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# INDEXING OF POWDER DIFFRACTION PATTERNS FOR LOW SYMMETRY LATTICES BY THE SUCCESSIVE DICHOTOMY METHOD

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# APPENDIX

## ANALYSIS OF BOUNDS $Q_-$ AND $Q_+$ FOR MONOCLINIC SYMMETRY WHEN THE PRODUCT $hl$ IS NEGATIVE

$Q_{hkl} (= 1/d^2_{hkl})$ is related to the direct parameters of the unit cell $(a, b, c, \beta)$ through

$$Q = f(A, C, \beta) + g(B), \tag{1}$$

where $f(A, C, \beta) = \dfrac{h^2}{A^2} + \dfrac{l^2}{C^2} - \dfrac{2\,hl\cos\beta}{AC}$ and $g(B) = \dfrac{k^2}{B^2}$,
with $A = a\sin\beta$, $B = b$ and $C = c\sin\beta$.

The variable of the $g$-function is independent of the variables in the $f$-function. The bounds $Q_-$ and $Q_+$ are then :

$$Q_- = f_{min} + g_{min} \quad \text{and} \quad Q_+ = f_{max} + g_{max}; \tag{2}$$

$f_{min}$ and $g_{min}$ are the smallest values taken by $f$ and $g$ in their respective defined ranges $F = [A_-, A_+] \times [C_-, C_+]$ and $G = [B_-, B_+]$ ; $f_{max}$ and $g_{max}$ are their greatest values.

### I. Values of $g_{min}$ and $g_{max}$

For the $g$- function, it is clear that :

$$g_{min} = \frac{k^2}{B_+^2} \quad \text{and} \quad g_{max} = \frac{k^2}{B_-^2}. \tag{3}$$

### II. Determination of the values of $f_{min}$ and $f_{max}$

#### II.1 Generalities

The determination of $f_{min}$ and $f_{max}$ is particularly laborious. First, note that the partial derivative $\dfrac{\partial f}{\partial \beta} = \dfrac{2\,hl\,\sin\beta}{AC}$ is always negative. Then, $f_{max}$ corresponds to $\beta = \beta_-$ and $f_{min}$ to

$\beta = \beta_+$ and also the $f$-function has no extremum in its domain $F$. Indeed, the value of $A$ and $C$ which should give these extrema must satisfy the following equations :

$$\begin{cases} \dfrac{\partial f}{\partial A} = 0 \\ \\ \dfrac{\partial f}{\partial C} = 0 \end{cases} \Leftrightarrow \begin{cases} \dfrac{h}{A} = \dfrac{l\cos\beta}{C} & (4) \\ \\ \dfrac{l}{C} = \dfrac{h\cos\beta}{A} & (5) \end{cases} \Rightarrow \cos^2\beta = 1 \Leftrightarrow \beta = 0° \text{ or } \beta = 180°$$

It is evident that these $\beta$ values have no physical sense. Consequently, $f_{min}$ and $f_{max}$ necessarily correspond to points on the boundaries $M_1M_2M_3M_4$ and $N_1N_2N_3N_4$, respectively, of the domain $F$ (Fig. 1).

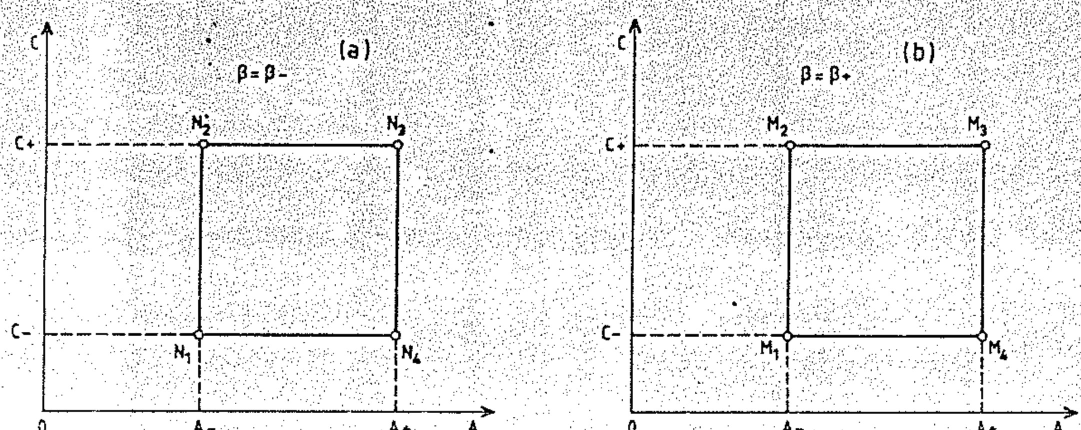


Fig. 1. Boundaries of the domain $F$ : (a) $\beta = \beta_-$, the point of the maximum is located on the full line $N_1N_2N_3N_4$ ; (b) $\beta = \beta_+$, the point of the minimum is located on the full line $M_1M_2M_3M_4$.

The extrema located on each of the segments $M_1M_2$, $M_3M_4$, $N_1N_2$ and $N_3N_4$ (Fig. 1) have coordinates $A$, $C$, $\beta$ which satisfy equation (5). Then :

$$\beta = \beta_o = \beta_\pm \; ; \; A = A_o = A_\pm \; ; \; C = C_e = \frac{l A_\pm}{h\cos\beta_\pm} \text{ (if } \beta_\pm \neq 90°\text{)} . \tag{6}$$

Likewise, if $\beta_\pm \neq 90°$, the coordinates of the extrema on the segments $M_1M_4$, $M_2M_4$, $N_1N_4$ and $N_2N_4$ are :

$$\beta = \beta_o = \beta_\pm \; ; \; A = A_e = \frac{h C_\pm}{l\cos\beta_\pm} \text{ [see (4)]} \; ; \; C = C_o = C_\pm . \tag{7}$$

At these points, the respective extrema have the value:

$$f_A = f(A_e, C_\pm, \beta_\pm) = \frac{l^2 \sin^2 \beta_\pm}{C_\pm^2} \quad and \quad f_C = f(A_\pm, C_e, \beta_\pm) = \frac{h^2 \sin^2 \beta_\pm}{A_\pm^2} . \tag{8}$$

If $\beta_\pm = 90°$ (only possible for $\beta_-$, because $\beta$ is an obtuse angle), the extrema $f_A$ and $f_C$ do not exist, since the equations (4) and (5) are not satisfied ($h$ and $l$ not equal to zero). In these cases, $f_{min}$ corresponds to one of the four corners $M_1, M_2, M_3, M_4$ (Fig. 1a) and $f_{max}$ to one of the four other corners $N_1, N_2, N_3, N_4$ (Fig. 1b).

Let us show that $f_A$ (or $f_C$) is a minimum and not a maximum. When $C$ and $\beta$ are fixed, $f$ becomes a single-variable function : $f(A, C_o, \beta_o) = \Phi(A)$. Then :

$$\frac{d\Phi}{dA} = - \frac{2\,h^2}{A^3} + \frac{2\,hl \cos \beta_o}{A^2 C_o} \; ;$$

$\frac{d\Phi}{dA}$ has the same sign as $\frac{A^3}{2\,h^2} \frac{d\Phi}{dA}$. Since $A_e$ is given by (7), it follows that :

$$\frac{A^3}{2\,h^2} \frac{d\Phi}{dA} = \frac{A}{A_e} - 1 \Rightarrow \frac{dF}{dA} > 0 \text{ when } A > A_e \text{ and } \frac{dF}{dA} < 0 \text{ when } A < A_e .$$

It can be seen that $f_A$ is thus a minimum. The minimum $f_A$ (or $f_C$) has only to be taken into account when $A_e$ (or $C_e$) is included in the range $[A_-, A_+]$ (or $[C_-; C_+]$).

It is now necessary to demonstrate that the values $A_e$ and the values $C_e$ [see (6) and (7)] cannot belong simultaneously to the domain $[A_-, A_+] \times [C_-, C_+]$. Indeed, in the reverse case, one should have :

$$\frac{h\, C_\pm}{l \cos \beta_o} \leq A_+ \tag{9}$$

$$\text{and} \quad \frac{l\, A_\pm}{h \cos \beta'_o} \leq C_+ \; , \tag{10}$$

where $\beta_o = \beta_+$ or $\beta_o = \beta_-$ and $\beta'_o = \beta_+$ or $\beta'_o = \beta_-$. (9) and (10) imply that :

$$(\cos\beta_o)\,(\cos\beta'_o) \geq \frac{C_\pm}{C_+}\,\frac{A_\pm}{A_+}$$

$$\Rightarrow |\cos\beta_+| \geq min\,(\frac{C_-}{C_+}, \frac{A_-}{A_+}). \qquad (11)$$

Let the minimum values of $\frac{C_-}{C_+}, \frac{A_-}{A_+} = \frac{X_-}{X_+} = \frac{X_-}{X_- + \varepsilon}$ be $\varphi$ ($X_-$), where $\varepsilon$ is the dichotomy step (the initial value is 0.4 Å). Then, to determine the smallest value of $\varphi(X)$ ,

$$\frac{d\varphi}{dX_-} = \frac{\varepsilon}{(X_- + \varepsilon)^2} > 0 \Rightarrow (\frac{X_-}{X_+})_{min} = \frac{x_{min}\sin\beta}{x_{min}\sin\beta + \varepsilon} = \frac{x_{min}}{x_{min} + \varepsilon/\sin\beta},$$

where $x_{min}$ is the minimum value of the dimensions of the direct unit cell. In the program, this value is fixed at 2.5 Å and the maximum value of the $\beta$ angle is fixed at 140° ; then

$$(\frac{X_-}{X_+})_{min} = 0.8007 \Rightarrow \beta > 143° .$$

Condition (11) is not possible for $\beta < 140°$, therefore $A_e$ and $C_e$ cannot both be in the domain $[A_-, A_+] \times [C_-, C_+]$. Note that inequalities (9) and (10) are not compatible.

After these general considerations, $f_{min}$ and $f_{max}$, will be determined for the different possible cases. It should be remembered that :

a) the product $hl$ is negative ;

b) the parameter $A$ is always greater than, equal to, parameter $C$ ;

c) the inequality (11) is impossible if $\beta < 140°$ ;

d) the inequalities (9) and (10) are inconsistent if $\beta < 140°$ ;

e) the $\beta$ coordinate of $f_{min}$ is $\beta_+$ ; likewise, the $\beta$ coordinate of $f_{max}$ is $\beta_-$ ;

f) because the extrema $f_A$ and $f_C$ considered above are minima, it can be deduced that :

(i) $f_{min}$ is either one of these extrema or the $f$ value at one of the four corners $M_1$, $M_2$, $M_3$ and $M_4$ (Fig. 1a),

(ii) $f_{max}$ necessarily occurs at one of the four corners $N_1$, $N_2$, $N_3$ and $N_4$ (Fig. 1b).

Let the boundaries be $M_1M_2M_3M_4$ and $N_1N_2N_3N_4$ (Fig. 1). The different possible cases will now be analysed.

## II.2 Calculation of $f_{min}$ and $f_{max}$ for the different cas

### II.2.1 Existence of the minimum point on the $M_2M_3$ segment

Let $f_{A_+}$ be this extremum : $f_{A_+} = \frac{l^2}{C_+^2}\sin^2\beta_+$ . By taking into account the above derivations, extremum points cannot exist on the segments $M_1M_2$, $M_3M_4$, $N_1N_2$ and $N_1N_4$.

Consequentely, $f_{min}$ is equal to $f_{A_+}$, since the other extremum $f_{A_-}$ ( $= \frac{l^2}{C_-^2}\sin^2\beta_+$) located on the line $M_1M_4$ is greater than $f_{A_+}$ ($f_{A_+}$ and $f_{A_-}$ are directly comparable) :

$$f_{min} = \frac{l^2}{C_+^2}\sin^2\beta_+ .$$

Morever the extremum point on $M_2M_3$ is located between $M_2$ and $M_3$ ; consequently :

$$\frac{h\,C_+}{l\cos\beta_+} \le A_+ \Rightarrow \cos\beta_+ \le \frac{h\,C_+}{l\,A_+} \Rightarrow \cos\beta_\pm \ge \frac{l\,A_\pm}{h\,C_\pm} \qquad \text{[see II.1(d)]}$$

$$\Rightarrow C_\pm \le \frac{l\,A_\pm}{h\cos\beta_\pm} ;$$

it can be concluded that the value of $f$-function at $N_1$ is greater than at $N_2$ (Fig. 2) ; in the same way its value at $N_4$ is greater than at $N_3$. Therefore $f_{max}$ corresponds to $C_-$.

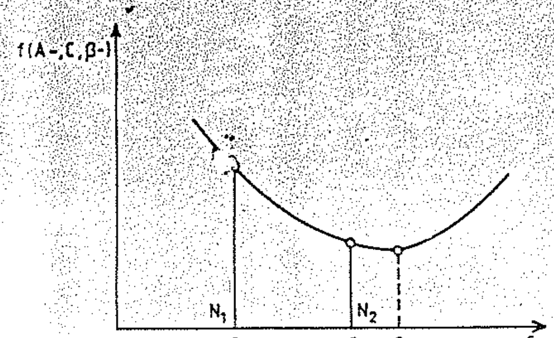


Fig. 2. Choice of the value of the maximum of $f$-function : $C_{e_-} = lA_-/h\cos\beta$ being the minimum point on line $N_1N_2$, the value of the $f$-function at $N_1$ is greater than at $N_2$.

In order to compare the values of the function $f$ at the points $N_1$ and $N_4$, a change in the variable $X = \frac{1}{A}$ can be made : $X_+ = \frac{1}{A_-}$ and $X_- = \frac{1}{A_+}$. At a point $M$, between $N_1$ and $N_4$ and having a coordinate $A$, it follows that :

$$f(A, C_-, \beta_-) = \frac{h^2}{A^2} + \frac{l^2}{C_-^2} - \frac{2\,hl\cos\beta_-}{AC_-} = h^2X^2 + \frac{l^2}{C_-^2} - \left(\frac{2\,hl\cos\beta_-}{C_-}\right)X = T(X).$$

If $X_o$ is the minimum point of this parabolic function $T(X)$, then :

- for $X_o > \frac{X_- + X_+}{2}$, the maximum of $f$ is obtained for $X_-$ (dotted line in Fig. 3),
- for $X_o < \frac{X_- + X_+}{2}$, the maximum of $f$ is obtained for $X_+$ (full line in Fig. 3).

With the original variable $A$, it follows that :

$$X_o = \frac{1}{A_e} = \frac{l\cos\beta_-}{hC_-} \; ; \; \frac{X_- + X_+}{2} = \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right).$$

$$f_{max} = f(A_+, C_-, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) < \frac{l\cos\beta_-}{hC_-}$$

$$\text{and} \quad f_{max} = f(A_-, C_-, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) \geq \frac{l\cos\beta_-}{hC_-}.$$

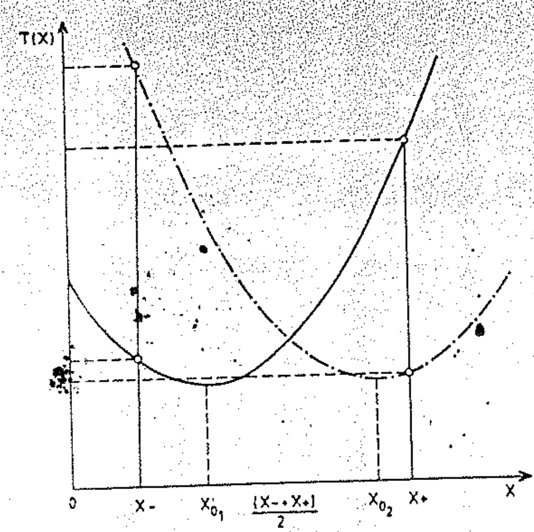


Fig. 3 - Determination of $f_{max}$ according to the position of $X_o$ with respect to $\frac{X_- + X_+}{2}$ ;

II.2.2 Existence of the minimum point on the $M_1M_4$ segment (and no extremum on $M_2M_3$)

Let $A_{e_-}$ be the coordinate $A$ of this extremum and $\chi(C) = f(A_{e_-}, C, \beta_+)$ (Fig. 4).

Then :

$$\frac{d\chi}{dC} = \left(\frac{\partial f}{\partial C}\right)_{A_{e_-},\beta_+} = -\frac{2l}{C^2}\left(\frac{l}{C} - \frac{\cos^2\beta_+}{A_{e_-}}\right) = -\frac{2l^2}{C^2}\left(\frac{l}{C} - \frac{\cos^2\beta_+}{C_-}\right)$$

$$\frac{d\chi}{dC} = 0 \Rightarrow C = C_1 = \frac{C_-}{\cos^2\beta_+} \quad (l \neq 0),$$

where $C_1$ is a minimum point for the function $\chi$. Morever, $C_+$ is lower than $C_1$, otherwise

$$C_+ \geq C_1 \Rightarrow C_+ \geq \frac{C_-}{\cos^2\beta_+} \Rightarrow \cos^2\beta_+ \geq \frac{C_-}{C_+} \Rightarrow |\cos\beta_+| > \frac{C_-}{C_+} \quad (|\cos\beta_+| < 1).$$

This inequality is impossible, as is the inequality (11) [see II.1(c)]. It follows that

$f(A_{e_-}, C_-, \beta_+) > f(A_{e_-}, C_+, \beta_+)$, which means that the minimum corresponds to $C_+$ and not to $C_-$. This minimum is either $f(A_-, C_+, \beta_+)$ or $f(A_+, C_+, \beta_+)$, depending on whether the value $A_{e_+} = \dfrac{h\,C_+}{l\cos\beta_+}$ is lower than $A_-$ or greater than $A_+$.

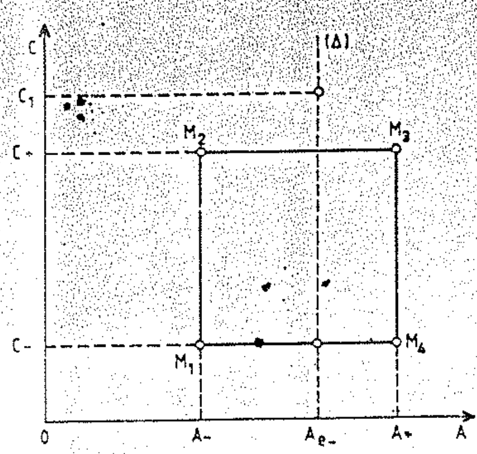


Fig. 4 - Comparison of $\chi(C_-)$ and $\chi(C_+)$. On the line $(\Delta)$ : $A = A_e$ = constant, the minimum of $\chi(C)$ is obtained from $C_1$ : $C_1 > C_+$ ; then $\chi(C_-) > \chi(C_+)$.

Now, the minimum point on $M_1M_4$ is located between $M_1$ and $M_4$ ; then :

$$\frac{hC_-}{l\cos\beta_+} > A_- \Rightarrow \frac{hC_+}{l\cos\beta_+} > A_- .$$

A graphical representation, as in Fig. 2, of the function $H(A) = f(A, C_+, \beta_+)$, should show that :

$$f_{min} = f(A_+, C_+, \beta_+).$$

The same demonstration as in case II.2.1, gives

$$f_{max} = f(A_+, C_-\beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) < \frac{l\cos\beta_-}{hC_-}$$

$$\text{and } f_{max} = f(A_-, C_-\beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) \geq \frac{l\cos\beta_-}{hC_-} .$$

II.2.3 Existence of the minimum point on the $M_3M_4$ segment (and no extremum on $M_2M_3$ and $M_1M_4$)

The value of this extremum is $f_{C_+} = \dfrac{h^2\sin^2\beta_+}{A_+^2}$ ; this is lower than the extremum $f_{C_-} = \dfrac{h^2\sin^2\beta_+}{A_-^2}$ , which exists on the line $M_1M_2$ ; $f_{C_+}$ and $f_{C_-}$ are lower than the values of the function at the points $M_1$, $M_2$, $M_3$ and $M_4$, because $f_{C_+}$ and $f_{C_-}$ are the minimum quantities on the segments $M_1M_2$ and $M_3M_4$, respectively. Consequently, $f_{min} = f_{C_+}$ , *ie* :

$$f_{min} = \frac{h^2\sin^2\beta_+}{A_+^2} .$$

Due to the symmetry of $C$ and $A$ in equation (1), a similar demonstration as in case II.2.1, applied to the parameter $C$, gives :

$$f_{max} = f(A_-, C_+, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{C_-} + \frac{1}{C_+}\right) < \frac{h\cos\beta_-}{lA_-}$$

$$\text{and } f_{max} = f(A_-, C_-, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{C_-} + \frac{1}{C_+}\right) \geq \frac{h\cos\beta_-}{lA_-} .$$

II.2.4 Case where the minimum point exists only on $M_1M_2$

The same demonstration as in case II.2.2 can be applied here. The results are :

$$f_{min} = f(A_+, C_+, \beta_+)$$

$$f_{max} = f(A_-, C_+, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{C_-} + \frac{1}{C_+}\right) < \frac{h\cos\beta_-}{lA_-}$$

$$\text{and} \quad f_{max} = f(A_-, C_-, \beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{C_-} + \frac{1}{C_+}\right) \geq \frac{h\cos\beta_-}{lA_-}.$$

II.2.5 Case where no minimum point exist on the line $M_1M_2M_3M_4$

To select between the points (corners) giving the lowest and the greatest value of $f$, two conditions have to be tested :

II.2.5.1 Case where $\cos\beta_- < \dfrac{lA_+}{hC_-}$ (12)

In this case, the following inequalities occur simultaneously :

$$C_- > \frac{lA_+}{h\cos\beta_-} \qquad \text{[see (12)]},$$

$$C_- > \frac{lA_-}{h\cos\beta_-} \qquad (A_- < A_+),$$

$$C_- > \frac{lA_+}{h\cos\beta_+} \qquad (|\cos\beta_+| > |\cos\beta_-|),$$

$$C_- > \frac{lA_-}{h\cos\beta_+} \qquad (A_- < A_+).$$

The two last expressions show that the minimum points on the lines $M_1M_2$ and $M_3M_4$ have coordinates $\dfrac{lA_-}{h\cos\beta_+}$ and $\dfrac{lA_+}{h\cos\beta_+}$ and lower than $C_-$. The graphic representations of $f(A_-, C, \beta_+)$ and $f(A_+, C, \beta_+)$, similar to Fig. 2, confirm that $f_{min}$ corresponds to $C_-$ and $f_{max}$ to

$C_+$. Morever, the relation $A_{e.} = \dfrac{h\,C_-}{l\cos\beta_+} < A_-$ is inconsistent with inequality (12) [see II.1(d)]. $A_{e.}$ is not within $[A_-, A_+]$, and is greater than $A_-$; consequentely, $A_{e.}$ is greater than $A_+$. Then

$$f_{min} = f(A_+, C_-, \beta_+).$$

Also, it follows that $\dfrac{h\,C_+}{l\cos\beta_-} > A_+$ and consequently

$$f_{max} = f(A_-, C_+, \beta_-).$$

II.2.5.2 Case where $\cos\beta_- \geq \dfrac{l\,A_+}{h\,C_-}$

i) If $\cos\beta_- \leq \dfrac{l\,A_-}{h\,C_+} \Rightarrow \cos\beta_+ \leq \dfrac{l\,A_-}{h\,C_+} \Rightarrow C_+ \geq \dfrac{l\,A_-}{h\cos\beta_+}$

$\Rightarrow C_- \geq \dfrac{l\,A_-}{h\cos\beta_+}$ [in the inverse case the minimum point $\dfrac{lA_-}{h\cos\beta_+}$ is on the segment $M_1M_2$ (Fig. 1)]

$\Rightarrow C_+ \geq \dfrac{l\,A_+}{h\cos\beta_+}$ [because $\dfrac{C_+}{A_+} > \dfrac{C_-}{A_-}$ given by II.1(b)]

$\Rightarrow C_- \geq \dfrac{lA_+}{h\cos\beta_+}$ [in the inverse case the minimum point is on the segment $M_3M_4$ (Fig.1)].

In other respects, hypothesis (i) imposes the condition : $\cos\beta_\pm \geq \dfrac{h\,C_\pm}{l\,A_\pm}$ [see II.1(d)]. Then, $A_\pm < \dfrac{h\,C_\pm}{l\cos\beta_\pm}$. Consequently, $f_{min}$ corresponds to $A_+$ and $f_{max}$ to $A_-$. This results combined with the hypothesis (i), gives

$$f_{min} = f(A_+, C_-, \beta_+),$$

$$f_{max} = f(A_-, C_+, \beta_-).$$

ii) If $\cos\beta_- > \dfrac{l A_-}{h C_+} \Rightarrow \cos\beta_- > \dfrac{l A_\pm}{h C_\pm}$ (because $\dfrac{l A_\pm}{h C_\pm} \le \dfrac{l A_-}{h C_+}$)

$$\Rightarrow C_\pm < \frac{l A_\pm}{h \cos\beta_-} .$$

The coordinates of the minimum points on the segment $N_1N_2$ and $N_3N_4$ ($\dfrac{l A_+}{h \cos\beta_-}$ *and* $\dfrac{l A_-}{h \cos\beta_-}$) are greater than $C+$. Then *fmax* corresponds to $C$-. In order to see if it is $A$- or $A$+ which gives this maximum, it is necessary to proceed as in II.2.1 :

$$f_{max} = f(A_+, C_-\beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) < \frac{l \cos\beta_-}{h C_-}$$

$$\text{and } f_{max} = f(A_-, C_-\beta_-) \quad \text{if} \quad \frac{1}{2}\left(\frac{1}{A_-} + \frac{1}{A_+}\right) \ge \frac{l \cos\beta_-}{h C_-} .$$

a) If $\cos\beta_+ < \dfrac{h C_+}{l A_-} \Rightarrow \cos\beta_\pm \ge \dfrac{l A_\pm}{h C_\pm}$ [see II.1(d)] ;

it follows that $f_{min}$ corresponds to $A_-$, *ie* :

$$f_{min} = f(A_-, C_+\beta_+).$$

b) If $\cos\beta_+ \ge \dfrac{h C_+}{l A_-} \Rightarrow A_- \le \dfrac{h C_+}{l \cos\beta_+}$

— if $\cos\beta_+ < \dfrac{l A_+}{h C_-} \Rightarrow \cos\beta_\pm \ge \dfrac{hC_\pm}{lA_\pm}$ [see II.1(d)] ; (13)

then $f_{min}$ corresponds to $A_+$. Taking into account this hypothesis, it follows that :

$$f_{min} = f(A_+, C_-, \beta_+).$$

Note : In this latter case, it is possible to deduce $f_{max}$ directly without a supplementary test. Indeed, from (13), $f_{max}$ corresponds to $A_-$ :

$$f_{max} = f(A_-, C_-, \beta_-).$$

– if $\cos\beta_+ \geq \frac{l A_+}{h C_-}$

$$\Rightarrow C_+ \leq \frac{l A_+}{h \cos\beta_+} \text{ (because the extremum } \frac{l A_-}{h \cos\beta_+} \notin [C_-, C_+]) \tag{14}$$

$$\Rightarrow C_- \leq \frac{l A_-}{h \cos\beta_+} \quad [\frac{C_-}{A_-} < \frac{C_+}{A_+} \text{ given by II.1(b)}]$$

$$\Rightarrow C_+ \leq \frac{l A_-}{h \cos\beta_+} \text{ [in the inverse case, the minimum point is on the segment } M_1M_2 \text{ (Fig. 1)]} \tag{15}$$

From (14) and (15) $f_{min}$ corresponds to $C_+$. This result used with the hypothesis (b) shows that $f_{min}$ corresponds to $A_+$:

$$f_{\min} = f(A_+, C_+, \beta_+).$$

To conclude, from the $f_{min}$ and $f_{max}$ expressions, rigorously derived for all possible cases when $hl < 0$ (§ II), and from the $g_{min}$ and $g_{max}$ expressions (§ I), the bounds $Q_-(hkl)$ and $Q_+(hkl)$ are calculated according to equations (2). The results of these mathematical calculations are summarised elsewhere in Table 1 and have been incorporated in the computer program DICVOL91.