

PROBABILITY CORRELATION OF Σ_1 RELATIONSHIPS AND THEIR TABLES OF 230 SPACE GROUPS

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ABSTRACT

In the present paper, using the structure factor algebra method, we discuss the correlation and the distinction between the conventionally used Σ_1 relationships and the probability value of $P_+(h_i)$ on the basis of the $P_+(h_i)$ of Hauptman's and Karle's Σ_1 relationship. The introduction of conception on equivalent point weight ω of h_1 and degeneracy ε_2 of h_2 makes the probability $P_+(h_i)$ expressed by Σ_1 relationships become more strict. There are a lot of interrelated Σ_1 relationships in all four high symmetry crystal systems. According to the results of this paper, what we need is only to retain a few independent Σ_1 relationships. Using the principle of linearization, we have completed the tables of the Σ_1 relationships for 156 space groups which belong to tetragonal, trigonal, hexagonal and cubic crystal systems. Now, we present the concise and perfect tables of 230 space groups of which 74 were accomplished by Hašek.

I. INTRODUCTION

In 1970's, based on various relationships, by means of the direct method, great achievements were gained in determining single crystal structures. The wide application of MULTAN is a prominent example. Those successful methods in the past were based almost wholly on the Σ_2 relationships, but usually, the Σ_1 and Σ_3 etc. relationships played a fair complementary part in the determination of crystal structures as well. In accordance with our experience of determining several structures experimentally, we consider it useful so that we put more phases accordingly as the probability, based on the Σ_1 and Σ_4 relationships (i.e. choosing a large starting set of phases). Therefore, the Σ_1 and Σ_4 relationships should play more important role in the direct method than that traditionally known before. Some principle formulae for calculation of the Σ_1 relationships are given in Vol. IV of the International Tables of X-ray Crystallography^[1], but it is not convenient to use them for concrete space groups directly. In order to calculate the Σ_1 relationships, Woolfson introduced restricted phases into MULTAN programme^[2], then he established an approximate method for the calculation of the Σ_1 formulae and this method is suitable for all space groups and also used practically. In 1974, Giacovazzo obtained a more strict formula for the calcula-

tion of Σ_1 relationships^[3], which is suitable for all space groups. In 1977, with the application of Giacovazzo's result, Hašek presented the table of the Σ_1 relationships of 74 space groups for the triclinic, monoclinic and orthorhombic crystal systems^[4].

In spite of the fact that these former authors had made great outstanding achievements in the respect of the Σ_1 relationships, there still remain some problems in the strict expression of $P_+(\mathbf{h}_1)$ the correlation between Σ_1 relationships and tabling Σ_1 relationships for four kinds of high symmetry crystal systems (excluding the low symmetry crystal systems). For example, 156 space groups of those four crystal systems are high symmetry, and their equivalent points are complex. One must meet with new difficulties in mathematics, crystallography and the large quantity of computation in making the tables of Σ_1 for high symmetry crystal systems. Thus, it is more necessary to choose the suitable method for calculation.

There are three methods for calculating the Σ_1 relationships, i.e. probability method^[5], algebra method^[6] and probability-algebra method^[3]. Comparing them with each other^[7], we prefer the last method. Since we have used and improved the restricted condition of the Σ_1 relationships which has universality, we can not only avoid the approximation caused by special phases adopted but also facilitate the realization of universal computation more easily.

II. $P_+(\mathbf{h}_1)$ AND CORRELATION BETWEEN THE Σ_1 RELATIONSHIPS

Based on the Σ_1 relationships, when the diffraction point phase of $\mathbf{h}_1$ is equal to 0 the probability expression can be written in the following form^[1,5]:

$$P_+(\mathbf{h}_1) \approx \frac{1}{2} + \frac{1}{2} \tanh \left\{ \frac{m_{12}n^{1/2}\sigma_3}{qm_{20}^{1/2}m_{02}\sigma_2^{3/2}} |E_{\mathbf{h}_1}| \sum (|E_{\mathbf{h}_1}|^2 - 1) \right\}. \quad (1)$$

In addition,

$$\xi_{\mathbf{h}} = \sum_j^n \exp 2\pi i \mathbf{h} \mathbf{C}_j \mathbf{r}, \quad (2)$$

$$\mathbf{C}_j \mathbf{r} = \mathbf{R}_j \mathbf{r} + \mathbf{t}_j, \quad (3)$$

according to the definition, the moment is

$$m_{20} = \langle \xi_{\mathbf{h}_1}^2 \rangle = \left\langle \sum_i^n \sum_j^n \exp 2\pi i \mathbf{h}_1 (\mathbf{C}_i - \mathbf{C}_j) \mathbf{r} \right\rangle,$$

where $\mathbf{C}_j$ is a symmetry operator of the j th equivalent transformation of the given space group; $\mathbf{r}$ is atomic coordinate in the real space, expressed as matrix; $\mathbf{R}_j$ is a rotation matrix of $\mathbf{C}_j$; $\mathbf{t}_j$ is a translation matrix of $\mathbf{C}_j$; $\mathbf{h}_1$ is the diffraction indices of the Σ_1 relationships to be determined, expressed as matrix; n is the number of the symmetry equivalent points in the real space; $\langle \rangle$ is the sign to calculate the average value, the other signs have the conventional meanings.

$$m_{20} = \left\langle \sum_i^n \sum_j^n \exp 2\pi i \mathbf{h}_1 (\mathbf{C}_i \mathbf{C}_j^{-1} \mathbf{C}_j - \mathbf{C}_j) \mathbf{r} \right\rangle$$

$$\begin{aligned}
&= \left\langle \sum_1^n \sum_j^n \exp 2\pi i \mathbf{h}_1 (\mathbf{C}_s - \mathbf{I}) \mathbf{C}_j \mathbf{r} \right\rangle \\
&= \left\langle \sum_1^n \sum_j^n \exp 2\pi i \mathbf{h}_1 \mathbf{t}_s \cdot \exp 2\pi i \mathbf{h}_1 (\mathbf{R}_s - \mathbf{I}) \mathbf{C}_j \mathbf{r} \right\rangle,
\end{aligned}$$

therefore

$$m_{20} = \left\langle \sum_1^n a_s(\mathbf{h}_1) \xi[\mathbf{h}_1(\mathbf{R}_s - \mathbf{I})] \right\rangle, \quad (4)$$

where

$$\mathbf{C}_s = \mathbf{C}_j \mathbf{C}_j^{-1}, \quad a_s(\mathbf{h}_1) = \exp 2\pi i \mathbf{h}_1 \mathbf{t}_s. \quad (5)$$

It will be seen from expression (4) that condition for $m_{20} \neq 0$ is

$$\mathbf{h}_1(\mathbf{R}_s - \mathbf{I}) = \mathbf{0}.$$

When $\mathbf{h}$ takes some special indices, their equivalent points of reciprocal space are degenerated, the numbers of the degenerated equivalent points are called degeneracy of reciprocal space of $\mathbf{h}$, therefore, when subscript s takes some values from 1 to n (amounts to numbers of ε_1), then we have

$$\mathbf{h}_1 \mathbf{R}_s = \mathbf{h}_1, \quad a_s(\mathbf{h}_1) = 1. \quad (6)$$

Therefore

$$m_{20} = \left\langle \sum_1^{\varepsilon_1} a_s(\mathbf{h}_1) \xi(\mathbf{0}) \right\rangle = \varepsilon_1 n. \quad (7)$$

Eq. (7) is identical with Iwasaki's result⁽⁸⁾. Similarly we have

$$m_{02} = \varepsilon_2 n. \quad (8)$$

Eqs. (7) and (8) show that both m_{20} and m_{02} are simple integrals, but the expression of the moment m_{12} is

$$\begin{aligned}
m_{12} &= \langle \xi_{\mathbf{h}_1} \xi_{\mathbf{h}_2}^* \rangle \\
&= \left\langle \sum_1^n \sum_j^n \sum_k^n \exp 2\pi i (\mathbf{h}_1 \mathbf{C}_i + \mathbf{h}_2 \mathbf{C}_j - \mathbf{h}_2 \mathbf{C}_k) \mathbf{r} \right\rangle \\
&= \left\langle \sum_1^n \sum_j^n \sum_k^n \exp 2\pi i (\mathbf{h}_1 \mathbf{C}_i \mathbf{C}_k^{-1} + \mathbf{h}_2 \mathbf{C}_j \mathbf{C}_k^{-1} - \mathbf{h}_2) \mathbf{C}_k \mathbf{r} \right\rangle \\
&= \left\langle \sum_1^n \sum_s^n \sum_k^n \exp 2\pi i [\mathbf{h}_1 \mathbf{C}_s + \mathbf{h}_2 (\mathbf{C}_s - \mathbf{I})] \mathbf{C}_k \mathbf{r} \right\rangle \\
&= \left\langle \sum_1^n \sum_s^n a_r(\mathbf{h}_1) a_s(\mathbf{h}_2) \xi[\mathbf{h}_1 \mathbf{R}_r + \mathbf{h}_2 (\mathbf{R}_s - \mathbf{I})] \right\rangle. \quad (9)
\end{aligned}$$

It will be seen from Eq. (9) that the restricted condition for $m_{12} \neq 0$ is

$$\mathbf{h}_1 \mathbf{R}_r - \mathbf{h}_2 (\mathbf{I} - \mathbf{R}_s) = \mathbf{0}. \quad (10)$$

Every r and s which satisfy Eq. (10) should take part in the calculation of proba-

bility for $P_+(\mathbf{h}_1)$ according to Formula (9), but the previous authors' treatment of the Σ_1 relationships is only a special circumstance in Formula (10).

(1) *Restricting the subscript r to satisfy the formula $\mathbf{h}_1\mathbf{R}_r = \mathbf{h}_1$*

According to Formula (9), when the subscript r varies from 1 to n , every one which satisfies the condition of Formula (10) should take part in calculation of Formula (9), but the previous authors' method brought the subscript r which only satisfies the formula $\mathbf{h}_1\mathbf{R}_r = \mathbf{h}_1$ into calculation of Formula (9), which decreased the range of numerical value which may be taken by the subscript r . In this case, Formula (10) becomes

$$\mathbf{h}_1 - \mathbf{h}_2(\mathbf{I} - \mathbf{R}_s) = \mathbf{0}. \quad (11)$$

Formula (11) is the restricted condition which is used in [4], then $a_r(\mathbf{h}_1) = 1$.

(2) *Taking the subscript s as a certain fixed value*

According to restricted condition of Formula (11), when the subscript s varies from 2 to n and the matrixes $\mathbf{h}_2(\mathbf{I} - \mathbf{R}_s)$ are calculated respectively, $(n - 1)$ single Σ_1 relationships consistently used can be obtained. Previous authors only took fixed one of the relationships to calculate the probability for $P_+(\mathbf{h}_1)$, that is, they took a certain selected numerical value from the subscript s ($s = 1, 2, \dots, n$) which satisfies the condition of Formula (11), which obviously decreases the range of numerical value which may be taken by the subscript s .

We call both the cases mentioned above the restricted condition of the single Σ_1 relationships. From this point of view, the expression of the moment m_{12} becomes

$$m_{12} = n\varepsilon_1 a_s(\mathbf{h}_2) \quad (12)$$

and coefficient of the Σ_1 relationships will be

$$W_0 = \frac{m_{12}n^{1/2}\sigma_3}{qm_{20}^{1/2}m_{02}\sigma_2^{3/2}} = \frac{\sigma_3\sqrt{\varepsilon_1}}{q\sigma_2^{3/2}\varepsilon_2} a_s(\mathbf{h}_2). \quad (13)$$

Both Formulae (11) and (13) are completely identical with the results reported by the previous authors^[3,4]. Making use of those results Hašek obtained the tables of the Σ_1 relationships of 74 space groups for low symmetry crystal systems^[4]. The concrete formula is

$$P_+(\mathbf{h}_1) \approx \frac{1}{2} + \frac{1}{2} \tanh[C \cdot S], \quad (14)$$

where

$$C = \frac{1}{q} \sigma_3 \sigma_2^{-\frac{3}{2}} \sqrt{\varepsilon_1} |E_{\mathbf{h}_1}|, \quad (15)$$

$$S = \sum (-1)^a (|E_{\mathbf{h}_2}|^2 - 1) / \varepsilon_2, \quad (16)$$

$$\mathbf{h}_1 = \mathbf{h}_2(\mathbf{I} - \mathbf{R}_s). \quad (11)$$

Next, we can obtain more strict formula for calculation of the probability $P_+(\mathbf{h}_1)$, by means of introducing both conceptions, the equivalent point weight ω of matrix $\mathbf{h}_1$ and the degeneracy weight ε_2 of matrix $\mathbf{h}_2$. It can be seen from both Formulae (9) and (10) that every subscript s which satisfies Formula (10) should join the calcu-

lation of Formula (9) for a given matrix R . Because the degeneracy of $\mathbf{h}_2$ is ε_2 , there are ε_2 numbers of subscripts s which satisfy Formula (10). In addition to that, when the subscript r varied from 1 to n , if there are ω numbers of equivalent points of $\mathbf{h}_1$ in $(n-1)$ single Σ_1 relationships, then ω numbers of them should all take part in the calculation of Formula (9), that is a inevitable outcome after taking account of correlation and distinction between the single Σ_1 relationships. Thus, using relevant crystallographic conditions, we obtain the moment m_{12} from both Formulae (9) and (10).

$$m_{12} = \varepsilon_1 \xi(\mathbf{0}) a_s(\mathbf{h}_2) \omega \varepsilon_2 = a_s(\mathbf{h}_2) n \omega \varepsilon_1 \varepsilon_2. \quad (17)$$

If Formula (17) is compared with (12), then a deduction can be obtained.

Deduction 1. When correlation and distinction among the single Σ_1 relationships are considered, the coefficient of the probability $P_+(\mathbf{h}_1)$ is $W = W_0 \omega \varepsilon_3$, that is,

$$W = \frac{\sigma_3}{q \sigma_2^{3/2}} \omega \sqrt{\varepsilon_1} a_s(\mathbf{h}_2). \quad (18)$$

Owing to the introduction of the equivalent point weight ω of $\mathbf{h}_1$ and the degeneracy weight ε_3 of $\mathbf{h}_2$, the calculation formula of the probability $P_+(\mathbf{h}_1)$ becomes

$$P_+(\mathbf{h}_1) \approx \frac{1}{2} + \frac{1}{2} \tanh[C \cdot S], \quad (14)$$

where

$$C = \frac{1}{q} \sigma_3 \sigma_2^{-\frac{1}{2}} \sqrt{\varepsilon_1} \omega |E_{\mathbf{h}_1}|, \quad (19)$$

$$S = \sum (-1)^a (|E_{\mathbf{h}_1}|^2 - 1). \quad (20)$$

The restricted conditions here are

$$\mathbf{h}_1 \mathbf{R}_r = \mathbf{h}_2 (\mathbf{I} - \mathbf{R}_r) \quad (21)$$

and

$$a_s(\mathbf{h}_2) = (-1)^a. \quad (22)$$

Formulae (14), (19), (20), (21) and (22) are main results obtained by us.

Other two deductions can be obtained further.

Deduction 2. There exist many single Σ_1 relationships which have correlation of fixed phase in the high symmetry crystal systems, we call them dependent single Σ_1 relationships.

There are ω relationships connected by the direct equivalent points in those dependent single Σ_1 relationships, therefore we should cancel $(\omega-1)$ relationships, and retain only one. In addition, only one of the relationships is retained, which is not connected directly with equivalent points, although they are dependent. But weight of the probability $P_+(\mathbf{h}_1)$ coefficient is not increased.

But in the calculation of the probability $P_+(\mathbf{h}_1)$ the weight ω probably varies for some diffraction indices $\mathbf{h}_2$ which is specially restricted, because the single Σ_1 relationships that are not, in general condition, direct equivalent points of $\mathbf{h}_1$, but can be

direct equivalent points of $\mathbf{h}_1$ when $\mathbf{h}_2$ has a certain special restriction. There is a small number of such $\mathbf{h}_2$ in the Σ_1 relationships, therefore there is little effect upon the calculation of the probability $P_+(\mathbf{h}_1)$.

Deduction 3. The principles to make a list of the Σ_1 relationships are

- 1) Write n number of matrixes $\mathbf{R}_s$ and $\mathbf{t}_s$ in the given space group in proper order.
- 2) Calculate $(n - 1)$ relationships from $\mathbf{h}_2(\mathbf{I} - \mathbf{R}_s)$ and obtain the Σ_1 relationship types of $\mathbf{h}_1$.
- 3) Determine corresponding freedom of $\mathbf{h}_2$ by each type of $\mathbf{h}_1$, thus finding out a sum method of $\mathbf{h}_2$.
- 4) Operate a rotation matrix $\mathbf{R}_r$ ($r = 2, 3, \dots, n$) for $(n - 1)$ single Σ_1 relationships, look for the number of the single Σ_1 relationships, ω , which is the direct equivalent points with each $\mathbf{h}_1$ to each other.
- 5) Retain only one of ω single Σ_1 relationships and cancel other $(\omega - 1)$, and those single Σ_1 relationships having no connection with direct equivalent points, although they are interrelated with $\mathbf{h}_1$.
- 6) List the tables of the independent Σ_1 relationships added by both weights ω and ε_1 .

The tables obtained in this way are concise and perfect ones. The total amount of the single Σ_1 relationships should be 337, but they are simplified into 130 in the tables.

III. TABLES OF THE Σ_1 RELATIONSHIPS

Instruction for the use of the tables

- 1) All the tables unitedly use Formulae (14), (19) and (20) for the calculation of the probability $P_+(\mathbf{h}_1)$.
- 2) For all space groups, the original points are chosen according to Vol. I of *International Tables for X-ray Crystallography*^[9], but for centrosymmetric space groups, the original points are chosen from the center of symmetry.
- 3) For monoclinic space groups, axis b is selected as the unique axis^[4].
- 4) All space groups with the lattice R for trigonal crystal system are described by the coordinate system H .
- 5) The weight ω in the tables takes general value given by Deduction 2. There is no need to check the table of ε , when the value $\omega \cdot \sqrt{\varepsilon_1}$ is used directly.
- 6) All the Σ_1 relationships in the tables are independent. It is noted that there can exist not only one relation suitable for the calculation of Σ_1 when $\mathbf{h}_1$ takes some special values. Under these circumstances, the probability $P_+(\mathbf{h}_1)$ is calculated again after adding the values calculated respectively.
- 7) Each sum sign represents a independent sum relation. If $\mathbf{h}_1$ is restricted such that a function relation appears among h , k and l , then the independent sum

Tables of the Σ_i Relationships
Table 1
Tetragonal Space Groups

Point Group	Reflexion Type for Determination of $P_+(h_i)$	Expression for S	$\omega\sqrt{\epsilon_1}$	No. of Space Group Exponent	75	76	77	78	79	80
4	$2h \quad 2k \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	1	α_1	0	l	0	l	0	0
	$h+k \quad k-h \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	2	α_2	0	l/2	l	l/2	0	$k+l/2$
$\bar{4}$	$2h \quad 2k \quad 0$	$\sum_l Q_{hkl}$	1		81	82				
	$0 \quad 0 \quad 2l$ $h+k \quad k-h \quad 0$	Q_{00l} Q_{hko}	$2\sqrt{2}$ 2							
4/m	$2h \quad 2k \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	$\sqrt{2}$		83	84	85	86	87	88
	$0 \quad 0 \quad 2l$	$\sum_k (-1)^{a_k} Q_{hkl}$	2	α_1	0	0	$h+k$	$h+k$	0	k
	$2h \quad 2k \quad 2l$	Q_{hkl}	1	α_2	0	l	h	$k+l$	0	$(3h+k+l)/2$
	$h-k \quad h+k \quad 0$ $h-k \quad h+k \quad 2l$	$\sum_l (-1)^{a_l} Q_{hkl}$ $(-1)^{a_l} Q_{hkl}$	$2\sqrt{2}$ 2	α_3	0	l	k	$h+l$	0	$3(h+k+l)/2$
422	$2h \quad 2k \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	1		89	90	91	92	93	94
	$2h \quad 0 \quad 2l$	$\sum_k (-1)^{a_k} Q_{hkl}$	1	α_1	0	0	l	l	0	0
	$h+k \quad h+k \quad 2l$	$\sum_{h(k)} (-1)^{a_k} Q_{hkl}$	1	α_2	0	$h+k$	0	$h+k+l$	0	$h+k+l$
	$h-k \quad h+k \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	2	α_3	0	0	l/2	l	l/2	0
4mm	$2h \quad 2k \quad 0$	$\sum_l Q_{hkl}$	1	α_4	0	$h+k$	l/2	$h+k+l$	l	$h+k+l$
	$2h \quad 0 \quad 0$	$\sum_k (-1)^{a_k} Q_{hkl}$	$\sqrt{2}$		99	100	101	102	103	104
	$h+k \quad h+k \quad 0$	$\sum_l (-1)^{a_l} Q_{hkl}$	$\sqrt{2}$	α_1	0	$h+k$	l	$h+k+l$	l	$h+k+l$
	$h-k \quad h+k \quad 0$	$\sum_{h(k)} (-1)^{a_k} Q_{hkl}$	2	α_2	0	$h+k$	0	0	l	$h+k+l$
				α_3	0	0	l	$h+k+l$	0	0
					105	106	107	108	109	110

42m	2h	2k	0	$\sum_l Q_{hkl}$	1	α_1	0	h+k	0	h+k	0	l				
	2h	0	2l	$\sum_k (-1)^a Q_{hkl}$	1	α_2	l	h+k+l	0	h+k	k + $\frac{l}{2}$	k + $\frac{l}{2}$				
	h-k	h+k	0	Q_{hko}	2	α_3	l	0	0	0	k + $\frac{l}{2}$	k + $\frac{l}{2}$				
	h+k	h+k	0	$\sum_{h(k)} (-1)^a Q_{hkl}$	$\sqrt{2}$											
	2h	2k	0	$\sum_l Q_{hkl}$	1	α	0	l	h+k	h+k+l	0	l				
	2h	0	0	$\sum_k (-1)^a Q_{hkl}$	$\sqrt{2}$											
	h-k	h+k	0	Q_{hko}	2											
	h+k	h+k	2l	$\sum_{h(k)} (-1)^a Q_{hkl}$	1											
4/mmm	2h	2k	0	$\sum_l (-1)^a Q_{hkl}$	$\sqrt{2}$		123	124	125	126	127	128	129	130	131	132
	0	0	2l	$\sum_h \sum_k (-1)^a Q_{hkl}$	$2\sqrt{2}$	α_1	0	0	h+k	h+k	0	0	h+k	h+k	0	0
	2h	2k	2l	Q_{hkl}	1	α_2	0	l	k	k+l	h+k	h+k+l	h	h+l	0	l
	2h	0	0	$\sum_k \sum_l (-1)^a Q_{hkl}$	2	α_3	0	0	h	h+l	h+k	h+k+l	k	k+l	0	l
	2h	0	2l	$\sum_k \sum_l (-1)^a Q_{hkl}$	$\sqrt{2}$	α_4	0	0	h	h	0	0	h	h	l	l
	h-k	h+k	0	$\sum_k (-1)^a Q_{hkl}$	$2\sqrt{2}$	α_5	0	l	0	k	0	0	k	k	l	l
	h-k	h+k	0	$\sum_l (-1)^a Q_{hkl}$	$2\sqrt{2}$	α_6	0	l	0	l	h+k	h+k+l	h+k	h+k+l	l	0
	h+k	h+k	0	$\sum_l (-1)^a Q_{hkl}$	2	α_7	0	l	h+k	h+k+l	h+k	h+k+l	0	l	l	0
	h+k	h+k	0	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	2		133	134	135	136	137	138	139	140	141	142
	h+k	h+k	2l	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	$\sqrt{2}$	α_1	h+k	h+k	0	0	h+k	h+k	0	0	k	k
					α_2	k	k+l	h+k	h+k+l	h	h+l	0	l	0	l	
					α_3	h	h+l	h+k	h+k+l	k	k+l	0	l	k	k+l	
					α_4	h+l	h+l	l	h+k+l	h+l	h+l	0	0	(3h+k+3l)/2	(3h+k+3l)/2	
					α_5	k+l	k+l	l	h+k+l	k+l	k+l	0	0	(3h+3k+l)/2	(3h+3k+l)/2	
					α_6	l	0	h+k+l	0	h+k+l	h+k	0	l	(3h+k+l)/2	(3h+k+l)/2	
					α_7	h+k+l	h+k	h+k+l	0	l	0	0	l	(3h+3k+l)/2	3(h+k+l)/2	

Table 2
Trigonal Space Groups

Point Group	Reflexion Type for determination of $P_+(h_i)$	Expression for S	$\omega\sqrt{\varepsilon_i}$	No. of Space Group Exponent	
$\bar{3}$	$2h \quad 2k \quad 2l$	Q_{hkl}	1		147 148
	$h-k \quad h+2k \quad 0$	$\sum_l Q_{hkl}$	2		
	$h+k \quad -h \quad 2l$	Q_{hkl}	2		
32	$h+k \quad h+k \quad 2l$	$\sum_{h(k)} (-1)^a Q_{hkl}$	1		149 151 153
	$h \quad h \quad 0$	$\sum_l (-1)^a Q_{h0l}$	2	α	$0 \quad \frac{2}{3}l \quad \frac{2}{3}l$
	$-k \quad 2k \quad 2l$	$\sum_h (-1)^a Q_{hkl}$	1		
	$3h \quad -3h \quad 0$	$\sum_l (-1)^a Q_{h,-2h,l}$	2		150 152 154 155
	$h-k \quad k-h \quad 2l$	$\sum_{h(k)} Q_{hkl}$	1	α	$0 \quad \frac{2}{3}l \quad \frac{2}{3}l \quad 0$
	$2h+k \quad 0 \quad 2l$	$\sum_{h(k)} (-1)^a Q_{hkl}$	1		
	$h+k \quad h+k \quad 0$	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	1	α	156 158 160 161
	$h-k \quad k-h \quad 0$	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	1	α	0 l 0 l
	$h-k \quad k-h \quad 0$	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	1	α	157 159 0 l
$\bar{3}m$	$2h \quad 2k \quad 2l$	Q_{hkl}	1		162 163
	$h-k \quad k-h \quad 0$	$\sum_{h(k)} \sum_l (-1)^a Q_{hkl}$	$\sqrt{2}$	α	0 l
	$h+k \quad h+k \quad 2l$	$\sum_{h(k)} (-1)^a Q_{hkl}$	$\sqrt{2}$		
	$h-k \quad h+2k \quad 0$	$\sum_l Q_{hkl}$	2		
	$h+k \quad -h \quad 2l$	Q_{hkl}	2		
	$2h \quad 2k \quad 2l$	Q_{hkl}	1		164 165 166 167
	$h-k \quad k-h \quad 2l$	$\sum_{h(k)} (-1)^a Q_{hkl}$	$\sqrt{2}$	α	0 l 0 l
	$h-k \quad h+2k \quad 0$	$\sum_l Q_{hkl}$	2		
	$h+k \quad -h \quad 2l$	Q_{hkl}	2		
	$2h \quad -h \quad 0$	$\sum_k \sum_l (-1)^a Q_{hkl}$	$\sqrt{2}$		

Table 3
Hexagonal Space Groups

Point Group	Reflection Type for Determination of $P_+(h_i)$	Expression for S	$\omega\sqrt{\varepsilon_1}$	No. of Space Group Expo- nent	168 169 170 171 172 173
6	$h - k \quad h + 2k \quad 0$	$\sum_l (-1)^{\sigma_1} Q_{hkl}$	2	α_1	$0 \quad \frac{2}{3}l \quad \frac{2}{3}l \quad \frac{2}{3}l \quad \frac{2}{3}l \quad 0$
	$h + k \quad -h \quad 0$	$\sum_l (-1)^{\sigma_2} Q_{hkl}$	2	α_2	$0 \quad l/3 \quad l/3 \quad \frac{2}{3}l \quad \frac{2}{3}l \quad l$
$\bar{6}$	$0 \quad 0 \quad 2l$	$\sum_h \sum_k Q_{hkl}$	$\sqrt{3}$		174
6/m	$0 \quad 0 \quad 2l$	$\sum_h \sum_k (-1)^{\sigma} Q_{hkl}$	$\sqrt{6}$	α	175 176
	$h - k \quad h + 2k \quad 0$	$\sum_l Q_{hkl}$	$2\sqrt{2}$		$0 \quad l$
	$h + k \quad -h \quad 2l$	Q_{hkl}	$\frac{2}{2\sqrt{2}}$		
	$h + k \quad -h \quad 0$	$\sum_l (-1)^{\sigma} Q_{hkl}$	$2\sqrt{2}$		
	$h - k \quad h + 2k \quad 2l$	$(-1)^{\sigma} Q_{hkl}$	2		
622	$h - k \quad k - h \quad 2l$	$\sum_{h(k)} (-1)^{\sigma_1} Q_{hkl}$	1	α_1	177 178 179 180 181 182
	$h - k \quad h + 2k \quad 0$	$\sum_l (-1)^{\sigma_1} Q_{hkl}$	2		$0 \quad \frac{2}{3}l \quad \frac{2}{3}l \quad \frac{2}{3}l \quad \frac{2}{3}l \quad 0$
	$h + k \quad -h \quad 0$	$\sum_l (-1)^{\sigma_2} Q_{hkl}$	2		$0 \quad l/3 \quad l/3 \quad \frac{2}{3}l \quad \frac{2}{3}l \quad l$
	$-k \quad 2k \quad 2l$	$\sum_h (-1)^{\sigma_2} Q_{hkl}$	1	α_2	
6mm	$h - k \quad k - h \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma_2} Q_{hkl}$	$\sqrt{2}$	α_1	183 184 185 186
	$h + k \quad h + k \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma_3} Q_{hkl}$	$\sqrt{2}$		$0 \quad 0 \quad l \quad l$
	$h - k \quad h + 2k \quad 0$	$\sum_l Q_{hkl}$	2	α_2	$0 \quad l \quad 0 \quad l$
	$h + k \quad -h \quad 0$	$\sum_l (-1)^{\sigma_1} Q_{hkl}$	2	α_3	$0 \quad l \quad l \quad 0$
$\bar{6}m2$	$0 \quad 0 \quad 2l$	$\sum_h \sum_k (-1)^{\sigma} Q_{hkl}$	$\sqrt{6}$	α	187 188
	$h + k \quad h + k \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma} Q_{hkl}$	$\sqrt{2}$		$0 \quad l$
	$h + k \quad h + k \quad 2l$	$\sum_{h(k)} Q_{hkl}$	1		
	$0 \quad 0 \quad 2l$	$\sum_h \sum_k (-1)^{\sigma} Q_{hkl}$	$\sqrt{6}$	α	189 190
	$h - k \quad k - h \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma} Q_{hkl}$	$\sqrt{2}$		$0 \quad l$
	$h - k \quad k - h \quad 2l$	$\sum_{h(k)} Q_{hkl}$	1		
6/mmm	$0 \quad 0 \quad 2l$	$\sum_h \sum_k (-1)^{\sigma_1} Q_{hkl}$	$2\sqrt{3}$	α_1	191 192 193 194
	$h - k \quad h + 2k \quad 0$	$\sum_l Q_{hkl}$	$2\sqrt{2}$		$0 \quad 0 \quad l \quad l$
	$h + k \quad -h \quad 0$	$\sum_l (-1)^{\sigma_1} Q_{hkl}$	$2\sqrt{2}$		$0 \quad l \quad 0 \quad l$
	$h - k \quad h + 2k \quad 2l$	$(-1)^{\sigma_1} Q_{hkl}$	2		$0 \quad l \quad l \quad 0$
	$h + k \quad -h \quad 2l$	Q_{hkl}	2		
	$h - k \quad k - h \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma_2} Q_{hkl}$	2		
	$h + k \quad h + k \quad 0$	$\sum_{h(k)} \sum_l (-1)^{\sigma_3} Q_{hkl}$	2		
	$h - k \quad k - h \quad 2l$	$\sum_{h(k)} (-1)^{\sigma_3} Q_{hkl}$	$\sqrt{2}$		
	$h + k \quad h + k \quad 2l$	$\sum_{h(k)} (-1)^{\sigma_2} Q_{hkl}$	$\sqrt{2}$		

43m	0	2k	2l	$\sum_h (-1)^a Q_{hkl}$	1	α_1	215	216	217	218	219	220				
	0	k-l	l-k	$\sum_h (-1)^a Q_{hkl}$	$\sqrt{2}$	α_1	0	0	0	0	0	h+k				
	0	k+l	l-k	$\sum_h (-1)^a Q_{hkl}$	$\sqrt{2}$	α_2	0	0	0	h+k+l	l	(h+k+l)/2				
	0	k+l	l-k	$\sum_h (-1)^a Q_{hkl}$	1	α_3	0	0	0	k+l	l	(3k+l)/2				
m3m	2h	2k	2l	Q_{hkl}	1	α_1	221	222	223	224	225	226	227	228	229	230
	0	2k	2l	$\sum_h (-1)^a Q_{hkl}$	$\sqrt{2}$	α_1	0	k+l	0	k+l	0	0	$\frac{k+l}{2}$	$\frac{k+l}{2}$	0	h+k
	0	0	2l	$\sum_h (-1)^a Q_{hkl}$	$2\sqrt{2}$	α_2	0	h+k	0	h+k	0	0	$\frac{h+k}{2}$	$\frac{h+k}{2}$	0	h+l
	h-k	k-l	l-h	$\sum_{h(k,l)} Q_{hkl}$	2	α_3	0	h+k+l	h+k+l	0	0	l	0	l	0	$\frac{h+k+l}{2}$
	h+k	k+l	l+h	Q_{hkl}	2	α_4	0	h	h+k+l	k+l	0	l	$\frac{k+l}{2}$	$\frac{k+3l}{2}$	0	$\frac{3h+k+3l}{2}$
	0	k-l	l-k	$\sum_h (-1)^a Q_{hkl}$	2											
	2h	k+l	k+l	$\sum_{k(l)} (-1)^a Q_{hkl}$	$\sqrt{2}$											
	h+k	k-h	2l	$\sum_h (-1)^a Q_{hkl}$	2											
	h-k	h+k	0	$\sum_l (-1)^a Q_{hkl}$	$2\sqrt{2}$											

Appendix

Tables of the Σ , Relationships (Triclinic, Monoclinic and Orthorhombic Space Groups)

Point Group	Reflection Type for Determination of $P_+(h_0)$	Expression for S	$\omega\sqrt{\epsilon_1}$	Expo- nent	No. of Space Group
Triclinic space groups					
$\bar{1}$	$2h$ $2k$ $2l$	Q_{hkl}	1	α	2
Monoclinic space groups					
2	$2h$ 0 $2l$	$\sum_k (-1)^k Q_{hkl}$	1	α	3 4 5
					0 k 0
m	0 $2k$ 0	$\sum_k \sum_l (-1)^k Q_{hkl}$	1	α	6 7 8 9
					0 l 0 l
	$2h$ $2k$ $2l$	Q_{hkl}	1	α	10 11 12 13 14 15
$2/m$	$2h$ 0 $2l$	$\sum_k (-1)^k Q_{hkl}$	$\sqrt{2}$	α	0 k 0 l $k+l$ l
	0 $2k$ 0	$\sum_k \sum_l (-1)^k Q_{hkl}$	$\sqrt{2}$		
Orthorhombic space groups					
222	$2h$ $2k$ 0	$\sum_l (-1)^l Q_{hkl}$	1	α_1	16 17 18 19 20 21 22 23 24
	$2h$ 0 $2l$	$\sum_k (-1)^k Q_{hkl}$	1	α_2	0 l 0 $h+l$ l 0 0 0 $h+l$
	0 $2k$ $2l$	$\sum_h \sum_l (-1)^k Q_{hkl}$	1	α_3	0 l $h+k$ $k+l$ l 0 0 0 $k+l$
					0 0 $h+k$ $h+k$ 0 0 0 $h+k$

	$2h$	$2k$	0	$\sum_i (-1)^{\sigma_i} Q_{hki}$		1	α_1	25	26	27	28	29	30	31	32	33	34	35
mm $\bar{2}$	$2h$	0	0	$\sum_k \sum_i (-1)^{\sigma_i} Q_{hki}$	α_1	$\sqrt{2}$	α_1	0	l	0	0	l	0	$h+l$	0	l	0	0
	$2h$	0	0	$\sum_k \sum_i (-1)^{\sigma_i} Q_{hki}$	α_2	$\sqrt{2}$	α_2	0	0	l	h	$h+l$	$k+l$	0	$h+k$	$h+k+l$	$h+k+l$	0
	0	$2k$	0	$\sum_k \sum_i (-1)^{\sigma_i} Q_{hki}$	α_3	$\sqrt{2}$	α_3	0	l	l	h	h	$k+l$	$h+l$	$h+k$	$h+k+l$	$h+k+l$	0
								36	37	38	39	40	41	42	43	44	45	46
					α_1		α_1	l	0	0	0	0	0	0	0	0	0	0
mmm					α_2		α_2	0	l	0	k	h	$h+k$	0	$(h+k+l)/2$	0	l	h
					α_3		α_3	l	l	0	k	h	$h+k$	0	$(h+k+l)/2$	0	l	h
	$2h$	$2k$	$2l$	Q_{hkl}		1		47	48	49	50	51	52	53	54	55	56	57
	0	$2k$	$2l$	$\sum_h \sum_i (-1)^{\sigma_i} Q_{hki}$	α_1	$\sqrt{2}$	α_1	0	$k+l$	l	k	h	$k+l$	0	$h+l$	$h+k$	$h+l$	k
	$2h$	0	0	$\sum_k \sum_i (-1)^{\sigma_i} Q_{hki}$	α_2	$\sqrt{2}$	α_2	0	$h+l$	l	h	0	$h+k+l$	$h+l$	l	$h+k$	$k+l$	$k+l$
	$2h$	0	$2l$	$\sum_k \sum_i (-1)^{\sigma_i} Q_{hki}$	α_3	$\sqrt{2}$	α_3	0	$h+k$	0	$h+k$	h	h	$h+l$	h	0	$h+k$	l
	0	$2k$	0	$\sum_h \sum_i (-1)^{\sigma_i} Q_{hki}$		$\sqrt{2}$		58	59	60	61	62	63	64	65	66	67	68
	$2h$	$2k$	0	$\sum_i \sum_k (-1)^{\sigma_i} Q_{hki}$	α_1	$\sqrt{2}$	α_1	$h+k+l$	h	$h+k$	$h+k$	$h+k+l$	0	0	0	l	0	$h+l$
	$2h$	0	0	$\sum_i \sum_k (-1)^{\sigma_i} Q_{hki}$	α_2	$\sqrt{2}$	α_2	$h+k+l$	k	l	$k+l$	k	l	$k+l$	0	l	h	$h+k+l$
	0	0	$2l$	$\sum_h \sum_k (-1)^{\sigma_i} Q_{hki}$	α_3	$\sqrt{2}$	α_3	0	$h+k$	$h+k+l$	$h+l$	$h+l$	l	$k+l$	0	0	h	k
								69	70	71	72	73	74					
					α_1		α_1	0	$(k+l)/2$	0	l	l	0					
					α_2		α_2	0	$(h+l)/2$	0	l	h	k					
					α_3		α_3	0	$(h+k)/2$	0	0	k	k					

variable is written down with the sum sign Σ , other diffraction index varying with it is indicated by bracket (), for example, $\sum_{h(k)}$ represents that k does not keep constant during the summation of h .

8) There are 5 space groups without Σ_1 relationships, namely No. 1, 143, 144, 145 and 146.

9) When the reflection type of the space group No. 121 is $2h\ 0\ 2l$ and $h+k$ $h+k\ 0$, l must be even.

10) All the reflection types listed in the tables satisfy the requirements of both the centrosymmetric reflections and the structure seminvariants.

11) The tables of the Σ_1 relationships from No. 1 to 74 have been finished by Hašek. In fact, there are no Σ_1 relationships being direct equivalent points to $\mathbf{h}_1$. Therefore, Hašek's tables are correct⁽⁴⁾. We quote them in appendix in the unified form, and consider that the unified formulae should be used for the calculation of the probability $P_+(\mathbf{h}_1)$.

We corrected three typographic errors in Hašek's tables, i.e.

1) Exponents for space group Ima2 are $\alpha=0$, $\beta=h$ and $\gamma=h$ rather than $\alpha=0$, $\beta=k$ and $\gamma=k$.

2) The s expression of $0\ 2k\ 0$ of the point group $2/m$ is $\sum_h \sum_l (-1)^a Q_{hkl}$ rather than $\sum_k \sum_l (-1)^a Q_{hkl}$.

3) Reflection type in Table 6c $h\ h\ 0$ should be corrected into $h\ k\ 0$.

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