Lewis Dot Structures

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A Primer on Lewis Dot Structures

Before we can really begin to understand the Lewis dot structure and what we can learn from it, we should first learn how to construct them. To begin, let's illustrate the steps involved in generating a Lewis dot structure for cyanic acid, HCNO...
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First, determine the number of valence electrons in each of the atomic species in a given compound. The group number (as indicated on your periodic table) is useful here... (Remember: He is an exception as it has only 2 valence electrons)

<table>
<thead>
<tr>
<th>Atomic Species</th>
<th>Group</th>
<th>Valence Electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxygen (O)</td>
<td>Group VI</td>
<td>6e^-</td>
</tr>
<tr>
<td>Nitrogen (N)</td>
<td>Group V</td>
<td>5e^-</td>
</tr>
<tr>
<td>Carbon (C)</td>
<td>Group IV</td>
<td>4e^-</td>
</tr>
<tr>
<td>Hydrogen (H)</td>
<td>Group I</td>
<td>1e^-</td>
</tr>
</tbody>
</table>

TOTAL: 16e^- 

In our case, oxygen (O) has 6 valence electrons, carbon (C) has 4 valence electrons, nitrogen (N) has 5 valence electrons, and hydrogen (H) has only 1 valence electron.
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Next, determine the "spatial arrangement" of the atoms in a molecule. Sometimes, the central atom in the structure is written first (as in CO$_2$ or CH$_4$). In organic chemistry, the central atom is almost always some type of carbon. When all else fails, guess...

In our case, let's try the following structure...

\[ H \quad N \quad C \quad O \]
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Once a proposed structure has been found, begin by filling in the electrons, as determined in step 1. To guide you along, there are four simple rules...

In our case, let's begin with the following arrangement...

\[
\text{H} : \ddot{\text{N}} :: \text{C} :: \ddot{\text{O}}
\]

You may find yourself asking, "Why the double bonds?"...
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RULE 1: "Structures in which all first row atoms have filled octets are more important than structures with unfilled octets."

By forming a double bond with carbon (sharing 2 e-'s, rather than one, with carbon), oxygen completes it's octet. Much like oxygen, the central carbon atom will bond doubly to nitrogen. Lastly, as our model shows, nitrogen and hydrogen share one electron each to complete the nitrogen octet. Note how hydrogen needs only two electrons to reach stability...

Are we done yet? Well, not exactly. There are three more rules of Lewis octet theory that need to be covered.
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RULE 2: "Quantum theory states that paired electrons are lower in energy than unpaired electrons."

Let's examine our dot structure to see if it satisfies this aspect of Lewis octet theory...

H : Ñ : C : O

As you can see (hopefully...), all of the electrons in the above structure for cyanic acid are paired.
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RULE 3: "Internal charges are carried such that more electronegative atoms carry more negative charge and more electropositive atoms carry more positive charge."

To determine a formal charge, we use a simple formula...

\[
\text{FORMAL CHARGE} = \text{GROUP NO.} - [\text{NO. OF BONDS} + \text{NO. OF LONE PAIR ELECTRONS}]
\]

\[
\begin{align*}
1-1=0 & \quad \text{H} : \overset{\cdot}{\text{N}} : \overset{\cdot}{\text{C}} : \text{O} \\
4-4=0 & \quad 5-5=0 \\
6-6=0 & 
\end{align*}
\]

So, in this instance, there are no formal charges in our structure. Note here that the net internal charge equals the net external charge.
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There is one more aspect of quantum mechanics that is involved in Lewis octet theory, and necessarily, the generation of Lewis dot structures.

**Resonance**, or movement of electrons about the atoms of a molecule can have various effects on the properties of the compound.

In our case, let's migrate the lone pair electrons on nitrogen to carbon, while simultaneously migrating two electrons from the C=O bond solely to oxygen.

Note that only *pairs* of electrons were moved, keeping in line with Rule 2 of octet theory. In addition, all of our octets remain filled, keeping in check with Rule 1, as well. Now, let's consider what happens to our formal charges by "resonating" a bond...
Note that our resonance structure now has formal charges of -1 on oxygen and +1 on nitrogen. Still, as expected, the net internal charge equals the net external charge as -1+0+1+0=0. We know from periodicity that oxygen is more electronegative than nitrogen, so we would expect it would prefer to bear a negative charge compared to nitrogen.

Now then, from these two choices, how then would we determine which structure contributes most to the actual compound cyanic acid?
RULE 4: "Any resonance structure containing the least amount of charge separation is the most stable for a given compound."

With this in mind, we can, with confidence, say that the BEST (notice we do not say ONLY!!) Lewis dot structure for cyanic acid is the species found on the left...