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**A model for a three-dimensional representation of
crystallographic space groups**

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Mineralogia. — *A model for a three-dimensional representation of crystallographic space groups* (*). Nota di ROMANO MEZZETTI e LODOVICO RIVA DI SANSEVERINO, presentata (**) dal Socio P. GALITELLI.

RIASSUNTO. — Viene descritto un modello per la rappresentazione di gruppi spaziali monoclinali e rombici; la sua costruzione è stata suggerita dalla difficoltà di immaginare la disposizione dei punti in una cella elementare, partendo dalla simbologia del gruppo spaziale.

Si sottolineano i dettagli e le possibilità di impiego del modello.

INTRODUCTION.

Symmetry and its representation is the first subject for the normal course in Mineralogy and a very important one in that of Crystallography.

From the classification of the possible combinations for the "macroscopic" symmetry elements (the 32 classes), a step forward is made by introducing the translation within the cell ("microscopic" symmetry). In this way the possible combinations reach the number of 230 groups, the crystallographic space groups.

Although most textbooks bear wide explanations and clear illustrations of the symmetry involved and the International Tables for Crystallography, vol. I, report the complete disposition of symmetry elements in every space group, it is a result of common experience that the three-dimensional view of the whole cell content is often difficult. In fact the position, reached by a point to be submitted to one or more symmetry operations, is not realized by anyone but the most experienced crystallographer.

This process, to replace the "image" with the "vision" specially for beginners, has been brought forward by several Authors, who have stressed this point recently (Mathieson 1962, de Camargo 1963, Joel and Ward 1963, Cunningham and Ng-Yelim 1965, 1968, Riva di Sanseverino 1967, Zussman 1967). A flourishing field of didactic applications is also the structural building of mineral and organic substances (among others Meyer 1960, Smith 1960, Beevers 1963, 1966, Gottardi 1965, Gibbs and Grender 1968).

It is here intended to visualize the subject of the first crystallographic steps, giving design and details of a teaching model representing the monoclinic and various orthorhombic space groups in three dimensions.

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TECHNICAL DETAILS.

The crystallographic cell content is interpreted by very small lamps: it is convenient that they have an asymmetric shape. They are connected to the symmetrically related lamps by switches, bearing a maximum of 8 simultaneous contacts.

The whole model, illustrated in Tab. I, fig. 1, consists (a) of a base under which the switches used for symmetry plane operations are attached, (b) of a box, repeating just more than 1/2 of the cell volume, on which the diad axes are mounted, connected with their own switches and possibly turned by knobs, and (c) of a crystallographic cell, built in galvanized iron wire along the external sides and in transparent plastic rods along the central part.

There are 22 lamps, and 16 switches corresponding to as many symmetry elements.

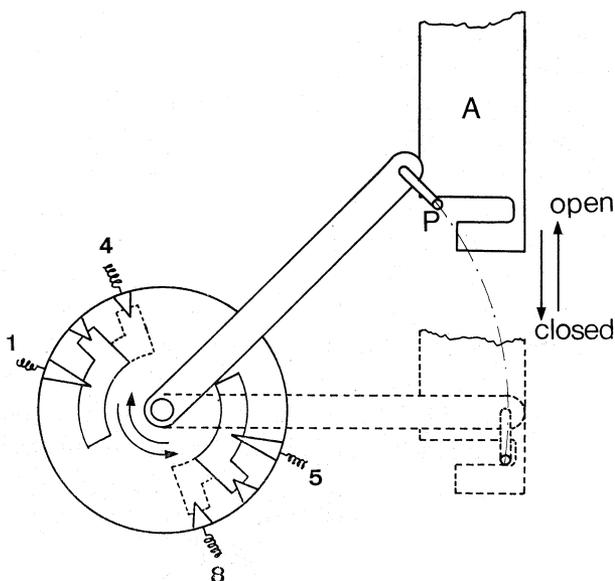


Fig. 1. - Device for "symmetry plane" contacts. By fitting the transparent sheet, the small foot A lowers pivot P (and closes 1-4 and 5-8 circuits, see step (c) in Tab. I, fig. 2), through the hole previously made in the base.

This arrangement produces an actual picture of the cell including the symmetry elements. Obviously, while the planes, as flat plexiglas sheets, are being fitted in (see fig. 1), the axes cannot be fixed along the proper directions in the cell: rotation axes acting upon the box have therefore to be transferred ideally to the cell, parallel to themselves.

Although more synthetic conventions have been newly suggested (Belov and Kletsova 1959 a, b, Menzer 1960), the space group symbology has been taken from the International Tables for Crystallography, vol. I. The monoclinic system has been given a β of 90° . Non primitive Bravais lattices

have been limited to C lattices, the centering being controlled by an independent switch, attached to lamp 7.

Lamp 1 is on, being the general position xyz ; any action on a symmetry element (indicated by the space group symbol) will light up a second lamp; a successive action will light up two further lamps and so on.

A translation $z + 1$ has also been considered for lamps 17 and 17', 18 and 18', 21 and 21', to fix this unnecessary but relevant component of space groups.

USE OF THE MODEL.

The purpose of the entire design is to answer the problem: "Given a space group symbol, say $Cmm2$, where will a *general* point be found, whenever it undergoes the symmetry operations involved?"

Starting from the symbology, it would be useful to *act* with the indicated symmetry elements and to *see* where the point given is repeated, i.e. to find the equivalent positions from the initial coordinates xyz .

To underline the *action* the model is completed by $8 + 2$ transparent planes and by 8 rotating knobs. In the case of $Cmm2$ a reflection plane m normal to x and a second plane m normal to y will be fitted, and then a knob (diad axis 2) might be turned along z (its action being in this case useless). The switch C will finally show the face centering (Tab. I, fig. 2).

All monoclinic and those orthorhombic space groups listed in Table II have been included. Some limitations, due to the technical realization and to the fact that most substances crystallize in these systems, have restricted the project. Nevertheless no hindrance seems to exist in building a second model for cubic and tetragonal space groups. More than for a complete description of crystallographic systems, the model has been planned as such for a representation of symmetry operations and of point distributions.

TABLE II.

The orthorhombic space groups interpreted by the model.

$P 222$	$P mm2$	$P ca2_1$	$P na2_1$
$P 222_1$	$P mc2_1$	$P nc2$	$P nn2$
$C 222$	$P cc2$	$P mn2_1$	$C mm2$
$C 222_1$	$P ma2$	$P ba2$	$C mc2_1$
			$C cc2$

For the monoclinic system the symmetry elements, indicated by the space group symbol, may be used in any order; for the orthorhombic system, owing to the rigidity of the proposed design, it is mandatory to follow the order strictly.

For example, while $C_{2/c}$ disposition will be obtained beginning either by using the non-primitive element C , or by turning the knob 2 along the y axis, or else by placing the glide plane perpendicularly to the y axis, for the space group Cmm_2 to be verified, the order has to be obeyed. Only thereafter one might start from the diad axis, as its position in the cell will now be known.

Two possible positions might in fact be taken by the diad axis 2 (or also by 2_1) along the z axis, in the orthorhombic system (Table III): generally, a rigid model requires fixed positions for all symmetry elements.

TABLE III.

Scheme of fixed positions.

An axis position is indicated by the two-dimensional coordinates of the intersection in a plane normal to the axis. The position for a plane is defined by the unidimensional coordinate of the intersection with an axis normal to the plane. The alternative for axes is limited to those along z , in orthorhombic space groups (see text).

Symmetry element	Class	Symbol	Position
Axes	even	2	1/2, 1/2 (or 1/4, 1/4)
	odd	2_1	1/4, 1/2 (or 1/2, 1/4)
Planes	even	m, n	1/2
	odd	a, b, c	both 1/4 and 3/4

While performing the project, the necessity of unifying the possible positions for axes and planes became evident: the International Tables for Crystallography, vol. I, show a random disposition of some symmetry elements: for example, a glide plane normal to y may be found at $y = 1/2$ in a space group and at $y = 1/4$ in another space group, and so on for other elements.

This is evidently related to the advantages given by a simpler formula for the structure factor calculation. The model has not got any duty in this respect, and its rigidity has often imposed to change the origin of space group as chosen in the International Tables.

Also the reciprocal positioning could not be settled arbitrarily: to overcome the eventual confusion, a sort of definition, satisfying both to the symmetry showed by any space group among those here included and to the exigence of a stable position for a certain symmetry element, has been found.

Provided that symmetry elements are divided into two classes as shown by Table III, then the following rule is experimentally derived: “*Even*

symmetry elements occupy even positions, odd symmetry elements occupy odd positions”. This is the basic operational instruction for the model, valid only for the space groups here included.

Special care has been taken regarding economic problems; the cost in material has been reckoned at about Lire 10,000 and a technician had to spend six days to perform constructional and electrical connections.

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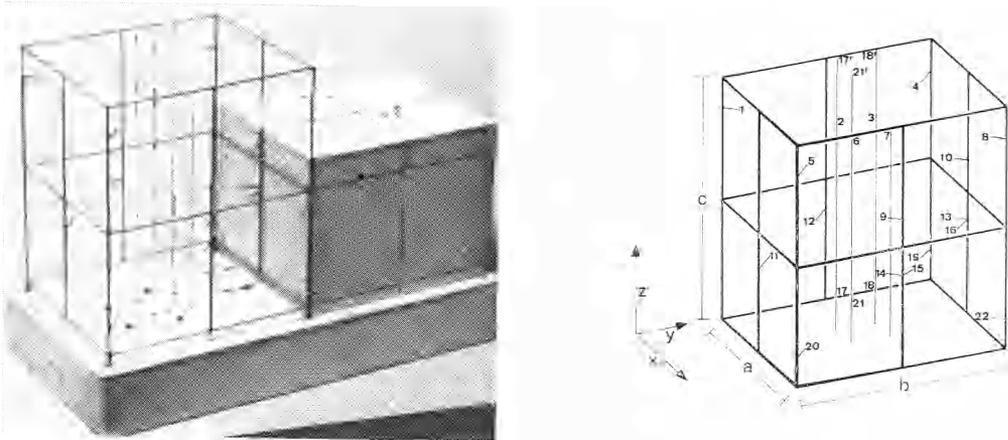


Fig. 1. – The model and a schematic view of the 22 non equivalent positions. The numbering of lamps is arbitrary. The round holes in the box indicate positions for rotation axes (knobs). Note the translation $z + 1$ between lamps 17 and 17', 18 and 18', 21 and 21'.

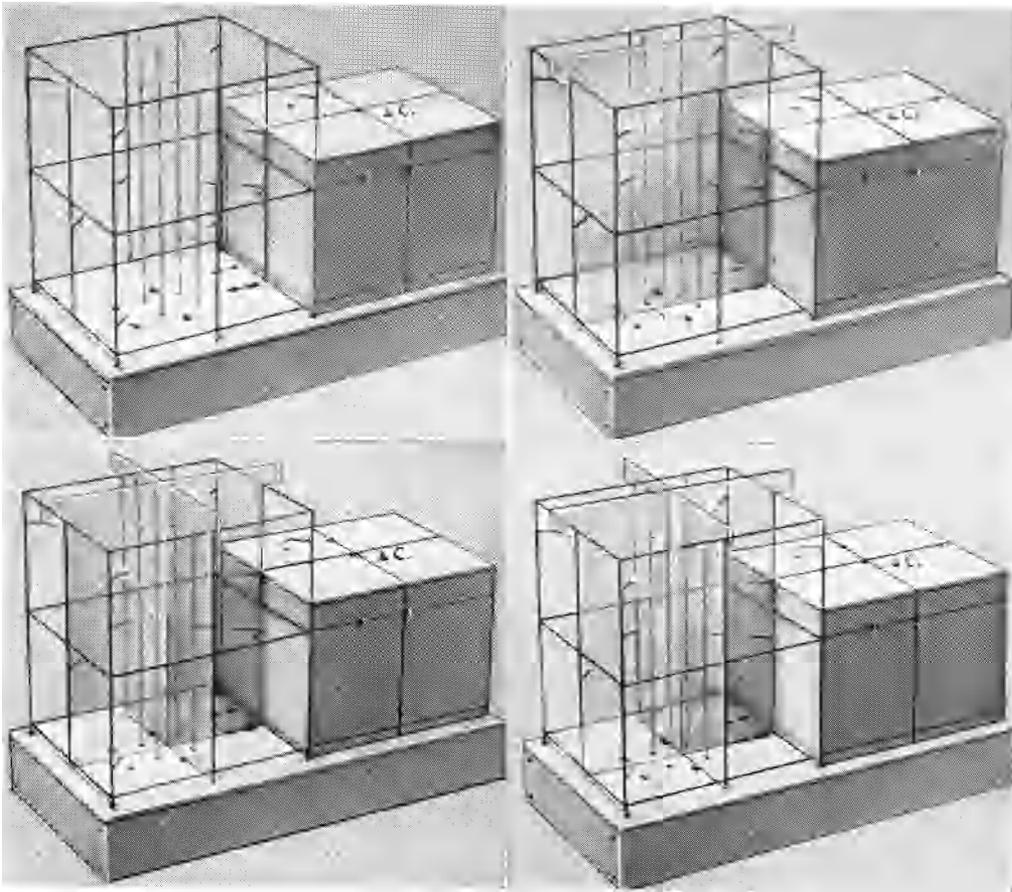


Fig. 2. – The space group $Cmm2$, showed by successive symmetry operations. *Upper left*: Lamp 1 is on; *Upper right*: Lamp 5 is lighted up by mirror plane m normal to x ; *Lower left*: The second mirror plane lights up lamps 4 and 8; *Lower right*: Switch C is hand-operated and lights up lamps 2, 3, 6 and 7.