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MATHEMATICS

Corresponding Member of the Academy of Sciences of the USSR B. N. DELONE

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Abstract

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ADDENDUM TO MY 1933 PAPER

ON THE PROPER SETTING OF A CRYSTAL

I have more than once received inquiries from foreign crystallographers as to how the vectors of a crystallographic Bravais frame (i.e., a frame formed by the edges of a Bravais parallelepiped) are expressed in terms of the vectors of an arbitrary initial fundamental frame of the lattice. In the present article I answer this question, and also solve the problem of the unambiguous choice of the Bravais frame in the case of monoclinic and triclinic lattices.

First of all I note that the following remarks must be made to the exposition of my method in ([1]) (as was pointed out at the time in ([2]) and ([3])).

1°. The syngonies in my terminology are called: cubic, tetragonal, orthorhombic, monoclinic, triclinic, rhombohedral, and hexagonal, and are denoted respectively by the letters (boldface) K, Q, O, M, T, R, H (all of which are distinct).

The individual kinds (out of 24) of lattices of one and the same syngony are further indicated by subscripts attached to these letters, for example: M_1, M_2, M_3, ⋯, M_6, chosen by me conventionally.

2°. In carrying out the reduction of a tetradric symbol, at each step one must simultaneously transform its vectors according to the rule: **add the vector corresponding to the bold-marked vertex of the marked edge to both vectors whose vertices do not belong to this edge, and replace that vector itself by its opposite.**

Example:

[diagram]

The vectors corresponding to the reduced symbol, in the present case $-a,\ -3a-2b-c,\ 2a+b+c,\ 3a+2b+c+d$, are the vectors of the reduced Selling frame. In all that follows we shall denote by a, b, c, d precisely these reduced vectors.

3°. If the reduced symbol (i.e., the symbol on which there are no positive parameters) is one of the following:

[diagram]

O_4 O_5 M_4 M_5

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one must make one more additional step of reduction with respect to the marked zero edge and the vertex (which only permutes among themselves the nonzero edges meeting at this vertex) and pass to symbols:

[diagrams]

4°. The tetrahedral symbol must be thought of spatially. It may be "rotated" within itself; in doing so the arrangement of the quantities of the parameters P, Q, R, S, T, U, standing on its edges, changes.

The letters a, b, c, δ, however, we always leave in their usual places (i.e., a at the lower left, b at the lower right, etc.). In the case of the first 5 monoclinic sorts, as is easily seen, by such "rotation" one can achieve that the inequalities written in the table in parentheses next to the symbol (one or two) are satisfied. In the case M_6, in order to achieve the written inequalities, it will sometimes be necessary to make one more step of transformation through a zero edge

[diagrams]

or

[diagrams]

The reduced symbol, treated as indicated in 3° and 4°, we shall call prepared, and we shall assume that this has always been done.

5°. In the cases O_2, O_3, O_4, δ is the length of the smallest diagonal of the faces, d the length of the largest edge.

6°. A, B, C are the vectors of the Bravais frame; a, b, c are their lengths; α is the angle of the monoclinic parallelepiped.

The unambiguous choice of the base-centered monoclinic Bravais parallelepiped is made as follows: the lateral edge B in all monoclinic sorts is in essence specified uniquely; as the edge A of the base, which is at the same time an edge of the centered lateral face, one chooses the smallest possible such edge; as the other edge C of the base one chooses that which forms the smallest obtuse angle α with A. In the case of a primitive monoclinic Bravais parallelepiped (i.e., in the sort M_6), as the edges A and C of the base one chooses the smallest vector in the lattice lying in the plane of the base, and the smallest noncollinear vector to it forming with it an obtuse angle.

With the aid of not entirely simple arguments one can show that, if one uses the prepared reduced symbol, then in all 6 monoclinic cases the formulas of the table give precisely the vectors of the Bravais parallelepiped chosen unambiguously in this way (as just indicated).

For triclinic cases, as the fundamental frame of the lattice we take the one made up of its shortest vector A, the shortest vector B noncollinear with it, and the shortest vector C noncoplanar with A and B. Moreover, as was shown in (3), either 1) such vectors are three of the four reduced vectors a, b, c, δ of Selling (and then all three angles between them are not acute), or 2) one of them is one

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of the "sum vectors" $\lambda = b + c$, $\mu = c + a$, $\nu = a + b$, and the other two are two of Selling' s vectors, of which one is one of those entering into the corresponding "sum," and the other does not enter into it and is taken with the opposite sign, for exam-

In the figure:

- K_1:

$$A = \delta + \lambda, \qquad B = \delta + \nu, \qquad C = \alpha + \delta,$$
$$a = b = c = 2\sqrt{-P}.$$

- K_2:

$$A = \delta - \alpha, \qquad B = \gamma - \nu, \qquad C = \alpha + \delta,$$
$$A = \alpha, \qquad B = \delta, \qquad C = \gamma,$$
$$a = b = c = 2\sqrt{-P}.$$

- K_3:

$$a = b = c = \sqrt{-S},$$
$$A = \alpha, \qquad B = \delta, \qquad C = \gamma.$$

- R_1 ($\alpha > 90^\circ$):

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma,$$
$$a = b = c = \sqrt{-2P - S},$$
$$\cos\alpha = \frac{P}{-2P - S}.$$

- R_2 ($\alpha < 90^\circ$):

$$A = \delta, \qquad B = \delta + \gamma, \qquad C = -\nu,$$
$$a = b = c = \sqrt{-P - S},$$
$$\cos\alpha = \frac{-S}{-P - S}.$$

- H:

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma,$$
$$a = b = \sqrt{-2Q}, \qquad c = \sqrt{-T}.$$

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- Q_1 $(c < a\sqrt{2})$:

$$A = \delta + \gamma, \qquad B = \delta + \nu, \qquad C = \alpha + \delta,$$
$$a = b = \sqrt{-2P - 2Q}, \qquad c = 2\sqrt{-P}.$$

- Q_2 $(c > a\sqrt{2})$:

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma - \nu,$$
$$a = b = \sqrt{-2P}, \qquad c = 2\sqrt{-P - T}.$$

- Q_3:

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma,$$
$$a = b = \sqrt{-S}, \qquad c = \sqrt{-T}.$$

- O_1:

$$A = \alpha - \delta, \qquad B = \gamma - \nu, \qquad C = \alpha + \delta,$$
$$a = 2\sqrt{-P - Q}, \qquad b = 2\sqrt{-P - T}, \qquad c = 2\sqrt{-P}.$$

- O_2 $(\delta > d)$:

$$A = \delta + \gamma, \qquad B = \delta + \nu, \qquad C = \alpha + \delta,$$
$$a = \sqrt{-2P - 2Q}, \qquad b = \sqrt{-2Q - 2R}, \qquad c = \sqrt{-2R - 2P}.$$

- O_3 $(\delta < d)$:

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma - \nu,$$
$$c = \sqrt{-2P - 2R - 4T}, \qquad a = \sqrt{-2P}, \qquad b = \sqrt{-2R}.$$

- O_4 $(\delta = d)$:

$$A = \delta + \gamma, \qquad B = \delta + \nu, \qquad C = \alpha + \delta,$$
$$a = \sqrt{-2P}, \qquad b = \sqrt{-2R}, \qquad c = \sqrt{-2P - 2R}.$$

- O_5:

$$A = \alpha - \delta, \qquad B = \alpha + \delta, \qquad C = \gamma,$$
$$a = \sqrt{-2S - 4Q}, \qquad b = \sqrt{-2S}, \qquad c = \sqrt{-T}.$$

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- O_6:

$$A = \alpha, \qquad B = \delta, \qquad C = \gamma,$$
$$a = \sqrt{-U}, \qquad b = \sqrt{-S}, \qquad c = \sqrt{-T}.$$

for example, the vectors $\lambda, c, -a$ (and then all three angles formed by them are not obtuse). The lengths of these seven vectors are calculated by the formulas:

$$a^2 = -P - Q - U, \qquad b^2 = -Q - R - S, \qquad c^2 = P - R - T,$$

$$\delta^2 = -S - T - U,$$

$$\lambda^2 = -P - Q - S - T, \qquad \mu^2 = -Q - R - T - U, \qquad \nu^2 = -P - R - S - U.$$

$$M_1 \quad (a < b), \qquad |P| < |R|,$$
$$A = \varepsilon + \vartheta, \qquad B = \varepsilon - \vartheta, \qquad C = u,$$
$$a = \sqrt{-2P - 2R}, \qquad b = \sqrt{-2P - 2R - 4T}, \qquad c = \sqrt{-2P - Q},$$
$$\cos\alpha = \frac{2P}{ac}.$$

$$M_2 \quad (a > b), \qquad |Q| < |T|, \quad |P| < |R|,$$
$$A = u - \vartheta, \qquad B = \varepsilon + \vartheta, \qquad C = \vartheta + \varepsilon,$$
$$\cos\alpha = \frac{2P + 2Q}{ac},$$
$$a = \sqrt{-2R - 2P - 4Q}, \qquad b = \sqrt{-2P - 2R}, \qquad c = \sqrt{-2P - Q - T}.$$

$$M_3 \quad (a > b), \qquad |U| < |S|,$$
$$A = 2u + \varepsilon, \qquad B = -\varepsilon, \qquad C = \vartheta,$$
$$a = \sqrt{-2P - 4Q - 4U}, \qquad b = \sqrt{-2P}, \qquad c = \sqrt{-S - U},$$
$$\cos\alpha = \frac{2U}{ac}.$$

$$M_4 \quad (a = b), \qquad |P| < |S|,$$
$$A = u + \vartheta, \qquad B = u - \vartheta, \qquad C = \varepsilon,$$
$$a = \sqrt{-2P - 2S}, \qquad b = \sqrt{-2P - 2S}, \qquad c = \sqrt{-2P - T},$$
$$\cos\alpha = \frac{2P}{ac}.$$

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$$M_5 \quad (a > b), \qquad |R| < |P|,$$
$$A = 2\vartheta + \nu, \qquad B = -\nu, \qquad C = \varepsilon,$$
$$a = \sqrt{-4R - 2S}, \qquad b = \sqrt{-2S}, \qquad c = \sqrt{-P - R},$$
$$\cos\alpha = \frac{2R}{ac}.$$

$$M_6 \qquad |P| < |T|, \quad |P| < |U|,$$
$$A = u, \qquad B = \vartheta, \qquad C = \varepsilon,$$
$$a = \sqrt{-P - U}, \qquad b = \sqrt{-S}, \qquad c = \sqrt{-P - T},$$
$$\cos\alpha = \frac{P}{ac}.$$

$$T_1$$

$$T_2$$

$$T_3$$

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Cited Literature

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Note: Figure translations are in progress. See original paper for figures.

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