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Quintets: a Sequence of Nested Neighborhoods of the Structure Invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$

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A sequence of nested neighborhoods of the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$ is derived. Each neighborhood is a subset of the succeeding ones and consists of the small number of structure factor magnitudes $|E|$ upon which, in favorable cases, the value of φ mostly depends.

1. Introduction

Although the neighborhood concept was introduced only a year ago (Hauptman, 1975*a*, *b*), its important role in identifying the small set of magnitudes $|E|$ on which the value of a given structure invariant or seminvariant φ mostly depends is now firmly established (Hauptman, 1976; Green & Hauptman, 1976). In the present paper a sequence of nested neighborhoods of the five-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$ is obtained. In subsequent work the related probability distributions are derived, and these in turn lead to explicit estimates for φ in terms of magnitudes $|E|$. In the accompanying papers (Fortier & Hauptman, 1977; Hauptman & Fortier, 1977) the conditional probability distribution of φ, given the 15 magnitudes in the second neighborhood, is derived for the space group $P1$.

2. The first neighborhood

Let **h**, **k**, **l**, **m**, **n** be reciprocal vectors which satisfy

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=0\,. \tag{2.1}$$

Then the linear combination of phases

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}} \tag{2.2}$$

is a structure invariant. In analogy with earlier work (Hauptman, 1975*a*, *b*) the first neighborhood of φ is defined to consist of the five magnitudes

$$|E_{\mathbf{h}}|,\ |E_{\mathbf{k}}|,\ |E_{\mathbf{l}}|,\ |E_{\mathbf{m}}|,\ |E_{\mathbf{n}}|, \tag{2.3}$$

shown schematically as the first shell in Fig. 1. [Also see Schenk (1975) for the identity of the first two neighborhoods.]

3. The second neighborhood

Assume that the six magnitudes

$$|E_{\mathbf{h}}|,\ |E_{\mathbf{k}}|,\ |E_{\mathbf{l}}|,\ |E_{\mathbf{m}}|,\ |E_{\mathbf{n}}|,\ |E_{\mathbf{h}+\mathbf{k}}| \tag{3.1}$$

are all large. Then it is known that the structure invariant

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}\simeq 0\,. \tag{3.2}$$

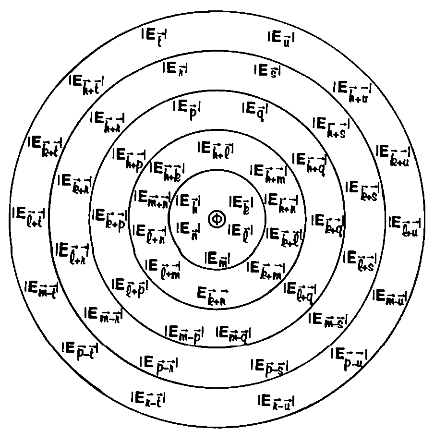

Fig. 1. A sequence of nested neighborhoods for the five-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$. The reciprocal vectors **h, k, l, m, n, p, q, r, s, t, u** satisfy $\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{p}+\mathbf{q}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{r}+\mathbf{s}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{t}+\mathbf{u}=0$, but are otherwise arbitrary. In the applications it is best that $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{n}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$, $|E_{\mathbf{t}}|$, $|E_{\mathbf{u}}|$ be large.

Also (Hauptman, 1975*a*, *b*), according as the three magnitudes

$$|E_{\mathbf{l}+\mathbf{m}}|,\ |E_{\mathbf{l}+\mathbf{n}}|,\ |E_{\mathbf{m}+\mathbf{n}}| \tag{3.3}$$

are all large or all small, the structure invariant

$$\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{h}+\mathbf{k}}\simeq 0 \text{ or } \pi\,, \tag{3.4}$$

respectively. Addition of (3.2) and (3.4) then yields

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}\simeq 0 \text{ or } \pi \tag{3.5}$$

in the respective cases. In this way rows 1 and 11 of Table 1 are obtained. In a similar way the remaining rows of Table 1 are found.

Inspection of Table 1 shows that certain rows are mutually reinforcing. Thus rows 1–10 of Table 1 are combined to yield the first row of Table 2. The second row of Table 2 is obtained by combining the rows 11–14 of Table 1 which are mutually reinforcing; the seventh row of Table 2 is obtained by combining rows 11, 12 and 15 of Table 1, *etc.* Thus the second (15-magnitude) neighborhood of φ is obtained by adding to the five magnitudes (2.3) of the first neighborhood the additional ten magnitudes

$$|E_{\mathbf{h}+\mathbf{k}}|,\ |E_{\mathbf{h}+\mathbf{l}}|,\ |E_{\mathbf{h}+\mathbf{m}}|,\ |E_{\mathbf{h}+\mathbf{n}}|,\ |E_{\mathbf{k}+\mathbf{l}}|,$$
$$|E_{\mathbf{k}+\mathbf{m}}|,\ |E_{\mathbf{k}+\mathbf{n}}|,\ |E_{\mathbf{l}+\mathbf{m}}|,\ |E_{\mathbf{l}+\mathbf{n}}|,\ |E_{\mathbf{m}+\mathbf{n}}|, \tag{3.6}$$

shown schematically as the second shell of Fig. 1. Furthermore, the value of φ is probably 0 or π in accordance with the entries of Table 2.

4. The third neighborhoods of the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$

Let **p** and **q** be arbitrary reciprocal vectors satisfying

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{p}+\mathbf{q}=0\,. \tag{4.1}$$

Then

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}} \tag{4.2}$$

is a structure invariant and, in view of (2.1),

$$\mathbf{m}+\mathbf{n}-\mathbf{p}-\mathbf{q}=0 \tag{4.3}$$

so that

$$\psi_{pq}=\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}-\varphi_{\mathbf{p}}-\varphi_{\mathbf{q}} \tag{4.4}$$

is also a structure invariant. In view of § 3, φ is estimated by means of the 15 magnitudes (2.3) and (3.6) in its second neighborhood, φ_{pq} by means of the 15 magnitudes in its second neighborhood,

$$|E_{\mathbf{h}}|,\ |E_{\mathbf{k}}|,\ |E_{\mathbf{l}}|,\ |E_{\mathbf{p}}|,\ |E_{\mathbf{q}}|;$$
$$|E_{\mathbf{h}+\mathbf{k}}|,\ |E_{\mathbf{h}+\mathbf{l}}|,\ |E_{\mathbf{h}+\mathbf{p}}|,\ |E_{\mathbf{h}+\mathbf{q}}|,\ |E_{\mathbf{k}+\mathbf{l}}|,$$
$$|E_{\mathbf{k}+\mathbf{p}}|,\ |E_{\mathbf{k}+\mathbf{q}}|,\ |E_{\mathbf{l}+\mathbf{p}}|,\ |E_{\mathbf{l}+\mathbf{q}}|,\ |E_{\mathbf{p}+\mathbf{q}}|, \tag{4.5}$$

Table 1. *The probable values of the structure invariant* $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$; *L means large, S means small*

		Magnitudes |E|													
Row	φ	h	k	ℓ	m	n	|h+k|	|h+ℓ|	|h+m|	|h+n|	|k+ℓ|	|k+m|	|k+n|	|ℓ+m|	|ℓ+n|	|m+n|
1	0	L	L	L	L	L	L							L	L	L
2	0	L	L	L	L	L		L				L	L			L
3	0	L	L	L	L	L			L		L		L		L	
4	0	L	L	L	L	L				L	L	L		L		
5	0	L	L	L	L	L			L	L	L					L
6	0	L	L	L	L	L		L		L		L			L	
7	0	L	L	L	L	L		L	L				L	L		
8	0	L	L	L	L	L	L			L			L	L		
9	0	L	L	L	L	L	L		L			L			L	
10	0	L	L	L	L	L	L	L			L					L
11	π	L	L	L	L	L	L							S	S	S
12	π	L	L	L	L	L		L				S	S			S
13	π	L	L	L	L	L			L		S		S		S	
14	π	L	L	L	L	L				L	S	S		S		
15	π	L	L	L	L	L			S	S	L					S
16	π	L	L	L	L	L		S		S		L			S	
17	π	L	L	L	L	L		S	S				L	S		
18	π	L	L	L	L	L	S			S			S	L		
19	π	L	L	L	L	L	S		S			S			L	
20	π	L	L	L	L	L	S	S			S					L

Table 2. *The probable values of the structure invariant* $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$, *given the* 15 *magnitudes in its second neighborhood; L means large, S means small; obtained by combining reinforcing rows in Table* 1

		Magnitudes |E|													
Derived from Rows of Table 1	φ	h	k	ℓ	m	n	|h+k|	|h+ℓ|	|h+m|	|h+n|	|k+ℓ|	|k+m|	|k+n|	|ℓ+m|	|ℓ+n|	|m+n|
1–10	0	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L
11, 12, 13, 14	π	L	L	L	L	L	L	L	L	L	S	S	S	S	S	S
11, 15, 16, 17	π	L	L	L	L	L	L	S	S	S	L	L	L	S	S	S
12, 15, 18, 19	π	L	L	L	L	L	S	L	S	S	L	S	S	L	L	S
13, 16, 18, 20	π	L	L	L	L	L	S	S	L	S	S	L	S	L	S	L
14, 17, 19, 20	π	L	L	L	L	L	S	S	S	L	S	S	L	S	L	L
11, 12, 15	π	L	L	L	L	L	L	L	S	S	L	S	S	S	S	S
11, 13, 16	π	L	L	L	L	L	L	S	L	S	S	L	S	S	S	S
11, 14, 17	π	L	L	L	L	L	L	S	S	L	S	S	L	S	S	S
12, 13, 18	π	L	L	L	L	L	S	L	L	S	S	S	S	L	S	S
12, 14, 19	π	L	L	L	L	L	S	L	S	L	S	S	S	S	L	S
13, 14, 20	π	L	L	L	L	L	S	S	L	L	S	S	S	S	S	L
15, 16, 18	π	L	L	L	L	L	S	S	S	S	L	L	S	L	S	S
15, 17, 19	π	L	L	L	L	L	S	S	S	S	L	S	L	S	L	S
16, 17, 20	π	L	L	L	L	L	S	S	S	S	S	L	L	S	S	L
18, 19, 20	π	L	L	L	L	L	S	S	S	S	S	S	S	L	L	L

and, from earlier work (Hauptman, 1975*b*), ψ_{pq} is estimated in terms of the seven magnitudes in its second neighborhood,

$$|E_{\mathbf{m}}|, |E_{\mathbf{n}}|, |E_{\mathbf{p}}|, |E_{\mathbf{q}}|; |E_{\mathbf{m}+\mathbf{n}}|, |E_{\mathbf{m}-\mathbf{p}}|, |E_{\mathbf{m}-\mathbf{q}}| . \quad (4.6)$$

However, from (2.2), (4.2) and (4.4) it is clear that the following identity holds:

$$\varphi - \varphi_{pq} - \psi_{pq} \equiv 0 . \quad (4.7)$$

It is therefore to be expected that in the favorable case that the 15-magnitude estimates for φ and φ_{pq}, and that the seven-magnitude estimate for ψ_{pq} yield values for φ, φ_{pq} and ψ_{pq} in accord with (4.7), then φ will be well estimated in terms of the 37 magnitudes (2.3), (3.6), (4.5) and (4.6), of which only the following 25 are distinct:

$$\begin{aligned}
&|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{n}}|;\\
&|E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{h}+\mathbf{l}}|, |E_{\mathbf{h}+\mathbf{m}}|, |E_{\mathbf{h}+\mathbf{n}}|, |E_{\mathbf{k}+\mathbf{l}}|,\\
&|E_{\mathbf{k}+\mathbf{m}}|, |E_{\mathbf{k}+\mathbf{n}}|, |E_{\mathbf{l}+\mathbf{m}}|, |E_{\mathbf{l}+\mathbf{n}}|, |E_{\mathbf{m}+\mathbf{n}}|;\\
&|E_{\mathbf{p}}|, |E_{\mathbf{q}}|, |E_{\mathbf{h}+\mathbf{p}}|, |E_{\mathbf{h}+\mathbf{q}}|, |E_{\mathbf{k}+\mathbf{p}}|, |E_{\mathbf{k}+\mathbf{q}}|,\\
&|E_{\mathbf{l}+\mathbf{p}}|, |E_{\mathbf{l}+\mathbf{q}}|, |E_{\mathbf{m}-\mathbf{p}}|, |E_{\mathbf{m}-\mathbf{q}}| . \quad (4.8)
\end{aligned}$$

Hence the third (25-magnitude) neighborhood of φ is obtained by adjoining to the second (15-magnitude) neighborhood (2.3) and (3.6) the additional ten magnitudes shown in the third shell of Fig. 1,

$$|E_{\mathbf{p}}|, |E_{\mathbf{q}}|, |E_{\mathbf{h}+\mathbf{p}}|, |E_{\mathbf{h}+\mathbf{q}}|, |E_{\mathbf{k}+\mathbf{p}}|, |E_{\mathbf{k}+\mathbf{q}}|, |E_{\mathbf{l}+\mathbf{p}}|, |E_{\mathbf{l}+\mathbf{q}}|, |E_{\mathbf{m}-\mathbf{p}}|, |E_{\mathbf{m}-\mathbf{q}}|, \quad (4.9)$$

where **p** and **q** are arbitrary reciprocal vectors satisfying (4.1). Hence there are many third neighborhoods.

One naturally anticipates that the conditional variance of the structure invariant φ, given the 25 magnitudes in its third neighborhood, will be particularly small if it should happen that the two 15-magnitude subsets and the 7-magnitude subset of the third neighborhood which are the respective second neighborhoods of the structure invariants φ, φ_{pq}, ψ_{pq} yield reliable estimates for the latter in accord with the identity (4.7). Thus, only those estimates are useful for which $|E_{\mathbf{p}}|$ and $|E_{\mathbf{q}}|$ are both large, where **p** and **q** satisfy (4.1). Table 3 illustrates the particularly favorable case that (row 1)

$$\varphi \simeq \varphi_{pq} \simeq \psi_{pq} \simeq 0 \quad (4.10)$$

or (rows 2–5)

$$\varphi \simeq \varphi_{pq} \simeq \pi, \ \psi_{pq} \simeq 0 \quad (4.11)$$

[both in accord with (4.7)] when it is expected that, with high probability, $\varphi = 0$ or π in the respective cases.

5. The fourth neighborhoods of the structure invariant $\varphi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} + \varphi_{\mathbf{n}}$

Proceed as in § 4 and denote by **r** and **s** two reciprocal vectors which satisfy

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{r}+\mathbf{s}=0 \quad (5.1)$$

so that

$$\varphi_{rs} = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{r}} + \varphi_{\mathbf{s}} \quad (5.2)$$

is a structure invariant. Now it follows from (2.1), (4.1) and (5.1) that

$$\mathbf{m}+\mathbf{n}-\mathbf{r}-\mathbf{s}=0 \quad (5.3)$$

and

$$\mathbf{p}+\mathbf{q}-\mathbf{r}-\mathbf{s}=0 \quad (5.4)$$

so that

$$\psi_{rs} = \varphi_{\mathbf{m}} + \varphi_{\mathbf{n}} - \varphi_{\mathbf{r}} - \varphi_{\mathbf{s}} \quad (5.5)$$

and

$$\chi_{rs} = \varphi_{\mathbf{p}} + \varphi_{\mathbf{q}} - \varphi_{\mathbf{r}} - \varphi_{\mathbf{s}} \quad (5.6)$$

are also structure invariants. The invariant φ_{rs} is approximated by means of the 15 magnitudes

$$\begin{aligned}
&|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{r}}|, |E_{\mathbf{s}}|,\\
&|E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{h}+\mathbf{l}}|, |E_{\mathbf{h}+\mathbf{r}}|, |E_{\mathbf{h}+\mathbf{s}}|, |E_{\mathbf{k}+\mathbf{l}}|,\\
&|E_{\mathbf{k}+\mathbf{r}}|, |E_{\mathbf{k}+\mathbf{s}}|, |E_{\mathbf{l}+\mathbf{r}}|, |E_{\mathbf{l}+\mathbf{s}}|, |E_{\mathbf{r}+\mathbf{s}}|, \quad (5.7)
\end{aligned}$$

in its second neighborhood, ψ_{rs} by means of the seven magnitudes

$$|E_{\mathbf{m}}|, |E_{\mathbf{n}}|, |E_{\mathbf{r}}|, |E_{\mathbf{s}}|; |E_{\mathbf{m}+\mathbf{n}}|, |E_{\mathbf{m}-\mathbf{r}}|, |E_{\mathbf{m}-\mathbf{s}}| \quad (5.8)$$

Table 3. *The probable values of the structure invariant* $\varphi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} + \varphi_{\mathbf{n}}$, *given the* 25 *magnitudes in its third neighborhood; L means large; S means small*

	Magnitudes $\|E\|$																								
ϕ	$\mathbf{h}$	$\mathbf{k}$	$\mathbf{l}$	$\mathbf{m}$	$\mathbf{n}$	$\mathbf{p}$	$\mathbf{q}$	$\mathbf{h+k}$	$\mathbf{h+l}$	$\mathbf{h+m}$	$\mathbf{h+n}$	$\mathbf{k+l}$	$\mathbf{k+m}$	$\mathbf{k+n}$	$\mathbf{l+m}$	$\mathbf{l+n}$	$\mathbf{m+n}$	$\mathbf{h+p}$	$\mathbf{h+q}$	$\mathbf{k+p}$	$\mathbf{k+q}$	$\mathbf{l+p}$	$\mathbf{l+q}$	$\mathbf{m-p}$	$\mathbf{m-q}$
0	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L
π	L	L	L	L	L	L	L	S	S	L	S	S	L	S	L	S	L	L	S	L	S	L	S	L	L
π	L	L	L	L	L	L	L	S	S	L	S	S	L	S	L	S	L	S	L	S	L	S	L	L	L
π	L	L	L	L	L	L	L	S	S	S	L	S	S	L	S	L	L	L	S	L	S	L	S	L	L
π	L	L	L	L	L	L	L	S	S	S	L	S	S	L	S	L	L	S	L	S	L	S	L	L	L

in its second neighborhood, and χ_{rs} by the seven magnitudes

$$|E_{\mathbf{p}}|, |E_{\mathbf{q}}|, |E_{\mathbf{r}}|, |E_{\mathbf{s}}|; |E_{\mathbf{p+q}}|, |E_{\mathbf{p-r}}|, |E_{\mathbf{p-s}}| \qquad (5.9)$$

in its second neighborhood. Now, in addition to the identity (4.7) there are the two additional identities

$$\varphi - \varphi_{rs} - \psi_{rs} \equiv 0 \qquad (5.10)$$

and

$$\varphi_{pq} - \varphi_{rs} - \chi_{rs} \equiv 0 \qquad (5.11)$$

which must be satisfied. Hence, in view of (5.7)–(5.9), the fourth (37-magnitude) neighborhood of φ is obtained from the 25-magnitude third neighborhood (2.3), (3.6) and (4.9) by adjoining the additional twelve magnitudes shown in the fourth shell of Fig. 1,

$$|E_{\mathbf{r}}|, |E_{\mathbf{s}}|, |E_{\mathbf{h+r}}|, |E_{\mathbf{h+s}}|, |E_{\mathbf{k+r}}|, |E_{\mathbf{k+s}}|, |E_{\mathbf{l+r}}|, |E_{\mathbf{l+s}}|, |E_{\mathbf{m-r}}|, |E_{\mathbf{m-s}}|, |E_{\mathbf{p-r}}|, |E_{\mathbf{p-s}}|, \qquad (5.12)$$

where **r** and **s** are arbitrary reciprocal vectors satisfying (5.1). Hence there are many fourth neighborhoods, but only those are useful for which $|E_{\mathbf{r}}|$ and $|E_{\mathbf{s}}|$ are large.

6. The remaining neighborhoods

One continues as in §§ 4 and 5 to derive the fifth and higher neighborhoods of φ. Thus the fifth (51-magnitude) neighborhoods are obtained from a fourth (37-magnitude) neighborhood by adjoining the 14 additional magnitudes

$$|E_{\mathbf{t}}|, |E_{\mathbf{u}}|, |E_{\mathbf{h+t}}|, |E_{\mathbf{h+u}}|, |E_{\mathbf{k+t}}|, |E_{\mathbf{k+u}}|, |E_{\mathbf{l+t}}|, |E_{\mathbf{l+u}}|, |E_{\mathbf{m-t}}|, |E_{\mathbf{m-u}}|, |E_{\mathbf{p-t}}|, |E_{\mathbf{p-u}}|, |E_{\mathbf{r-t}}|, |E_{\mathbf{r-u}}| \qquad (6.1)$$

where **t** and **u** are reciprocal vectors which satisfy

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{t}+\mathbf{u}=0 \qquad (6.2)$$

but are otherwise arbitrary, so that again there are many fifth neighborhoods; but only those are useful for which $|E_{\mathbf{t}}|$ and $|E_{\mathbf{u}}|$ are both large.

One continues in this way to obtain the sixth (67-magnitude) neighborhoods, *etc.* The first five of this sequence of nested neighborhoods are conveniently exhibited in Fig. 1 in which the five magnitudes of the first shell define the first neighborhood, the 15 magnitudes of the first two shells the second neighborhood, *etc.*

7. Concluding remarks

A sequence of nested neighborhoods of the quintet invariant φ has been obtained. There remains the task of deriving the associated conditional probability distributions and corresponding estimates for φ in the expectation that as more and more magnitudes $|E|$ are used the potential for obtaining more and more reliable estimates will be increased. In the accompanying papers (Fortier & Hauptman, 1977; Hauptman & Fortier, 1977) this task is begun in the space group $P1$ for the second neighborhood. It remains to derive analogous distributions in the remaining space groups and for the higher neighborhoods.

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