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Representing The World Around Us: Applications of Group Representation Theory to Molecular Orbital (MO) theory

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ABSTRACT

Molecular orbital (MO) theory is at the forefront of modern chemistry, allowing for accurate descriptions of the reactivity of molecules by using quantum mechanics to predict the location and energies of electrons within a molecule. The equations which govern their behavior, the Schrodinger equation, are often difficult to solve. Sometimes, we can only approximate a solution using numerical methods. This paper discusses a method that exploits a molecule's internal symmetry. Specifically, we use Group representation theory to help analyze and break down the molecular symmetry, and then use the analysis to help us find the MOs. First, we establish key results about irreducible representations and characters. We then establish a correspondence between MO's and irreducible representations. We then use the results obtained to perform MO calculations on water. We then compare the results obtained via our MO theory calculations and Valance Bond Theory (VBT). We conclude by showing these calculations are best used for rough work, being most useful for deciding which atomic orbitals they arose from, and each MO's energies relative to each other.

KEY WORDS: **Molecular Orbital (MO) theory, Group theory, Representation Theory, Symmetry-Adapted Linear Combination (SALC), Quantum Chemistry**

1 | INTRODUCTION

Molecular orbital (MO) theory is a theory in chemistry that describes the nature of chemical bonding. It assumes that all atoms that constitute a larger molecule combine their atomic orbitals to construct larger MOs (Galbraith et al., 2021). In essence, orbitals are 'regions of electron density.' These regions of density are dictated by the electron's wave function(s), which in turn are governed by the Schrodinger equation, given by (Miessler et al., 2022)

$$\widehat{H}\psi = E\psi$$

where $\widehat{H}$ is the Hamiltonian operator, ψ is our wave function, and E is the energy (eigenvalue) of the wave function. Solving it is quite difficult, as it typically involves second-order Partial Differential Equations (PDEs) with complicated boundary conditions. Sometimes, all we can do is approximate solutions. However, solutions to this equation allows us to gain insight into a molecule's electronic structure and thus its reactivity and is thus of great significance to chemists.

1.1 Group Theory and Abstract Algebra

Abstract algebra is a branch of mathematics which aims to study algebraic structures, like Groups, Rings, &Fields (Carter, 2021). This paper focuses on groups and their applications to problems in Chemistry, but they also appear in physics and computer science, among other disciplines (Carter, 2021).

At its core, Group theory is mathematical study of an object's symmetries (Carter, 2021). Before formally defining what groups are, we consider an example (Figure 1). Notice how we can combine 2 subsequent symmetries of the square to obtain another: for instance, if we reflect along the x axis, then reflect along the y axis, this is the same as rotating the square 180 degrees counterclockwise. There is also a way to 'undo' each symmetry: if you turn 90 degrees clockwise, turning counterclockwise 90 degrees undoes the original turn. Lastly, there is a 'home state': the configuration shown above. The set of symmetries associated with this square form a group (under composition).

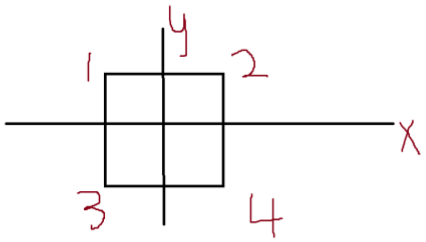


Figure 1: Square on the x-y plane, centered at the origin [self-generated]

Formally speaking, a group is a set G with a binary operation $*$ [a function/rule which takes pairs of elements in G and returns some element in G, with $*\ (a, b)$ denoted $a * b$ which satisfies the following properties:

1. There exists an identity element (typically denoted e) which satisfies $e * a = a = a * e$ for every $a \in G$
2. This binary operation is associative $a * (b * c) = (a * b) * c$ for any $a, b, c \in G$
3. Every element has an inverse: for every $a \in G$, there exists some $a^{-1} \in G$ such that $a * a^{-1} = a^{-1} * a = e$

Of course, we have only really scratched the surface of group theory and abstract algebra, with more details relegated to the appendix.

1.2 Representation Theory

Informally, representation theory is a way to associate elements of a group G to invertible matrices in such a way which preserves the group's algebraic structure. This allows us to use the tools of linear algebra and the mathematical theories associated with vector spaces to study our group G by encoding symmetries in terms of matrices. More formally, we define a representation of a group G as follows (Serre, 1977):

Definition 1*. A representation of a group G is a map $\rho: G \to GL(V)$ which is a homomorphisim [a homomorphism is a function between 2 groups which preserves the algebraic structure], Where $GL(V)$ denotes the group of invertible linear maps from a vector space V to itself. V is called the representation space.*

Here, if group theory and linear algebra are 2 different mathematical 'languages', then ρ behaves like a translator between the 2 'languages' and allows us to go between them. For simplicity, assume that all groups are finite, and that our vector spaces are complex and finite dimensional. This allows us to associate elements $g \in G$ to an invertible $n \times n$ matrix ρ_g with complex number entries, where $n < \infty$. In short, representation theory is a way to encode an object's symmetries in terms of matrices and linear algebra.

One important notion within representation theory is that of subrepresentations. These are representations which act on subspaces of the representation space V which are 'invariant' under the representation. By studying these sub-representations, we can use them to understand the whole. We formalize this notion as follows (Serre, 1977):

Definition 2*. Let G be a group and let $\rho: G \to GL(V)$ be a representation. Then W is a subrepresentation of G if*

1. *W is a subspace of V.*
2. *for any $g \in G$, we have that $\rho_g(W) \subseteq W$ (that is, elements in W get mapped to other elements in W under any ρ_g, and thus W is 'invariant').*

If the only such subspaces are $\{0\}$ and V itself, then our representation is said to be irreducible. Irreducible representations, sometimes called irreps or irreducibles, play a role analogous to that of prime numbers in $\mathbb{Z}$. Just like how an integer can be written as a product of prime number powers, we will show every representation can be written as a direct sum of (some number of copies of) irreducibles. Moreover, knowing an integer's prime factorization gives us information about that number, like its gcd (greatest common divisor) and lcm (lowest common multiple). Similarly, we will see that irreducible representations give us insight into a molecule such as the degeneracy of an MO, its relative energies, and which AOs formed it (Lowe & Peterson, 2011).

There are many representations of a group. However, it might be possible that two representations of G might end up encoding the same information, just in different ways. For instance, consider the representations ρ, ρ' of the group $C_2 = \{e, a\}$, where $a^2 = a * a = e$, given by:

$$p(a) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, p'(a) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

Both ρ and ρ′ encode a reflection but do it differently: ρ about the x axis, and ρ′ about the y axis. This notion of two different things having the same algebraic structure, and thus encoding the same information is an important mathematical idea known as isomorphism (Serre, 1977). In the context of group representations, isomorphism is defined as follows (Serre, 1977):

Definition 3*. Let $\rho: G \to GL(V)$, and $\rho': G \to GL(V')$ be two representations of G. we say that $\rho \cong \rho'$ [that is, ρ is isomorphic to ρ'] if there exists some invertible linear map $T: V \to V'$ such that for every $g \in G$, we have that:*

$$T \circ \rho_g \circ T^{-1} = \rho'_g$$

An important remark here is that this map T is the same for all the ρ_g. This notion, called simultaneously similar, is a stronger requirement than simply requiring each ρ_g to be similar to the ρ'_g, since we use the same 'similarity' matrix for all of them.

1.3 MO theory

To talk about MO theory, first, we need to talk about Atomic Orbitals (AO's), and our understanding of the atom. Our modern understanding of the atom consists of three types of particles: protons and neutrons packed together inside of a densely packed nucleus, with electrons flying around this nucleus (Sullivan & Musgrove, 2023). As our understanding of quantum mechanics started to improve, we could now predict where electrons were located within the atom. The wave nature of the electron gives a corresponding wave function that describes its behavior (Sullivan & Musgrove, 2023), which can be obtained by solving the following equation (Miessler et al., 2022):

$$\hat{H}\psi = E\psi$$

Where $\hat{H}$ is the Hamiltonian operator, ψ the wave function and E is the energy. The wave function ψ itself has no direct use, but $\psi * \overline{\psi} = ||\psi||^2$ does, being interpreted as the probability of finding an electron within a certain region of space/ 'electron density map.' These regions of electron density generated by $||\psi||^2$ are called orbitals. Although 'wavefunction' and 'orbital' are technically different, they will be used interchangeably.

Within an energy level, the angular momentum of electrons gives rise to sublevels, denoted s, p, d, and f (Sullivan & Musgrove 2023). In terms of their energies, we have s<p<d<f. These sublevels are shown in Figure 2.

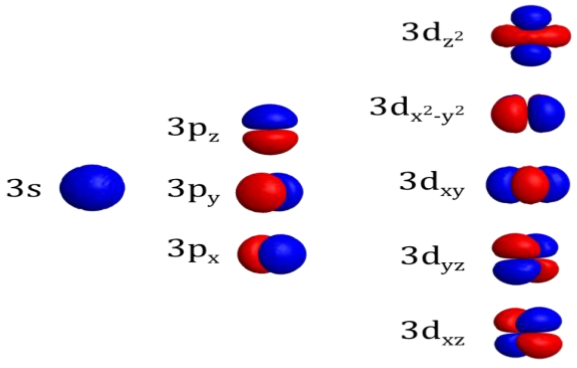


Figure 2: Various atomic orbitals [obtained (with permission to reproduce) from (Kennephol, n.d.)]

From the picture, we can observe some various symmetry within the sublevels, arising from the electron's angular momentum. For instance, the s orbital possesses spherical symmetry, and the p orbitals have a dumbbell-symmetry to them.

When atoms combine to create molecules, the highest energy atomic orbitals (valance orbitals) will overlap with each other to form MO's (Miessler et al.,2022). We aim to use representation theory to establish a correspondence between irreducible representations and these MO's.

2 | METHODS

Mathematical proof is the primary method of analysis for this paper. We first prove key results from representation theory concerning sub-representations and character theory. Then, we establish a correspondence between MO's and irreducible representations, before finally working through an example (a water molecule) of how we can use the SALC method to perform MO calculations.

To prove these results, we mostly use tools from linear algebra and a bit of group theory. While efforts to keep things accessible have been made, familiarity with the following linear algebra topics is ideal: span, linear independence, orthogonality in $\mathbb{R}^n$, projections, linear transformations, inner product spaces, spectral theory, Jordan normal form, and have some exposure to direct sums/tensor products. In addition, some knowledge of group theory is also useful:

knowledge of what groups are, their properties, homo/isomorphisms, conjugacy & the class equation.

3 | RESULTS

First, we (re)address some assumptions we make for this section: assume our groups G are of finite order, and vector spaces are finite-dimensional and complex, so we can associate elements $g \in G$ to an invertible $n \times n$ matrix ρ_g with complex number entries, with $n < \infty$. The goal of this section is to establish some results from representation theory needed to perform MO calculations, listed below:

1. Every representation has a decomposition into irreducibles.
2. Characters on irreducible representations give an orthonormal basis (which we need to find the above decomposition)

3.1 The role of irreducible representations

The goal of this subsection is to establish the first result on the above list. More formally, we can write that statement as follows:

***Theorem 4** (Maschke's theorem): Every representation is either irreducible or can be decomposed into a direct sum of irreducible representations (Serre, 1977).*

To prove this, we need to create subspaces which are invariant under the action of G (a subrepresentation). However, given some subrepresentation W, we can make another subrepresentation by averaging out the projection onto W over the group G. The following lemma goes through the details of this process (Serre, 1977):

***Lemma 5**. Let $\rho: G \to GL(V)$ be a representation of G, with representation space V, and a subrepresentation W. Then there exists some subspace W^c is also stable under the action of G (a subrepresentation) and satisfies $V = W \oplus W^C$.*

3.2 Proof of Lemma 5 [Adapted from (Serre, 1977)]:

First, let P be some projection from V onto W, and we use it to define a map, P°, which 'averages' the projection map over G:

$$P^\circ(x) = \left[\frac{1}{|G|}\sum_{g\in G} \rho_g\, P \rho_g^{-1}\right] x$$

We claim P° is a projection onto W. First, we show that that $P^\circ(x) = x$ for any $x \in W$ and any $g \in G$. Indeed, if we fix some $x \in W$ and $g \in G$, we see the result outlined below:

$$P^\circ(x) = \left[\frac{1}{|G|}\sum_{g\in G} \rho_g\, P \rho_g^{-1}\right] x$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_g \left(P\left(\rho_g^{-1}(x)\right)\right) = \frac{1}{|G|}\sum_{g\in G} \rho_g \left(\rho_g^{-1}(x)\right)$$

$$= \frac{1}{|G|}\sum_{g\in G} x = \mathrm{x}$$

Moreover, we remark that:

1. P° maps from V to W (since P is a projection onto W any $x \in V$ implies $P(x) \in W$, and W is an invariant subspace of ρ_g , so for all $x \in W$, we have $\rho_g(x) \in W$).
2. P° is the identity on W (since $P^\circ(x) = x$ for any $x \in W$).

Thus, we have that P° is a projection from V to W, for which it is the identity on W. Thus P° is a projection onto W. We also observe that for any $h \in G$, we have that $\rho_h P^\circ \rho_h^{-1} = P^\circ$ as we see that:

$$\rho_h P^\circ \rho_h^{-1} = \rho_h \left[\frac{1}{|G|}\sum_{g\in G} \rho_g\, P \rho_g^{-1}\right] \rho_h^{-1}$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_h\, \rho_g P \rho_g^{-1} \rho_h^{-1}$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_{hg}\, P \rho_{hg}^{-1}$$

$$= P^\circ$$

Since we have $\rho_h P^\circ \rho_h^{-1} = P^\circ$, it follows that $\rho_h P^\circ = P^\circ \rho_h$ for any $h \in G$. Thus, we take our new subrepresentation W^c to be $ker\ (P^\circ)$. This subspace is indeed stable under the action of G, since for any $y \in W^c$ and any , $g \in G$ we see that:

$$P^\circ\left(\rho_g(y)\right) = \rho_g\left(P^\circ(y)\right) = \rho_g(0) = 0$$
$$\Rightarrow P^\circ\left(\rho_g(y)\right) = 0$$

Thus, for any $g \in G$ and any $y \in W^c$, we have $\rho_g(y) \in W^c$. Lastly, because P° is a projection, we have that $V = ker(P^\circ) \oplus Im(P^\circ)$. Since we defined W^c to be the kernel of P°, and the image of P° is W, we have that $V = W \oplus W^C$. This completes the proof. This completes the results needed to prove theorem 4, done below.

3.3 Proof of Theorem 4: Maschke's theorem

This is again adapted from (Serre, 1977), proceeding by induction on $\dim(V)$. The base case of $\dim(V) = 0$ gives the 0-space, which is irreducible. To see this, consider what the subspaces of the 0-space are.

Now, suppose that we can decompose V into a direct sum of irreducible subrepresentations if $\dim(V) \leq n$, and we consider what happens if $\dim(V) = n + 1$. If V is irreducible, then there is nothing to check since it is irreducible. If V is reducible, then we have a proper subrepresentation W, and can apply Lemma 5 to find a subrepresentation W^c such that $V = W \oplus W^c$. Since W, W^c are subrepresentations and V is reducible they must be proper subspaces of V. Thus, we have that $\dim(W) < \dim(V)$ & $\dim(W^C) < \dim(V)$ and apply the induction hypothesis on W, W^c to complete the proof.

Thus, we have that every representation has a decomposition into irreducibles, analogous to how every integer has a prime factorization. However, we have not addressed how one finds a decomposition. Character theory seeks to address this issue.

3.4 Character Theory

Having established that we can decompose a representation into irreducibles, we aim to find a way to compute them. To do this, we need to introduce the notion of the character of a representation, defined below (Fulton & Harris, 2004):

Definition 6*. The Character χ_ρ of a representation ρ is a map from our group G to $\mathbb{C}$ given by $\chi_\rho(g) = Tr(\rho_g)$, where $Tr(M)$ denotes the trace of a square matrix M, the sum of diagonal entries.*

Trace is invariant under similarity of matrices. Thus, isomorphic representations have equal characters. However, this goes both ways, as representations that have equal characters are isomorphic (Schedler, n.d.). Thus, characters can be used to uniquely identify a representation of a group up to isomorphism.

When the context is clear, subscripts are dropped, with χ_ρ becoming χ. Moreover, if the representation is irreducible, its associated character is also said to be irreducible (Serre, 1977).

Given representations $\rho: G \to V, \rho': G \to GL(V')$, one can define direct sums $\rho \oplus \rho'$ by the map $\rho \oplus \rho': G \to V \oplus V'$ by sending $g \in G$ to the map which sends $(v, w) \in V \oplus W$ to $\left(\rho_g(v), {\rho'}_g(w)\right)$. One can also define $\rho \otimes \rho'$ in an analogous way on pure tensors. For dual spaces, one can define the dual of a representation ρ^* by $\rho^*(g) = \left(\rho_g^{-1}\right)^T$ on V^* (Fulton & Harris, 2004).

The following proposition establishes some basic properties of characters on direct sums and tensor products (Fulton & Harris, 2004).

Proposition 7*. let $\rho: G \to GL(V), \rho': G \to GL(V')$ be representations of G. Then we have that*

1. $\chi_{\rho\oplus\rho'} = \chi_\rho + {\chi_\rho}'$
2. $\chi_{\rho\otimes\rho'} = \chi_\rho * {\chi_\rho}'$
3. $\chi_{\rho^*} = \overline{\chi_\rho}$

Another property characters have is that group elements in the same conjugacy class have equal character, since if we have $a, b, g \in G$ such that $a = gbg^{-1}$ then:

$$\begin{gathered}\chi_\rho(a) = \chi_\rho(gbg^{-1}) = Tr\left(\rho_{gbg^{-1}}\right) \\ = Tr\left(\rho_g\left(\rho_b\rho_{g^{-1}}\right)\right) = Tr\left(\left(\rho_b\rho_{g^{-1}}\right)\rho_g\right) \\ = Tr(\rho_b) = \chi_\rho(b)\end{gathered}$$

Characters are thus constant on conjugacy classes, & are dubbed class functions (Serre, 1977). The set of all class functions associated with a fixed group G, C_G form a complex inner product space (Serre,1977), with addition/scalar multiplication is done pointwise, and the inner product given by (Serre, 1977):

$$\langle \chi_\rho, {\chi_\rho}' \rangle = \frac{1}{|G|} \sum_{g \in G} \overline{\chi_\rho(g)}\, {\chi_\rho}'(g)$$

Here, an inner product aims to give rise to the notion of distances and angles within an abstract vector space (Axler, 2024). In particular, this inner product gives us a way to talk about the length of a character or angles between 2 characters. Verification of all the relevant properties amounts to routine calculations and is thus left to the reader.

Since characters are class functions, if G has k conjugacy classes, we can index the sum by the conjugacy classes, and rewrite the inner product as:

$$\langle \chi_\rho, \chi_\rho{}' \rangle = \frac{1}{|G|}\sum_{i=1}^{k} n_i \, \overline{\chi_\rho(g_i)}\chi_\rho{}'(g_i)$$

where n_i denotes the number of elements in each conjugacy class, and g_i some representative.

Having now established what characters are, and some of their key properties, we work to prove the following:

Theorem 8*. Characters of irreducible representations (irreducible characters) form an orthonormal basis [a basis which all basis vectors are orthogonal to each other and have length 1] for* C_G*.*

However, we need to establish some preliminary results. The first of these gives a formula relating the dimension of a representation and its character (Fulton & Harris, 2004).

Lemma 9*. Let* $\rho: G \to GL(V)$ *be a representation with subrepresentation* $V^G = \{v \in V | \rho_g(v) = v \text{ for all } g \in G\}$*, and define a linear map* $\phi: V \to V$ *by* $\phi(v) = \frac{1}{|G|}\sum_{g\in G} \rho_g(v)$*. Then* ϕ *is a projection from* V *onto* V^G*.*

3.5 Proof of Lemma 9 [adapted from (Fulton & Harris, 2004)]:

We first show that $V^G = \mathrm{Im}(\phi)$, from which it follows V^G is a subrepresentation [when we prove Schur's lemma later, we will see that images of linear maps are subrepresentations]. We note that for any $v \in V^G$ we can observe that:

$$v = \frac{1}{|G|}|G|v = \frac{1}{|G|}\sum_{g\in G} v = \frac{1}{|G|}\sum_{g\in G} \rho_g(v) = \phi(v)$$

The 3rd equality is a result of rewriting $|G|$ as the sum of $|G|$ many 1's, and the fact that for any $g \in G \text{ and } v \in V^G, \text{we have } \rho_g(v) = v$. This shows that $\mathrm{Im}(\phi) \supseteq V^G$. For the other inclusion, let $v \in V$, and we show that $\phi(v) \in V^G$. Indeed, for any $h \in G$, we have that:

$$\rho_h(\phi(v)) = \rho_h\left(\frac{1}{|G|}\sum_{g\in G}\rho_g(v)\right) = \frac{1}{|G|}\sum_{g\in G}\rho_h\left(\rho_g(v)\right)$$
$$= \frac{1}{|G|}\sum_{g\in G}\rho_{hg}(v) = \phi(v)$$

Where the 2nd equality holds comes from distributing the matricies, the 3rd one is a result of ρ being a group homomorphisim, and the last equality holds as the h simply re-orders the terms in the sum. This gives us the desired equality of sets.

To show that $\phi \circ \phi = \phi$, all that one needs to do is evaluate the quantity $\phi\left(\phi(v)\right)$. The resulting double sum is straightforward but requires substantial amounts of calculation, so we leave it to the reader. Since ϕ is a projection, we have that $\dim\left(Im(\phi)\right) = Tr(\phi)$. To see this, consider the Jordan normal form, ϕ_J of ϕ. Since ϕ is a projection, there are 2 eigenvalues of ϕ: 0 and 1. For the Jordan block associated with eigenvalue 1, the eigenspace associated with it is just V^G, and consequently, the Jordan block for the eigenvalue 1 is simply the identity matrix of size $dim(V^G)$. For the block associated with eigenvalue 0, it is simply the 0 matrix of size $dim((V^G)^c)$, where $(V^G)^c$ is the orthogonal complement of V^G. We note that since $\mathrm{Im}(\phi) = V^G$, it follows that they agree in dimension, so we get $\dim(V^G) = dim\left(im(\phi_J)\right)$. Lastly, the trace of ϕ and ϕ_J are the same, as they are similar matrices. Thus, we have that $\dim(V^G) = \dim\left(\mathrm{Im}(\phi)\right) = \dim\left(\mathrm{Im}(\phi_J)\right) = \mathrm{Tr}(\phi_J) = Tr(\phi)$.

We note that since $\mathrm{Im}(\phi) = V^G$, it follows that they agree in dimension. Thus, we observe that:

$$\dim\left(\mathrm{Im}(\phi)\right) = \dim(V^G) = Tr(\phi)$$
$$= Tr\left(\frac{1}{|G|}\sum_{g\in G}\rho_g\right) = \frac{1}{|G|}\sum_{g\in G}Tr\left(\rho_g\right) = \frac{1}{|G|}\sum_{g\in G}\chi_\rho(g)$$

and thus obtain the formula below (denoted formula 4.1).

$$\dim(V^G) = \frac{1}{|G|}\sum_{g\in G}\chi_\rho(g)$$

We now prove the next lemma, aiming to classify the possible maps which go between any two irreducible representations:

Lemma 10 *(Schur's lemma). Let* $\rho: G \to GL(V), \rho': G \to GL(V')$ *be two different representations of a group G which* *are both irreducible and let* $f: V \to V'$ *be a linear map such that for any* $g \in G$, *we have* $f \circ \rho_g = \rho'_g \circ f$. *Then*

1. *if* $\rho \ncong \rho'$, *then* $f \equiv 0$
2. *if* $\rho \cong \rho'$ *and* $V = V'$, *then* $f = cI$, *where I denotes the identity map, and c is a constant.*

3.5 Proof of Lemma 10 [adapted from (Serre, 1977)]:

We prove each part separately. To prove the first part of Schur's lemma, we first need to show that $\ker(f)$ and $\mathrm{Im}(f)$ are G-invariant subspaces. For any $y = f(x) \in \mathrm{Im}(f)$, we see that

$$\rho'_g(y) = \rho'_g(f(x)) = f\left(\rho_g(x)\right)$$

$$\Rightarrow \rho'_g(y) \in \mathrm{Im}(f) \ \ [\text{Since } \rho_g(x) \in V]$$

and thus $\mathrm{Im}(f)$ is a subrepresentation. Similarly, for any $x \in ker(f)$, we see that:

$$f\left(\rho_g(x)\right) = \rho'_g(f(x)) = \rho'_g(0) = 0 \Rightarrow \rho_g(x) \in ker(f)$$

This shows that $\ker(f)$,$\mathrm{Im}(f)$ are subrepresentations of G (that is, they are G-invariant). Now, consider the chain of inclusions below:

$$\{0\} \subseteq \ker(f) \subseteq V$$
$$\{0\} \subseteq \mathrm{Im}(f) \subseteq V'$$

Since ρ, ρ' are irreducible, the only possibilities for $ker(f)$ and $\mathrm{Im}(f)$ are either $V = ker(f)$ and $\mathrm{Im}(f) = 0$ or $ker(f) = \{0\}$ and $\mathrm{Im}(f) = V'$. But $ker(f) = \{0\}$ and $\mathrm{Im}(f) = V'$ would imply f is invertible. Thus, from the fact that $f \circ \rho_g = \rho'_g \circ f$, we can obtain that $f \circ \rho_g \circ f^{-1} = \rho'_g$, for any $g \in G$, contradicting the assumption $\rho \ncong \rho'$. Thus $V = ker(f)$ which gives $f = 0$.

To address the second part, suppose that $\rho \cong \rho'$ and $V = V'$, and let $f: V \to V$ be linear. Since $\mathbb{C}$ is algebraically closed [every polynomial with complex coefficients has a complex root], f must have some eigenvalue λ. Thus, set $h = f - \lambda I$, and it follows that for any $g \in G$, we have $h \circ \rho_g = \rho'_g \circ h$. To see this, substitute h into one side, and make use of the fact $f \circ \rho_g = \rho'_g \circ f$ and $\lambda I \circ \rho_g = \rho'_g \circ \lambda I$. Since f has an eigenvalue, we have that $ker(h) \neq 0$. Thus, by the previous point, we must have that $h = 0$, from which it follows $f = \lambda I$.

Thus, given two irreducible representations $\rho: G \to GL(V)$ and $\rho': G \to GL(V')$, Schur's lemma allows us to give an explicit description of elements in the set $Hom_G(V, V')$. Here, $Hom_G(V, V')$ is the set of all linear maps $T: V \to V'$ which obey $\rho'_g \circ T = T \circ \rho_g$ for any $g \in G$ [that is, these maps intertwine/ "translate between" representations ρ & ρ′]. If $\rho \ncong \rho'$, then the only possible $T \in Hom_G(V, V')$ by part 1 of Schur's lemma is the 0 map, & $Hom_G(V, V') = \{0\}$.

If, $\rho \cong \rho'$ however, then any nonzero $\theta \in Hom_G(V, V')$ is invertible. Thus, for any nonzero maps $\phi, \theta \in Hom_G(V, V')$, we have that $\theta^{-1} \circ \phi \in Hom_G(V, V)$. But part 2 of Schur's lemma gives us that $\theta^{-1} \circ \phi = cI$ for some $c \in \mathbb{C}$. Thus, we compose by θ on both sides to obtain $\phi = c\theta$ (Chua, n.d.). We conclude that $Hom_G(V, V') = span\{\phi\}$ for some invertible linear map $\phi: V \to V'$ on irreducible representations. In short, we have that:

$$Hom_G(V, V') \cong \ \mathbb{C} \text{ if } \rho \cong \rho' \text{ and } \{0\} \text{ otherwise}$$

Given that $Hom_G(V, V') \cong V^* \otimes V'$ (Fulton & Harris, 2004), we have that $\chi_{Hom_G(V,V')} = \overline{\chi_\rho}\chi_{\rho'}$ by proposition 7. Since isomorphic vector spaces have the same dimension, we can apply formula 4.1, to obtain the following:

$$\dim\left(Hom_G(V, V')\right) = \frac{1}{|G|}\sum_{g \in G} \chi_{Hom_G(V,V')}$$
$$= \frac{1}{|G|}\sum_{g \in G} \overline{\chi_\rho(g)}\,\chi_{\rho'(g)}$$

Where χ_ρ is the character of $\rho: G \to GL(V)$, and $\chi_{\rho'}$ is the character of $\rho': G \to GL(V')$. Combining this with the observation that $\dim(Hom_G(V, V')$ is either 0 or 1 (on irreducible representations), by our above work, we get that:

$$\frac{1}{|G|}\sum_{g \in G} \overline{\chi_\rho(g)}\,\chi_{\rho'(g)} = 1$$
$$[\text{if } \rho \cong \rho' \ \text{ and is 0 otherwise}]$$

This work shows that the set of irreducible characters forms an orthonormal set in C_G, implying linear independence. Moreover, Theorem 4 shows that every representation can be decomposed into irreducibles, so the set of irreducible characters also forms a spanning set in C_G. Thus, the set of irreducible characters forms an orthonormal basis for C_G, which was precisely theorem 8.

Given our orthonormal basis, one can easily compute the decomposition into irreducibles by projecting onto each irreducible. This process is formalized below as proposition 11.

Proposition 11. *If* ρ *is a representation of a finite group* G *with character* χ, *and we have* $\rho = \bigoplus_{i=1}^{k} m_i\rho_i$, *with all* ρ_i

irreducible, and m_i *positive integers, then* $m_i = \frac{1}{|G|}\sum_{g\in G}\overline{\chi_\rho(g)}\,\chi_{\rho_i}(g)$ *for any* $1 \le i \le k$.

These scalars associated with the irreducible representations are called the multiplicities of an irreducible representation (Fulton & Harris, 2004). They give the 'number' of copies or times a certain irreducible representation occurs in our representations. Going back to the prime number analogy on page 4, they are analogous to the exponents in a prime factorization. Like with prime factorization, we ignore the irreducibles of multiplicity 0.

3.6 Proof of Proposition [adapted from (Bouchard, 2020)]:

Given that $\rho = \bigoplus_{i=1}^{k} m_i\rho_i$, we have that $\chi = \sum_{i=1}^{k} m_i\,\chi_i$. To this equation, we take the inner product of both sides with some fixed χ_j, and obtain that.

$$\langle \chi, \chi_j \rangle = \left\langle \sum_{i=1}^{k} m_i \chi_i \chi_j\,, \chi_j \right\rangle$$

$$= \sum_{i=1}^{k} m_i \langle \chi_i, \chi_j \rangle = m_j \langle \chi_j, \chi_j \rangle = m_j$$

Where the 2nd equality comes from the linearity of the inner product, and the 3rd the fact that $\langle \chi_i, \chi_j \rangle = 1$ if $i = j$ and is 0 otherwise. Thus, we obtain the following formula below

$$m_j = \langle \chi, \chi_j \rangle = \frac{1}{|G|}\sum_{g\in G}\overline{\chi_\rho(g)}\,\chi_{\rho_j}(g)$$

In the Chemistry context, this formula for the m_j is known as the 'reduction formula' (Miessler et al., 2022).

3.7 Chemical Results

Now that we have finished proving all the necessary mathematical results, we can start to put the pieces together. The goal of this section is to prove one more result (Lowe & Peterson, 2011):

Theorem 12*. One can associate each MO of a molecule with some irreducible representation of a molecule's point group.*

The importance of this theorem cannot be understated: This theorem allows us to deduce information about an MO, such as which atomic orbitals were used to form it, its relative shape, and energies by only knowing with which irreducible representation it is associated.

Before continuing, we first need to incorporate a group structure into our molecule. Fortunately, this is easy since many molecules have internal symmetry. For instance, take water, H_2O, pictured in Figure 3.

From left to right, we have an axis of rotation (labelled C_2), and the 2 internal planes of reflection. This set of symmetries forms a group under composition. This group of internal symmetries is called the point group of a molecule (Miessler et al., 2022), as we treat the atoms as points in 3d space centred about some fixed point. Typically, the 'central atom' of a molecule is the fixed point and is thus associated with the origin.

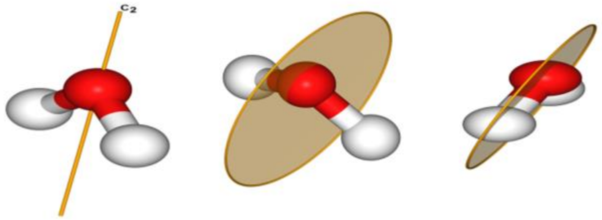


Figure 3: Water molecule with its various symmetries highlighted [obtained from (University, n.d.), with permission to reproduce]

In the case of water, all our symmetries above 'fix' the oxygen (red) atom, so we take it to be the origin. Convention also dictates that the main axis of rotation of a molecule (in the case of water, the C_2 axis) is the Z axis (Miessler et al., 2022).

We remark that since the MOs make up the molecule (and thus it is internal symmetry), we have that the set of all MOs for a given molecule is invariant under a molecule's point group. Put another way, the group of symmetries associated with the set of a molecule's MOs is the same as that molecule's point group. This observation is significant since finding a point group of a molecule is much easier than finding all a molecule's MOs (we will see this in the next section). Thus, by knowing the symmetries of the molecule, we know the symmetries of all our MOs. Thus, we can build a representation of this group of symmetries and thus can use the tools outlined in the previous sections to break that representation down and understand it. Theorem 12 will allow us to contextualize the results we have established about group representations in terms of our MOs.

Before proving Theorem 12, we need some more groundwork related to solutions to the Schrodinger equation, and general assumptions used in quantum mechanics: firstly, when we talk about things like the "norm of a wave function", we assume this norm is calculated with respect to the usual inner product on complex-valued functions on some domain $S, C(S)$, given by

$$\langle f, g\rangle = \int_S f(x)\overline{g(x)}dx$$

we also need to introduce the concept of degeneracy, defined below (Lowe & Peterson, 2011):

Definition 13*. 2 different orbitals (wave functions) are said to be degenerate if they are in the same energy level.*

If there are more than 2 degenerate orbitals, then the number of orbitals in a given energy level is called the degeneracy. Since orbitals are simply the square of wavefunctions, and these wavefunctions are eigenfunctions of the Hamiltonian operator (associated with some eigenvalue E), we can equivalently define degeneracy as the dimension of the eigenspace associated with E. We assume without loss of generality that these wavefunctions form an orthonormal set (if not, just apply Gram-Schmidt algorithm). With that, we are now ready to prove theorem 12.

3.8 Proof of Theorem 12 [Adapted from ("Molecular orbital theory and its symmetry 393 aspects", n.d.), (Vvednsky, n.d.)]:

The first thing one needs to show is that the Hamiltonian is invariant under each symmetry operation (Vvednsky, n.d.): that is, if R is some element in your point group, we have that $R\widehat{H} = \widehat{H}R$. The symmetry operations only interchange identical nuclei, and thus permute wavefunctions (by the symmetry of the molecule). From this, it follows that the Hamiltonian is invariant under our point group.

Thus, if ψ is the wave function associated with your orbital, it is an eigenfunction of the Hamiltonian. From the fact that $\widehat{H}$ and R commute, we conclude that $R\psi$ is also an eigenfunction of $\widehat{H}$, so we set $R\psi = c\psi$, where c is some constant. From here, we treat the cases of non-degenerate and degenerate wavefunctions separately.

In the case of a non-degenerate wave function, then the normalization conditions imposed on the wave function (the wave function has norm 1) imply that $R\psi = \pm\psi$, since if $R\psi = c\psi$ for some constant c, we have that

$$\langle c\psi, c\psi\rangle = 1 \Longrightarrow |c|^2\langle\psi,\psi\rangle = 1$$
$$\Longrightarrow |c|^2 = 1\ (\psi \text{ has norm } 1) \Longrightarrow c = \pm 1$$

Since $c\psi\overline{c\psi}$ is real-valued, and the group operations only re-orient $c\psi\overline{c\psi}$, and do not change the area enclosed by it, we have that $c \in \mathbb{R}$. (Lowe & Peterson, 2011). Thus, $|c|^2 = c^2$.

Thus, it follows that the wave function is either symmetric or anti-symmetric with regard to any symmetry operation of our point group. If it is symmetric, then the eigenvalue is +1, and if it is anti-symmetric, it is -1. Thus, an easy representation can be constructed by the matrices [1] and [-1], associating elements that are symmetric to [1], and those which are anti to [-1]. Notice how this representation is 1-dimensional and is thus irreducible. To see this, ask what the possible subspaces of a 1-dimensional space are.

The case involving degenerate wavefunctions of degeneracy n, where $n > 1$ is more involved, as the representation of these wavefunctions is more complicated (Vvednsky, n.d.). So, we let, $X = \{\psi_1, \psi_2, \dots, \psi_n\}$, be the set of all degenerate wavefunctions associated with some fixed energy eigenvalue E, where $n < \infty$. Moreover, assume X is the smallest set which contains all eigenfunctions and let $V = span(X)$.

We remark that X is a basis by the orthonormality of our wave functions. We will prove any representation of G with representation space V is irreducible via the method of contradiction.

Suppose we have some reducible representation of V. Since V is reducible, we can find some non-trivial subspace W which is stable under the action of G. Consequently, we can find some basis for this subspace, which we call A. We know that:

1. $A \subseteq V$,
2. Elements in A are eigenfunctions of $\widehat{H}$, since linear combinations of eigenfunctions associated with the same eigenvalue are eigenfunctions
3. $A \neq \emptyset$.

Since W is a subrepresentation and V is reducible, this implies that W is a proper, nontrivial subspace of V. Moreover, since W is invariant under the action of our point group, we know that our matrices given by the representation map elements in W to other elements in W. Thus, we can reduce the set of eigenfunctions of our Hamiltonian to the set A, and thus reduce the degeneracy of our wavefunctions to the set A. Since A is a basis for W, and W is a proper nonzero subspace of V, we conclude that $dim(W) < dim(V)$, which implies $|A| < |X|$. This contradicts the assumption that X was the smallest set which contains all our eigenfunctions (and was thus of minimal degeneracy). Thus, our representation of these wavefunctions must be irreducible.

Remark: The minimality condition meant we assumed the degeneracy was normal: that is, assuming all our eigenfunctions would be accounted for mathematically (Vvednsky, n.d.). However, experimental evidence might suggest we cannot always account for all degeneracy mathematically. In such cases, the degeneracy is accidental (Vvednsky, n.d.)

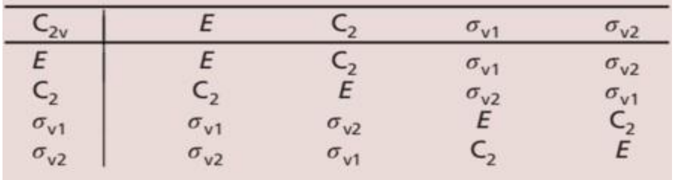
3.9 Worked example: $\boldsymbol{H_2O}$ (water)

Let us now, in detail, perform the MO calculations for water (H_2O) using the SALC method. In general, the process has 4 steps:

1. Find the point group of the molecule.
2. Find a representation of the point group (any representation will work)
3. Decompose the representation into irreducibles.
4. Form the MOs by matching atomic orbitals of the same irreducible representations.

Step 3 of this method relies on theorem 12 to ensure we can associate each MO with an irreducible representation and ensure that the set of all the MOs has a representation. From here, the sections regarding characters and irreducible representations ensure we both can break down this representation into irreducibles and provide us with a procedure by which to do so. This section aims to consolidate all the results we collected and show how they can be used in a real-world example.

First, we need to identify the point group of H_2O. This is easiest to do with point group identification flow charts (available on the internet and in many inorganic chemistry textbooks). These make point group identification easier by prompting the reader to identify key conjugacy classes. Using the flow chart given in (Miessler et al., 2022) to identify the point group of water, we get it is C_{2v}. C_{2v} has 4 elements: $E, C_2, \sigma_v, \sigma_{v'}$, which are the identity, rotation by 180 degrees, and the 2 reflections about the planes highlighted in Figure 2, respectively. These elements are related to each other via the multiplication table below. We include the multiplication table, shown in Figure 4, to be explicit in the description of C_{2v}, but in practice, people just tend to use character tables [more on these later] to pull whatever information they need about the group.



C_{2v}	E	C_2	σ_{v1}	σ_{v2}
E	E	C_2	σ_{v1}	σ_{v2}
C_2	C_2	E	σ_{v2}	σ_{v1}
σ_{v1}	σ_{v1}	σ_{v2}	E	C_2
σ_{v2}	σ_{v2}	σ_{v1}	C_2	E

Figure 4: Group multiplication table for C_{2v}, [obtained from (Pfennig, 2018), Creative Common License]

3.10 Finding a representation of our point group

Having identified our point group, we now seek to find a representation for it. Typically, chemists would find a representation in $\mathbb{R}^3$, but we can observe that our molecule is flat (see Figure 2) since there is a plane on which all 3 atoms lie. Thus, it suffices to find a representation in $\mathbb{R}^2$.

Conventions dictate we orient the molecule, so the origin is where our oxygen is, and the axis of rotational symmetry is the z-axis (Miessler et al., 2022). We placed the molecule on the xz plane, though placing it on the yz plane would make no difference. For each symmetry operation in our group, we aim to find a matrix that has the same corresponding geometric action in $\mathbb{R}^2$ as that group element and compute the corresponding trace. By doing this, we get a representation ρ of C_{2v} in $\mathbb{R}^2$ (Miessler et al., 2022) (Figure 5). Now, we collect traces to obtain the character of each element (Table 1).

$$\rho(E)=\begin{bmatrix}1&0\\0&1\end{bmatrix},\rho(C_2)=\begin{bmatrix}0&1\\1&0\end{bmatrix},\rho(\sigma_{v(xz)})=\begin{bmatrix}1&0\\0&1\end{bmatrix},\rho(\sigma_{v'(yz)})=\begin{bmatrix}0&1\\1&0\end{bmatrix}$$

Figure 5: Representation ρ of C_{2v} in $\mathbb{R}^2$ (Miessler et al., 2022).

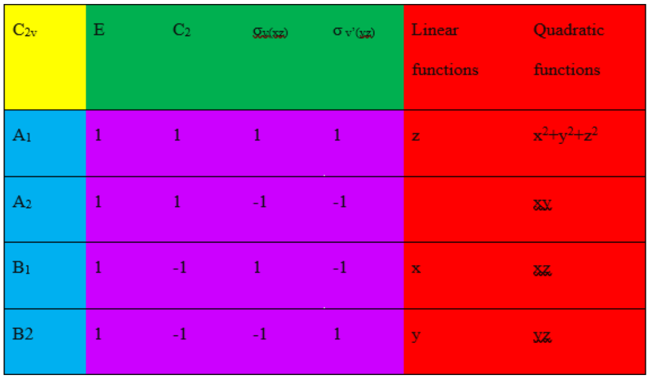
Table 1: Reducible representation of water molecule under its point group.

Conjugacy class representative	E	C_2	σ_v	$\sigma_{v'}$
Character of representative	2	0	2	0

Charcters are just maps from a group G to the complex numbers which are constant on conjugacy classes, so this table below is nothing more than a table of values of the character evaluated on all of the group's conjugacy classes. This table gives us a reducible representation of our point group.

Physically speaking, this reducible representation we have obtained does not say much. It just says that the set of all our MOs has these types of symmetries. But this is where the power of decomposing into irreducibles comes in.

By knowing the irreducible representations associated with each atomic orbital, which are easily deduced from character tables, then we know which atomic orbitals interacted to form bonding/antibonding MOs since they must be associated with irreducible representations that have non-zero multiplicity. From this, we know which MO an AO is associated with, since Noether's theorem states that conservation of symmetry is equivalent to conservation of some physical quantity, in this case, angular momentum (Baez, 2020). Thus, atomic orbitals will only overlap to form an MO if they have the same irreducible representations. Knowing the AOs involved in MO formation, we can deduce other MO properties such as energy, spectroscopic properties, and via the dimensionality of an irreducible, degeneracy. To help us decompose our representation into irreducibles, we make use of a character table (Figure 6).



C2v	E	C2	σv(xz)	σ v'(yz)	Linear functions	Quadratic functions
A1	1	1	1	1	z	$x^2+y^2+z^2$
A2	1	1	-1	-1		xy
B1	1	-1	1	-1	x	xz
B2	1	-1	-1	1	y	yz

Figure 6. Character table for C_{2v}, reproduced from (Kennephol, n.d.) with permission.

We have colour-coded the table for ease of reading, with each section of the table being described as follows (Miessler et al., 2022), (Lowe & Peterson, 2011):

1. Yellow corresponds to the point group.
2. Blue corresponds to the various irreducible representations of our point group, named with respect to the Mulliken symbol conventions (Lowe & Peterson, 2011)
3. Green corresponds to the different conjugacy classes (numbers, if there are any indicate size, and the E, C_n, σ, etc. being representatives. If there are no numbers, assume the number is 1)
4. Purple corresponds to the characters associated with an irreducible
5. Red corresponds to the linear and quadratic rotor functions, which is unimportant for our work

We use the fact that characters on irreducibles form a basis for the characters of all representations. The character table gives us all the information we need about our irreducibles, and Table 1 gives us the characters of our reducible representation we created in step 2. So, we apply the reduction formula to find the multiplicities of each irreducible.

For A_1 , one of the 1-dimensional (irreducible) subrepresentations of C_{2v} in our representation ρ of C_{2v}, we get:

$$m_{A_1} = \langle \chi, \chi_{A_1} \rangle = \frac{1}{|G|} \sum_{i=1}^{k} n_i \, \overline{\chi_\rho(g_i)} \chi_\rho{}'(g_i)$$

$$= \frac{1}{4}(2*1*1+0*1*1+2*1*1+0*1*1) = 1$$

Repeating this process with the other irreducibles, we get that $\rho = 1A_1 + 1B_1$. Thus, our MOs have components associated with the A_1 irreducible representation, and another to the B_1 irreducible.

3.12 Matching Atomic Orbitals

Now, we form the MOs from the atomic orbitals we started with, by determining which atomic orbitals interact with each other.

This is where the irreducible representations come in. We first find the irreducible representations associated with each atomic orbital under our point group, done the same way we did it for water. Then, we form the MOs by taking linear combinations of those atomic orbitals that have the same irreducible representation together, so we satisfy Noether's theorem, and by extension the physicists

Now that we know which atomic orbitals make up a given MO, we can form them by adding/subtracting the wavefunctions associated with those atomic orbitals, i.e., taking linear combinations of atomic orbitals. While we could technically take some scalar multiples when we do the LC process, the normalization conditions on wavefunctions make it so there is only 1 value for the scalars. For a set of n atomic orbitals which go on, we should yield n MOs in return, so as to not break physics (which would pose a big problem).

The result of this process yields the following MO diagram below, which has been color-coded. Orange is used to lump the orbitals of type B_1 symmetry, blue to lump those orbitals of type A_1 symmetry, and green to lump those orbitals of type B_2 symmetry. The arrows indicate the electrons that occupy a given MO. We start with the atoms and their orbitals on the edges (before bonding), and the middle has the resulting

MOs which form because of bonding, and we plot everything against their relative energies (**Figure 7**).

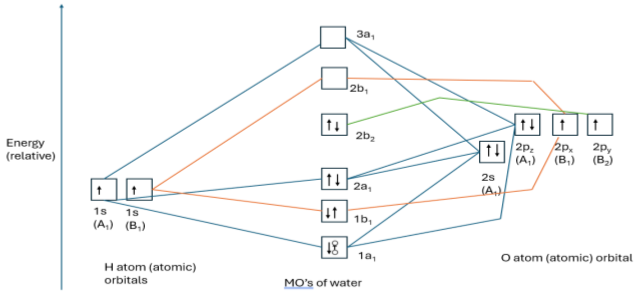


Figure 7: MO diagram for water

Here the energy scale is relative, based on the idea that bonding interactions (adding orbitals) stabilize electrons (and lower their energy), whereas anti-bonding (subtracting orbitals) interactions do the opposite. We use our knowledge of atomic orbitals to guess the extent of bonding/antibonding interactions. Note that we did not use the irreducible representations to assign energies, but merely used them to deduce the atomic orbitals which compose the MO. Only once we knew which AOs formed the MO did we make an educated guess as to their energies.

4 | DISCUSSION

We now aim to see if our mathematical model matches experimental evidence by comparing the predictions made by our MO theory calculations with predictions made by Valance Bond Theory (VBT), a different, but equivalent theory that is also used by chemists (Galbraith et al., 2021). The key difference is that VBT treats electrons as localized entities used to form chemical bonds, whereas MO theory treats them as distributed throughout an entire molecule, with individual wave functions (orbitals) forming the bonds between atoms (Galbraith et al., 2021). Put another way, MO theory treats a molecule as a whole and analyzes the individual parts, whereas VBT uses the parts to analyze the whole. It turns out that both approaches end up becoming equivalent (Galbraith et al., 2021), but both have their advantages and disadvantages.

An important remark here: when we draw Lewis diagrams for any molecule (**Figure 8**), the lines represent bonds, and the dots represent electrons. a pair of electrons is called a lone pair, which is highlighted in blue (Miessler et al., 2022), (Sullivan & Musgrove, 2023).

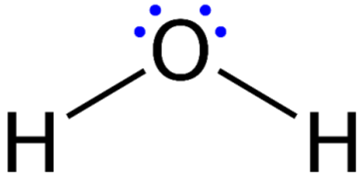


Figure 8: Lewis's structure of Water [Obtained from (*Lewis structure* 2024), Creative Commons license]

When it comes to molecular shape, VBT does seem to do a much better job, because of it is easy to conceptually grasp. Using VBT, one can expect the bond angle between the 2 hydrogen atoms to be approximately 109.5° (based on sp^3 hybridization) (Encyclopedia, 2022), whereas the experimental value turns out to be closer to 104.5° (Encyclopedia, 2022). VBT attempts to explain this observation by arguing that the lone pair electrons create more repulsion, but a more accurate explanation is given by Bent's rule (Encyclopedia, 2022).

While MO theory can use the shape of water, it involves testing various molecular geometries and finding one that minimizes the total energy (Kennephol, n.d.). This is best done by a computer. Our method is limited in this regard, requiring us to already know what this minimum energy configuration is beforehand. Fortunately, VBT often gets close enough to this minimum for most purposes, and thus acts as a good starting point.

Moreover, this method can only give us information regarding which atomic orbitals combine to form the MO and does not give us the proportion in which they are mixed, which is the physical interpretation of the coefficients in the linear combination. This requires using a computer to solve the Schrodinger equation. However, for rough calculations, this group-theoretic method provides a reasonable approximation.

However, VBT falls short when we consider spectroscopic evidence. VBT would predict that there were 2 bands in a photoelectric spectrum (PES) of water since it assumes both $O-H$ bonds and lone pairs are indistinguishable from each other (Encyclopedia, 2022). However, the PES of water gives 4 different bands, corresponding to energies of 12.6 eV, 14.7 eV, 18.5 eV, and 32.2 eV (Encyclopedia, 2022). Clearly, VBT disagrees with this experimental evidence.

Our group theoretic method produces an MO diagram that contains 4 MOs filled with electrons. These 4 orbitals which have electrons correspond nicely to the 4 bands in the PES of water. More crucially, our method is able to distinguish the energies of the two lone pairs, which VBT cannot.

We can use our MO diagram to correctly make predictions regarding (relative) MO energies for water and by extension the types of reactions water can undergo. For instance, the MO associated with 12.6 eV has high-energy electrons, which are consistent with compounds that are basic. Indeed, water can be seen acting as a base. When H_2SO_4 (sulfuric acid) is mixed with water, we get the following chemical equilibrium (Miessler et al., 2022):

$$H_2SO_4 + H_2O \rightleftharpoons HSO_4^- + H_3O^+$$

Of course, this method relies on our molecule having internal symmetry. Mathematically, this is always possible, since you can always have symmetry by 'doing nothing' and thus have the point group be the trivial one. However, our method really does not work well for molecules that have trivial symmetry, since there is nothing to exploit. However, this method works well for molecules that have non-trivial symmetry.

We were able to show that group theory can play a powerful role in simplifying otherwise complicated calculations involving molecular orbitals. These computations allowed us to make important predictions regarding relative electron energies and can also be used to predict regions of electron density, and thus reactivity on a molecule. However, this model has its limitations, since it only works if there is symmetry to exploit (the point group is non-trivial) and can only predict some molecular properties. Thus, the mathematical model presented in this paper should act as a supplement to more traditional computational methods, and not replace them entirely.

5 | ACKNOWLEDGEMENTS

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6 | CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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