

Experiment 16

Lewis Dot Structures and Geometry by VSEPR Theory

Pre-Lab Assignment

Before coming to lab:

- Read the lab thoroughly.
- Answer the pre-lab questions that appear at the end of this lab exercise.

Purpose

To determine the Lewis dot structures and VSEPR geometries of a variety of covalently bonded molecules and ions.

Background

While some atomic elements can be found in nature, most combine with other atoms to form larger groups called molecules. Lewis Theory states that atoms will form bonds with their valence electrons in order to fill their outer orbitals to mimic the electron configuration of the noble gases. Since the outer s and p orbitals can hold a total of eight electrons, almost all atoms on the periodic table will follow the Octet Rule, or "rule of eight". Exceptions to the Octet Rule include early elements, such as H and He that can hold only two, and elements in Period 3 or greater that have empty d orbitals that can hold more than eight electrons.

To bond, atoms can either share their electrons (in covalent compounds) or transfer them completely (in ionic compounds). For covalent compounds, the electrons in each bond form counts for both atoms towards satisfying their octet. For ionic compounds, the atoms are held together by electrostatic attraction between opposite charges.

Lewis structures are a two-dimensional representation of a molecule's connectivity. They represent the valence electrons present in the molecule as lone pairs (unshared electrons, drawn as dots) or bonds (shared electrons, drawn as lines). They give powerful information about the location of atoms in the molecule that can in turn determine many of the molecule's physical and chemical properties, including boiling and melting point, odor, viscosity, surface tension, and reactivity.

To Draw Lewis Structures:

1. Calculate the total number of valence electrons contributed to the molecule by each atom.
2. Draw a skeletal structure by connecting each atom to another by one bond. One bond represents two electrons.
 - More electronegative elements prefer to be terminal.
 - Less electronegative elements prefer to be central.
 - H is always terminal.
3. Distribute the remaining electrons as lone pairs on each atom to satisfy their octets.
4. If there are fewer electrons in Steps 2 and 3 than in Step 1, add multiple bonds.

- If there are more electrons in Steps 2 and 3 than in Step 1, add them to any Period 3 or greater elements.
- Check formal charges on each atom. The most stable Lewis structures will have the smallest/fewest formal charges, with the most stable compounds having no formal charges. Negative formal charges are more stable on more electronegative atoms. The sum of the formal charges in the molecule should equal the overall charge of the molecule.

$$\text{Formal Charge} = \# \text{ of valence electrons the atom brought} - \# \text{ of bonds} - \# \text{ of lone pairs}$$

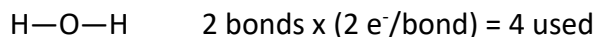
Example Problem: Drawing Lewis Structures

Draw the Lewis structure for H₂O.

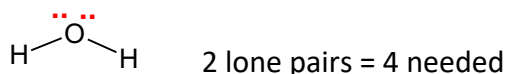
Step 1: Count the total number of valence electrons

$$2 \times (1 \text{ e}^- \text{ from H}) + 1 \times (6 \text{ e}^- \text{ from O}) = 8 \text{ total}$$

Step 2: Draw a skeletal structure of the molecule



Step 3: Distribute the remaining electrons as lone pairs to satisfy the octet for each atom



No Step 4 or 5 needed.

Step 6: Check formal charges

$$\text{H} = (1 \text{ valence e}^-) - (1 \text{ e}^- \text{ from bond}) = 0 \text{ for each}$$

$$\text{O} = (6 \text{ valence e}^-) - (2 \text{ e}^- \text{ from bonds} + 4 \text{ e}^- \text{ from lone pairs}) = 0$$

Atoms that hold *fewer* than eight valence electrons are said to have an incomplete octet. This is most often seen for early period elements such as Be (2 e⁻) or B (4 e⁻), and especially for H and He that hold only two electrons each due to having only a 1s orbital available. Atoms that can hold *more* than eight valence electrons are said to have an expanded octet. This is possible only for elements in period 3 or greater due to their empty d-orbitals (recall that electrons fill the 4s orbitals before the 3d). For some molecules, expanding the central atom's octet can minimize formal charges, making the overall molecule more stable than if the Octet Rule was obeyed.

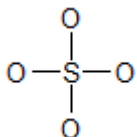
Example Problem: Drawing Lewis Structures

Draw the Lewis structure for SO_4^{2-} .

Step 1: Count the total number of valence electrons

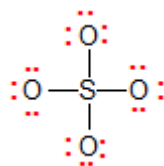
$$1 \times (6 \text{ e}^- \text{ from S}) + 4 \times (6 \text{ e}^- \text{ from O}) + 2 \text{ e}^- \text{ (from charge)} = 32 \text{ total}$$

Step 2: Draw a skeletal structure of the molecule



$$4 \text{ bonds} \times (2 \text{ e}^-/\text{bond}) = 8 \text{ used}$$

Step 3: Distribute the remaining electrons as lone pairs to satisfy the octet for each atom



$$12 \text{ lone pairs} = 24 \text{ needed}$$

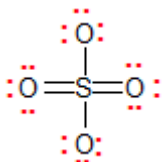
No Step 4 or 5 needed.

Step 6: Check formal charges

$$\text{S} = (6 \text{ valence e}^-) - (4 \text{ e}^- \text{ from bonds}) = +2$$

$$\text{O} = (6 \text{ valence e}^-) - (1 \text{ e}^- \text{ from bonds} + 6 \text{ e}^- \text{ from lone pairs}) = -1$$

Step 7: Minimize formal charges by expanding octets for period 3 or greater elements. Keep negative formal charges on more electronegative atoms.



$$\text{S} = (6 \text{ valence e}^-) - (6 \text{ e}^- \text{ from bonds}) = 0$$

$$\text{O} = (6 \text{ valence e}^-) - (2 \text{ e}^- \text{ from bonds} + 4 \text{ e}^- \text{ from lone pairs}) = 0$$

$$\text{O} = (6 \text{ valence e}^-) - (1 \text{ e}^- \text{ from bonds} + 6 \text{ e}^- \text{ from lone pairs}) = -1$$

Whenever more than one Lewis structure can be drawn for a molecule which satisfies the Octet Rule **and** keeps the atoms in the same positions, the difference structures are said to be resonance forms (or resonance isomers). The actual molecule is a mixture, or resonance hybrid, of each of its resonance forms where its moving electrons are shared (called delocalized) between multiple lone pairs and bonds. The example of SO_4^{2-} above has **six** resonance structures.

Resonance structures involve the spreading of electrons, not the moving of atoms. Atomic rearrangement creates geometric isomers which are considered different molecules from the originals.

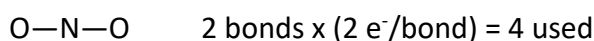
Example Problem: Drawing Lewis Structures

Draw the Lewis structure for NO_2^- .

Step 1: Count the total number of valence electrons

$$1 \times (5 \text{ e}^- \text{ from N}) + 2 \times (6 \text{ e}^- \text{ from O}) + 1 \text{ e}^- \text{ from negative charge} = 18 \text{ total}$$

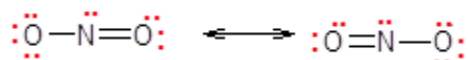
Step 2: Draw a skeletal structure of the molecule



Step 3: Distribute the remaining electrons as lone pairs to satisfy the octet for each atom



Step 4: If there are too few electrons, add multiple bonds



Step 6: Check formal charges

$$\text{N} = (5 \text{ valence e}^-) - (3 \text{ e}^- \text{ from bonds} + 2 \text{ e}^- \text{ from lone pairs}) = 0$$

$$\text{O (left)} = (6 \text{ valence e}^-) - (1 \text{ e}^- \text{ from bonds} + 6 \text{ e}^- \text{ from lone pairs}) = -1$$

$$\text{O (right)} = (6 \text{ valence e}^-) - (2 \text{ e}^- \text{ from bonds} + 4 \text{ e}^- \text{ from lone pairs}) = 0$$

N and O are in period 2 so cannot expand their octets.

While Lewis structures represent the connectivity and structure of molecules, they fail to show their three-dimensional shape due to their limitations. In the late 1950's and 60's, Dr. R. J. Gillespie proposed that the geometry of simple molecules can be determined based on electronic repulsions (Valence Shell Repulsion Theory, or VSEPR Theory). Geometries are determined around the central atom of a molecule, or any atom that has at least two neighbors. Around the central atom, regions of high electron density, such as bonds or lone pairs, are placed as far apart as possible in order to minimize the repulsion between them. Each lone pair is considered an electron region or electron domain. Since multiple bonds occupy the same physical side of an atom, single, double, and triple bonds are treated equally and considered as a single electron region. If more than one central atom is present, then the geometry can be determined separately at each.

Electronic geometry is the simplest form of a molecule's shape as it only takes into account the total number of electron regions. However, since lone pairs are free on individual atoms, they repel other electron regions more strongly than bonding. Molecular geometry more accurately

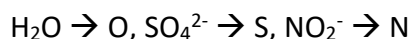
represents a molecule's physical shape as it takes this extra repulsion into account. If the central atom has no lone pairs, then its electronic and molecular geometries will be identical.

Total Electron Regions	Bonding Electron Regions	Nonbonding Electron Regions	Electronic Geometry	Molecular Geometry
2	2	0	linear	linear
3	3	0	trigonal planar	trigonal planar
	2	1		bent
4	4	0	tetrahedral	tetrahedral
	3	1		trigonal pyramidal
	2	2		bent
5	5	0	trigonal bipyramidal	trigonal bipyramidal
	4	1		see-saw
	3	2		T-shaped
	2	3		linear
6	6	0	octahedral	octahedral
	5	1		square pyramidal
	4	2		square planar

Example Problem: Determining VSEPR Geometry

Determine the electronic and molecular geometry of H_2O , SO_4^{2-} , and NO_2^- .

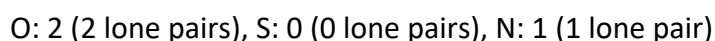
Step 1: Find the central atom.



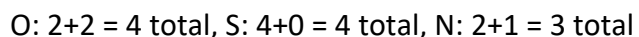
Step 2: Count the bonding electron domains around each atom.



Step 3: Count the nonbonding electron domains around each atom.



Step 4: Count the total electron domains.



Step 5: Use the table to assign the geometries to each.

H_2O : tetrahedral, bent

SO_4^{2-} : tetrahedral, tetrahedral

NO_2^- : trigonal planar, bent

Electronegativity is a property individual to each element that measures its attractiveness to an additional electron (Fig. 1). Fluorine is the most electronegative element on the periodic table with an assigned value of 4.0, indicating its strong pull on electrons. When different elements are bonded, the difference between their electronegativities can be used to classify the bond as either nonpolar covalent, polar covalent, or ionic (Table 1).

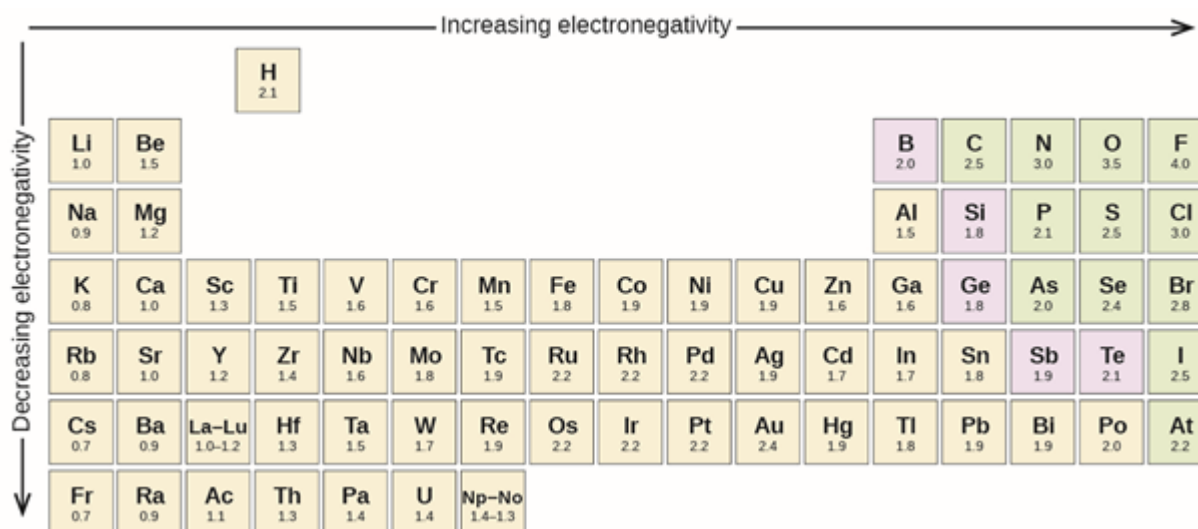


Figure 1: Electronegativity values of elements

Table 1: Bond Classifications

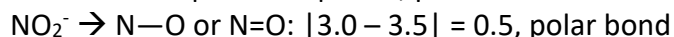
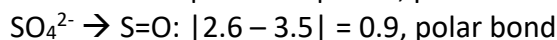
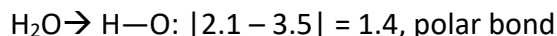
Bond Type	Nonpolar Covalent	Polar Covalent	Ionic
ΔeN	0-0.4	0.5-2.0	>2.0
Description	evenly shared	unevenly shared	exchanged

Polar bonds form dipoles where the more electronegative element pulls extra electron density away from the less electronegative element and creates partial negative and positive charges on each, respectively. Polarity is the measure of how unevenly electron density is shared in a molecule due to the presence of polar bonds. Molecules in which all bonds are nonpolar are said to be overall nonpolar and have even distribution of electron density throughout. Molecules that contain polar bonds can be either overall polar or nonpolar depending on how those bonds are oriented. If the molecule is **symmetric** (i.e., equal dipoles are opposite in direction with no lone pairs on the central atom and therefore cancel), then it is said to be overall nonpolar. If the molecule is **asymmetric** (i.e., the dipoles are not opposite in direction or not equal or the central atom has a lone pair and therefore do not cancel), then it is said to be overall polar. The overall polarity of a molecule has a great effect on its macroscopic properties, such as solubility, boiling and melting points, and viscosity.

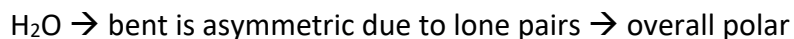
Example Problem: Determining the Polarity of a Molecule

Determine whether H_2O , SO_4^{2-} , and NO_2^- are overall polar or nonpolar.

Step 1: Calculate ΔeN to find any polar bonds.



Step 2: Use the molecular geometry to determine whether the dipoles cancel.



Procedure

Part I: Molecular Models and Lewis Structures

1. Draw the correct Lewis structures for each molecule or ion indicated on the following data sheets. Be sure to check all formal charges and be alert for any exceptions to the Octet Rule. If the molecule has resonance structures, indicate "Y" in the resonance column. If no resonance structures exist, indicate "N".
2. Using the provided molecular model kit pieces, build the model for each molecule on the following data sheets. Show your Lewis structures and models to your instructor for sign-off. Correct any mistakes.

White (matte or shiny, 1 hole) = Hydrogen

Black (matte or shiny, 4 hole) = Carbon

Blue (matte or shiny, 4 hole) = Nitrogen

Red (matte or shiny, 2 hole) = Oxygen

Green (matte or shiny, 1 hole), Purple (shiny, 1 hole), Orange (shiny, 1 hole),

Grey (matte, 1 hole) = Halogens

Purple (matte or shiny, 4 hole) = Phosphorous

Yellow (shiny, 4 hole or matte, 6 hole) = Sulfur

Rust (shiny, 5 hole) or Silver (shiny, 6 hole) = any expanded octet

Note: use shiny bonds in shiny atoms and matte bonds in matte atoms.

Part II: VSEPR Geometry and Polarity

1. Using your corrected Lewis structures from Part I, count the bonding, nonbonding, and total electron domains and determine the electronic and molecular geometries for each molecule and ion indicated on your data sheets.
2. Calculate the difference in electronegativity for each unique bond and indicate whether the bond is polar or nonpolar.
3. Indicate whether the molecule is symmetric or asymmetric around the central atom.
4. Determine whether the molecule is overall polar or nonpolar.

Experiment 16—Data Sheet

Name: _____

NO₃¹⁻	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: N = O () = O () = O () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		
NF₃	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: N = F () = F () = F () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

ICl₃ iodine trichloride	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: I = Cl () = Cl () = Cl () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>	Symmetric or Asymmetric?	Overall Polar or Nonpolar?			

IF₅	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: I = F () = F () = F () = F () = F () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>	Symmetric or Asymmetric?	Overall Polar or Nonpolar?			

SCl₆ sulfur hexachloride	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: S = Cl () = Cl () = Cl () = Cl () = Cl () = Cl () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		
PO₄³⁻	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: P = O () = O () = O () = O () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

OF₂	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: O = F () = F () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

CO₂	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: C = O () = O () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

XeF₂	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: Xe = F () = F () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

XeCl₄ xenon tetrachloride	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: Xe = Cl () = Cl () = Cl () = Cl () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

H₂CO	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: C = O = H () = H () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		
SiF₅¹⁻	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: Si = F () = F () = F () = F () = F () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

SeO₂	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
			Bonding	Lone Prs.	Total
Total number of valence e⁻:		Formal Charges: Se = O () = O () =	Electronic Shape:		
			Molecular Shape:		
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

SO₃	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
			Bonding	Lone Prs.	Total
Total number of valence e⁻:		Formal Charges: S = O () = O () = O () =	Electronic Shape:		
			Molecular Shape:		
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

SeBr₄	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: Se = Br () = Br () = Br () = Br () =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		
CH₃CHO	Lewis Structure:	Resonance? Yes or No	# of e⁻ groups on central atom		
		Formal Charges: Cx = Cy () = H () = H () = H () = H () = O =	Bonding	Lone Prs.	Total
Electronic Shape:					
Molecular Shape:					
Total number of valence e⁻:					
ΔeN for Bonds (indicate polar or nonpolar): <i>show calculations:</i>		Symmetric or Asymmetric?	Overall Polar or Nonpolar?		

Treat each carbon separately – label each C with X or Y subscript to differentiate them.

Experiment 16—Post-Lab Assignment

1. Nitrous oxide (N_2O) has two possible arrangements: (i) NON or (ii) NNO.

a. Draw Lewis structures for (i) NON and (ii) NNO.

b. Calculate the formal charges for each atom in the structures in (a).

c. Which structure (i) or (ii) is more stable? Explain.

2. Acetic acid (CH_3COOH) is diluted and sold commercially as vinegar.

a. Draw the Lewis structure for CH_3COOH .

b. Circle **each** central atom (hint: there are three).

c. Determine the electronic and molecular geometries around each central atom in (b).

Experiment 16—Pre-Lab Assignment

Name: _____

1. Ozone, O_3 , is present in earth's atmosphere and absorbs UV radiation.

a. Draw the Lewis structure for O_3 . Show formal charges for **all** atoms and include any possible resonance structures.

b. Determine the VSEPR geometries for O_3 .

Electronic Geometry: _____

Molecular Geometry: _____

2. Draw the Lewis structures for (a) C_2H_6 , (b) C_2H_4O , and (c) CH_5N . Show formal charges for **all** atoms and determine the VSEPR geometries for each.

a. C_2H_6

Electronic Geometry for C_1 : _____

Electronic Geometry for C_2 : _____

Molecular Geometry for C_1 : _____

Molecular Geometry for C_2 : _____

b. C_2H_4O

Electronic Geometry for C_1 : _____

Electronic Geometry for C_2 : _____

Molecular Geometry for C_1 : _____

Molecular Geometry for C_2 : _____

c. CH_5N

Electronic Geometry for C: _____

Electronic Geometry for N: _____

Molecular Geometry for C: _____

Molecular Geometry for N: _____