Chemical Bonding and Structural Representation of Molecules

- 1. Write the ground state electron configuration of each of the following atoms. For each atom, identify the valence electrons and the core electrons.
 - (a) Al (b) S (c) O (d) N (e) F
- 2. Which of the following formula contains at least one ionic bond?

| (a) H ₂ | (b) NaCl | (c) NaOH | (d) CH₃ONa | (e) CH4 |
|----------------------------|-------------|---|---------------|---------|
| (f) HOCH₂CH₃ | (g) LiNHCH₃ | (h) CH ₃ CH ₂ CO ₂ K | (i) C₀H₅NH₃CI | |

- 3. Rank the following in order of increasing negative partial charge (δ -) <u>on carbon</u>, assuming that a covalent bond exists between the atoms indicated.
 - (a) CH₃-CH₃ (b) CH₃-Li (c) CH₃-F (d) CH₃-OH (e) CH₃-NH₂
- 4. Draw Lewis structures for each of the following molecules:
 - (a) CH_5N (contains a σ bond between C and N)
 - (b) CH_3NO_2 (contains a σ bond between C and N but no bonds between C and O. At least a double bond between N and one of O's)
 - (c) CH₂O
 - (d) CH₂Cl₂
 - (e) BrCN
- 5. Draw the following Lewis structures using <u>condensed</u> formulas.



- 6. Draw the molecules in Problem 5 using <u>bond-line</u> formulas.
- 7. Draw Lewis structures for the following molecules. Include all lone pairs and H atoms.



- 8. Draw each of the species in Problem 7 as a <u>condensed</u> formula.
- 9. Convert each of the compounds given in condensed structures, first, into dash-line structures and, finally, into bond-line structures. Include lone-pair electrons and formal charges, where necessary.
- 10. Re-write the following cyclic compounds in bond-line formula.





- 12. Convert each of the compounds given in condensed structures, first, into dash-line structures and, finally, into bond-line structures. Include lone-pair electrons and formal charges, where necessary.
 - (a) $CH_3CH_2CH_2OCH_3$ (b) $(CH_3CH_2)_2CH(CH_2)_2NH_2$ (c) $(CH_3)_2C=CHCH_2CH_3$ (d) CH_3COCH_3 (e) $(CH_3CH_2CH_2)_3COCH_2CH_2CH=CHCH_2CH_2OC(CH_2CH_3)_3$ (wow!)
- 13. For each bond-line structure, a) draw the missing lone-pair electrons on atoms, b) determine the number of C atoms present, and c) determine the total number of H atoms connected to the C atoms.



14. The molecule shown is the bond-line structure of cholesterol. Re-draw the given structure as a condensed formula. What advantages do bond-line structures have?



15. Each chemical transformation below shows a starting material (*i.e.* reactant) being converted into a product. For each reaction, determine whether the product has more, fewer or the same number of C atoms as the starting material.



16. Draw Lewis structures for each of the following ions. One atom in each ion has a formal charge that is not zero. Determine which atom it is, and what the formal charge is.



17. Complete the Lewis structure for each of the following molecules by adding enough H atoms to complete the tetravalence (*N.B.* octet) of each carbon. Then, re-draw the molecule in bond-line formula, including lone-pair electrons and formal charge on atoms, where necessary.



18. Complete the Lewis structure for each of the following molecules. You may assume that no formal charges exist on any atoms. (All H atoms are shown; add only bonds and lone pairs of electrons.)



- 19. For each molecule, fill in the missing lone-pair electrons and identify all C atoms that you expect will be deficient in electron density (partial positive, δ +) by writing δ + next to them.
- (a) Br





(c)

(c)



- 20. For each of the following compounds, identify any <u>polar covalent</u> bonds. For the covalent bonds identified, place δ + and δ symbols in the appropriate locations.
- **(**a)

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21. Atoms having a partial positive charge (δ +) within a compound are the places most likely to be attacked by an anion, such as hydroxide (OH⁻), when a chemical reaction takes place. In the compound shown, identify TWO carbon atoms that are most likely to be attacked by a hydroxide ion.

(b)



22. Identify the formal charge on each atom in the following species. Assume that all valence electrons are shown.





24. Determine the formal charge on O and N atoms below.



25. In the methoxide anion (CH₃O⁻), is it possible for a double bond to exist between C and O, given that the negative charge resides on O? Explain why or why not by drawing the Lewis structure of the molecule, and assigning the formal charge on all atoms.



26. The following is a skeleton of a molecular anion having the overall formula $C_6H_6NO^2$. The hydrogen atoms are not shown.



- (a) Draw a complete Lewis structure of the species in which -1 formal charge is on N. Include all H atoms and lone-pair electrons
- (b) Do the same for the species with the -1 formal charge on O.
- (c) Do the same for the species with the -1 formal charge on the C atom that is bonded to three other C atoms.
- 27. Re-draw the following structure of glucose as a bond-line structure including the lone-pair electrons. Indicate the formal charge on atoms, where necessary.







Curved-Arrows

29. (a) Draw curved arrows to show how each chemical reaction is taking place. (b) Indicate which bonds are formed and broken as a result of the chemical reaction. (*N.B.* It is always advised that you fill in missing lone-pair electrons before starting to draw curved-arrows)



30. For each reaction, (a) provide bond-line structures of reactants and products, including lone-pair electrons now shown. (b) using curved-arrows, show how the reaction is taking place. (c) Indicate which bonds are broken and formed as a result of the chemical reaction.

| (a) | $NH_4^+ + OH^- \rightarrow NH_3 + H_2O$ |
|-----|--|
| (b) | $CH_3COO^- + CH_3NH_3^+ \rightarrow CH_3COOH + CH_3NH_2$ |
| (c) | $CH_3CH_2O^-$ + NH_4^+ \rightarrow CH_3CH_2OH + NH_3 |
| (d) | $CH_3CH_2CH_2NH_3{}^{\scriptscriptstyle +} \ + \ OH^{\scriptscriptstyle -} \ \ CH_3CH_2CH_2NH_2 \ + \ H_2O$ |

31. For each set of reactants to be used in the following acid-base reactions, a) identify the electrophile and the nucleophile. b) provide the bond-line structures of the expected products including lone-pair electrons and formal charges on atoms. c) Use curved arrows to show how the reaction is taking place. d) Identify which bonds are broken and newly generated as a result of the chemical reaction.

(a) $NH_3 + HCI \rightarrow$ (b) $HCO_3^- + OH^- \rightarrow$

(c)
$$CH_3CH_2O^- + HCI \rightarrow$$

(d) $CH_3COO^- + NH_4^+ \rightarrow$

Resonance

32. Which of the following pairs are not resonance structures of one another? All lone-pair electrons may or may not be shown. Identify where each lone-pair that is not shown belongs.



33. Draw all important resonance structures for each of the following molecules or ions. Be sure to include the curved arrows that indicate which pairs of electrons are shifted in going from one resonance structure to the next.

| (a) CH₃NO₂ | (b) CH₃CO₂ ⁻ | (c) CH₃CHCHCH₂⁺ (the ion has two C-C single bonds) | (d) C₅H₅N (a ring is formed by the C and N atoms, and each H is bonding to C) | (e) C₄H₅N (a ring is formed by the C and N atoms, the N is bonded to one H, each C is |
|------------|-------------------------|--|---|--|
| | | | | bonded to one H) |

34. Draw all important resonance structures for each of the following ions. Be sure to include the curved arrows that indicate which pairs of electrons are shifted in going from one resonance structure to the next. What is the resonance hybrid of each species?



- 35. (a) Draw all significant resonance structures of the following ion. In drawing each additional resonance structure, use curved arrows to indicate which pairs of electrons are being shifted.(b) What is the resonance hybrid of the ion?
 - (c) Which C-C bond is the longest?
- (a) Draw all significant resonance structures for the following ion.
 Show how the electrons are moved using curved-arrow notation.
 - (b) What is the resonance hybrid of the ion?



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- 37. The two species A and B shown are structurally very similar. Draw all important resonance structures for each species and determine which is more stable. Explain.
- 38. The two species C and D shown are structurally very similar. Draw all important resonance structures for each species and determine which is more stable. Explain.





Solutions

1. Write the ground state electron configuration of each of the following atoms. For each atoms, identify the valence electrons and the core electrons.

| | | Ground-state Electronic Configuration | The number of Valence Electrons (in Red) |
|-----|----|---|--|
| (a) | AI | 1s²2s²2p ⁶ 3s²3p¹ | 3 |
| (b) | S | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁴ | 6 |
| (c) | 0 | 1s ² 2s ² 2p ⁴ | 6 |
| (d) | Ν | 1s ² 2s ² 2p ³ | 5 |
| (e) | F | 1s ² 2s ² 2p ⁵ | 7 |

2. Which of the following formula contains at least one ionic bond?

Molecules (b), (c), (d), (g), (h) and (i) contain at least an ionic bond.

- 3. Rank the following in order of increasing negative partial charge (δ -) <u>on carbon</u>, assuming that a covalent bond exists between the atoms indicated.
 - (a) CH₃-CH₃ (b) CH₃-MgBr (c) CH₃-Li (d) CH₃-F (e) CH₃-OH (f) CH₃-NH₂

Ranking (Least negative) D < E < F < A < B (Most Negative)

4. Draw Lewis structures for each of the following molecules:



5 + 6 Draw the following Lewis structures using <u>condensed</u> and <u>bond-line</u> formulas.

Bond Line Formula

- (a) $CH_3CH_2CH_2CH_3$
- (b) CH₃CH=CHCH₃ or CH₃CHCHCH₃ (No double bond drawn)
- (c) $CH_3C(CH_3)=CHCH_3 \text{ or } CH_3C(CH_3)CHCH_3$ (No double bond drawn)



7 + 8 Draw Lewis structures and condensed formula for the following molecules. Include all lone pairs and H atoms.





9. Convert each of the compounds given in condensed structures, first, into dash-line structures and, finally, into bond-line structures. Include lone-pair electrons and formal charges, where necessary.



10. Re-write the following cyclic compounds in bond-line formula.



11. Provide a condensed structure for each compound given below.

| | Bond-line structures | Condensed structures |
|-----|-------------------------|--|
| (a) | | (CH ₃) ₂ CHCH ₂ OH |
| (b) | OH O | (CH ₃) ₂ CHC(=O)CH(CH ₃) ₂ |
| (c) | | CH ₃ CH ₂ CH=CHCH=CHCH ₃ |
| (d) | ∕_N∕_ H | (CH ₃ CH ₂) ₂ NH |

Bond-line structures

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... .0

- 12. Convert each of the compounds given in condensed structures, first, into dash-line structures and, finally, into bond-line structures. Include lone-pair electrons and formal charges, where necessary.
 - (a) $CH_3CH_2CH_2OCH_3$
 - (b) (CH₃CH₂)₂CH(CH₂)₂NH₂
 - (c) $(CH_3)_2C=CHCH_2CH_3$
 - (d) CH₃COCH₃
 - $(e) \qquad (CH_3CH_2CH_2)_3COCH_2CH_2CH=CHCH_2CH_2OC(CH_2CH_3)_3$

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13. For each bond-line structure, a) draw the missing lone-pair electrons on atoms, b) determine the number of C atoms present, and c) determine the total number of H atoms connected to the C atoms.



14. The molecule shown is the bond-line structure of cholesterol. Re-draw the given structure as a condensed formula. What advantages do bond-line structures have?



The bond-line structure avoids writing of C and H atoms, drawing of C-H bonds and clutter; thereby, allowing quicker drawing of the molecule. 15. Each chemical transformation below shows a starting material (*i.e.* reactant) being converted into a product. For each reaction, determine whether the product has more, fewer or the same number of C atoms as the starting material.



16. Draw Lewis structures for each of the following ions. One atom in each ion has a formal charge that is not zero. Determine which atom it is, and what the formal charge is.

| | (a) | (b) | (C) | (d) | (e) |
|-----------------|-----------------------------------|--------------------|---------------------------------|----------------------|---|
| | The C_2H_5 anion | The CH₃O cation | The CH ₆ N cation | The CH₅O cation | The C ₃ H ₃ anion |
| Lewis structure | H H H-C-C: [©] H H | , C=0,⊕ H H | H H | H H H-C-O: H H | H _ H-C-C≡C : H |

17. Complete the Lewis structure for each of the following molecules by adding enough H atoms to complete the tetravalence (*N.B.* octet) of each carbon. Then, re-draw the molecule in bond-line formula, including lone-pair electrons and formal charge on atoms, where necessary.



18. Complete the Lewis structure for each of the following molecules. You may assume that no formal charges exist on any atoms. (All H atoms are shown; add only bonds and lone pairs of electrons.)



19. For each molecule, fill in the missing lone-pair electrons and identify all C atoms that you expect will be deficient in electron density (partial positive, δ +) by writing δ + next to them.



- 20. For each of the following compounds, identify any <u>polar covalent</u> bonds. For the covalent bonds identified, place δ + and δ symbols in the appropriate locations.
 - (a) δ^{-} δ^{+} δ^{+} δ^{+} δ^{+} Polar covalent bonds are

Polar covalent bonds are indicated in red Polar covalent bonds are indicated in red

- Polar covalent bonds are indicated in red
- 21. Atoms having a partial positive charge (δ+) within a compound are the places most likely to be attacked by an anion, such as hydroxide (OH⁻), when a chemical reaction takes place. In the compound shown, identify TWO carbon atoms that are most likely to be attacked by a hydroxide ion.

(b)

 δ^+ δ^+ Cl:

22. Identify the formal charge on each atom in the following species. Assume that all valence electrons are shown.

As for formal charges, only two atoms in Red have formal charges as shown in the left structure. All other atoms have the formal charge of zero (and shown to be neutral).

23. Inspect each structure carefully and draw right numbers of lone-pair electrons on C, N and O atoms to satisfy the formal charges indicated. If no charges given on an atom, it means the formal charge of zero.









24. Determine the formal charge on O and N atoms below.



25. In the methoxide anion (CH₃O⁻), is it possible for a double bond to exist between C and O, given that the negative charge resides on O? Explain why or why not by drawing the Lewis structure of the molecule, and assigning the formal charge on all atoms.



26. The following is a skeleton of a molecular anion having the overall formula $C_6H_6NO^2$. The hydrogen atoms are not shown.







Curved-Arrows

29. (a) Draw curved arrows to show how each chemical reaction is taking place. (b) Indicate which bonds are formed and broken as a result of the chemical reaction. (*N.B.* It is always advised that you fill in missing lone-pair electrons before starting to draw curved-arrows)



30. For each reaction, (a) provide bond-line structures of reactants and products, including lone-pair electrons now shown. (b) using curved-arrows, show how the reaction is taking place. (c) Indicate which bonds are broken and formed as a result of the chemical reaction.



31. For each set of reactants to be used in the following acid-base reactions, a) identify the electrophile and the nucleophile. b) provide the bond-line structures of the expected products including lone-pair electrons and formal charges on atoms. c) Use curved arrows to show how the reaction is taking place. d) Identify which bonds are broken and newly generated as a result of the chemical reaction.



Resonance

32. Which of the following pairs are not resonance structures of one another? All lone-pair electrons may or may not be shown. Identify where each lone-pair that is not shown belongs.

202-DCP-05



Only pairs C, D and E are considered resonance structures of one another.

33. Draw all important resonance structures for each of the following molecules or ions. Be sure to include the curved arrows that indicate which pairs of electrons are shifted in going from one resonance structure to the next.



34. Draw all important resonance structures for each of the following ions. Be sure to include the curved arrows that indicate which pairs of electrons are shifted in going from one resonance structure to the next. What is the resonance hybrid of each species?



35. (a) Draw all significant resonance structures of the following ion. In drawing each additional resonance structure, use curved arrows to indicate which pairs of electrons are being shifted.(b) What is the resonance hybrid of the ion?

(c) Which C-C bond is the longest?





The resonance hybrid is the combination of the four structures.

This bond (in red) is the longest C-C bond as it is not a part of electron delocalization and excluded from the resonance stabilization.

- (a) Draw all significant resonance structures for the following ion. Show how the electrons are moved using curved-arrow notation.
 - (b) What is the resonance hybrid of the ion?





37. The two species A and B shown are structurally very similar. Draw all important resonance structures for each species and determine which is more stable. Explain.





Structure A has more resonance structures; therefore, gains a greater amount of resonance stabilization (More stable)

38. The two species C and D shown are structurally very similar. Draw all important resonance structures for each species and determine which is more stable. Explain.





Structure D has more resonance structures; therefore, gains a greater amount of resonance stabilization (More stable)