conform with the alternative position of the magnesium atoms.

It is to be noted that in both varieties in this projection one set of oxygen atoms at the base of the silicate layer lies almost exactly over the hydroxyl groups of the layer below, while the other set of oxygen atoms at the base of the silicate layer lies almost exactly over points half way between the hydroxyl groups of the layer below. How exactly this relationship is obeyed cannot be stated with certainty until the further refinement of the structures has been completed. In the projection down [010] one of the oxygen atoms involved is not resolved from the adjacent silicon atom, but the other oxygen atom in both varieties is at present determined to be 0·1 Å from the point exactly opposite the hydroxyl group of the next layer. In other minerals of the kaolin-type whose detailed structure is known this distance exceeds 0·4 Å. The difference is presumably associated with the inter-layer disorder along [010] which must result from the cylindrical structure revealed by the electron microscope (Noll & Kircher, 1951). On account of their different radii, successive layers must be completely out of register in the [010] direction, and the basal oxygen atoms of one layer will therefore be unable to take up the two-

dimensionally most favourable positions with respect to the hydroxyl groups of the layer below. Rather, they will be constrained to take up appropriate positions with respect to the rows of hydroxyl groups which, considered statistically, will have the same effect as corrugations running round the circumference of the cylinder. Then, if the two sets of basal oxygen atoms have slightly different elevations in a direction perpendicular to the layers, one will lie over the 'grooves' between the hydroxyl groups and the other will lie over the 'ridges' of hydroxyl groups. Just such a difference in the elevations of the oxygen atoms is in fact indicated by the Fourier projections.

References

ARUJA, E. (1943). Ph.D. Thesis, Cambridge.
NOLL, W. & KIRCHER, H. (1951). N. Jb. Min. **10**, 219.
WHITTAKER, E. J. W. (1951). Acta Cryst. **4**, 187.
WHITTAKER, E. J. W. (1953). Acta Cryst. **6**, 93.

A contribution to the vector-algebraic method for the interpretation of the Patterson synthesis. By A. BEZJAK, *Laboratory for General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia*

Recently Lindqvist (1952) described and successfully applied a new 'vector-algebraic method' for the interpretation of the Patterson synthesis in the case of centrosymmetrical structures. In this note a modification and further development of his method is described.

If in the centrosymmetrical lattice two atoms are chosen at the points $A(x_i, y_i, z_i)$ and $B(x_j, y_j, z_j)$, then in the Patterson function the maxima with the coordinates

$$M_1(2x_i, 2y_i, 2z_i); \quad M_2(2x_j, 2y_j, 2z_j);$$
$$M_3(x_i+x_j, y_i+y_j, z_i+z_j); \quad M_4(x_i-x_j, y_i-y_j, z_i-z_j)$$

are to be found. These maxima belong to the interatomic vectors r_1, r_2, r_3 and r_4, respectively (Fig. 1). If the atoms are of the same scattering power the maxima M_3 and M_4 are twice as large as the maxima M_1 and M_2.
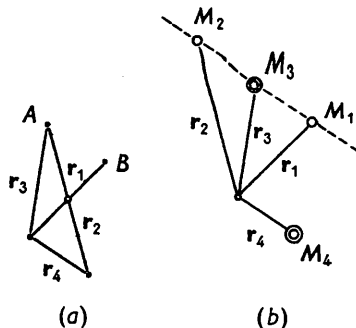

Fig. 1.

The vectors r_1 and r_2 are the diagonals and the vectors r_3 and r_4 are the sides of a parallelogram; they are therefore related by the equations

$$r_1 = r_3 + r_4, \quad r_2 = r_3 - r_4,$$

upon which Lindqvist based his method.

Evidently, the maxima M_1, M_2 and M_3 are located on a straight line with M_3 exactly at the mid point of the length M_1M_2 (Fig. 1(b)). Moreover, the maximum M_4 is to be found on the terminal of the vector r_4, the length of which is equal to the length M_2M_3 (or M_3M_1) and is in the same direction.

If, therefore, the positions of two atoms are to be determined from a Patterson projection, three maxima (1, 2, 1) located on a straight line must be found with a doubly-weighted maximum (2) at the mid point. On the straight line parallel to the first but passing through the origin a doubly-weighted maximum at a distance 1–2 from the origin must also be found. Consequently, the real positions of the atoms in the projection are at the mid points of the lines joining the origin to the singly-weighted maxima.

If the positions of three atoms are to be found from the Patterson projection, then the singly-weighted maxima would be located on the corners of a triangle with the doubly-weighted maxima at the mid points of its sides. On the straight lines parallel to each side of this triangle and passing through the origin the corresponding doubly-weighted maxima would also appear (Fig. 2).

It follows that for n atoms (of the same scattering power) the singly-weighted maxima would make in the

Patterson projection a polygon of the nth order, with doubly-weighted maxima at the mid points of each side
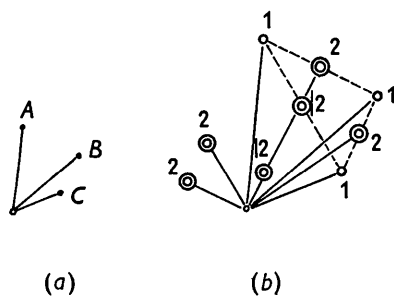

Fig. 2.

and on the straight lines passing through the origin parallel to these sides. The order of the polygon depends upon the multiplicity of the space group (e.g. in the plane group pg the polygon is of the $2n$th order).

The method was successfully applied in the structure determination of mercury oxychloride, $2HgCl_2.HgO$, which has been undertaken in this laboratory (Grdenić & Šćavničar, 1952). The crystals of this compound belong to the symmetry group T^4-P2_13 with 4 formula units in the elementary cell. The interpretation of the Patterson projection in this case could obviously be restricted only to the Hg–Hg maxima. Using the method described a 'triangle' was found (Fig. 3) from which the probable preliminary mercury parameters were derived, and subse-

quently confirmed by the symmetry relations and by finding a corresponding 'hexagon' in the Patterson projection.
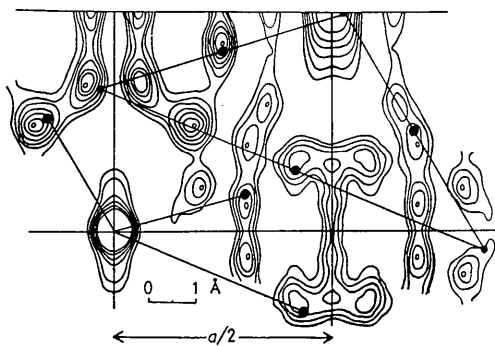

Fig. 3.

In conclusion I wish to thank Dr D. Grdenić for a very helpful discussion and also S. Šćavničar for supplying me with all data and allowing me to publish the Patterson projection in Fig. 3.

References

GRDENIĆ, D. & ŠĆAVNIČAR, S. (1952). To be published. Presented at the 1st Congress of Pure and Applied Chemistry of the People's Republic of Croatia, Zagreb, October 1952.
LINDQVIST, I. (1952). *Acta Cryst.* **5**, 667.

Acta Cryst. (1953). **6**, 749

International Union of Crystallography

Third General Assembly and International Congress, Paris, 21-28 July 1954

By kind invitation of the French Government the Third General Assembly and International Congress of the Union will be held in Paris from 21 to 28 July 1954.

Membership

Delegates to the General Assembly, which will be concerned with the formal business of the Union, will be nominated by the National Committees. Crystallographers throughout the world are, however, cordially invited to attend the International Congress; it is particularly hoped that they will assist the Union by bringing the Congress to the notice of their colleagues, by press announcements and otherwise, so that the attendance may be large and fully representative of crystallographic research in all countries. The Union is unfortunately not in a position to provide funds to assist delegates in meeting travelling expenses.

The membership fee will be 3000 francs for crystallographers and 2000 francs for their friends.

Programme

The subjects selected for consideration are:

1. Instruments and Measurements.
2. New Developments in Structure Determination.
3. Mineral Structures, including Synthetic Minerals and Ceramics.
4. Metal Structures.
5. Inorganic Structures.
6. Organic Structures.
7. Proteins and Related Structures.
8. Random and Deformed Structures.
9. Liquids and Liquid Crystals.
10. Glasses.
11. Thermal Transformations.
12. Diffuse Scattering.
13. Crystal Growth.
14. Neutron Diffraction.
15. Miscellaneous.

The Executive Committee has decided that no report of the Congress shall be published, it being felt that most of the contributions will find their way into the scientific literature in the normal manner and that the expense of separate publication would not be warranted. Full abstracts of the contributions will, however, be distributed in advance; speakers will then be expected to present their papers quite briefly at the Congress in order that ample time may be available for discussion.

The Programme Committee expects that a large num-