Theoret. chim. Acta (Berl.) 31, 221—230 (1973)

The Use of Site Symmetry in Constructing Symmetry Adapted Functions

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Received March 5, 1973

It is shown that the application of a projection operator from a given group to a function is equivalent to the successive application of projection operators from factor groups of the starting group to that function. When used with the factor groups representing the site symmetry of a position and the simplest group of interchanges of positions, this concept provides a very simple method for obtaining symmetry adapted linear combinations of basis functions.

Key words: Symmetry adapted functions – Site symmetry – Projection operators – Factor groups

Introduction

One of the most important uses of group theory by chemists lies in the construction of symmetry adapted linear combinations of basis functions. For most of the axial point groups (those with no more than one principal axis) the procedure involves a very simple explicit or implicit application of projection operators [1–3]. The procedure becomes more difficult for cubic and higher symmetries.

Frequently, symmetry adapted functions are constructed from subgroups of the point groups of the molecule under consideration (as, for example, in the use of the C_6 group rather than D_{6h} for constructing the π molecular orbitals of benzene). In the axial point groups, the feasibility of such a process, and the appropriate choice of the subgroups is usually intuitively obvious to an experienced worker (and completely baffling to a neophyte). Again in the non-axial groups the process is much more difficult.

The purpose of this paper is to put the factorization process on a theoretically sound footing and to outline a simple systematic procedure for constructing symmetry adapted linear combinations (which, following Cotton [1], we will call SALC's) of the basis functions within any symmetry group. The method, which draws on the work of Altmann [4, 5], can be applied equally well to point groups of high symmetry (cubic, isosahedral, etc.), the symmetry groups of non-rigid molecules [6, 7], space groups, or any other problem where the group describing the system can be factored into appropriate subgroups.

The procedure will involve expressing the projection operators for the group under consideration as products of projection operators of two subgroups, the subgroup corresponding to the site symmetry of a basis function or set of basis functions and the subgroup corresponding to the simplest interchange of equivalent sites. Melvin [8] and Altmann [4, 5], have previously considered factorization of the projection operator; however, their factorizations are more restrictive than that presented here. The work of Melvin requires the concept of a "kernel" subgroup within a given irreducible representation; *i.e.*, a subgroup onto which the irreducible representation under consideration maps as the totally symmetric irreducible representation. The factorization used by Altmann uses the concept of the poles of a rotation to derive an invariant subgroup of the group under consideration. The present work does not require either of these concepts.

Groups as Products of Subgroups

Groups having more than one independent generator (*i.e.* more than one independent type of symmetry element) can be expressed as products of subgroups. (The product of two groups N, consisting of the set of elements $\{N_i\}$ and C, consisting of the set of elements $\{C_j\}$, is the set of all products of elements $\{N_i C_j\}$.) The point group for any three-dimensional object can be expressed as the product of, at most, three independent subgroups. For systems with high symmetry, the factoring is usually not unique. The independent subgroups may themselves have more than one independent generator. Ultimately, however, the factoring can be continued until each subgroup has only one generator. These one-generator subgroups are cyclic in form, and consequently abelian.

In constructing a group as the product of two subgroups, two types of product are usually considered (see Altmann [4] for proofs); the direct product and the semidirect product. The direct product occurs when every element of one subgroup commutes with every element of the other. In semidirect products, the complete set of elements of one subgroup (the invariant subgroup) will commute with every element of the other subgroup. The notations are:

$$\text{Direct product} \quad G = N \times C \tag{1}$$

$$\text{Semidirect product} \quad G = N \wedge C \tag{2}$$

where in (2) N is the invariant subgroup. In the present work, we propose to construct a specific binary product structure for the point group and then to construct the SALC's in the full symmetry by building them up from the subgroups. The product, however, will not necessarily be constructed so that either group is invariant. It is, in fact, what is commonly called the "weak direct product". The direct product and semidirect product are special cases of this.

The proposed approach is to express the point group as the product of the site-symmetry group [9] of a given atom G_S and the simplest group which interchanges the considered atom with those equivalent to it, G_I.

$$G = G_I \cdot G_S\,. \tag{3}$$

Note that a "dot" has been used to indicate the product since, depending upon the specific case, either a direct, a semidirect, or a weak direct product may be involved, and, if semidirect, either G_S or G_I may be invariant. Note also that the order of the group G_I is just equal to the number of equivalent atoms. The utility of this factorization comes from the fact that in the simplest group of order n which interchanges n equivalent functions, *i.e.* functions which are identical except for interchange of origins (the group G_I in this case), each function generates a regular representation of the group [10]. Furthermore, every irreducible representation of a group is contained m_Γ times (where m_Γ is the dimension of the irreducible representation) in the regular representation of the group [11]. Thus, if every equivalent atom contained only one basis function, the irreducible representations of G_I would immediately yield the SALC's. This is the case, for example, for the π molecular orbitals of benzene.

Unfortunately, most cases of interest have more than one basis function centered on each atom. However, we shall show that all that is required to produce SALC's over the full group is to project independent functions within G_S and then combine these using the regular representation of G_I. The only "trick" is that *all* equivalent or degenerate basis functions must be generated by the operation of the elements of G_I on any one of the equivalent set.

Projection Operators as Products of Projection Operators of Subgroups

Consider the form of the projection operator $\hat{\boldsymbol{P}}^{(\Gamma)}$ for the irreducible representation Γ in the group G

$$\hat{\boldsymbol{P}}^{(\Gamma)} = \sum_R \chi_R^{*(\Gamma)} \hat{\boldsymbol{R}} \tag{4}$$

where $\chi_R^{(\Gamma)}$ is the character of element R in representation Γ and $\hat{\boldsymbol{R}}$ is the corresponding group operation. $\chi_R^{(\Gamma)}$ is defined as the trace of the matrix representing the operation R in the representation Γ

$$\chi_R^{(\Gamma)} = \operatorname{Tr} R^{(\Gamma)} = \sum_i R_{ii}^{(\Gamma)} . \tag{5}$$

Now if G is a product of G_I (having the operations $\hat{\boldsymbol{S}}$) and G_S (having the operations $\hat{\boldsymbol{T}}$) then

$$\hat{\boldsymbol{R}} = \hat{\boldsymbol{S}}\hat{\boldsymbol{T}} \tag{6}$$

and $R^{(\Gamma)}$, the matrix representing $\hat{\boldsymbol{R}}$ in Γ, is the matrix direct product (outer or Kronecker product) of the matrices representing $\hat{\boldsymbol{S}}$ and $\hat{\boldsymbol{T}}$ in some representations, say Γ' and Γ'' [12]

$$R^{(\Gamma)} = S^{(\Gamma')} \times T^{(\Gamma'')} . \tag{7}$$

From the properties of an outer product

$$\operatorname{Tr} R^{(\Gamma)} = \operatorname{Tr} S^{(\Gamma')} \operatorname{Tr} T^{(\Gamma'')} \tag{8}$$

Thus,

$$\operatorname{Tr} R^{(\Gamma)} = \sum_k \sum_l S_{kk}^{(\Gamma')} T_{ll}^{(\Gamma'')} . \tag{9}$$

Substituting Eqs. (6) and (9) into Eq. (4), and recognizing that the summation over R may be replaced by the double summation over S and T, we obtain

$$\hat{\boldsymbol{P}}^{(\Gamma)} = \sum_S \sum_T \sum_k \sum_l S_{kk}^{*(\Gamma')} T_{ll}^{*(\Gamma'')} \hat{\boldsymbol{S}}\hat{\boldsymbol{T}} \tag{10}$$

Table 1. Site symmetry and interchange groups for some selected systems

Point group	Molecule	Ligand	G_S	G_I
C_{3v}	AX_3	X	C_s	C_3
	AX_3Y	Y	C_{3v}	C_1
C_{4v}	AX_4	X	C_s	C_4
	AX_4YZ	$Y(Z)$	C_{4v}	C_1
C_{nv}	AX_n	X	C_s	C_n
D_{2h}	$AX_2Y_2Z_2$	$X(Y, Z)$	C_{2v}	C_2
D_{2d}	AX_2Y_2	$X(Y)$	C_s	D_2
D_{3h}	AX_3	X	C_{2v}	C_3
	AX_3Y_2	Y	C_{3v}	C_2
D_{3d}	AX_6	X	C_s	S_6
D_{4h}	AX_4	X	C_{2v}	C_4
	AX_4Y_2	Y	C_{4v}	C_2
D_{6h}	X_6	X	C_{2v}	C_6
T_d	AX_4	X	C_{3v}	D_2
O_h	AX_6	X	C_{4v}	S_6

which may be refactored to give

$$\begin{aligned} \hat{P}^{(\Gamma)} &= \sum_S \sum_k S_{kk}^{*(\Gamma')} \hat{S} \sum_T \sum_l T_{ll}^{*(\Gamma'')} \hat{T} \\ &= \sum_S \chi_S^{*(\Gamma')} \hat{S} \sum_T \chi_T^{*(\Gamma'')} \hat{T} \\ &= \hat{P}_{G_I}^{(\Gamma')} \hat{P}_{G_S}^{(\Gamma'')} . \end{aligned} \tag{11}$$

Any SALC in G can be constructed by first projecting out the independent functions within the site-symmetry group G_S and then operating on this by the appropriate projection operator in the group of the simplest interchanges, G_I. However, we have already stated that, because of the generation of the regular representation, each irreducible representation of G_I occurs in a predetermined fashion. If degenerate functions in the starting basis set remain both degenerate and unique under the operations of G_S, the group G_I will have to be expanded to interchange all equivalent functions, and the site symmetry correspondingly reduced to a lower symmetry group. Such a situation occurs, for example, for p_x and p_y orbitals if a C_4 site symmetry axis is present. The projection $P^{(E)} p_x$ gives back pure p_x and similarly for p_y.

Once all degeneracies have been broken, the correlation theorem [13] and correlation tables can be used to immediately write down the desired SALC's.

Applications

The systematic application of Eq. (11) for constructing SALC's will be outlined stepwise. As a specific example we will construct the molecular orbitals arising from the p-type atomic orbitals on the ligands in an AX_6 octahedral complex.

Step 1: *Factor the point group of the molecule into the product of* G_I *and* G_S. In the octahedral complex (O_h point group) the ligand positions have C_{4v} site symmetry (four planes of symmetry and a C_4 axis pass through each ligand). The

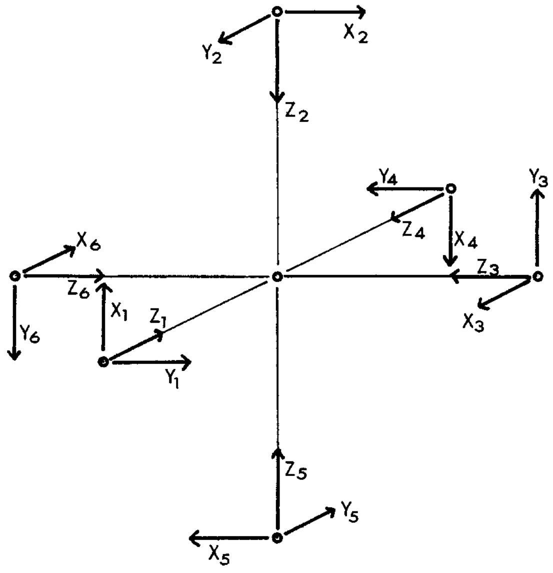

Fig. 1. Set of ligand p_x, p_y and p_z orbitals in an octahedral complex

six ligands are interchanged by the operations of a group of order 6, the S_6 group. G_S is simply the group of the symmetry elements which pass through the site. G_I may be found by factoring G into a product of abelian groups, by extracting G_S from this and by obtaining G_I from what is left. The usual product structure for O_h is [5]

$$O_h = D_2 \wedge D_3' \times C_i \,. \tag{12}$$

Factoring into abelian groups yields

$$O_h = C_2 \wedge C_2' \wedge C_3' \wedge C_2'' \times C_i \,. \tag{13}$$

The group C_{4v} is not immediately obvious from this; however,

$$C_{4v} \times C_i = D_{4h} = C_2 \wedge C_2' \wedge C_2'' \times C_i \,. \tag{14}$$

Thus

$$\begin{aligned} O_h &= C_3' \cdot C_i \cdot C_{4v} \\ &= S_6 \cdot C_{4v} \,. \end{aligned} \tag{15}$$

(Note that the invariance properties are lost when the C_2 groups are commuted with the C_3' group; consequently, the weak direct product must be used in Eq. (15).) Table 1 lists G_I and G_S for some selected structures.

Step 2: *Orient the basis functions on each site so that equivalent functions are interchanged by the elements of G_I.* If there are degeneracies in the basis functions which are not lifted by G_S, the orientations will not be unique. More will be said about this point later. A suitable choice for the p-type ligand atomic orbitals in the example is shown in Fig. 1.

Table 2. Correlation of the irreducible representations of O_h with those of the site-symmetry and interchange groups

O_h	S_6	C_{4v}	D_{3d}	C_{2v}
A_{1g}	A_g	A_1	A_{1g}	A_1
A_{2g}	A_g	B_1	A_{2g}	B_1
E_g	E_g	A_1+B_1	E_g	A_2+B_2
T_{1g}	A_g+E_g	A_2+E	$A_{2g}+E_g$	$A_2+B_1+B_2$
T_{2g}	A_g+E_g	B_2+E	$A_{1g}+E_g$	$A_1+A_2+B_2$
A_{1u}	A_u	A_2	A_{1u}	A_2
A_{2u}	A_u	B_2	A_{2u}	B_2
E_u	E_u	A_2+B_2	E_u	A_1+B_1
T_{1u}	A_u+E_u	A_1+E	$A_{2u}+E_u$	$A_1+B_1+B_2$
T_{2u}	A_u+E_u	B_1+E	$A_{1u}+E_u$	$A_1+A_2+B_1$

If degeneracies not lifted by G_S are associated with basis functions which are not mixed by the appropriate representations in G_S, G_I must be expanded to interchange all equivalent functions. In the example, the p_x and p_y degeneracy is not removed by C_{4v}, nor are p_x and p_y mixed by $\hat{P}^{(E)}$. Thus, there are twelve equivalent basis functions which must be combined by G_I. G_I must be expanded to a group of order twelve. The group $S_6 \cdot C_2'$, where the axis in C_2' bisects adjacent pairs of ligands, has the proper order. If this C_2 axis lies between ligands 1 and 2, it converts p_{x_1} into p_{y_2} and p_{y_1} into $-p_{x_2}$. The new G_I is D_{3d}. The new G_S, C_{2v}, is the group which reflects the site symmetry of the newly introduced C_2 axis.

Step 3: *Find the correlations of the irreducible representations of G_I and G_S with those of the complete group.* For the example, these are shown in Table 2.

Step 4: *Using the correlation theorem, find the irreducible representations of the* SALC'*s which are expected to be derived from each type of basis function.* The correlation theorem [13], which is, in fact, a simple application of the ideas of induced and subduced representations and the Frobenius reciprocity theorem, states that the irreducible representations in a group G spanned by a function, or set of functions, located at a site of lower symmetry G_S can be found by finding the irreducible representations spanned by the function in G_S and then correlating these with the irreducible representations of G. Each function having symmetry Γ' in G_S will contribute to every Γ in G which correlates with Γ'. From Table 2 it is seen that the A_1 representation of C_{4v} correlates with the A_{1g}, E_g and T_{1u} representations: thus the p_z ligand functions will appear in molecular orbitals of these symmetries. The E representation of C_{4v} correlates with the T_{1g}, T_{2g}, T_{1u} and T_{2u} representations of O_h. The p_x and p_y ligand orbitals will give rise to molecular orbitals of these symmetries.

Step 5: *Find the independent basis functions within G_S.* For the O_h system we are using, the p_z orbitals can be used directly in the $S_6 \cdot C_{4v}$ factorization. They transform as the A_1 representation within C_{4v}, and, being non-degenerate, are independent. The p_x and p_y orbitals transform as the E representation and are not

Table 3. Character tables for S_6 and D_{3d} with correlations to O_h

a) S_6 (real form)

O_h	S_6	E	$2C_3$	i	$2S_6$
A_{1g}	A_g	1	1	1	1
E_g	E_g	2	-1	2	-1
	A_u	1	1	-1	-1
	E_u	2	-1	-2	1
T_{1u}	A_u+E_u	3	0	-3	0

b) D_{3d}

O_h	D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$
	A_{1g}	1	1	1	1	1	1
	A_{2g}	1	1	-1	1	1	-1
	E_g	2	-1	0	2	-1	0
	A_{1u}	1	1	1	-1	-1	-1
	A_{2u}	1	1	-1	-1	-1	1
	E_u	2	-1	0	-2	1	0
T_{1g}	$A_{2g}+E_g$	3	0	-1	3	0	-1
T_{2g}	$A_{1g}+E_g$	3	0	1	3	0	1
T_{1u}	$A_{2u}+E_u$	3	0	-1	-3	0	1
T_{2u}	$A_{1u}+E_u$	3	0	1	-3	0	-1

independent. In the $D_{3d} \cdot C_{2v}$ factorization, the projection operators from $C_{2v}(G_S)$ must be used. We have, operating on say p_{x_1} and p_{y_1}

$$\begin{aligned} \hat{P}^{(A_1)}\, p_{x_1} &= p_{x_1} + p_{y_2} = \chi_{A_1} \\ \hat{P}^{(A_2)}\, p_{y_1} &= p_{y_1} - p_{x_2} = \chi_{A_2} \\ \hat{P}^{(B_1)}\, p_{x_1} &= p_{x_1} - p_{y_2} = \chi_{B_1} \\ \hat{P}^{(B_2)}\, p_{y_1} &= p_{y_1} + p_{x_2} = \chi_{B_2}\,. \end{aligned} \tag{16}$$

Step 6: *Construct* SALC's *by using the projection operators from G_I and the functions from G_S obtained in step 5.* The appropriate representations within G_I are obtained from the correlation tables obtained in step 3. The character tables for S_6 and D_{3d} are given in Table 3, along with the representations leading to the desired representations in O_h. The results of applying the projection operators are (unnormalized):

For the p_z orbitals with $G_I = S_6$

$$\begin{aligned} \phi(a_{1g}) &= \hat{P}^{(A_g)}\, p_{z_1} = p_{z_1} + p_{z_2} + p_{z_3} + p_{z_4} + p_{z_5} + p_{z_6} \\ \phi(e_g) &= \hat{P}^{(E_g)}\, p_{z_1} = 2p_{z_1} - p_{z_2} - p_{z_3} + 2p_{z_4} - p_{z_5} - p_{z_6} \\ \phi(t_{1u}) &= \hat{P}^{(A_u+E_u)}\, p_{z_1} = 3p_{z_1} - 3p_{z_4}\,. \end{aligned} \tag{17}$$

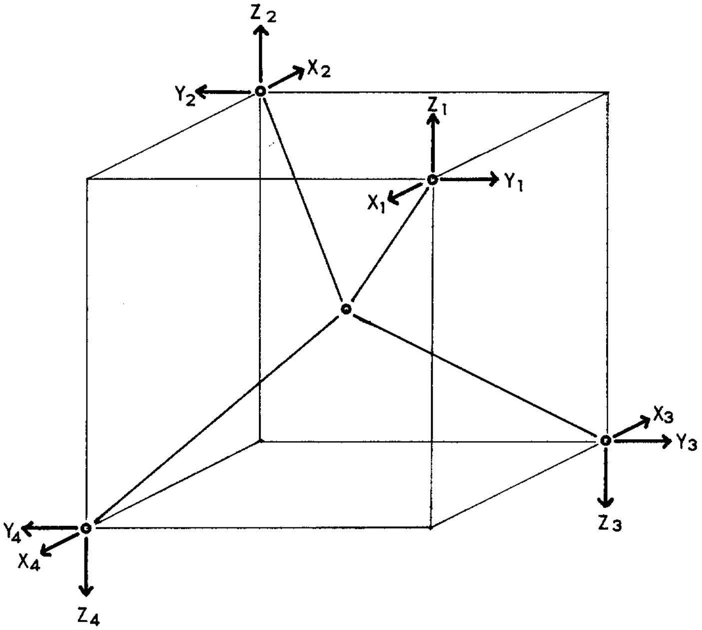

Fig. 2. Starting set of hydrogen centered basis vectors for the normal vibrations of methane

For the p_x and p_y orbitals with $G_I = D_{3d}$ (the x_i and y_i represent the corresponding p_x and p_y orbitals)

$$\begin{aligned}
\phi(t_{1g}) &= \hat{P}^{(A_{2g}+E_g)}\chi_{B_1} \\
&= 2(x_1 - y_2) + y_1 - x_2 - x_3 + y_3 + 2(x_4 - y_5) + y_4 - x_5 - x_6 + y_6 \\
\phi(t_{2g}) &= \hat{P}^{(A_{1g}+E_g)}\chi_{A_1} \\
&= 4(x_1 + y_2) + y_1 + x_2 + x_3 + y_3 + 4(x_4 + y_5) + y_4 + x_5 + x_6 + y_6 \\
\phi(t_{1u}) &= \hat{P}^{(A_{2u}+E_u)}\chi_{B_2} \\
&= 4(y_1 + x_2) + x_1 + y_2 + x_3 + y_3 - 4(y_4 + x_5) - x_4 - y_5 - x_6 - y_6 \\
\phi(t_{2u}) &= \hat{P}^{(A_{1u}+E_u)}\chi_{A_2} \\
&= 2(y_1 - x_2) + x_1 - y_2 + x_3 - y_3 - 2(y_4 - x_5) - x_4 + y_5 - x_6 + y_6 .
\end{aligned} \tag{18}$$

These, of course, are not unique. In the present case, the use of the S_6 subgroup of D_{3d} leads to a simpler, but equivalent set of functions.

$$\begin{aligned}
\phi'(t_{1g}) &= \hat{P}^{(A_g+E_g)}\chi_{B_1} = 3(x_1 - y_2) + 3(x_4 - y_5) \\
\phi'(t_{2g}) &= \hat{P}^{(A_g+E_g)}\chi_{A_1} = 3(x_1 + y_2) + 3(x_4 + y_5) \\
\phi'(t_{1u}) &= \hat{P}^{(A_u+E_u)}\chi_{B_2} = 3(y_1 + x_2) - 3(y_4 + x_5) \\
\phi'(t_{2u}) &= \hat{P}^{(A_u+E_u)}\chi_{A_2} = 3(y_1 - x_2) - 3(y_4 - x_5) .
\end{aligned} \tag{19}$$

These are in the form presented by Gray and Beach [14].

As a second example, consider the normal coordinates of methane. We will consider only the motions of the hydrogens relative to the carbon. The total

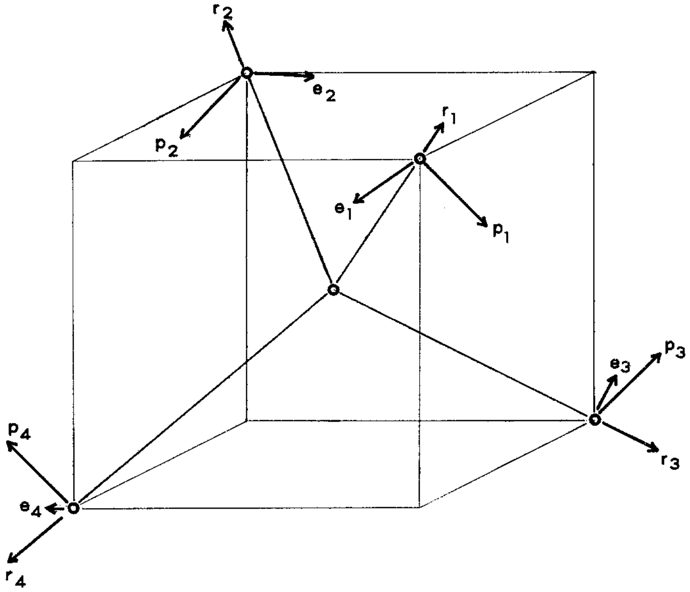

Fig. 3. Site-symmetry adapted hydrogen displacement vectors for methane

representation for a set of cartesian displacement vectors situated on the five atoms is $A_1 + E + T_1 + 3T_2$ [9]. Of these, one T_2 represents a translation of the entire molecule. This is the representation of the displacement vectors on the carbon; consequently, ignoring the carbon eliminates this from consideration. Of the remaining representations, which can all be obtained from the vectors on the four hydrogens, the T_1 represents a rotation of the entire molecule. The vibrational representations are thus $A_1 + E + 2T_2$.

The steps are as follows:

1. The point group of the molecule is T_d. This can be factored into $D_2 \wedge C_{3v}$. The D_2 is G_I and C_{3v} is G_S.

2. A suitable orientation for the displacement vectors is shown in Fig. 2. This orientation has been chosen so that the basis vectors match the site symmetry.

3. The correlations of D_2 and C_{3v} with T_d are shown in Table 4.

4. From Table 4 it is seen that the A_1 representation of C_{3v} correlates with the A_1 and T_2 representations of T_d while the E representation of C_{3v} correlates with the E, T_1 and T_2 representations. The T_1 representation is the representation of the rotations, therefore, we need not concern ourselves with it.

Table 4. Correlation of D_2 and C_{3v} with T_d

T_d	D_2	C_{3v}
A_1	A	A_1
A_2	A	A_2
E	$2A$	E
T_1	$B_1 + B_2 + B_3$	$A_2 + E$
T_2	$B_1 + B_2 + B_3$	$A_1 + E$

5. The independent basis vectors within C_{3v} are

$$\begin{aligned}\hat{P}^{(A_1)}X_1 &= X_1+Y_1+Z_1=r_1\\ \hat{P}^{(E)}X_1 &= 2X_1-Y_1-Z_1=e_1\\ \hat{P}^{(E)}(Y_1-Z_1) &= Y_1-Z_1=p_1\,.\end{aligned}\tag{20}$$

These are shown in Fig. 3.

6. The final vibrational functions are (only one component of each degenerate function is given):

$$\phi(a_1)=\hat{P}^{(A)}r_1 \qquad =r_1+r_2+r_3+r_4\,, \tag{21a}$$

$$\phi_1(t_2)=\hat{P}^{(B_1+B_2+B_3)}r_1=3r_1-r_2-r_3-r_4\,, \tag{21b}$$

$$\phi(e)=\hat{P}^{(A)}e_1 \qquad =e_1+e_2+e_3+e_4\,, \tag{21c}$$

$$\phi_2(t_2)=\hat{P}^{(B_1+B_2+B_3)}e_1=3e_1-e_2-e_3-e_4\,. \tag{21d}$$

The functions represented by Eqs. (21a), (21b) and (21c) are completely equivalent to the functions ν_1, ν_{3b} and ν_{2a} given by Herzberg [15]. That of Eq. (21d) does not look like one of his forms. However, using the projection operator for only the B_3 representation of D_2 yields

$$\phi_2'(t_2)=\hat{P}^{(B_3)}e_1=e_1-e_2-e_3+e_4\,. \tag{22}$$

This is one of the ν_4 vibrations listed by Herzberg.

Acknowledgement. The author would like to thank Dr. T. H. Siddall, III and his students for calling attention to this problem.

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