Workshop: Modeling Benzene using the Particles in a Two-Dimensional Box

Physical Chemistry I
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1. Benzene is an iconic molecule for organic chemists. The π molecular orbital diagram is well known. A mnemonic for the pattern of the pi energy levels is the Frost circle (see http://chemistry.umeche.maine.edu/CHY556/Frost.html, or the original paper: A. A. Frost [J. Chem. Phys., **1953**, *21*, 572]). Sketch the energy levels for benzene based on the Frost circle.

2. Now let's model the wave functions for the pi electrons in benzene assuming it is a square. Given that the CC bond length in benzene is 1.40 Å, what should the edge length of the square be? There are several ways to estimate this. It might be useful to recall that the distance from the center of a regular hexagon to the vertices is the same as the edge length. What simplifications are we making here?

3. Following the same logic we did for the particle in a 3-dimensional box, what is the wave function for a particle confined to a square two dimensional box?

4. Write an expression for the energy for the square box. How many independent quantum numbers are there?

5. Now, using the box size you choose above, compute the energies of the first 6 states of your benzene-sized box. Predict the HOMO-LUMO transition energy. What wavelength of light does this correspond to? Where does this fall in the spectrum?

6. Experimentally, the HOMO-LUMO transition in benzene falls at about 200 nm, how does this compare with your prediction? Would making the box bigger or smaller improve the agreement? Can you ustify changing the box size in this way? What might be a better model than a square box?

The Culture of Chemistry

Kathleen Lonsdale Dame Kathleen Lonsdale was an Irish crystallographer who showed that benzene had a regular hexagonal structure. She was the first woman to be elected to the Royal Society. Bryn Mawr trivia: Prof. Lonsdale was a good friend of Prof. Donnay's mother (Gai Donnay, another eminent woman crystallographer), and was godmother to Prof. Donnay's brother, Albert.

The audience for this in-class workshop is pairs of students in a junior physical chemistry course, in the very early stages of the semester.

Big question: how do we create and modify simple quantum mechanical models for complex molecules?
Big idea: wavefunctions for systems of independent particles can be built from single particle functions
What does success look like?
Students create an energy level diagram for the pi electrons based on their model and compute a HOMO-LUMO gap, expressed in terms of the wavelength.
Students can articulate ways to assess the quality of the model and how to alter the model in ways likely to improve it.
Students can explain how to generally solve the Schrödinger equation for independent particles in higher dimensions.

Map the exercise onto Bloom's taxonomy. Assess overall on scale of 1 (weakly maps onto the taxonomy) to 3 (strongly maps onto the taxonomy).

Bloom's taxonomy
Remember: recall facts
Understand: explain ideas or concepts
Apply: Use information in new situations
Analyze: Draw connections among ideas
Evaluate: Justify a stand or decision
Create: Produce new or original work