1. Hello and welcome to this short animated pencast on molecular group theory. (4.3s)
2. Today we will discuss benzene. (2.5s)
3. More specifically, we will discuss the symmetry of the basis set consisting of benzene’s pz orbitals. (6s)
4. Benzene belongs to the D6h point group, which means we will make use of the D6h point group character table to find out which symmetry operations can be applied to benzene. (9s)
5. We will then use this information to construct the character of our basis set, under these transformations. (5s)
6. Finally, we will use the little orthogonality theorem to find out which irreps make up the trace of our basis set. That is, the irreps whose linear combination equals the trace of the basis set. (11s)
7. But first, some rules. (2s)
8. When constructing the trace, we apply each symmetry operation to the entire benzene molecule. Then we observe if any orbital stays in the place where it started. If that is the case, we attach the value of 1 to that orbital. Orbitals that stay in place will be highlighted with a glowing animation. (14s)
9. If the orbital stays in place but in a different orientation such that the positive and negative lobes swap places, then the orbital is attributed a value of -1. (9s)
10. Finally, if the orbital leaves its starting position during the symmetry operation, a value of zero is attributed to it. Orbitals that leave their starting position become transparent(9s).
11. With this, we can start considering each symmetry operation on the basis set. For this we consider all symmetry operations of the D6h point group. (8s)
12. We start with the E operation. As you can see, all orbitals stay in place. The coefficient associated with each orbital is therefore 1, adding up to a total of 6(9s).
13. Finally, the vertical mirror planes all cross 2 atoms each, which stay in place with unchanged orientation after the transformation, giving this symmetry operation a total trace of 6 (9s)
14. With this we have seen all symmetry operations of benzene applied to the basis set consisting of its pz orbitals. Now we can construct the overall trace for this basis set and express it in terms of its constituent irreps (11s).
15. To do this, we count how many times each irrep appears in the trace. This can be done with the little orthogonality theorem. That is, by taking the dot product between each irrep with the trace and dividing by the square of the length of both vectors, as can be seen with the A1g irrep. (14s)
16. This operation gives 0, but that is not the case for all irreps. In any case, the application of the little orthogonality theorem for all irreps can be found here. Feel free to pause and check all of them by yourself (11s):
17. Carrying on this computation to all irreps reveals that our trace can be decomposed into the following linear combination of irreps (you can check this by adding them up) (10s):

Show the linear combination

With this we have reached our objective of finding the irreducible representations that fully describe the symmetry of the basis set made up by the pz orbitals in the carbon atoms of the benzene molecule.

But we are not done just yet. Though I won’t go into the details in this video, I think it is very interesting to note that once the irreps are known, further processing can be done to find out which linear combinations of atomic orbitals would have the symmetries described by each irrep. These of course, can be plotted to show the possible symmetries hidden in the basis set we started with.

First, I show you a graphical depiction of what these linear combinations would look like when each atomic orbital is considered in isolation.

As you can see, the A and B irreps each pertain to a single linear combination, while the degenerate E irreps pertain to two.

Finally, I want to show you what these would look like if the vector fields associated with each orbitals were added up to then construct the molecular isosurface:

Though in practice the coefficients used on each atomic orbital would have been optimized for lowering electron repulsion, it is still interesting to see the shapes that arise from adding these fields of electron density and how they relate to the images I showed before.

Thank you very much for watching!

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