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A COMPUTERIZED PROGRAM FOR FINDING THE SYMMETRIES OF THE MOLECULAR NORMAL MODES OF VIBRATION

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A Method and a Program for finding the Symmetries of the Molecular Normal Modes of Vibration is presented. It is based on the attachment of three-versors-to-each-atom scheme followed by deriving the corresponding reducible representation and its decomposition into the irreducible ones. Applications are presented and discussed, including the newly proposed pseudo-finite groups for linear molecules.

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1. Introduction

The electronic, vibrational, and Raman spectra are all connected, one way or another, with the vibrations of the atoms that are forming molecules, complexes, etc.

In the case of the electronic spectra, vibrational movements of the molecular atoms are producing broadening and/or fine structure of the bands.

The pure vibrational spectra of the molecules (complexes) are associated with the permanent electric-dipole variation (Infrared domain, IR); some of those connected with the induced electric-quadrupol variation (Raman domain) are also vibrational in nature.

It follows from the above that a great deal of spectral behavior of atomic associations are due to atomic vibrations around their equilibrium positions.

The main problems of the vibrational movements consist in the correct description of the corresponding energy levels (wave functions, w.f.) and of the transitions between these states (selection rules). Both these operations are, sometimes, difficult and time consuming. Knowing the symmetry of the molecules and of the atomic movements during their vibrations is of a great help in optical spectroscopy.

A method of exquisite elegance and efficiency in such cases is that of the *finite punctual group formalism.* This instrument is more than adequate for finding the symmetries of the *normal modes of vibration* (n.m.v.) of the considered molecules. Finding the spatial, exact, form of the n.m.v. is, in principle, simple but in most cases, very difficult in practice. Hopefully there is no need, for solving the just mentioned spectral problems, to know the exact pattern of the n.m.v. (like dimension and orientation of the vectors representing the atomic movement during vibration). Their symmetry is enough.

The first item to be known here, for solving the two mentioned problems, is the molecular symmetry and its association with one of the known punctual groups.

In the case of the w.f., describing the energy levels, the group formalism will tell us which of the elementary atomic orbitals (s, p, d, ….) may combine and with a simple algebra, in what proportions, for building molecular hybrids, adequate for describing the molecular spectral states.

When transitions (or selection rules) are considered, we look for the intensity of a spectral band, which is proportional to the *moment of transition*, π, equal to an integral over the Ψ_1 and Ψ_2

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w.f. describing the two states, and the implied operator, P, connected with different physical quantities, which are changing in the process:

$$\pi = \int \Psi_1 P \Psi_2 \, d\tau \tag{1}$$

Such an integral cannot depend on the position of the molecule in a coordinate system, in other words, its value is invariant to any symmetrical changes in the molecule's orientation. This means that a series of coordinate transformation can be made (like reflections, rotations, and inversion) without altering the internal (energy) states of that molecule. These operations form a specific *group* for any kind of molecule, and the elemental, atomic, orbitals (out of which hybrid orbitals are formed), as well as the mentioned operators, are bases for the irreducible representations describing that molecule. The hybrid orbitals are bases for a reducible representation in the same group.

All elemental w.f. and all operators needed to deal with most of the optical spectroscopy problems are represented directly by simple, products, or squared Cartesian coordinates, as well as by the sense of rotation around some of the symmetry axes.

All we have to know, to find the elemental (atomic) w.f. needed to form a given hybrid (molecular) orbital, is the form of the hybrid orbital (orientation of its lobes), that is a rather simple task. The form of the molecule indicates them. Using these hybrids as a base, a reducible representation is generated in the molecule's group, and subsequently reduced to its irreducible representations. Now a rule is applied: only those elemental orbitals will enter as components in the hybrid orbital that have the symmetries of the just found irreducible representations. As for the quantities of each of them, the group formalism is also an extremely useful instrument, but we will not deal with it here. We are only interested now in finding the symmetries.

The other mentioned problem, of transitions, is again very simple. The transition between two energy levels of a molecule is represented, as mentioned before, by the corresponding transition moment, π. A second rule is applied: the product of the three factors of the π integral must be the basis for the totally symmetric representation of the group the considered molecule belongs to (or at least one of its components should do so after reduction), otherwise the integral will be zero (zero intensity, i.e., no transition). This conclusion can be illustrated by the following example. Let us take a molecule and try one of the specific symmetry operations. For simplicity (not affecting generality) imagine that the Ψ_1 and Ψ_2 w.f. of the implied levels, are non-degenerate, the changing operator is P, and take as the symmetry operation the inversion, I. Before doing any symmetry operation let us calculate the value of the transition moment, π. Presume the found value is A. Then we do the inversion in the central point of the molecule. There are the following possibilities: all factors of the integrand are symmetric to inversion. In this case the value of π remains the same: A. This means that the integrand will generate the totally symmetric representation (i.e. transition is permitted). If one of the factors is antisymmetric to inversion then we get –A. What we have done (inversion) is a symmetry operation and the value (or sign) of π cannot change under such a transformation, meaning A=-A must be true and that is not possible unless A=0 (transition is forbidden). If two of the factors are antysymmetric then, again, π = A (transition permitted) and so on (the +*+ = +, +*- = - rule). The game is played by the symmetry to inversion (in this case) of the integrand's factors.

The above mentioned facts are the motives for which symmetry and the group formalism is of an exquisite importance in optical spectroscopy, in general.

2. Models, n.m.v symmetry determination

Let us concentrate now on how it works in practice and what are the steps to be taken for finding the symmetry of the n.m.v. of a molecule.

1. The first step consists in establishing the symmetry of the considered molecule and the punctual group it belongs to. This is an easy task for someone familiar with the group theory. There are many articles and books treating the subject [1-5].

2. Step two: the attachment of a set of three mutually orthogonal versors to each one of the atoms in the molecule. These sets can be oriented in any direction, but for simplifying calculations, they should be oriented conveniently against the symmetry elements of the molecule: see the following examples.

3. The third step: application of all the operations in the group (one in each class) to all the versors, generating a reducible representation for the molecule. The result is, in fact, a set of characters of the representation (the trace of the representation matrices, or matrices of symmetry transformations).

4. Step four: reduction (decomposition) of the representation found at point 3, into its irreducible representations of the group (this part is accomplished by the computer program proposed in this paper).

The so found representations are directly connected with all the movements of all the atoms in the molecule, including translation and rotation of that molecule as a whole; therefore they are not real vibrations and must be eliminated from the list found at point 4. To do this we have simply to look at the character table of the group the molecule belongs to. Some of the irreducible representations, that have x, y, and z, as well as R_x, R_y and R_z, as bases, are representing translations and rotations, respectively. Not all the representations generated by these bases are due to translations and rotations: the program will take care of this, eliminating just the false vibrations. What remains after this elimination are the symmetries of the real normal modes of vibration of the considered molecule, the final result given by the program.

We should mention one more item: the number of the n.m.v. For any molecule having N atoms, is 3N-5, or 3N-6 depending on the fact that the molecule is linear or non-linear (for a linear molecule the molecular, axis - usually z - has no symmetry significance, so, we do not subtract R_z , therefore the number of the n.m.v. is 3N-5).

Some other features should be observed, connected with easing the operation of finding the reducible representation: a) if a set of versors are changing the position of their origin (the corresponding atom is moved to another equivalent position) during a symmetry operation, then that set of versors will not have any contribution to the character we are looking for, since in the transformation matrices there will be no non-zero diagonal elements; b) only versors, which are preserving their origin, will be transformed into themselves (+1 or –1), or into combination of themselves, giving projections that are generating non-zero diagonal elements; c) if the initial orientation of the versors is not convenient, they can freely be reoriented conveniently, for each symmetry operation; d) there is always a control of the correctness of the orientation by the fact that the product of the reducible representation with each of the irreducible ones (reduction operation) divided by the order of the group, an integer must be obtained (except for the new $\underline{C}_{9v}$ and $\underline{D}_{9h}$ groups, since here the characters are expressed in fractional values, but even in these cases the corresponding ratios are very near to an integer the error being, usually, less than 1 %). A computer rounding eliminates all ambiguity.

3. Application examples

Let us take some concrete examples (in the figures each type of atoms is colored differently).

1. A pyramidal, A-B_3 molecule, Fig. 1. This molecule belongs to the $\underline{C}_{3v}$ group. Its characters are given in Table 1. We will designate the symmetry elements (point, axes, planes) by lower case letters (i, c, σ), while the corresponding group elements (symmetry operations) by upper case letters (I, C, Σ).

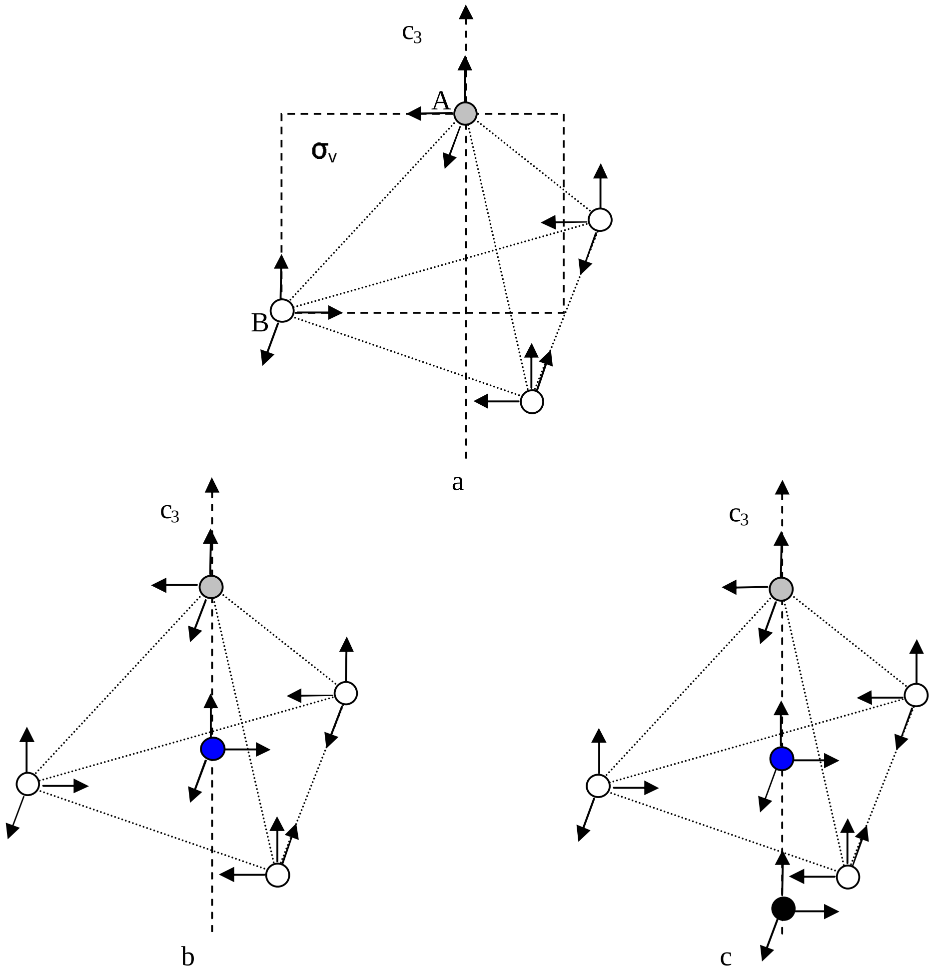

Fig. 1. a, b, c. Molecules having $\underline{C}_{3v}$ symmetry.

Table 1.

$\underline{C}_{3v}$	E	$2C_3$	$3\Sigma_v$	linear bases	bilinear bases
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	(x,y) (R_x, R_y)	(x^2-y^2, xy) (xz,yz)
Γ_a	12	0	2	4* (x,y,z)	
Γ_b	15	0	3	5* (x,y,z)	
Γ_c	18	0	4	6* (x,y,z)	

First we look for the characters the 3N versors are generating under all the operations in the mentioned group:

The E operation (in each and every group) is simple to apply: “no operation” means a character, $\chi(E)$, equal to the number of all versors, namely 3N. In this case, four atomic molecule, $\chi(E)=12$. The transformation matrix (12*12) has all diagonal elements equal to 1 and all the others are zero (each versor is transformed into itself).

The C_3 operation, around the z-axis (the highest order c_n-axis, in all groups, is always oriented vertically along the z-axis, by convention) affects only the versors of one atom, A, since all B atoms are changing places and do not have non-zero diagonal elements in the corresponding matrix of transformation. A rotation around a c_3-axis, of the three versors, in any group, gives a zero character, as follows (presuming x, y, z, and x', y', z', the old and new coordinate, respectively):

$$\begin{aligned} x' &= x\cos(120^0) - y\sin(120^0) + 0z \\ y' &= x\sin(120^0) + y\cos(120^0) + 0z \\ z' &= 0x \quad +0y \quad + 1z \end{aligned} \tag{2}$$

and the transformation matrix is,

$$\begin{bmatrix} \cos(120^0) & -\sin(120^0) & 0 \\ \sin(120^0) & \cos(120^0) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} -1/2 & 1/2 & 0 \\ 1/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3}$$

whose trace is zero, i.e., its character is $\chi\,(C_3) = 0$.

The Σ_v operation affects two atoms (A and one B) whose z-versors are in that plan. It is convenient to take one of the x and y versors in the same σ_v plane. Let us take y in that plane. So reflection, for any one atom, will reproduce z and y into themselves and change x into minus x. The corresponding matrix is,

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{4}$$

and the character $\chi(\Sigma_v)$ is equal to 1. Again, this is true in any group: reflection in a plane of a set of three versors gives 1. But there are two atoms on that plane, so, $\chi(\Sigma_v) = 2$ in the reducible representation. These characters are given in the fifth line of Table 1, as Γ_a.

It is easy to see that the cases illustrated by Fig. 1b and 1c, with 5 and 6 atoms, respectively, for the same group, have three and four atoms on the c_3-axis and four and five atoms on the σ_v-plane, in the two cases. The corresponding characters are given in the sixth and seventh lines of Table 1, as Γ_b and Γ_c respectively.

The $\underline{C}_{2h}$ – group, Fig 2. This molecule is a planar (horizontal) one, obviously, $\chi(E) = 12$. $\chi(C_2) = 0$, since there is no atom on the c_2-axis. The same is true for I-operation: $\chi(I) = 0$. There are 8 versors in the Σ_h plane and 4 perpendiculars to it. That means eight are reproduced, preserving their magnitude and orientation and four are changing their sign in the process: $\chi(\Sigma_h) = 4$. All these are given in the sixth line of Table 2.

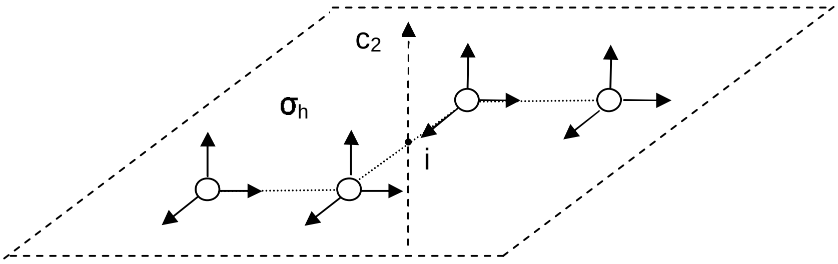

Fig. 2. The planar A_4 molecule, $\underline{C}_{2h}$ symmetry.

Table 2.

$\underline{C}_{2h}$	E	C_2	I	Σ_h	linear bases	bilinear bases
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	(R_x, R_y)	(xz,yz)
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	(x,y)	
Γ	12	0	0	4	4* (x,y,z)	

Let us take now three different molecules all having $\underline{D}_{3h}$ symmetry, Fig. 3 a, b and c. The results of the transformations imposed by the symmetry operations of this group are given in Table 3, lines 8, 9 and 10.

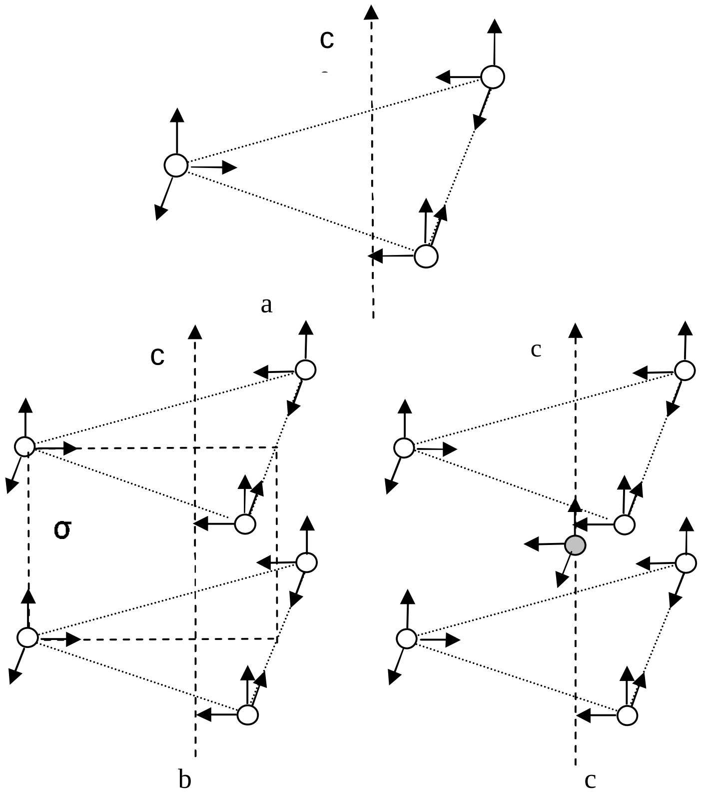

Fig. 3. a, b, c. Molecules having $\underline{D}_{3h}$ symmetry.

Table 3.

$\underline{D}_{3h}$	E	$2C_3$	$3C_2$	Σ_h	$2S_3$	$3\Sigma_v$	linear bases	bilinear bases
A_1’	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2’	1	1	-1	1	1	-1	R_z	
E’	2	-1	0	2	-1	0	(x,y)	$(x^2 - y^2, xy)$
A_1”	1	1	1	-1	-1	-1		
A_2”	1	1	-1	-1	-1	1	z	
E”	2	-1	0	-2	1	0	(R_x, R_y)	(xz,yz)
Γ_a	9	0	-1	3	0	1	3* (x,y,z)	
Γ_b	18	0	0	0	0	2	6* (x,y,z)	
Γ_c	21	0	-1	1	-2	3	7* (x,y,z)	

The $\underline{D}_{3d}$ case, Fig. 4, a b, and Table 4, is illustrated by two molecules, slightly different, in order to emphasize the already mentioned fact that position of the atoms on the symmetry elements are very important. The feint atom triangles are copies of the opposite, real atom triangles, to emphasize their relative positions.

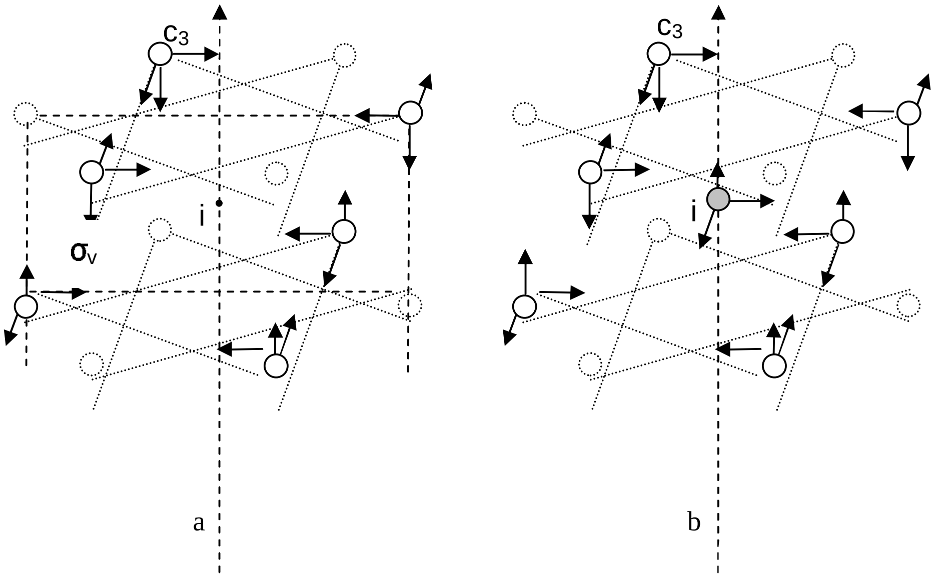

Fig. 4. a, b. The $\underline{D}_{3d}$ symmetry molecules.

Table 4.

$\underline{D}_{3d}$	E	$2C_3$	$3C_2$	I	$2S_6$	$2\Sigma_d$	linear bases	bilinear bases
A_{1g}	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	-1	1	1	-1	R_z	
E_g	2	-1	0	2	-1	0	(R_x, R_y)	$(x^2 - y^2, xy)$ (xz,yz)
A_{1u}	1	1	1	-1	-1	-1		
A_{2u}	1	1	-1	-1	-1	1	z	
E_u	2	-1	0	-2	1	0	(x,y)	
Γ_a	18	0	0	0	0	2	6*(x,y,z)	
Γ_b	21	0	-1	-3	0	3	7*(x,y,z)	

The following cases, $\underline{T}_d$, Fig, 5, Table 5, and $\underline{O}_h$, Fig. 6, Table 6, are given for the only reason of showing the correct answers and may be used for exercises by those interested in verifying the method.

Table 5.

$\underline{T}_d$	E	$8C_3$	$3C_2$	$6S_4$	$6\Sigma_d$	linear bases	bilinear bases
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x,y,z)	(xy,xz,yz)
Γ	15	0	-1	-1	3	5*(x,y,z)	

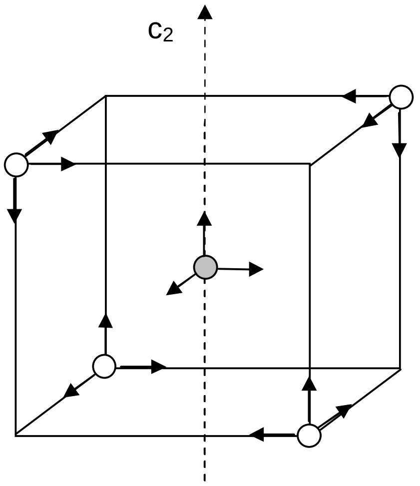

Fig. 5. The $\underline{T}_d$ symmetry species.

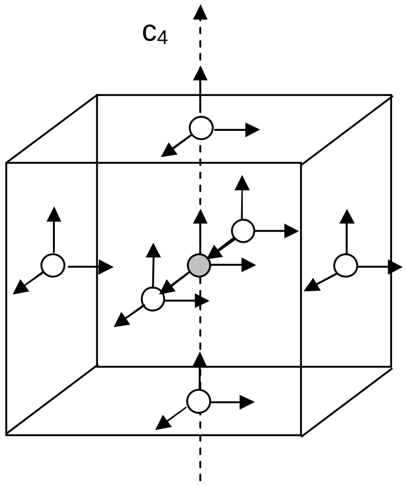

Fig. 6. The $\underline{O}_h$ symmetry species.

Table 6.

$\underline{O}_h$	E	$8C_3$	$6C_2$	$6C_4$	$3C_2$	I	$6S_4$	$8S_6$	$3\Sigma_h$	$6\Sigma_d$	linear bases	bilinear bases
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	3	0	-1	1	-1	3	1	1	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xy,xz,yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x,y,z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		
Γ	21	0	-1	3	-3	-3	-1	0	5	3	7*(x,y,z)	

Finally, the new, $\underline{C}^{\infty}_{9v}$ group, [6] for linear, unsymmetrical, molecules is presented in Fig. 7 a, b and Table 7. The $\underline{D}^{\infty}_{9h}$ shape and character table are not given or discussed here, since this group is simply the product: $\underline{C}_i * \underline{C}^{\infty}_{9v} = \underline{D}^{\infty}_{9h}$ and, consequently very easy to derive.

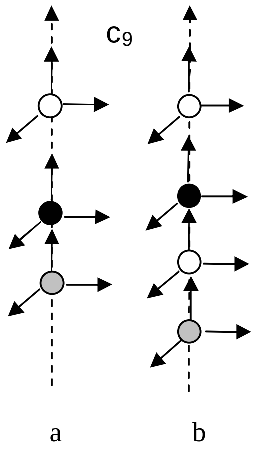

Fig.7. a, b. Linear, $\underline{C}^{\infty}_{9v}$ Symmetry

Table 7.

$\underline{C}^{\infty}_{9v}$	E	$2C_9$	$2C_9^2$	$2C_9^3$	$2C_9^4$	$9\Sigma_v$	linear bases	bilinear bases
$A_1 \equiv \Sigma^+$	1	1	1	1	1	1	z	x^2+y^2, z^2
$A_2 \equiv \Sigma^-$	1	1	1	1	1	-1	R_z	
$E_1 \equiv \Pi$	2	1.532	0.347	-1	-1.879	0	(x,y) (R_x , R_y)	(xz,yz)
$E_2 \equiv \Delta$	2	0.347	-1.879	-1	1.532	0		(x^2-y^2,xy)
$E_3 \equiv \Phi$	2	-1	-1	2	-1	0		
$E_4 \equiv \Gamma$	2	-1.879	1.532	-1	0.347	0		
Γ_a	9	7.596	4.041	0	-2.637	3	3*(x,y,z)	
Γ_b	12	10.128	5.388	0	-3.516	4	4*(x,y,z)	

4. Discussion

The nonlinear molecules do not need further discussion.

The linear molecules, however, must be treated a little deeper because we are using the recently proposed, pseudo-finite groups ($\underline{C}^{\infty}_{9v}$ and $\underline{D}^{\infty}_{9h}$) [6], which are limited, but rather efficient. Namely, they are transformed $\underline{C}_{\infty v}$ and $\underline{D}_{\infty h}$ infinite groups into pseudo-finite ones. This has been made by giving φ, the rotation angle around the molecular axis, finite, discrete values. The only problem with these groups is that they are not closed. This inconvenience is only bad for higher representations. We found that 9 is a good enough order for n, covering correctly and completely, all operations concerning representations up to E_2 (Δ). To this level these groups are working perfectly like any other finite group, in all respects as much as the n.m.v. are concerned. There is no need, in what we are doing here, to go to a higher group. In fact, all elements necessary for the n.m.v. symmetry determination are not going over E_1 (Π). If higher orders are, nevertheless necessary, in other problems, like transitions, hybrid orbital construction, etc., these groups can easily be extended to n=17, for example.

The characters of the reducible representations can be found, in this case, by inspecting the character tables of the $\underline{C}^{\infty}_{9v}$ (or $\underline{D}^{\infty}_{9h}$) group. They are the characters generated by the x, y and z coordinates (bases). The three-versors-to-each-atom model is valid here like in any other case (group) except that now the characters are not integers, i.e., less comfortable to work with. So, we should use another, simpler, method: add the irreducible characters that are generated by x, y and z bases, and multiply that sum by the number of atoms in the molecule we are interested in, separately for every class of the group. The result will be the characters of the reducible matrix of transformations of the 3N versors on the molecule, to be introduced into P.C. when asked by the program. This way of finding the reducible characters is possible only because all the atoms are simultaneously on all the symmetry elements of the (linear) molecules. (This method can be used with nonlinear molecules if the above mentioned sum of characters is multiplied by the number of atoms on each element of symmetry involved in each specific operation, and not by 3N). The so found symmetry species are also containing false vibrations: (translations and rotations) of the molecule. The program, presented here, as mentioned before, will eliminate these species and give the symmetries of the real vibrations only, so, there is no need to bather with them at all.

We have recently published two alternate, empiric, methods for finding the n.m.v. symmetries of the linear molecules [6,7].

5. Conclusion

Just a few cases have been discussed here, to show how the program works and to present some possible variations, but the method can be applied to any other group. All we have to do is to; a) consider the form of the molecule we are interested in; b) find the corresponding group; c) attach a set of three mutually orthogonal versors to each atom; d) generate the reducible representation by yourself. The program will ask you to introduce the name of the group the considered molecule belongs to, then to introduce the characters of the just found reducible matrices. It will find the irreducible representations, eliminate the false vibrations, and give the symmetries (representations) of the real n.m.v. of the molecule (how many of each species).

It should be stressed that point d) is solved differently for the linear molecules compared to all the others. In fact, in this case we do not even need the three-versors-to-each-atom model, but use directly the character tables of the two pseudo-finite groups, as an easier way.

The program is written in GWBASIC since it is simple, friendly and everybody has it. Comments are included in the program. Being simple, it can be easily translated into any other language (Appendix A).

Data are the characters of the irreducible representations of the analyzed groups multiplied by the number of operations in each class, followed by the symbols of those representations.

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Appendix A

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10 REM Program:"nmv-symm".bas, for finding the symmetries of the molecular
normal modes of vibration (n.m.v).

15 LET A$="choose the group (c3v, c2h, d3h, d3d, td, oh, c9v)"
20 PRINT A$: INPUT "A$";A$
25 IF A$<>"c3v" AND A$<>"c2h" AND A$<>"d3h" AND A$<>"d3d" AND A$<>"td"
AND A$<>"oh" AND A$<>"c9v" THEN GOTO 15
30 IF A$="c3v" THEN C=3: REM C= number of classes (representations) in the
group.
35 IF A$="c3v" THEN H=6: REM H= order of the group.
40 IF A$="c3v" THEN RESTORE 430
45 IF A$="c2h" THEN C=4
50 IF A$="c2h" THEN H=4
55 IF A$="c2h" THEN RESTORE 455
60 IF A$="d3h" THEN C=6
65 IF A$="d3h" THEN H=12
70 IF A$="d3h" THEN RESTORE 485
75 IF A$="d3d" THEN C=6
80 IF A$="d3d" THEN H=12
85 IF A$="d3d" THEN RESTORE 525
90 IF A$="td"  THEN C=5
95 IF A$="td"  THEN H=24
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100 IF A$="td" THEN RESTORE 565
105 IF A$="oh" THEN C=10
110 IF A$="oh" THEN H=48
115 IF A$="oh" THEN RESTORE 600
120 IF A$="c9v" THEN C=6
125 IF A$="c9v" THEN H=18
130 IF A$="c9v" THEN RESTORE 660
135 DIM A(C,C)
140 FOR N=1 TO C
145 FOR M=1 TO C
150 READ D: REM D= DATA= X(R)*g(R); g(R)= number of operations in the class.
155 A(N,M)=D
160 NEXT M,N
165 DIM B(C)
170 FOR M=1 TO C
175 PRINT M;"  ";
180 INPUT "B=";B: REM B= the characters of the reducible representation.
185 B(M)=B
190 NEXT M
195 DIM Y(C)

200 FOR I=1 TO C
205 Y=0
210 FOR M=1 TO C
215 Y(M)=A(I,M)*B(M)
220 Y=Y+Y(M)
225 NEXT M
230 PRINT " I = "; I,
235 READ B$: PRINT B$; " = "; : REM B$= symbols of the irred. representations.
240 Z=CINT(Y)/H
245 IF A$="c3v" THEN GOTO 280
250 IF A$="c2h" THEN GOTO 300
255 IF A$="d3h" THEN GOTO 325
260 IF A$="d3d" THEN GOTO 350
265 IF A$="td" THEN GOTO 375
270 IF A$="oh" THEN GOTO 390
275 IF A$="c9v" THEN GOTO 405
280 IF I=1 THEN Z=Z-1: REM Lines 285-415: subtraction of the false n.m.v.
285 IF I=2 THEN Z=Z-1
290 IF I=3 THEN Z=Z-2
295 GOTO 415
300 IF I=1 THEN Z=Z-1
305 IF I=2 THEN Z=Z-2
310 IF I=3 THEN Z=Z-1
315 IF I=4 THEN Z=Z-2
320 GOTO 415
325 IF I=2 THEN Z=Z-1
330 IF I=3 THEN Z=Z-1
335 IF I=5 THEN Z=Z-1
340 IF I=6 THEN Z=Z-1
345 GOTO 415
```

```
350 IF I=2 THEN Z=Z-1
355 IF I=3 THEN Z=Z-1
360 IF I=5 THEN Z=Z-1
365 IF I=6 THEN Z=Z-1
370 GOTO 415
375 IF I=4 THEN Z=Z-1
380 IF I=5 THEN Z=Z-1
385 GOTO 415
390 IF I=4 THEN Z=Z-1
395 IF I=9 THEN Z=Z-1
400 GOTO 415
405 IF I=1 THEN Z=Z-1
410 IF I=3 THEN Z=Z-2
415 PRINT CINT(Z)
420 NEXT I

425 REM The c3v-group:
430 DATA     1,   2,   3
435 DATA     1,   2,  -3
440 DATA     2,  -2,   0
445 DATA       A1, A2, E
450 REM The c2h-group:
455 DATA     1,  1,  1,  1
460 DATA     1, -1,  1, -1
465 DATA     1,  1, -1, -1
470 DATA     1, -1, -1,  1
475 DATA       Ag, Bg, Au, Bu
480 REM The d3h-group:
485 DATA     1,  2,  3,  1,  2,  3
490 DATA     1,  2, -3,  1,  2, -3
495 DATA     2, -2,  0,  2, -2,  0
500 DATA     1,  2,  3, -1, -2, -3
505 DATA     1,  2, -3, -1, -2,  3
510 DATA     2, -2,  0, -2,  2,  0
515 DATA       A'1, A'2, E', A"1, A"2, E"
520 REM The d3d-group:
525 DATA     1,  2,  3,  1,  2,  3
530 DATA     1,  2, -3,  1,  2, -3
535 DATA     2, -2,  0,  2, -2,  0
540 DATA     1,  2,  3, -1, -2, -3
545 DATA     1,  2, -3, -1, -2,  3
550 DATA     2, -2,  0, -2,  2,  0
555 DATA       A1g, A2g, Eg, A1u, A2u, Eu
560 REM The td-group:
565 DATA     1,  8,  3,  6,  6
570 DATA     1,  8,  3, -6, -6
575 DATA     2, -8,  6,  0,  0
580 DATA     3,  0, -3,  6, -6
585 DATA     3,  0, -3, -6,  6
590 DATA       A1, A2, E, T1, T2
595 REM The oh-group:
```

```
600 DATA     1,  8,  6,  6,  3,  1,  6,  8,  3,  6
605 DATA     1,  8, -6, -6,  3,  1, -6,  8,  3, -6
610 DATA     2, -8,  0,  0,  6,  2,  0, -8,  6,  0
615 DATA     3,  0, -6,  6, -3,  3,  6,  0, -3, -6
620 DATA     3,  0,  6, -6, -3,  3, -6,  0, -3,  6
625 DATA     1,  8,  6,  6,  3, -1, -6, -8, -3, -6
630 DATA     1,  8, -6, -6,  3, -1,  6, -8, -3,  6
635 DATA     2, -8,  0,  0,  6, -2,  0,  8, -6,  0
640 DATA     3,  0, -6,  6, -3, -3, -6,  0,  3,  6
645 DATA     3,  0,  6, -6, -3, -3,  6,  0,  3, -6
650 DATA       A1g, A2g, Eg, T1g, T2g, A1u, A2u, Eu, T1u, T2u

655 REM The c9v-group:
660 DATA     1,      2,        2,       2,     2,       9
665 DATA     1,      2,        2,       2,     2,      -9
670 DATA     2,   3.064,   0.694,   -2,  -3.758,   0
675 DATA     2,   0.694,  -3.758,   -2,   3.064,   0
680 DATA     2,     -2,       -2,       4,    -2,       0
685 DATA     2,  -3.758,   3.064,   -2,   0.694,   0
690 DATA       A1,  A2,  E1,  E2,  E3,  E4

695 REM
700 REM Finding the reducible representations with the three-versors-to-each-atom
technique, for real, finite, groups is a direct, easy, task when the characters
of the ireducible representations are integers, as it is in many cases.

705 REM
710 REM With the pseudo-finite groups, C9v and D9h, the sum of the irreducible
characters, generated by the x,y and z, multiplied by the number of atoms, in each
class, are to be taken for finding the characters of the reducible representation.
```