the structure determination could then proceed in a straightforward manner. More detailed descriptions of these applications will be published later (Sjölin, Alenljung, Svensson & Prince, 1988; Sjölin & Svensson, 1988).

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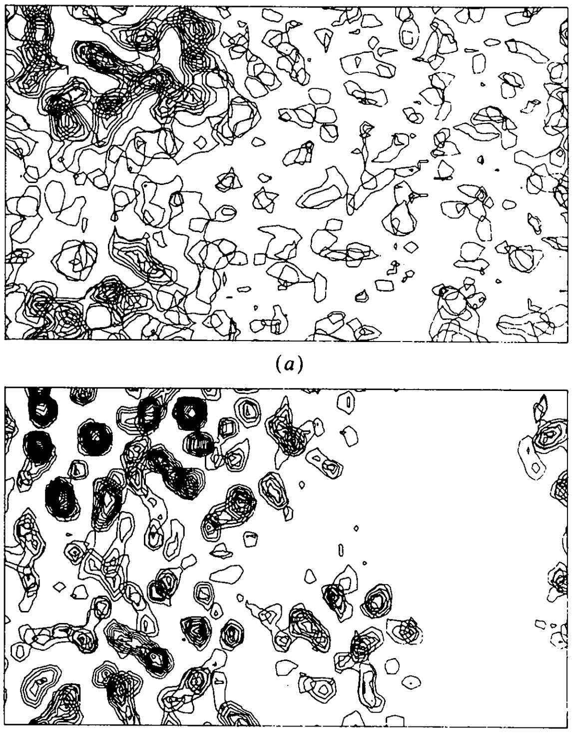

(a)

(b)

Fig. 4. Overlaid sections of electron density maps for calcium-containing fragment 1 of bovine prothrombin. (a) An F_o map with MIR phases to 3·2 Å. (b) Map with phases extended to 2·4 Å by solvent flattening and maximum entropy. Noise level in both maps set at 1σ level.

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Some Thoughts on Harker–Kasper Inequalities

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Abstract

The approach by Harker & Kasper [*Acta Cryst.* (1948), **1**, 70-75] which led to the first inequality relationships between structure factors has not previously been applied to the space group $P1$ and there seems to have been a view that it could not give useful results for that space group. The idea has also been advanced that Harker–Kasper inequalities are contained within the complete set of determinantal

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inequalities derived by Karle & Hauptman [*Acta Cryst.* (1950), **3**, 181–187]. It is shown that the Harker–Kasper approach can be applied in space group $P1$ and gives inequality relationships which are distinct, at least in form, from those derived from determinants. Indeed, in some cases, a simple Harker–Kasper inequality can be more effective than an equally simple determinantal inequality in restricting the allowed values of three-phase invariants.

Introduction

The first steps in direct methods were made by Harker & Kasper (1948) who applied the Cauchy inequality

$$\left|\sum_{j=1}^{N} a_j b_j\right|^2 \le \sum_{j=1}^{N} |a_j|^2 \sum_{j=1}^{N} |b_j|^2 \tag{1}$$

to derive inequality relationships between structure factors. They found useful relationships for determining the signs of real structure factors for both centrosymmetric and non-centrosymmetric structures but the procedures for finding inequality relationships were not very systematic. The more complete and systematic approach of Karle & Hauptman (1950) in deriving determinantal inequalities was much preferred; indeed the view has been expressed that determinantal inequalities 'include' those obtained by the Harker & Kasper approach and also that the latter approach gave no useful information for the space group $P1$.

Although inequality relationships offer very little these days in practical approaches to structure solution they do offer useful insights into the factors which govern phase-estimating probabilistic formulae. For this reason it seems worthwhile to look again at Harker–Kasper inequalities, especially for the least restrictive and most general of all space groups, $P1$.

Harker–Kasper inequalities for P1

In the usual notation we write the unitary structure factor for space group $P1$ as

$$U(\mathbf{h}) = \sum_{j=1}^{N} n_j \exp 2\pi i \mathbf{h}\,.\,\mathbf{r}_j. \tag{2}$$

For the sum of two structure factors we may write

$$U(\mathbf{h}) + U(\mathbf{k}) = \sum_{j=1}^{N} n_j(\exp 2\pi i \mathbf{h}\,.\,\mathbf{r}_j + \exp 2\pi i \mathbf{k}\,.\,\mathbf{r}_j) \tag{3}$$

which by simple manipulation becomes

$$U(\mathbf{h}) + U(\mathbf{k}) = 2\sum_{j=1}^{N} n_j \exp \pi i(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}_j \times \cos \pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}_j. \tag{4}$$

We now apply the Cauchy inequality (1) with

$$a_j = n_j^{1/2} \exp \pi i(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}_j;$$
$$b_j = 2n_j^{1/2} \cos \pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}_j.$$

Then

$$\sum_{j=1}^{N} |a_j|^2 = \sum_{j=1}^{N} n_j = 1 \tag{5a}$$

and

$$\begin{aligned}\sum_{j=1}^{N} |b_j|^2 &= 4\sum_{j=1}^{N} n_j \cos^2 \pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}_j \\ &= 2\sum_{j=1}^{N} n_j[1+\cos 2\pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}_j] \\ &= 2[1+|U(\mathbf{h}-\mathbf{k})|\cos \varphi(\mathbf{h}-\mathbf{k})].\end{aligned} \tag{5b}$$

This gives the simplest inequality

$$|U(\mathbf{h}) + U(\mathbf{k})|^2 \le 2[1+|U(\mathbf{h}-\mathbf{k})| \cos \varphi(\mathbf{h}-\mathbf{k})], \tag{6a}$$

which has a curious form involving the isolated phase angle $\varphi(\mathbf{h}-\mathbf{k})$ which is not a structure invariant. The first version of this paper then stated: 'However, the phases $\varphi(\mathbf{h})$ and $\varphi(\mathbf{k})$ are implicit in the sum of the complex quantities $U(\mathbf{h})$ and $U(\mathbf{k})$ which appears on the left-hand side so that in some opaque way a three-phase invariant is involved.' One of the referees investigated this point and found that the statement was incorrect. The referee recast inequality (6a) in the form

$$|U(\mathbf{h}) + U(\mathbf{k})|^2 - 2[1+|U(\mathbf{h}-\mathbf{k})| \cos \varphi(\mathbf{h}-\mathbf{k})] \le 0 \tag{6b}$$

and by computer examined the value of the left-hand side with change of origin. It was found that, while the value was always less than zero, it did nevertheless change with the origin. Apparently an inequality relationship derived by the Harker–Kasper approach does not need to involve structure-invariant quantities, a misconception which this author and, perhaps, many others have had.

The next case we consider is when the index triples $\mathbf{h}$ and $\mathbf{k}$ are linearly independent. In that case there can always be chosen at least one origin for which

$$\varphi(\mathbf{h}) = \varphi(\mathbf{k}) = 0. \tag{7}$$

In this case both the structure factors are real and positive so that

$$\begin{aligned}|U(\mathbf{h})| + |U(\mathbf{k})| &= \sum_{j=1}^{N} n_j(\cos 2\pi \mathbf{h}\,.\,\mathbf{r}_j + \cos 2\pi \mathbf{k}\,.\,\mathbf{r}_j) \\ &= 2\sum_{j=1}^{N} n_j \cos \pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}_j \times \cos \pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}_j.\end{aligned} \tag{8}$$

Applying the Cauchy inequality with

$$a_j = (2n_j)^{1/2} \cos \pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j;$$
$$b_j = (2n_j)^{1/2} \cos \pi(\mathbf{h}-\mathbf{k}) \cdot \mathbf{r}_j$$

and using (5b) gives

$$[|U(\mathbf{h})|+|U(\mathbf{k})|]^2 \leq [1+|U(\mathbf{h}+\mathbf{k})| \cos \varphi(\mathbf{h}+\mathbf{k})] \times [1+|U(\mathbf{h}-\mathbf{k})| \cos \varphi(\mathbf{h}-\mathbf{k})]. \quad (9)$$

Again the phases $\varphi(\mathbf{h}+\mathbf{k})$ and $\varphi(\mathbf{h}-\mathbf{k})$ stand in isolation, but given condition (7) the values of two three-phase invariants are implicitly contained in inequality (9).

A more general treatment is possible without the need for the linear independence of **h** and **k**. We now write

$$|U(\mathbf{h})| = U(\mathbf{h}) \exp[-i\varphi(\mathbf{h})] = \sum_{j=1}^{N} n_j \cos[2\pi\mathbf{h} \cdot \mathbf{r}_j - \varphi(\mathbf{h})]. \quad (10)$$

Then

$$|U(\mathbf{h})|+|U(\mathbf{k})| = \sum_{j=1}^{N} n_j\{\cos[2\pi\mathbf{h} \cdot \mathbf{r}_j - \varphi(\mathbf{h})] + \cos[2\pi\mathbf{k} \cdot \mathbf{r}_j - \varphi(\mathbf{k})]\} \quad (11a)$$

$$= \sum_{j=1}^{N} 2n_j \cos\{\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j - \tfrac{1}{2}[\varphi(\mathbf{h})+\varphi(\mathbf{k})]\} \times \cos\{\pi(\mathbf{h}-\mathbf{k}) \cdot \mathbf{r}_j - \tfrac{1}{2}[\varphi(\mathbf{h})-\varphi(\mathbf{k})]\} \quad (11b)$$

If one takes

$$a_j = (2n_j)^{1/2} \cos\{\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j - \tfrac{1}{2}[\varphi(\mathbf{h})+\varphi(\mathbf{k})]\}$$

then

$$|a_j|^2 = n_j\{1+\cos[2\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j - \varphi(\mathbf{h}) - \varphi(\mathbf{k})]\}. \quad (12)$$

Now

$$\sum_{j=1}^{N} n_j \cos[2\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j - \varphi(\mathbf{h}) - \varphi(\mathbf{k})]$$
$$= \cos[\varphi(\mathbf{h})+\varphi(\mathbf{k})] \sum_{j=1}^{N} n_j \cos 2\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j + \sin[\varphi(\mathbf{h})+\varphi(\mathbf{k})] \sum_{j=1}^{N} n_j \sin 2\pi(\mathbf{h}+\mathbf{k}) \cdot \mathbf{r}_j$$
$$= |U(\mathbf{h}+\mathbf{k})| \cos \varphi(\mathbf{h}+\mathbf{k}) \cos[\varphi(\mathbf{h})+\varphi(\mathbf{k})] + |U(\mathbf{h}+\mathbf{k})| \sin \varphi(\mathbf{h}+\mathbf{k}) \sin[\varphi(\mathbf{h})+\varphi(\mathbf{k})]$$
$$= |U(\mathbf{h}+\mathbf{k})| \cos \varphi_3(\mathbf{h}, \mathbf{k}) \quad (13)$$

where

$$\varphi_3(\mathbf{h}, \mathbf{k}) = \varphi(\mathbf{h}) + \varphi(\mathbf{k}) - \varphi(\mathbf{h}+\mathbf{k}). \quad (14a)$$

Combining results (11b), (12) and (13) and with, similarly to (14a),

$$\varphi_3(\mathbf{h}, \bar{\mathbf{k}}) = \varphi(\mathbf{h}) - \varphi(\mathbf{k}) - \varphi(\mathbf{h}-\mathbf{k}), \quad (14b)$$

we find the most general Harker-Kasper inequality for space group $P1$,

$$[|U(\mathbf{h})|+|U(\mathbf{k})|]^2 \leq [1+|U(\mathbf{h}+\mathbf{k})| \cos \varphi_3(\mathbf{h}, \mathbf{k})] \times [1+|U(\mathbf{h}-\mathbf{k})| \cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}})] \quad (15)$$

which involves two three-phase invariants.

A comparison with determinantal inequalities

The simplest determinantal inequality involving a three-phase invariant is

$$\begin{vmatrix} 1 & U(\mathbf{h}) & U(\mathbf{k}) \\ U(\bar{\mathbf{h}}) & 1 & U(\mathbf{k}-\mathbf{h}) \\ U(\bar{\mathbf{k}}) & U(\mathbf{h}-\mathbf{k}) & 1 \end{vmatrix} \geq 0 \quad (16a)$$

or

$$1-|U(\mathbf{h})|^2-|U(\mathbf{k})|^2-|U(\mathbf{h}-\mathbf{k})|^2 + 2|U(\mathbf{h})U(\mathbf{k})U(\mathbf{h}-\mathbf{k})| \cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq 0. \quad (16b)$$

Usually, but not always, a knowledge of $|U(\mathbf{h}+\mathbf{k})|$ makes (15) a stronger inequality than (16b). For example, with

$$|U(\mathbf{h})| = |U(\mathbf{k})| = |U(\mathbf{h}+\mathbf{k})| = |U(\mathbf{h}-\mathbf{k})| = 0{\cdot}5$$

then (16b) gives $\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq -1$ which contains no new information; on the other hand with inequality (15), assuming that the first factor on the right-hand side equals 1·5, its maximum possible value, gives $\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq -2/3$, which is new information.

The power of expression (15) in restricting the value of $\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}})$ is stronger as $|U(\mathbf{h}+\mathbf{k})|$ becomes smaller so that if in the case just considered $|U(\mathbf{h}+\mathbf{k})| = 0$ then $\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq 0$. However, if we take

$$|U(\mathbf{h})| = |U(\mathbf{k})| = |U(\mathbf{h}-\mathbf{k})| = 0{\cdot}6; \quad |U(\mathbf{h}+\mathbf{k})| = 1$$

then the Harker-Kasper inequality (15) gives

$$\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq -0{\cdot}47,$$

while the determinantal inequality gives

$$\cos \varphi_3(\mathbf{h}, \bar{\mathbf{k}}) \geq 0{\cdot}185$$

which is more restrictive. The general rule seems to be that if $|U(\mathbf{h}+\mathbf{k})|$ is small then the Harker-Kasper inequality gives more information but if $|U(\mathbf{h}+\mathbf{k})|$ is large then the determinantal inequality is the stronger.

There is an order-four determinantal inequality which involves the four structure factors $U(\mathbf{h})$, $U(\mathbf{k})$, $U(\mathbf{h}+\mathbf{k})$ and $U(\mathbf{h}-\mathbf{k})$ and should be stronger still.

This is

$$\begin{vmatrix} 1 & U(\mathbf{h}) & U(\mathbf{k}) & U(\mathbf{h}+\mathbf{k}) \\ U(\bar{\mathbf{h}}) & 1 & U(\mathbf{k}-\mathbf{h}) & U(\mathbf{k}) \\ U(\bar{\mathbf{k}}) & U(\mathbf{h}-\mathbf{k}) & 1 & U(\mathbf{h}) \\ U(\bar{\mathbf{h}}+\bar{\mathbf{k}}) & U(\bar{\mathbf{k}}) & U(\bar{\mathbf{h}}) & 1 \end{vmatrix} \geq 0. \qquad (17)$$

An expansion of this determinant involves three-phase and four-phase invariants and it is more difficult to extract phase information from it than from inequalities (15) or (16*b*).

Another inequality from *P*1

Starting with (11*a*) and taking

$$a_j = (n_j)^{1/2}$$
$$b_j = (n_j)^{1/2}\{\cos[2\pi\mathbf{h}\,.\,\mathbf{r}_j - \varphi(\mathbf{h})] + \cos[2\pi\mathbf{k}\,.\,\mathbf{r}_j - \varphi(\mathbf{k})]\}$$

one finds

$$\begin{aligned}[|U(\mathbf{h})| + |U(\mathbf{k})|]^2 \leq 1 &+ \tfrac{1}{2}|U(2\mathbf{h})|\cos[\varphi(2\mathbf{h}) - 2\varphi(\mathbf{h})] \\ &+ \tfrac{1}{2}|U(2\mathbf{k})|\cos[\varphi(2\mathbf{k}) - 2\varphi(\mathbf{k})] \\ &+ |U(\mathbf{h}+\mathbf{k})|\cos\varphi_3(\mathbf{h},\mathbf{k}) \\ &+ |U(\mathbf{h}-\mathbf{k})|\cos\varphi_3(\mathbf{h},\bar{\mathbf{k}}). \qquad (18)\end{aligned}$$

There can be sets of magnitudes for which inequality (18) would restrict $\cos\varphi_3(\mathbf{h},\bar{\mathbf{k}})$ more than did either of inequalities (15) or (16*b*). Thus with

$$|U(\mathbf{h})| = |U(\mathbf{k})| = |U(\mathbf{h}-\mathbf{k})| = 0{\cdot}6$$
$$|U(2\mathbf{h})| = |U(2\mathbf{k})| = 0; \qquad |U(\mathbf{h}+\mathbf{k})| = 0{\cdot}2,$$

inequality (18) gives

$$\cos\varphi_3(\mathbf{h},\bar{\mathbf{k}}) \geq 0{\cdot}73,$$

inequality (15) gives

$$\cos\varphi_3(\mathbf{h},\bar{\mathbf{k}}) \geq 0{\cdot}33$$

and inequality (16*b*) gives

$$\cos\varphi_3(\mathbf{h},\bar{\mathbf{k}}) \geq 0{\cdot}185.$$

It is clear that a knowledge of magnitudes other than the three directly related to $\varphi_3(\mathbf{h},\bar{\mathbf{k}})$ gives additional information about the restrictions on the three-phase invariant. What is true for inequalities will also hold for probability relationships and distributions and this is the basis of the neighbourhood concept (Hauptman, 1976). The way in which the magnitudes apply the extra restrictions is clearly seen in the context of inequality relationships.

Concluding remarks

Simple inequality relationships which come from the Harker–Kasper formulation and from Karle–Hauptman determinants are seen to differ in their structure and to have a relative power which depends on whether certain sets of magnitudes are large or small. Thus inequality (15) involves the four unitary structure factors $U(\mathbf{h})$, $U(\mathbf{k})$, $U(\mathbf{h}-\mathbf{k})$, $U(\mathbf{h}+\mathbf{k})$; the determinantal inequality (16*b*) involves only the first three of these while inequality (17) involves the same structure factors in a rather more complicated way. In their original paper Karle & Hauptman (1950) stated that the set of determinantal inequalities was 'complete' in the sense that no other completely independent inequality relationships could be found on the basis of the non-negativity of electron density. However, the fact that inequality (6*b*), derived from the Cauchy inequality, involves a quantity which is not a structure invariant while the Karle–Hauptman determinants, by their very nature, are structure invariants suggests that the two approaches may not formally have the same basis. The necessary and sufficient condition for the Harker–Kasper approach is that the normalized scattering factor for each atom should be real and non-negative so that $|n^{1/2}|^2 = n$, a condition which does not necessarily imply non-negative electron density. Whether the Karle & Hauptman statement applies to Harker–Kasper inequalities or not, what can be said with confidence is that no simple manipulations of determinants will yield inequality (15).

Equally, it must also be said that, while the Harker–Kasper inequalities have some kind of separate identity, they are probably less useful than determinantal inequalities on the whole but can be more useful in particular situations.

We may also conclude that the Harker–Kasper approach *can* be applied to the space group *P*1 and gives insights into the magnitudes influencing the probable values of $\varphi_3(\mathbf{h},\bar{\mathbf{k}})$.

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Improving the Interpretation of Translation Functions by a Simple Map-Correlation Procedure

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Abstract

A procedure for improving the reliability of the Q (translation) functions is presented. The procedure involves correlating between maps calculated using different sections of the reflection data, these being spherical shells divided according to d spacing. The peaks in the Q function representing the true shifts of the fragment are found to be the most stable under such a correlation procedure. The modification has been incorporated into a computer program.

Introduction

Traditionally the weakest part of Patterson-function interpretation procedures for crystal structure solution has been the location of oriented fragments in the cell. Much effort has been put into improving the reliability of translation functions and several techniques have been employed to do so (Karle, 1972; Langs, 1975; Doesburg & Beurskens, 1983; Bruins Slot & Beurskens, 1984; Egert, 1983).

In our own Patterson-method routines (Wilson & Tollin, 1985, 1986) we use the Q functions of Tollin (Tollin & Cochran, 1964; Tollin, 1966) and perform the calculations in reciprocal space. These functions find the location of an oriented fragment with respect to symmetry elements individually. For certain space groups, therefore, there is a built-in degeneracy in the Q-function determination, *e.g.* in $P2_12_12_1$ three Q functions determine six coordinates and hence each shift is located with twofold degeneracy.

This degeneracy can be exploited in the interpretation of the maps by using cross comparison between them. Often such an interpretive procedure can eliminate ambiguities in the Q-function calculations. However, the intrinsic problems of translation functions mean that even such a procedure can give incorrect answers, owing to the coincidence of spurious peaks from each of the maps. Further, if no such degeneracy exists, there is no means to check the results indicated by a Q function other than by trial and error of the resulting model in Fourier or tangent-recycling procedures.

We have found that in unfavourable circumstances the correct translational shifts in a Q-function calculation may not correspond to the highest peak in the map. Indeed, the solution representing the correct shifts can sometimes be well down the peak list. Even in degenerate cases this situation can arise, as will be shown below.

In this paper we discuss ways of improving the interpretation of Q maps, thus reducing the possibility of an incorrect translation being indicated and used in an attempted structural solution.

'Improving' Q maps

As was noticed by Karle (1972) and ourselves (Wilson & Tollin, 1985), some improvement is often gained in the calculation of translation functions (in our case the Q functions) when only the outer half [higher $(\sin\theta)/\lambda$, smaller d spacing] of the data, or some outer portion, is used in the calculations. Such data will be referred to as 'cut-off' data. The effect on the appearance of a Q map resulting from the use of cut-off data will now be discussed.

A typical feature of the Q functions is the appearance of bands of density in the map, regions of considerable linear extent where positive density is found (Fig. 1*a*). These are not universal, but are very common, especially when the model being used is small in relation to the asymmetric unit. The peaks in the Q map representing the required shifts arise from this general plateau region.

However, when cut-off data are used, these bands tend to break up and to become narrower (Fig. 1*b*). In the new map the peaks will be more likely to appear as islands in a sea of negative density, and are thus qualitatively more obvious. In this sense, the maps calculated with cut-off data are improved. A rationale for this improvement is now given.

The Q functions (Tollin & Cochran, 1964; Tollin, 1966) are defined as

$$Q(\mathbf{R}_0)=\sum_{\mathbf{h}}|F_s(\mathbf{h})|^2\sum_{j,j'=1}^{n}\cos 2\pi\mathbf{h}\,.\,[\mathbf{r}_j+\mathbf{R}_0 - T(\mathbf{r}_{j'}+\mathbf{R}_0)],$$

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