one may take a generating set with the smallest possible value of n or prefer a set with larger n if it is more symmetric. Different choices of n will lead to different abstract groups.

(b) The n vectors $\mathbf{v}^{(i)}$ give a representation of the point group by n-dimensional matrices (of integers):

$$g\mathbf{v}^{(i)} = \sum \mathbf{v}^{(j)} D^{ji}(g). \qquad (A.1)$$

(c) Because the phase functions are linear to within additive integers, it is enough to specify their values at the n generating vectors. For each point-group operation g these values constitute an n-vector Φ_g with components

$$\Phi_g^{(i)} = \Phi_g(\mathbf{v}^{(i)}). \qquad (A.2)$$

(d) Because each component of a given phase-function vector Φ_g is determined only to within an additive integer, Φ_g can be represented by any member of the entire n-dimensional set S_g of vectors whose components differ from those of Φ_g by integers.

(e) Given any two representatives Φ_g and Φ_h from S_g and S_h, it follows from (3.6) that a vector from S_{gh} is given by

$$\Phi_{gh} = \Phi_g D(h) + \Phi_h. \qquad (A.3)$$

(f) Elements of the space group consist of ordered pairs (g, Φ_g), (g, Φ'_g), (g, Φ''_g), ... where g is any point-group element and $\Phi_g, \Phi'_g, \Phi''_g, \ldots$ are all the vectors in S_g. The combination law for two such pairs is the semidirect product

$$(g, \Phi_g)(h, \Phi_h) = (gh, \Phi_g D(h) + \Phi_h). \qquad (A.4)$$

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The Program *SAPI* and its Applications. I. Automatic Search of Pseudo-Systematic Extinction for Solving Superstructures

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Abstract

The name *SAPI* is an abbreviation of 'structure analysis programs with intelligent control'. It may also be read inversely as 'Institute of Physics, Academia Sinica'. *SAPI* is based on *MULTAN*80, but differs from it by a number of features. These will be described in a series of papers. The present paper describes an algorithm which can distinguish superstructures from ordinary structures by automatically discovering the pseudo-systematic extinction rule in reciprocal space. This algorithm enables *SAPI* to handle superstructures in a fully automatic way, leading to a complete solution in favourable cases.

Introduction

Superstructures are distinguished by their pseudo-translational symmetry, which leads to the effect of pseudo-systematic extinction, *i.e.* there exists two classes of reflections, one systematically strong, the

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other systematically weak. The phases of the second class of reflections are usually very difficult to determine. A direct method (Fan Hai-fu, Yao Jia-xing, Main & Woolfson, 1983) has been proposed and incorporated into the *MULTAN*80 program (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). With the modified *MULTAN*80, superstructures can be solved by inputing the pseudo-systematic extinction rule into the program. In order to make the procedure fully automatic, an algorithm was recently developed to search automatically for the pseudo-systematic extinction rule in reciprocal space. The philosophy of this algorithm and some examples are given in this paper.

Index relations for the systematically strong reflections

We consider only the pseudo-systematic extinction due to the existence of a sublattice. If several possible sublattices exist simultaneously, only one of them should be considered. If all the possible sublattices are compatible with each other, the one with the smallest unit cell will be accepted. If the possible sublattices are incompatible, we should consider that one which results in the lowest average intensity of the systematically weak reflections.

A sublattice can be described by three primitive translation vectors, $\mathbf{t}_1$, $\mathbf{t}_2$ and $\mathbf{t}_3$, at least one of which should be a pseudo-translation vector of the true lattice, *i.e.*

$$\mathbf{t} = \mathbf{T}/p, \tag{1}$$

where $\mathbf{T} = m_1\mathbf{a} + m_2\mathbf{b} + m_3\mathbf{c}$ is the shortest lattice vector parallel to $\mathbf{t}$, and p is an integer greater than 1. Accordingly (see Fan Hai-fu & Zheng Qi-tai, 1982) all reflections with $\mathbf{H}.\mathbf{t}$ ($\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$) not equal to an integer will be systematically weak, leading to an effect of pseudo-systematic extinction. In other words all the strong reflections will satisfy the relation

$$\mathbf{H}.\mathbf{t} = n, \tag{2}$$

where n denotes an arbitrary integer. Equivalently we have

$$m_1h + m_2k + m_3l = pn, \tag{3}$$

where m_1, m_2 and m_3 are integers without a common divisor other than 1. This is the index relation that should be satisfied by all the systematically strong reflections.

Since three vectors are sufficient to define a sublattice, no more than three index relations should be used for defining the group of 'strong' reflections.

Finding index relations for the systematically strong reflections

There are three kinds of index relations, which, respectively, are those with one, two or three of the coefficients m_1, m_2 and m_3 not equal to zero. We should try firstly to find those index relations having only one coefficient not equal to zero. This is done as follows.

Calculate the average E^2 values for different indices h. Reject those h's with average E^2 smaller than a certain limit; in our program the default value of this limit is set to 0·5. Find the greatest common divisor p for all the remaining h's. If there exist several incompatible values of p, only the one giving the smallest average E^2 value for the systematically weak reflections should be accepted. Repeat the above process to find index relations of the types $k = p'n$ and $l = p''n$.

Index relations with two or three coefficients not equal to zero can be found as follows:

(1) Calculate the index difference, Δh, for each pair of reflections having k and l in common.

(2) Sum the E^2 values for all pairs of reflections having the same Δh. Reject those Δh's corresponding to an average E^2 smaller than a certain limit.

(3) Find the greatest common divisor p_1 for the remaining Δh's.

(4) Use a similar procedure to find p_2 for Δk and p_3 for Δl respectively.

(5) If two or more of p_1, p_2 and p_3 equal 1, then there will be no index relation with two or three coefficients not equal to zero for the 'strong' reflections.

(6) If only two of p_1, p_2 and p_3, say p_1 and p_3, are greater than 1, then there are two possible relations, *i.e.*

$$m_1h + m_3l = pn \quad \text{or} \quad m_1h - m_3l = pn,$$

where $m_1 = p/p_1$, $m_3 = p/p_3$. Calculate the average E^2 for the 'weak' reflections corresponding to each of the above relations. Reject any relation which makes the average E^2 greater than a certain limit, or reject the one which results in a larger average E^2 when both average E^2's are smaller than the limit.

(7) If p_1, p_2 and p_3 are all greater than 1, then the following relations are all possible:

$$m_1h + m_2k + m_3l = pn$$
$$m_1h + m_2k = pn$$
$$m_1h + m_3l = pn$$
$$m_2k + m_3l = pn.$$

Reject any one of the above relations if the corresponding average E^2 for the 'weak' reflections is greater than a certain limit.

Before any relation is finally accepted, it should be checked for independence. This includes the following considerations:

(1) One-index relations are the most fundamental relations and should be accepted first.

(2) If there already exists a one-index relation, say $h = p_1 n$, then any multi-index relation including h, say $m_1 h + m_2 k + m_3 l = pn$ with m_1 not equal to zero, should not be accepted, provided $p_1 = p/m_1$.

(3) Since the combination of a two-index relation and a three-index relation gives rise to a one-index relation, they are not allowed to be accepted simultaneously. The one resulting in a larger average E^2 for the 'weak'°reflections should be rejected.

(4) After the above considerations, any index relation should be rejected if it can be a result of the centred lattice or of other relations not yet rejected.

Set up index relations for the systematically weak reflections

Suppose that the index relations found for the 'strong' group are

$$m_1 h + m_2 k + m_3 l = p_1 n$$
$$m_4 h + m_5 k + m_6 l = p_2 n$$
$$m_7 h + m_8 k + m_9 l = p_3 n;$$

then there will be at most $p_1 p_2 p_3 - 1$ 'weak' groups.

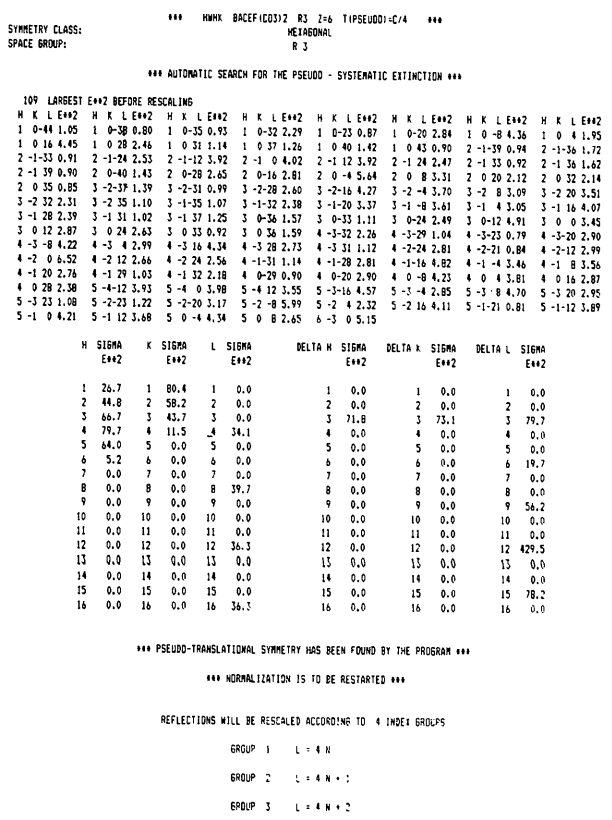

Fig. 1. Result for the structure of HWHK, $BaCeF(CO_3)_2$: $t = c/4$.

The index relations for each 'weak' group can be

$$m_1 h + m_2 k + m_3 l = p_1 n + p_1'$$
$$m_4 h + m_5 k + m_6 l = p_2 n + p_2'$$
$$m_7 h + m_8 k + m_9 l = p_3 n + p_3'$$

where p_1', p_2' and p_3' are integers equal to or less than p_1, p_2 and p_3 respectively. In addition, there should not be more than two of p_1', p_2' and p_3' equal to the corresponding value of p_1, p_2 and p_3.

Finally, some 'weak' reflection group found as above may actually contain no reflections in it. Such a group will be rejected after a final check.

The above algorithm has been included in *SAPI*85 (Yao Jia-xing, Zheng Chao-de, Qian Jin-zi, Han Fu-sen, Gu Yuan-xin & Fan Hai-fu, 1985) as a subroutine named *AUTOGP*.*

* A listing of the subroutine *AUTOGP* has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44885 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

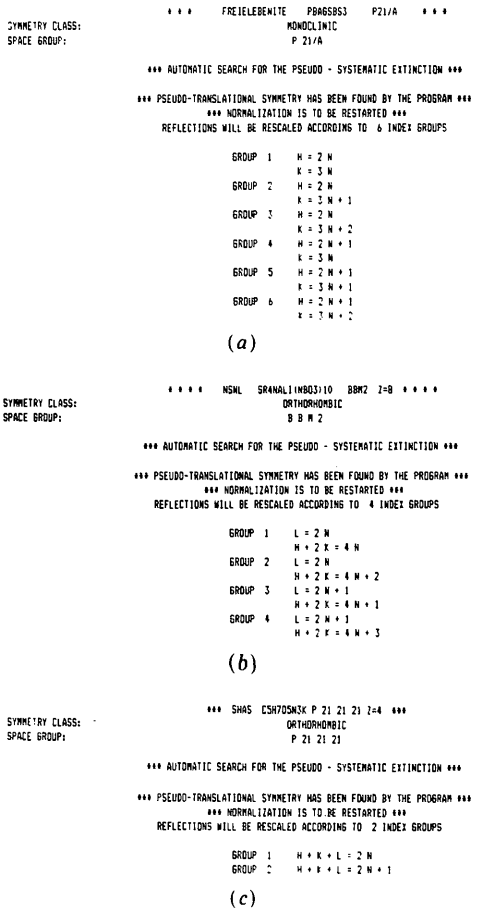

Fig. 2. Results for (*a*) freielebenite, $AgPbSbS_3$: $t_1 = a/2$, $t_2 = b/3$; (*b*) NSNL, $LiNaSr_4(NbO_3)_{10}$: $t_1 = c/2$, $t_2 = a/4 + b/2$; (*c*) SHAS, $C_5H_7KN_3O_5$: $t = a/2 + b/2 + c/2$.

Some examples are shown in Figs. 1 and 2. In these examples the user needs only to input the diffraction intensities, space-group symbol, chemical formula and cell dimensions in the usual way. The program can then tell what kind of pseudo-systematic extinction exists.

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The Program *SAPI* and its Applications. II. The Combination of Patterson Superposition and Direct Methods

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Abstract

A minimum-function subroutine is included in the *SAPI* program. This enables the superposition of either two Patterson maps or a Patterson map with an E map. Both kinds of superposition can effectively combine Patterson and direct methods leading to results better than those from either of the two alone. Practical examples are given to elucidate the efficiency of such a combination.

The Patterson superposition method is very powerful if a few atoms, especially heavy atoms, in the asymmetric unit are known with certainty. On the other hand, direct methods are very efficient in obtaining an E map with the highest peaks corresponding to true atoms. However, an E map often contains some spurious peaks which cause trouble in the interpretation. Hence Patterson superposition based on an E map may be a powerful procedure for fragment development, especially when the known part of the structure cannot dominate the phases.

There are two ways to combine the information from an E map and the Patterson map:

(1) Calculate a Patterson minimum function according to some Harker and non-Harker peaks, the positions of which are derived from a few highest peaks on the E map (minimum Patterson Patterson, MPP).

(2) Calculate a minimum function by superimposing a Patterson map onto an E map with the Patterson origin coinciding successively with the highest peaks of the E map (minimum E map Patterson, MEP). Schenk (1972) first proposed such a kind of combination.

*SAPI*85 (Yao Jia-xing, Zheng Chao-de, Qian Jin-zi, Han Fu-sen, Gu Yuan-xin & Fan Hai-fu, 1985) provides facilities for both the above procedures, which are best explained using the following three examples.

Example 1. *MPP on eight known atoms*

Crystal data: chemical formula $C_{52}H_{24}Fe_8O_{28}$, space group $P1$, unit-cell parameters $a = 14{\cdot}660$, $b = 12{\cdot}919$, $c = 9{\cdot}086$ Å, $\alpha = 92{\cdot}48$, $\beta = 115{\cdot}20$, $\gamma = 112{\cdot}02°$, $Z = 1$. In this structure there are eight heavy atoms (Fe) in the asymmetric unit. A default run of *SAPI*85 was first executed. In the resulting E map, the eight highest peaks all correspond to true atoms but one of them was not iron. The largest spurious peak appeared as the tenth peak, and there are 12 spurious peaks within the top 33 peaks on the E map. Hence the E map is difficult to interpret. A Patterson minimum function was then calculated according to the positions of the eight highest peaks on the E map. This resulted in a much improved map, in which the eight highest peaks all correspond to Fe atoms, and the largest spurious peak appeared as the 34th peak. In other words, all the top 33 largest peaks correspond to true atoms. For comparison, a weighted Fourier map was calculated with phases from the eight highest peaks of the E map, all assumed to be Fe atoms. It resulted in a map with 11 spurious peaks within the top 33 peaks and the largest spurious peak appeared as the 13th peak. The above results are summarized

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