This consists of two possibilities, namely F_P and F_P^c having the same or opposite signs, so that separating out these two, we have

$$P(F_P^c;\, F_P) = \frac{1}{\sqrt{2\pi\sigma_2^2(1-D^2)}}\left[\exp\left\{\frac{(|F_P^c|-D|F_P|)^2}{2\sigma_P^2(1-D^2)}\right\} + \exp\left\{-\frac{(|F_P^c|+D|F_P|)^2}{2\sigma_P^2(1-D^2)}\right\}\right] \quad (A7)$$

$$= \sqrt{\frac{2}{\pi}}\frac{1}{[\sigma_P^2(1-D^2)]^{\frac{1}{2}}}\exp\left\{-\frac{|F_P^c|^2+D^2|F_P|^2}{2\sigma_P^2(1-D^2)}\right\} \times \cosh\left[\frac{D|F_P|\,|F_P^c|}{\sigma_P^2(1-D^2)}\right]. \quad (A8)$$

Since this involves only the magnitudes $|F_P^c|$ and $|F_P|$ it is seen that this is also the distribution, $P(F_P^c|;\, |F_P|)$.

Making the usual transformation in (*A*8), namely writing $y_N = |F_N|/\sigma_N$ and $y_P^c = |F_P|^c/\sigma_P$, we obtain expression (17) given in the text.

APPENDIX III

The desired integral (18) can be written:

$$\frac{2}{\pi\sigma_2(1-D^2)}\exp\left\{-\frac{(1-D^2)\,y_N^2+\sigma_2^2D^2\,y_P^{c2}}{2\sigma_2^2(1-D^2)}\right\} \times \int_0^\infty \exp\left\{-\frac{[(1-D^2)\,\sigma_1^2+\sigma_2^2]\,y_P^2}{2\sigma_2^2(1-D^2)}\right\}\cosh\left[\frac{y_N y_P\,\sigma_1}{\sigma_2^2}\right] \times \cosh\left[\frac{y_P^c y_P D}{(1-D^2)}\right] dy_P\,. \quad (A9)$$

The integral in (*A*9) above is of the form

$$\int_0^\infty \exp(-p^2x^2)\cosh(ax)\cosh(bx)\,dx\,, \quad (A10)$$

where

$$p^2 = \frac{(1-D^2)\,\sigma_1^2+\sigma_2^2}{2\sigma_2^2(1-D^2)},\quad a = \sigma_1 y_N/\sigma_2^2,\quad b = y_P^c D/(1-D^2)\,.$$

Since we have the relation

$$I_{-1/2}(z) = \sqrt{\frac{2}{\pi z}}\cosh z\,, \quad (A11)$$

(*A*10) can be written in the form

$$\frac{\pi}{2}\sqrt{ab}\int_0^\infty \exp(-p^2x^2)\,I_{-1/2}(ax)\,I_{-1/2}(bx)\,x\,dx\,. \quad (A12)$$

The integral in (*A*12) is similar to (*A*2) considered in Appendix I, with the only difference that the order of the Bessel function is $-\frac{1}{2}$ in the former, while it is zero in the latter. Thus, using the same result (*A*3) of Appendix I, (*A*12) reduces to

$$\frac{\pi}{2}\sqrt{ab}\,\frac{1}{2p^2}\exp\left\{\frac{a^2+b^2}{4p^2}\right\} I_{-1/2}\left(\frac{ab}{2p^2}\right). \quad (A13)$$

Again making use of (*A*1) in (*A*13) and substituting for *a*, *b*, p^2, *etc.*, we obtain the expression (19) given in the text.

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The Absorption Correction in Crystal Structure Analysis

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An exact method for computing the absorption correction for any polyhedral crystal is described. First an analytical formula is derived for the contribution to the diffracted intensity from a tetrahedron in which the path length of the rays is a linear function of the coordinates of the diffracting element, and it is then shown how the crystal is to be divided into such tetrahedra. A computer program for the IBM 1620 machine to compute the absorption correction is described.

Introduction

In crystal-structure analysis the basic observed quantities are the intensities of the *hkl* reflexions. A number of corrections (Lorentz and polarization factors, absorption correction) have to be applied to the observed intensities before they can be used as the basis of a structure determination. The absorption correction

takes account of the fact that the intensity of the beams, both the incident and the diffracted beam, is lowered by absorption on its passage through the crystal; the extent of this absorption depends for a given crystal on the mean path within the crystal and is thus a function of the shape of the crystal and its orientation, in other words of h, k, and l.

No fully satisfactory method of evaluating the absorption correction for the general case has so far been described; the position up to 1958 is well summarized in *International Tables for X-ray Crystallography* (1959). The methods described there are based on numerical or graphical approximations, mostly for special cases, and are, with one exception, applicable only to the two-dimensional case or the equatorial reflexions of prisms. The exception is the technique developed by Busing & Levy (1957), who use three-dimensional numerical integration based on the eight-point Gauss formula to evaluate the integral (1) given below. Sands (1958), quoted in Zalkin & Sands (1958), has written a program for the IBM 650 computer, using essentially Busing & Levy's technique, but only for the two-dimensional case. Since then, several papers dealing with the problem have appeared; Ferrari, Braibanti & Tiripicchio (1961) treat again the two-dimensional case; for strongly absorbing crystals Fitzwater (1961) has evaluated the transmission for crystals of elliptical shape by developing the exponential in (1) into a series and integrating it term by term.

It is the purpose of this paper to develop an analytical method for the three-dimensional case without making any restriction on the value of the absorption and to describe its application.

Let I_μ be the intensity of the diffracted beam issuing from a crystal with absorption coefficient μ and let I_0 be the corresponding intensity for $\mu=0$. Then the transmission $T(=I_\mu/I_0)$ is given by $T=A/V$, where

$$A=\int \exp(-\mu L)dV\,. \tag{1}$$

The total path length L equals l_1+l_2, where l_1 is the length of the path of the incident ray from its point of entry into the crystal up to the volume element dV and l_2 the corresponding length of the path of the beam diffracted in dV. The integration is to be carried out over the volume V of the crystal, which we assume to be bounded by plane surfaces, *i.e.* to be a polyhedron; we further assume the polyhedron to be convex. The basis of our method of computing the integral A is to divide the crystal first in a manner similar to that used by Howells (1950) into a number of elementary polyhedra throughout each of which L is a linear function of the coordinates of dV. As each of these polyhedra is convex, each can be subdivided into a number of tetrahedra. An analytical expression is derived for A_T, the contribution from one such tetrahedron and from this A can be obtained by summing over all tetrahedra. The major part of the work in computing A is to find the elementary polyhedra, but the keystone of our method is the analytical expression for A_T.

Analytical considerations

We derive first the expression for A_T. We take one of the vertices of the tetrahedron as origin of the coordinates and the three edges passing through this vertex as axes of coordinates x, y and z. The tetrahedron is thus bounded by the three coordinate planes and a fourth plane, whose equation we write in the form

$$\frac{x}{u}+\frac{y}{v}+\frac{z}{w}=1\,.$$

The four vertices are then (0, 0, 0), (u, 0, 0), (0, v, 0) and (0, 0, w). Since L is assumed to be a linear function of the coordinates, we can write

$$\mu L=g=px+qy+rz+s\;;$$

also $dV=K\,dx\,dy\,dz$. The sheets of constant attenuation, $g=$const., are not necessarily related in any way to the edges or faces of the tetrahedron. Then

$$A_T=\int \exp(-\mu L)dV=\iiint \exp[-(px+qy+rz+s)]$$
$$\times K\,dx\,dy\,dz=K\exp(-s)\int_0^u\int_0^{v(1-x/u)}\int_0^{w(1-x/u-y/v)}$$
$$\times\exp(-rz)dz\exp(-qy)dy\exp(-px)dx\,.$$

The evaluation of this integral is straightforward; the result is obtained in terms of u, v, w, p, q, r, and s. We can replace these parameters by the values of g at the four vertices

$$g_1=s,\; g_2=pu+s,\; g_3=qv+s,\; g_4=rw+s$$

and by $Kuvw=6V_T$. After some algebraic manipulation we obtain

$$A_T=6V_T\left\{\frac{\exp(-g_1)}{(g_2-g_1)(g_3-g_1)(g_4-g_1)}\right.$$
$$+\frac{\exp(-g_2)}{(g_1-g_2)(g_3-g_2)(g_4-g_2)}+\frac{\exp(-g_3)}{(g_1-g_3)(g_2-g_3)(g_4-g_3)}$$
$$\left.+\frac{\exp(-g_4)}{(g_1-g_4)(g_2-g_4)(g_3-g_4)}\right\}. \tag{2}$$

i.e. A is a sum of terms, one for each vertex, and depends, apart from the volume, only on the four g_i values. This expression can also be written as the ratio of two determinants

$$A_T=-6V_T\cdot\begin{vmatrix}\exp(-g_1) & g_1^2 & g_1 & 1\\ \exp(-g_2) & g_2^2 & g_2 & 1\\ \exp(-g_3) & g_3^2 & g_3 & 1\\ \exp(-g_4) & g_4^2 & g_4 & 1\end{vmatrix}\Bigg/\begin{vmatrix}g_1^3 & g_1^2 & g_1 & 1\\ g_2^3 & g_2^2 & g_2 & 1\\ g_3^3 & g_3^2 & g_3 & 1\\ g_4^3 & g_4^2 & g_4 & 1\end{vmatrix}.$$

Expression (2) is not suitable for numerical computation since one or more of the differences (g_i-g_j) in the denominators can be zero if the plane of constant attenuation is parallel to one or more edges of the tetrahedron .The following artifices enable us to circumvent this difficulty.

We introduce a function $h(u)=[1-\exp(-u)]/u$. Then (2) can be rearranged to give

$$A_T = 6V_T \exp(-g_1)\left\{\frac{h(g_2-g_1)}{(g_3-g_2)(g_4-g_2)} - \frac{h(g_3-g_1)}{(g_3-g_2)(g_4-g_3)} + \frac{h(g_4-g_1)}{(g_4-g_2)(g_4-g_3)}\right\}$$

$$= 6V_T \exp(-g)\left\{\frac{\dfrac{h(\Delta g_2)-h(\Delta g_3)}{\Delta g_3-\Delta g_2} \quad \dfrac{h(\Delta g_3)-h(\Delta g_4)}{\Delta g_4-\Delta g_3}}{\Delta g_4-\Delta g_2}\right\} \tag{3}$$

with $g=g_1$, $\Delta g_i=g_i-g_1$. Now $\Delta g_i=0$ presents no problem, since $h(0)=1$; if $\Delta g_3=\Delta g_2$ ($g_3=g_2$) or $\Delta g_4=\Delta g_3$ ($g_4=g_3$), the corresponding fraction in the numerator of (3) tends to $-h'$, where $-h'(u)=[1-h(u)]/u-h(u)$ and $-h'(0)=\frac{1}{2}$. Finally, the difficulty arising from $\Delta g_2=\Delta g_4(g_2=g_4)$ can be circumvented by assuming that the g_i are ordered so that $g_1\leq g_2\leq g_3\leq g_4$; in this case $g_2=g_4$ implies $g_2=g_3$ and $g_3=g_4$, and the double fraction in (3) tends to $\frac{1}{2}h''(\Delta g_2)$, with $\frac{1}{2}h''(0)=\frac{1}{6}$, so that $A_T=V_T\exp(-g)$ for $g_1=g_2=g_3=g_4$, as is physically evident.

To compute the transmission T of a crystal for given directions of the incident and diffracted rays, it is thus necessary to divide it into its Howells polyhedra and then to subdivide each of these into tetrahedra. For each tetrahedron A_T and V_T are computed using (3) and its differential analogues: and these are cumulated to give

$$T=\Sigma A_T/\Sigma V_T\,.$$

Geometrical considerations

Let us illustrate the procedure on a two-dimensional case (Fig. 1); let $ABCD$ represent the crystal and let the directions of the incident and diffracted beams be as indicated on the diagram. This example also represents the case of a prismatic crystal with cross-section $ABCD$ for beams as indicated. The incident ray through A and the diffracted ray through B divide the parallelogram into four Howells polygons, in this case two triangles ABR and AQR and two quadrilaterals $BCPR$ and $DPRQ$; after division of the two latter into two triangles each, *e.g.* as indicated by the dotted lines, six triangles are obtained. If we consider the direction of the diffracted beam to be reversed, the distinction between incident and diffracted directions becomes irrelevant for the purposes of this computation. Each Howells polygon is characterized by having all its incident rays arriving through one side and all diffracted rays leaving through one (possibly even the same) side.

The vertices of the Howells polygons are the vertices, A, B, C, D of the parallelogram, the intersections P, Q of the rays through the vertices 'in the light' with sides 'in the shade', and the intersection R of these rays. We shall refer to elements in the light and in the shade as being l and s, respectively.

To compute T on the basis of the preceding arguments, one could first take a side l with respect to direction 1 ($l1$) and one l with respect to direction 2 ($l2$), evaluate the corresponding Howells polygon, split it into triangles and compute the contribution A_{Tr} for each triangle; all Howells polygons are obtained by combining each side $l1$ with each side $l2$ and T is obtained from the sum of all A_{Tr}. It might be preferable to evaluate first all possible vertices of Howells polygons and to select then the sets belonging to successive Howells polygons. For more complex crystals some combinations of sides will not give a Howells polygon.

These considerations can be extended easily to the three-dimensional case. We illustrate this by the example of a crystal in the shape of a cube (Fig. 2) in which the first direction (incident ray) is given by EX, the second (diffracted ray reversed) by FU. Each Howells polyhedron is the intersection within the crystal of two prisms, one based on a face $l1$, with generators parallel to the first direction, and one based on a face $l2$, with generators parallel to the second direction. Since there are three faces $l1$ (those meeting in E) and three $l2$ (those meeting in F) there can be nine Howells polyhedra; in fact, one of them has only an edge in common with the crystal.

Fig. 2 shows the division of the cube into the eight finite Howells polyhedra. Their vertices are points of four different types, apart from the vertices of the

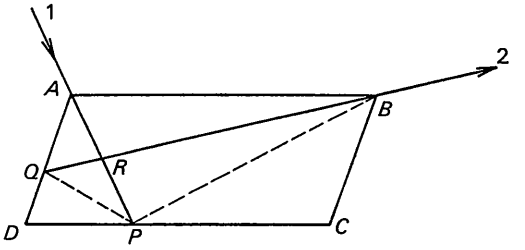

Fig. 1. Decomposition of a parallelogram into Howells polygons and triangles; 1: direction of incident beam, 2: direction of diffracted beam.

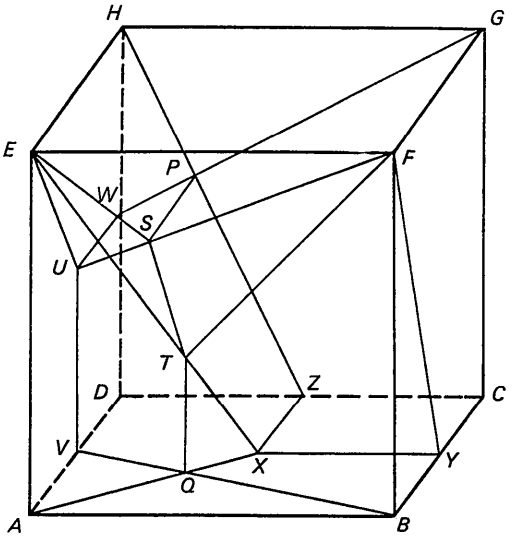

Fig. 2. Decomposition of a cube into elementary polyhedra.

crystal: they may be points at which the ray through a vertex *l* intersects an opposite face *s*, in other words, the projection of a vertex *l* onto an opposite face *s*, like points *X* and *U*; they may be points at which the ray through a vertex *l* intersects a plane of light passing through an edge *l* in the other direction, such as *T* (ray through *E* and plane of light through *BF*) and *S* (ray through *F* and plane of light through *EH*); they may be points in which planes of light through an edge *l* cut an opposite edge *s*, such as *Y* (intersection of plane through *EF* with *BC*), *Z* (*EH* and *CD*), *V* (*BF* and *AD*), and *W* (*FG* and *DH*), and finally they may be points at which the projections of an edge *l*1 and edge *l*2 onto the same face *s*1 and *s*2 intersect, such as *P* (intersection of *HZ* and *GW*) and *Q* (intersection of *AX* and *BV*).

The vertices of the Howells polyhedra based on the different faces *l* are given in the table below.

Face *l*2	*ABEF*	*BCFG*	*EFGH*
*l*1			
ABEF	*ABQEFT*	*BYXQFT*	*EF*
ADEH	*AQVETSU*	*VQXZDUSTPW*	*USPWEH*
EFGH	*EFST*	*XYCZSTFGP*	*EFGHSP*

Computer program

A computer program (ERA 304) has been written for the IBM 1620 data-processing system in the symbolic programming language to compute the transmission of a crystal of any shape for any directions of the two beams. The program works as follows.

The crystal is assumed to be given in terms of the equations of its faces referred to an arbitrary system of Cartesian coordinates. An auxiliary program (ERA 193) written in FORTRAN computes the coordinates of the vertices and the coincidences of faces, edges, and vertices from the equations of the faces and these serve as 'crystal data' for the main program. After they have been read, the volume of the crystal is computed and the direction cosines of the incident and diffracted beams are read; the coordinates of points of types *X*, *T*, and *Y* in both directions and then of points of type *P* are computed. The vertices of the polyhedra belonging to a pair of faces *l*1 and *l*2, respectively, are collected and the Howells polyhedra built up systematically: any four points are taken to form the first tetrahedron and further tetrahedra are found by taking successive points. For each tetrahedron, the volume V_T and the contribution A_T to the integral A are computed and both are cumulated. When all possible combinations of pairs of faces *l*1 and *l*2 have been examined, $V=\Sigma V_T$ is compared with the volume of the crystal computed in the first phase and if the difference is within a predetermined limit of precision, $T=\Sigma A_T/\Sigma V_T$ is computed and *T*, *V* and identifications of the crystal and the two directions are punched.

Owing to the limited storage capacity of the standard IBM 1620 computer (20000 decimal digits) all computations are carried out with four-digit fixed-point numbers; accidental coincidences can thus occur and some of the Howells polyhedra are then not computed correctly. If ΣV_T differs significantly from the volume first computed the program changes the directions by amounts which are physically not significant and the computation is repeated, up to a maximum of four times; if no agreement is obtained, an error indication is punched instead of *T*.

The function $h(u)$ of equation (3) is computed by expanding it into a series of Chebyshev polynomials; the coefficients of this expansion have been obtained essentially as described by Clenshaw (1962) from the differential equation

$$uh'(u)+(1+u)h(u)=1\ .$$

The largest crystal the program can handle in the standard 1620 computer must not contain more than 20 faces or more than 25 vertices.

Another program (ERA 341) has been written in FORTRAN to evaluate the transmission of a parallelogram in the two-dimensional case represented in Fig. 1. Equation (4), the two-dimensional analogue of equation (3)

$$A_{Tr}=2F_{Tr}\exp(-g)\frac{h(\Delta g_2)-h(\Delta g_3)}{\Delta g_3-\Delta g_2}, \qquad (4)$$

where F_{Tr} is the area of the triangle and A_{Tr} its contribution to the integral A, is used to compute A_{Tr} but the decomposition of the parallelogram into Howells polygons is carried out by a logical sequence of considerations of the different possibilities.

The following tests were carried out to confirm that the program computes the transmission correctly and to obtain an estimate of the average error.

An imaginary crystal was constructed consisting of a prism on a square base and limited above by four octahedral planes (9 faces, 13 vertices). It was assumed that the crystal belongs to the cubic system, with the crystallographic axes parallel to the main axes of the crystal and with $\lambda/a=0{\cdot}36$. The directions of the incident and refracted rays were computed for all 407 possible sets of *hkl* with non-negative *h* and with the condition that the two directions make equal angles with the *c* axis, excluding the 00*l* reflexions, for which the above condition is not sufficient to define the directions of the beams uniquely. The 407 values of the transmission were computed twice, once with the crystal referred to a system of coordinates parallel to the crystallographic axes and a second time referred to a system rotated around an arbitrary direction by an arbitrary amount. The product of the absorption coefficient and the edge of the square was taken to be 2.

Except for one pair of directions the values of *T* agreed to within 0·1%; the mean difference was 0·02% of the average value of *T*, the standard deviation from the mean 0·03%.

As a second test *T* was computed for a dodecahedron with the same set of 407 pairs of directions; the values obtained were sorted according to $\sin\theta$ and it was

found that the value of T was within 15% of the mean for that value of $\sin\theta$ while the value at $\sin\theta=1$ was three times that at $\sin\theta=0$. The values of T obtained were compared with those for three spheres, computed by a separate program (ERA 325) by numerical integration of (1) over the sphere; the three spheres chosen were the circumscribed sphere, the sphere passing through the midpoints of the edges of the dodecahedron and the inscribed sphere. The values of T for the dodecahedron lay always between those for the latter two spheres and were spread around the estimated value for the sphere with the same volume as the dodecahedron. That the values of T were computed correctly for the three spheres was checked against the values computed separately for $\theta=0°$, 45°, and 90° and against those of Evans & Ekstein (1952).

As a third test, the values of T were computed for the cube and the directions of the beams used as illustration in Fig. 2; the cube edge was taken to be two, the value of μ was varied from zero to ten. For small values of μ, T approaches unity; a limiting value of T for high absorption can be obtained as follows: the only significant contribution to A arises from volume elements near faces which are both $l1$ and $l2$ and an approximate value for A is then

$$A=\sum_m F_m\int_0^\infty \exp\left[-\mu t\left(\frac{1}{\cos\varphi_m}+\frac{1}{\cos\psi_m}\right)\right]dt$$
$$=\frac{1}{\mu}\sum_m \frac{F_m}{\frac{1}{\cos\varphi_m}+\frac{1}{\cos\psi_m}} \qquad (5)$$

where the sum is to be taken over all faces both $l1$ and $l2$; F_m is the area of such a face, φ_m and ψ_m the angles of the perpendicular to the face with the two ray directions.

The table below gives the values of T as a function of μ both as computed by the program and as obtained from (5), T(lim).

μ	0·001	0·01	0·1	1	2	5	10
T	0·9983	0·9829	0·8446	0·2704	0·1337	0·0506	0·0246
T(lim)				0·2381	0·1191	0·0476	0·0238

Finally, as a fourth test, values of T were computed for a comparison with the program of Sands. Sands illustrates his method on a parallelogram with $a\mu=7{\cdot}035$, $b\mu=3{\cdot}015$. Six series of computations were made by program ERA 304 for the sets of directions used by Sands for his parallelogram, with his values of $a\mu$ and $b\mu$ and with $c\mu=1$; the value of μ was varied between 1 and 2, changing the size of the crystal appropriately to obtain always the quoted values of $a\mu$, $b\mu$, and $c\mu$. A seventh series was computed on a crystal referred to a different system of coordinates and values of the transmission were also computed by program ERA 341.

The values obtained by ERA 304 agreed on the whole (*i.e.* in 95% of all cases) within 0·1% with the values given by ERA 341, but agreement with the values of Sands was not so good: in 59 of the 168 cases the relative difference exceeded 1%, in 15 cases 3%, and in one case it was 6·3%. This illustrates the lack of reliability in methods of numerical integration when, as in this case, the integrand is not a smooth function of the argument. We have confirmed this behaviour by independent computations, trying to obtain the transmission by six-point or eight-point Gaussian integration across the area of the parallelogram, and found that large errors appear when the values of $a\mu$ and $b\mu$ exceed a few units.

The computation of A_T from equation (3) is for reasons of precision carried out with six places of decimals. A second version, program ERA 304 A, has been written, in which A_T is computed with four places of decimals, but since there is an error of several units in the fourth place in the results, the precision is not satisfactory if the value of T is below say 0·1.

The average time required to compute the transmission is 52 sec for a cube, 175 sec for the crystal used in the first test, and 400 sec for the dodecahedron; the corresponding figures for program ERA 304A are 45, 155, and 350 sec.

A computer program (ERA 426) based on the principles presented here has also been written in the FORTRAN language for the two-dimensional case.

We are indebted to Mr G. S. D. King for having aroused our interest in the problem of the absorption correction and for helpful discussions; we are also indebted to the operating staff of our IBM 1620 computer, Mrs L. De Keukelære, Mrs E. Provis and Mr A. Vosse for many hours of patient effort. We are grateful to the referee, Dr D. Rogers, for a careful revision of the text.

Note added in proof. – Since the completion of the manuscript of this paper two further papers dealing with the absorption correction have appeared: Ferrari, Braibanti & Tiripicchio (1965) and Braibanti & Tiripicchio, (1965).

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