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MAGNETICALLY SENSITIVE ELECTRICAL RESISTOR MATERIAL

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ABSTRACT

The isothermal galvanomagnetic tensor components associated with the Hall effect and the magneto resistance effect are analyzed for arbitrary orientation of the crystal axes in the sample, arbitrary orientation of the magnetic field $\underline{B}$, and arbitrary crystal symmetry. The conductivity components in suitable coordinates are expanded in powers of the components of $\underline{B}$. The coefficients are the galvanomagnetic material constants, called "brackets"; they are defined in Equation 10. By means of Onsager's relations it is shown that the magneto resistance effect is always even in $\underline{B}$, whereas the Hall effect is odd in $\underline{B}$ only with special geometry (Section 2). Further, the Hall effect is even or zero for some geometric and crystallographic conditions. The effects of the crystal symmetry on the brackets are covered by the theorem of Section 3. The resultant dependencies between the brackets are tabulated completely for all powers of $\underline{B}$ for the crystal classes other than the trigonal and hexagonal ones. For the latter the bracket relations are given up to the sixth power of B. Formulas for the number of independent brackets up to any power of B are given for all crystal symmetries in Section 4. Explicit forms of the galvanomagnetic tensor components in terms of the brackets for all arbitrary conditions, up to B^2, are tabulated in Section 5. The significance of the results obtained is pointed out in Section 6.

OBJECTIVE

This project aims at developing the understanding of the magneto resistance effect (change of electrical resistivity in a magnetic field) by theoretical and experimental research, with the ultimate aim of developing materials with more favorable magneto resistance properties than are available at present.

A. INTRODUCTION

Owing to administrative circumstances, the present report follows the previous one at an interval of approximately ten months. The work done during this period requires a relatively large amount of reporting. In order to distribute the burden of writing over a reasonable amount of time, it was found to be expedient to report presently on the progress made in this period with the theoretical work. The next report will consist of a similar comprehensive report on the experimental progress without a theoretical part.

Regarding the theoretical work reported here, the following remarks are appropriate.

1. Many of the problems which remained to be brought to conclusion in the phenomenological theory as sketched in previous reports have since been finished and are reported here.

2. Several additional viewpoints, simplifications, and shorter proofs have been found and are presented.

3. In order to make the report a self-consistent unit, a number of items which have been previously reported are included again. This is true of the main theorem. The bracket relations, which were formerly given up to $n \leq 4$, are now available for $n \leq 6$ and for many crystals for any value of n.

4. The authors expect to publish the same material in practically the same form very soon.

5. The theoretical developments presented here are, we feel, a good step forward of whatever theoretical material is available in this area of research at present and will be of considerable assistance in the experimental work of our own group and others.

6. Plans for theoretical work in the immediate future are primarily directed towards further development of the electron theoretical part of the theory (see the diagram, Figure 1, of the previous report).

B. THEORETICAL PART

1. INTRODUCTION

Consider a volume element of an anisotropic isothermal* homogeneous single crystal of arbitrary shape, placed in a homogeneous magnetic field $\underline{B}$. In the crystal is maintained a constant current density $\underline{J}$ by means of a suitable electric field $\underline{F}$ (see Figure 1).

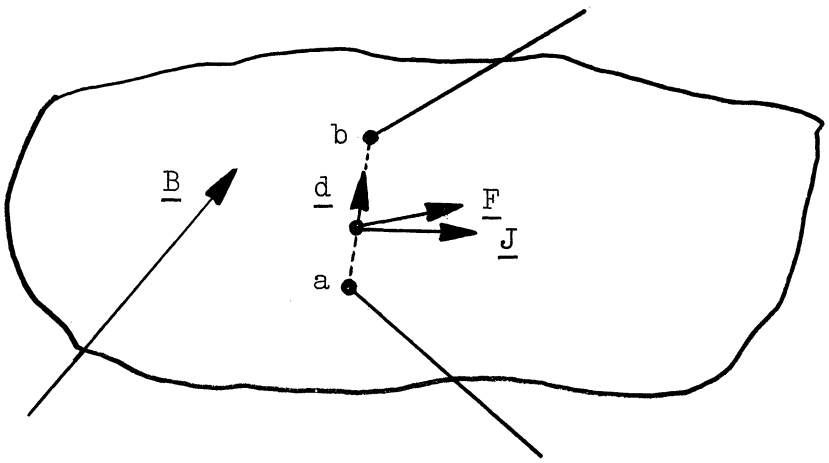

Figure 1. Orientation of vectors $\underline{J}$, $\underline{F}$, $\underline{B}$ and probes ab in an anisotropic single crystal.

Evidently $\underline{F}$ will be a vector function of $\underline{J}$ and $\underline{B}$,

$$\underline{F} = \underline{F}\,(\underline{J},\underline{B})^{**} \quad . \tag{1}$$

The dependence of $\underline{F}$ on $\underline{B}$ represents the galvanomagnetic effect. The crystal symmetry and other physical laws will, in general, restrict the possible forms of (1). It is the purpose of the present paper to find the proper description of $\underline{F}$ for all possible crystal symmetries, all orientations and magnitudes of $\underline{J}$ and $\underline{B}$ with respect to the symmetry axes of the crystal, under the restriction that Ohm's law is valid for fixed $\underline{B}$.

*Isothermal conditions are assumed throughout this paper without further explicit statement.

**Throughout this paper we restrict ourselves to nonferromagnetic substances.

The vector F can be determined experimentally for any given J and B by measuring the components $F_{1,2,3}$ of F in three independent directions. In a direction d one can measure F_d by measuring the potential difference V_{ab} between two probes a and b, without drawing current, and dividing by the distance ab. If d is taken along J, the resulting dependence of $F_{\parallel}$ (J,B) is called the magneto resistance effect; if d is normal to J, then $F_{\perp}$ (J,B) is called a Hall effect. Both are special cases of the galvanomagnetic effect. Other special cases, such as the Corbino effect, imply a geometry and boundary conditions which are again different.

Historically, Lord Kelvin[1] first discovered the magneto resistance effect for Fe in 1856 and also predicted the Hall effect in 1851. After many tries by various workers Hall[1] discovered it in 1879. The first empirical formula connecting the two effects was proposed by Beattie in 1896.[1] The name "galvanomagnetic effect" appeared in the literature, meaning the Hall, the magneto resistance effect, as well as some other effects such as the Corbino effect.

The dependence of the Hall effect on the magnetic field and on the temperature was studied by many investigators. In 1883 Righi[1] studied the influence of the crystal orientation of the Hall effect. Extensive summaries were given by Campbell[1] in 1923 and by Meissner[2] in 1935. Briefly, the findings[3] of all this work are that the Hall effect depends on the crystal orientation, and that it is not adequately described by a constant Hall coefficient. The Hall effect is not always an odd function of the magnetic field, contrary to a suggestion by Casimir[4] in 1945.

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1. L. L. Campbell, Galvanomagnetic and Thermomagnetic Effects, Longmans, Green and Co., Inc., 1923.

2. W. Meissner, Handbuch der Experimentalphysik, vol. XI, pt. 2, Leipzig, 1935.

3. See, for example, J. K. Logan and J. A. Marcus, Phys. Rev., 88:1234 (1952); R. K. Willardson, T. C. Harman, and A. C. Beer, ibid., 96:1512 (1954).

4. H. B. G. Casimir, Rev. Mod. Phys., 17:343 (1945); H. B. G. Casimir and A. N. Gerritsen, Physica, 8:1107 (1941).

Numerous authors extended Lord Kelvin's work on magneto resistance to nonferromagnetic materials. Grunmach and Wiedert[1] published in 1906-07 the first extensive study for various elements at room temperature. In 1928-30 Kapitza[5] went to lower temperatures and higher magnetic fields. In 1897 Van Everdingen[1] had discovered the influence of the crystal orientation on the magneto resistance. The effect was studied further by Schubnikow and de Haas,[6] Stierstadt,[7] Justi[8] and co-workers, Blom,[9] and others.[10] Schubnikow and de Haas, Stierstadt, and, more systematically, Blom, tried to analyze the angular dependence of the magneto resistance on the orientation of the magnetic field relative to the sample by a Fourier analysis. Briefly, findings[11] of all this work are that the magneto resistance depends markedly on the crystal orientation, especially at low temperatures; that for low magnetic fields (say less than 1 kilogauss) the magneto resistance is proportional to the square of the field, whereas at high fields the relation is a more complicated function of the field. According to most results, this function is even. In 1905 Voigt[12] laid the foundation for an appropriate description of the anisotropy of the Hall and magneto resistance

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5. P. Kapitza, Proc. Roy. Soc. London(A), 123:292 (1929).

6. L. Schubnikow and W. J. de Haas, Comm. Leiden Nr. 207, a,c,d (1930); Comm. Leiden Nr. 210, a,b (1930).

7. O. Stierstadt, Z. f. Phys., 80:636 (1933); 85:310, 697 (1933).

8. E. Justi, Leitfähigkeit und Leitungsmechanismus fester Stoffe, Chapter I, Vandenhoeck and Ruprecht, Göttingen, 1948.

9. J. W. Blom, Magnetoresistance for Crystals of Gallium, The Hague, Martinus Nijhoff, 1950.

10. R. Schulze, Phys. Z., 42:297 (1941); Y. Tanabe, Tohoku Univ. Res. Inst. Sci. Rep. I:275 (1949); E. Grueneisen and H. Adenstedt, Ann. Phys., 31:714 (1937); B. G. Lazarev, N. M. Nakhimovich, and E. A. Parfenova, C. R. Moskau (N.S.), 24:855 (1939).

11. For recent works see, for example, G. L. Pearson and H. Suhl, Phys. Rev., 83:768 (1951); G. L. Pearson and C. Herring, Physica, 20:975 (1954).

12. W. Voigt, Lehrbuch der Kristallphysik, Teubner, Leipzig and Berlin, 1928.

effects. Further contributions to the phenomenological theory were made by Kohler,[13] Casimir,[4] Seitz,[14] Juretschke,[15] and other workers.

The present paper attempts to give an explicit development and broadening of the general phenomenological theory, which is required for the interpretation of isothermal galvanomagnetic measurements in terms of true isothermal galvanomagnetic material constants.[16] In Section 2 the proper galvanomagnetic constants are defined, the dependence of F on the orientation of J and B is discussed, and some general relations are established. In Section 3 a general method is developed by means of which the effects of crystal symmetry are properly taken into account. In Section 4 formulas are given for the number of independent galvanomagnetic constants for the various crystal classes. In Section 5 explicit forms are given for F up to terms quadratic in the components of B for the various crystal symmetries, while the corresponding forms for higher powers can be elaborated from there on without essential difficulties. The significance of the results obtained is pointed out in Section 6.

The objective and plan of attack of the present work is as follows. The ultimate aim of the theory of the galvanomagnetic effects is to describe the function (1) completely in terms of the electronic properties of the material concerned. This task can be divided into two parts. In the first or phenomenological part the function (1) is described in terms of a number—finite or infinite—of appropriate constants that are characteristic for the material. In the second or electron-theoretical part these constants are interpreted in terms of electronic properties. The present paper is only concerned with the phenomenological part.

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13. M. Kohler, Ann. Physik, 20:878,891 (1934); 95:365 (1935).

14. F. Seitz, Phys. Rev., 79:372 (1950).

15. H. J. Juretschke, Acta Cryst., 8:716 (1955).

16. The essentials of the present paper were first given in a contract report, with the U. S. Signal Corps Engineering Laboratories, of November, 1954, by E. Katz, entitled: Magnetically Sensitive Electrical Resistor Material.

Here again the work can be divided into several steps. First, proper coordinates will be defined. Second, the galvanomagnetic function (1) must be put in the simplest form consistent with general principles and with arbitrary orientation of $\underline{B}$, arbitrary crystal symmetry, etc. This form must then be expressed in terms of functions that are characteristic for the material. Third, these functions must be described by a number—finite or infinite—of constants which are amenable to discussion by the electron theory. Fourth, the restrictions imposed on these constants by the crystal symmetry are to be established, and the number of independent nonvanishing constants should be found. Fifth, the information so obtained must be synthesized; the galvanomagnetic effect, measured under the most general conditions, is then expressed in terms of material constants ready for interpretation by the electron theory.

2. DEFINITIONS AND GENERAL RELATIONS

<u>a</u>. <u>Coordinate Systems</u>.—Two sets of orthogonal coordinate systems will be used.

(1) The symmetry coordinates k_i ($i = 1,2,3$). These are adapted to the crystal symmetry* as follows:

For the groups C_1, S_1 the directions of the coordinate axes are arbitrary. For the groups S_2, S_4, S_6, C_2, C_3, C_4, C_6, C_{2h}, C_{3h}, C_{4h}, C_{6h}, the k_3 axis is taken along the axis of rotation;** the other axes have one degree of freedom.

For the groups T, T_h, T_d, the coordinate axes are taken along the twofold rotation axes.

For all other classes, k_3 is taken along the rotation axis of highest order, k_1 along a rotation axis** normal to k_3, and k_2 accord-

*Only the macroscopic symmetry of the crystal, i.e., to which of the 32 crystallographic point groups it belongs, need here be considered.

**The axis of an improper rotation is understood here as the normal to the corresponding reflection plane.

ingly. Vector or tensor components with respect to these symmetry coordinates will carry Latin subscripts.

(2) The laboratory coordinates x^α ($\alpha = 1,2,3$) with x^1 along the current density $\underline{J}$, x^2 in the plane of $\underline{J}$ and $\underline{d}$, and x^3 accordingly. In the case of magneto resistance, $\underline{d}$ is along $\underline{J}$, allowing one degree of freedom for x^2 and x^3 in the plane normal to x^1. Vector and tensor components with respect to the laboratory coordinates will carry Greek superscripts. No confusion between superscripts and exponents should arise in practice.

The definition of the laboratory system implies

$$J^2 = J^3 = 0 \quad . \tag{2}$$

Denoting the direction cosines between the two coordinate systems by ℓ_i^α and using the summation convention for repeated indices, we have

$$\left.\begin{aligned} J^\alpha &= J_i \ell_i^\alpha \\ J_i &= J^\alpha \ell_i^\alpha \\ F^\beta &= F_j \ell_j^\beta \\ F_j &= F^\beta \ell_j^\beta \quad . \end{aligned}\right\} \tag{3}$$

b. Assumption I. Ohm's Law.—We assume Ohm's law to be valid for any constant applied magnetic field $\underline{B}$, i.e., the current density $\underline{J}$ is a homogeneous linear vector function of $\underline{F}$. Thus, in symmetry coordinates:

$$\left.\begin{aligned} J_i &= \sigma_{ij}\,(\underline{B})\,F_j \\ F_j &= \rho_{ji}\,(\underline{B})\,J_i \quad , \end{aligned}\right\} \tag{4}$$

where the conductivity tensor components σ_{ij} and the resistivity components ρ_{ji} are both functions of $\underline{B}$ and are related by

$$\rho_{ji} = \Delta_{ij}/\Delta \quad . \tag{5}$$

Here Δ is the determinant of the σ_{ij} and Δ_{ij} is the cofactor of σ_{ij} in Δ. The functions $\sigma_{ij}(\underline{B})$ and $\rho_{ji}(\underline{B})$ are characteristic of the material at any given temperature and independent of the geometry of galvanomagnetic measurements. The effects of crystal symmetry are to place restrictions on these functions. However, the direction of current flow $\underline{J}$ has, in general, no particularly simple relation to the symmetry coordinates, and the results of measurements are most directly expressed in terms of laboratory coordinates. Ohm's law, restated in laboratory coordinates, is

$$F^{\alpha} = \rho^{\alpha 1}(\underline{B})J^{1}$$

where

$$\rho^{\alpha 1}(\underline{B}) = \rho_{ji}(\underline{B})\ell_j^{\alpha}\ell_i^{1} = \Delta_{ij}(\underline{B})\ell_i^{1}\ell_j^{\alpha}/\Delta(\underline{B}) \quad . \qquad (6)$$

For $\alpha = 1$ these equations describe the magneto resistance effect; for $\alpha = 2$ or 3 they represent the Hall effect. The latter form expresses these galvanomagnetic effects in terms of the conductivity components in symmetry coordinates.

c. Assumption II. Onsager's Relations.—The validity of Onsager's relations is assumed:

$$\rho_{ji}(\underline{B}) = \rho_{ij}(-\underline{B})$$

and, consequently,

$$\sigma_{ji}(\underline{B}) = \sigma_{ij}(-\underline{B}) \qquad (7)$$

as well as

$$\rho^{\alpha\beta}(\underline{B}) = \rho^{\beta\alpha}(-B) \quad . \qquad (8)$$

d. The Parity of the Magneto Resistance Effect.—Equation (8) states that

$$\rho^{11}(\underline{B}) = \rho^{11}(-\underline{B}) \quad , \qquad (9)$$

which proves the theorem that the magneto resistance effect is even in $\underline{B}$. In the literature [17] there has been some controversy about the evenness of ρ^{11}, but the above argument shows that under the very broad assumptions stated, ρ^{11}

17. References 11, 4; D. Shoenberg, Proc. Camb. Phil. Soc., 31:271 (1935); J. Meixner, Ann. Phys., 36:105 (1939); ibid., 40:105 (1941); B. Donovan and G. K. T. Conn, Phil. Mag., 41:770 (1950).

must be an even function in B without exception.

e. Parity of the Hall Effect.—The Hall effect as defined by (6) with $\alpha \neq 1$ implies that the Hall electrodes are normal to the current. We shall adhere to this definition, though some experimenters prefer to define the Hall effect as measured with the Hall electrodes on an equipotential when B = 0.

In general the Hall effect is neither an odd nor an even function of B. This is true for either definition. However, in a number of special configurations the crystal symmetry may impose a special parity on the Hall effect. The complete list of such configurations is as follows. Consider the crystallographic point group, obtained from that of the crystal by augmenting it with an inversion center. The physical significance of this augmented group is explained in Section 3. Then one can easily prove with respect to this augmented group:

(1) If B lies along a 3-, 4-, or 6-fold axis and either J or d is normal to B, then the Hall effect is odd.

(2) If B is normal to a 2-, 4-, or 6-fold axis and either J or d is along that axis, then the Hall effect is odd.

(3) If B lies along any 2-, 3-, 4-, or 6-fold rotation axis and is coplanar with J and d, then the Hall effect is even.

(4) If B, J, and d are normal to the same 2-, 4-, or 6-fold axis, then the Hall effect is even.

(5) If B and either J or d lie along any 2-, 3-, 4-, or 6-fold rotation axis, then the Hall effect vanishes.

There are no other cases in which the Hall effect is purely even, odd, or zero as a function of B. The "new" galvanomagnetic effect reported by Goldberg and Davis,[18] for example, is a case illustrating points (4) and (5). In their Fig-

18. C. Goldberg and R. E. Davis, Phys. Rev., 94:1121 (1955).

ure 1 the slight discrepancy between the axis direction and the direction of zero Hall effect must be due to an experimental error of imperfect alignment.

f. Assumption III. Power Series Expansion of $\sigma_{ij}(\underline{B})$.—Most galvanomagnetic measurements suggest that $\sigma_{ij}(\underline{B})$ can be expanded as a series in powers of the components B_k. One of many typical examples is reproduced by A. H. Wilson[19] from work by Justi and Scheffers on gold. If a Fourier analysis of polar diagrams of this sort involves significant terms with arguments of the sines or cosines up to $n\phi$, then, it is easily shown, significant contributions to the conductivity components σ_{ij} arise from terms proportional to the n^{th} power of B and vice versa.

There is an observed limitation to the appropriateness of a power-series expansion for galvanomagnetic effects. Experiments[20] have shown that the Hall voltage and the magneto resistance at low temperatures contain oscillating terms which presumably are connected with the van Alphen - de Haas effect and are proportional to B sin B_o/B. Such terms do not possess a derivative with respect to B at B = 0 and hence cannot be expanded in powers of B. Consequently, the development presented here does not apply to that part of the galvanomagnetic effects which arisesfrom terms of such a nature.

As the third assumption, we write

$$\sigma_{ij}(\underline{B}) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{p=0}^{m} [m-p,p,n-m]_{ij} B_1^{m-p} B_2^{p} B_3^{n-m} \tag{10}$$

or, introducing the direction cosines γ_i of $\underline{B}$ with respect to the symmetry coordinates,

19. A. H. Wilson, The Theory of Metals, Univ. Press, Cambridge, 1953, p. 318.

20. See, for example, P. B. Alers and R. T. Webber, Phys. Rev., 91:1060 (1953); T. G. Berlincourt and J. K. Logan, Phys. Rev., 93:348 (1954); T. G. Berlincourt and M. C. Steele, Phys. Rev., 98:956 (1955); M. C. Steele, Phys. Rev., 99:1751 (1955).

$$\sigma_{ij}(\underline{B}) = \sum_{n=0}^{\infty} B^n \sum_{m=0}^{n} \sum_{p=0}^{m} [m-p,p,n-m]_{ij}\, \gamma_1^{m-p}\gamma_2^{p}\gamma_3^{n-m} \quad . \tag{10a}$$

The coefficients in this expansion are designated by the bracket symbols and are independent of $\underline{B}$. They are the true phenomenological material constants characterizing the galvanomagnetic behavior of any particular material. They are sums of components of tensors of rank 2n + 2 since the axial vector $\underline{B}$ is an antisymmetric tensor of rank two.*

Onsager's relations imply

$$[m-p,p,n-m]_{ij} = (-)^n\, [m-p,p,n-m]_{ji} \quad . \tag{11}$$

Consequently, it is sufficient to consider ij values of 11, 22, 33, 23, 31, 12, only. This will always be done unless stated otherwise. Another consequence of (11) is that all brackets with n = odd and i = j vanish. Denoting by ω an arbitrary odd number:

$$[m-p,p,\omega-m]_{ii} = 0 \quad . \tag{11a}$$

The restrictions imposed on the brackets by the crystal symmetry will be described in the next section. The fact that (6) is simpler in terms of ρ_{ij} then in terms of σ_{ij} would suggest a power-series expansion of the former. The latter was chosen since the brackets so obtained permit a simpler electron theoretical interpretation. However, the contents of all that follows are applicable without any modification to ρ-brackets and σ-brackets alike.

3. THE EFFECTS OF CRYSTAL SYMMETRY

a. Only Eleven Point Groups Need Analysis.—Tensor components that are material constants must be invariant under the operations of the crystallo-

*In order to set the tensor character in evidence, the brackets will sometimes be denoted by $[(23)^{m-p},(31)^{p},(12)^{n-m}]_{ij}$. The quantities (23), (31), (12) will be referred to as the pairs of inner indices and ij as the outer indices.

graphic point group of the crystal considered. If the tensor components are of even rank, they transform identically into themselves under inversion. Consequently, all tensor components of even rank that are material constants must be invariant under the operations of the point group that is obtained by augmenting the point group of the crystal considered by an inversion center. This is obviously also true for the brackets. Any point group augmented by an inversion center becomes one of the eleven well-known crystallographic point groups which possess such a center. Thus, it suffices to analyze these eleven point groups. They can all be generated by at most two rotations in addition to the inversion center. We shall generate the eleven point groups by means of the elements shown in Table I. In the second row are listed the twenty-one point groups without inversion center which go over into those of the first row by the addition of an inversion center.

TABLE I

GENERATING THE ELEVEN POINT GROUPS

Point Group	S_2	C_{2h}	C_{3i}	C_{4h}	C_{6h}	D_{2h}	D_{3i}	D_{4h}	D_{6h}	T_h	O_h
Equivalent	C_1	C_2	C_3	C_4	C_{3h}	C_{2v}	C_{3v}	D_{2d}	D_{3h}	T	T_d
Point		C_s		S_4	C_6	D_2	D_3	C_{4v}	C_{6v}		O
Groups								D_4	D_6		
Generating*											
Elements											
axis along k_3	-	2	3	4	6	2	3	4	6	2	4
axis along k_1	-	-	-	-	-	2	2	2	2	-	-
axis along [111]	-	-	-	-	-	-	-	-	-	3	3

*If an axis is taken as a generating element, its multiplicity N is listed at the appropriate place. The inversion center which is a common generating element of all groups is not listed.

Under a general rotation each bracket is transformed into a linear combination of other brackets. If the rotation be a covering operation, and thus requires invariance of the bracket, then certain relations must hold between the brackets.

Under inversion each bracket is transformed identically into itself. Hence, no relations between brackets can be derived from the requirement of invariance under inversion.

b. A Theorem Concerning the Effect of an N-Fold Rotation Axis Along k_3.—The effects of an N-fold rotation axis along k_3 are covered by a theorem which states that certain linear equations must hold between the brackets. In order to express these combinations concisely, some notations are introduced. Let s be the number of non-threes among a given ij and let θ be the number of twos minus the number of ones in ij. The numbers s,θ define uniquely one of the six independent pairs of indices ij, and vice versa. Table II gives the relation explicitly for further reference. We write

$$[m-p,p,n-m]_{ij} \equiv [m-p,p,n-m]_{(s,\theta)} \quad . \qquad (12)$$

TABLE II

TABLE OF s AND θ VALUES

ij	s	θ
33	0	0
31	1	-1
23	1	+1
11	2	-2
12	2	0
22	2	+2

Let z denote a nonnegative integer $\leq$ s and w a nonnegative integer $\leq$ m. Each of the linear equations referred to by the theorem will be labeled by five integers n, m, s, z, w. All brackets occurring in one equation have the same n,m,s, but may differ in p,θ. The parameters z,w serve to label the various equations with the same n,m,s, involving the same brackets with different coefficients.

Theorem

For an N-fold rotation axis along k_3, the brackets satisfy the equations

$$\sum_{\Theta} \sum_{p=0}^{m} g(m,p,w)\, \epsilon(s,\Theta,z)\, [m-p,p,n-m]_{(s,\Theta)} = 0 \quad , \tag{13}$$

provided the inequality

$$h \equiv m+s - 2(w+z) \not\equiv kN \qquad (k=0,\pm1,\pm2\ldots) \tag{14}$$

holds; in other words, h is not a multiple of N.

The summation over Θ is meant to include all ij combimations with constant s. The coefficient g(m,p,w) is defined in terms of binomial coefficients by

$$g(m,p,w) \equiv i^p \sum_{q=0} (-)^q \binom{m-p}{q}\binom{p}{w-q} \quad . \tag{15}$$

The factor ε(s,Θ,z) is given in Table III for all values for which it is defined. The proof of this basic theorem is given in Appendix I. In Appendix II it is shown that the only solution for the complete set (13) for given n,m,s, is that all brackets involved vanish. A consequence is that the equations (13) with the condition (14) represent a complete description of the symmetry properties of the brackets.

For finding the relations between brackets of given n,m,s, one will first list all brackets of this set according to their p and Θ values, next establish their coefficients gε for all possible values of the parameters w,z, and finally write down one equation of the type (13) for each set of w,z values compatible with (14). Shortcuts to this procedure will be explained after some corollaries of the theorem have been proved.

c. Some Consequences of the Theorem.—In formulating the fundamental theorem a rotation axis was taken along k_3. It is simple to apply the theorem

TABLE III

THE VALUES OF $\epsilon(s,\theta,z)$

			n = even			n = odd		
s	θ	ij z→	0	1	2	0	1	2
0	0	33	1	-	-	-	-	-
1	-1	31	1	1	-	1	1	-
1	1	23	i	-i	-	-i	i	-
2	-2	11	1	1	1	-	-	-
2	0	12	2i	0	-2i	0	2i	0
2	2	22	-1	1	-1	-	-	-

to a rotation axis along k_1 or k_2 by permutation of both inner and outer indices. The effect of a threefold axis along the [111] direction can be taken into account by requiring invariance for the brackets under cyclic permutation of the indices 1,2,3 both in and outside any bracket. Thus the effect of symmetry for the eleven point groups is completely described by the theorem with these generalizations.

However, in a number of cases the application of the theorem is greatly simplified by means of some corollaries.

Corollary I

For N = even (2,4,6) about k_3, all brackets for which the index 3 occurs an odd number of times (inside plus outside) are zero.

Proof

In any particular bracket, the index 3 occurs 2-s+m times. Thus it must be shown that all brackets with (m+s) odd vanish. If (m+s) is odd then h cannot be an integral multiple of the even number N. Thus all equations provided by the general theorem are valid. According to the theorem, given in

Appendix II, all brackets concerned must now vanish.

q.e.d.

In preparation of Corollary II let two brackets be called "adjoint" with respect to k_3, if they can be obtained from one another by interchanging the indices 1 and 2*), both inside and outside, and writing the resulting pairs of indices in the conventional order. For example, the brackets

$$[m-p,p,n-m]_{23} \quad \text{and} \quad [p,m-p,n-m]_{31}$$

are adjoint. Indeed the first bracket can be written as $[(23)^{m-p},(31)^{p},(12)^{n-m}]_{23}$. Upon interchanging 1 and 2 this becomes $[(32)^{p},(13)^{m-p},(21)^{n-m}]_{13}$. All pairs must now be interchanged in order to appear in the conventional order. The n inner pairs each give a minus sign. The outer pair gives $(-)^n$ according to Onsager's relation (11). The result is always a plus sign. The resulting bracket is $[(23)^{p},(31)^{m-p},(12)^{n-m}]_{31}$, which is the same as $[p,m-p,n-m]_{31}$. Thus the adjoining operation with respect to k_3 transforms one bracket into another one, by interchanging p with m-p and Θ with $-\Theta$.

Corollary II

For N = 4 about k_3, nonvanishing adjoint brackets are either equal or opposite. They are equal if the number of occurrences of the index 2 is even, opposite if this number is odd.

Proof

Under a fourfold rotation about k_3, k_1 transforms into k_2' and k_2 into $-k_1'$. Thus the result of this rotation differs from the operation "adjoining" only by a factor (-) to the power of the number of occurrences of the index 2. If the index 2 occurs an even number of times the factor is +1, otherwise -1. Since the fourfold rotation is a covering operation the corollary is proved.

*Similarly we define adjoint with respect to k_1 (or k_2) by interchanging the indices 2 and 3 (or 3 and 1).

The indices 1 and 2 occur both even or both odd. Indeed the total number of indices 1, 2, and 3 is even, and the occurrence of the index 3 is even according to Corollary I. Thus the corollary is symmetric with respect to the indices 1 and 2.

q.e.d.

Corollary III

If in an equation of the type (13) each bracket $[m-p,p,n-m]_{ij}$ is replaced by $[m-p,p,n'-m]_{ij}$, where n' has the same parity as n, the resulting equation also belongs to the set (13) and has the same h.

Proof

The corollary is essentially due to the fact that k_3 is the rotation axis. In equation (13) n occurs only in two places: in the brackets, all brackets in one equation having the same n, and in ϵ (see Table III). In the latter the influence of n enters only through its parity, hence different values of n with the same parity lead to similar equations. Since the definition (14) of h does not contain n, the h-values of such equations are equal.

q.e.d.

A consequence of this corollary is that a change from n to n' with the same parity in any bracket relation leads to another valid relation, i.e., bracket relations for given values of m,s need to be tabulated only for n = even and for n = odd, a fact which has permitted great simplification in the tables of bracket relations that follow.

Corollary IV

Two equations of the type (13) with equal n,m,s having parameter values w,z and w'=m-w, z'=s-z, i.e., h'=-h, are conjugate complex.

Proof

One must prove that the coefficient $g\epsilon$ is transformed into its conjugate complex by changing from w,z to w',z'. According to (15) it is easily shown that $g(m,p,w) = (-)^{m+p} g(m,p,m-w)$. Since the definition of g contains a factor i^p,

$$g(m,p,w) = (-)^m g^*(m,p,w') \quad , \tag{16}$$

the asterisk denoting the complex conjugate. Likewise, Table III shows that

$$\epsilon(s,\theta,z) = \epsilon^*(s,\theta,z') \quad . \tag{16a}$$

Thus by changing from w,z to w',z' the equation is multiplied through by the constant factor $(-)^m$ and each coefficient changes to its complex conjugate.

q.e.d.

The occurrence of the equations (13) in complex conjugate pairs permits a simplification in listing or surveying all such equations. If the real and imaginary part of each equation is taken separately, one need only consider one equation of each conjugate complex pair and maintain all self-conjugate equations. This can be done in two ways. In the first way one restricts the range of w to values satisfying the selection rule:

$$m - 2w \geq 0 \quad ,$$

and leaving $0 \leq z \leq s$ free. In this way only equations with $h \geq 0$ are selected, and this procedure is most practical for the making of tables of bracket relations. In the second way one restricts the range of z to values satisfying the selection rule:

$$s - 2z \geq 0 \quad ,$$

and leaving $0 \leq w \leq m$ free. This way is useful for proving some general relations, for example, those of Appendix III. It is evident that for self-conjugate equations

$$m - 2w = s - 2z = 0$$

is a necessary and sufficient condition. The number of real equations so obtained is equal to the number of original complex equations.

Corollary V

If in an equation of the type (13) each bracket is replaced by its adjoint, the resulting equation also belongs to the set (13) and has the same $|h|$.

Proof

Each equation (13) contains adjoint pairs of brackets, characterized by p,θ and $p'=m-p,\theta'=-\theta$, since summations over p and θ occur.

The coefficients of adjoint brackets in one equation are $g(m,p,w)$ $\epsilon(s,\theta,z)$ and $g(m,p',w)$ $\epsilon(s,\theta',z)$. Thus, replacing all brackets by their adjoints is equivalent to interchanging the above coefficients without changing the brackets. We shall prove that, apart from a constant factor, this change in coefficients transforms the equation into its conjugate complex, which according to Corollary IV also belongs to the set and has opposite h.

It follows directly from equation (15) that

$$g(m,p,w) = (-)^{m+w} i^{-m} g^*(m,p',w) \quad , \tag{17}$$

where $p'=m-p$. It is also easy to verify in Table III that

$$\epsilon(s,\theta,z) = (-)^{n+z} i^{s} \epsilon^*(s,\theta',z) \quad , \tag{17a}$$

where $\theta' = -\theta$. Thus by changing from p,θ to p',θ', the coefficients are multiplied by the constant factor $(-)^n i^h$ and change to their conjugate complex.

q.e.d.

A consequence of this corollary is: For any real relation between brackets its adjoint relation is also valid with the same coefficients. This fact is extensively used in constructing the tables of bracket relations which follow.

A number of other corollaries follow from the symmetry of g and ϵ. The principal ones are listed below, proofs being left to the reader. They are useful for checking relations among brackets.

Corollary VI

Any relation between brackets with $s = 1$ ($\Theta = \pm 1$) is invariant for the substitution $\Theta' = -\Theta$ followed by reversal of the sign of the coefficients of all terms with $\Theta' = -1$.

Corollary VII

Any relation between brackets with $s = 2$ is invariant for the substitution $\Theta' = -\Theta$ followed by reversal of the sign of the coefficients of all terms with $\Theta = 0$.

Corollary VIII

Any relation between brackets for $s = 1$, n = even, is transformed to a valid relation for n = odd by changing the sign of all brackets with $\Theta = + 1$, and vice versa.

Corollary IX

For m = odd any relation between brackets is invariant for the substitution $m' = m-p$ followed by reversal of the sign of the coefficients of all terms with outer indices 31 and 12.

d. The Procedure for Tabulating the Bracket Relations.—It was stated that the brackets are linear combinations of components of tensors of even rank. Thus the analysis can be restricted to eleven out of thirty-two point groups. Moreover, Onsager's relations permit one to use only six pairs of indices ij, with equations (11) and (11a) valid for all point groups. The theorem, given by equations (13) and (14), allows complete tabulation of all bracket relations for all these groups. Often the application of the corollaries, especially I and II, is helpful in obtaining the tables for certain groups from those of other groups. The brackets of the group S_2 can be tabulated completely by using equations (11) and (11a) only. It is to be remembered that all the tables that follow are constructed according to the convention that k_3 is taken along the rotation axis of highest order and k_1 along a rotation axis normal to k_3, if there be one.

TABLE IV

PROCEDURE FOR TABULATING BRACKET RELATIONS

Table of Group	+ Corollary I About k_3	+ Corollary I About k_1	+ Corollary II About k_3	+ Invariance Under Cyclic Permutation	Yields Table of Group
S_2	+				C_{2h}
C_{2h}		+			D_{2h}
C_{2h}			+		C_{4h}
D_{2h}			+		D_{4h}
D_{2h}				+	T_h
D_{4h}				+	O_h
C_{3i}		+			D_{3i}
C_{3i}	+				C_{6h}
C_{6h}		+			D_{6h}

The first six groups of the last column of Table IV are seen to be completely derivable from the Corollaries I and II and the invariance under cyclic permutation, as indicated by the + signs. The groups D_{3i}, C_{6h}, D_{6h} are based on C_{3i}, which required the direct application of the general theorem, assisted by the various corollaries. We have not found any simple rule yielding the complete tabulation for C_{3i}.

_e_. _Bracket Relations for C_{2h} and D_{2h}_.—Table V for C_{2h} and D_{2h} is constructed on the basis of Corollary I. The effect of symmetry is manifest entirely in the vanishing of certain brackets; all nonvanishing brackets are independent. Thus, we have used three symbols to indicate the state of a bracket whose inner part is given by the second column and whose outer indices appear in the first row. The inner parts of brackets contain the symbols e for an arbitrary even number and ω for an arbitrary odd one.

+ means the bracket is independent both for C_{2h} and D_{2h}.

⊕ means the bracket is independent for C_{2h} but vanishes for D_{2h}.

0 means the bracket vanishes both for C_{2h} and for D_{2h}.

Examples: $[203]_{23}$ is found to be zero as shown by $[ee\omega]_{23}$ in the eighth row,

$[204]_{12}$ is found to be independent for C_{2h} and zero for D_{2h} as shown by [eee] in the first row.

The outer indices 11, 22, 33 cannot occur with n = odd, according to equation (12). Table V is complete for all n.

TABLE V

BRACKET RELATIONS FOR C_{2h} AND D_{2h}

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	⊕	+	+	+
	[eωω]	+	⊕	0	0	0	0
	[ωeω]	⊕	+	0	0	0	0
	[ωωe]	0	0	+	⊕	⊕	⊕
n = odd	[ωωω]	0	0	⊕			
	[ωee]	+	⊕	0			
	[eωe]	⊕	+	0			
	[eeω]	0	0	+			

+ means bracket independent for C_{2h} and D_{2h}.
⊕ means bracket independent for C_{2h}, zero for D_{2h}.
0 means bracket zero for C_{2h} and D_{2h}.

f. Bracket Relations for C_{4h} and D_{4h}.—The effect of symmetry is manifested in two ways: either a bracket is zero or it is equal to plus or minus its adjoint (as defined in Corollary II of the theorem). Of each such pair of adjoint brackets, one bracket can be chosen as independent. In the first, fourth, fifth, and eighth or last row self-adjoint brackets may occur. A self-adjoint bracket may be forced to vanish if it must be minus its adjoint. Thus it turns out that four symbols are needed, whose meaning is explained under the Table VI, which gives the complete bracket relations for all n.

Examples: $[202]_{12}$ = $-[022]_{12}$ for C_{4h}, zero for D_{4h} (first row).

$[220]_{12}$ = self-adjoint and $-[220]_{12}$, hence zero for C_{4h} and D_{4h}.

$[202]_{11}$ = $+[022]_{22}$; one of the pair is independent, both for C_{4h} and D_{4h}.

TABLE VI

BRACKET RELATIONS FOR C_{4h} AND D_{4h}

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	⊖̇	† ---	--- †	†
	[eωω]	†	⊖	0	0	0	0
	[ωeω]	⊖	†	0	0	0	0
	[ωωe]	0	0	†	⊖ ---	--- ⊖	⊖̇
n = odd	[ωωω]	0	0	⊖̇			
	[ωee]	†	⊖	0			
	[eωe]	⊖	†	0			
	[eeω]	0	0	†			

† means bracket is one of an independent pair and equal to its adjoint for C_{4h} and D_{4h}.

⊖ means bracket is one of an independent pair and equal to minus its adjoint for C_{4h}, zero for D_{4h}.

⊖̇ means ⊖ and in addition zero if self-adjoint.

0 means zero for C_{4h} and for D_{4h}.

Dotted lines connect adjoint places.

g. Bracket Relations for T_h and O_h.—Table VII for these groups is derived from Table V for D_{2h} and Table VI for D_{4h} by requiring that brackets remain invariant under cyclic permutation of all indices. The six permutations of the indices 1,2,3 fall into two groups of three cyclic permutations. Brackets belonging to two such cyclic groups are pairwise adjoint with respect to k_1, k_2, and k_3. If adjoint brackets are to be equal, such as happens in O_h, or if brackets are pairwise self-adjoint, the two cyclic groups coincide. For example, we have for T_h a cyclic group of three equal brackets, obtained by cyclic interchange of inner and outer indices from the first one:

$$[202]_{11} = [220]_{22} = [022]_{33} \quad .$$

The other cyclic group of three equal brackets can be obtained from these by a transposition of two indices. Thus by interchanging 1 and 2, i.e., adjoining with respect to k_3, one obtains:

$$[022]_{22} = [220]_{11} = [202]_{33} \quad .$$

For O_h all six are equal. On the other hand, the bracket $[220]_{33}$ is self-adjoint with respect to k_3, hence there is only one cyclic group of three brackets derived from it and they are equal both for T_h and O_h, namely:

$$[220]_{33} = [022]_{11} = [202]_{22} \quad .$$

h. The Bracket Relations for C_{3i}, D_{3i}, C_{6h}, D_{6h}.—No simple rules for the complete tabulation are available and the theorem plus corollaries will be used. In order to obtain the most compact form for the results, the following scheme has been adopted.

For any particular bracket we must first decide whether or not it is zero. For C_{3i} all zero brackets are listed in Table VIII. The proof that these brackets are zeros for C_{3i} is given in Appendix III. The groups D_{3i}, C_{6h}, and D_{6h} have the same zeros and the additional zeros listed in Table IX. The latter was obtained from Tables V, VI, and VII according to the procedure shown in Table IV.

TABLE VII

BRACKET RELATIONS FOR T_h AND O_h

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	0	+	+	+
	[eωω]	+	0	0	0	0	0
	[ωeω]	0	+	0	0	0	0
	[ωωe]	0	0	+	0	0	0
n = odd	[ωωω]	0	0	0			
	[ωee]	+	0	0			
	[eωe]	0	+	0			
	[eeω]	0	0	+			

+ means nonvanishing bracket for T_h and for O_h.

0 means zero bracket for T_h and O_h.

In T_h + is one of an independent cyclic set of three equal brackets.

In O_h + is one of an independent permuted set of three or six equal brackets (three, if brackets are pairwise self-adjoint).

Dotted lines indicate places of brackets of the same set.

If a bracket does not vanish according to Tables VIII and IX, then its relations to other brackets are shown in Table X, up to m = 6 inclusive.

Table X is arranged in three parts, according to s = 0, 1, or 2. Each part consists of seven sub-tables for m = 0, 1, ... 6. The sub-tables, except the simplest ones, have the form of a core array of coefficients bordered by brackets. This arrangement represents a double-entry table, similar to the familiar trigonometric tables: brackets on the left are equal to the linear combinations of those at the top, with the listed coefficients, whereas brackets on the right use these same coefficients with those at the bottom. That this arrangement, in which adjoint brackets stand at opposite ends of

TABLE VIII

ZERO BRACKETS FOR C_{3i}, D_{3i}, C_{6h}, D_{6h}

	ij →	23	31	12	11	22	33
n = even	[eee]	[ooe]	[ooe]	[ooe]			
	[eωω]						[o1ω]
	[ωeω]						[1oω]
	[ωωe]						[11e] [31e] [13e]
n = odd	[ωωω]			[11ω] [31ω] [13ω]	—	—	—
	[ωee]			[1oe]	—	—	—
	[eωe]			[o1e]	—	—	—
	[eeω]	[ooω]	[ooω]		—	—	—

TABLE IX

ZERO BRACKETS FOR D_{3i}, C_{6h}, D_{6h}

	ij →	23	31	12	11	22	33
n = even	[eee]	*̇	*Δ	Δ̊			
	[eωω]		Δ	*Δ	*	*	*̇
	[ωeω]	Δ		*	*Δ	*Δ	*Δ
	[ωωe]	*Δ	*		Δ	Δ	Δ̊
n = odd	[ωωω]	*	*Δ	Δ̊	—	—	—
	[ωee]		Δ	*Δ	—	—	—
	[eωe]	Δ		*̇	—	—	—
	[eeω]	*Δ	*̇		—	—	—

Δ means zero bracket for D_{3i} and for D_{6h}.
* means zero bracket for C_{6h} and for D_{6h}.
· is a reminder to check Table VIII.

rows and columns, is possible is due to Corollary V. For example, for s = 1, m = 4 we have

$$[31e]_{23} = [40e]_{31} + 3[04e]_{31}$$

$$[13e]_{31} = 3[40e]_{23} + [04e]_{23}$$

The two equations are adjoint with respect to k_3.

TABLE X

RELATIONS FOR NONVANISHING BRACKETS FOR C_{3i}, D_{3i}, C_{6h}, D_{6h}

s = 0

m	
0	$[00e]_{33}$
1	---
2	$[20e]_{33} = [02e]_{33}$
3	$[12\omega]_{33} = -3[30\omega]_{33}$ $[21\omega]_{33} = -3[03\omega]_{33}$
4	$2[40e]_{33} = [22e]_{33} = 2[04e]_{33}$
5	$[50\omega]_{33}$ $[32\omega]_{33}$ -2 $[23\omega]_{33}$ $[14\omega]_{33}$ -3 $[41\omega]_{33}$ $[05\omega]_{33}$
6	$[60e]_{33}$ $[33e]_{33}$ $[06e]_{33}$ $[51e]_{33}$ 0 -3/10 0 $[15e]_{33}$ $[42e]_{33}$ -6 0 9 $[24e]_{33}$ $[06e]_{33}$ $[33e]_{33}$ $[60e]_{33}$

TABLE X (Continued)

$s = 1 \quad n = \text{even}^*$

m	
0	---
1	$[10\omega]_{31} = [01\omega]_{23}$ $[01\omega]_{31} = -[10\omega]_{23}$
2	$2[20e]_{31} = -[11e]_{23} = -2[02e]_{31}$ $2[20e]_{23} = [11e]_{31} = -2[02e]_{23}$
3	$[30\omega]_{31} = [12\omega]_{31} = [21\omega]_{23} = [03\omega]_{23}$ $-[30\omega]_{23} = -[12\omega]_{23} = [21\omega]_{31} = [03\omega]_{31}$
4	$[40e]_{31} \quad [04e]_{31}$ $[31e]_{23} \quad 1 \quad 3 \quad [13e]_{31}$ $[22e]_{31} \quad -3 \quad -3 \quad [22e]_{23}$ $[13e]_{23} \quad -3 \quad -1 \quad [31e]_{31}$ $[04e]_{23} \quad [40e]_{23}$
5	$[50\omega]_{31} \quad [05\omega]_{23}$ | $[50\omega]_{23} \quad [05\omega]_{31}$ $[41\omega]_{23} \quad -2 \quad 3 \quad [14\omega]_{31}$ | $[41\omega]_{31} \quad 2 \quad 3 \quad [14\omega]_{23}$ $[32\omega]_{31} \quad -4 \quad 6 \quad [23\omega]_{23}$ | $[32\omega]_{23} \quad -4 \quad -6 \quad [23\omega]_{31}$ $[05\omega]_{23} \quad [50\omega]_{31}$ | $[05\omega]_{31} \quad [50\omega]_{23}$
6	$[60e]_{31} \quad [06e]_{31}$ $[51e]_{23} \quad 1 \quad 3 \quad [15e]_{31}$ $[42e]_{31} \quad -2 \quad -3 \quad [24e]_{23}$ $[33e]_{23} \quad -2 \quad 2 \quad [33e]_{31}$ $[24e]_{31} \quad -3 \quad -2 \quad [42e]_{23}$ $[15e]_{23} \quad -3 \quad -1 \quad [51e]_{31}$ $[06e]_{23} \quad [60e]_{23}$

*The same table can be used for n = odd if each bracket with outer indices 23 receives a minus sign, according to Corollary VII.

TABLE X (Continued)

$s = 2 \qquad n = \text{even}$

m									
0	$[00e]_{11} = [00e]_{22}$								
1	$[10\omega]_{11} = [01\omega]_{12} = [10\omega]_{22}$								
	$[01\omega]_{22} = -[10\omega]_{12} = [01\omega]_{11}$								
2	$[11e]_{12} = [20e]_{11} - [20e]_{22}$								
	$[02e]_{11} = [20e]_{22}$								
	$[02e]_{22} = [20e]_{11}$								
	$[11e]_{11} = -[11e]_{22} = 2[20e]_{12} = -2[02e]_{12}$								
3	$[30\omega]_{11}$ $[30\omega]_{22}$								
	$[21\omega]_{12}$	-1/2	1/2		$[12\omega]_{12}$				
	$[12\omega]_{11}$	-1	-2		$[21\omega]_{22}$				
	$[12\omega]_{22}$	-2	-1		$[21\omega]_{11}$				
	$[03\omega]_{12}$	-1/2	1/2		$[30\omega]_{12}$				
	$[03\omega]_{22}$ $[03\omega]_{11}$								
4	$[40e]_{11}$ $([04e]_{11} + [40e]_{22})$ $[04e]_{22}$					$[40e]_{12}$ $[04e]_{12}$			
	$[31e]_{12}$	-3/2	-1/2	5/2	$[13e]_{12}$	$[31e]_{11}$	1	3	$[13e]_{22}$
	$[22e]_{11}$	-5/2	1/2	7/2	$[22e]_{22}$	$[31e]_{22}$	-1	-3	$[13e]_{11}$
	$[04e]_{11}$	1/2	1/2	-1/2	$[40e]_{22}$	$[22e]_{12}$	-3	-3	$[22e]_{12}$
	$[04e]_{22}$ $([40e]_{22} + [04e]_{11})$ $[40e]_{11}$					$[04e]_{12}$ $[40e]_{12}$			
5	$[50\omega]_{11}$ $[05\omega]_{12}$ $[50\omega]_{22}$								
	$[41\omega]_{12}$	1	3	-1	$[14\omega]_{12}$				
	$[32\omega]_{11}$	-3	-6	1	$[23\omega]_{22}$				
	$[32\omega]_{22}$	1	6	-3	$[23\omega]_{11}$				
	$[23\omega]_{12}$	-3	-4	3	$[32\omega]_{12}$				
	$[14\omega]_{11}$	0	2	-3	$[41\omega]_{22}$				
	$[14\omega]_{22}$	-3	-2	0	$[41\omega]_{11}$				
	$[05\omega]_{22}$ $[50\omega]_{12}$ $[05\omega]_{11}$								

6	$[60e]_{11}$	$[60e]_{22}$	$[06e]_{11}$	$[06e]_{22}$			$[60e]_{12}$	$[06e]_{12}$	$[33e]_{11}$	
$[51e]_{12}$	-1	1	-3	3	$[15e]_{12}$	$[51e]_{11}$	2/5	18/5	-3/10	$[15e]_{22}$
$[42e]_{11}$	-4	-2	3	6	$[24e]_{22}$	$[51e]_{22}$	-8/5	-12/5	-3/10	$[15e]_{11}$
$[42e]_{22}$	-2	-4	6	3	$[24e]_{11}$	$[42e]_{12}$	-2	-3	0	$[24e]_{12}$
$[33e]_{12}$	2	-2	-2	2	$[33e]_{12}$	$[33e]_{22}$	4	-4	1	$[33e]_{11}$
	$[06e]_{22}$	$[06e]_{11}$	$[60e]_{22}$	$[60e]_{11}$			$[06e]_{12}$	$[60e]_{12}$	$[33e]_{22}$	

$s = 2 \quad n = \text{odd}$

m	
0	$[00\omega]_{12}$
1	---
2	$[02\omega]_{12} = [20\omega]_{12}$
3	$[21e]_{12} = -3[03e]_{12}$ $[12e]_{12} = -3[30e]_{12}$
4	$2[40\omega]_{12} = [22\omega]_{12} = 2[04\omega]_{12}$
5	$2[41e]_{12} = 3[23e]_{12} = -[05e]_{12}$ $2[14e]_{12} = 3[32e]_{12} = -[50e]_{12}$
6	$[51\omega]_{12} = -3/10[33\omega]_{12} = [15\omega]_{12}$ $[42\omega]_{12} = -6[60\omega]_{12} + 9[06\omega]_{12}$ $[24\omega]_{12} = 9[60\omega]_{12} - 6[06\omega]_{12}$

4. THE NUMBER OF NONVANISHING INDEPENDENT BRACKETS

Let I(n) be the number of nonvanishing independent brackets for each point group as a function of n; further let P(n) be the number of possible brackets, $E^*(n)$ the number of valid equations (13) between them, E(n) the number of equations (13), valid and nonvalid, and K(n) the number of nonvalid equations (13) corresponding to $h = kN$. Then evidently

$$I(n) = P(n) - E^{*}(n) = P(n) - E(n) + K(n) \quad . \qquad (18)$$

Case 1. Groups C_N $(N = 1,2,3,4,6)$

It will be shown in Appendix II that $P_C(n) = E_C(n)$ for a rotation axis along k_3, reducing (18) to

$$I_{C_N}(n) = K_{C_N}(n) \quad . \qquad (19)$$

In order to evaluate $K_{C_N}(n)$, a counting diagram as shown in Figure 2 can be used. For any of the six allowed combinations of s,z when n is even (three when n is odd), each possible equation (13) is represented by a point in the h,m plane. The equations for a given value of n are represented by lattice points $m \leq n$. Since by definition $0 \leq w \leq m$, we have $-m + (s-2z) \leq h \leq +m + (s-2z)$; hence, for each s,z pair (subgraph), the points fill a triangular array. For purposes of counting it is convenient to think of each point as the center of a one-by-two rectangle, the rectangles filling the area. The points (equations) satisfying $h = kN$ lie on a series of equidistant horizontal lines spaced by a distance N.

For the group C_1 all the points must be counted as a function of n, i.e., up to $m = n$ inclusive, leading to

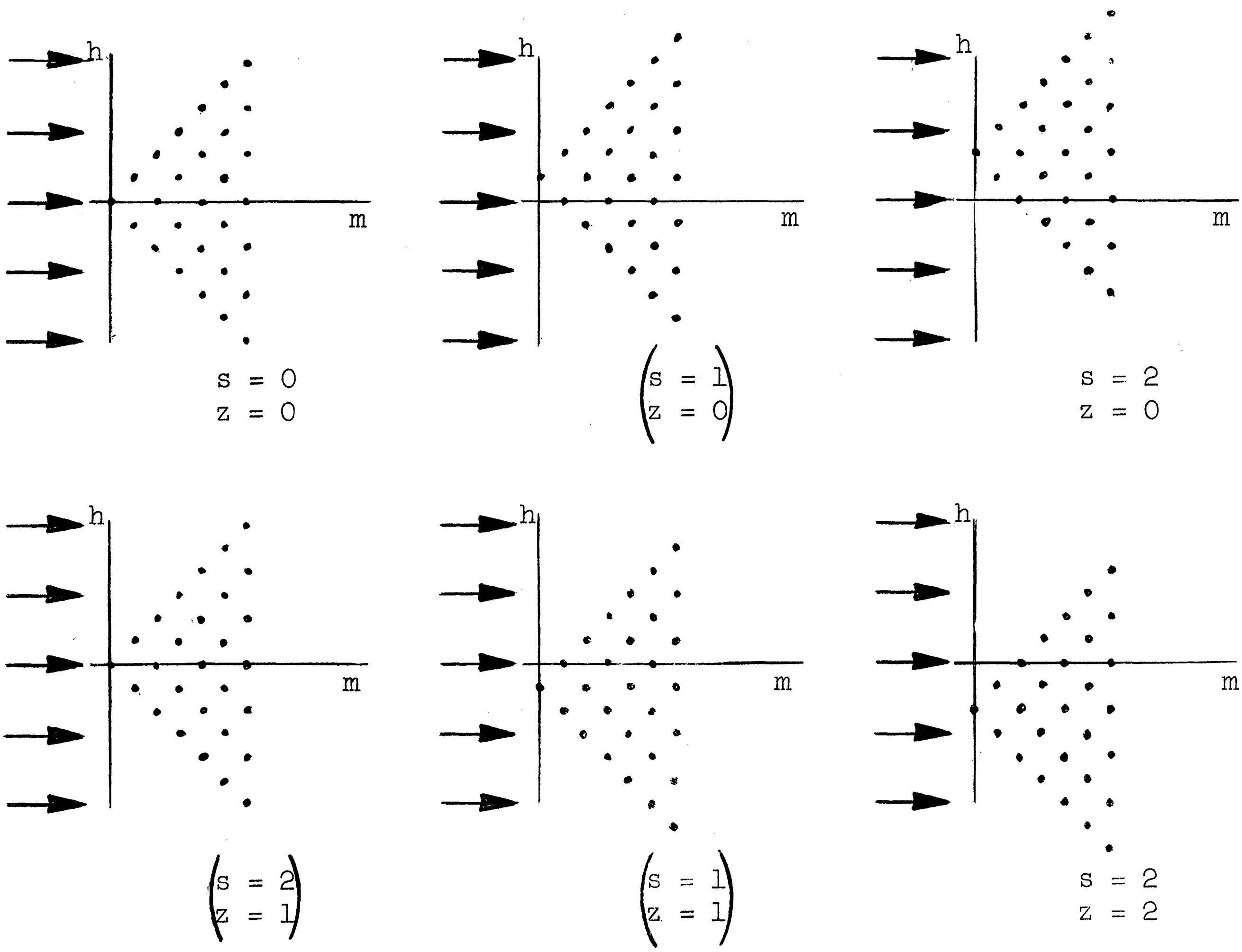
$$I_{C_1}(n) = P_C(n) = E_C(n) = K_{C_1}(n) = a_o n^2 + b_o n + c_o \quad , \qquad (20)$$

where, for n = even, $a_o = 3$, $b_o = 9$, $c_o = 6$, and, for n = odd, $a_o = 3/2$, $b_o = 9/2$, $c_o = 3$.

For $C_N (N > 1)$ the number of points lying on the horizontal lines $h = kN$ must be counted and is easily seen to be of the form $an^2 + bn + c$, where

$$a = a_o/N \qquad (21)$$

stems from the main triangle area covered by these lines (i.e., the rectangles of the lattice points on these lines) while



Points represent E-equations (13) in h,m plane for the various possible combinations of s and z. Arrows indicate K-equations for which h = kN. The case illustrated is N = 3. For n = even all six diagrams are valid; for n = odd, only those with parentheses.

Figure 2. Counting diagram.

$$\left.\begin{array}{llll} b & = & b_o/N & \text{for } N = \text{odd} \\ b & = & (b_o + 1)/N & \text{for } N = \text{even},\ n = \text{even} \\ b & = & (b_o + 1/2)/N & \text{for } N = \text{even},\ n = \text{odd} \end{array}\right\} \quad (22)$$

stems from circumference points with $h = kN$ whose rectangle areas stick out beyond the main triangle area. The values of c are most easily evaluated in practice by solving for c for some low value of n for which I_{C_N} has been counted. In this way the formulas of Table XI for the C classes result.

Case 2. Groups D_N $(N = 2,3,4,6)$

The quantities on the right-hand side of (18) will now be interpreted after the effect of a binary axis along k_1 has been taken into account. This effect is manifest in two ways: certain brackets vanish, reducing $P(n)$, and certain equations about k_3 must be dropped, reducing $E(n)$, as will now be shown.

According to Corollary I, all brackets for which the index 1 occurs an odd number of times vanish. In any bracket the index 1 occurs $p + n - m$ times inside and $1/2(s - \theta)$ times outside, together $p + n - m + 1/2\ (s - \theta)$ times. On the other hand, any equation (13) about k_3 contains brackets with the same n,m,s, but different p,θ. The coefficient $g\epsilon$ of any such bracket is $i^{p+1/2(s-\theta)}\ i^s$ times a real factor. Thus, if $n - m + s$ is even, then all brackets with imaginary coefficients in the equations (13) about k_3 vanish due to the binary axis about k_1, while if $n - m + s$ is odd, those with real coefficients vanish. Thus, every equation (13) about k_3 becomes equivalent to its complex conjugate, and in order to find $E^*_{D_N}(n)$ it is only necessary to count points $h \neq kN$ for which $h > 0$, i.e., the upper half of the counting diagram of Figure 2. Consequently

$$E^*_{D_N}(n) = 1/2\ E^*_{C_N}(n) \quad . \qquad (23)$$

The number of possible brackets after introducing the binary axis k_1 is clearly

$$P_{D_N}(n) = I_{C_{2h}}(n) \quad , \qquad (23a)$$

or with (18) and (20)

$$I_{D_N}(n) \;=\; I_{C_{2h}}(n) - 1/2\,[I_{C_1}(n) - I_{C_N}(n)] \;. \qquad (24)$$

Substituting the results found under Case 1 for $I_{C_{2h}}$ and I_{C_1}, we have for

$$n = \text{even} \qquad I_{D_N}(n) \;=\; 1/2\, I_{C_N}(n) + 1/2\, n + 1 \qquad (24a)$$

$$n = \text{odd} \qquad I_{D_N}(n) \;=\; 1/2\, I_{C_N}(n) + 1/4\, n + 1/4 \qquad (24b)$$

Case 3. Groups T_h, O_h and the Isotropic Case

For the class T_h, analysis of the effect of cyclic permutations leads immediately to

$$I_{T_h} \;=\; 1/3\; I_{D_{2h}} \;,$$

while for O_h case various simple ways of counting yield the results of Table XI.

5. EXPLICIT FORMS OF THE GALVANOMAGNETIC TENSOR UP TO B^2

For the practical purpose of reading off the explicit form of the galvanomagnetic tensor component $\rho^{\alpha 1} = F^{\alpha}/J^{1}$ in terms of the brackets, the tables of this section have been compiled. These give $\rho^{\alpha 1}$ for arbitrary orientation of the sample and the magnetic field with respect to the crystal axes and for all crystal structures except S_2.

It was shown in Section 2b that

$$\rho^{\alpha 1} \;=\; \rho_{ji}\, \ell_i^{\alpha}\, \ell_j^{1} \;=\; \frac{\Delta_{ij}}{\Delta}\, \ell_i^{\alpha}\, \ell_j^{1} \;, \qquad (25)$$

where Δ_{ij} is the cofactor of σ_{ij} in $\Delta = \det \sigma_{ij}$, and ℓ_i^{α} is the direction cosine of the laboratory coordinate axis α with respect to the symmetry coordinate axis i. For $\alpha = 1$ the equation represents the magneto resistance, for $\alpha \neq 1$ the Hall effect, and this is true for all that follows. The expansion of all σ_{ij} in powers of B leads to

TABLE XI

THE NUMBER OF NONVANISHING INDEPENDENT BRACKETS $an^2 + bn + c$

Group	n	a	b	c
$C_1=S_2$	even	3	9	6
	odd	3/2	9/2	3
C_{2h}	even	3/2	5	4
	odd	3/4	5/2	7/4
C_{3i}	even	1	3	2
	odd	1/2	3/2	1
C_{4h}	even	3/4	5/2	2
	4k+1	3/8	5/4	11/8
	4k-1	3/8	5/4	7/8
C_{6h}	6k-2	1/2	5/3	4/3
	6k			2
	6k+2			8/3
	6k-1	1/4	5/6	7/12
	6k+1			23/12
	6k+3			5/4
D_{2h}	even	3/4	3	3
	odd	3/8	3/2	9/8
D_{3i}	even	1/2	2	2
	odd	1/4	1	3/4
D_{4h}	even	3/8	7/4	2
	4k+1	3/16	7/8	15/16
	4k-1	3/16	7/8	11/16
D_{6h}	6k-2	1/4	4/3	5/3
	6k			2
	6k+2			7/3
	6k-1	1/8	2/3	13/24
	6k+1			29/24
	6k+3			7/8
T_h	even	1/4	1	1
	odd	1/8	1/2	3/8
O_h	even	1/8	3/4	1
	4k+1	1/16	3/8	9/16
	4k-1	1/16	3/8	5/16

$$\rho^{\alpha 1} \equiv \left(\sum_{\eta} \rho^{\alpha 1}_{2\eta} B^{2\eta} + \sum_{\eta} Q^{\alpha 1}_{2\eta+1} B^{2\eta+1} \right) \Big/ \sum_{\eta} M_{2\eta} B^{2\eta}$$

$$= \frac{1}{M_o} \left(P_o^{\alpha 1} + Q_1^{\alpha 1} B + \left(P_2^{\alpha 1} - \frac{P_o^{\alpha 1}}{M_o} M_2 \right) B^2 --- \right) . \tag{26}$$

Table XII gives M_o. Table XIII gives the nonvanishing coefficients of $\ell_i^1 \ell_j^{\alpha}$ in $P_o^{\alpha 1}$. Table XIV gives the coefficients of γ_k, the direction cosines of $\underline{B}$ in the crystal coordinate system, resulting in $Q_1^{\alpha 1}$. For the purpose of tabulating the coefficient of B^2 we write

$$\left(P_2^{\alpha 1} - \frac{P_o^{\alpha 1}}{M_o} M_2 \right) = R_2^{\alpha 1} = R_{k\ell}^{\alpha 1} \gamma_k \gamma_\ell . \tag{27}$$

Tables XV, XVI, and XVII give the $R_{k\ell}^{\alpha 1}$ for the various classes. Coefficients for higher powers than B^2 can be obtained similarly if needed. These tables are useful, for example, in determining what measurements must be made in order to determine all the independent brackets (material constants). In principle, a number of measurements at least equal to the number of independent brackets is needed. It is expedient to choose these with care. For example, no matter how many magneto resistance measurements are made, even with different samples, allowing variation of ℓ_i^{α} and γ_k, one cannot obtain all brackets individually. Combinations of Hall and magneto resistance measurements work most efficiently.

In Table XIV ℓ_k^{β} has been used as an abbreviation defined by

$$\ell_k^{\beta} \equiv \ell_i^1 \ell_j^{\alpha} - \ell_j^1 \ell_i^{\alpha} ,$$

where, if $\alpha = 1$, ℓ_k^{β} automatically vanishes in agreement with the evenness of the magneto resistance, while, if $\alpha \neq 1$, the subscripts ijk must be a permutation of 123 of the same parity as the superscripts $1\alpha\beta$. In that case ℓ_k^{β} is the direction cosine between the symmetry axis k and the laboratory axis β.

TABLE XII

THE EXPLICIT FORM OF M_o

C_{2h}	$[ooo]_{33}([ooo]_{11}[ooo]_{22} - [ooo]_{12}^2)$
D_{2h}	$[ooo]_{33}[ooo]_{11}[ooo]_{22}$
C_{3i}, D_{3i}, C_{4h}, D_{4h}, C_{6h}, D_{6h}	$[ooo]_{33}[ooo]_{11}^2$
T_h, O_h	$[ooo]_{11}^3$

TABLE XIII

THE EXPLICIT FORM OF $P_o^{\alpha 1}$

	$\ell_1^1 \ell_1^\alpha$	$\ell_2^1 \ell_2^\alpha$	$\ell_3^1 \ell_3^\alpha$	$\ell_1^1 \ell_2^\alpha + \ell_2^1 \ell_1^\alpha$
C_{2h}	$[ooo]_{22}[ooo]_{33}$	$[ooo]_{33}[ooo]_{11}$	$[ooo]_{11}[ooo]_{22} - [ooo]_{12}^2$	$-[ooo]_{33}[ooo]_{12}$
D_{2h}	$[ooo]_{22}[ooo]_{33}$	$[ooo]_{33}[ooo]_{11}$	$[ooo]_{11}[ooo]_{22}$	
C_{3i}, D_{3i}, C_{4h}, D_{4h}, C_{6h}, D_{6h}	$[ooo]_{11}[ooo]_{33}$	$[ooo]_{11}[ooo]_{33}$	$[ooo]_{11}^2$	
T_h, O_h	$[ooo]_{11}^2$	$[ooo]_{11}^2$	$[ooo]_{11}^2$	

TABLE XIV

THE EXPLICIT FORM OF $Q_1^{\alpha_1}$

	γ_1	γ_2	γ_3
C_{2h}	$\ell_1^\beta([100]_{23}[000]_{11}+[100]_{31}[000]_{12})$ $+\ell_2^\beta([100]_{31}[000]_{22}+[100]_{23}[000]_{12})$	$\ell_1^\beta([010]_{23}[000]_{11}+[010]_{31}[000]_{12})$ $+\ell_2^\beta([010]_{31}[000]_{22}+[010]_{23}[000]_{12})$	$\ell_3^\beta[001]_{12}[000]_{33}$
D_{2h}	$\ell_1^\beta[100]_{23}[000]_{11}$	$\ell_2^\beta[010]_{31}[000]_{22}$	$\ell_3^\beta[001]_{12}[000]_{33}$
C_{3i}, C_{4h}, C_{6h}	$\ell_1^\beta[100]_{23}[000]_{11}-\ell_2^\beta[010]_{23}[000]_{22}$	$\ell_1^\beta[010]_{23}[000]_{11}+\ell_2^\beta[100]_{23}[000]_{11}$	$\ell_3^\beta[001]_{12}[000]_{33}$
D_{3i}, D_{4h}, D_{6h} / T_h, O_h	$\ell_1^\beta[100]_{23}[000]_{11}$	$\ell_2^\beta[100]_{23}[000]_{11}$	$\ell_3^\beta[001]_{12}[000]_{33}$

TABLE XV

THE EXPLICIT FORM OF R_2 FOR C_{2h}, D_{2h}

$-R_{11}^{\alpha 1}$	$l_1^{\alpha} l_1^{1} \{ ([000]_{33} [200]_{11} + [100]_{31}^{2*}) A/B + 2([100]_{23} [100]_{31} - [000]_{33} [200]_{12}) A + ([000]_{33} [200]_{22} + [100]_{23}^{2}) AB \} +$ $+ l_2^{\alpha} l_2^{1} \{ ([000]_{33} [200]_{22} + [100]_{23}^{2}) B/A + 2([100]_{23} [100]_{31} - [000]_{33} [200]_{12}) B + ([000]_{11} [200]_{33} + [100]_{31}^{2}) AB \} +$ $+ l_3^{\alpha} l_3^{1} \{ [000]_{11} [000]_{22} [200]_{33} + [000]_{11} [100]_{23}^{2} + [000]_{22} [100]_{31}^{2*} + (2[100]_{23} [100]_{31} - [000]_{12} [200]_{33}) (1 - AB) [000]_{12}^{*} \} / [000]_{33} +$ $+ (l_1^{\alpha} l_2^{1} + l_2^{\alpha} l_1^{1}) \{ ([000]_{33} [200]_{12} - [100]_{23} [100]_{31}) (1 + AB) - ([000]_{33} [200]_{11} + [100]_{31}^{2}) A - ([000]_{33} [200]_{22} + [100]_{23}^{2}) B \}^{*}$
$-R_{22}^{\alpha 1}$	$l_1^{\alpha} l_1^{1} \{ ([000]_{33} [020]_{11} + [010]_{31}^{2}) A/B + 2([010]_{31} [010]_{23} - [000]_{33} [020]_{12}) A + ([000]_{33} [020]_{22} + [010]_{23}^{2}) AB \} +$ $+ l_2^{\alpha} l_2^{1} \{ ([000]_{33} [020]_{22} + [010]_{23}^{2*}) B/A + 2([010]_{31} [010]_{23} - [000]_{33} [020]_{12}) B + ([000]_{11} [020]_{33} + [010]_{31}^{2}) AB \} +$ $+ l_3^{\alpha} l_3^{1} \{ ([000]_{22} [020]_{33} [000]_{11} + [000]_{11} [010]_{23}^{2*} + [000]_{22} [010]_{31}^{2}) + (2[010]_{23} [010]_{31} - [000]_{12} [020]_{33}) (1 - AB) [000]_{12}^{*} \} / [000]_{33} +$ $+ (l_1^{\alpha} l_2^{1} + l_2^{\alpha} l_1^{1}) \{ ([000]_{33} [020]_{12} - [010]_{31} [010]_{23}) (1 + AB) - ([000]_{33} [020]_{11} + [010]_{31}^{2}) A - ([000]_{33} [020]_{22} + [010]_{23}^{2}) B \}^{*}$
$R_{33}^{\alpha 1}$	$l_1^{\alpha} l_1^{1} \{ ([000]_{22} [002]_{11} + [001]_{12}^{2}) / [000]_{11} - 2[002]_{12} A + [002]_{22} AB \} [000]_{33} +$ $+ l_2^{\alpha} l_2^{1} \{ ([000]_{11} [002]_{22} + [001]_{12}^{2}) / [000]_{22} - 2[002]_{12} B + [002]_{11} AB \} [000]_{33} +$ $+ l_3^{\alpha} l_3^{1} (1 - AB)^2 [002]_{33} [000]_{11} [000]_{22} / [000]_{33} +$ $+ (l_1^{\alpha} l_2^{1} + l_2^{\alpha} l_1^{1}) \{ (1 + AB) [002]_{12} - ([000]_{22} [002]_{11} + [000]_{11} [002]_{22} + [001]_{12}^{2}) A / [000]_{22} \}^{*} [000]_{33}$
$-(R_{23}^{\alpha 1} + R_{32}^{\alpha 1})$	$(l_2^{\alpha} l_3^{1} + l_3^{\alpha} l_2^{1}) ([000]_{11} [011]_{23} - [001]_{12} [010]_{31} - [000]_{12} [011]_{31}^{*}) + (l_3^{\alpha} l_1^{1} + l_1^{\alpha} l_3^{1}) ([000]_{22} [011]_{31} - [001]_{12} [010]_{23} - [000]_{12} [011]_{23})^{*} (1 - AB)$
$-(R_{31}^{\alpha 1} + R_{13}^{\alpha 1})$	$(l_2^{\alpha} l_3^{1} + l_3^{\alpha} l_2^{1}) ([000]_{11} [101]_{23} - [001]_{12} [100]_{31} - [000]_{12} [101]_{31})^{*} + (l_3^{\alpha} l_1^{1} + l_1^{\alpha} l_3^{1}) ([000]_{22} [101]_{31} - [001]_{12} [100]_{23} - [000]_{12} [101]_{23}^{*}) (1 - AB)$
$-(R_{12}^{\alpha 1} + R_{21}^{\alpha 1})$	$l_1^{\alpha} l_1^{1} \{ ([000]_{33} [110]_{11} + 2[010]_{31} [100]_{31}) A/B + (2[100]_{23} [010]_{31} + 2[010]_{23} [100]_{31} - [000]_{33} [110]_{12}) A +$ $+ ([000]_{22} [110]_{33} + [000]_{33} [110]_{22} + 2[100]_{23} [010]_{23}) AB \}^{*} +$ $+ l_2^{\alpha} l_2^{1} \{ ([000]_{33} [110]_{22} + 2[100]_{23} [010]_{23}) B/A + (2[100]_{23} [010]_{31} + 2[010]_{23} [100]_{31} - [000]_{33} [110]_{12}) B +$ $+ ([000]_{11} [110]_{33} + [000]_{33} [110]_{11} + 2[100]_{31} [010]_{31}) AB \}^{*} +$ $+ l_3^{\alpha} l_3^{1} \{ ([000]_{22} [110]_{33} [000]_{11} + 2[000]_{22} [100]_{31} [010]_{31} + 2[100]_{23} [010]_{23} [000]_{11}) +$ $+ (2[100]_{23} [010]_{31} + 2[010]_{23} [100]_{31} - [000]_{12} [110]_{33}) (1 - AB) [000]_{12} \}^{*} / [000]_{33} +$ $+ (l_1^{\alpha} l_2^{1} + l_2^{\alpha} l_1^{1}) \{ ([000]_{33} [110]_{12} - [100]_{23} [010]_{31} - [010]_{23} [100]_{31}) (1 + AB) -$ $- ([000]_{33} [110]_{11} + 2[010]_{31} [100]_{31}) A - ([000]_{33} [110]_{22} + 2[100]_{23} [010]_{23}) B \}$

A $\quad [000]_{12}^{*}/[000]_{11}$ $\qquad$ $A/B = 1/(B/A) = [000]_{22}/[000]_{11}$

B $\quad [000]_{12}^{*}/[000]_{22}$ $\qquad$ * means zero for D_{2h}

TABLE XVI

THE EXPLICIT FORM OF R_2 FOR C_{3i}, C_{4h}, C_{6h}, D_{3i}, D_{4h}, D_{6h}

$-R_{11}^{\alpha 1}$	$\ell_1^{\alpha}\ell_1^{1}([200]_{11}\,[000]_{33} + [100]_{31}^{2*}) + (\ell_2^{\alpha}\ell_3^{1} + \ell_3^{\alpha}\ell_2^{1})\,[000]_{11}\,[200]_{23}^{\Delta}$ $+ \ell_2^{\alpha}\ell_2^{1}([200]_{22}\,[000]_{33} + [100]_{23}^{2}) + (\ell_3^{\alpha}\ell_1^{1} + \ell_1^{\alpha}\ell_3^{1})\,[000]_{11}\,[200]_{31}^{\Delta *}$ $+ \ell_3^{\alpha}\ell_3^{1}([200]_{33}\,[000]_{11} + [100]_{23}^{2} + [100]_{31}^{2*})\,[000]_{11}/[000]_{33} + (\ell_1^{\alpha}\ell_2^{1} + \ell_2^{\alpha}\ell_1^{1})\,([000]_{33}\,[200]_{12}$
$-R_{22}^{\alpha 1}$	$\ell_1^{\alpha}\ell_1^{1}([200]_{22}\,[000]_{33} + [100]_{23}^{2}) - (\ell_2^{\alpha}\ell_3^{1} + \ell_3^{\alpha}\ell_2^{1})\,[000]_{11}\,[200]_{23}^{\Delta}$ $+ \ell_2^{\alpha}\ell_2^{1}([200]_{11}\,[000]_{33} + [100]_{31}^{2*}) - (\ell_3^{\alpha}\ell_1^{1} + \ell_1^{\alpha}\ell_3^{1})\,[000]_{11}\,[200]_{31}^{\Delta *}$ $+ \ell_3^{\alpha}\ell_3^{1}([200]_{33}\,[000]_{11} + [100]_{23}^{2} + [100]_{31}^{2*})\,[000]_{11}/[000]_{33} - (\ell_1^{\alpha}\ell_2^{1} + \ell_2^{\alpha}\ell_1^{1})\,([000]_{33}\,[200]_{12}$
$-R_{33}^{\alpha 1}$	$(\ell_1^{\alpha}\ell_1^{1} + \ell_2^{\alpha}\ell_2^{1})\,([002]_{11}\,[000]_{33} + [001]_{12}^{2}\,[000]_{33}/[000]_{11}) + \ell_3^{\alpha}\ell_3^{1}[002]_{33}\,[000]_{11}^{2}/[000]_{33}$
$-(R_{23}^{\alpha 1} + R_{32}^{\alpha 1})$	$(\ell_1^{\alpha}\ell_1^{1} - \ell_2^{\alpha}\ell_2^{1})\,[000]_{33}\,[011]_{11}^{\Delta} + (\ell_2^{\alpha}\ell_3^{1} + \ell_3^{\alpha}\ell_2^{1})\,([011]_{23}\,[000]_{11} - [100]_{23}\,[001]_{12})$ $+ (\ell_3^{\alpha}\ell_1^{1} + \ell_1^{\alpha}\ell_3^{1})\,([011]_{31}\,[000]_{11} + [100]_{31}\,[001]_{12})^{*} - (\ell_1^{\alpha}\ell_2^{1} + \ell_2^{\alpha}\ell_1^{1})\,[000]_{33}\,[101]_{11}^{\Delta *}$
$-(R_{31}^{\alpha 1} + R_{13}^{\alpha 1})$	$(\ell_1^{\alpha}\ell_1^{1} - \ell_2^{\alpha}\ell_2^{1})\,[000]_{33}\,[101]_{11}^{\Delta *} - (\ell_2^{\alpha}\ell_3^{1} + \ell_3^{\alpha}\ell_2^{1})\,([011]_{31}\,[000]_{11} + [100]_{31}\,[001]_{12})^{*}$ $+ (\ell_3^{\alpha}\ell_1^{1} + \ell_1^{\alpha}\ell_3^{1})([011]_{23}\,[000]_{11} - [100]_{23}\,[001]_{12}) + (\ell_1^{\alpha}\ell_2^{1} + \ell_2^{\alpha}\ell_1^{1})\,[000]_{33}\,[011]_{11}^{\Delta}$
$-(R_{12}^{\alpha 1} + R_{21}^{\alpha 1})$	$\ell_1^{\alpha}\ell_1^{1}([000]_{33}\,[110]_{11}^{\dagger} + 2[100]_{23}\,[100]_{31})^{*} + (\ell_1^{\alpha}\ell_2^{1} + \ell_2^{\alpha}\ell_1^{1})\,([000]_{33}\,[110]_{12}^{\ddagger} - [100]_{23}^{2} + [1$ $- \ell_2^{\alpha}\ell_2^{1}([000]_{33}\,[110]_{11} + 2[100]_{23}\,[100]_{31})^{*} - 2(\ell_2^{\alpha}\ell_3^{1} + \ell_3^{\alpha}\ell_2^{1})\,[000]_{11}\,[200]_{31}^{\Delta *} + 2(\ell_3^{\alpha}\ell_1^{1} + \ell_1^{\alpha}\ell$

* means zero for D_{3i}, D_{4h}, D_{6h}.

Δ means zero for C_{4h}, C_{6h}, D_{4h}, D_{6h}.

$\dagger$ means $[110]_{11} = -2[200]_{12}$ } for C_{3i}, C_{6h}, D_{3i}, D_{6h}.

$\ddagger$ means $[110]_{12} = [200]_{11} - [200]_{22}$ } for C_{3i}, C_{6h}, D_{3i}, D_{6h}.

TABLE XVII

THE EXPLICIT FORM OF R_2 FOR T_h AND O_h

$-R_{11}^{\alpha 1}$	$\ell_1^1 \ell_1^\alpha [200]_{11} [000]_{11} + \ell_2^1 \ell_2^\alpha ([200]_{22} [000]_{11} + [100]_{23}^2) + \ell_3^1 \ell_3^\alpha ([200]_{33}^* [000]_{11} + [100]_{23}^2)$
$-R_{22}^{\alpha 1}$	$\ell_1^1 \ell_1^\alpha ([200]_{33}^* [000]_{11} + [100]_{23}^2) + \ell_2^1 \ell_2^\alpha [200]_{11} [000]_{11} + \ell_3^1 \ell_3^\alpha ([200]_{22} [000]_{11} + [100]_{23}^2)$
$-R_{33}^{\alpha 1}$	$\ell_1^1 \ell_1^\alpha ([200]_{22} [000]_{11} + [100]_{23}^2) + \ell_2^1 \ell_2^\alpha ([200]_{33}^* [000]_{11} + [100]_{23}^2) + \ell_3^1 \ell_3^\alpha [200]_{11} [000]_{11}$
$-(R_{23}^{\alpha 1}+R_{32}^{\alpha 1})$	$(\ell_2^1 \ell_3^\alpha + \ell_3^1 \ell_2^\alpha)([011]_{23} [000]_{11} - [100]_{23}^2)$
$-(R_{31}^{\alpha 1}+R_{13}^{\alpha 1})$	$(\ell_3^1 \ell_1^\alpha + \ell_1^\alpha \ell_3^1)([011]_{23} [000]_{11} - [100]_{23}^2)$
$-(R_{12}^{\alpha 1}+R_{21}^{\alpha 1})$	$(\ell_1^1 \ell_2^\alpha + \ell_2^\alpha \ell_1^1)([011]_{23} [000]_{11} - [100]_{23}^2)$

For O_h * means $[200]_{33} = [200]_{22}$

For O_h Table XVII can be reduced to the following simplified form:

$$-R_2 = ([200]_{22} [000]_{11} + [100]_{23}^2)\, \delta^{\alpha 1} + ([100]_{23}^2 - [011]_{23} [000]_{11}) \left(\sum_{i=1,2,3} \gamma_i \ell_i^\alpha \right) \left(\sum_{j=1,2,3} \gamma_j \ell_j^1 \right)$$
$$+ [000]_{11} ([200]_{11} - [200]_{22} - [011]_{23}) \sum_{i=1,2,3} \gamma_i^2 \ell_i^\alpha \ell_i^1$$

with $\delta^{\alpha 1} = \begin{cases} 1 \text{ if } \alpha = 1 \\ 0 \text{ otherwise} \end{cases}$.

When $\alpha = 1$, this simplified form becomes identical, except a multiplying constant, to equation (5) given by Pearson and Suhl (Ref. 11); see Table XVIII.

6. DISCUSSION

The anisotropy of galvanomagnetic effects, first studied by Righi in 1883, appeared in many works from time to time. However, the crystallographic effects have never been taken into account comprehensively. An overall investigation of the crystallographic effects of the 32 point groups upon the isothermal galvanomagnetic effects is attempted in the present paper. The results include as special cases the work of Voigt and of Juretschke concerning the tables of brackets, the work of Seitz, Pearson and Suhl, and Goldberg and Davis concerning the formulas for cubic crystals, and some of the work of Kohler, insofar as it is concordant with Onsager's relations.

For D_{3i} and $m \leq 4$, Juretschke's[15] results agree completely with ours presented in Table X, except for a different notation. In order to facilitate the comparison of our bracket notation with the notations used by Seitz and by Pearson and Suhl for the case O_h, Table XVIII has been prepared.

TABLE XVIII

NOTATIONS OF VARIOUS AUTHORS

Seitz's Notation	Pearson and Suhl's Notation	Bracket Notation
$\sigma_0 = 1/\rho_0$		$[000]_{11}$
α		$[100]_{23} = [001]_{12}$
β		$[200]_{22} = [002]_{11}$
γ		$[011]_{23} = [110]_{12}$
$\beta + \gamma + \delta$		$[200]_{11} = [002]_{33}$
	a	$[100]_{23}/[000]_{11}$
	b	$([200]_{22}[000]_{11}+[100]_{23}^2)/[000]_{11}^2$
	c	$([100]_{23}^2-[011]_{23}[000]_{11})/[000]_{11}^2$
	d	$([200]_{11}-[200]_{22}-[011]_{23})/[000]_{11}$

The methods developed here can be extended to all thermo-galvanomagnetic effects. We hope to follow up this paper by one which gives the electron theoretical definition of the brackets and further developments regarding the effects of crystallographic symmetry by means of the electron theory of solids.

Many investigators limit themselves to cases where the magnetic field is either parallel or normal to the current, or in the plane of the current and the Hall probes. Such limitations seem unnecessary with the broadened definitions of the galvanomagnetic effects, which permit the magnetic field to be arbitrarily oriented (Seitz did this for the magneto resistance of cubic crystals including terms up to B^2). Therefore all the galvanomagnetic effects bearing various conventional names, such as the transverse and longitudinal magneto resistance, the Hall effect, the "planar Hall field," and the Corbino effect, are included as special cases. They can all be analyzed in terms of an ascending power series of the magnetic field; the only known exception is the oscillatory behavior at very low temperatures. The Corbiho effect, about which, to the best of our knowledge no work has been done on single crystals, will be dealt with in a separate paper.

We have also brought to light certain properties regarding the parity of the galvanomagnetic effects, about which a certain lack of consistency is to be found in the literature. In particular, the magneto resistance is necessarily an even function of the magnetic field, while, contrary to the odd-Hall-effect convention, it was proved here that the Hall effect is in general neither an odd nor an even function of B, but can be purely odd or purely even or zero when proper conditions are satisfied. These contentions are firmly supported by experiments, for example by Logan and Marcus, and by Goldberg and Davis.

APPENDIX I

Proof of the Theorem Concerning an N-Fold Rotation Axis Along k_3

Let $k_1'k_2'k_3'$ be a set of symmetry coordinates of a point and let $k_1''k_2''k_3''$ be the transformed set of the <u>same</u> point after rotation of the coordinate axes through an angle $\phi = 2\pi/N$ about k_3. With respect to these two systems of axes the components of a tensor T of arbitrary rank are related by

$$T''_{ij\ldots\ell} = \sum_{\lambda\mu\ldots\tau} a_{i\lambda}\, a_{j\mu} \ldots a_{\ell\tau}\, T'_{\lambda\mu\ldots\tau} \, , \tag{A.1}$$

where

$$a_{i\lambda} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{A.2}$$

This is true in particular for the components of the position vector $\underline{k}$ of a point, of the components of the magnetic field vector B, and of the components σ_{ij} of the second-rank conductivity tensor. Thus by such a rotation of coordinate axes any equation between singly primed tensor components is transformed into one with doubly primed tensor components. If the rotation is a "covering" operation of the crystal, then the equation must be invariant, i.e., its form in terms of singly primed quantities must be identical to that in terms of doubly primed quantities. This principle can be applied to equation (10). Thus, for a covering operation the coefficients (brackets) in the singly primed and doubly primed forms of (10) must be identical, hence can be written without any primes.

Now the doubly primed forms of equations (10) can be transformed by applying the equations A.1 and A.2 to the doubly primed components of σ and B. The transformed equations so obtained in terms of singly primed components must be equivalent to equations (10) in their direct singly primed form. This equivalence requirement yields certain identities between the brackets. It will be shown that these identities are just described by equations (13) and (14). In order to simplify the proof we shall not apply the above reasoning to the Cartesian components of the tensors involved but rather refer to a pair of coordinate systems of a different type (complex, nonorthogonal) defined by

$$\left.\begin{aligned} \overline{k_1'} &= k_1' + i\,k_2' \\ \overline{k_2'} &= k_1' - i\,k_2' \\ \overline{k_3'} &= k_3' \end{aligned}\right\} \quad (A.3)$$

and likewise for double primes. Quantities referring to the complex coordinates will be marked by a bar throughout. We define the complex components of $\underline{B}$ by

$$\left.\begin{aligned} \overline{B_1'} &= B_1' + i\,B_2' \\ \overline{B_2'} &= B_1' - i\,B_2' \\ \overline{B_3'} &= B_3' \end{aligned}\right\} \quad (A.4)$$

and likewise for double primes. The complex components of the second-rank conductivity tensor are defined by*

*For a tensor of arbitrary rank n the complex component $\overline{T}_{ij\ldots\ell}$ is defined as follows.

a. Replace every index in the given order by a symbol according to this scheme: the index one by (1_1+i_2), the index two by (1_1-i_2), the index three by (1_3).
b. Multiply the n-fold product of symbols so obtained according to the associative and distributive law, but do not use the commutative law.
c. Replace each "term" of the symbolic polynomial so obtained by T with the indices of that term in the given order and with a coefficient equal to the product of the coefficient parts (upper parts) of the "factors" of that term. The resulting polynomial in T is the desired expression.

For example, one wants to find the appropriate definition of $\overline{T}_{123}$. According to (a) he writes the symbol $(1_1+i_2)(1_1-i_2)(1_3)$. According to (b) he obtains the symbolic polynomial $(1_1)(1_1)(1_3) - (1_1)(i_2)(1_3) + (i_2)(1_1)(1_3) - (i_2)(i_2)(1_3)$. According to (c) the definition is now $\overline{T}_{123} = T_{113} - i\,T_{123} + i\,T_{213} + T_{223}$.

$$\overline{\sigma_{ij}} = \begin{pmatrix} \sigma_{11} - \sigma_{22} + i(\sigma_{12} + \sigma_{21}) & \sigma_{11} + \sigma_{22} - i(\sigma_{12} - \sigma_{21}) & \sigma_{13} + i\sigma_{23} \\ \sigma_{11} + \sigma_{22} + i(\sigma_{12} - \sigma_{21}) & \sigma_{11} - \sigma_{22} - i(\sigma_{12} + \sigma_{21}) & \sigma_{13} - i\sigma_{23} \\ \sigma_{31} + i\sigma_{32} & \sigma_{31} - i\sigma_{32} & \sigma_{33} \end{pmatrix} \quad (A.5)$$

According to Onsager's relation

$$\overline{\sigma_{ij}}(\underline{B}) = \overline{\sigma_{ji}}(-\underline{B}) \quad , \qquad (A.6)$$

hence terms below the diagonal of A.5 are dependent and it suffices to consider those above the diagonal.

For convenience we shall now introduce another notation. Let s denote the number of ones and twos together, and z the number of twos, among the indices of a $\overline{\sigma_{ij}}$. This definition of z is consistent with that given in Section 3b. The numbers s,z define uniquely one of the six independent pairs of indices ij and vice versa. We write (note the indices between parentheses):

$$\overline{\sigma_{(s,z)}} \equiv \overline{\sigma_{ij}} \quad . \qquad (A.7)$$

Thus, for example, $\overline{\sigma_{(11)}}$ is another notation for $\overline{\sigma_{23}}$. It can be verified by direct substitution of these definitions and comparison with A.1 and A.2 that the complex tensor components as defined transform under a rotation of coordinates about k_3 according to

$$\overline{T''_{ij\ldots\ell}} = \sum_{\lambda\mu\ldots\tau} \overline{a_{i\lambda}}\,\overline{a_{j\mu}} \cdots \overline{a_{\ell\tau}}\,\overline{T'_{\lambda\mu\ldots\tau}} \qquad (A.8)$$

with the diagonalized matrix

$$\overline{a_{i\lambda}} = \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & e^{i\phi} & 0 \\ 0 & 0 & 1 \end{pmatrix} . \qquad (A.9)$$

In particular,

$$\left.\begin{aligned}\overline{B_1''} &= \overline{B_1'}\ e^{-i\phi}\\ \overline{B_2''} &= \overline{B_2'}\ e^{i\phi}\\ \overline{B_3''} &= \overline{B_3'}\\ \overline{\sigma''}_{(s,z)}(\underline{B}) &= \overline{\sigma'}_{(s,z)}(\underline{B})\ e^{-i\phi(s-2z)} \quad .\end{aligned}\right\} \quad (A.10)$$

We are now ready to apply the invariance principle. The equations to which it will be applied are the expansions of $\overline{\sigma'}_{(s,z)}$ and $\overline{\sigma''}_{(s,z)}$ in powers of $\overline{B_k'}$ and $\overline{B_k''}$, respectively, analogous to equation (10):

$$\overline{\sigma'}_{(s,z)}(\underline{B}) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{w=0}^{m} \overline{C'}_{(s,z)}(n,m,w)\ \overline{B_1'}^{w}\ \overline{B_2'}^{m-w}\ \overline{B_3'}^{n-m} \quad . \qquad (A.11)$$

Comparison of A.11 with equations (10) and (11) yields

$$\overline{C'}_{(s,z)}(n,m,w) \equiv (1/2)^m\ (-)^w \sum_{p=0}^{m} \sum_{\Theta} g(m,p,w)\ \epsilon(s,\Theta,z)\ [m-p,p,n-m]_{(s,\Theta)}, \qquad (A.12)$$

where g and ϵ are the functions defined in the text by equation (15) and Table III. Equations of identical form, but with double primes, hold for the components with respect to the doubly primed coordinate system.

From the equality of singly and doubly primed brackets for a covering operation of the crystal, arrived at earlier, it follows now that

$$\overline{C''}_{(s,z)}(n,m,w) = \overline{C'}_{(s,z)}(n,m,w) \quad . \qquad (A.13)$$

According to the plan outlined at the beginning of this section, one must now express the doubly primed components of $\overline{\sigma''}_{(s,z)}$ and $\overline{B_k''}$ in the doubly primed analog of A.11 in terms of the singly primed ones by means of A.10.

We obtain

$$\overline{\sigma'}_{(s,z)} = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{w=0}^{m} \overline{C''}_{(s,z)}(n,m,w)\ e^{i\phi h}\ \overline{B_1'}^{w}\ \overline{B_2'}^{m-w}\ \overline{B_3'}^{n-m} \qquad (A.14)$$

with $h = m + s - 2(w + z)$. Comparing A.14 with A.11 it is seen in view of A.13 that the two results are only compatible if

$$\left.\begin{array}{lll} \text{either} & \overline{C''}_{(s,z)}(n,m,w) & = 0 \\ \text{or} & e^{i\phi h} & = 1 \ . \end{array}\right\} \quad (A.15)$$

In connection with A.12, the equations A.15 are identical with (13) and (14) in the text, and the theorem is proved.

APPENDIX II

Completeness of the Equations (13)

Consider the complete set of equations (13) for given n,m,s, that is, the equations (13) for all values of $0 \leq w \leq m$ and $0 \leq z \leq s$, regardless of the value of h.

Theorem

The only solution of the complete set of equations (13) for given n,m,s is that all the brackets with the given n,m,s vanish.

Proof

In the power-series expansion (10) the brackets for given n,m,s, with the six independent pairs of outer indices, are independent constants (as long as no symmetry restrictions are introduced).

The moduli of the transformations from B_i to $\overline{B_i}$ and from σ_{ij} to $\overline{\sigma_{ij}}$ or $\overline{\sigma}_{(s,z)}$ are nonvanishing, according to A.4 and A.5. Consequently, in the power-series expansion A.11 the constants $C_{(s,z)}$ for given n,m,s, are independent constants and the equations A.12 for given n,m,s can be inverted, leading to homogeneous expressions of the brackets in terms of the C's.

The complete set of equations (13) for given n,m,s, states that all C's vanish; consequently, all brackets with these n,m,s values vanish.

q.e.d.

In this proof use has been made of the fact that for given n,m,s, the number of brackets $[m-p,p,n-m]_{(s,\theta)}$ is equal to the number of constants $C_{(s,z)}$ (n,m,w), hence equal to the number of equations (13) [without (14)]. This equality is easily verified. Indeed, the number of equations for given n,m,s, is determined by the ranges of the integers w and z, given by $0 \leq w \leq m$ and $0 \leq z \leq s$, while the number of brackets is determined by the ranges of the integers p and $1/2(s - \Theta)$, given by $0 \leq p \leq m$ and $0 \leq 1/2(s - \Theta) \leq s$.

The theorem of this appendix is useful in spotting vanishing brackets and in counting nonvanishing ones. It also follows from this theorem and Appendix I that the symmetry properties of the brackets are completely described by the equations (13) with the condition (14).

APPENDIX III

Proof of Table VIII - Zero Brackets for a Threefold Axis of Symmetry

Consider the set of equations (13) for given values of n,m,s and different w,z. According to Corollary IV and the remarks made immediately thereafter, it is expedient to select from the original complex equations those satisfying the selection rule

$$s - 2z \geq 0 \tag{C.1}$$

and equating their real and imaginary parts to zero. The number of real equations so obtained is equal to the number of the original complex equations with $s - 2z$ unrestricted by C.1. It is also equal to the number of brackets having the given values n,m,s that occur in these equations (see Appendix II).

A first type of zero bracket arises through the application of the theorem of Appendix II. If no equation of the set is invalidated by $h = kN$, then all the brackets of the set vanish. The h values of the equations, for any particular value of $s - 2z$, range from $m + s - 2z$ downward in steps of two for the various values of $0 \leq w \leq m$. In order to avoid $h = 0$, this type of analysis is restricted to $m + s$ = odd. In order to avoid $h = \pm 3$ as well, it is necessary that

$$m + s - 2z = 1 \tag{C.2}$$

for all values of z, compatible with the given n,m,s values and C.1. This condition can only be realized in three ways. First, $m = 1$, $s - 2z = 0$, and $s = 0$; consequently, $z = 0$ and n must be even. Second, $m = 1$, $s - 2z = 0$, and $s = 2$; consequently, $z = 1$ must be the only compatible z value, necessitating n = odd (see Table III). Third, $m = 0$, $s - 2z = 1$; consequently, $s = 1$, and the only z value compatible with C.1 is $z = 0$. The corresponding zero brackets are, respectively,

$$\left.\begin{array}{l} [1 0 \omega]_{33}\ [0 1 \omega]_{33} \\ [1 0 e]_{12}\ [0 1 e]_{12} \\ [o o n]_{23}\ [o o n]_{31} \quad . \end{array}\right\} \quad (C.3)$$

A second type of zero brackets can arise for m + s = even. According to the definitions of g and ϵ, the coefficients $g\epsilon$ of any bracket in the complex equations are $i^{p+1/2(s-\Theta)} \cdot i^s$ times a real number. Thus, all the real parts of the equations with given n,m,s, contain only brackets of one parity of p', defined by

$$p' = p + 1/2(s - \Theta) \quad , \qquad (C.4)$$

and all the imaginary parts of these equations contain only brackets of the other parity of p'. The brackets with given n,m,s thus fall into two subgroups according to the parity of p'. In each subgroup there are as many real independent equations as there are brackets. There is one way in which the condition h = kN can affect one of these two subgroups without affecting the other. The brackets in the unaffected subgroup must then vanish on the same grounds, as before the condition h = kN was applied. In order that h = kN shall affect only one subgroup, it is necessary and sufficient that it affect only self-conjugate complex equations. According to Corollary IV, these occur only for h = 0; namely, if both

$$\left.\begin{array}{l} (s - 2z) = 0 \\ (m - 2w) = 0 \quad , \end{array}\right\} \quad (C.5)$$

hence m,s, and m + s are all even. Since h = 6 is inadmissible, the possible values of m are 0,2,4. These can be realized in three ways, compatible with C.5. First, s = 0; consequently, z = 0 and n = even. The case m = 0 must here be excluded since the remaining subgroup is empty. Second, s = 2, n = odd; consequently, z = 1. On the same grounds as in the first case, m = 0 is excluded.

Third, $s = 2$, n = even; consequently, $z = 1$ according to C.5. But the equations with $s = 2$, $z = 0$ must now also be admitted, while no equation that is not self-conjugate complex should be ruled out by $h = k.3$. This configuration allows only $m = 0$. The corresponding zero brackets are:

$$\left.\begin{array}{l} [11e]_{33}\ [31e]_{33}\ [13e]_{33} \\ [11\omega]_{12}\ [31\omega]_{12}\ [13\omega]_{12} \\ [ooe]_{12}\quad . \end{array}\right\} \quad (C.6)$$

It can be shown that a threefold axis produces no other zero brackets than those listed in C.3 and C.6.