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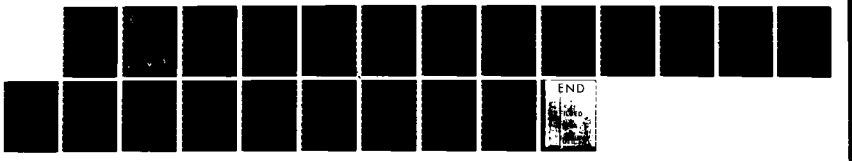

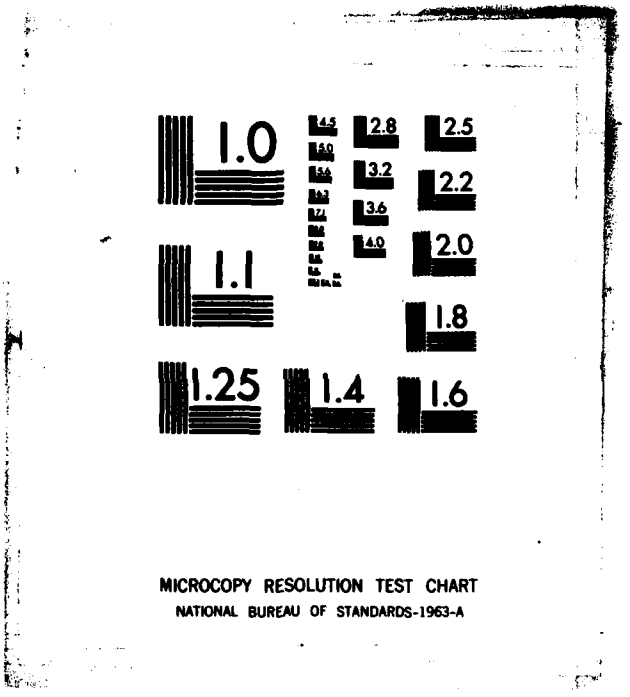
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TECHNICAL REPORT ARCSL-TR-83043

THE ELEMENTS OF THE ROTATION MATRICES IN TERMS OF RODRIGUEZ'S PARAMETERS

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The elements of the rotation matrices, $D^{L}_{M'M}$ for arbitrary L, as well as those of the matrix S which rotates the cartesian coordinates, are expressed in terms of Rodriguez's parameters, *viz.*, the direction cosines of the axis, lambda nu upsilon λ, μ, ν, and the angle of rotation, omega ω.

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PREFACE

The work described in this report is based on work supported in part by the US Army European Research Office through contract DAJA37-81-C-0895, and in part by the Centro Nazionale Ricerche (CNR) (National Center for Research) through the Gruppo Nazionale Struttura della Materia (GNSM) (National Group for the Structure of the Matter). This work was started in 1978 and is on-going.

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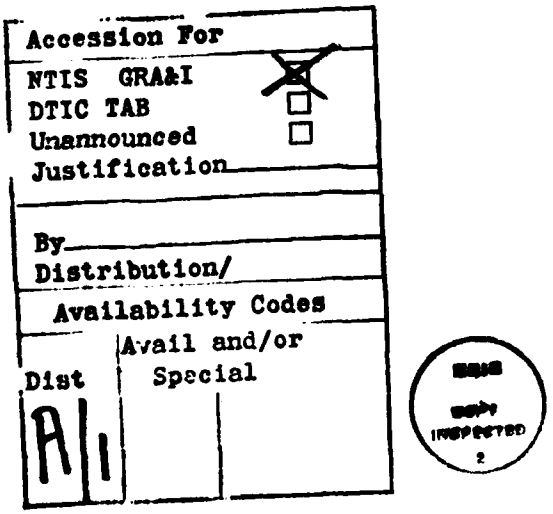

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THE ELEMENTS OF THE ROTATION MATRICES IN TERMS OF RODRIGUEZ'S PARAMETERS

1. INTRODUCTION

In quantum mechanics and group theory, the elements of the rotation matrices $\underset{\sim}{D}^J$ are expressed in terms of the eulerian angles whose mutual independence offer undoubted advantages. However, there is one application in which expressing the elements of $\underset{\sim}{D}^J$ in terms of Rodriguez's parameters,[1] viz., the direction cosines of the axis, λ, μ, ν, and the angle of rotation, ω, may be very useful. The application we are thinking of is the calculation of symmetrized combinations of irreducible spherical tensors,[2] particularly scalar and vector spherical harmonics. In this case, while their use to describe the rotations is rather instinctive, the lack of mutual independence of Rodriguez's parameters does not matter.

2. DISCUSSION

Bassani and Pastori-Parravicini,[3] who restrict their analysis to two-component spinors, have used Rodriguez's parameters to study the rotational properties of functions. We will obtain general expressions for the elements of the matrices $\underset{\sim}{D}^J$, for arbitrary J, and, particularly for the elements of the matrix $\underset{\sim}{S}$ describing the rotation of the cartesian coordinates:

$$x_i' = \sum_j S_{ij} x_j \tag{1}$$

Recalling that the matrices $\underset{\sim}{D}^J$ form an irreducible representation of order 2J+1 of the rotation group in three dimensions on a basis of simultaneous eigenvectors of J^2 and J_z

$$D^J_{M'M}(\underset{\sim}{\omega}) = \langle J,M' \mid e^{i \underset{\sim}{\omega} \cdot \underset{\sim}{J}} \mid J,M \rangle \tag{2}$$

where $\underset{\sim}{\omega}$ is the vector angle of rotation, and the explicit expression for the elements $D^{J}_{M'M}$ is given (e.g., by Hammermesh)[4] in terms of the Kayley-Klein[5] parameters, a and b, as

$$D^{J}_{M'M}(a,b) = \sum_{k} \frac{[(J+M)!(J-M)!(J+M')!(J-M')!]^{\frac{1}{2}}}{(J+M-k)!k!(J-M'-k)!(M'-M+k)!} \times a^{J+M-k}\,(a^*)^{J-M'-k}\,b^{k}\,(-b^*)^{M'-M+k} \tag{3}$$

It is well known that the Kayley-Klein parameters are used in classical mechanics as a tool to integrate gyroscopic problems; but for present purposes, they are better related to the elements of $\underset{\sim}{D}^{\frac{1}{2}}$:

$$\underset{\sim}{D}^{\frac{1}{2}} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

Therefore, once it is shown that a and b can be expressed in terms of λ, μ, ν, and ω, the task will be done. To this end, notice that for $J = \frac{1}{2}$, Equation 2 yields:

$$D^{\frac{1}{2}}_{M'M} = \left\langle \frac{1}{2}, M' \middle| e^{i\,\underset{\sim}{\omega}\cdot\underset{\sim}{J}} \middle| \frac{1}{2}, M' \right\rangle = \left\{ \exp\left[i\frac{\omega}{2}\left(\lambda\,\underset{\sim}{\sigma}_x + \mu\,\underset{\sim}{\sigma}_y + \nu\,\underset{\sim}{\sigma}_z\right)\right]\right\}_{M'M} \tag{4}$$

where the $\underset{\sim}{\sigma}$'s are the Pauli spin matrices. Now, let us put

$$\mathbb{P} = \lambda\,\underset{\sim}{\sigma}_x + \mu\,\underset{\sim}{\sigma}_y + \nu\,\underset{\sim}{\sigma}_z = \begin{pmatrix} \nu & \lambda - i\mu \\ \lambda + i\mu & -\nu \end{pmatrix}$$

then, by substituting into Equation (4), we get

$$\underset{\sim}{t} = \exp\left(i\frac{\omega}{2}\mathbb{P}\right) = \sum_{k}\left(\frac{i\omega}{2}\right)^{k}\frac{1}{k!}\mathbb{P}^{k} \tag{5}$$

according to the customary definition of the functions of a matrix. Since it is immediately verified that

$$\mathbb{P}^{2k} = \mathbb{1}; \qquad \mathbb{P}^{2k+1} = \mathbb{P}$$

Equation (5) can be rewritten as

$$\underset{\approx}{D}^{\frac{1}{2}} = \sum_k \left[\left(\frac{i\omega}{2} \right)^{2k} \frac{1}{(2k)!} \mathbb{P}^{2k} + \left(\frac{i\omega}{2} \right)^{2k+1} \frac{1}{(2k+1)!} \mathbb{P}^{2k+1} \right]$$

$$= \mathbb{1} \cos \frac{\omega}{2} + i \mathbb{P} \sin \frac{\omega}{2} \tag{6}$$

Therefore, the expression for $\underset{\approx}{D}^{\frac{1}{2}}$ becomes

$$\underset{\approx}{D}^{\frac{1}{2}} = \begin{pmatrix} \cos \frac{\omega}{2} + i\nu \sin \frac{\omega}{2} & i(\lambda - i\mu) \sin \frac{\omega}{2} \\ i(\lambda + i\mu) \sin \frac{\omega}{2} & \cos \frac{\omega}{2} - i\nu \sin \frac{\omega}{2} \end{pmatrix}$$

and the Kayley-Klein parameters take on the desired form

$$a = \cos \frac{\omega}{2} + i\nu \sin \frac{\omega}{2} \tag{7a}$$

$$b = i(\lambda - i\mu) \sin \frac{\omega}{2} \tag{7b}$$

When dealing with symmetry properties of sets of spherical tensors centered at molecular or crystal sites, the site coordinates have to be rotated in order to get the permutations induced by the group operations. This can be done easily through the use of the matrix $\underset{\approx}{S}$ of Equation (1), whose expression has been given by Goldstein[5] in terms of a and b:

$$\underset{\approx}{S} = \begin{bmatrix} \frac{1}{2}(a^2 + a^{*2} - b^2 - b^{*2}) & \frac{1}{2}(b^{*2} - b^2 - a^2 + a^{*2}) & -(a\,b + a^*\,b^*) \\ \frac{1}{2}(a^2 - a^{*2} - b^2 + b^{*2}) & \frac{1}{2}(a^2 + a^{*2} + b^2 + b^{*2}) & -i(a\,b - a^*\,b^*) \\ a\,b^* + a^*\,b & i\,(b\,a^* - a\,b^*) & a\,a^* - b\,b^* \end{bmatrix} \tag{8}$$

Substituting Equation (6) into Equation (7) then yields

$$\underset{\approx}{S} = \begin{bmatrix} \lambda^2 + (1-\lambda^2)\cos\omega & \lambda\mu\,(1-\cos\omega) - \nu\sin\omega & \nu\lambda\,(1-\cos\omega) + \mu\sin\omega \\ \lambda\mu\,(1-\cos\omega) + \nu\sin\omega & \mu^2 + (1-\mu^2)\cos\omega & \mu\nu\,(1-\cos\omega) - \lambda\sin\omega \\ \nu\lambda\,(1-\cos\omega) - \mu\sin\omega & \mu\nu\,(1-\cos\omega) + \lambda\sin\omega & \nu^2 + (1-\nu^2)\cos\omega \end{bmatrix} \tag{9}$$

3. CONCLUSION

In conclusion, it is pointed out that Equation (9) has been successfully coded with Equation (3) with a and b given by Equation (7) as part of a program to get symmetrized combinations of spherical multipoles centered at the sites of a molecule. In spite of the occurrence of complex quantities, we were also able to implement the coding to reduce the request for complex computer algebra to a minimum.

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