Construction of the C_{2v} character table

The character table C_{2v} has the following form:

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

We will consider how the various basis functions x, y, z and others in the right hand columns map onto the basis Vectors of the space (also known as irreducible representations). These are the A_1, A_2, B_1 and B_2.

The totally symmetric basis vector

As an example we will consider the C_{2v} point group, which corresponds to the H_2O molecule for instance. We can call the totally symmetry basis vector A_1 as shown in Table 1. A_1 is just a name like, X, Y or Z for the Cartesian space.

$\mathbf{C_{2v}}$	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1

The basis vectors must be normalized and orthogonal. Normalization is like saying that these are unit vectors in the space. The dimensionality of the basis must also equal the dimensionality of the space. The C_{2v} point group is 4-dimensional (i.e. there are four symmetry elements). To determine the dimensionality of any point group we need only count the symmetry operations.

The normalization condition

Is A_1 normalized (i.e. does it have a length of 1)? We will sum over the square of the contribution for each symmetry element and then divide by the dimension of the group h. The length L is

$$|S|^2 = \frac{1}{h}\sum_{i=1}^{h} \chi_i^2$$

where S is the *basis vector name and* χ *is the character or value of each symmetry operation for that particular basis vector.*
We can see that A_1 *is normalized.*

$$|A_1|^2 = \frac{1}{4}(1^2 + 1^2 + 1^2 + 1^2) = 1$$

The other basis vectors must be orthogonal to A_1 and also normalized. We could find these vectors using four equations and four unknowns.

Starting point for construction

We will call the remaining vectors A_2, B_1 and B_2. Based on the information we have up to now we can construct a table of the basis vectors that looks like this.

$\mathbf{C_{2v}}$	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1
A_2	1			
B_1	1			
B_2	1			

One formal way to find the remaining elements of the table is to use 9 unknown values that fill the table and then to set up nine equations based normalization, orthogonality and the sum rule that each column (except E) sums to zero. However, we will invoke an intuitive approach to find the basis vectors.

The normalization condition for A_2

The subscript refers to whether a basis vector changes sign upon reflection. The letter describes whether it changes sign upon rotation. A does not change upon rotation, but B does. 1 does not change sign upon reflection, but 2 does. Thus, A_2 does not change sign upon rotation ($C_2 = 1$), but it does change sign upon reflection, i.e $\sigma_{v(xz)} = \sigma_{v(yz)} = -1$

$\mathbf{C_{2v}}$	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1			
B_2	1			

We can see that A_2 is normalized sine

$$|A_2|^2 = \frac{1}{4}(1^2 + 1^2 + (-1)^2 + (-1)^2) = 1$$

The orthogonality is given by

$$|S_1||S_2| = \frac{1}{h}\sum_{i=1}^{h} \chi_{1i}\chi_{2i}$$

which is explicitly given by

$$|A_1||A_2| = \frac{1}{4}\big((1)(1) + (1)(1) + (1)(-1) + (1)(-1)\big) = 0$$

Next we consider the B basis vectors, which should change sign upon rotation.

C_{2v}	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1		
B_2	1	-1		

The orthonormal basis in C_{2v}

$\mathbf{C_{2v}}$	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

Mulliken symbols for irreps:

- "A"—symmetric *wrt* rotation about principle axis ($\chi[C_n(z)] = +1$)
- "B"— irrep is antisymmetric *wrt* rotation about the principle axis ($\chi[C_n(z)] = -1$)
- "E" —doubly degenerate irrep ($d = 2 \Rightarrow \chi(E) = 2$)
- "T"—triply degenerate irrep ($d = 3 \Rightarrow \chi(E) = 3$)

Construction of the C_{3v} character table

The character tables C_{3v} has the following form:

C_{3v}	E	$2C_3$	$3\sigma_v$		
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)

This character table contains a two-dimensional representation called E. This is because the x and y dimensions are coupled in this point group.

Let's generate the C_{3v} point group.

The operations of C_{3v} are E, $2C_3$, $3\sigma_v$ (h=6, m=3)

$d_1^2 + d_2^2 + d_3^2 = 6$
$d_1 = d_2 = 1$ and $d_3 = 2$.

Since the dimensions of the irreps are the $\chi(E)$ and every group contains the totally symmetric irrep,

C_{3v}	**1**E	**2**C_3	**3**σ_v
Γ_1	1	1	1
Γ_2	1	j	k
Γ_3	2	m	n

Orthogonality of Γ_1 & Γ_2: (**1**)(1)(1) + (**2**)(1)(j) + (**3**)(1)(k) = 0

1 + 2j + 3k = 0

Normalization of Γ_2 requires $(1)(1)^2 + 2(j)^2 + 3(k)^2 = 6$

j = +1 and k = -1

Orthogonality of Γ_1 & Γ_3: (**1**)(1)(2) + (**2**)(1)(m) + (**3**)(1)(n) = 0

2 + 2m + 3n = 0

Normalization of Γ_3 means $(1)(2)^2 + 2(m)^2 + 3(n)^2 = 6$

m = -1 and n =0.

C_{3v}	**1**E	**2**C_3	**3**σ_v
Γ_1	1	1	1
Γ_2	1	j	k
Γ_3	2	m	n

Mulliken symbols for C_{3v}

C_{3v}	**1**E	**2**C_3	**3**σ_v
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Treating rotations and binary products as before, we can represent the C3v point group as

C_{3v}	E	$2C_3$	$3\sigma_v$		
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)

The x2-y2 and xy orbitals are also degenerate as are the xz and yz orbitals

In many instances there are more than one A, B, E , etc. irreps present in the point group so subscripts and superscripts are used

g or ***u*** subscripts are used in point groups with centers of symmetry (i) to denote ***g****erade* (symmetric) and ***u****ngerade* (antisymmetric) with respect to inversion

' and " are used to designate symmetric and antisymmetric with respect to inversion through a σ_h plane

numerical subscripts are used otherwise