $D_{3h}^3(i)$.
	$\sigma \to \sigma_h$	$D_{4h}^1(p,q)$, $D_{4h}^2(m)$, $D_{4h}^5(i,j)$, $D_{4h}^6(h)$, $D_{4h}^9(q)$, $D_{4h}^{10}(n)$, $D_{4h}^{13}(h)$, $D_{4h}^{14}(i)$, $D_{4h}^{17}(l)$, $D_{4h}^{18}(k)$.
D_{4h}	$\sigma \to \sigma_v$	$D_{4h}^1(s,t)$, $D_{4h}^7(i)$, $D_{4h}^9(o,p)$, $D_{4h}^{15}(g)$, $D_{4h}^{17}(n)$, $D_{4h}^{19}(h)$.
	$\sigma \to \sigma_d$	$D_{4h}^1(r)$, $D_{4h}^3(m)$, $D_{4h}^5(k)$, $D_{4h}^7(j)$, $D_{4h}^{10}(o)$, $D_{4h}^{12}(m)$, $D_{4h}^{14}(j)$, $D_{4h}^{16}(i)$, $D_{4h}^{17}(m)$, $D_{4h}^{18}(l)$.
	$\sigma \to \sigma_h$	$D_{6h}^1(p,q)$, $D_{6h}^2(l)$, $D_{6h}^3(j)$, $D_{6h}^4(j)$.
D_{6h}	$\sigma \to \sigma_v$	$D_{6h}^1(n)$, $D_{6h}^3(k)$.
	$\sigma \to \sigma_d$	$D_{6h}^1(o)$, $D_{6h}^4(k)$.
O_h	$\sigma \to \sigma_h$	$O_h^1(k,l)$, $O_h^3(k)$, $O_h^5(j)$, $O_h^6(i)$, $O_h^9(j)$.
	$\sigma \to \sigma_d$	$O_h^1(m)$, $O_h^4(k)$, $O_h^5(k)$, $O_h^7(g)$, $O_h^9(k)$.

Table 3. *Orientation of C_{2h} sites in crystals*

Supergroup	Orientation	Wyckoff sites
	$C_2 \to C_2^z$	$D_{2h}^{3}(a,b,c,d)$, $D_{2h}^{9}(a,b,c,d)$, $D_{2h}^{12}(a,b,c,d)$, $D_{2h}^{19}(e,f)$, $D_{2h}^{20}(c,d,e,f)$, $D_{2h}^{23}(e)$, $D_{2h}^{26}(c,d)$.
D_{2h}	$C_2 \to C_2^y$	$D_{2h}^{5}(a,b,c,d)$, $D_{2h}^{21}(e,f)$, $D_{2h}^{23}(d)$, $D_{2h}^{28}(c,d)$.
	$C_2 \to C_2^x$	$D_{2h}^{7}(a,b,c,d)$, $D_{2h}^{17}(a,b)$, $D_{2h}^{18}(a,b)$, $D_{2h}^{21}(c,d)$, $D_{2h}^{23}(c)$, $D_{2h}^{28}(a,b)$
	$C_2 \to C_2$	$D_{4h}^{2}(e)$, $D_{4h}^{6}(c)$, $D_{4h}^{10}(f)$, $D_{4h}^{13}(a,c)$, $D_{4h}^{14}(c)$.
D_{4h}	$C_2 \to C_2'$	$D_{4h}^{19}(c,d)$.
	$C_2 \to C_2''$	$D_{4h}^{3}(e,f)$, $D_{4h}^{7}(d,e)$, $D_{4h}^{12}(e,f)$, $D_{4h}^{16}(c,d)$, $D_{4h}^{17}(f)$, $D_{4h}^{18}(e)$.
	$C_2 \to C_2$	$D_{6h}^{2}(g)$.
D_{6h}	$C_2 \to C_2'$	$D_{6h}^{4}(g)$.
	$C_2 \to C_2''$	$D_{6h}^{3}(f)$.

Table 4. *Orientation of C_{2v} sites in crystals*

Supergroup	Orientation	Wyckoff sites
C_{4v}	$\sigma_v \to \sigma_v$	$C_{4v}^{1}(c)$, $C_{4v}^{7}(a,b,c)$, $C_{4v}^{9}(b)$, $C_{4v}^{11}(a)$.
	$\sigma_v \to \sigma_d$	$C_{4v}^{2}(b)$, $C_{4v}^{3}(a,b)$, $C_{4v}^{4}(a)$, $C_{4v}^{10}(b)$.
	$C_2 \to C_2^z$	$D_{2h}^{1}(q,r,s,t)$, $D_{2h}^{5}(e,f)$, $D_{2h}^{13}(a,b)$, $D_{2h}^{19}(k,l)$, $D_{2h}^{21}(g)$, $D_{2h}^{23}(i)$, $D_{2h}^{25}(i,j)$, $D_{2h}^{28}(e)$.
D_{2h}	$C_2 \to C_2^y$	$D_{2h}^{1}(m,n,o,p)$, $D_{2h}^{17}(c)$, $D_{2h}^{19}(i,j)$, $D_{2h}^{23}(h)$, $D_{2h}^{25}(g,h)$.
	$C_2 \to C_2^x$	$D_{2h}^{1}(i,j,k,l)$, $D_{2h}^{19}(g,h)$, $D_{2h}^{23}(g)$, $D_{2h}^{25}(e,f)$.
	$2\sigma_v \to 2\sigma_v$	$D_{4h}^{1}(i)$, $D_{4h}^{7}(f)$, $D_{4h}^{9}(g,h,i)$, $D_{4h}^{15}(c,d)$, $D_{4h}^{17}(g)$, $D_{4h}^{19}(e)$.
D_{4h}	$2\sigma_v \to 2\sigma_d$	$D_{4h}^{3}(h)$, $D_{4h}^{5}(f)$, $D_{4h}^{10}(g,h)$, $D_{4h}^{12}(g)$, $D_{4h}^{14}(e)$, $D_{4h}^{16}(e)$, $D_{4h}^{18}(g)$.
	$2\sigma_v \to \sigma_h+\sigma_v$	$D_{4h}^{1}(l,m,n,o)$, $D_{4h}^{9}(j,k,l,m)$, $D_{4h}^{17}(i,j)$.
	$2\sigma_v \to \sigma_h+\sigma_d$	$D_{4h}^{1}(j,k)$, $D_{4h}^{5}(g,h)$, $D_{4h}^{10}(i,j)$, $D_{4h}^{14}(f,g)$, $D_{4h}^{17}(h)$, $D_{4h}^{18}(h)$.
	$C_2 \to C_2$	$D_{6h}^{1}(i)$.
D_{6h}	$C_2 \to C_2'$	$D_{6h}^{1}(j,k)$, $D_{6h}^{3}(g)$.
	$C_2 \to C_2''$	$D_{6h}^{1}(l,m)$, $D_{6h}^{4}(h)$.
	$2\sigma_v \to 2\sigma_h$	$O_h^{1}(h)$, $O_h^{3}(f,g,h)$, $O_h^{5}(g)$, $O_h^{6}(e)$, $O_h^{7}(f)$, $O_h^{9}(g)$.
O_h	$2\sigma_v \to 2\sigma_d$	$O_h^{4}(g)$.
	$2\sigma_v \to \sigma_h+\sigma_d$	$O_h^{1}(i,j)$, $O_h^{5}(h,i)$, $O_h^{9}(h)$.

Table 5. *Orientation of C_{3v} sites in crystals*

Supergroup	Orientation	Wyckoff sites
C_{6v}	$\sigma_v \to \sigma_v$	$C_{6v}^{1}(b)$, $C_{6v}^{4}(a,b)$.
	$\sigma_v \to \sigma_d$	$C_{6v}^{3}(a)$.
D_{6h}	$\sigma_v \to \sigma_v$	none
	$\sigma_v \to \sigma_d$	$D_{6h}^{1}(h)$, $D_{6h}^{4}(e,f)$.

Table 6. *Orientation of D_2 sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_4	$3C_2 \to C_2+2C_2'$	$D_4^{1}(e,f)$, $D_4^{5}(a,b,c,d)$, $D_4^{9}(c)$.
	$3C_2 \to C_2+2C_2''$	$D_4^{2}(a,b)$, $D_4^{5}(e,f)$, $D_4^{6}(a,b)$, $D_4^{9}(d)$, $D_4^{10}(a,b)$.
D_{4h}	$3C_2 \to C_2+2C_2'$	$D_{4h}^{2}(f)$, $D_{4h}^{4}(c)$, $D_{4h}^{10}(e)$, $D_{4h}^{11}(a,b)$, $D_{4h}^{12}(c)$.
	$3C_2 \to C_2+2C_2''$	$D_{4h}^{6}(d)$, $D_{4h}^{8}(a)$, $D_{4h}^{11}(c)$, $D_{4h}^{12}(d)$, $D_{4h}^{13}(d)$, $D_{4h}^{16}(a)$, $D_{4h}^{20}(b)$.
O	$3C_2 \to C_2+2C_2'$	$O^{2}(e,f)$, $O^{3}(d)$, $O^{5}(d)$, $O^{8}(c,d)$.
	$3C_2 \to 3C_2$	$O^{2}(d)$.
O_h	$3C_2 \to C_2+2C_2'$	$O_h^{4}(f)$.
	$3C_2 \to 3C_2$	$O_h^{10}(c)$.

Table 7. *Orientation of D_3 sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_6	$C_2' \to C_2'$	$D_6^{6}(a)$.
	$C_2' \to C_2''$	$D_6^{1}(c,d)$, $D_6^{6}(b,c,d)$.
D_{6h}	$C_2' \to C_2'$	none
	$C_2' \to C_2''$	$D_{6h}^{2}(c)$, $D_{6h}^{3}(d)$.

Table 8. *Orientation of D_{2d} sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_{4h}	$\sigma_d \rightarrow \sigma_v$	$D_{4h}^7(a,b)$, $D_{4h}^9(e,f)$, $D_{4h}^{15}(a,b)$, $D_{4h}^{17}(d)$, $D_{4h}^{19}(a,b)$.
	$\sigma_d \rightarrow \sigma_d$	$D_{4h}^3(c,d)$, $D_{4h}^{10}(b,d)$, $D_{4h}^{12}(a,b)$, $D_{4h}^{18}(b)$.
O_h	$\sigma_d \rightarrow \sigma_h$	$O_h^3(c,d)$, $O_h^6(c)$, $O_h^9(d)$.
	$\sigma_d \rightarrow \sigma_d$	$O_h^4(d)$.

Table 9. *Orientation of D_{3d} sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_{6h}	$C_2 \rightarrow C_2'$	$D_{6h}^4(a)$.
	$C_2 \rightarrow C_2''$	$D_{6h}^3(b)$.

Table 10. *Orientation of D_{2h} sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_{4h}	$3C_2 \rightarrow C_2+2C_2'$	$D_{4h}^1(e,f)$, $D_{4h}^9(a,b,c,d)$, $D_{4h}^{17}(c)$.
	$3C_2 \rightarrow C_2+2C_2''$	$D_{4h}^5(c,d)$, $D_{4h}^{10}(a,c)$, $D_{4h}^{14}(a,b)$ $D_{4h}^{18}(d)$.
O_h	$3C_2 \rightarrow C_2+2C_2'$	$O_h^5(d)$.
	$3C_2 \rightarrow 3C_2$	$O_h^3(b)$.

Table 11. *Orientation of D_{3h} sites in crystals*

Supergroup	Orientation	Wyckoff sites
D_{6h}	$\sigma_v \rightarrow \sigma_v$	$D_{6h}^3(a)$.
	$\sigma_v \rightarrow \sigma_d$	$D_{6h}^1(c,d)$, $D_{6h}^4(b,c,d)$.

C_2^x	D_2	C_2^y	D_2	C_2^z	D_2
A	$A+B_3$	A	$A+B_2$	A	$A+B_1$
B	B_1+B_2	B	B_1+B_3	B	B_2+B_3

Examination of *International Tables for X-ray Crystallography* (1969, p. 102) shows that in the case of space group No. 16, $D_2^1 = P222$, Wyckoff sites *i–l* are on the x axis, *m–p* are on the y axis, and *q–t* are on the z axis. In more difficult cases the analysis can be quite tedious and the author is grateful to Dr D. M. Adams and Mr D. C. Newton of the University of Leicester for a copy of some computations on Wyckoff sites which were carried out in connexion with the Bhagavantam–Venkatarayudu method for the analysis of lattice vibrations. It was quite easy to recognize the different possible orientations of sites from their tables and the results are recorded in Tables 1 to 11.

Ambiguities of the kind described above arise when similar elements of symmetry occur in more than one group-theoretical class of elements of the point group. In all crystallographic cases, choice is restricted to sets of reflexion planes and/or twofold axes of symmetry. Correspondingly, the only site groups requiring attention are $C_2, C_{1h}, C_{2h}, C_{2v}, C_{3v}, D_2, D_3, D_{2d}, D_{3d}, D_{2h}$, and D_{3h}. In the Tables, the various crystal classes (referred to as supergroups) for which orientational differences occur are listed together with the relationship between key elements of site group and supergroup and then a list of Wyckoff sites (given in parentheses after the Schönflies symbol for the space group). It will be seen that there are never more than four distinguishable orientations and so it is fairly easy to find the orientation of any Wyckoff site by inspection. It should be noted that, where relevant, the crystallographic z axis was chosen as the principal axis and in the case of dihedral point groups the x axis was chosen to be a C_2' axis. The remaining elements of symmetry then followed in accordance with current conventions.

Reference

International Tables for X-ray Crystallography (1969). Vol. I, 3rd ed. Birmingham: Kynoch Press.