Short Communications

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On an application of inequality methods to centrosymmetric crystals with partly known structures.

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The use of inequality methods for structure determination has been recently emphasised by many authors. We wish to show in our present paper a modified application of inequality methods to crystals with partly known structures. This happens when some of the atoms lie in special positions by space-group requirements or when some atoms have already been fixed by Patterson function or by other methods.

The unitary structure factor U_{hkl} for crystals with centres of symmetry can be written as follows:

$$U_{hkl} = \sum_{i'} n'_i \cos 2\pi(hx'_i+ky'_i+lz'_i) + \sum_{i''} n''_i \cos 2\pi(hx''_i+ky''_i+lz''_i) = U'_{hkl}+U''_{hkl}\,, \qquad (1)$$

where, the notation being the same as in our previous paper (1952*b*), $n_i = Z_i/F_{000}$, Z_i being the number of electrons in the *i*th atom, and single primes refer to the atoms in known and double primes to those in unknown positions. If the part U''_{hkl} is modified as follows:

$$\hat{U}''_{hkl} = \frac{U''_{hkl}}{\sum_{i''} n''_i} \equiv \frac{U_{hkl}-\sum_{i'} n_i \cos 2\pi(hx'_i+ky'_i+lz'_i)}{1-\sum_{i'} n'_i}\,, \qquad (2)$$

this should of course satisfy the inequalities of Harker & Kasper or ours, and, being intensified by $1/\sum_{i''} n''_i$ as compared with original U''_{hkl}, will be more adequate for the application of the inequality methods. Although we cannot obtain directly the value of $\hat{U}''_{hkl}$ if the sign of U_{hkl} is unknown, still $\hat{U}''_{hkl}$ should possess either

$$\frac{|U_{hkl}|-\sum_{i'} n'_i \cos 2\pi(hx'_i+ky'_i+lz'_i)}{1-\sum_{i'} n'_i}$$

or

$$\frac{-|U_{hkl}|-\sum_{i'} n'_i \cos 2\pi(hx'_i+ky'_i+lz'_i)}{1-\sum_{i'} n'_i}\,,$$

the inadequate alternative being possibly precluded by the use of the inequality methods and leading thus to the knowledge of the correct sign of U_{hkl}. Obviously, if one of the alternatives comes out to be of absolute value greater than unity, this should be excluded and the sign of U_{hkl} will thus be determined directly. It may be added that, in subtracting the effect of the known part U'_{hkl} from U_{hkl}, one should be careful to adjust the arbitrary parameters (Okaya & Nitta, 1952*a*, *b*), due to choice of the origin, between the expressions U_{hkl} and $\sum_{i'} n'_i \cos 2\pi(hx'_i+ky'_i+lz'_i)$.

Actual examples of the application of this method will be given later.

In conclusion, the authors wish to thank Mr Y. Tomiie for his valuable suggestions on the present problem.

References

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Application of our linear inequalities and some remarks on B. S. Magdoff's paper on 'Forbidden reflections in the Harker–Kasper inequalities'.

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Magdoff (1951) had made some useful and interesting applications of the Harker–Kasper inequalities for space-group extinctions and for half odd indices, using the 'sum and difference' inequality of Harker & Kasper (1947, 1948). By the linear inequalities for crystals with centres of symmetry which we have found recently (Okaya & Nitta, 1952*b*), we can obtain analogous but more convenient inequality relations. The inequality (18) in our paper (Okaya & Nitta, 1952*b*),

$$p^2+q^2+2r^2+p^2U_{2h,\,2k,\,2l}+q^2U_{2h',\,2k',\,2l'} + 2pq(U_{h+h',\,k+k',\,l+l'}+U_{h-h',\,k-k',\,l-l'}) \geqq 4r|pU_{hkl}+qU_{h'k'l'}|, \quad r \geqq 0\,, \qquad (1)$$

can be modified to the following form by putting $r=0$:

$$p^2+q^2+p^2U_{2h,\,2k,\,2l}+q^2U_{2h',\,2k',\,2l'} \pm 2pq(U_{h+h',\,k+k',\,l+l'}+U_{h-h',\,k-k',\,l-l'}) \geqq 0\times|pU_{hkl}\pm qU_{h'k'l'}|\,. \qquad (2)$$