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## A computer procedure for the systematic application of Sayre's equation for solving the phase problem for the analysis of centrosymmetric structures.

By P. T. BEURSKENS,* *Crystallography Laboratory, University of Pittsburgh, Pittsburgh* 13, *Pa., U.S.A.*

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The Sayre equation (Sayre, 1952)

$$s(\mathbf{h}+\mathbf{h}') \sim s(\mathbf{h}).s(\mathbf{h}') \qquad (1)$$

has been used to generate many signs from a set of known signs, and to find relations among signs from which further signs may be deduced, (Zachariasen, 1952; Woolfson, 1957; Grant, Howells & Rogers, 1957; De Vries, 1963). In the sign correlation method presented here, several reflexions numbered 1, 2, ...$i$... are given an arbitrarily chosen sign and these are used together with the origin determining signs to generate other signs with relation (1). The generated signs are determined relative to the arbitrarily chosen signs and this dependency is traced. From the degree of consistency of the generated signs it is deduced whether or not the arbitrary choices were correct.

The following notation is used:

[0] is a set of reflexions [0]**h** of which the signs are independent of any of the arbitrary choices,

[$i$] is a set of reflexions [$i$]**h** of which the signs depend only on the $i$th arbitrary choice (the $i$th arbitrary choice is included),

[$i, j, \ldots$] is a set of reflexions [$i, j, \ldots$]**h** of which every one of the signs depends upon the choices $i, j, \ldots$,

[$x$] is an abbreviation for [$i, j, \ldots$], so $x$ stands for 0, or $i$, or any combination $i, j, \ldots$. A set [$x$] is called a *correlation set.*

The *combination rule* is defined as:

$$[x, x'] = [x].[x'] \qquad (2)$$

in which '$i, i$' is replaced by '0' and '$i$, 0' is replaced by '$i$'.

A reflexion (**h**+**h**′) which is generated by Sayre's equation (1) from two reflexions [$x$]**h** and [$x'$]**h**′ is registered in the set [$x, x'$] according to the combination rule (2). Thus Sayre's equation is formulated:

$$s[x, x']\mathbf{h}+\mathbf{h} \sim s[x]\mathbf{h}.s[x']\mathbf{h}'. \qquad (3)$$

A relation among the arbitrary choices is obtained if a reflexion **h** is present in set [$x$] as well as in set [$x'$];

$$\text{if } s[x]\mathbf{h} = \; s[x']\mathbf{h}, \text{ then } [x, x'] \cong [0] \qquad (4a)$$

$$\text{if } s[x]\mathbf{h} = -s[x']\mathbf{h}, \text{ then } [x, x'] \cong [0]\,. \qquad (4b)$$

(4$a$) expresses that all reflexions of set [$x, x'$] probably have absolute correct signs, and (4$b$) that the signs of these reflexions have to be reversed. These relations (4) are called correlation equations.†

A correlation equation is assumed to be correct if it is found many times with a high probability. Consequently, one arbitrary choice can be expressed in terms of the other choices using the combination rule (2). The number of possible sign combinations of the original arbitrary choices is thus reduced by a factor 2.

The sign correlation method has been programmed for an IBM 1620 computer for triclinic, monoclinic, and orthorhombic space groups, was tested on potassium fluoride tetrahydrate (Beurskens & Jeffrey, 1964), and was used successfully by other members of this laboratory to give a single set of signs for the structure determination of orthonitroperbenzoic acid, peroxypelargonic acid, and allantoin, all in space group $P2_1/c$.

A more detailed description of the method is given in the IBM 1620 computer description (Beurskens, 1963) which is available upon request.

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* Present address: Laboratorium voor Kristalchemie, Rijks Universiteit, Utrecht, The Netherlands.

† Some of the relations $s[i, j]\mathbf{h} = \pm s[i, k]\mathbf{h}$ or $s[i, j]\mathbf{h} = \pm s[k, l]\mathbf{h}$ are equivalent to coincidences (Grant *et al.*, 1957) or coincidences of the second kind (DeVries, 1963, who introduced the name 'correlation equation' for sign relations restricted for four reflexions).

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## Crystallographic data for modifications of mesotartaric acid.

By G. A. BOOTSMA and J. C. SCHOONE, *Laboratorium voor Kristalchemie, Rijksuniversiteit, Utrecht, The Netherlands*

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Four different modifications of mesotartaric acid were obtained by crystallization from water (Table 1).

Prism-shaped crystals of I were obtained by slowly evaporating a solution at about 70 °C, prism-shaped crystals of the normal monohydrate form III by evaporating a saturated solution at room temperature. Crystals