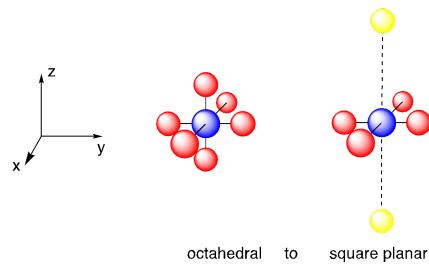


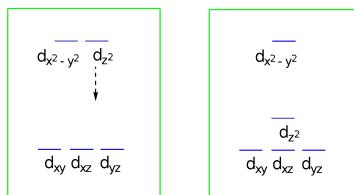
10.3.5: Square-Planar Complexes

Square planar geometry is much less common than octahedral, but square planar complexes assert their importance through their frequent appearance in key catalytic processes and other settings. Furthermore, having learned something about bonding in octahedral complexes, we can make some educated guesses about metal-orbital interactions in square planar complexes. Both geometries are nicely described by Cartesian coordinates and so it is relatively easy to draw comparisons between the two.

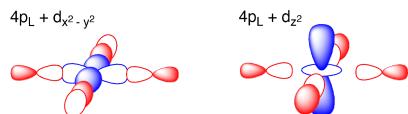
We can imagine how we might arrive at a square planar geometry simply by taking an octahedral geometry and removing two axial ligands. The four remaining equatorial ligands form a square planar complex.



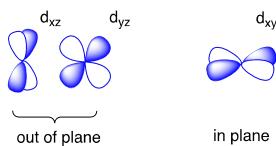
Since we already know something about the d orbital splitting diagram in an octahedral case, we can draw some rational conclusions about the consequence of this change. The axially-oriented d_{z^2} orbital drops in energy because it is no longer forming the antibonding combination with ligand orbitals along the z axis.



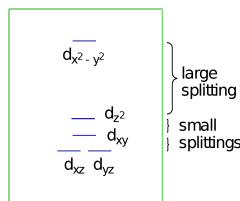
The d_{z^2} orbital does not drop all the way to the non-bonding level, however, because the toroid (the donut around the central node of the orbital) is still in plane with ligand orbitals along the x and y axes. Nevertheless, the d_{z^2} orbital overlaps with these ligand orbitals to a much lesser extent than the $d_{x^2-y^2}$ orbitals, so it drops to a level well below the $d_{x^2-y^2}$ orbital.



The d orbital splitting diagram shown above is not the one you will normally see for a square planar complex. The three non-bonding orbitals, d_{xy} , d_{xz} and d_{yz} , are degenerate in an octahedral geometry but not in a square planar one. The d_{xy} orbital is in the plane of the metal and ligands whereas the d_{xz} and d_{yz} are above and below that plane.



We therefore might not expect all three of these orbitals to be at the exact same energy level in the square planar coordination environment. We usually think of the d_{xy} orbital as lying at higher energy than the d_{xz} , d_{yz} pair because of the potential for interaction with the ligands that lie in the same plane as the d_{xy} orbital. The typical drawing of a d orbital splitting diagram reflects that subtle difference, showing the five metal d orbitals lying at four different energy levels with just one degenerate set (the d_{xz} , d_{yz} pair).



Note that there is a large splitting and two smaller splittings between the d orbitals, rather than the single splitting observed in an octahedral environment. As a result, when we talk about possible high spin and low spin electron population in the square planar environment, we are generally concerned with whether the electrons can surmount the large splitting and occupy the top orbital, the $d_{x^2-y^2}$.

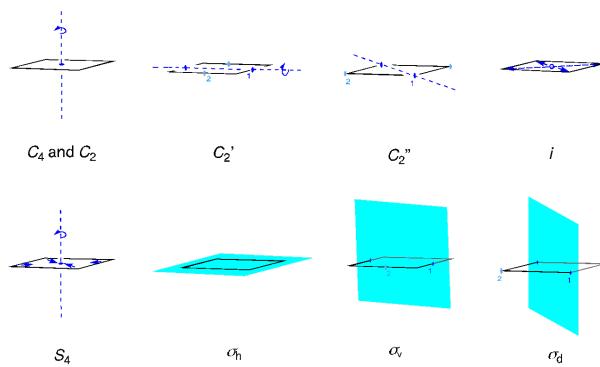
Sometimes, square planar d orbital splitting diagrams show the d_{xy} orbital above the d_{z^2} orbital and sometimes *vice versa*; the exact order varies with the ligands involved. The reasons for these differences are somewhat complicated. For example, this order can reflect the importance of pi bonding in a particular complex, as we will see later.

Group Theory Treatment of Square Planar Complexes

In octahedral coordination, we were able to use group theory to confirm the bonding picture we had arrived at through simple observation. We can do the same thing in the square planar case. This time, we need to use a character table for D_{4h} symmetry.

D_{4h}	E	$2C_4$	C_2	$2C_{2'}$	$2C_{2''}$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	
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	R_z
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	$x^2 - y^2$
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1	xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y) (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	z
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1	
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1	
E_u	2	0	-2	0	0	-1	0	2	0	0	(x, y)

The ten symmetry elements listed in this table may be easier to grasp than the ones in the higher-symmetry octahedral point group. In this case, we see several two- or four-fold axes and some mirror planes. They are illustrated below.



If we consider only sigma bonding from the ligands, which was the initial consideration we thought about earlier, then we could look at how this picture operates when transformed by these symmetry elements:



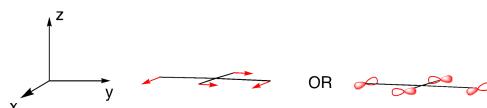
In that case, we obtain a reducible representation that can be reduced to the following:

$$\Gamma_{\sigma} = A_{1g} + B_{1g} + Eu$$

Returning to the character table, we find that the matching orbitals on the metal include the d_{z^2} and the $d_{x^2-y^2}$, as well as the s (represented by x^2+y^2), the p_x and p_y . If we are just interested in the d orbital splitting diagram, that gives us the picture that we had obtained before. Two d orbitals display some antibonding character whereas the other three are non-bonding. Of course, this treatment does not take into account the subtly different interactions of the ligands with the d_{z^2} and the $d_{x^2-y^2}$ orbitals. Although they are of like symmetry, these orbitals overlap with the ligands to different extents.

Pi Bonding

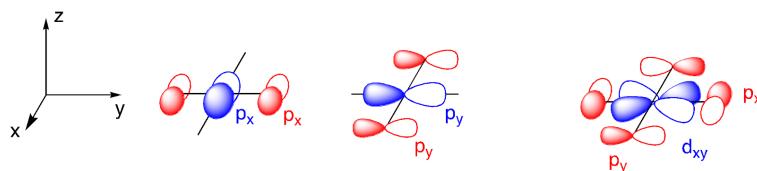
If we also want to include pi bonding in our understanding of these complexes, we have to think about two different orientations of the ligand p orbitals, which are not symmetrically equivalent in this case. The first orientation is parallel to the plane of the metal-ligand complex. It looks like this:



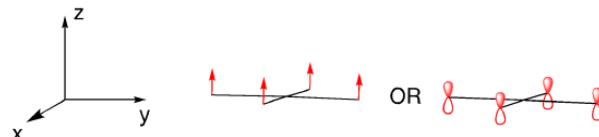
Treatment of those vectors with the symmetry elements leads to a reducible representation that can be represented by this one:

$$\Gamma_{\pi \parallel} = A_{2g} + B_{2g} + E_u$$

Consulting the character table, we find that the corresponding orbitals on the central atom are d_{xy} , p_x and p_y . In reality, the interaction with the d_{xy} is likely to be much more pronounced than with either the p_x or the p_y because of stronger overlap between the d_{xy} and the ligand p orbital.



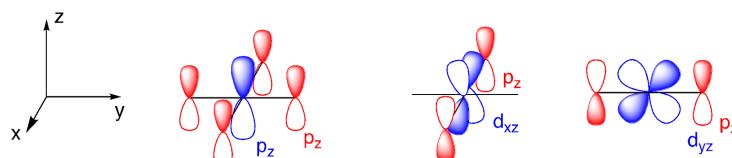
The second orientation is perpendicular to the plane of the complex.



This time, the irreducible representation is as follows:

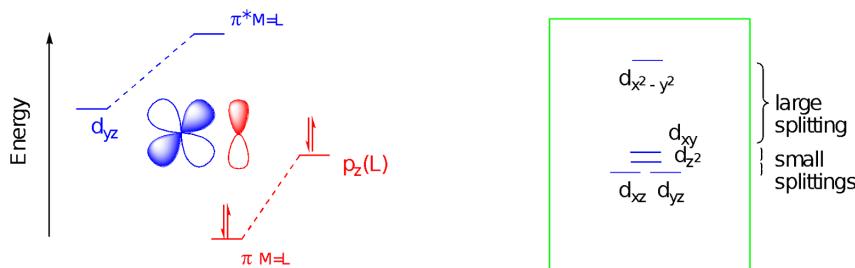
$$\Gamma_{\pi \perp} = A_{2g} + B_{2g} + E_u$$

According to the character table, this time the corresponding orbitals on the central atom are d_{xz} , d_{yz} , and p_z . Once again, because of stronger overlap between the d_{xy} or d_{yz} with the ligand p orbital compared to ligand overlap with the metal p_z , the former case is likely to be much more important than the latter.

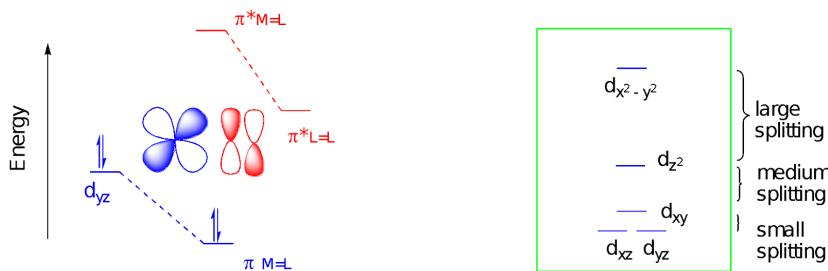


Thus, we see that the d orbitals that were not originally involved in sigma bonding have the potential to be involved in pi bonding. Which ones will actually be involved depends on the orientations of the ligands that are capable of pi bonding with these orbitals. That may be all of them in a more symmetric case (such as a homoleptic complex, in which all four ligands are the same as each other). It may be fewer in a complex with lower symmetry, in which the overall D_{4h} symmetry is broken by different ligands.

The nature of the ligands is probably of greater significance in terms of the magnitude of splittings in the d orbital diagram. If the metal forms a pi bond with the ligand via interaction with a p orbital on the ligand, then the resulting pi bond will be closer in both energy and character to the lower-energy ligand p orbital. We still think of that orbital as largely based on the more electronegative ligand. That means that the corresponding antibonding combination is more like the metal orbital in energy and character. It is still mostly a d orbital, for example. That results in a decrease in the splittings between d orbitals as the otherwise non-bonding set is pushed up in energy. We might even see the d_{xy} orbital at a higher energy level than the nominally sigma-antibonding d_{z^2} orbital, given a strong enough pi-bonding interaction.



On the other hand, if the metal orbital interacts with the empty π^* orbital of a ligand such as cyanide or carbon monoxide, this situation will be reversed. Because of its antibonding nature, the ligand π^* orbital lies above the metal d orbital in energy. When the two orbitals combine, the ligand π^* orbital becomes the metal-ligand π^* orbital. The metal d orbital drops in energy to form the metal-ligand bonding combination. Consequently, the metal orbitals involved in pi bonding to a pi acceptor drop in energy and splittings get larger. In particular, the gap between the pi bonding metal orbitals and the purely sigma bonding metal orbitals grows wider in this case.



The difference in overall splitting in these cases can be quite significant. For example, the differences between energy levels, denoted $\Delta 1$ and $\Delta 2$ below, are about 50% greater with the strongly pi-accepting cyanide ligand than with the pi-donating chloride in the corresponding homoleptic palladium complexes.¹

	PdCl ₄ ²⁻	Pd(CN) ₄ ²⁻
$\Delta 1$	19,150 cm ⁻¹	>30,000 cm ⁻¹
$\Delta 2$	6,200	10,800
$\Delta 3$	1,450	50

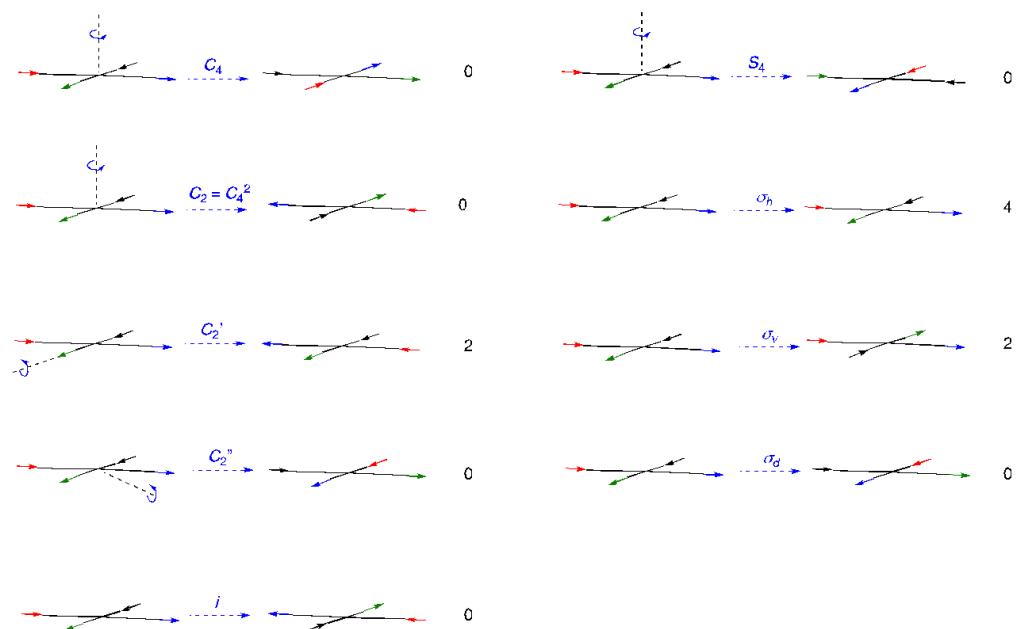
In all of these cases, the splitting between the highest-lying $d_{x^2-y^2}$ orbital and the next highest is much larger than the other splittings. That factor leads to square planar complexes generally adopting a low-spin configuration, which in this case means the lower orbitals are all occupied before the $d_{x^2-y^2}$. Square planar complexes are most often observed with d^7 or d^8 metal ions, which avoids populating that highest-energy d orbital.

Problems

1. a) Demonstrate how to arrive at the reducible representation for sigma bonding under the D_{4h} symmetry of a square planar complex.
- b) Determine the irreducible representation.
2. a) Demonstrate how to arrive at the reducible representation for pi bonding in the plane of the complex under the D_{4h} symmetry of a square planar complex.
- b) Determine the irreducible representation.

Solutions.

1. a) There are 4 unchanged vectors for E . For the others:



- b) Γ_σ : Remember, $a_i = \frac{1}{h} \text{QN} \cdot \chi(R) \cdot \chi(R) Q$

$$A_{1g}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1] = \frac{1}{16} [4 + 4 + 4 + 4] = \frac{1}{16}(16) = 1$$

$$A_{2g}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1)] = \frac{1}{16} [4 - 4 + 4 - 4] = \frac{1}{16}(0) = 0$$

$$B_{1g}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1)] = \frac{1}{16} [4 + 4 + 4 + 4] = \frac{1}{16}(16) = 1$$

$$B_{2g}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1] = \frac{1}{16} [4 - 4 + 4 - 4] = \frac{1}{16}(0) = 0$$

$$E_g: a_i = \frac{1}{16} [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 4 \cdot (-2) + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0] = \frac{1}{16} [8 - 8] = \frac{1}{16}(0) = 0$$

$$A_{1u}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot (-1) + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1)] = \frac{1}{16} [4 + 4 - 4 - 4] = \frac{1}{16}(0) = 0$$

$$A_{2u}: a_i = \frac{1}{16} [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot (-1) + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1] = \frac{1}{16} [4 - 4 - 4 + 4] = \frac{1}{16}(0) = 0$$

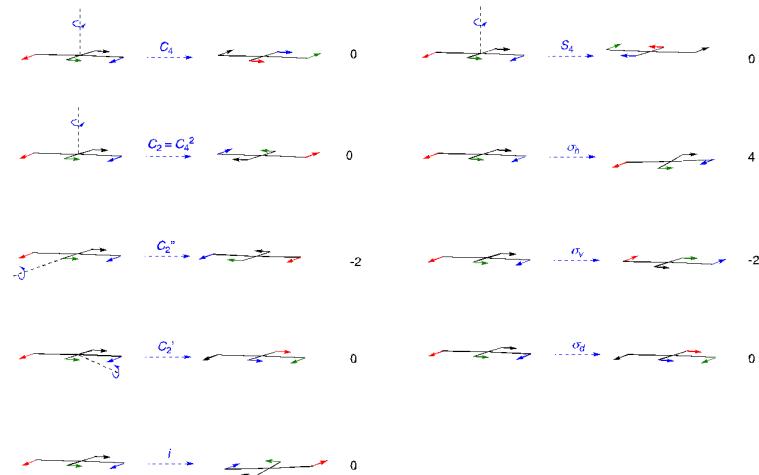
$$B_{1u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot (-1) + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1] = 1/16 [4 + 4 - 4 - 4] = 1/16(0) = 0$$

$$B_{2u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot (-1) + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1)] = 1/16 [4 - 4 - 4 + 4] = 1/16(0) = 0$$

$$E_u: ai = 1/16 [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot 0 \cdot 0 + 1 \cdot 4 \cdot 2 + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0] = 1/16 [8 + 8] = 1/16(16) = 1$$

$$\Gamma_\sigma = A_{1g} + B_{1g} + E_u$$

2. a) There are 4 unchanged vectors for E . For the others:



b) $\Gamma_{\pi||}$:

$$A_{1g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1] = 1/16 [4 - 4 + 4 - 4] = 1/16(0) = 0$$

$$A_{2g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1)] = 1/16 [4 + 4 + 4 + 4] = 1/16(16) = 1$$

$$B_{1g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1)] = 1/16 [4 - 4 + 4 - 4] = 1/16(0) = 0$$

$$B_{2g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1] = 1/16 [4 - 4 + 4 - 4] = 1/16(16) = 1$$

$$E_g: ai = 1/16 [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 4 \cdot (-2) + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0] = 1/16 [8 - 8] = 1/16(0) = 0$$

$$A_{1u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot (-1) + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1)] = 1/16 [4 - 4 - 4 + 4] = 1/16(0) = 0$$

$$A_{2u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 4 \cdot (-1) + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1] = 1/16 [4 + 4 - 4 - 4] = 1/16(0) = 0$$

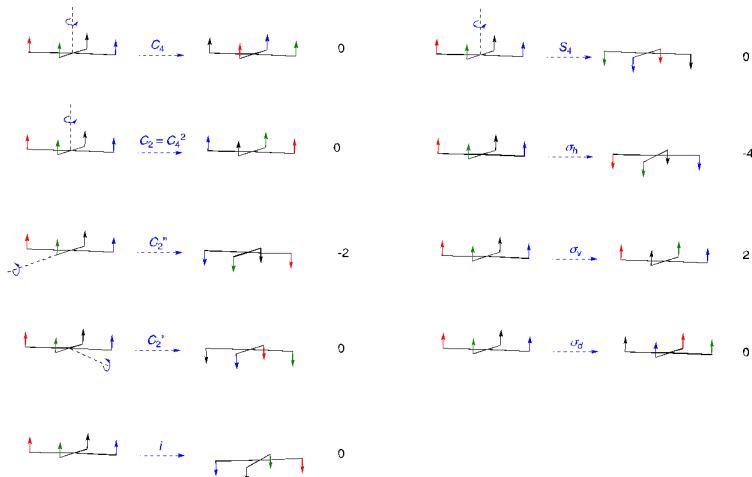
$$B_{1u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot (-1) + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1] = 1/16 [4 - 4 - 4 + 4] = 1/16(0) = 0$$

$$B_{2u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 4 \cdot (-1) + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1)] = 1/16 [4 + 4 - 4 - 4] = 1/16(0) = 0$$

$$E_u: ai = 1/16 [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot 0 \cdot 0 + 1 \cdot 4 \cdot 2 + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0] = 1/16 [8 + 8] = 1/16(16) = 1$$

$$\Gamma_{\pi||} = A_{2g} + B_{2g} + E_u$$

3. a) There are 4 unchanged vectors for E . For the others:



b) $\Gamma_{\pi \perp}$:

$$A_{1g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot (-4) \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1] = 1/16 [4 - 4 - 4 + 4] = 1/16(0) = 0$$

$$A_{2g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot (-4) \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1)] = 1/16 [4 + 4 - 4 - 4] = 1/16(0) = 0$$

$$B_{1g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot (-4) \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1)] = 1/16 [4 - 4 - 4 + 4] = 1/16(0) = 0$$

$$B_{2g}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot (-4) \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1] = 1/16 [4 + 4 - 4 - 4] = 1/16(0) = 0$$

$$E_g: ai = 1/16 [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot (-4) \cdot (-2) + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0] = 1/16 [8 + 8] = 1/16(16) = 1$$

$$A_{1u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot (-4) \cdot (-1) + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot (-1)] = 1/16 [4 - 4 + 4 - 4] = 1/16(0) = 0$$

$$A_{2u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot (-1) + 1 \cdot (-4) \cdot (-1) + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1] = 1/16 [4 + 4 + 4 + 4] = 1/16(16) = 1$$

$$B_{1u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot (-4) \cdot (-1) + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1] = 1/16 [4 - 4 + 4 - 4] = 1/16(0) = 0$$

$$B_{2u}: ai = 1/16 [1 \cdot 4 \cdot 1 + 2 \cdot 0 \cdot (-1) + 1 \cdot 0 \cdot 1 + 2 \cdot (-2) \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot 0 \cdot (-1) + 2 \cdot 0 \cdot 1 + 1 \cdot (-4) \cdot (-1) + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1)] = 1/16 [4 + 4 + 4 + 4] = 1/16(16) = 1$$

$$E_u: ai = 1/16 [1 \cdot 4 \cdot 2 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot (-2) \cdot 0 + 2 \cdot 0 \cdot 0 + 1 \cdot 0 \cdot (-2) + 2 \cdot 0 \cdot 0 + 1 \cdot (-4) \cdot 2 + 2 \cdot 2 \cdot 0 + 2 \cdot 0 \cdot 0] = 1/16 [8 - 8] = 1/16(0) = 0$$

$$\Gamma_{\pi \perp} = A_{2u} + B_{2u} + E_g$$

References

- Gray, H. B.; Ballhausen, C. J. *J. Am. Chem. Soc.* **1963**, 85, 260-264.

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