

V. SINIVEE

## ENSEMBLE AVERAGES OF MOLECULAR SPHERICAL TENSORS

In various branches of molecular physics one has to deal with the calculation of quantities defined as ensemble averages of tensors associated with a representative molecule. The chemical shifts,  $g$ -factors of free radicals, direct nuclear dipole-dipole interaction tensor and hyperfine interaction tensors may serve as examples of such quantities well known in the NMR and EPR of liquids. If the liquid (considered as an ensemble of molecules) is homogeneous and isotropic, the calculation of averages of molecular tensors is trivial. This is not the case if the liquid is homogeneous but anisotropic. In this case the liquid consists of partially oriented molecules and thus the knowledge of the distribution function of molecular orientations [1] is needed in order to calculate average molecular tensors.

External electric and magnetic fields as well as ultrasonic waves may be used in order to induce partial orientation of molecules. Liquid crystals and solid matrixes supply us with species possessing great anisotropy. In developing theories of physical phenomena taking place in such media, several authors have introduced methods for calculating average tensors associated with an axially symmetric distribution of molecules. The present paper is an extended approach, in which useful mathematical properties of spherical tensors [2] and of generic spherical functions [3] are utilized.

We consider the calculation of ensemble averages of spherical (irreducible) tensors rigidly bound with the molecule and rotating together with the latter. The distribution function is assumed to be an arbitrary continuous single valued function. Then, symmetrical distributions considered by Saupe [4] and Buckingham and McLauchlan [1,5] are easily treated as special cases (Section 2). Mathematical quantities used in this paper are briefly reviewed in the Appendix.

### 1. General

Let  $\mathbf{e}_j$  ( $j = x, y, z$ ) denote the unit vectors of a Cartesian reference system (the  $e$ -system) rigidly bound with the molecule. Let  $\mathbf{a}_j$  denote unit vectors of a similar system (the  $a$ -system) bound with measuring device. A second laboratory reference system  $\mathbf{b}_j$  (the  $b$ -system) relative to which the distribution function has a simple form will be introduced in order to describe symmetrical distributions.

The choice of a reference system allows one to establish a correspondence between mathematical quantities like the vectors and the physical ones. In order to expand this correspondence to ordinary tensors one associates with each reference system an orthonormalized basis

defined in the tensorial space. This basis is composed of direct products of unite vectors of the reference system like  $\mathbf{a}_x \mathbf{a}_y$ . Now the tensor may be described in terms of its components. We consider the tensor as an invariant quantity, whereas its components will depend upon the choice of the reference system. Especially, if  $T_{xy}$  denotes a component of a tensor  $\mathbf{T}$  (of second degree) defined relative to the  $a$ -system,  $T'_{xy}$  will denote the corresponding component defined relative to the  $b$ -system. A further diversity of representations of a tensor is introduced by considering tensors with complex components. In this case one associates with each reference system several orthonormalized basis sets differing by the choice of phase factors. We are especially interested in canonical basis sets (see Appendix). The one associated, say, with the  $a$ -system is composed of unite tensors  $\mathbf{a}_m^l$ . Thus, the second degree tensor  $\mathbf{T}$  may be described (relative to  $a$ -system) by one of the equalities

$$\mathbf{T} = \sum_{j_1} \sum_{j_2} T_{j_1 j_2} \mathbf{a}_{j_1} \mathbf{a}_{j_2} = \sum_{l=0}^2 \sum_m T_m^l \mathbf{a}_m^l. \quad (1.1)$$

The quantities  $T_{j_1 j_2}$  will be referred to Cartesian components of the tensor, the  $T_m^l$  denote the canonical ones. The  $2l+1$  components  $T_m^l$  describe a spherical tensor  $\mathbf{T}^{(l)}$  of the order  $l$ . The spherical tensors may be defined with or without the reference to an ordinary tensor  $\mathbf{T}$  of the degree  $q$ . In the former case one speaks about spherical components  $\mathbf{T}^{(l)}$   $l=1; 2; \dots q$  of the ordinary tensor.

The orientation of the  $e$ -system (of the molecule) relative to the  $a$ -system is given by Euler angles  $\psi, \theta, \varphi$ . Similarly, the orientation of the  $e$ -system relative to the  $b$ -system is denoted by  $\psi', \theta', \varphi'$  and that of the  $b$ -system relative to the  $a$ -system by  $\psi^0, \theta^0, \varphi^0$ . In some cases we use  $\theta, \alpha$  in order to denote the spherical coordinates of the vector  $\mathbf{e}_z$  relative to the  $a$ -system.

The relative orientation of two reference systems may also be described by the rotation needed to bring one system in coincidence with the other. Thus, we define

$$\hat{\Omega} \mathbf{a}_j = \mathbf{e}_j, \quad \hat{\Omega}' \mathbf{b}_j = \mathbf{e}_j, \quad \hat{\Omega}^0 \mathbf{a}_j = \mathbf{b}_j, \quad (1.2)$$

with the relation

$$\hat{\Omega} = \hat{\Omega}' \hat{\Omega}^0. \quad (1.3)$$

The entities  $\hat{\Omega}, \hat{\Omega}', \hat{\Omega}^0$  are linear operators defined in the vector space. We often use symbols like  $\Omega$  to denote the set of Euler angles  $\psi, \theta, \varphi$ .

The rotation  $\hat{\Omega}$  of the vector space induces a corresponding unitary transformation  $\hat{D}(\Omega)$  in the tensor space. One is led to the tensor representation of the rotational group [2, 3]. The representation associates an operator relation

$$\hat{D}(\Omega) = \hat{D}(\Omega') \hat{D}(\Omega^0) \quad (1.4)$$

with each equation of the kind (1.3). There are, of course, many equivalent ways to define the representation in a unitary space. The tensor representation is given by

$$\hat{D}(\Omega) \mathbf{a}_{j_1} \mathbf{a}_{j_2} = \sum_{k_1} \sum_{k_2} \Omega_{k_1 j_1} \Omega_{k_2 j_2} \mathbf{a}_{k_1} \mathbf{a}_{k_2}, \quad (1.5)$$

where the matrix elements of  $\hat{\Omega}$  are given by scalar products

$$\Omega_{jk} = (\hat{\Omega} \mathbf{a}_k, \mathbf{a}_j). \quad (1.6)$$

As in the case of equations (1.1), (1.6), we often select the case of a second degree tensor and of the  $a$ -system in order to clarify a general convention or relation.

Equation (1.5) may also be expressed in relation to the canonical basis. In this case one obtains the equation

$$\hat{D}(\Omega) \mathbf{a}_m^i = \sum_n D_{nm}^i(\Omega) \mathbf{a}_n^i \quad (1.7)$$

with  $m, n = 0; \pm 1; \dots \pm l$ . The functions  $D_{mn}^i(\Omega) = D_{mn}^i(\psi, \theta, \varphi)$  are known as generic spherical functions [3] or Wigner transformation matrix elements (see Appendix). A useful relation between the generic spherical functions defined relative to different reference systems is given by

$$D_{mn}^i(\Omega) = \sum_k D_{mk}^i(\Omega^0) D_{kn}^i(\Omega'). \quad (1.8)$$

Equation (1.8) represents the operator equation (1.4) in the matrix form.

Physical quantities like the electric dipole moment of the molecule or the dipole-dipole interaction tensor of two nuclei of the molecule may be described by tensors rigidly bound with the molecule. If the molecule rotates, such quantities become functions of the orientation of the molecule. The analytical form of such functions depend upon the choice of the reference system. If  $L(\Omega)$  describes  $L$  relative to the  $a$ -system and  $L'(\Omega')$  relative to the  $b$ -system the equation

$$L(\Omega) = L'(\Omega') = L(\Omega' \Omega^0) \quad (1.9)$$

establishes the relation between both functions. The quantity  $L$  itself may be a scalar, vector, tensor, operator, etc.

The dependence of spherical tensors bound with the molecule upon the orientation may be derived as follows. Let originally the  $e$ -system coincide with, say, the  $a$ -system. Rotate, now, the  $e$ -system to its actual place. Then, the transformation of the tensor  $\mathbf{T}^{(l)}$  is given by

$$\mathbf{T}^{(l)}(\Omega) = \hat{D}(\Omega) \mathbf{T}, \quad (1.10)$$

where  $\mathbf{T}$  corresponds to zero Euler angles. If the Eq. (1.10) is expressed in terms of canonical components, one obtains

$$T_m^i(\Omega) = \sum_n D_{mn}^i(\Omega) T_n^i. \quad (1.11)$$

Note that in this case  $T_n^i$  equals to canonical components defined relative to the  $e$ -system. The equations (1.10), (1.11) are related to the  $a$ -system. With reference to the  $b$ -system one obtains similarly the equation

$$T_m^{i'}(\Omega') = \sum_n D_{mn}^i(\Omega') T_n^i, \quad (1.12)$$

where  $T_n^i$  has the value mentioned above. The relation between both functions of orientation is easily derived on the basis of equations (1.8), (1.11), (1.12). One obtains

$$T_m^i(\Omega) = \sum_n D_{mn}^i(\Omega^0) T_n^{i'}(\Omega'). \quad (1.13)$$

The distribution of orientations of molecules of the ensemble is given

by the singlet orientation distribution function [1]  $P(\Omega)$ . The normalization of the latter is given by

$$(P, P) = \int |P(\Omega)|^2 d\Omega = 1, \quad (1.14)$$

where

$$d\Omega = (1/8\pi^2) \sin \vartheta d\vartheta d\varphi d\phi. \quad (1.15)$$

The distribution function  $P'(\Omega')$  defined relative to the  $b$ -system is given by the general relation (1.9).

If the distribution function is known relative to a laboratory reference system, the ensemble average  $\langle L \rangle$  of a function of orientation  $L(\Omega)$  defined relative to the same reference system is given by

$$\langle L \rangle = \int L(\Omega) P(\Omega) d\Omega. \quad (1.16)$$

The distribution function is expected to be continuous and single-valued. The manifold of all such functions of orientation (including those with complex values) forms a unitary Hilbert space. In this space the generic spherical functions with  $l=0; 1; 2; \dots$  form a complete set of orthogonal (but not normalized) basis functions. Thus, one can expand the distribution functions in series

$$P(\Omega) = \sum_l \sum_m \sum_n (2l+1) \bar{S}_{mn}^l D_{mn}^l(\Omega), \quad (1.17)$$

$$P'(\Omega') = \sum_l \sum_m \sum_n (2l+1) \bar{S}_{mn}^{l'} D_{mn}^l(\Omega'), \quad (1.18)$$

where

$$S_{mn}^l = \langle D_{mn}^l(\Omega) \rangle, \quad (1.19)$$

$$S_{mn}^{l'} = \langle D_{mn}^l(\Omega') \rangle. \quad (1.20)$$

Applying the definition of averages (1.16) to a component (1.11) of spherical tensor one obtains the equation

$$\langle T_m^l \rangle = \sum_n S_{mn}^l T_n^l. \quad (1.21)$$

For components defined relative to the  $b$ -system, the similar equation is given by

$$\langle T_m^{l'} \rangle = \sum_n S_{mn}^{l'} T_n^l. \quad (1.22)$$

The following transformation law of the quantities  $S_{mn}^l$  given by

$$S_{mn}^l = \sum_k D_{mk}^l(\Omega^0) S_{kn}^{l'}. \quad (1.23)$$

may be verified with help of equations (1.17), (1.8), (1.18). Insertion of Eq. (1.23) into the Eq. (1.21) yields the transformation law

$$\langle T_m^l \rangle = \sum_n D_{mn}^l(\Omega^0) \langle T_n^{l'} \rangle. \quad (1.24)$$

Comparing Eq. (1.24) with Eq. (1.13) one concludes: the average of a spherical tensor is itself a spherical tensor of the same order. If the distribution of molecular orientations is symmetric, one chooses such a  $b$ -system that  $P'(\Omega')$  has a simple analytical form. With the help of Eq. (1.22) one calculates at first  $\langle T_n^{l'} \rangle$  and then transforms the results to the  $a$ -system making use of Eq. (1.24).

Equation (1.21) is the basic result of this paper. It clarifies the sensitivity of averages of spherical tensors of different order to the analytical form of the distribution function  $P(\Omega)$ . The average of a spherical tensor of the order  $l$  "feels" only that part of the distribution function which is the projection of  $P(\Omega)$  into the  $(2l+1)^2$  dimensional subspace of the Hilbert space associated with the value  $l$ . The average of an ordinary tensor of the degree  $q$  "feels" a much broader subspace spanned over a set of previously mentioned subspaces with  $l=0; 1; \dots q$ . Since ordinary tensors up to the degree two are most commonly observed, much information about the distribution function is lost. Thus, the measurement of higher order tensors like the nonlinear polarizabilities is important.

If the components of the spherical tensor  $T_n^l$  defined relative to the  $e$ -system are known, the calculation of the average tensor requires the knowledge of the quantities  $S_{mn}^l$  only. The latter form a  $(2l+1)^2$  matrix called ordnungsmatrix. This matrix is indeed a generalization of the ordnungsmatrix introduced by Saupe [4] and of  $S$ -coefficients of Buckingham [4, 5]. Since  $P(\Omega)$  is real, the equation

$$\bar{S}_{mn}^l = (-1)^{m+n} S_{-m, -n}^l \quad (1.25)$$

holds. The change of the laboratory reference system induces independent transformation of elements of the ordnungsmatrix belonging to different columns. As shown by Eq. (1.23), the transformation law of the column is that of a spherical tensor of the order  $l$ . The normalization equation (1.14) establishes an upper limit to the absolute value of  $S_{mn}^l$ . Since

$$\sum_l \sum_m \sum_n (2l+1) |S_{mn}^l|^2 = 1, \quad (1.26)$$

one concludes

$$|S_{mn}^l| \leq 1/\sqrt{2l+1}. \quad (1.27)$$

Therefore, experimental determination of low order ordnungsmatrixes enables to appreciate the importance or unimportance of higher order parts of the distribution function.

## 2. Symmetrical Distributions

The distribution function  $P(\Omega)$  is called symmetric if there exists a nonunitary transformation establishing a correspondence between orientations with equal probability. The symmetry transformation is expected to preserve the continuity of  $P(\Omega)$  and the value of  $d\Omega$ . The symmetry of the distribution function can be due to symmetry properties of intermolecular forces. More commonly the origin of symmetrical distributions lies in the symmetry of macroscopic environment. Distribution functions belonging to a group of symmetry transformations will be spanned over invariant subspaces of the Hilbert space. As a consequence, the ordnungsmatrixes are greatly reduced, and the properties of the average spherical tensors are correspondingly affected.

The isotropic distribution is described by

$$P(\Omega) = 1. \quad (2.1)$$

Only  $S_{00}^0$  does not vanish. There is only one nonvanishing component of average spherical tensors given by

$$\langle T_0^0 \rangle = T_0^0. \quad (2.2)$$

The distribution is called axially symmetric if the symmetry group consists of rotations around a fixed axis. Let the direction of this axis coincide with  $\mathbf{b}_z$ . Then

$$P'(\Omega') = P'(\vartheta', \varphi'). \quad (2.3)$$

The nonzero elements of the ordnungsmatrix are now  $S'_{0n}$ . From the point of view of the  $b$ -system each average spherical tensor has only one nonvanishing component given by

$$\langle T_0^l \rangle = \sum_n S'_{0n} T_n^l. \quad (2.4)$$

The components of the average tensor defined relative to the  $a$ -system depend upon the direction of  $\mathbf{b}_z$  as given by

$$\langle T_m^l \rangle = D_{m0}^l(\Omega^0) \langle T_0^l \rangle. \quad (2.5)$$

Especially, the angular dependence of a first order spherical tensor is given by

$$\begin{aligned} D_{00}^1 &= \cos \vartheta^0, \\ D_{\pm 1,0}^1 &= \pm (1/\sqrt{2}) \sin \vartheta^0 \exp(\mp i\alpha^0), \end{aligned} \quad (2.6)$$

where  $\vartheta^0$ ,  $\alpha^0 = \varphi^0 + (3\pi/2)$  denote the spherical coordinates of the vector  $\mathbf{b}_z$ . The corresponding transformation functions of a second order average spherical tensor are

$$\begin{aligned} D_{00}^2 &= \frac{1}{2}(3 \cos^2 \vartheta^0 - 1), \\ D_{\pm 1,0}^2 &= \pm \sqrt{\frac{3}{2}} \sin \vartheta^0 \cos \vartheta^0 \exp(\mp i\alpha^0), \\ D_{\pm 2,0}^2 &= \sqrt{\frac{3}{8}} \sin^2 \vartheta^0 \exp(\mp i2\alpha^0). \end{aligned} \quad (2.7)$$

Thus, the axially symmetric distribution is described by the direction  $\mathbf{b}_z$  and by ordnungsmatrixes  $S'_{0n}$ , each of which contains only  $l+1$  independent complex quantities. Since the definition of the canonical basis includes an arbitrary phase factor for each irreducible subspace, the number of independent real numbers reduces to  $2l+1$ .

Another kind of distribution functions which can actually be expanded on the basis of spherical harmonics is given by

$$P(\Omega) = P(\psi, \theta). \quad (2.8)$$

The distribution given by Eq. (2.8) is invariant relative to rotations of the molecule around an axis bound with the molecule. This axis has been chosen as the  $\mathbf{e}_z$  vector of the molecular reference system. Now only the matrix elements  $S_{m0}^l$  do not vanish. The average of a spherical tensor is given by

$$\langle T_m^l \rangle = S_{m0}^l T_0^l. \quad (2.9)$$

An axially symmetric distribution which also possesses invariance with respect to rotations around the  $\mathbf{e}_z$  axis is described by

$$P'(\Omega') = P'(\theta'). \quad (2.10)$$

Each ordnungsmatrix of the distribution function (2.10) has only one nonvanishing element  $S'_{00}$  — the degree of orientation (Ordnungsgrad). Equation (1.18) gives now an expansion on the basis of Legendre polynomials. Nonvanishing components of average tensors are given by

$$\langle T'_{0l} \rangle = S'_{00} T'_{0l}. \quad (2.11)$$

Since the equation (2.5) remains valid, a measurement of angular dependence of average spherical tensors does not detect a difference between this distribution and the more general one given by Eq. (2.3). However, the knowledge of several spherical tensors defined relative to the  $e$ -system allows one to solve this problem. For this purpose Eq. (1.27) can be helpful.

### Appendix

In this paper a Cartesian tensor of the degree  $q$  is considered as an element of a  $3^q$  dimensional unitary space (of the tensor space). In this space the scalar product of two tensors  $\mathbf{T}$ ,  $\mathbf{Q}$  is defined by

$$(\mathbf{T}, \mathbf{Q}) = \sum_j T_j \bar{Q}_j \quad (A.1)$$

where barred symbols denote complex conjugate quantities.  $T_j$  and  $Q_j$  ( $j=1; \dots; 3^q$ ) are components of the tensors defined relative to an orthonormalized basis.

The tensor space is the direct product of  $q$  vector spaces, each of which is expanded by introducing complex numbers. A Cartesian component of the tensor  $\mathbf{T}$  is now described by  $q$  labels

$$T_{j_1 j_2 \dots j_q}, \quad j_1; j_2; \dots; j_q = x; y; z. \quad (A.2)$$

The formation of direct product is an operation specific for the tensor algebra. Another property, considered as an essential part of the definition of the tensor, is the tensor representation of the rotational group given by Eq. (1.5). Especially, the rotation around a unite vector  $\mathbf{n}$  by an infinitesimal angle  $d\beta$  is characterized by the Hermitean operator

$$\hat{I}_n = \left( \frac{\partial \hat{D}(\mathbf{n}, \beta)}{\partial \beta} \right)_{\beta=0} \quad (A.3)$$

defined in the tensor space. In particular  $\hat{I}_x, \hat{I}_y, \hat{I}_z$  are associated with infinitesimal rotations around  $\mathbf{a}_x, \mathbf{a}_y$  and  $\mathbf{a}_z$ , respectively. Further,

$$\hat{I}^2 = \hat{I}_x^2 + \hat{I}_y^2 + \hat{I}_z^2, \quad \hat{I}_{\pm} = \hat{I}_x \pm i\hat{I}_y. \quad (A.4)$$

The canonical basis of the tensor space is now defined by

$$\begin{aligned} \hat{I}^2 \mathbf{a}_m^l &= l(l+1) \mathbf{a}_m^l, \\ \hat{I}_z \mathbf{a}_m^l &= m \mathbf{a}_m^l, \\ \hat{I}_{\pm} \mathbf{a}_m^l &= \sqrt{(l \mp m)(l \pm m + 1)} \mathbf{a}_{m \pm 1}^l. \end{aligned} \quad (A.5)$$

The canonical components of the tensor  $\mathbf{T}$  are denoted by  $T_m^l$ . The development of a Cartesian tensor into its spherical components corresponds to the reduction of the tensor space into irreducible subspaces. In each subspace Eq. (A.5) defines the canonical basis up to an arbitrary phase factor. If  $q > 2$ , the reduction of the tensorial space is ambiguous. In this case the equation (1.1) should be replaced by

$$(1.1) \quad \mathbf{T} = \sum_l \sum_m \sum_v T_m^{lv} \mathbf{a}_m^{lv}, \quad (\text{A.6})$$

where  $v=1; 2; \dots g_l$ . Each  $\mathbf{a}_m^{lv}$  satisfies Eq. (A.5). Each transforms according to Eq. (1.11). Thus, the ordnungsmatrix does not depend upon  $v$ . Eq. (1.21) should be replaced by

$$(1.21) \quad \langle T_m^{lv} \rangle = \sum_n S_{mn}^l T_n^{lv}. \quad (\text{A.7})$$

Therefore, an additional convention is needed in order to choose a canonical basis.

For tensors of the degree one, the relation between Cartesian and canonical components is given by

$$(A.8) \quad T_0^1 = T_z,$$

$$T_{\pm 1}^1 = \mp (1/\sqrt{2}) (T_x \mp iT_y).$$

For tensors of the degree two, one has the following relations

$$(A.9) \quad T_0^2 = (1/\sqrt{3}) (T_{xx} + T_{yy} + T_{zz}),$$

$$T_0^1 = (i/\sqrt{2}) (T_{xy} - T_{yx}),$$

$$(A.10) \quad T_{\pm 1}^1 = -\frac{1}{2} [(T_{zx} - T_{xz}) \mp i(T_{zy} - T_{yz})],$$

$$T_0^2 = (1/\sqrt{6}) (2T_{zz} - T_{xx} - T_{yy}),$$

$$(A.11) \quad T_{\pm 1}^2 = \mp \frac{1}{2} [(T_{zx} + T_{xz}) \mp i(T_{zy} + T_{yz})],$$

$$T_{\pm 2}^2 = \frac{1}{2} [(T_{xx} - T_{yy}) \mp i(T_{xy} + T_{yx})].$$

Spherical harmonics used in this paper are given by

$$(A.12) \quad Y_l^m(\vartheta, \alpha) = (1/2\pi) P_l^m(\cos \vartheta) \exp(im\alpha),$$

where  $P_l^m(\mu)$ ,  $\mu = \cos \vartheta$  denote normalized adjungated Legendre polynomials. The normalization is defined by

$$(A.13) \quad \int_{-1}^{+1} |P_l^m(\mu)|^2 d\mu = 1.$$

Generic spherical functions are given by

$$(A.14) \quad D_{mn}^l(\psi, \vartheta, \varphi) = e^{-im\psi} P_{mn}^l(\mu) e^{-in\varphi}.$$

The functions  $P_{mn}^l(\mu)$  are defined in [3]. The Euler angles correspond



to the rotation of a right-hand screw. The scalar product of generic spherical functions is given by

$$(D^l_{mn}, D^l_{mn}) = \int |D^l_{mn}(\Omega)|^2 d\Omega = \frac{1}{2l+1}. \quad (\text{A.15})$$

The following special cases of generic spherical functions are used in this paper

$$D^l_{m0}(\vartheta, \vartheta) = (-1)^m \sqrt{\frac{4\pi}{2l+1}} Y_l^{-m}(\vartheta, \alpha), \quad (\text{A.16})$$

$$D^l_{00}(\vartheta) = P_l(\mu), \quad (\text{A.17})$$

where  $\vartheta$ ,  $\alpha$  denote spherical coordinates of  $\mathbf{a}_z$ . The ordinary (un-normalized) Lagrange polynomials are denoted by  $P_l(\mu)$ .

#### REFERENCES

1. Buckingham A. D., Disc. Faraday Soc. **43**, 205 (1967).
2. Любарский Г. Я., Теория групп и ее применения в физике, М., 1957.
3. Гельфанд И. М., Минлос Р. А., Шапиро З. Я., Представления группы вращений и группы Лоренца, М., 1958.
4. Saure A., Z. Naturforschung, **19a**, 161 (1964).
5. Buckingham A. D., McLauchlan K. A., Prog. NMR Spectr., **2**, 63 (1967).

Academy of Sciences of the Estonian SSR,  
Institute of Cybernetics

Received  
Apr. 28, 1972

#### V. SINIVEE

##### MOLEKULAARSETE SFÄÄRILISTE TENSORITE KESKVÄÄRTUSED

Sfäärilisi tensoreid, mis on seotud molekuliga ja roteeruvad koos viimasega, nime-tatakse molekulaarseteks. Käsitletakse säärase tensorite keskvaärtuste arvutamist juhul, kui molekulide orientatsioonide jaotus on meelevaldne ühetähenduslik funktsioon.

#### B. СИНИВЕЭ

##### СРЕДНИЕ МОЛЕКУЛЯРНЫЕ СФЕРИЧЕСКИЕ ТЕНЗОРЫ

Молекулярными названы сферические тензоры, которые связаны с молекулой и вращаются вместе с ней. Рассматривается расчет средних значений таких тензоров при допущении произвольного, непрерывного, однозначного статического распределе-ния ориентаций молекул.