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ROTATED ELASTIC AND PIEZOELECTRIC COEFFICIENTS OF AMMONIUM DIHYDROGEN PHOSPHATE

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ABSTRACT

By applying transformation equations to Mason's experimental results, the elastic and piezoelectric coefficients of ammonium dihydrogen phosphate (ADP) are computed for separate rotations about the crystallographic axes. Young's modulus for the long bar is similarly treated. Expressions are derived for the Mason D' piezoelectric coefficient and for k, the electromechanical coupling, of the Z-cut long bar.

PROBLEM STATUS

This is a final report on a small portion of the larger problem; work on the larger problem, a general study of vibrations in piezoelectric crystals, still continues.

AUTHORIZATION

NRL Problem No. S01-09R

ROTATED ELASTIC AND PIEZOELECTRIC COEFFICIENTS OF AMMONIUM DIHYDROGEN PHOSPHATE

INTRODUCTION

Since the great majority of piezoelectric crystals find their most frequent applications in orientations which are rotated with respect to the conventional crystallographic axes, it becomes worthwhile to investigate the behavior of a crystal's properties as it undergoes an arbitrary rotation. In this article, the elastic and piezoelectric properties of ammonium dihydrogen phosphate, $NH_4 H_2 PO_4$ (hereinafter called ADP), will be considered.

ADP is of particular interest because of its extensive use in electroacoustic transducers for the generation and reception of sound signals in water.

ADP is a member of the tetragonal scalenohedral class, termed Vd in the Schönflies crystallographic notation, and $\bar{4}$ 2m in the Hermann-Mauguin convention, and crystallizes with the habit illustrated in Figure 1. The original unrotated system will be considered right-handed and will be specified by the axes, X, Y, and Z. The Z axis lies along the long dimension of the crystal and is an axis of fourfold alternating symmetry. The X and Y axes possess twofold symmetry. The piezoelectric axes, P_1 and P_2, are diagonal axes located at angles of 45° with X and Y. A positive stress, i.e. a tension, acting along P_1 produces a positive charge at the positive end of the Z axis. The latest convention for directions of crystallographic axes suggested by the I.R.E. Technical Committee on Piezoelectric Crystals[1,10]* is adopted.

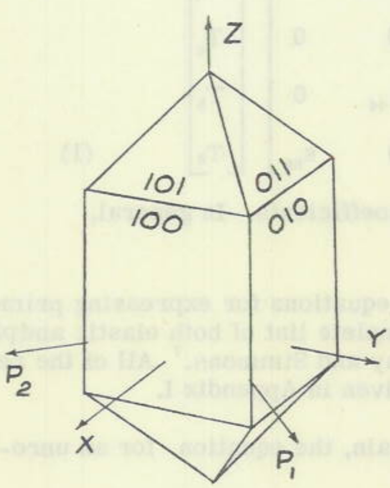

Figure 1 - Growth habit for ADP

The transformed orientation following a rotation about any single axis may be specified by X, Y′, Z′ for a rotation about X; X′, Y, Z′ for a rotation about Y; and X′ Y′ Z for a rotation about Z. These are the types of rotation to be considered here since they are most often encountered in practice. The angle of rotation is taken as positive when it appears counterclockwise to an observer looking back toward the origin from the positive end of the axis of rotation.

The values of the elastic and piezoelectric coefficients for an unrotated orientation are taken from Mason.[2] In an unpublished report, Baerwald[3] disagrees slightly with Mason's figures but this discrepancy is not serious enough to affect the results which follow.

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* *Superior numbers indicate references which are listed after the appendices.*

The coefficients to be considered are the elastic compliance and stiffness constants, and the piezoelectric strain and stress coefficients, i.e., the "s" and "c," and the "d" and "e" constants of Cady[4] respectively. The unprimed coefficients apply in the original unrotated orientation; after a given rotation, the primed coefficients will be employed.

ELASTIC PROPERTIES OF ADP

The stress matrix T is written as

$$T = \left\{X_x, Y_y, Z_z, Y_z, Z_x, X_y\right\}.$$

The first three terms of the column matrix denote the normal stress components; the latter three the shear stress components. In like manner, the strain matrix S is

$$S = \left\{x_x, y_y, z_z, y_z, z_x, x_y\right\}$$

where the first three terms are normal strains and the latter three are shear strains.

According to the generalized form of Hooke's Law, the elastic equation for an unrotated ADP crystal is

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} \qquad (1)$$

where $[s_{hk}]$ represents the matrix of elastic compliance coefficients. In general, $s_{hk} = s_{kh}$ where h = 1 to 6 and k = 1 to 6.

Voigt[5] and Cady[6] have given several of the transform equations for expressing primed constants in terms of the unprimed constants alone. A complete list of both elastic and piezoelectric relations has been previously presented by Faraday and Simmons.[7] All of the required transformation equations for the compliances are given in Appendix I.

If the stress components are written in terms of the strain, the equation for an unrotated ADP crystal will be

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \end{bmatrix} \qquad (2)$$

where $[c_{hk}]$ is the matrix of elastic stiffness coefficients. In general, $c_{hk} = c_{kh}$ where $h = 1$ to 6 and $k = 1$ to 6.

Since the s matrix of (1) and the c matrix of (2) are reciprocals of one another, the stiffness coefficients can immediately be written in terms of the compliances as follows:

$$c_{11} = \frac{|\Delta_{11}|}{|\Delta|}, \qquad c_{12} = \frac{|\Delta_{12}|}{|\Delta|}, \text{ etc.} \tag{3}$$

where $|\Delta_{11}|$ refers to the minor of the s_{11} term, i.e.,

$$|\Delta_{11}| = \begin{vmatrix} s_{11} & s_{13} \\ s_{13} & s_{33} \end{vmatrix} \quad \text{and} \quad \Delta_{11} = \begin{vmatrix} s_{11} & s_{12} & s_{13} \\ s_{12} & s_{11} & s_{13} \\ s_{13} & s_{13} & s_{33} \end{vmatrix}$$

Also

$$c_{44} = 1/s_{44} \quad \text{and} \quad c_{66} = 1/s_{66} \tag{4}$$

As before, the primed elastic stiffness coefficients can readily be written with the aid of the transformation expressions. All of the necessary equations are included in Appendix II.

It is now possible to compute all of the elastic compliance and stiffness coefficients as functions of the angle of rotation for arbitrary rotations about the X, the Y, or the Z axis.

Mason[2] has measured values for the compliance coefficients of a plated ADP crystal for an unrotated orientation. The elastic constants considered in this article are all understood to have the superscript E to indicate that they were measured with the applied field constant or equal to zero. These are termed by Cady the "isagric" constants in contrast to constants measured with the surface charge equal to zero.

Values of the compliance coefficients s_{hk} are taken at 20°C which is considered to be normal room temperature and are expressed in terms of cm²/dyne in cgs units. They are as follows:

$$s_{11} = s_{22} = 1.70 \times 10^{-12}$$

$$s_{12} = 0.65 \times 10^{-12}$$

$$s_{13} = s_{23} = -1.10 \times 10^{-12}$$

$$s_{33} = 4.35 \times 10^{-12}$$

$$s_{44} = s_{55} = 11.50 \times 10^{-12}$$

$$s_{66} = 16.30 \times 10^{-12}$$

The use of the rationalized mks system will change the units to m²/newton and the multiplying factor 10^{-12} will become 10^{-11}.

Employing (3) and (4), the stiffness coefficients c_{hk} are readily computed for an unrotated orientation and are expressed in terms of dyne/cm² in cgs units. They are given as follows:

$$c_{11} = c_{22} = 75.5 \times 10^{10}$$

$$c_{12} = -19.8 \times 10^{10}$$

$$c_{13} = c_{23} = 14.1 \times 10^{10}$$

$$c_{33} = 30.1 \times 10^{10}$$

$$c_{44} = c_{55} = 8.7 \times 10^{10}$$

$$c_{66} = 6.1 \times 10^{10}$$

In rationalized mks units these are expressed in newton/m^2 and the multiplying factor becomes 10^9.

The transform equations are now applied and values for each of the elastic coefficients are computed for a 360^0 rotation about each of the axes.

As an illustration, Table 1 shows the variation of the s'_{hk} constants with a positive rotation about the Z axis. The value in each case is understood to be multiplied by 10^{-12} cm^2/dyne for cgs units and by 10^{-11} m^2/newton for rationalized mks units.

TABLE 1

Angle of Rotation θ	$s'_{11} = s'_{22}$	s'_{12}	$s'_{16} = -s'_{26}$	s'_{66}
0^0	1.70	0.65	0	16.30
5^0	1.80	0.54	1.21	15.87
10^0	2.10	0.24	2.28	14.64
15^0	2.57	-0.24	3.07	12.75
20^0	3.14	-0.82	3.50	10.43
25^0	3.74	-1.43	3.50	7.97
30^0	4.31	-2.01	3.07	5.65
35^0	4.77	-2.48	2.28	3.76
40^0	5.07	-2.79	1.21	2.53
45^0	5.17	-2.90	0	2.10

The coefficients $s'_{13} = s'_{23}$, s'_{33}, and $s'_{44} = s'_{55}$ remain invariant for the entire rotation in the XY plane. The values of $s'_{11} = s'_{22}$, s'_{12}, and s'_{66} are symmetrical about $\theta = 45^0$ in the XY plane; so from 45^0 to 90^0 these coefficients will repeat their values. In the case of s'_{16} and s'_{26} a change of sign takes place though their absolute magnitudes are once more repeated from 45° to 90°. Also, each coefficient remains invariant for a rotation of $\pi/2$, whence each value will be repeated in exactly the same fashion for each of the four quadrants.

Tables 2 and 3 serve as an index for the polar plots of all of the elastic coefficients for separate rotations about each axis. As before, the s'_{hk} values shown are understood to be multiplied by 10^{-12} cm^2/dyne for cgs units and by 10^{-11} m^2/newton for rationalized mks units. In like manner, the c'_{hk} values shown are to be multiplied by 10^{10} dyne/cm^2 in the cgs system and by 10^9 newton/m^2 in the rationalized mks system.

TABLE 2

Figure No.	Rotation About Axis	Elastic Compliance Coefficients, s'_{hk}
2	X	A, s'_{11} ; B, s'_{22} ; C, s'_{33}
3	X	D, s'_{55} ; E, s'_{44} ; F, s'_{66}
4	X	G, s'_{12} ; H, s'_{13} ; J, s'_{23}
5	X	K, s'_{14} ; L, s'_{24} ; M, s'_{34} ; N, s'_{56}
2	Y	B, s'_{11} ; A, s'_{22} ; C, s'_{33}
3	Y	D, s'_{44} ; E, s'_{55} ; F, s'_{66}
4	Y	G, s'_{12} ; J, s'_{13} ; H, s'_{23}
6	Y	O, s'_{15} ; P, s'_{25} ; Q, s'_{35} ; R, s'_{46}
7	Z	S, $s'_{11} = s'_{22}$; T, s'_{33}
8	Z	U, $s'_{44} = s'_{55}$; V, s'_{66}
9	Z	A', s'_{12} ; B', $s'_{13} = s'_{23}$
10	Z	C', s'_{16} ; D', s'_{26}

TABLE 3

Figure No.	Rotation About Axis	Elastic Stiffness Coefficients, c'_{hk}
11	X	A, c'_{11} ; B, c'_{22} ; C , c'_{33}
12	X	D, c'_{44} ; E, c'_{55} ; F, c'_{66}
13	X	G, c'_{12} ; H, c'_{13} ; J, c'_{23} ; K, c'_{14}
14	X	L, c'_{24} ; M, c'_{34} ; N, c'_{56}
11	Y	B, c'_{11} ; A, c'_{22} ; C, c'_{33}
12	Y	E, c'_{44} ; D, c'_{55} , F, c'_{66}
13	Y	G, c'_{12} ; J, c'_{13} ; H, c'_{23}
15	Y	O, c'_{15} ; P, c'_{25} ; Q, c'_{35} ; R, c'_{46}
16	Z	S, $c'_{11} = c'_{22}$; T, c'_{33}
17	Z	U, $c'_{44} = c'_{55}$; V, c'_{66} ; A', $c'_{13} = c'_{23}$
18	Z	B', c'_{12} ; C', c'_{16} ; D', c'_{26}

The fourfold symmetry of ADP about the Z axis is readily evidenced by Figures 7, 8, 9, and 10 for the compliances and by Figures 15, 16, 17, and 18 for the stiffnesses.

It is of interest to note that the diminution of the number of elastic coefficients in the XY plane as well as the invariance under rotation about the Z axis of some of the coefficients eliminates some of the undesirable modes of vibration of the ADP crystal. As a result, it is possible to excite an almost purely longitudinal mode in a 45° Z-cut crystal bar the width and thickness of which are negligible compared to length. Only the s'_{11} coefficient makes a contribution in this case and the frequency of a plated ADP bar vibrating in this mode is given by Mason[2] as

$$f_r = (1/2l)\,(1/\rho s'_{11})^{\frac{1}{2}}$$

where f_r is the fundamental resonant frequency, l the length of the bar, ρ the density (1.804) and s'_{11} is 5.17 x 10^{-12} cm^2/dyne. It will be shown later that s'_{11} is the reciprocal of Young's modulus for the Z-cut bar.

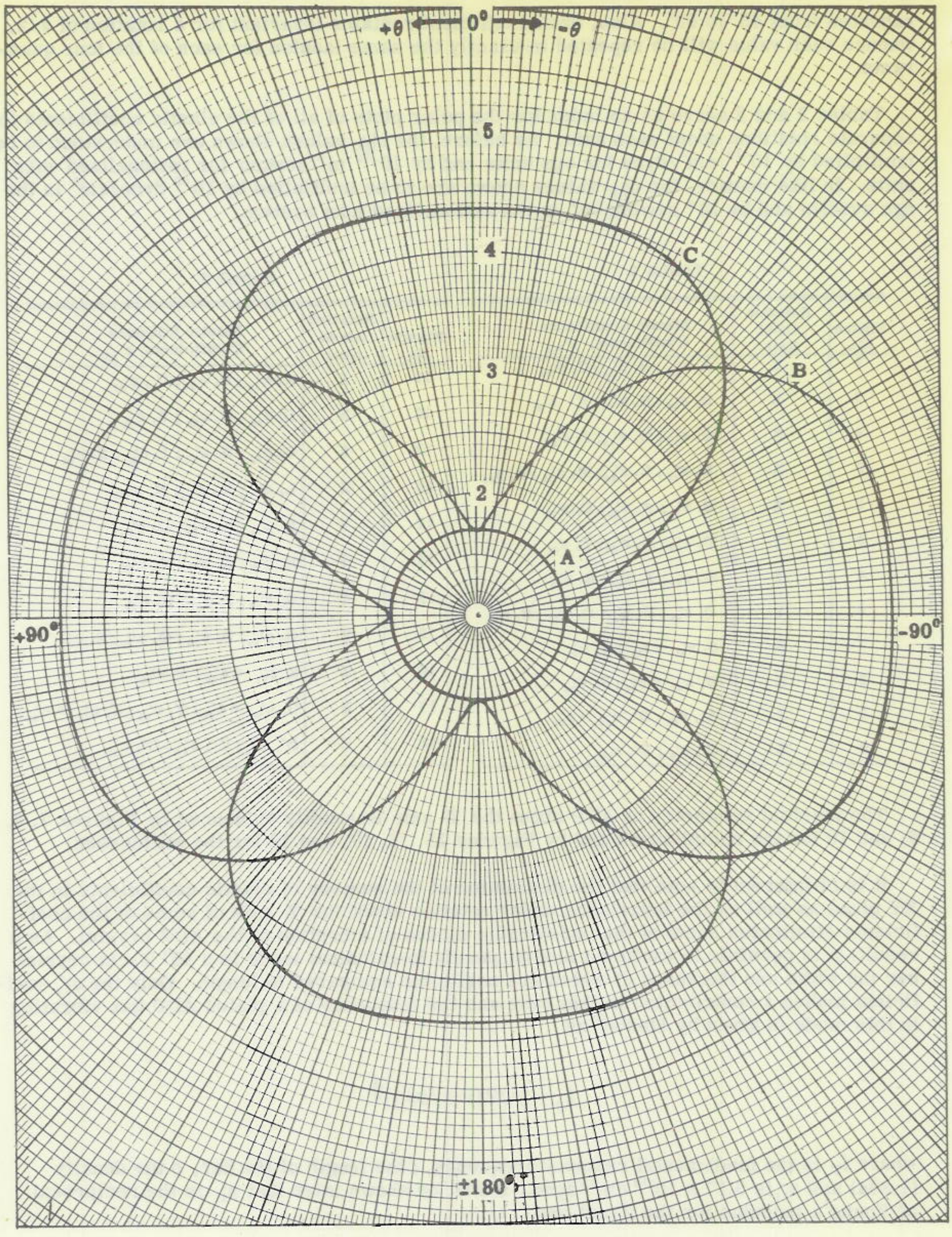
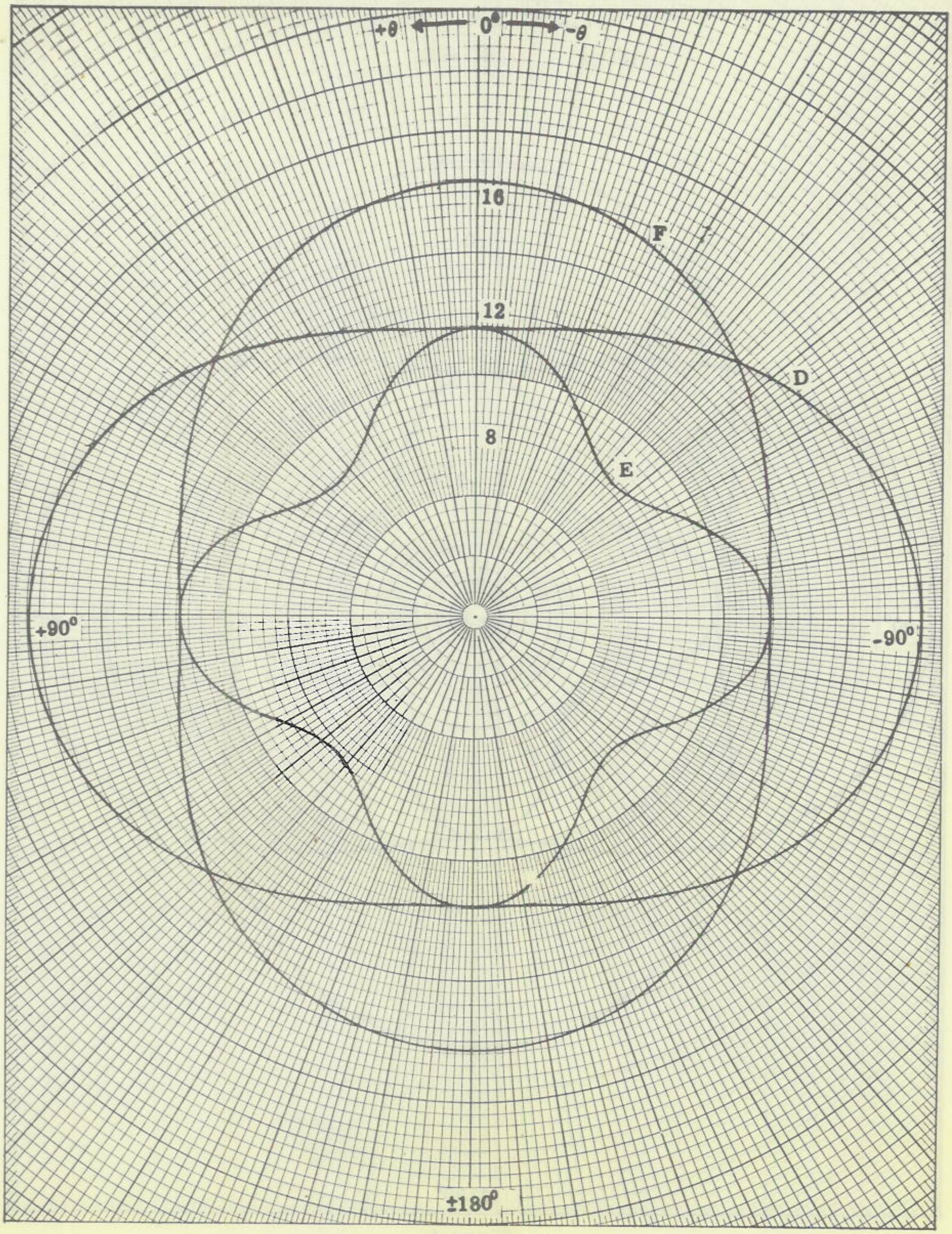


Figure 2



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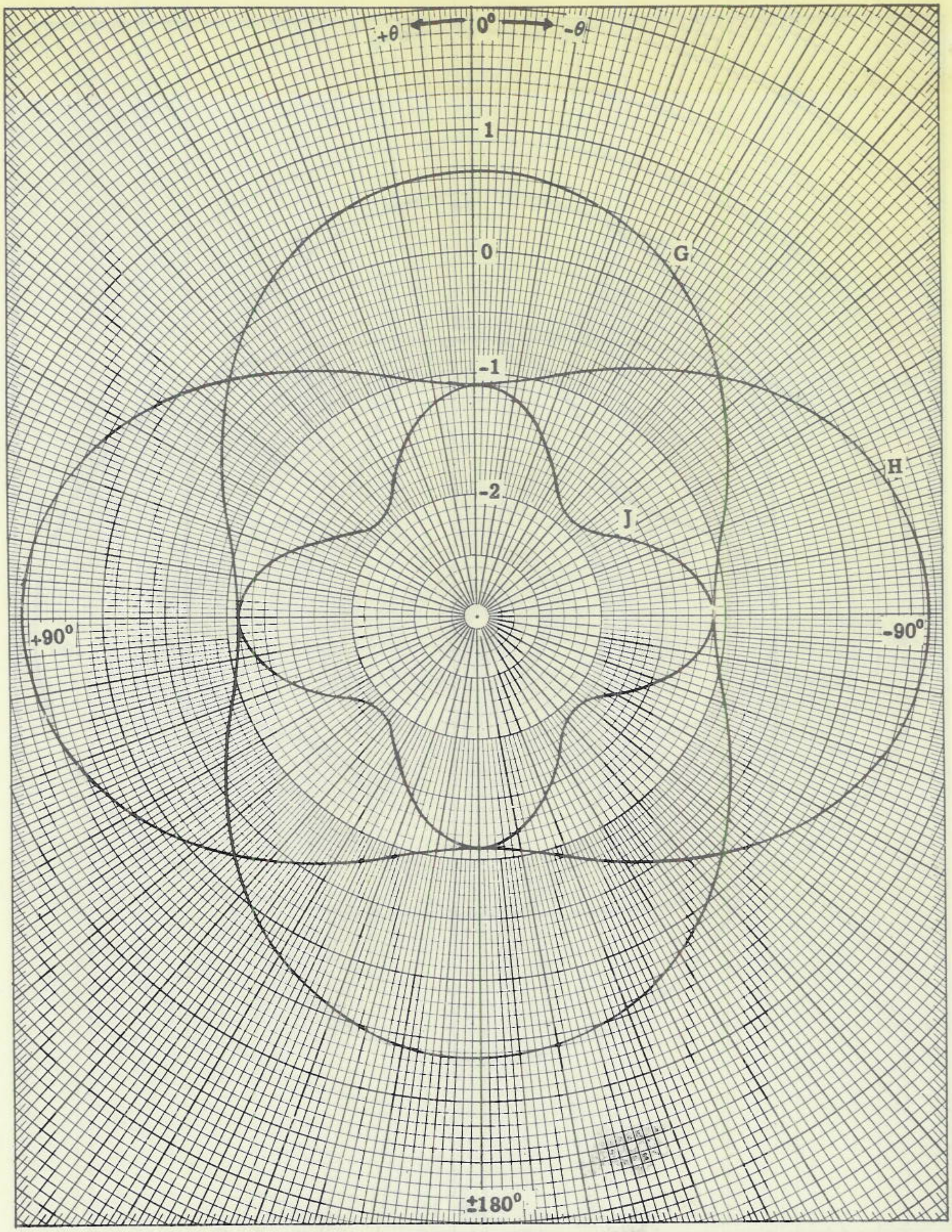


Figure 4

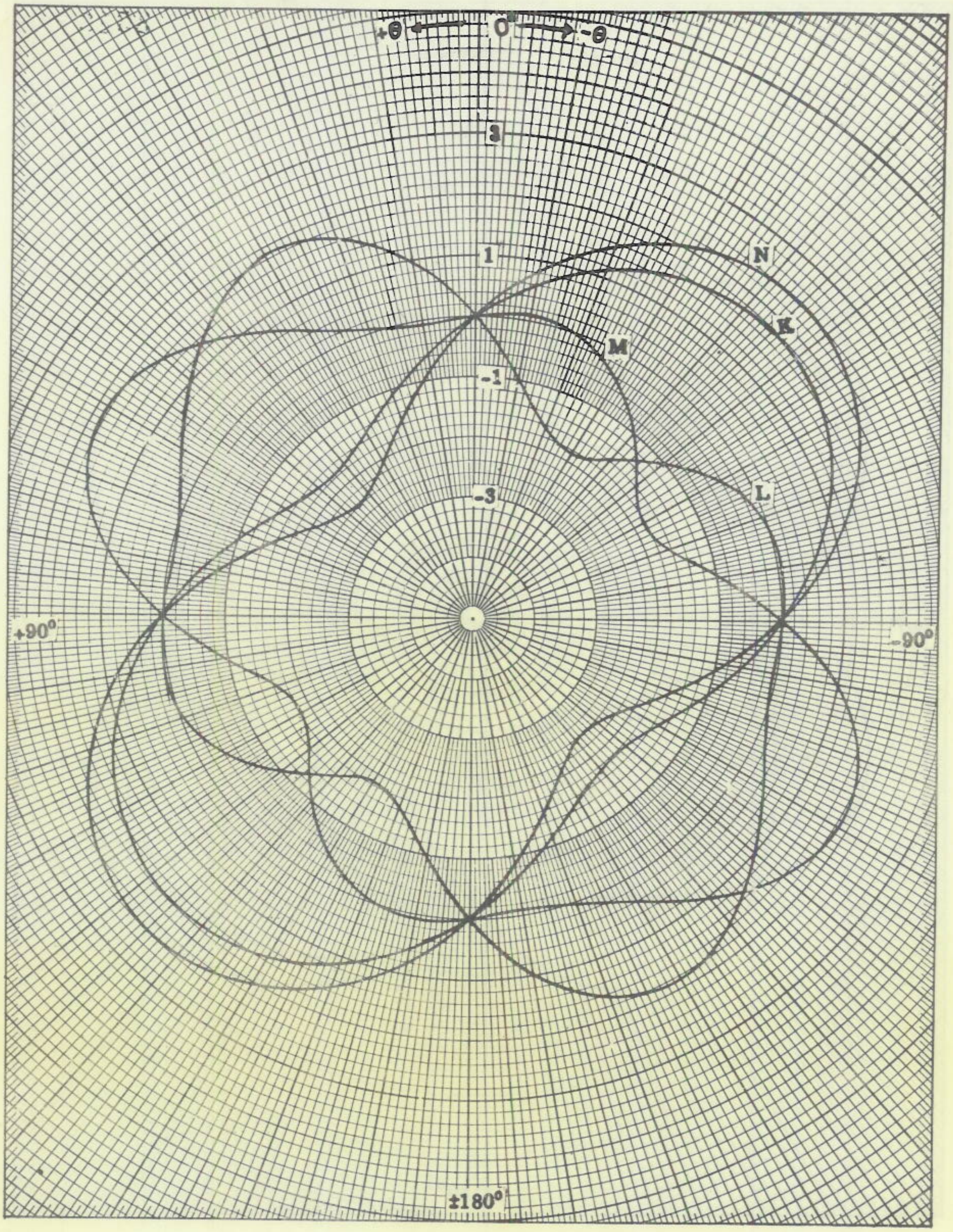


Figure 5

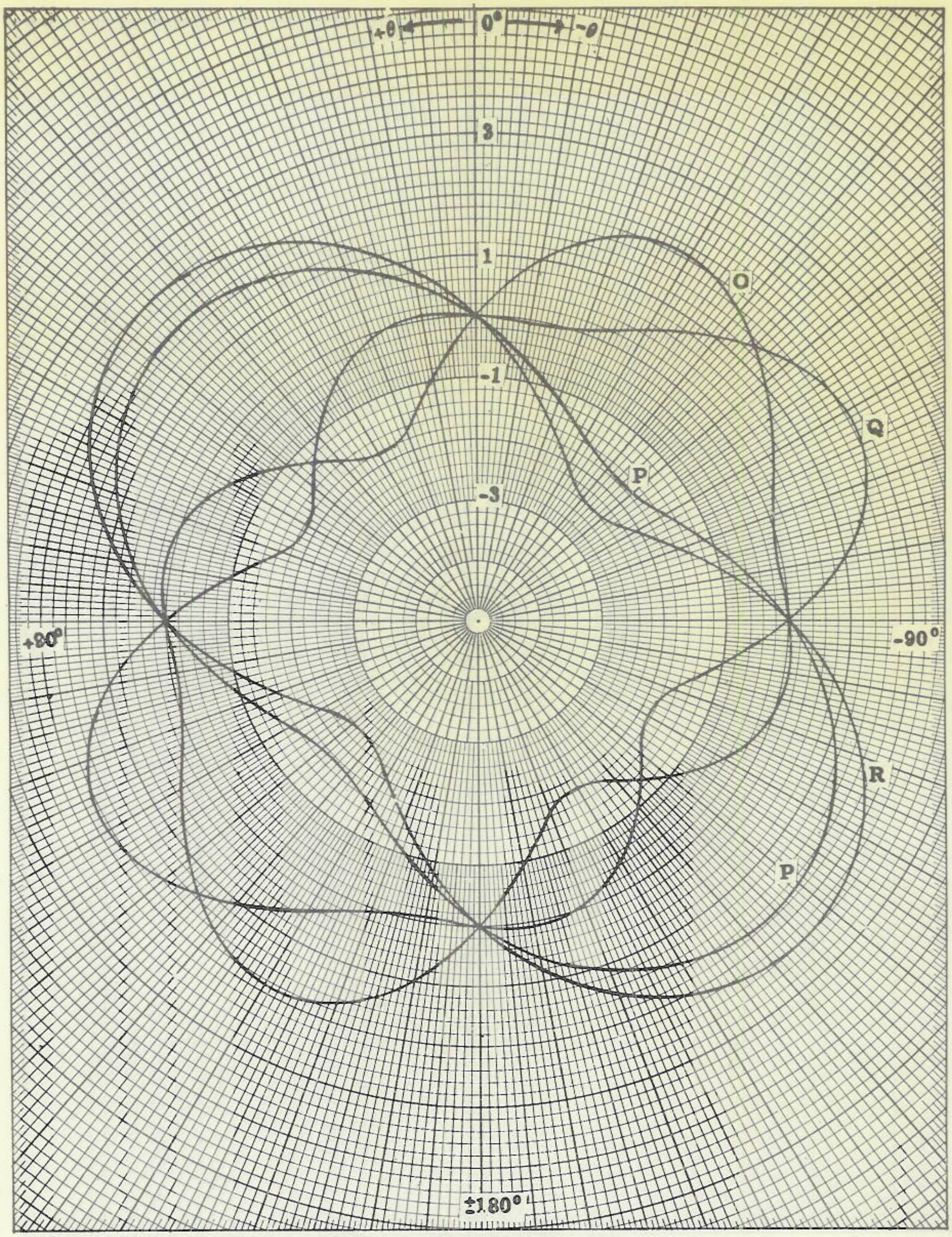
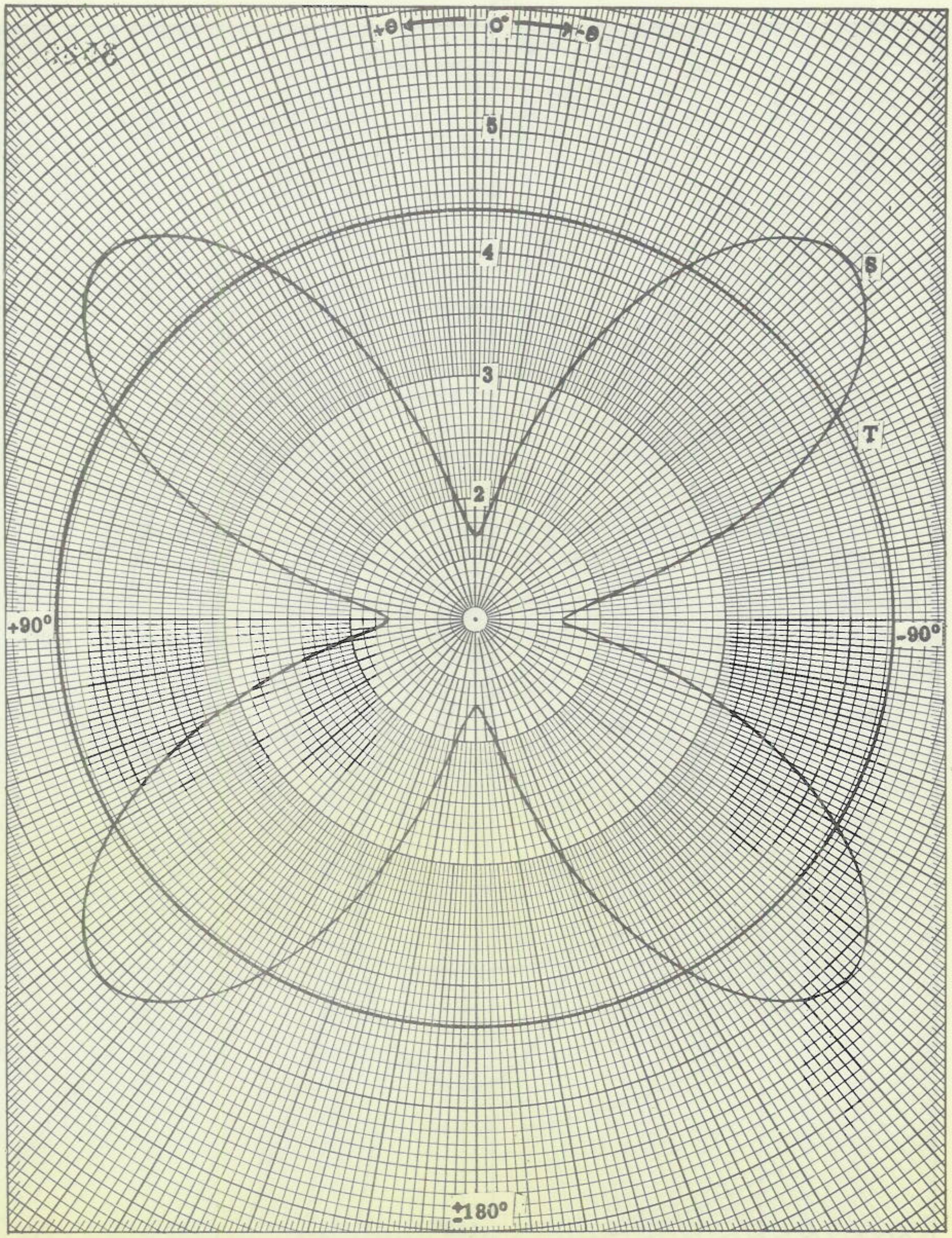


Figure 6



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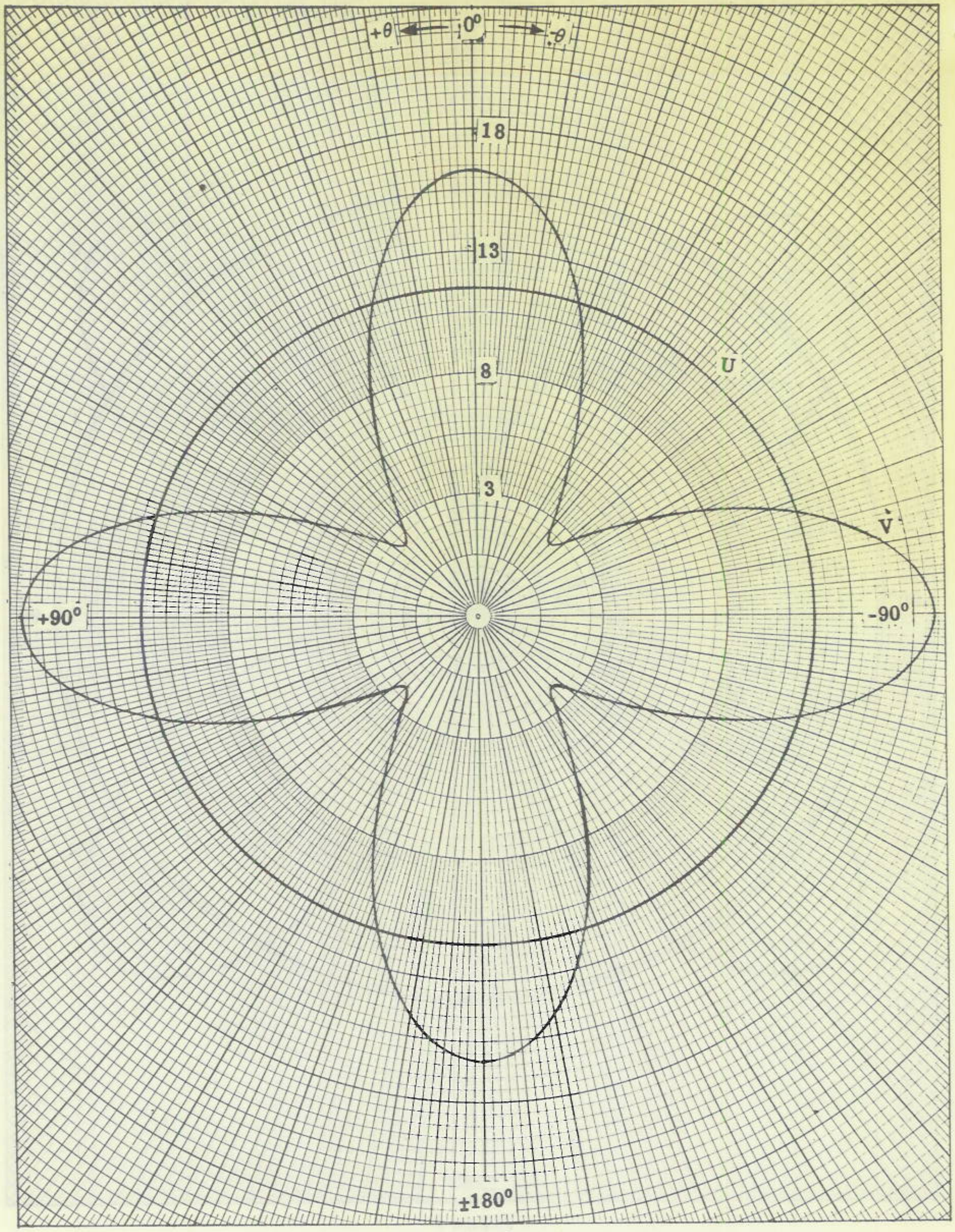

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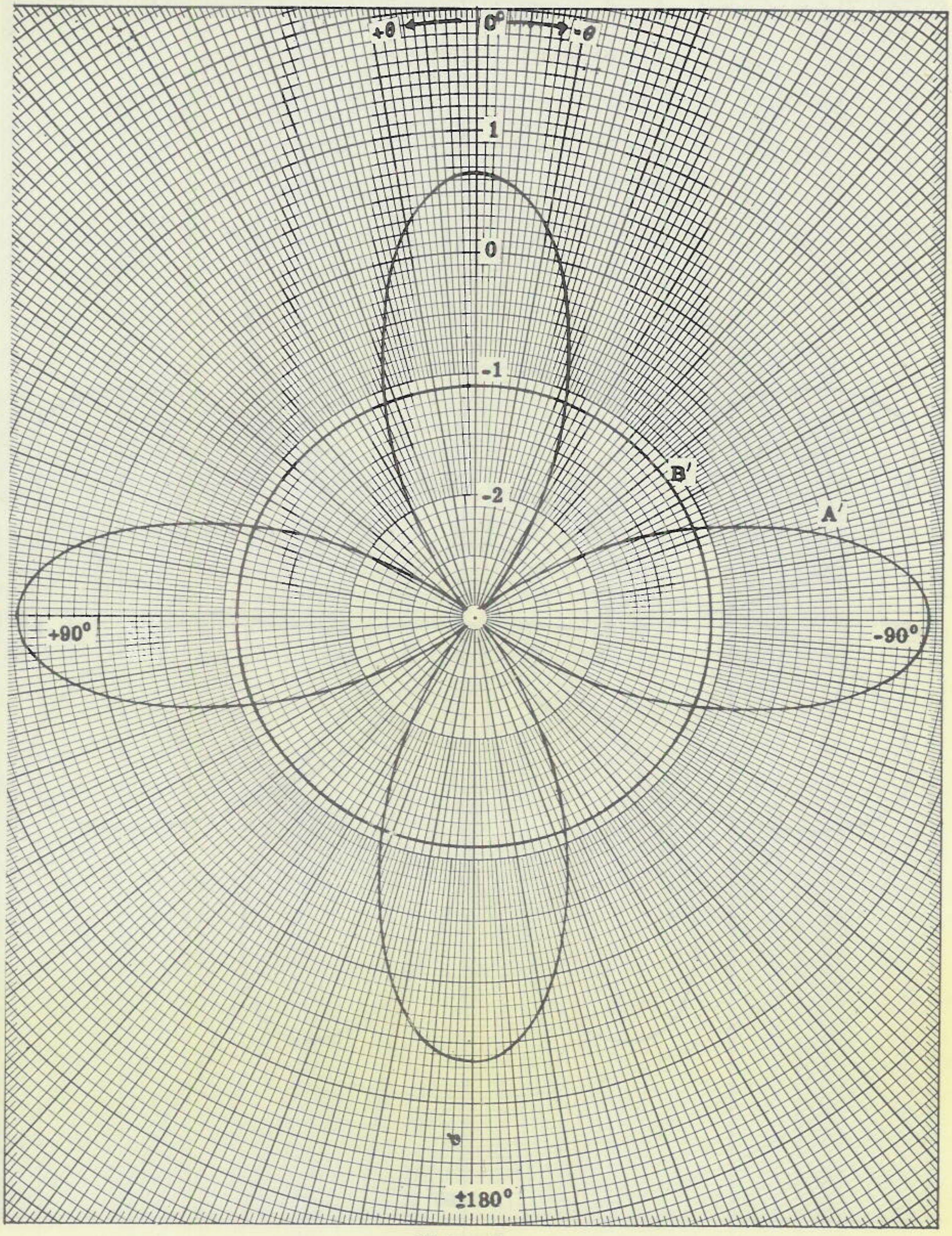

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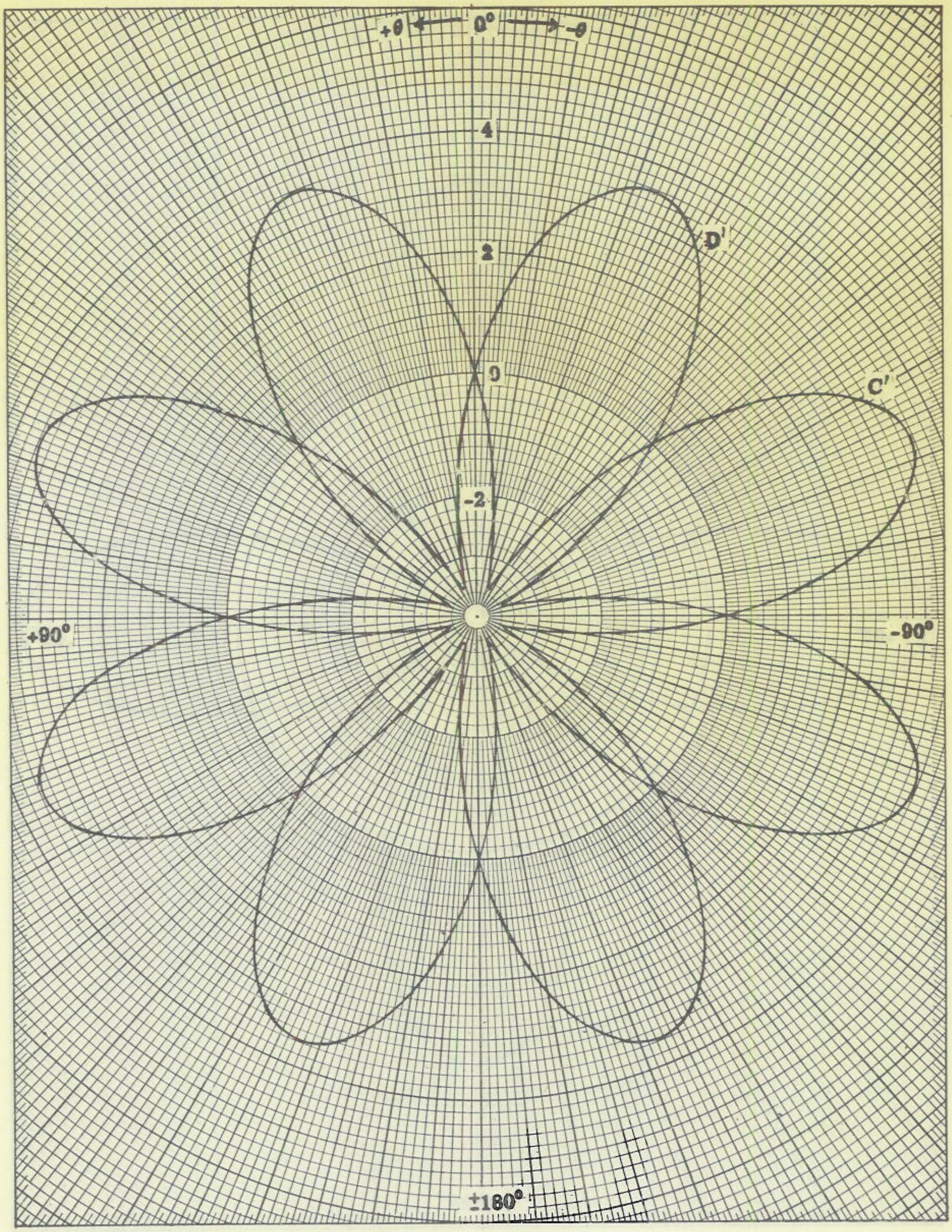


Figure 10

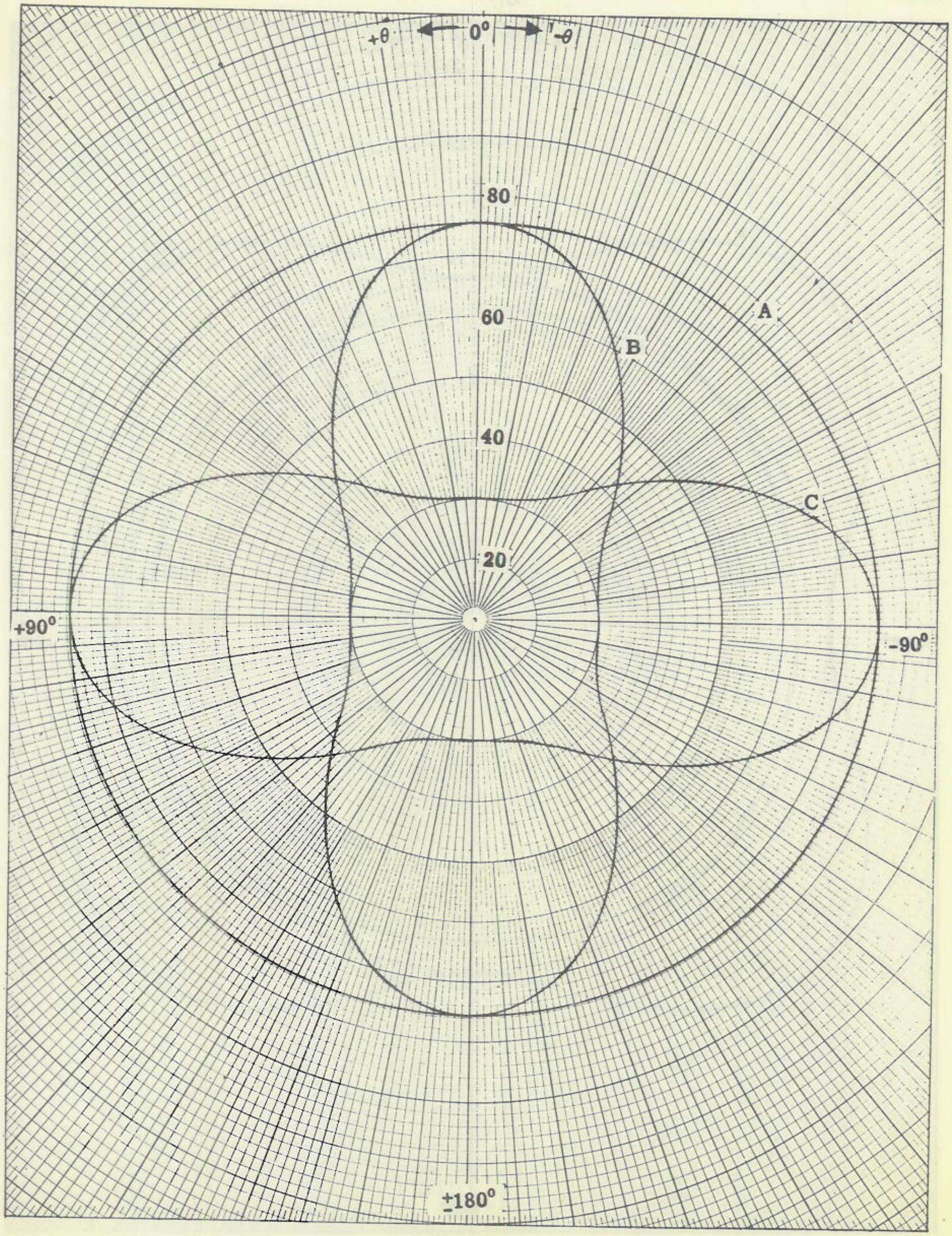
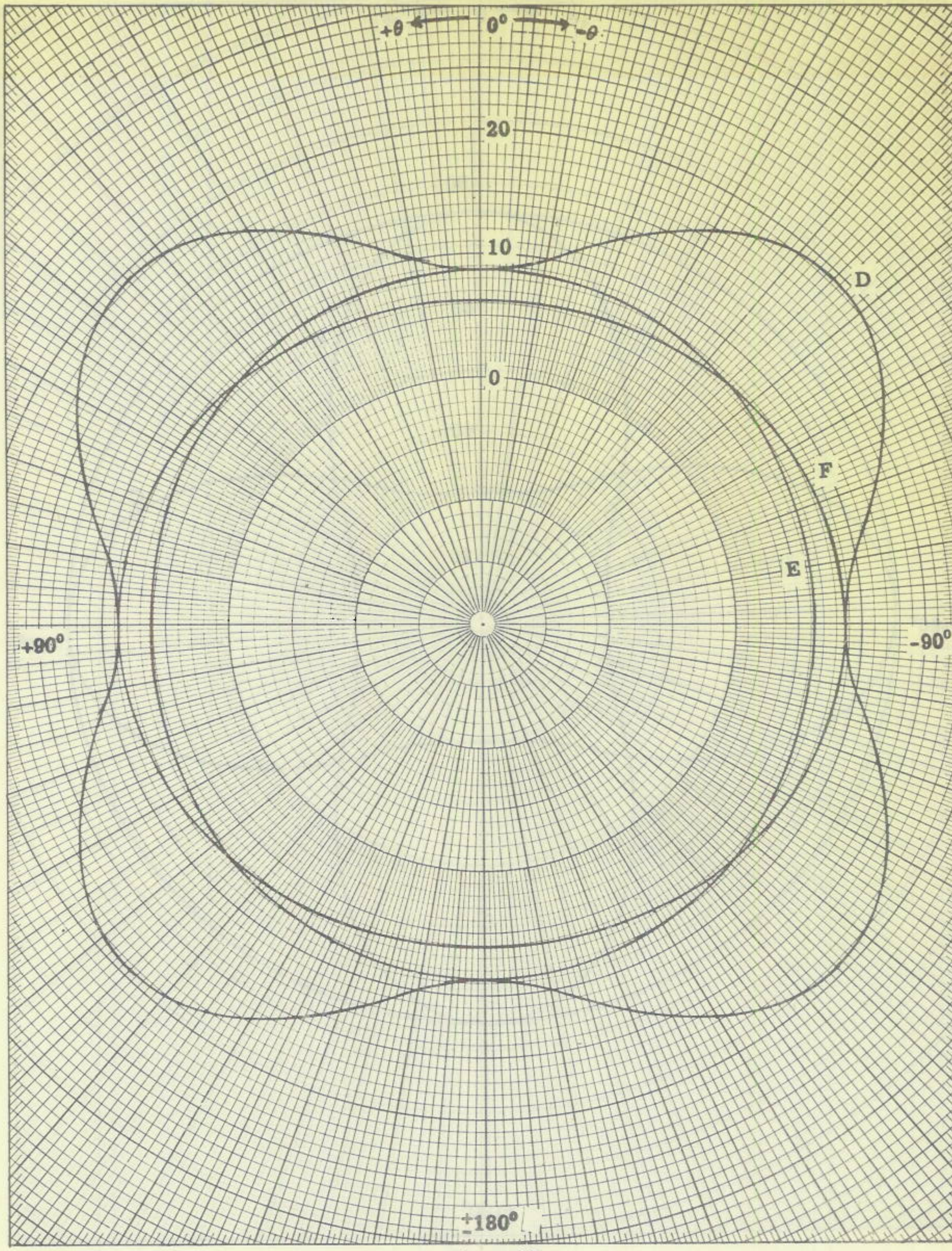


Figure 11



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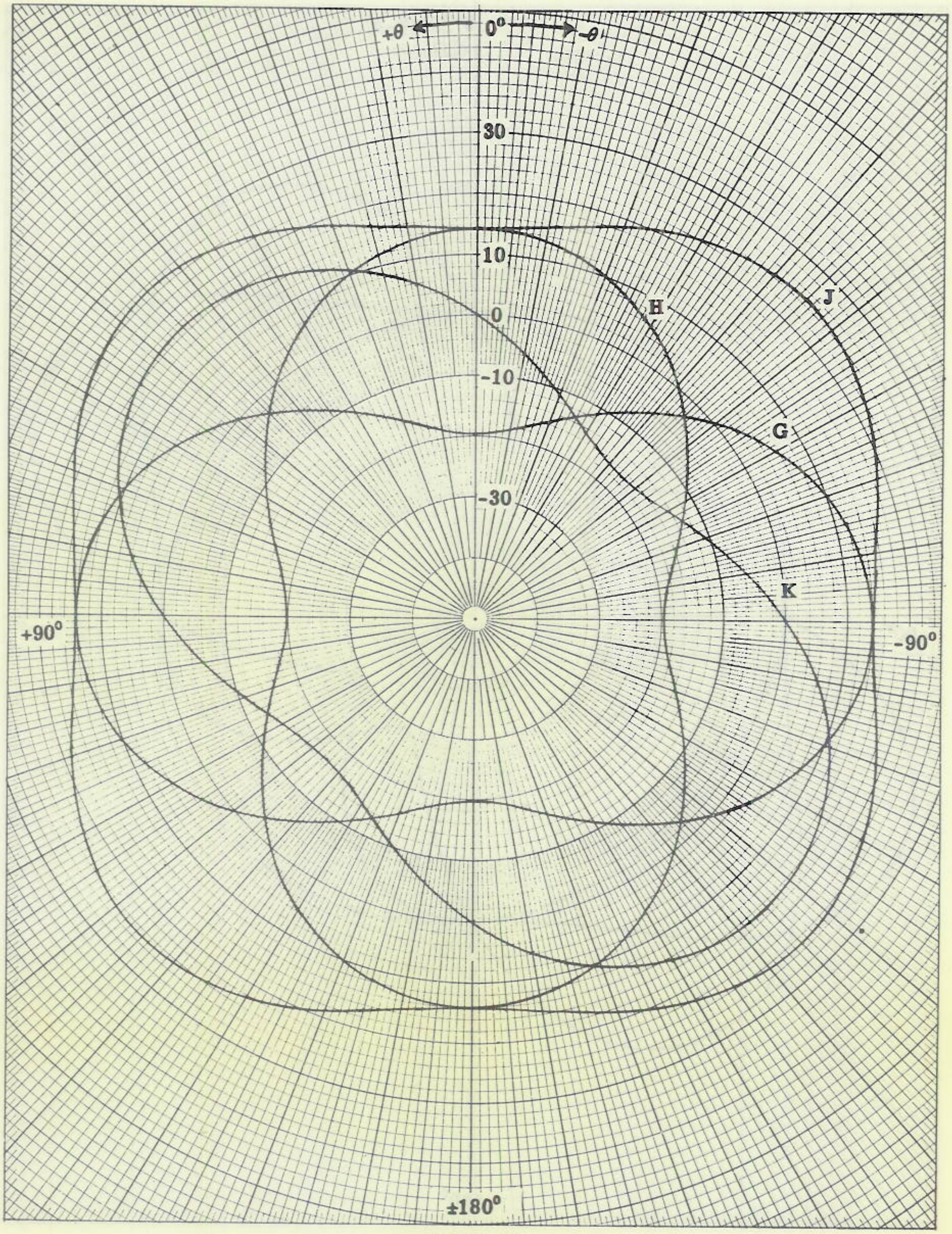

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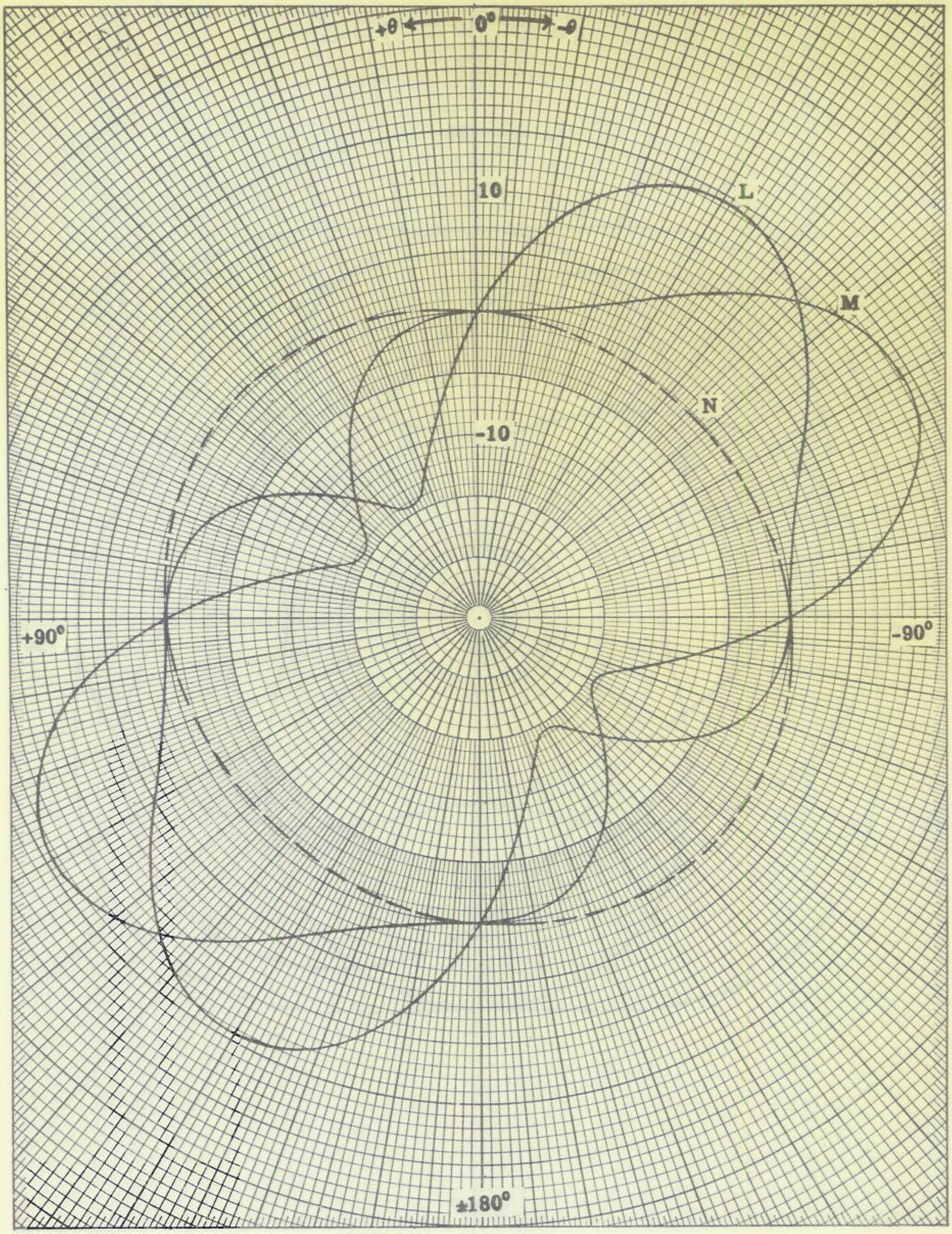

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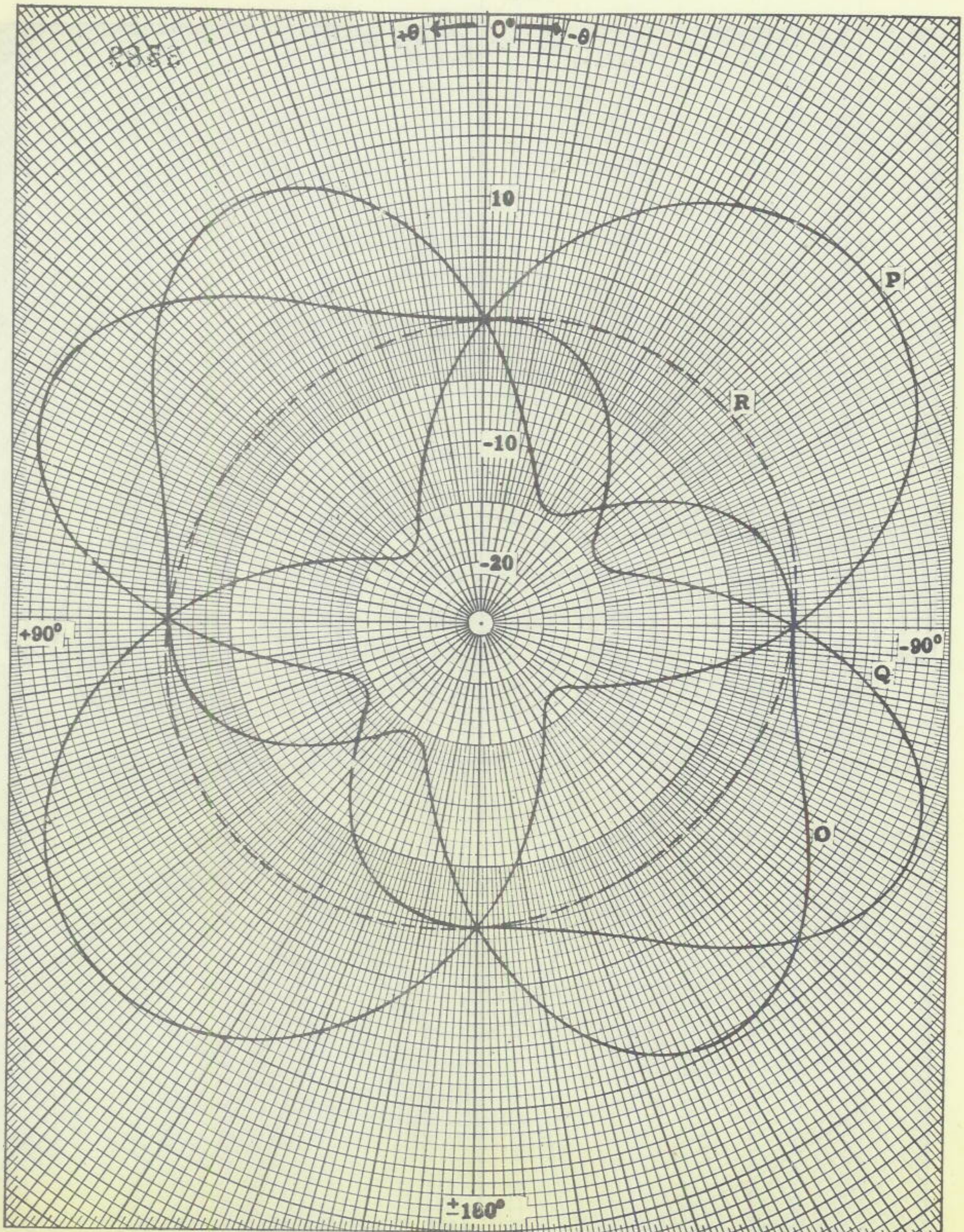

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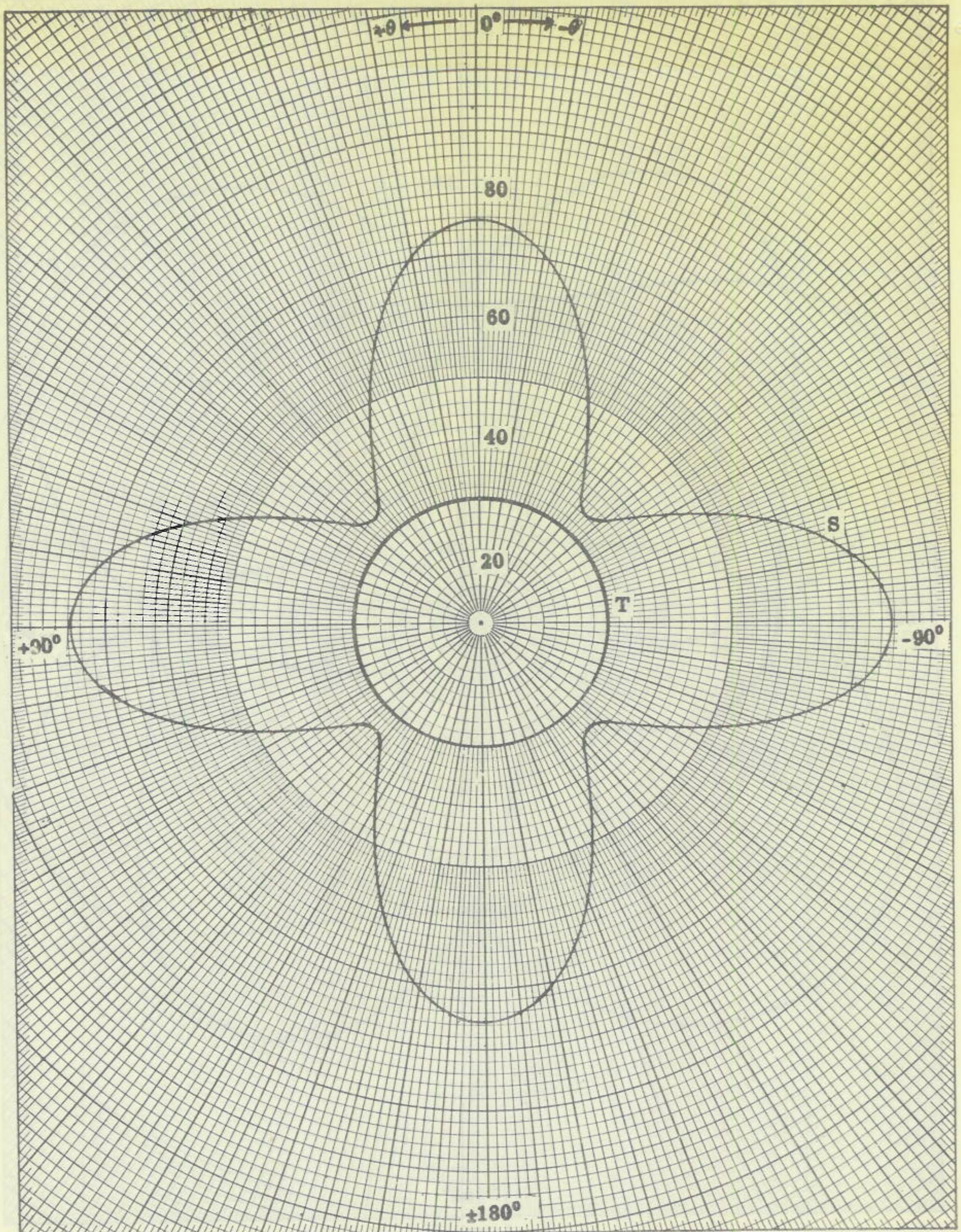
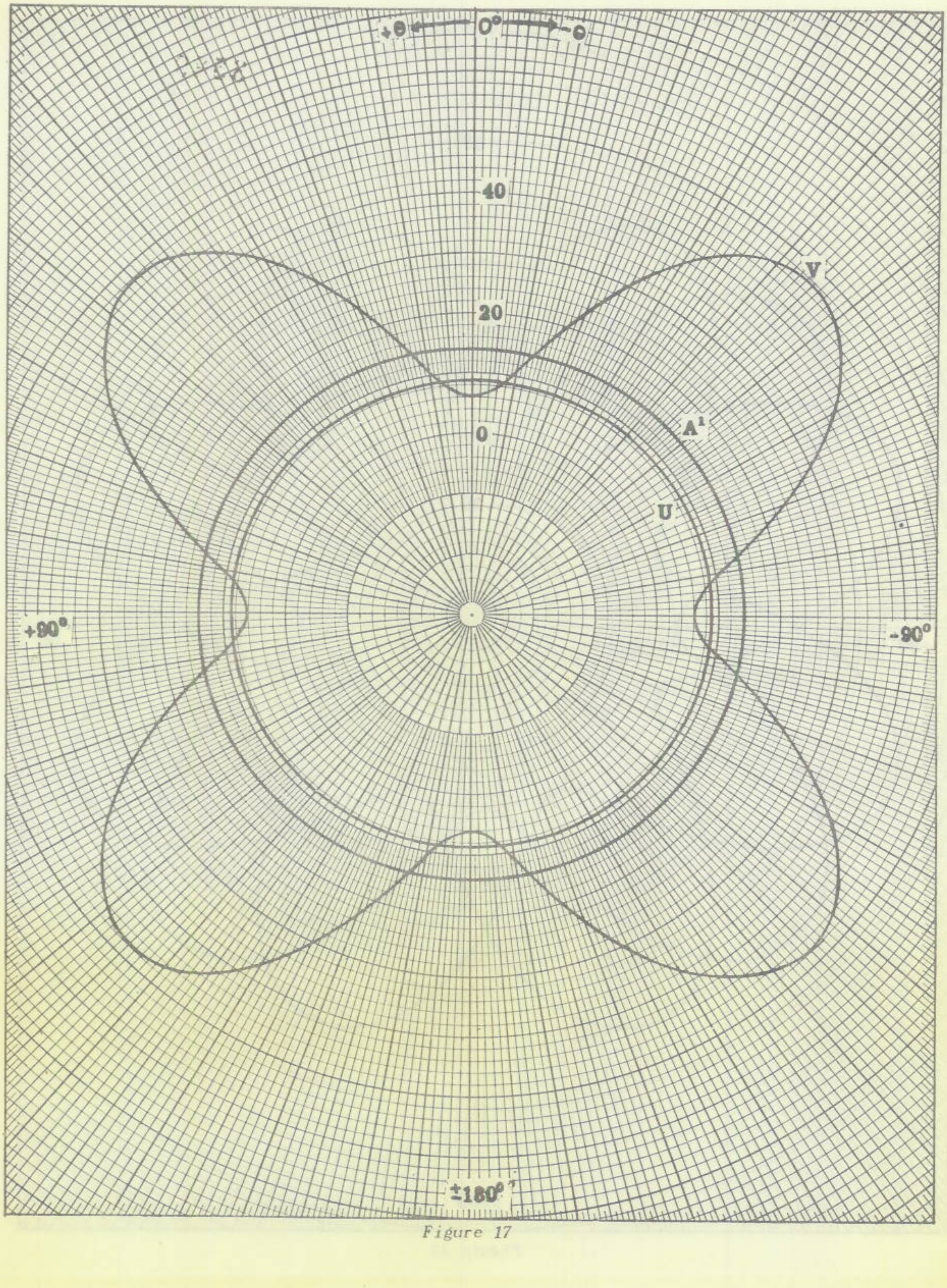


Figure 16



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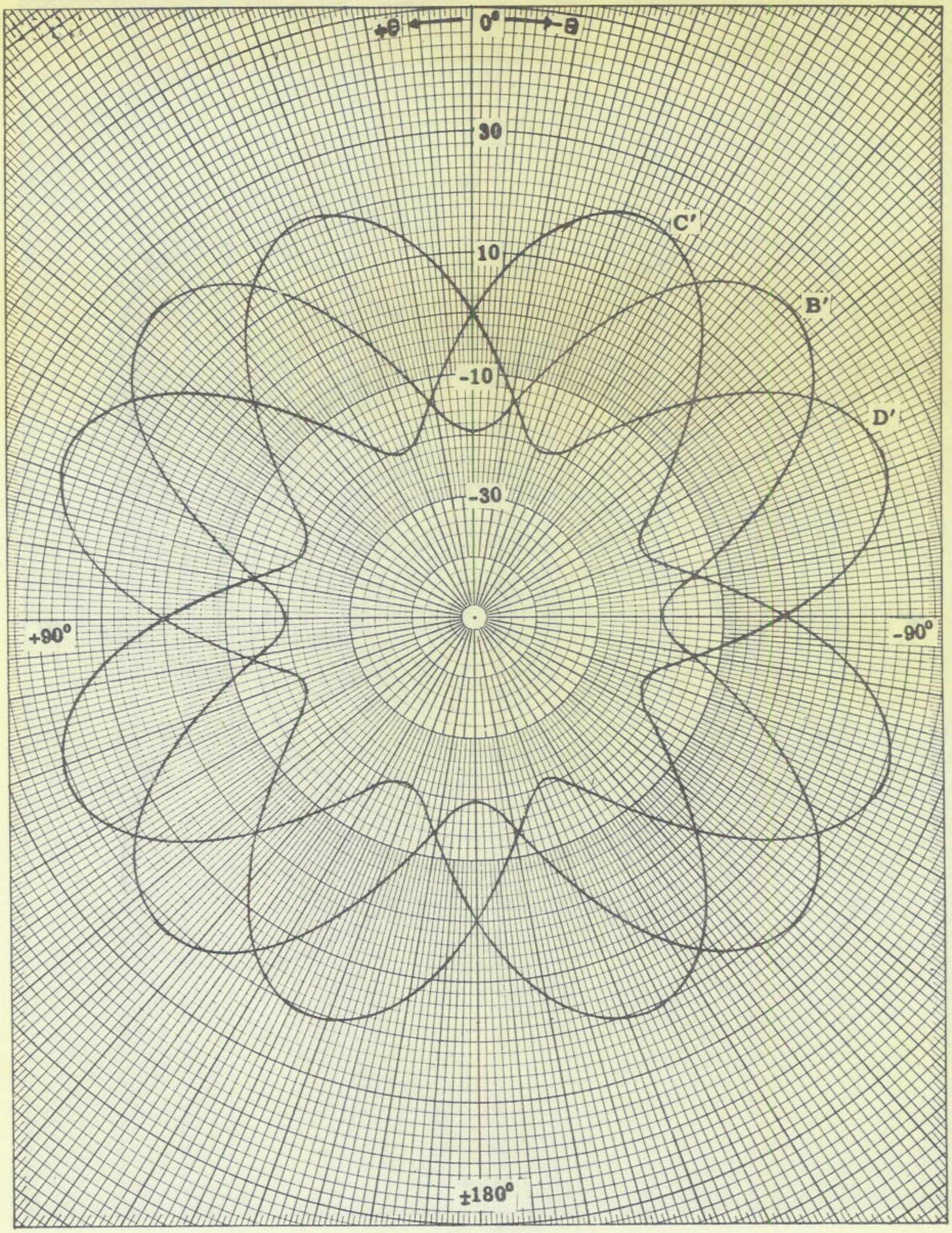

Figure 18

PIEZOELECTRIC PROPERTIES OF ADP

For the direct piezoelectric effect, a polarization results from a mechanical stress in the absence of an electric field. For the converse effect, an impressed field gives rise to mechanical strains and internal stresses. The effects resulting from mechanical forces may be added to these by the process of superposition.

In matrix form the converse effect for an unrotated ADP crystal may be written as

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ d_{14} & 0 & 0 \\ 0 & d_{14} & 0 \\ 0 & 0 & d_{36} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \qquad (5)$$

where $[d_{jk}]_t$ is the transpose of $[d_{jk}]$, the matrix of the piezoelectric strain coefficients in accordance with Cady's terminology.[4] In general $d_{jk} \neq d_{kj}$ where j = 1, 2, 3; and k = 1 to 6. E_1, E_2 and E_3 refer to the impressed fields in the X, Y, and Z directions respectively.

The procedure for determining d'_{jk} for rotated orientations is identical with that followed above for the elastic compliance coefficients. Appendix III gives a complete list of equations for the required transformation of the "d" constants.

The equation for the internal stresses existing in an unrotated ADP crystal is given by

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ -e_{14} & 0 & 0 \\ 0 & -e_{14} & 0 \\ 0 & 0 & -e_{36} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \qquad (6)$$

where $[e_{jk}]_t$ is the transpose of $[e_{jk}]$, the matrix of the piezoelectric stress coefficients.[4] In general $e_{jk} \neq e_{kj}$ where j = 1, 2, 3; and k = 1 to 6.

The values of the "e" constants are readily determined once the "d" constants are known. For, in the case of the direct piezoelectric effect, when a crystal at any arbitrary orientation is subjected to a mechanical stress in the absence of an electric field, an electric displacement is produced according to the equations.

$$D' = e'S' \quad (7) \quad \text{and} \qquad D' = d'T' \qquad (8)$$

where D′ is the displacement matrix, d′ and e′, the matrices of the piezoelectric strain and stress coefficients respectively, S′, the strain matrix and T′, the stress matrix.

So, combining (7) and (8)

$$s' = d'T'S'^{-1} \tag{9}$$

and from Hooke's Law

$$T' = c'S'$$

or

$$c' = T'S'^{-1} \tag{10}$$

Whence, from (9) and (10)

$$e' = d'c' \tag{11}$$

Since the piezoelectric strain coefficients and the elastic stiffness coefficients have already been computed for each rotation, it is a simple matter to determine the piezoelectric stress coefficients. The complete list of expressions required for this calculation for ADP is given in Appendix IV.

The experimental values for d_{jk} at 20^0 C are given by Mason.[2] In cgs units they are expressed as statcoulombs/dyne and are as follows:

$$d_{14} = d_{25} = 5.0 \times 10^{-8}$$

$$d_{36} = 148.0 \times 10^{-8}$$

In the rationalized mks system they are given in terms of coulombs/newton and the multiplying factor 10^{-8} becomes $1/3 \times 10^{-12}$

The transform equations of Appendix III are now applied and values for each of the piezoelectric strain coefficients are computed for a 360^0 rotation about each of the X, Y, and Z axes. Table 4 serves as an index for these polar plots.

The piezoelectric stress coefficients for a 360^0 rotation about each of the crystallographic axes are next computed by employing the method of Appendix IV. They are expressed as statcoulombs/cm^2 in cgs units and are given for an unrotated ADP crystal as

$$e_{14} = e_{25} = 4.35 \times 10^3$$

$$e_{36} = 90.3 \times 10^3$$

In rationalized mks units they are expressed as coulombs/m^2 and the multiplying factor 10^3 becomes $1/3 \times 10^{-2}$.

Table 5 serves as an index for the polar plots of e'_{jk}.

Figures 19 - 31 readily illustrate the twofold symmetry of the piezoelectric coefficients of ADP.

TABLE 4

Figure No.	Rotation About Axis	Piezoelectric Strain Coefficients, d'_{jk}
19	X	A, d'_{12}; B, d'_{13}
20	X	C, d'_{14}
21	X	D, d'_{25}
22	X	E, d'_{26}; F, d'_{35}
23	X	G, d'_{36}
21	Y	D, d'_{14}
22	Y	F, d'_{16} ; E, d'_{34}
19	Y	B, d'_{21}; A, d'_{23}
20	Y	C, d'_{25}
23	Y	G, d'_{36}
20	Z	C, $d'_{14} = d'_{25}$
24	Z	H, d'_{15}; J, d'_{24}
25	Z	K, d'_{31}; L, d'_{32}
26	Z	M, d'_{36}

TABLE 5

Figure No.	Rotation About Axis	Piezoelectric Stress Coefficients, e'_{jk}
27	X	A, e'_{12} ; B, e'_{13}; C, e'_{14}
28	X	D, e'_{25} ; E, e'_{36}
29	X	F, e'_{26} ; G, e'_{35}
28	Y	D, e'_{14} ; E, e'_{36}
29	Y	G, e'_{16} ; F, e'_{34}
27	Y	B, e'_{21} ; A, e'_{23}; C, e'_{25}
27	Z	C, $e'_{14} = e'_{25}$
30	Z	H, e'_{15} ; J, e'_{24}
31	Z	K, e'_{31} ; L, e'_{32} ; M, e'_{36}

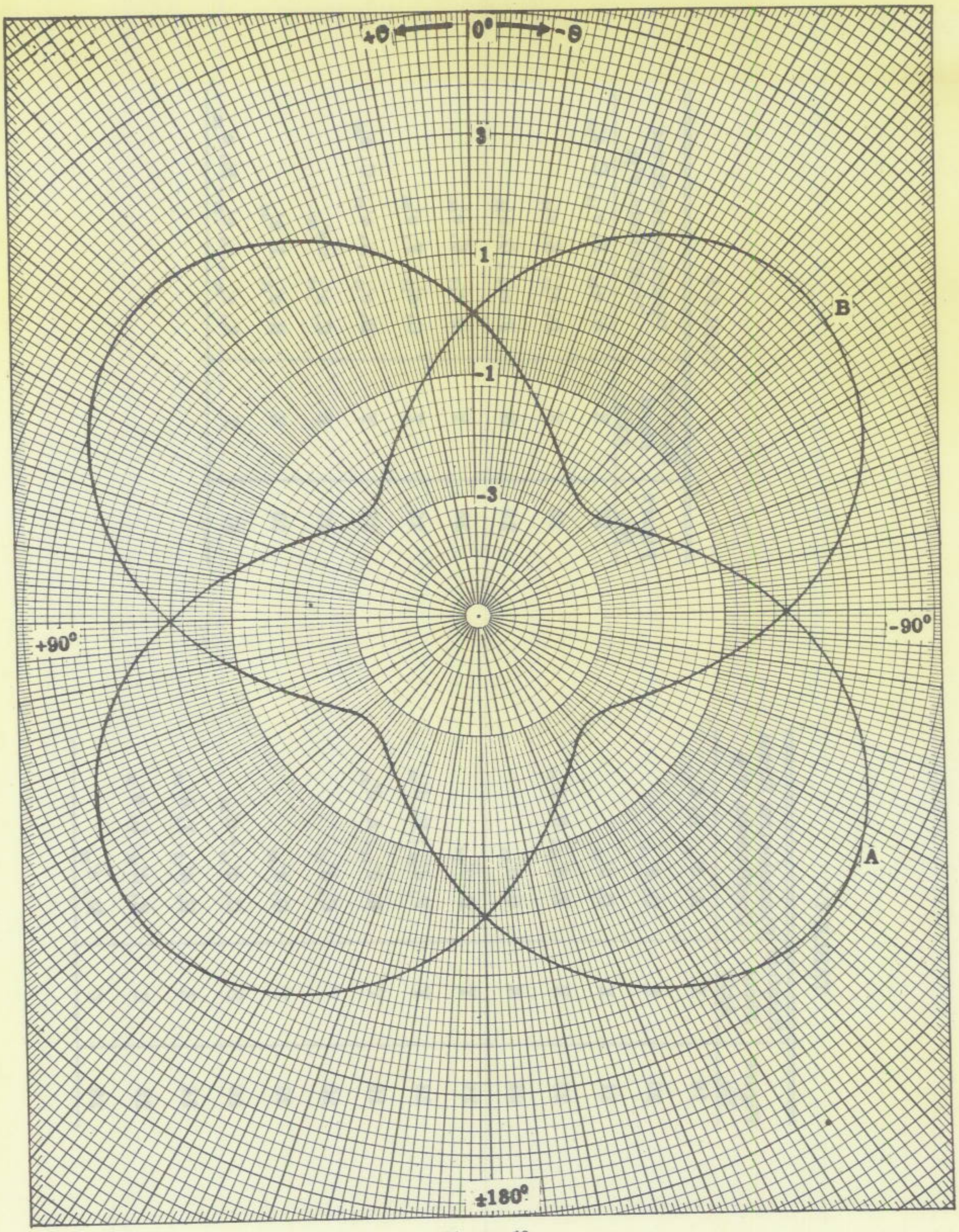

Figure 19

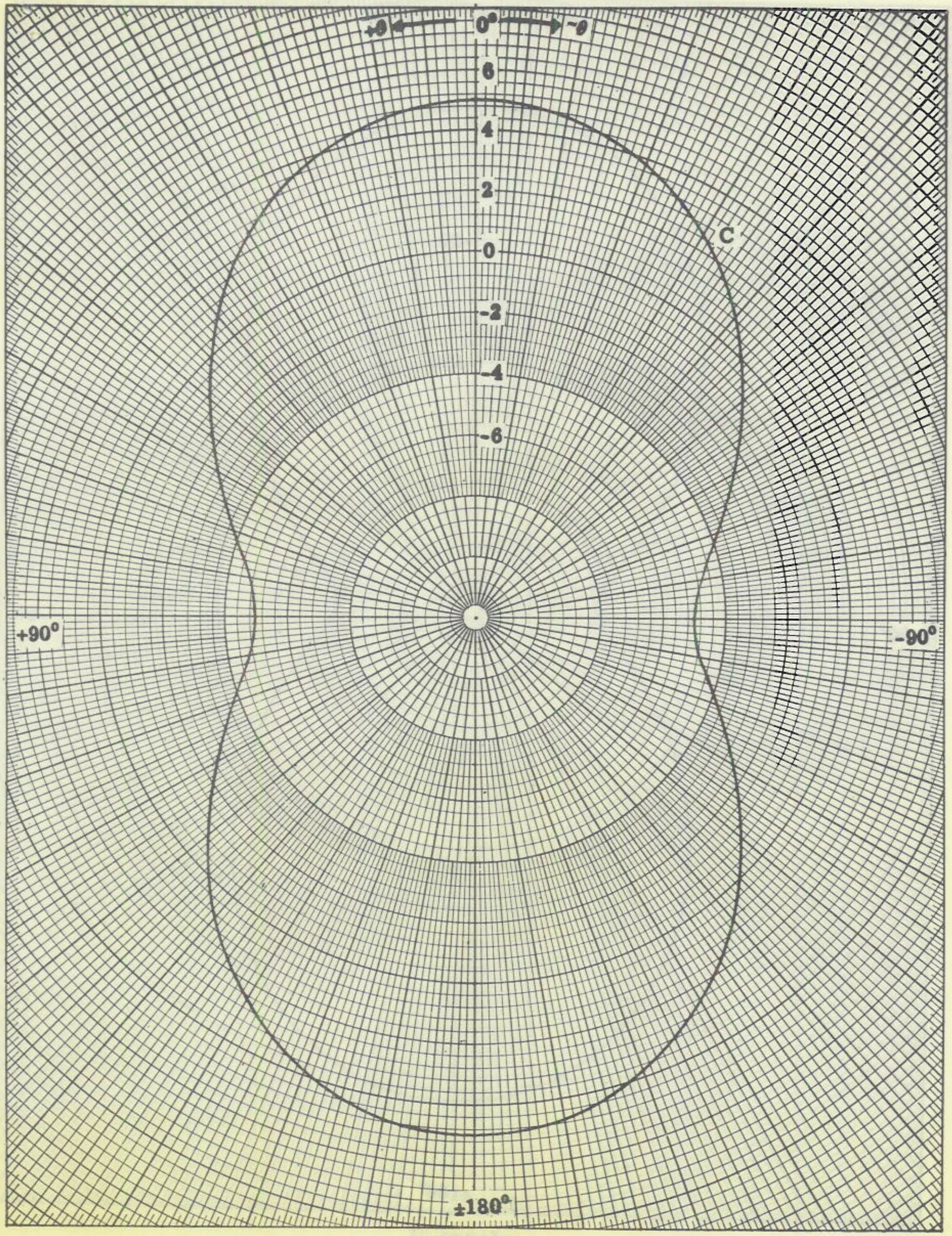

Figure 20

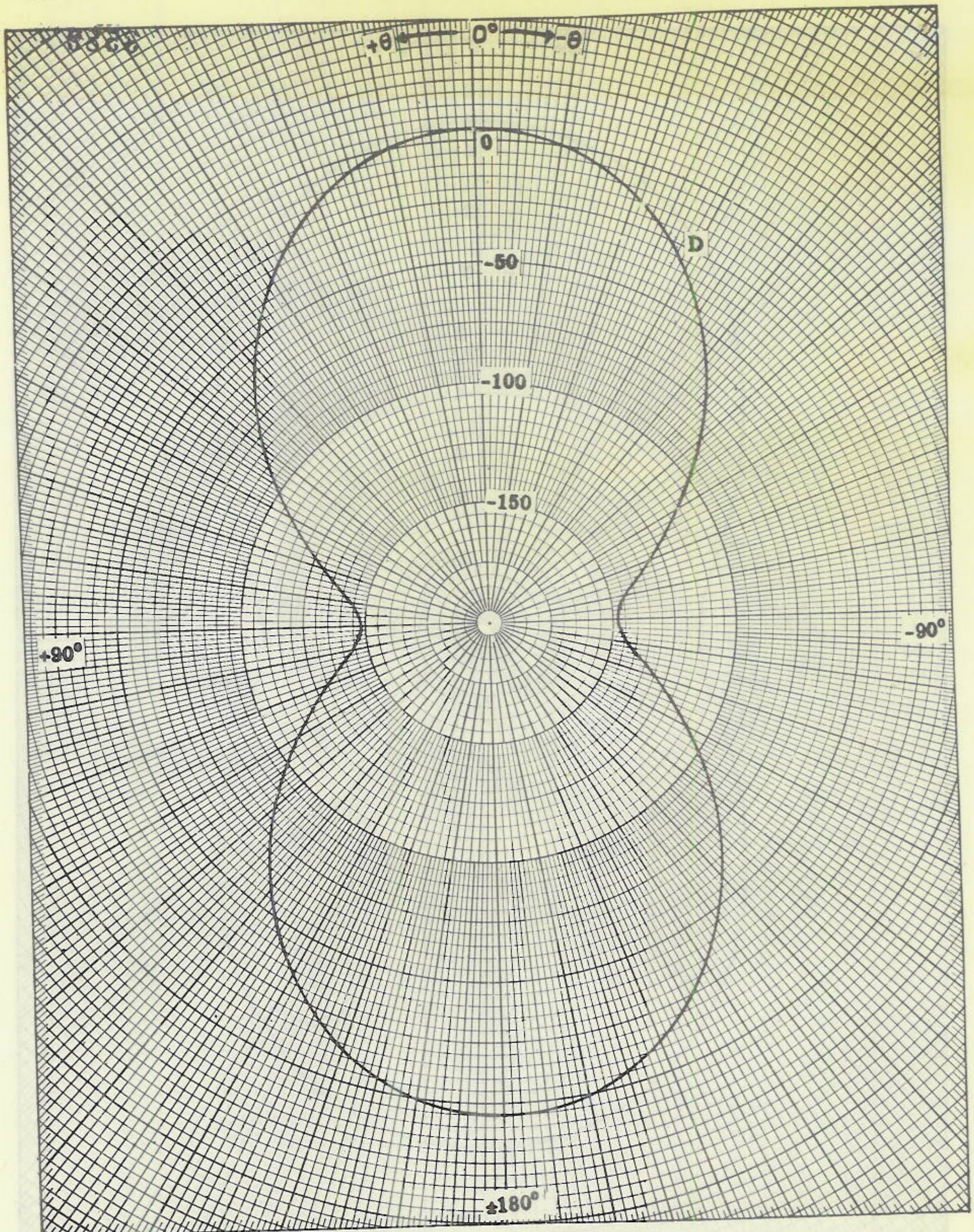

Figure 21

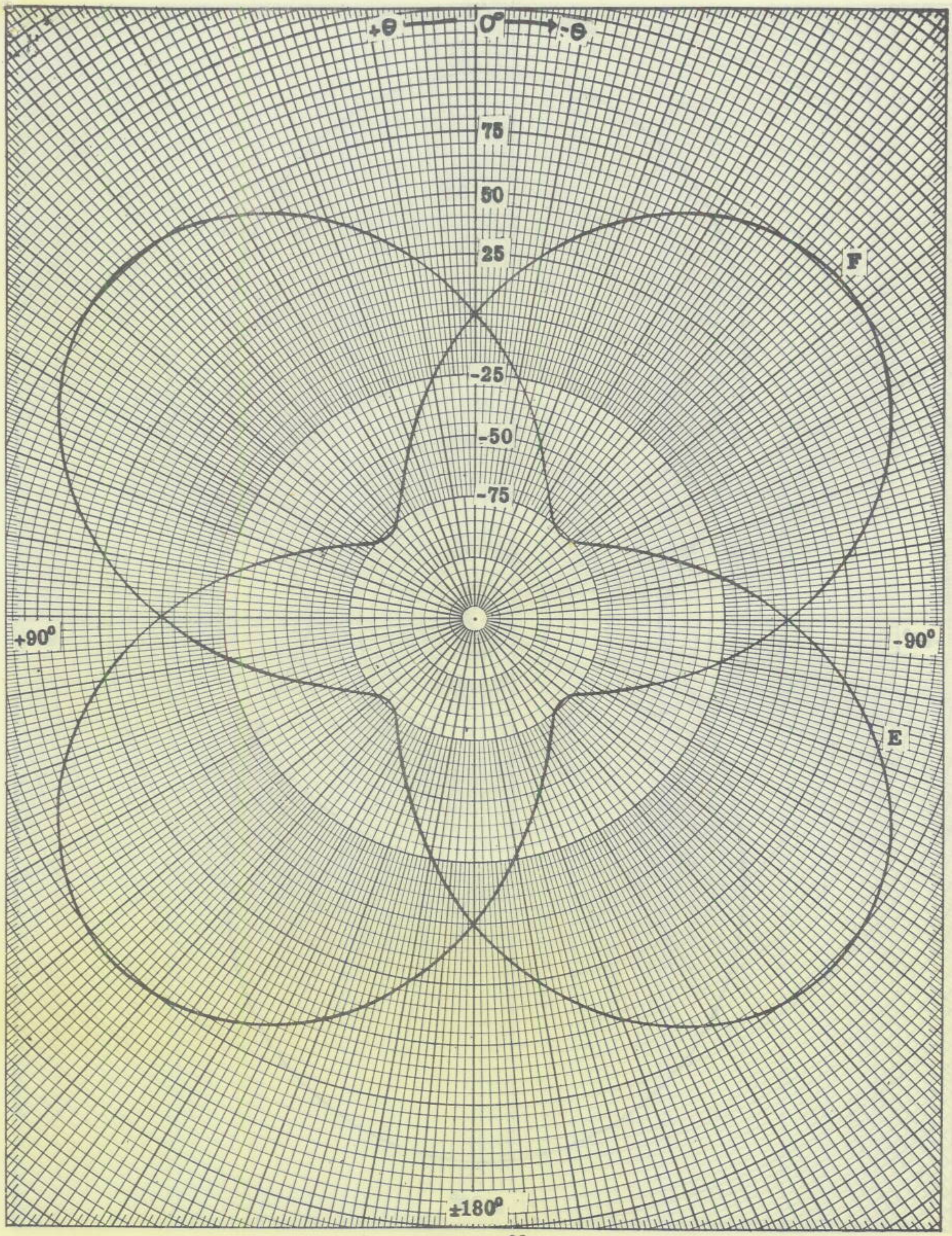

Figure 22

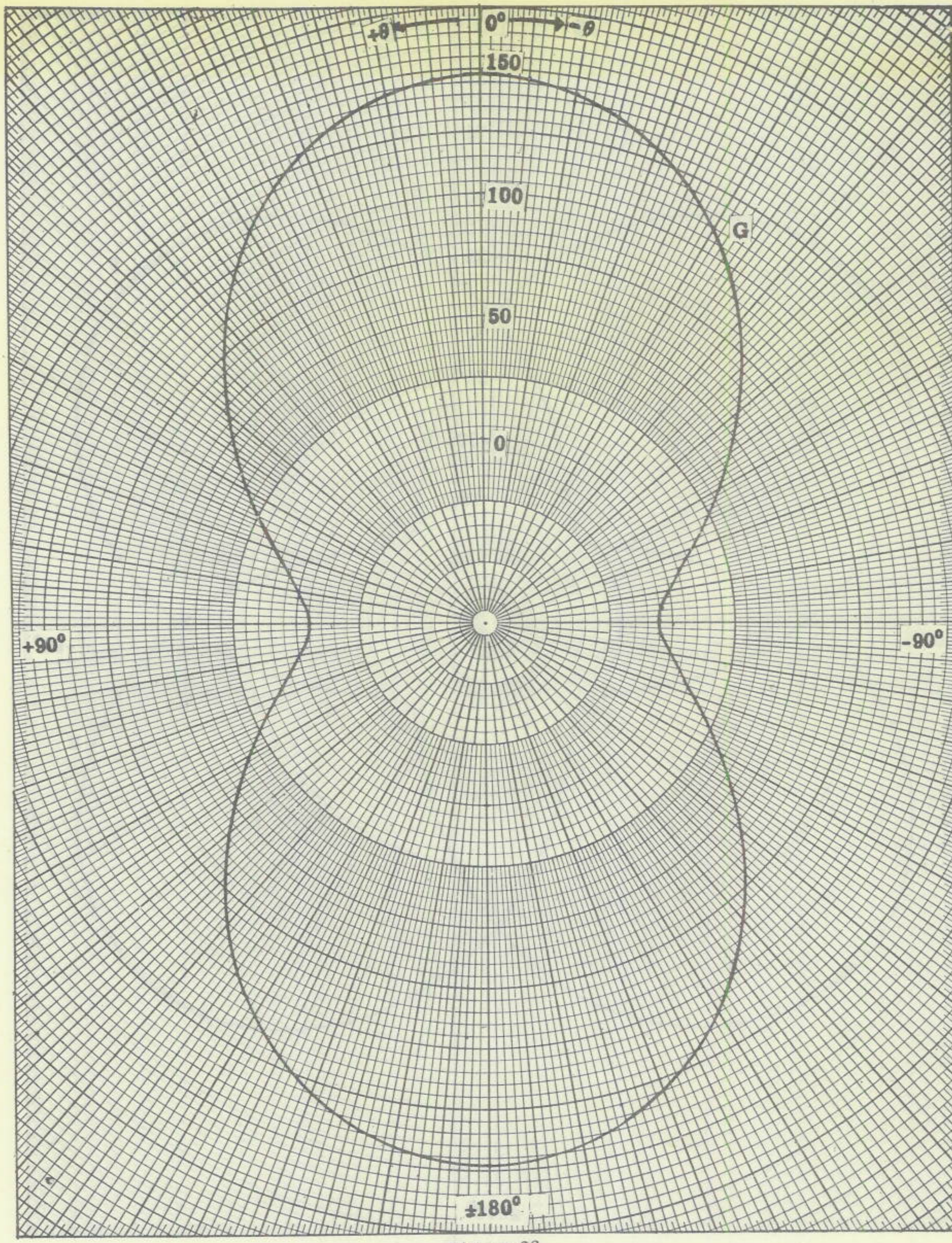

Figure 23

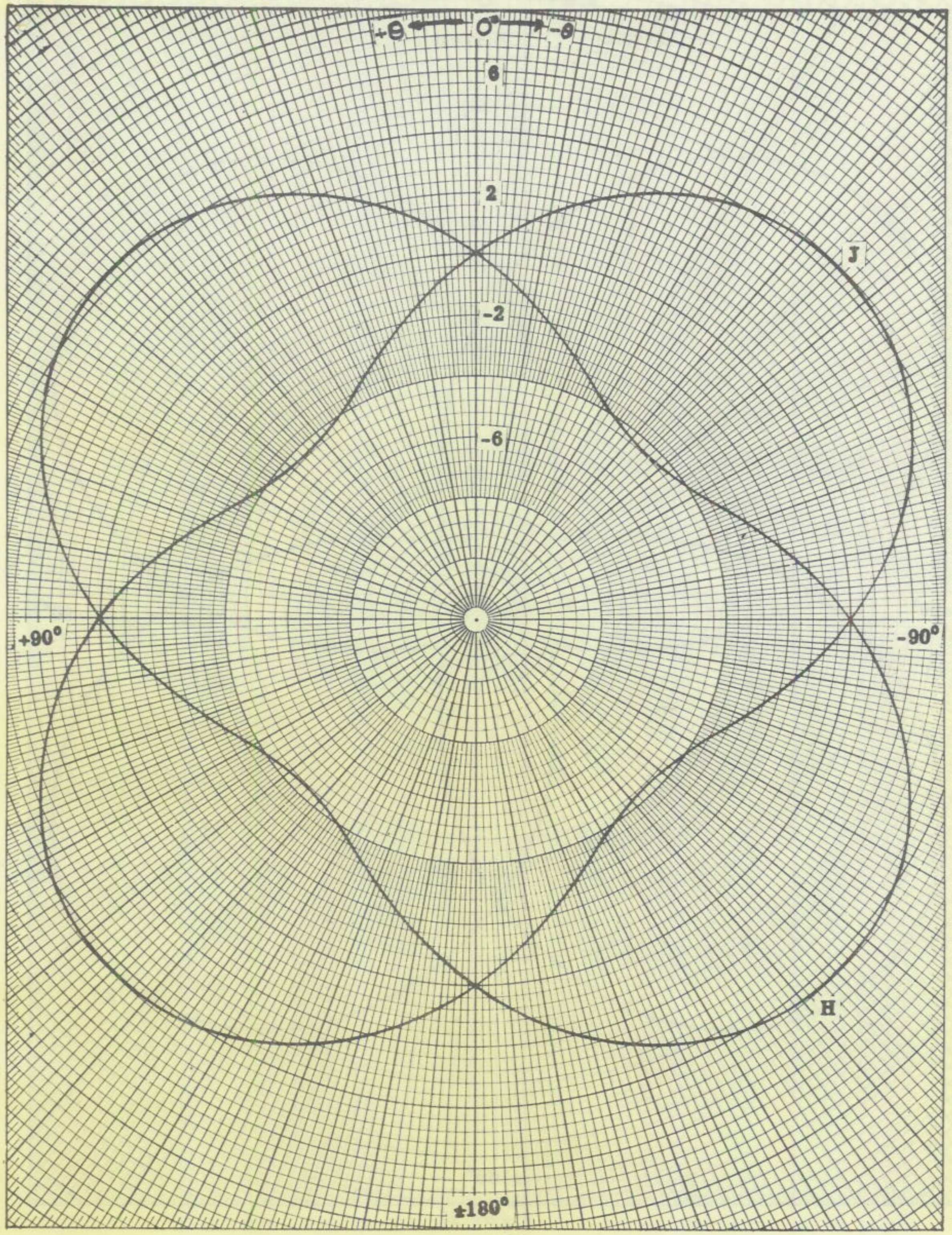

Figure 24

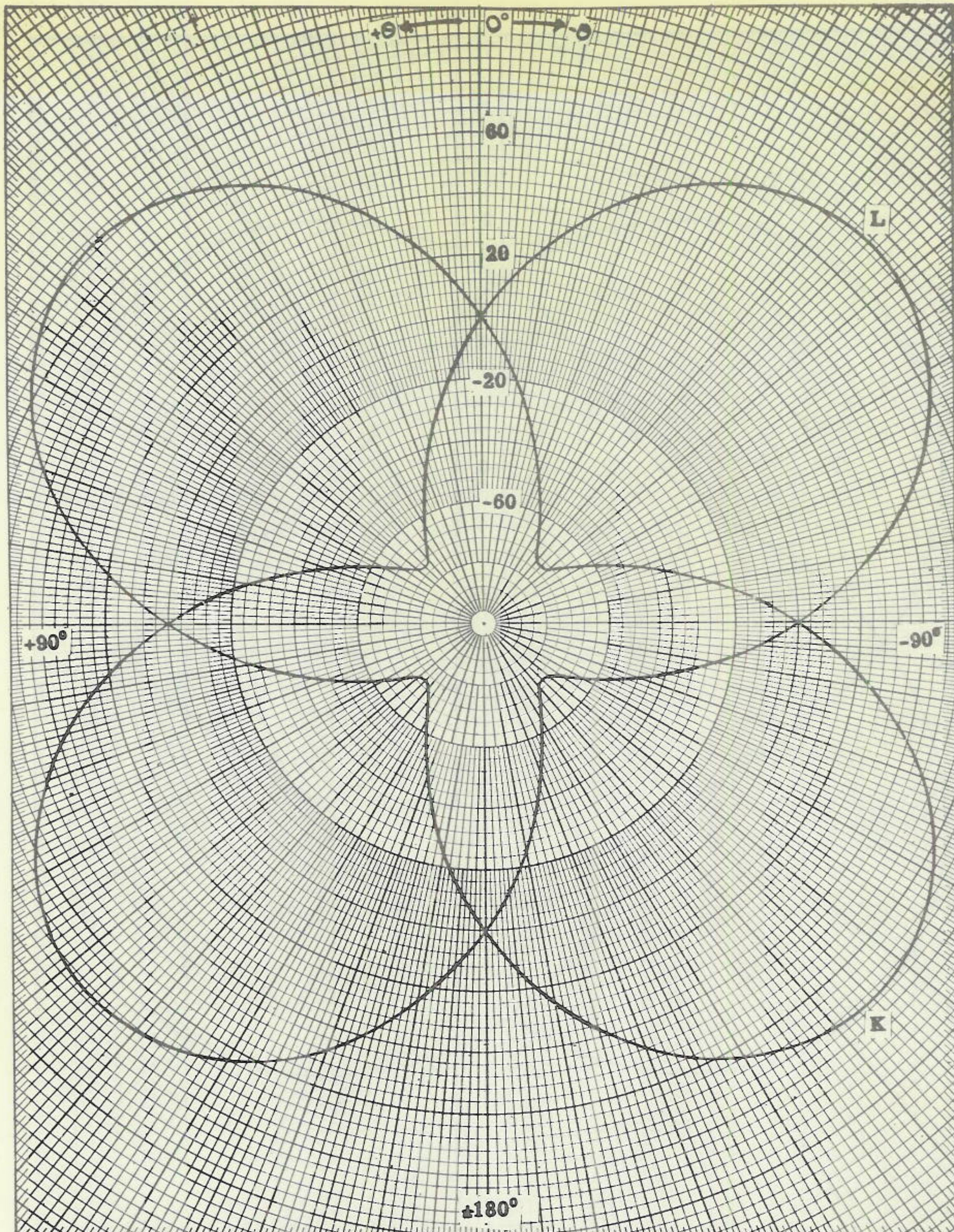

Figure 25

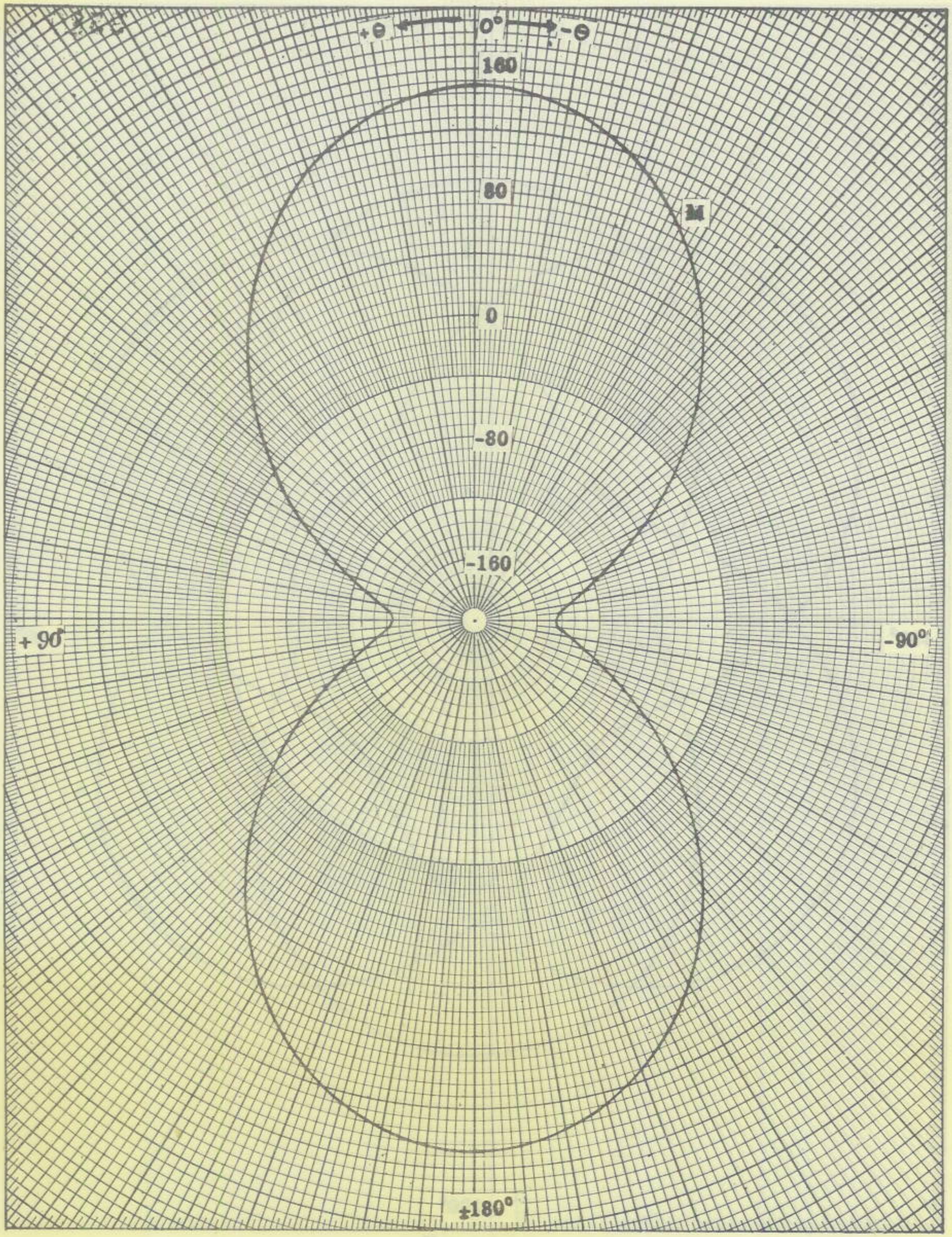

Figure 26

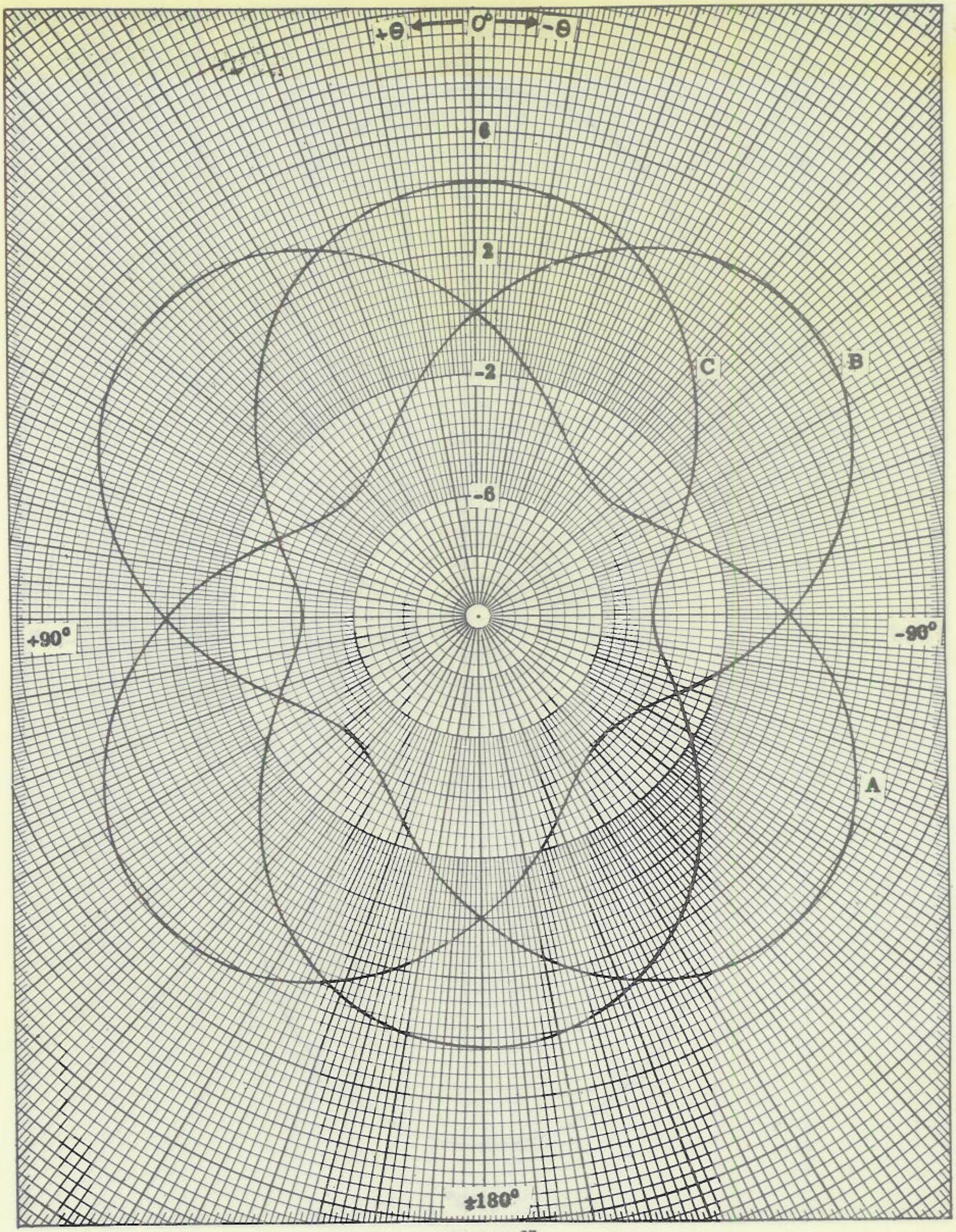

Figure 27

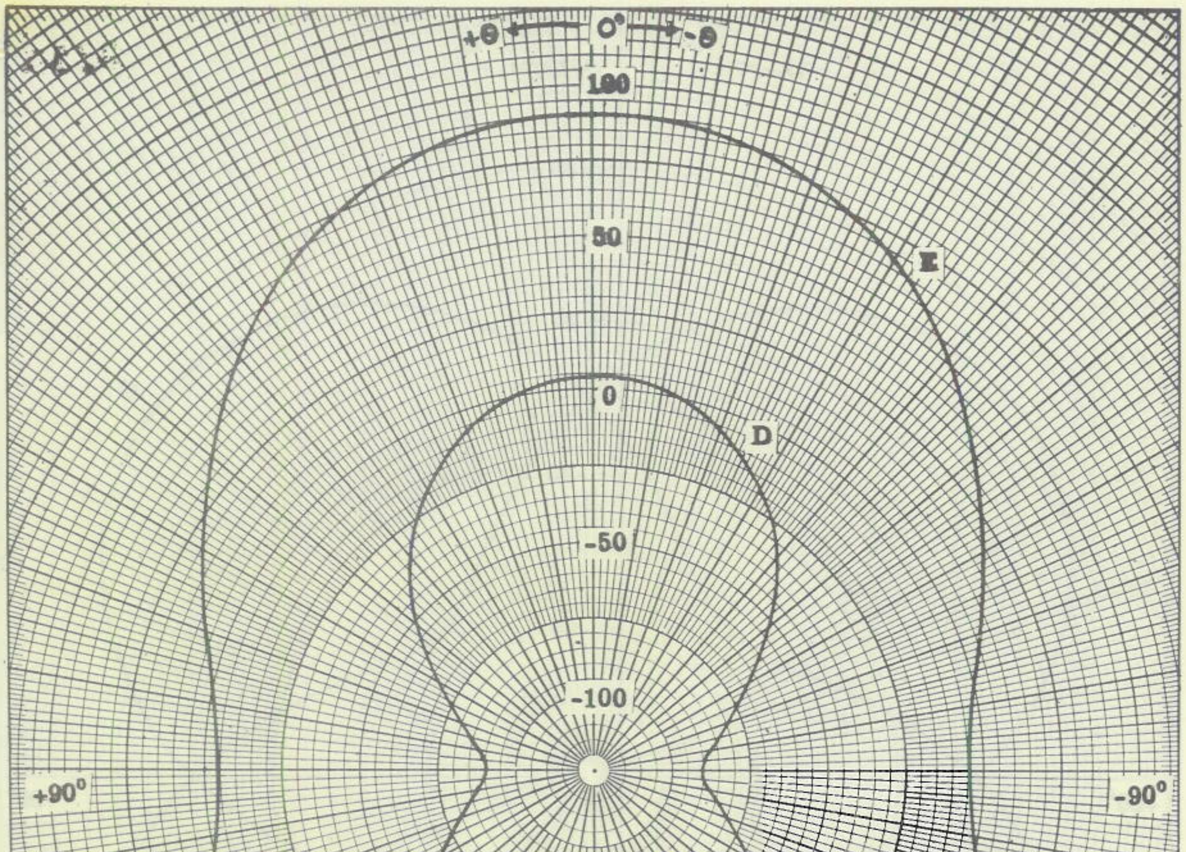

Figure 28

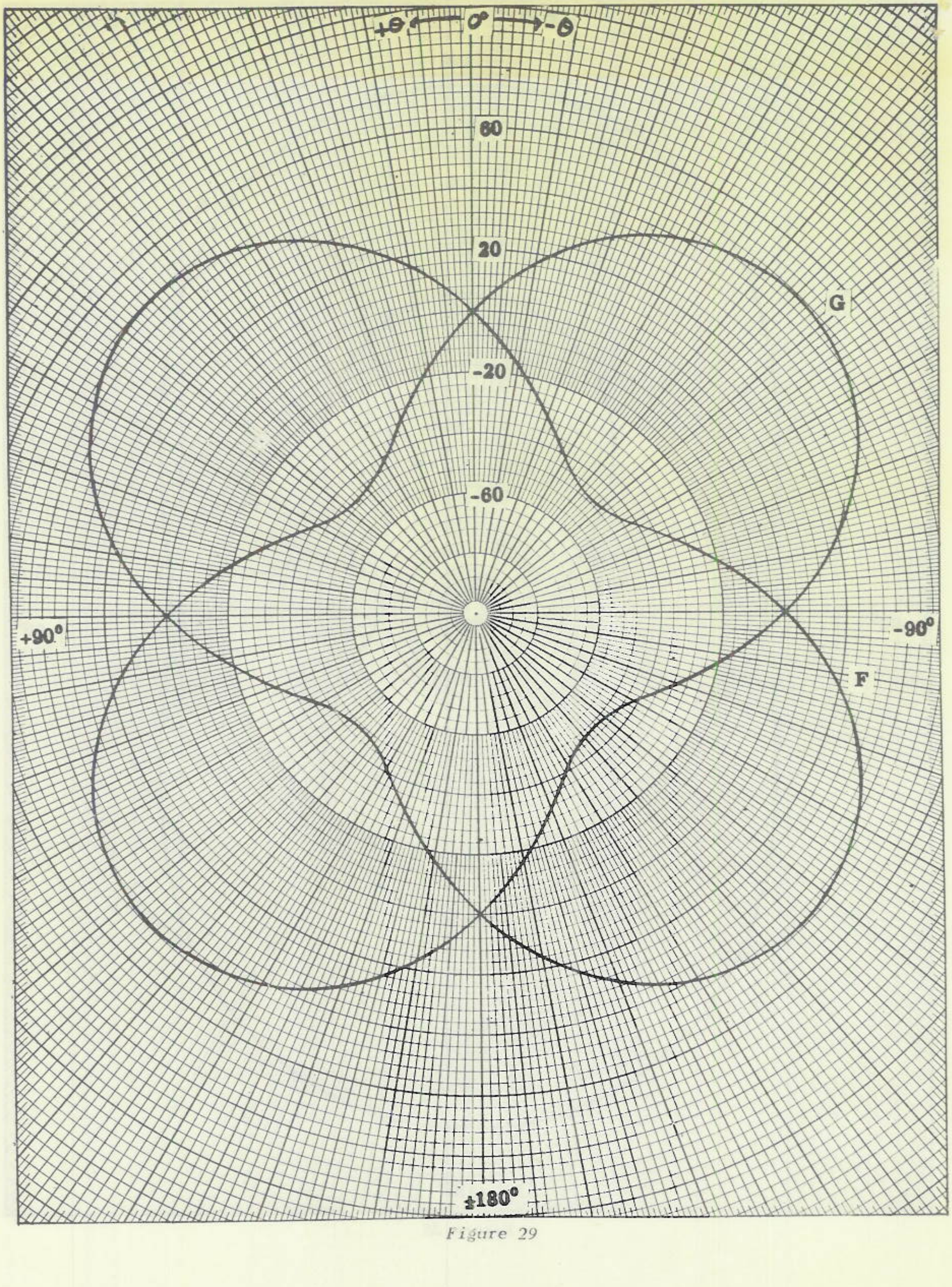

Figure 29

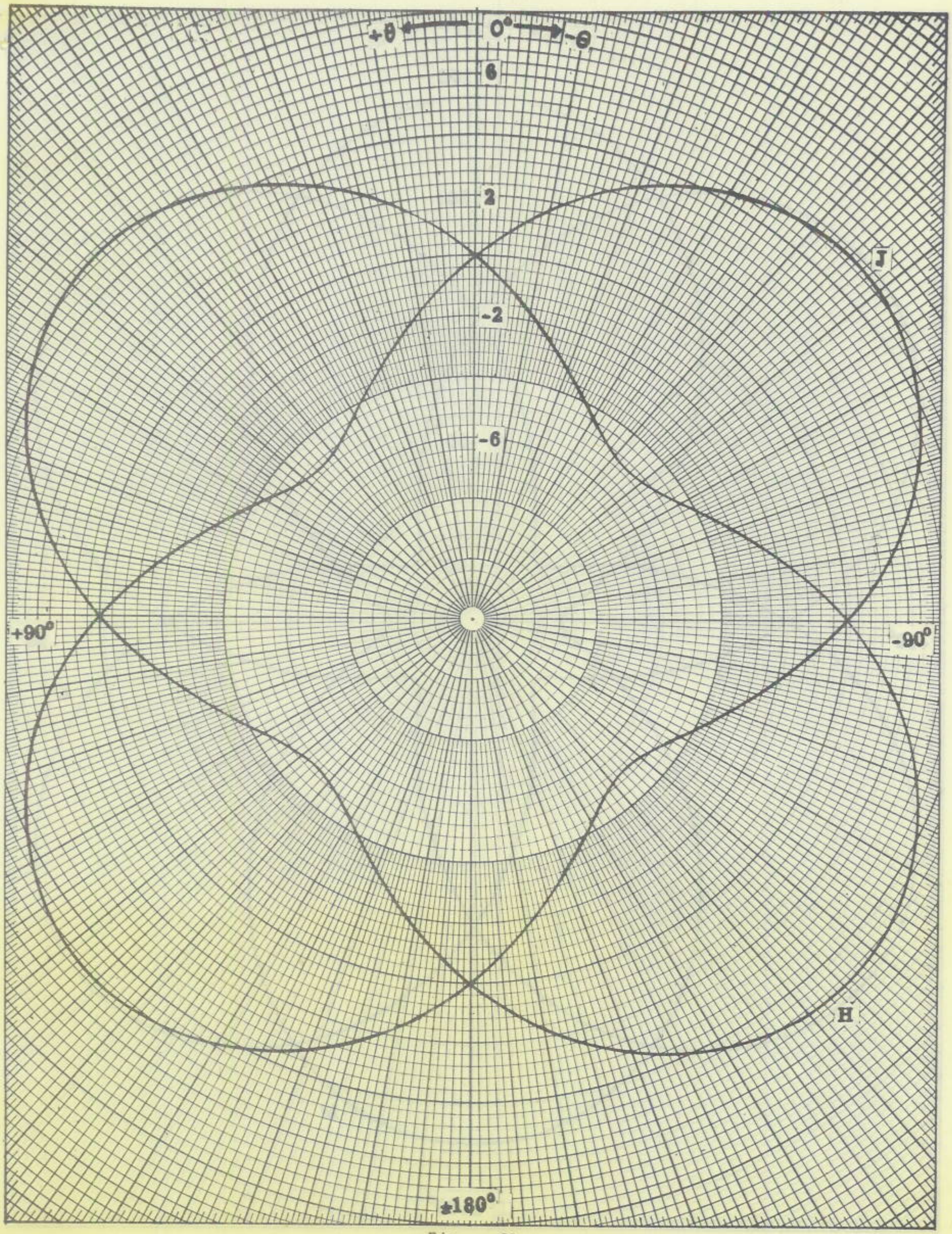

Figure 30

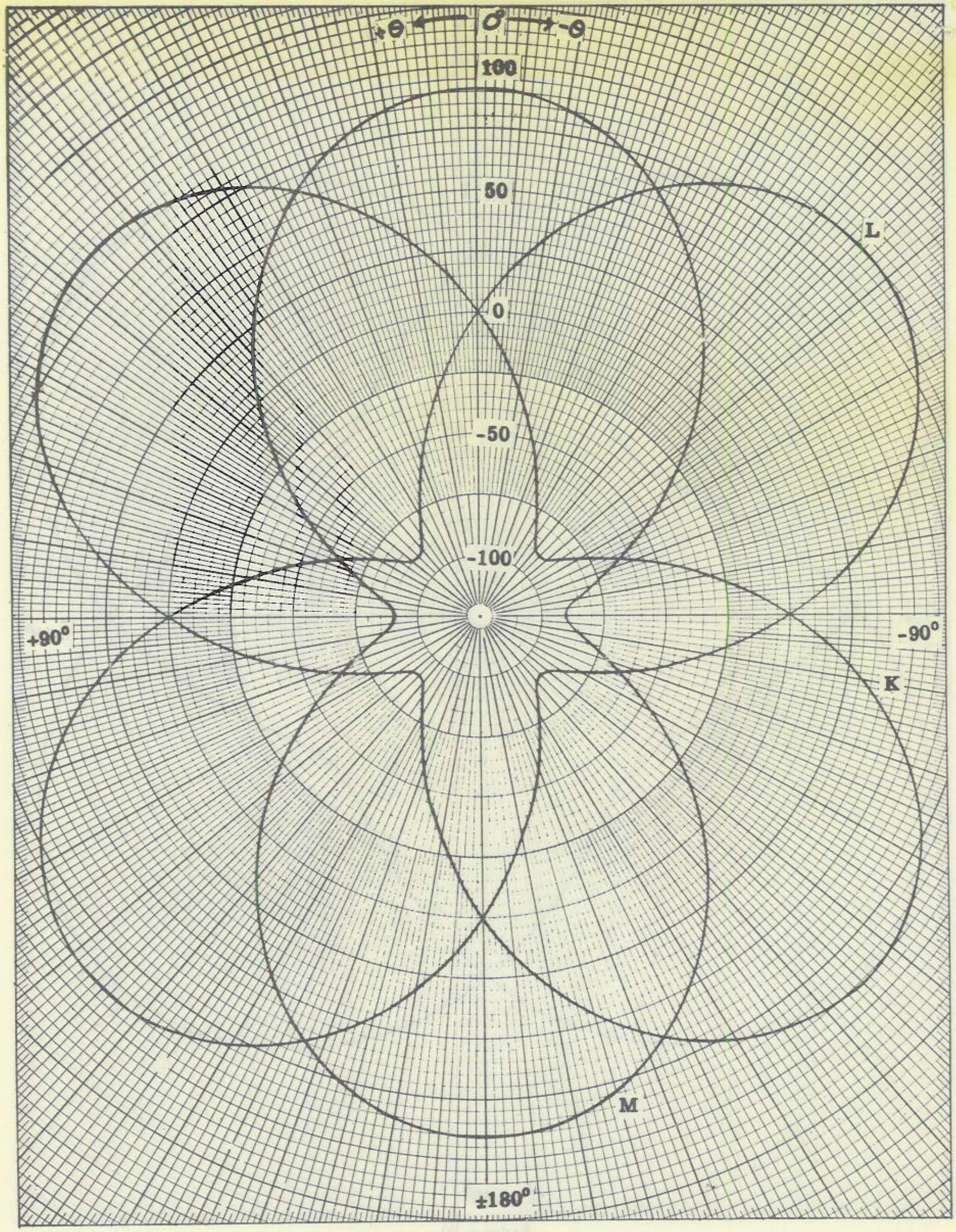

Figure 31

YOUNG'S MODULUS FOR THE LONG BAR

It is of interest to investigate the variation of Young's modulus for a long crystal bar with angular rotation about the various axes. Koga[8] has given an equation which is convenient for calculation. For any orientation having the conventional direction cosines l, m, n, this expression is written as

$$\begin{aligned}1/Y_0' = {} & l^2(l^2 s_{11} + m^2 s_{12} + n^2 s_{13} + mn\, s_{14} + nl\, s_{15} + lm\, s_{16}) \\ & + m^2(l^2 s_{12} + m^2 s_{22} + n^2 s_{23} + mn\, s_{24} + nl\, s_{25} + lm\, s_{26}) \\ & + n^2(l^2 s_{13} + m^2 s_{23} + n^2 s_{33} + mn\, s_{34} + nl\, s_{35} + lm\, s_{36}) \\ & + mn(l^2 s_{14} + m^2 s_{24} + n^2 s_{34} + mn\, s_{44} + nl\, s_{45} + lm\, s_{46}) \\ & + nl(l^2 s_{15} + m^2 s_{25} + n^2 s_{35} + mn\, s_{45} + nl\, s_{55} + lm\, s_{56}) \\ & + lm(l^2 s_{16} + m^2 s_{26} + n^2 s_{36} + mn\, s_{46} + nl\, s_{56} + lm\, s_{66})\end{aligned} \quad (12)$$

where Y_0' is Young's modulus along the length of the crystal.

For a crystal bar rotated about the X axis, $l = 0$, $m = \cos\theta = c$, $n = \sin\theta = s$. So Equation (12) reduces to

$$1/Y_0' = c^4 s_{22} + 2c^3 s\, s_{24} + c^2 s^2(2s_{23} + s_{44}) + 2cs^3 s_{34} + s^4 s_{33} \quad (13)$$

But for ADP, $s_{11} = s_{22}$, $s_{13} = s_{23}$, and $s_{24} = s_{34} = 0$

and (13) becomes $1/Y_0' = c^4 s_{11} + c^2 s^2(2s_{13} + s_{44}) + s^4 s_{33}$

or $Y_0' = 1/s'_{22}$.

In like manner, a rotation about the Y axis yields $Y_0' = 1/s'_{33}$.

For a rotation about the Z axis, $Y_0' = 1/s'_{11}$.

The appropriate values for ADP at 20° C are plotted on Figure 32. Each value is to be multiplied by 10^{11} dyne/cm^2 for cgs units and by 10^{10} newton/m^2 for rationalized mks units. Curve A shows a rotation about the X axis, B about the Y axis, and C about the Z axis.

THE D' PIEZOELECTRIC COEFFICIENT AND THE ELECTROMECHANICAL COUPLING FOR THE Z-CUT BAR

Mason[9] has suggested an alternative method of writing the piezoelastic relations. This proves to be of particular use in the design of electroacoustic transducers. Since the Z-cut ADP crystal has the most extensive application, this type will be treated in Mason's notation.

For the plated Z-cut ADP crystal at an arbitrary orientation, the following relations apply:

$$\begin{aligned} T'_1 &= c'_{11} S'_1 + c'_{12} S'_2 + c'_{13} S'_3 + c'_{16} S'_6 - f'_{31} Q_3 \\ T'_2 &= c'_{12} S'_1 + c'_{11} S'_2 + c'_{13} S'_3 - c'_{16} S'_6 + f'_{31} Q_3 \\ T'_3 &= c'_{13} S'_1 + c'_{13} S'_2 + c'_{33} S'_3 \\ T'_6 &= c'_{16} S'_1 - c'_{16} S'_2 + c'_{66} S'_6 - f'_{36} Q_3 \\ E_3 &= f'_{31} S'_1 - f'_{31} S'_2 + f'_{36} S'_6 - \frac{4\pi}{K_3^C} Q_3 \end{aligned} \quad (14)$$

where f'_{jk} are piezoelectric coefficients related to the "e" constants and to K_j^C, the clamped dielectric constants along the crystallographic axes, by the relation

$$f'_{jk} = \frac{4\pi e'_{jk}}{K_j^C}$$

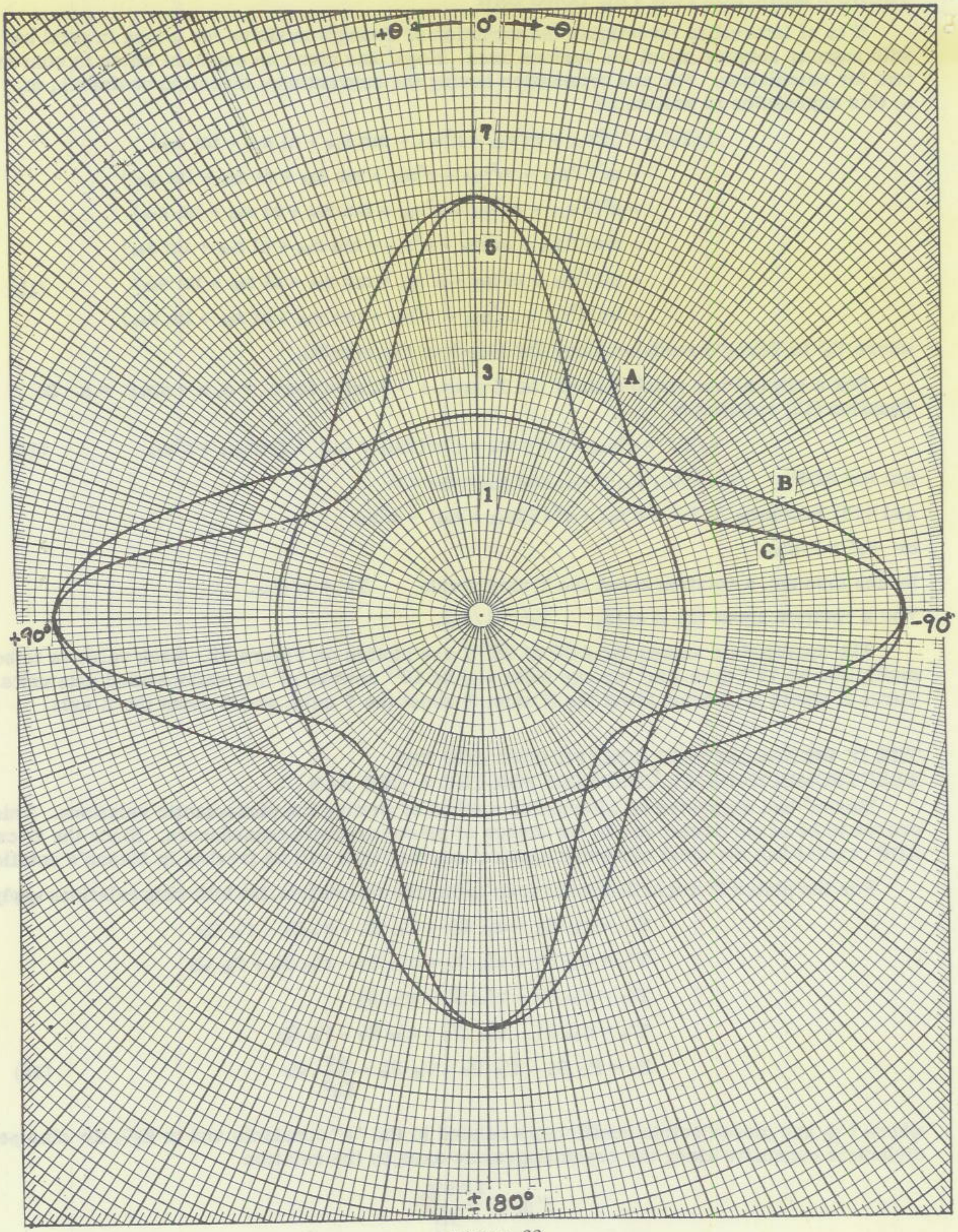

Figure 32

and Q_3 is the charge per unit area on the surface of the crystal, being related to the field and polarization in the Z direction by

$$Q_3 = \frac{E_3}{4\pi} + P_3$$

For the case of the Z-cut long bar, having thickness and width dimensions which are negligible with respect to the length, the boundary conditions that $T'_2 = T'_3 = T'_6 = 0$ apply. After S'_2, S'_3 and S'_6 are eliminated, (14) may be written in cgs units as follows:

$$T'_1 = Y_0' S'_1 - D' Q_3$$

$$E_3 = \frac{4\pi}{K'^{\,LC}_3} Q_3 - D' S'_1 \qquad (15)$$

where Y_0' is the Young's modulus of the long bar in the direction of the rotated X' axis, D' is a piezoelectric coefficient which varies with the type of crystal and orientation and K'^{LC}_3 is the dielectric constant along the Z direction when the crystal is longitudinally clamped, i.e., constrained from moving along the length but not the thickness or width. These variables are expressed as follows:

$$Y_0' = \frac{\begin{vmatrix} c'_{11} & c'_{12} & c'_{13} & c'_{16} \\ c'_{12} & c'_{11} & c'_{13} & -c'_{16} \\ c'_{13} & c'_{13} & c'_{33} & 0 \\ c'_{16} & -c'_{16} & 0 & c'_{66} \end{vmatrix}}{\begin{vmatrix} c'_{11} & c'_{13} & -c'_{16} \\ c'_{13} & c'_{33} & 0 \\ -c'_{16} & 0 & c'_{66} \end{vmatrix}} = \frac{1}{s'_{11}}$$

$$D' = \left[f'_{31} - \frac{c'_{16}}{c'_{66}} f'_{36} \right] \left[\frac{s'_{11} - s'_{12}}{s'_{11}} \right]$$

$$\frac{4\pi}{K'^{\,LC}_3} = \frac{4\pi}{K_3^{\,C}} - \frac{\left(f'_{31} - \frac{c'_{16}}{c'_{66}} f'_{36} \right)^2}{c'_{11} - \frac{c'^{\,2}_{13}}{c'_{33}} - \frac{c'^{\,2}_{16}}{c'_{66}}}$$

Mason[2] gives the value of K_3^C at 20° C as 14.0. Figure 33 shows the plot for the variation of D' as the crystal bar undergoes a complete rotation about the Z axis. D' is expressed in 10^4 statcoulombs/cm^2 in cgs units and $1/3 \times 10^{-1}$ coulombs/m^2 in rationalized mks units.

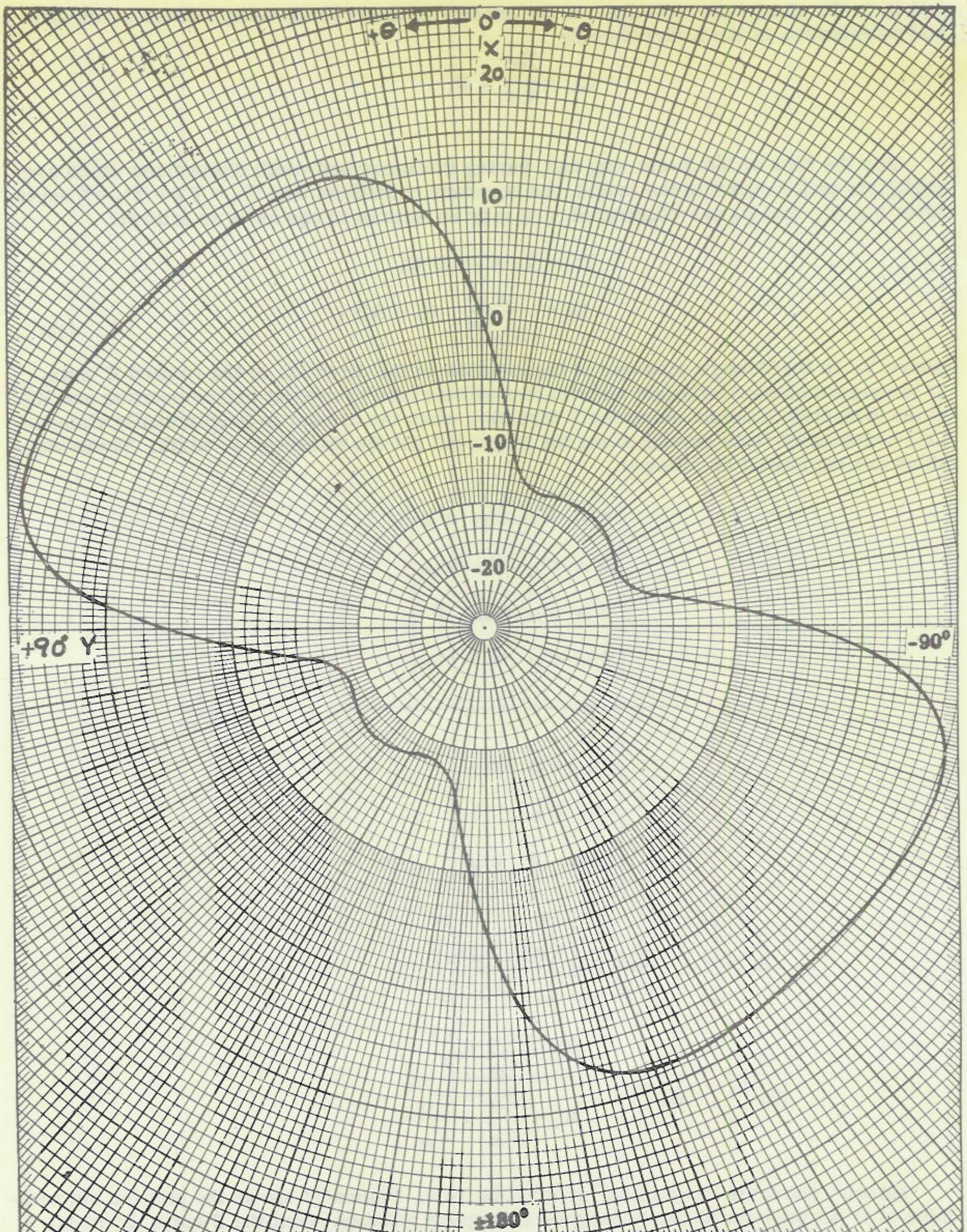

Figure 33 - The D' piezoelectric coefficient of a Z-cut ADP bar rotated about the Z axis

Another quantity of particular interest in design is k, the electromechanical coupling. For the Z-cut crystal bar, it is defined as

$$k^2 = \frac{D'^2 K'_3{}^{LC}}{4\pi Y_0'} \tag{16}$$

In a form convenient for computation, it is expressed as

$$k^2 = \frac{4\pi e_{36}^2 K'_3{}^{LC}}{s'_{11} (K_3{}^C)^2} \left[\left(\sin 2\theta - \frac{c'_{16}}{c'_{66}} \cos 2\theta\right) (s'_{11} - s'_{12}) \right]^2$$

for a rotation of angle θ about the Z axis. Convention dictates the choice of the positive value for k.

This is readily computed from the previous data. Figure 34 is a polar plot for a rotation about the Z axis while Figure 35 is a linear plot for a rotation from 0° to 45° in the X'Y' plane.

Of particular interest is the case where θ is 45°. The values of the quantities appearing in Equation (16) for this case are:

$k = 0.31$

$D' = 12.66 \times 10^4$ statcoulombs/cm^2

$K'_3{}^{LC} = 14.39$

$Y_0' = 1.93 \times 10^{11}$ dyne/cm^2

ACKNOWLEDGMENTS

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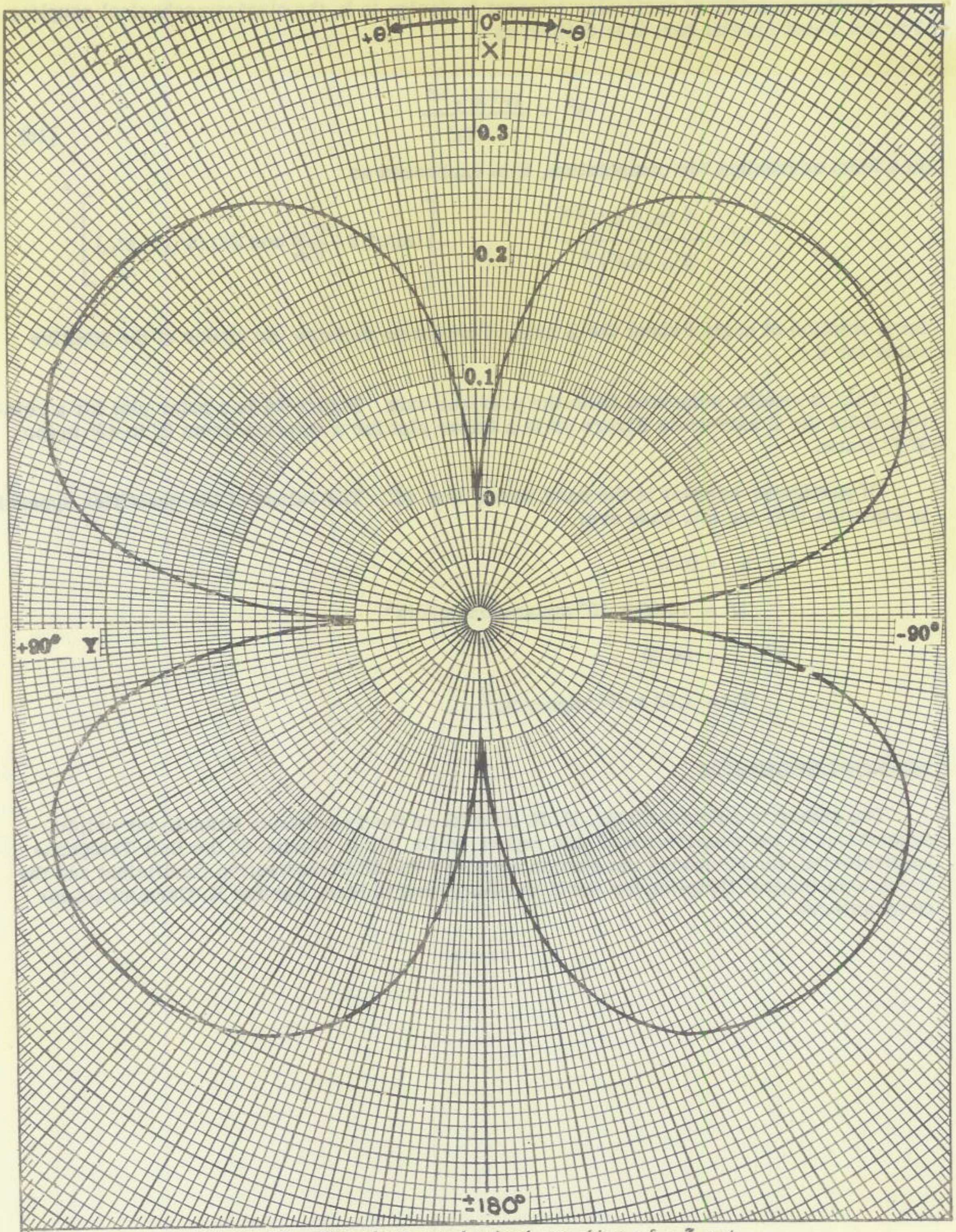

Figure 34 - The electromechanical coupling of a Z-cut ADP bar rotated about the Z axis

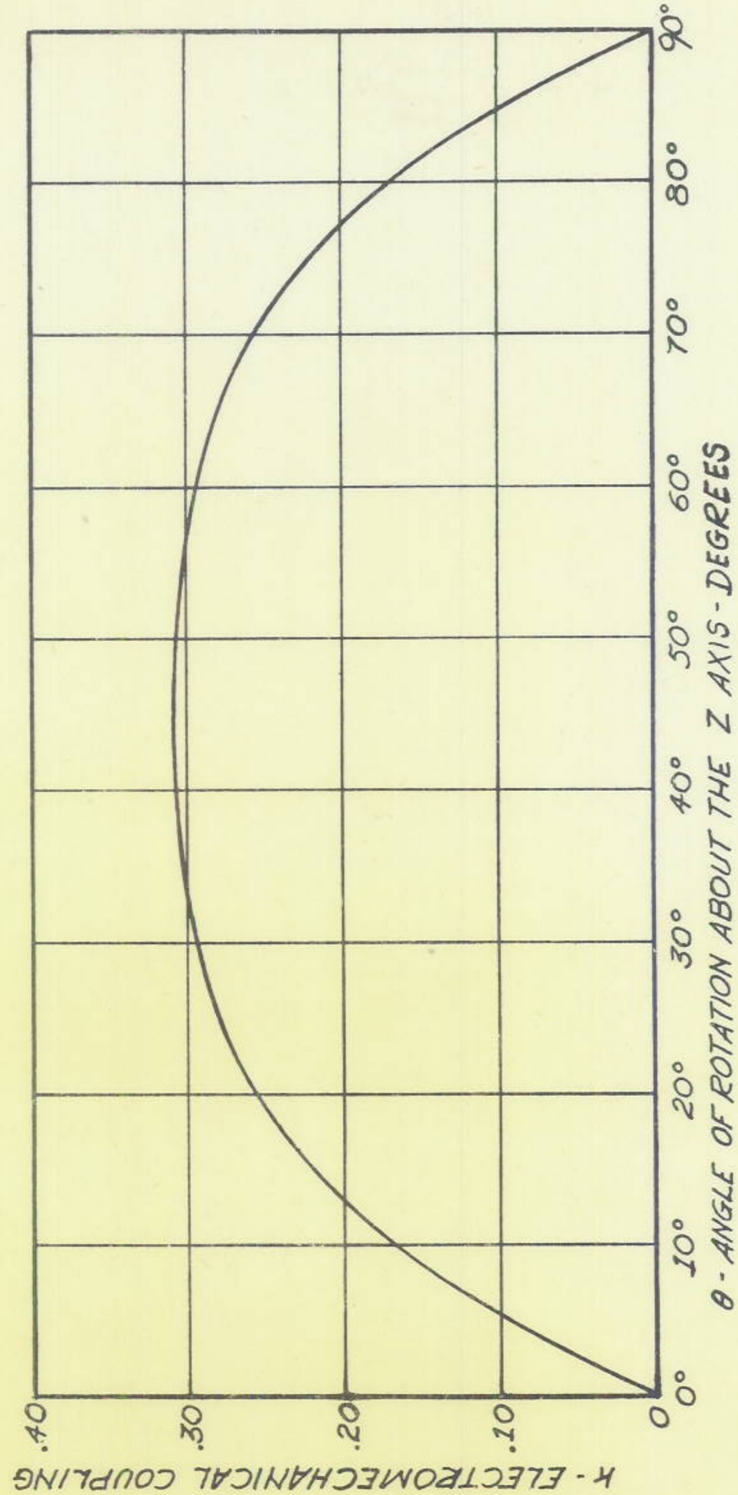

Figure 35 - The electromechanical coupling of a Z-cut ADP bar rotated about the Z axis

APPENDIX I

Elastic Compliance Coefficient Transformations

For a rotation of an arbitrary angle θ about the X axis, if $c = \cos\theta$ and $s = \sin\theta$, the primed expressions for the compliance coefficients of ADP are written:

$$s'_{11} = s_{11}$$

$$s'_{12} = c^2 s_{12} + s^2 s_{13}$$

$$s'_{13} = s^2 s_{12} + c^2 s_{13}$$

$$s'_{14} = 2\,cs\,(s_{13} - s_{12})$$

$$s'_{22} = c^4 s_{22} + c^2 s^2\,(2s_{23} + s_{44}) + s^4 s_{33}$$

$$s'_{23} = c^2 s^2\,(s_{22} + s_{33} - s_{44}) + (c^4 + s^4)\,s_{23}$$

$$s'_{24} = -2c^3 s\, s_{22} + cs\,(c^2 - s^2)\,(2s_{23} + s_{44}) + 2\,cs^3 s_{33}$$

$$s'_{33} = s^4 s_{22} + c^2 s^2\,(2\,s_{23} + s_{44}) + c^4 s_{33}$$

$$s'_{34} = -2\,cs^3 s_{22} - cs\,(c^2 - s^2)\,(2\,s_{23} + s_{44}) + 2\,c^3 s\; s_{33}$$

$$s'_{44} = 4c^2 s^2\,(s_{22} + s_{33} - 2s_{23}) + (c^2 - s^2)^2 s_{44}$$

$$s'_{55} = c^2 s_{55} + s^2 s_{66}$$

$$s'_{56} = cs\,(s_{55} - s_{66})$$

$$s'_{66} = s^2 s_{55} + c^2 s_{66}$$

For a rotation about the Y and Z axes, the appropriate expressions are obtained by a simple permutation of the subscripts on each side of the equations above. 1 is added for the Y rotation and 2 is added for the Z rotation. So 1, 2, 3 become 2, 3, 1 for a Y rotation and 3, 1, 2 for a Z rotation. Similarly for the 4, 5, 6 subscripts.

Thus for a rotation about Y, the compliance coefficients become:

$$s'_{11} = s^4 s_{33} + c^2 s^2\,(2\,s_{13} + s_{55}) + c^4 s_{11}$$

$$s'_{12} = s^2 s_{23} + c^2 s_{12} \quad \text{etc.}$$

and for a rotation about Z

$$s'_{11} = c^4 s_{11} + c^2 s^2\,(2\,s_{12} + s_{66}) + s^4 s_{22}$$

$$s'_{12} = c^2 s^2\,(s_{11} + s_{22} - s_{66}) + (c^4 + s^4)\,s_{12} \qquad \text{etc.}$$

* * *

APPENDIX II
Elastic Stiffness Coefficient Transformations

For a rotation about the X axis, the primed expressions for the stiffness coefficients of ADP are written:

$$c'_{11} = c_{11}$$

$$c'_{12} = c^2 c_{12} + s^2 c_{13}$$

$$c'_{13} = s^2 c_{12} + c^2 c_{13}$$

$$c'_{14} = cs\,(c_{13} - c_{12})$$

$$c'_{22} = c^4 c_{22} + 2c^2 s^2 (c_{23} + 2c_{44}) + s^4 c_{33}$$

$$c'_{23} = c^2 s^2 (c_{22} + c_{33} - 4c_{44}) + (c^4 + s^4)\, c_{23}$$

$$c'_{24} = -c^3 s c_{22} + cs\,(c^2 - s^2)(c_{23} + 2c_{44}) + cs^3 c_{33}$$

$$c'_{33} = s^4 c_{22} + 2c^2 s^2 (c_{23} + 2c_{44}) + c^4 c_{33}$$

$$c'_{34} = -cs^3 c_{22} - cs\,(c^2 - s^2)(c_{23} + 2c_{44}) + c^3 s c_{33}$$

$$c'_{44} = c^2 s^2 (c_{22} + c_{33} - 2c_{23}) + (c^2 - s^2)^2 c_{44}$$

$$c'_{55} = c^2 c_{55} + s^2 c_{66}$$

$$c'_{56} = cs\,(c_{55} - c_{66})$$

$$c'_{66} = s^2 c_{55} + c^2 c_{66}$$

For a rotation about the Y and Z axes, the appropriate expressions are obtained by applying the rule given in Appendix I.

* * *

APPENDIX III
Piezoelectric Strain Coefficient Transformations

For a rotation about the X axis, the primed expressions for the piezoelectric strain coefficients of ADP are written:

$$d'_{12} = cs\, d_{14}$$

$$d'_{13} = -cs\, d_{14}$$

$$d'_{14} = (c^2 - s^2)\, d_{14}$$

$$d'_{25} = c^2 d_{25} - s^2 d_{36}$$

$$d'_{26} = cs(d_{25} + d_{36})$$

$$d'_{35} = -cs(d_{25} + d_{36})$$

$$d'_{36} = c^2 d_{36} - s^2 d_{25}$$

For a rotation about the Y and Z axes, the appropriate expressions are obtained by the rule given above in Appendix I.

Thus, for a rotation about Y, the piezoelectric strain coefficients become:

$$d'_{14} = c^2 d_{14} - s^2 d_{36}$$

$$d'_{16} = -cs(d_{36} + d_{14}) \quad \text{etc.}$$

and for a rotation about Z

$$d'_{14} = c^2 d_{14} - s^2 d_{25}$$

$$d'_{15} = cs(d_{14} + d_{25}) \quad \text{etc.}$$

* * *

APPENDIX IV
Equations for Piezoelectric Stress Coefficients

Assuming all of the piezoelectric stress coefficients to be present for the general case, (11) is written

$$\begin{bmatrix} e'_{11} & e'_{12} & e'_{13} & e'_{14} & e'_{15} & e'_{16} \\ e'_{21} & e'_{22} & e'_{23} & e'_{24} & e'_{25} & e'_{26} \\ e'_{31} & e'_{32} & e'_{33} & e'_{34} & e'_{35} & e'_{36} \end{bmatrix} = \begin{bmatrix} d'_{11} & d'_{12} & d'_{13} & d'_{14} & d'_{15} & d'_{16} \\ d'_{21} & d'_{22} & d'_{23} & d'_{24} & d'_{25} & d'_{26} \\ d'_{31} & d'_{32} & d'_{33} & d'_{34} & d'_{35} & d'_{36} \end{bmatrix} \begin{bmatrix} c'_{11} & c'_{12} & c'_{13} & c'_{14} & c'_{15} & c'_{16} \\ c'_{12} & c'_{22} & c'_{23} & c'_{24} & c'_{25} & c'_{26} \\ c'_{13} & c'_{23} & c'_{33} & c'_{34} & c'_{35} & c'_{36} \\ c'_{14} & c'_{24} & c'_{34} & c'_{44} & c'_{45} & c'_{46} \\ c'_{15} & c'_{25} & c'_{35} & c'_{45} & c'_{55} & c'_{56} \\ c'_{16} & c'_{26} & c'_{36} & c'_{46} & c'_{56} & c'_{66} \end{bmatrix}$$

Each primed piezoelectric stress coefficient can be readily obtained by matrix multiplication. For an X axis rotation, e'_{12} beomes

$$e'_{12} = d'_{11}c'_{12} + d'_{12}c'_{22} + d'_{13}c'_{23} + d'_{14}c'_{24} + d'_{15}c'_{25} + d'_{16}c'_{26} \qquad (16)$$

Since d'_{11}, d'_{15}, d'_{16}, c'_{25} and c'_{26} vanish for this rotation,

$$e'_{12} = d'_{12}c'_{22} + d'_{13}c'_{23} + d'_{14}c'_{24} \qquad (17)$$

Furthermore, d'_{21}, d'_{22}, d'_{23}, d'_{24}, d'_{31}, d'_{32}, d'_{33}, d'_{34}, c'_{15}, c'_{16}, c'_{35}, c'_{36}, c'_{45}, and c'_{46} also vanish. So the complete primed expressions become

$$e'_{12} = d'_{12}c'_{22} + d'_{13}c'_{23} + d'_{14}c'_{24}$$

$$e'_{13} = d'_{12}c'_{23} + d'_{13}c'_{33} + d'_{14}c'_{34}$$

$$e'_{14} = d'_{12}c'_{24} + d'_{13}c'_{34} + d'_{14}c'_{44}$$

$$e'_{25} = d'_{25}c'_{55} + d'_{26}c'_{56}$$

$$e'_{26} = d'_{25}c'_{56} + d'_{26}c'_{66}$$

$$e'_{35} = d'_{35}c'_{55} + d'_{36}c'_{56}$$

$$e'_{36} = d'_{35}c'_{56} + d'_{36}c'_{66}$$

It is of interest to note that e'_{11} vanishes for a rotation about the X axis. In expanded form

$$e'_{11} = d'_{12}c'_{12} + d'_{13}c'_{13} + d'_{14}c'_{14}$$

Appendices II and III give the transformed expressions for the primed piezoelectric strain coefficients and the stiffnesses. Then

$$e'_{11} = (cs\ d_{14})(c^2 c_{12} + s^2 c_{13}) - (cs\ d_{14})(s^2 c_{12} + c^2 c_{13})$$

$$+ (c^2 - s^2)\, d_{14} \quad \left[cs(c_{13} - c_{12})\right] = 0$$

To compute e'_{12} for an angle of rotation of 10^0 about the X axis, for example, the values of c'_{22}, c'_{23}, c'_{24}, d'_{12}, d'_{13}, and d'_{14} for a 10^0 rotation about X are taken from Figures 11, 13, 14, 19 and 20 respectively. The required multiplication and summation are then carried out.

For rotations about the Y axis or about Z, the appropriate expressions are obtained by the rule given in Appendix I. Hence for a rotation about Y, e'_{12} is obtained from Equation (17), as follows:

$$e'_{23} = d'_{22}\, c'_{23} + d'_{23} c'_{33} + d'_{21} c'_{13} + d'_{25} c'_{35} + d'_{26} c'_{36} + d'_{24} c'_{34}$$

Since d'_{22}, d'_{24}, d'_{26}, c'_{34}, and c'_{36} vanish for such a rotation,

$$e'_{23} = d'_{23} c'_{33} + d'_{21} c'_{13} + d'_{25} c'_{35}$$

Likewise d'_{11}, d'_{12}, d'_{13}, d'_{15}, d'_{31}, d'_{32}, d'_{33}, d'_{35}, c'_{14}, c'_{16}, c'_{24}, c'_{26}, c'_{45}, and c'_{56} also vanish. So

$$e'_{14} = d'_{16} c'_{46} + d'_{14} c'_{44}$$

$$e'_{21} = d'_{23} c'_{13} + d'_{21} c'_{11} + d'_{25}\, c'_{15} \qquad \text{etc.}$$

A rotation about the Z axis may be treated similarly. In this case d'_{11}, d'_{12}, d'_{16}, d'_{21}, d'_{22}, d'_{23}, d'_{26}, d'_{33}, d'_{34}, d'_{35}, c'_{14}, c'_{15}, c'_{24}, c'_{25}, c'_{34}, c'_{35}, c'_{36}, c'_{45}, c'_{46}, and c'_{56}, all vanish. Then

$$e'_{14} = d'_{14} c'_{44}$$

$$e'_{31} = d'_{31} c'_{11} + d'_{32} c'_{12} + d'_{36} c'_{16} \qquad \text{etc.}$$

* * *

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