Indexing of powder diffraction patterns for low-symmetry lattices by the successive dichotomy method

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

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APPENDIX

ANALYSIS OF BOUNDS \( Q_{\pm} \) FOR MONOCLINIC SYMMETRY WHEN THE PRODUCT \( hl \) IS NEGATIVE

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

\[
Q = f(A, C, \beta) + g(B),
\]

where

\[
f(A, C, \beta) = \frac{k^2}{A^2} + \frac{l^2 - 2 \chi \cos \beta}{C^2} \quad \text{and} \quad g(\beta) = \frac{k^2}{B^2},
\]

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:

\[
Q_- = f_{\min} + g_{\min} \quad \text{and} \quad Q_+ = f_{\max} + g_{\max}.
\]

\( f_{\min} \) 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:

\[
g_{\min} = \frac{k^2}{B^2} \quad \text{and} \quad g_{\max} = \frac{k^2}{B^2}.
\]

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

\[
\frac{\partial f}{\partial \beta} = \frac{2 \chi \sin \beta}{AC}
\]

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:

$$
\begin{align*}
\frac{\partial f}{\partial A} &= 0, \\
\frac{\partial f}{\partial C} &= 0
\end{align*}
\quad \iff 
\begin{align*}
\frac{h}{A} &= \frac{l \cos \beta}{C} \\
\frac{l}{C} &= \frac{h \cos \beta}{A}
\end{align*}
$$

(4)

(5)

It is evident that these $\beta$ values have no physical sense. Consequently, $f_{\text{min}}$ and $f_{\text{max}}$ 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 $F$.](image)

Figs. 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) $\beta = \beta_0$, 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:

$$
\beta = \beta_0 = \beta_+; \quad A = A_0 = A_+; \quad C = C_0 = \frac{l A_\pm}{h \cos \beta_\pm} \quad (\text{if } \beta_\pm \neq 90^\circ).
$$

(6)

Likewise, if $\beta_\pm \neq 90^\circ$, the coordinates of the extrema on the segments $M_1M_4$, $M_2M_4$, $N_1N_4$ and $N_3N_4$ are:

$$
\beta = \beta_0; \quad A = A_+ = \frac{h C_\pm}{l \cos \beta_\pm} \quad [\text{see (4)}]; \quad C = C_0 = C_\pm.
$$

(7)
At these points, the respective extrema have the value:

\[ f_A = f(A_+, C_+, \beta_+), \quad f_C = f(A_-, C_-, \beta_-) = \frac{h^2 \sin^2 \beta_-}{A_-^2} \quad \text{and} \quad f_C = f(A_+, C_+, \beta_+) = \frac{h^2 \sin^2 \beta_+}{A_+^2}. \]

If \( \beta_\pm = 90^\circ \) (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, \( f_{\text{min}} \) corresponds to one of the four corners \( M_1, M_2, M_3, M_4 \) (Fig. 1a) and \( f_{\text{max}} \) 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: \( f(A, C_\rho, \beta_\rho) = \Phi(A) \). Then:

\[ \frac{d\Phi}{dA} = -\frac{2h^2}{A^3} + \frac{2hl \cos \beta_\rho}{A^2 C_\rho}. \]

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

\[ \frac{A^3}{2h^2} \frac{d\Phi}{dA} = \frac{A}{A_\rho} - 1 \Rightarrow \frac{dF}{dA} > 0 \quad \text{when} \quad A > A_\rho \quad \text{and} \quad \frac{dF}{dA} < 0 \quad \text{when} \quad A < A_\rho. \]

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 \( A_\rho \) (or \( C_\rho \)) is included in the range \([A_-, A_+] \times [C_-, C_+]\).

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

\[ \frac{h C_\pm}{l \cos \beta_\rho} \leq A_+ \]

and

\[ \frac{1 A_\pm}{h \cos \beta_\rho'} \leq C_+. \]

where \( \beta_\rho = \beta_+ \) or \( \beta_\rho = \beta_- \) and \( \beta_\rho' = \beta_+ \) or \( \beta_\rho' = \beta_- \). (9) and (10) imply that:
\begin{align*}
\left( \cos \beta \right) \left( \cos \beta' \right) & \geq \frac{C_+}{C_+} \frac{A_+}{A_+} \\
\Rightarrow \left| \cos \beta \right| & \geq \min \left( \frac{C_+}{C_+}, \frac{A_+}{A_+} \right). \tag{11}
\end{align*}

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

\[ \frac{d\varphi}{dX} = \frac{\varepsilon}{(X + \varepsilon)^2} > 0 \Rightarrow \left( \frac{X}{X_{+ \text{min}}} \right) = \frac{x_{\text{min}} \sin \beta}{x_{\text{min}} \sin \beta + \varepsilon} = \frac{x_{\text{min}}}{x_{\text{min}} + \varepsilon \sin \beta}, \]

where \( x_{\text{min}} \) 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

\[ \left( \frac{X}{X_{+ \text{min}}} \right) = 0.8007 \Rightarrow \beta > 143°. \]

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

After these general considerations, \( f_{\text{min}} \) and \( f_{\text{max}} \) 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 \( f_{\text{min}} \) is \( \beta_+ \); likewise, the \( \beta \) coordinate of \( f_{\text{max}} \) is \( \beta \);
f) because the extrema \( f_A \) and \( f_C \) considered above are minima, it can be deduced that:

(i) \( f_{\text{min}} \) 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) \( f_{\text{max}} \) 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 cases

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 $N_1N_4$. Consequently, $f_{min}$ 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):

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

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

$$\frac{h \cdot c}{l \cos \beta_+} \leq A_+ \Rightarrow \cos \beta_+ \leq \frac{h \cdot c}{l A_+} \Rightarrow \cos \beta_+ \geq \frac{l A_+}{h \cdot c}$$  \quad \text{[see II.1(d)]}

$$\Rightarrow C_+ \leq \frac{l A_+}{h \cdot \cos \beta_+}$$

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 $N_3$ is greater than at $N_4$. Therefore $f_{max}$ corresponds to $C_-$.

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

\[ \text{\small $0$ $c_-$ $c_+$ $2c_-$ $2c_+$} \]
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:

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

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:

$$X_o = \frac{1}{A_o} = \frac{l \cos \beta}{hC} = \frac{X_+ + X_-}{2} - \frac{1}{2} \left(\frac{1}{A} + \frac{1}{A_+}\right).$$

$$f_{max} = f(A_+, C, \beta) \quad \text{if} \quad \frac{1}{2} \left(\frac{1}{A} + \frac{1}{A_+}\right) < \frac{l \cos \beta}{hC}$$

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

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

Then:

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

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

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

$$C_+ > C_1 \Rightarrow C_+ > \frac{C}{\cos^2 \beta_\varepsilon} \Rightarrow \cos^2 \beta_\varepsilon > \frac{C}{C_+} \Rightarrow k \cos \beta_\varepsilon > \frac{C}{C_+} \quad (k \cos \beta_\varepsilon < 1).$$

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

$f(A_{\varepsilon}, C_+, \beta_\varepsilon) > f(A_{\varepsilon}, C_+, \beta_\varepsilon)$, which means that the minimum corresponds to $C_+$ and not to $C_-$. This minimum is either $f(A_{\varepsilon}, C_+, \beta_\varepsilon)$ or $f(A_{\varepsilon}, C_+, \beta_\varepsilon)$, depending on whether the value

$$A_{\varepsilon} = \frac{h C_+}{l \cos \beta_\varepsilon}$$

is lower than $A_-$ or greater than $A_+.$

Fig. 4 - Comparison of $\chi(C_+)$ and $\chi(C_-).$ On the line $(A): A = A_{\varepsilon}$ 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:

\[
\frac{h \cos \beta_+}{l \cos \beta_+} > A \quad \Rightarrow \quad \frac{h C_+}{l \cos \beta_+} > A
\]

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:

\[
f_{max} = f(A_+, C, \beta) \quad \text{if} \quad \frac{1}{2} \left( \frac{1}{A_+} + \frac{1}{A} \right) < \frac{l \cos \beta}{h C_+},
\]

and \[
f_{max} = f(A_+, C, \beta) \quad \text{if} \quad \frac{1}{2} \left( \frac{1}{A_+} + \frac{1}{A} \right) \geq \frac{l \cos \beta}{h C_+}.
\]

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 \( f_{C_+} = \frac{h^2 \sin^2 \beta_+}{A_+^2} \); this is lower than the extremum \( f_C = \frac{h^2 \sin^2 \beta_+}{A^2} \), 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, \( f_{min} = f_{C_+} \), i.e.:

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

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:

\[
f_{max} = f(A_+, C_+, \beta) \quad \text{if} \quad \frac{1}{2} \left( \frac{1}{C_+} + \frac{1}{C} \right) < \frac{h \cos \beta}{l A_+},
\]

and \[
f_{max} = f(A_+, C, \beta) \quad \text{if} \quad \frac{1}{2} \left( \frac{1}{C_+} + \frac{1}{C} \right) \geq \frac{h \cos \beta}{l A_+}.
\]
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:

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

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

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.2.5 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 $\cos \beta < \frac{lA_+}{hC}$

In this case, the following inequalities occur simultaneously:

\[ C_+ > \frac{lA_+}{h \cos \beta_+} \quad \text{[see (12)]} \]

\[ C_+ > \frac{lA_+}{h \cos \beta} \quad (A_- < A_+) \]

\[ C_+ > \frac{lA_+}{h \cos \beta_+} \quad (|\cos \beta| > |\cos \beta_+|) \]

\[ C_+ > \frac{lA_+}{h \cos \beta_+} \quad (A_+ < A_+) \]

The two last expressions show that the minimum points on the lines $M_1M_2$ and $M_3M_4$ have coordinates $\frac{lA_+}{h \cos \beta_+}$ and $\frac{lA_+}{h \cos \beta_+}$ 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
Moreover, the relation \( A_+ = \frac{hC_+}{\cos \beta_+} < A_+ \) is inconsistent with inequality (12) [see II.1(d)].

\( A_+ \) is not within \([A_-, A_+]\) and is greater than \( A_- \); consequently, \( A_+ \) is greater than \( A_+ \). Then

\[
\sigma'_{\text{min}} = f(A_+, C_+, \beta_+).
\]

Also, it follows that \( \frac{hC_+}{\cos \beta_+} > A_+ \) and consequently

\[
\sigma'_{\text{max}} = f(A_+, C_+, \beta_+).
\]

II.2.5.2 Case where \( \cos \beta_+ \geq \frac{IA_+}{hc} \)

1) If \( \cos \beta_+ \leq \frac{IA_+}{hC_+} \Rightarrow \cos \beta_+ \leq \frac{IA_+}{hC_+} \Rightarrow C_+ \geq \frac{IA_+}{h \cos \beta_+} \[
\]
   \( \Rightarrow C_+ \geq \frac{IA_+}{h \cos \beta_+} \) [in the inverse case the minimum point \( \frac{IA_+}{h \cos \beta_+} \) is on the segment \( M_1M_2 \) (Fig. 1)]

\[
\Rightarrow C_+ \geq \frac{IA_+}{h \cos \beta_+} \) [because \( C_+ > \frac{C_+}{A_+} \) given by II.1(b)]

\[
\Rightarrow C_+ \geq \frac{IA_+}{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 \( \cos \beta_+ \geq \frac{hC_+}{IA_+} \) [see II.1(d)]. Then, \( A_+ < \frac{hC_+}{\cos \beta_+} \). Consequently, \( \sigma'_{\text{min}} \) corresponds to \( A_+ \) and \( \sigma'_{\text{max}} \) to \( A_- \). This results combined with the hypothesis (i), gives

\[
\sigma'_{\text{min}} = f(A_+, C_+, \beta_+),
\]

\[
\sigma'_{\text{max}} = f(A_-, C_+, \beta_+).
\]
ii) If \( \cos \beta_+ \rightarrow \frac{IA}{hC_+} \Rightarrow \cos \beta_+ \geq \frac{IA_\pm}{hC_\pm} \) (because \( \frac{IA_\pm}{hC_\pm} \leq \frac{IA}{hC_+} \))

\[ \Rightarrow C_\pm < \frac{IA_\pm}{h \cos \beta} \]

The coordinates of the minimum points on the segment \( N_1N_2 \) and \( N_3N_4 \) (\( \frac{IA_+}{h \cos \beta_+} \) and \( \frac{IA_-}{h \cos \beta_-} \)) are greater than \( C_+ \). Then \( f_{\text{max}} \) 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:

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

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

a) If \( \cos \beta_+ < \frac{hC_+}{IA_+} \Rightarrow \cos \beta_+ \geq \frac{IA_\pm}{hC_\pm} \) [see II.1(d)]

it follows that \( f_{\text{min}} \) corresponds to \( A_+ \), i.e.

\[ f_{\text{min}} = f(A_+, C_+, \beta) \]

b) If \( \cos \beta_+ \geq \frac{hC_+}{IA_+} \Rightarrow A_\pm \leq \frac{hC_+}{\cos \beta_+} \)

\[ \text{-- if } \cos \beta_+ < \frac{IA_\pm}{hC_-} \Rightarrow \cos \beta_+ \geq \frac{hC_\pm}{IA_\pm} \] [see II.1(d)]

(13)

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

\[ f_{\text{min}} = f(A_+, C_+, \beta_+) \]

Note: In this latter case, it is possible to deduce \( f_{\text{max}} \) directly without a supplementary test.

Indeed, from (13), \( f_{\text{max}} \) corresponds to \( A_- \):

\[ f_{\text{max}} = f(A_-, C_-, \beta_-) \]
\[
\text{if} \quad \cos \beta_+ \geq \frac{1A_+}{h C_+} \quad \Rightarrow \quad C_+ \leq \frac{1A_+}{h \cos \beta_+} \quad \text{(because the extremum} \quad \frac{1A_+}{h \cos \beta_+} \in [C_-, C_+])
\]

(14)  

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

(15)  

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

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

\[
f_{\text{min}} = f(A_+, C_+, \beta_+).
\]

To conclude, from the \( f_{\text{min}} \) and \( f_{\text{max}} \) expressions, rigorously derived for all possible cases when \( h \ell < 0 \) (§ II), and from the \( q_{\text{min}} \) and \( q_{\text{max}} \) expressions (§ I), the bounds \( Q_+(h\ell t) \) and \( Q_+(h\ell t) \) 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.