Developing a Holistic Understanding of Hybridization and Resonance

by
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"Are you making that for me?" Gavin exclaimed as he peeped into the kitchen on his way to the laundry room. His sister Maya was baking a marble cake.

"Yes, Gavin. Hey, can you please pass me the baking soda from the top shelf?" Maya asked. Gavin winked at her as he set down his laundry basket. Maya was only 4 feet 11 inches tall. Gavin had surpassed her in height two years ago, despite being three years younger.

Maya's "little" brother then asked, "What's the purpose of adding baking soda to the cake batter?"

"It makes the cake fluffy."

"How so?"

"I think by making bubbles."

"The packaging says the main ingredient is sodium bicarbonate. Hmmm…wait a minute." Gavin took up his bottle of laundry detergent. "This one contains sodium carbonate, not sodium bicarbonate. Maybe this one makes foam?"

That evening, when Gavin was studying for his organic chemistry quiz, he looked up the structure of sodium bicarbonate ($NaHCO_3$) and sodium carbonate (Na_2CO_3) online. There was a lot of information available. Sodium bicarbonate or "baking soda" acts as a rising agent by releasing carbon dioxide (CO_2). That is what would make baked goods become soft and fluffy. Sodium carbonate or "washing soda" softened the water to help laundry detergents lather more effectively. Gavin continued to read and learned about a lot of other interesting uses for both compounds. He also studied their chemical structures.

The next day Gavin excitedly told his organic chemistry professor, Dr. Corey, about his newfound knowledge concerning sodium bicarbonate and sodium carbonate, and the similarities of their chemical structures. Dr. Corey told Gavin that each compound was very interesting in its own right, but together they could be used to learn about the concepts of resonance and hybridization. Gavin had learned about these topics in his general chemistry lecture, but he didn't understand how they were related. "How so?" Gavin asked. Dr. Corey in turn asked him what he knew about resonance.

"I was taught that resonance is the delocalization of electrons that will give you another valid Lewis dot structure. But I'm not sure how hybridization ties in with the topic of resonance."

"I'll explain, but you will have to do some work on the blackboard," Dr. Corey said. "For the sake of simplicity, let's work with sodium carbonate, ok?" Dr. Corey then asked Gavin to draw the Lewis dot structure for sodium carbonate and identify the formal charges, which he correctly did on the blackboard (Figure 1).

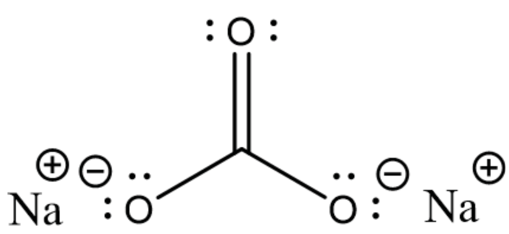


Figure 1. Lewis dot structure and formal charges for sodium carbonate.

Dr. Corey then asked Gavin to figure out the hybridization of each atom (other than sodium) of sodium carbonate. Gavin recalled that he had to think about hybridization in terms of a formula:

Electron group number = number of sigma bonds + lone pairs

Accordingly, he annotated the Lewis dot structure of sodium carbonate with hybridization information (see Figure 2; note that he made some mistakes, which are highlighted in red font).

Dr. Corey gently pointed out that Gavin made a common mistake (identifying two of the oxygen atoms as *sp3* hybridized), primarily due to how he learnt about hybridization—that is, without relating it to resonance. Dr. Corey then went up to the blackboard and drew all the resonance forms of sodium carbonate, and asked Gavin to add the arrows. (Gavin made some more mistakes, which are highlighted in red font in Figure 3).

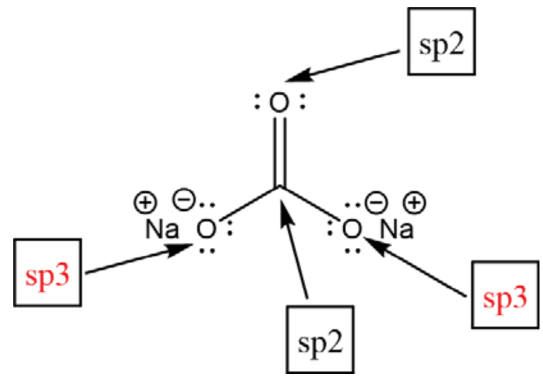


Figure 2. Lewis dot structure and formal charges for sodium bicarbonate annotated with hybridization information *(incorrect).*

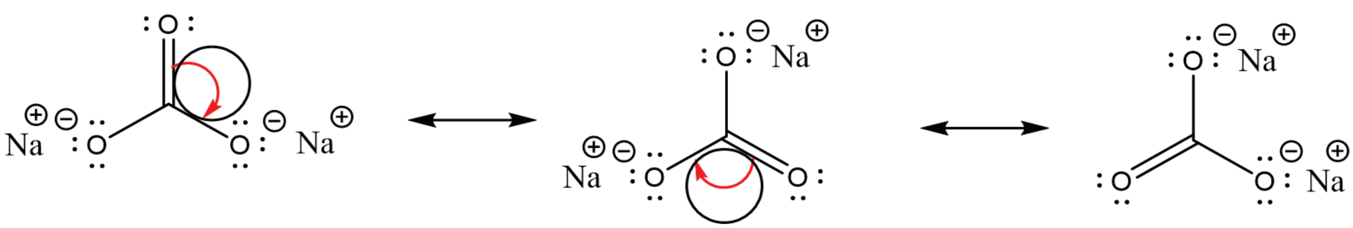


Figure 3. Resonance forms of sodium carbonate *(incorrect arrows).*

Dr. Corey then asked Gavin to examine his arrows in Figure 3. "This is another common misconception students struggle with," Dr. Corey said. "If you were moving arrows in that direction, wouldn't you be exceeding the octet on the oxygen? The movement of arrows is always from an electron-rich species to an electron-deficient species." Gavin understood and then corrected the arrows (Figure 4.)

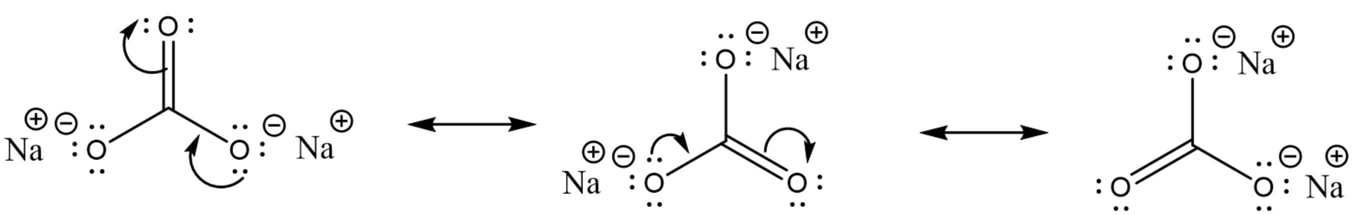


Figure 4. Resonance forms of sodium carbonate *(corrected arrows).*

Dr. Corey directed Gavin's attention to the specific oxygen atoms that were involved in resonance and hinted that they must have an unhybrid *p*-orbital in order to delocalize the electrons. Dr. Corey then urged Gavin to reconsider his approach at identifying the hybridization of each atom (other than sodium) of sodium carbonate.

Gavin caught on. By thinking about resonance, he then realized the mistake he had made and updated Figure 2 as follows (Figure 5).

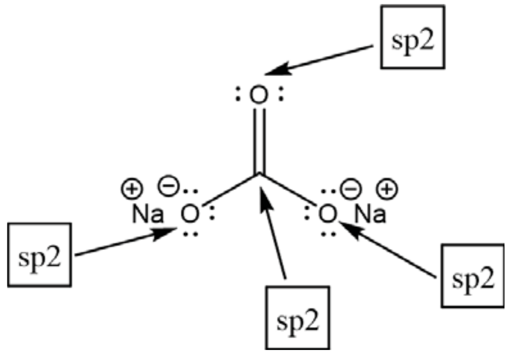
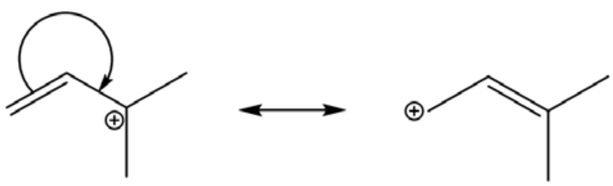


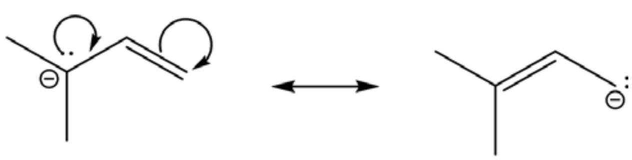
Figure 5. Lewis dot structure and formal charges for sodium carbonate annotated with hybridization information *(corrected).*

"Perfect," Dr. Corey exclaimed. "By thinking about resonance, you understood that all atoms (except sodium) should have an *sp2* hybridization, although they may seem to have different formal charges. Delocalization of electrons, or resonance can occur only if electrons are in *p*-orbital. And that is possible for atoms only when they are *sp2* or *sp* hybridized.

"That's not all," the professor continued. "When you learn about reactions of electrophilic aromatic substitution reactions or about reactions of conjugated systems in your advanced organic chemistry course, thinking about both hybridization and resonance will be immensely helpful. Here, try another one—draw the resonance structures of each of the species, A and B."



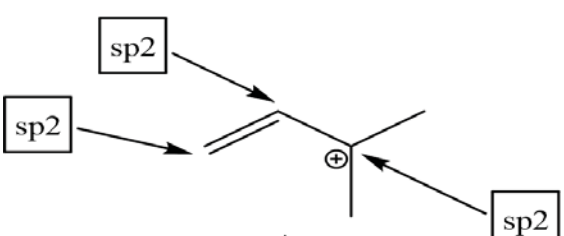
A



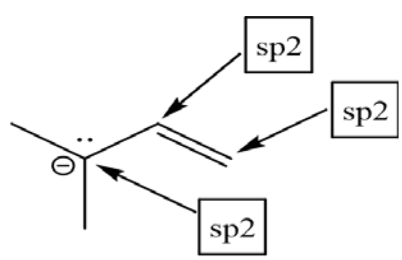
B

Figure 6. Resonance structures of species A and B.

Gavin confidently assigned the correct hybridization to each of the atoms involved in resonance (Figure 7):



A



B

Figure 7. Assignment of hybridization to atoms involved in resonance of species A and B.

Exercise

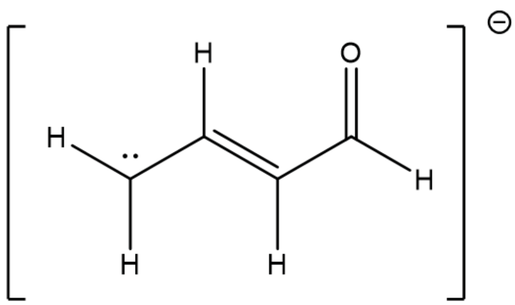
For each of the species below:

i. Draw the Lewis dot structure
ii. Specify which atom will have the non-zero formal charge.
iii. Using arrows draw all important resonance contributing structure. If any of the structure is lowest energy, circle it and explain why it is major.
iv. Specify hybridization of all non-hydrogen atoms.
v. What is the hybridization of all the atoms whose electrons are taking part in resonance?

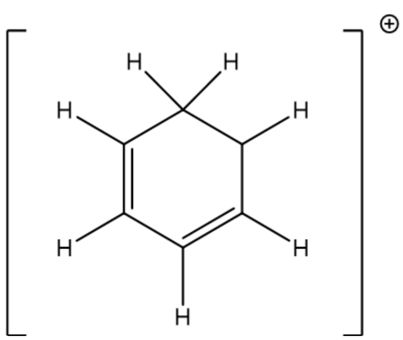
A.

$NO_3^{\ominus}$

B.



C.



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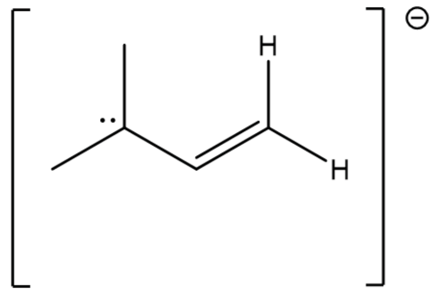
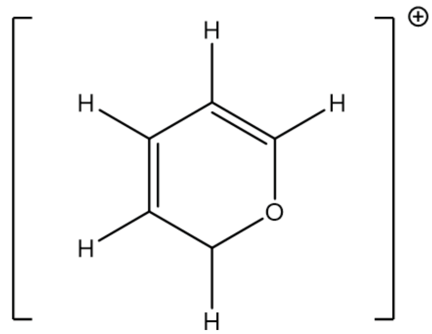


E.



F.