THE THUMB RULE REVEALS: FACILITATING THE TRANSITION FROM ELECTRON GEOMETRY TO MOLECULAR GEOMETRY AND VICE VERSA

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ABSTRACT

Both 1st and 2nd semester students of General Chemistry are introduced to the concepts of electron and molecular geometry as part of a chapter concerning "Chemical Bonding" (sections following Valence Shell Electron Pair Repulsion Theory). Often, instructors note that students encounter difficulties discriminating between the electron geometry and the molecular geometry of a molecule which is dependent on the presence of lone pairs on the central atom. We propose a "thumb rule" that is designed to "reveal" any difference between the two said geometries and thereby facilitates the transition from electron to molecular geometry and vice versa. The use of this technique is additionally advantageous since it is simple to apply and does not require any materials (and is therefore free of charge). Importantly, it is a fun exercise that facilitates learning. *[African Journal of Chemical Education—AJCE 7(3), Special Issue, October 2017]*

INTRODUCTION

Freshmen college students learn about the "shapes" of molecules towards the end of a General Chemistry I syllabus or at the very beginning of General Chemistry II [1]. They are taught that the spatial shapes adopted by molecules are often very different than that which might have been rendered on paper to-date (Fig 1).

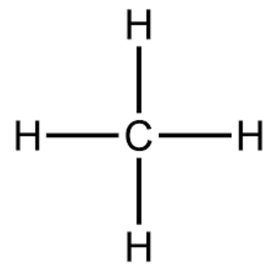


Figure 1. Typical representation of methane by students of General Chemistry prior to becoming familiar with "shapes of molecules".

The repulsive forces exerted by electron pairs around the central atom in the molecule, be they bonding pairs or lone pairs, is key to the three-dimensional geometry adopted by every molecule. The Introduction to the Valence Shell Electron Pair Repulsion (VSEPR) theory helps students recognize that electron pair repulsion needs to be minimized [2]. According to this theory, single, double and triple bonds each represent only a "single region" of electron density [3]. Furthermore, the repulsive forces around a lone pair are greater than that exerted around bonding pairs. Nevertheless, in each case, the objective is to minimize the repulsive forces between the regions of electron density be they from lone pairs or bonding pairs or a combination of the two.

To achieve this, each bond in a molecule is placed farthest from the neighboring bonding in three dimensional space. The same principle applies when a lone pair of electrons is present. Except, the lone pair exerts a greater repulsion on neighboring regions of electron density than do bonding pairs.

Based on VSEPR principles, students need to be able to render the geometries of molecules. For example, methane contains four bonding pairs via four single bonds around the central carbon. These four regions of electron density repel one another. Therefore, the mechanism that must be adopted to achieve maximum distance between these regions of repulsion is one of a tetrahedral placement of the bonds around the central carbon. The student recognizes then that the bond angles are all equal and that the geometry of methane is that of a tetrahedron (or that methane is tetrahedral).

At this stage, the student of chemistry learns about the possibility of a difference between the electron geometry of a molecule and its molecular geometry [4-6]. An understanding of both electron and molecular geometries are critical. Both geometries impact the chemical and physical properties of the molecule. They influence its ability to not only participate in chemical reactions but also impact other properties such as molecular polarity, it's "state" (solid, liquid or gas), color, magnetic tendency and biological activity (if any). Knowledge of both geometries is key not only to the student of General Chemistry but is a basis for organic reactions, and higher progress in Chemistry, Physics and Biology and a career in the STEM fields.

Electron geometry refers to the positions (arrangement) of the regions of electron density around the central atom [1]. Thus, since both bonding pairs and lone pairs represent regions of electron density, their combined presence, if any, would need to be accounted for when discussing its electron geometry.

Molecular geometry only takes into consideration the presence of other atoms that are bonded to central atom in the 3-D structure of the molecule [1, 4-6]. Thus, only bonding pairs need to be accounted for whereas lone pairs do not participate.

Central atoms that do not contain one or more lone pairs would have identical electron and molecular geometries since there are no lone pairs to be excluded when contributions to the molecular geometry are to be considered [1]. However, when the central atom possesses one or more lone pairs, then the molecular geometry differs considerable from the electron geometry.

It is here that students often find application of the concepts confusing. Particularly, they are often unable to correctly transition from one geometrical representation to the other (electron to molecular, and vice versa) whether or not such a difference exists (due to the presence or absence of lone pair(s).

We propose a simple, manual, tool that helps facilitate the student of General Chemistry to transition from one geometry to the other, viz., the "Thumb rule".

METHODOLOGY/EXPERIMENTAL

The Thumb Rule

Elements of the rule

1. Render the 3-D electron configuration structure of the molecule based on VSEPR rule

To transit from electron geometry to the molecular geometry:

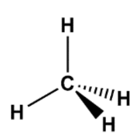
2. Inspect the Lewis structure for the presence of lone pairs on the central atom. If no lone pairs exist, the electron and molecular geometries are the same
3. If a lone pair is present on the central atom, use your thumb to conceal it and re-examine the structure of the molecule. At this stage, only bonding pairs of electrons should be visualized (These link the central atom to the partner atoms). The geometry of the molecule is now representative of the molecular geometry.
4. If the central atom possesses more than one lone pair, apply rule (3) so that all lone pairs on the central atom are concealed. Along with your dominant hand thumb, you could avail of the other thumb or take the help of a friend to conceal additional lone pairs.

To transit from molecular geometry to the electron geometry

5. Remove the concealed lone pair on the central atom by retracting your opposable digit from its position in (3). This should reveal the lone pair. If the central atom possesses more than one lone pair, retract the thumbs so that all lone pairs are no longer obscured. The electron geometry now becomes apparent since the lone pairs become exposed along with the previously visible bonding pairs. I.e. all regions of electron density on the central atom are visible, permitting the student to transition from the molecular geometry to the electron geometry.

RESULTS AND DISCUSSION

Consider a molecule such as methane. The student is instructed to draw the Lewis structure of the said molecule and inspect it for lone pairs. If no lone pairs exist, the molecular and electron geometries coincide and are to be rendered taking into account the VSEPR rules.



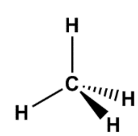


Figure 2. Representation of methane by students of General Chemistry after becoming familiar with the “shapes of molecules”. Left: Electron geometry (Tethrahedral); Right: Molecular geometry (Tethrahedral)

The molecule is re-examined, by applying the Thumb rule.

In methane, the search for lone pairs reveals the absence of the same. Therefore, rule 2 (from methods) applies and the electron and molecular geometries of methane are the same.

Next, consider a molecule with a lone pair such as ammonia. The central nitrogen atom possesses four regions of electron density. Three of these manifest themselves as bonding pairs of electrons (N-H bonds) and one as a lone pair. The electron geometry of ammonia is tetrahedral whereas the molecular geometry is trigonal pyramidal.

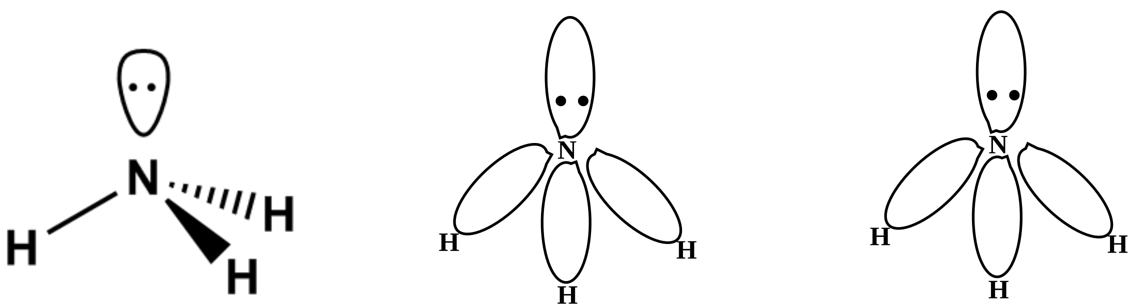


Figure 3. Left: Representation of ammonia based on Lewis structure and principles of VSEPR theory. Middle: Electron geometry of ammonia (Tetrahedral). Right: Molecular geometry of ammonia (Trigonal pyramidal)

Note: The ability to differentiate between the electron and molecular geometry in ammonia is not very obvious to the student. The molecules are re-examined now, by applying the Thumb rule

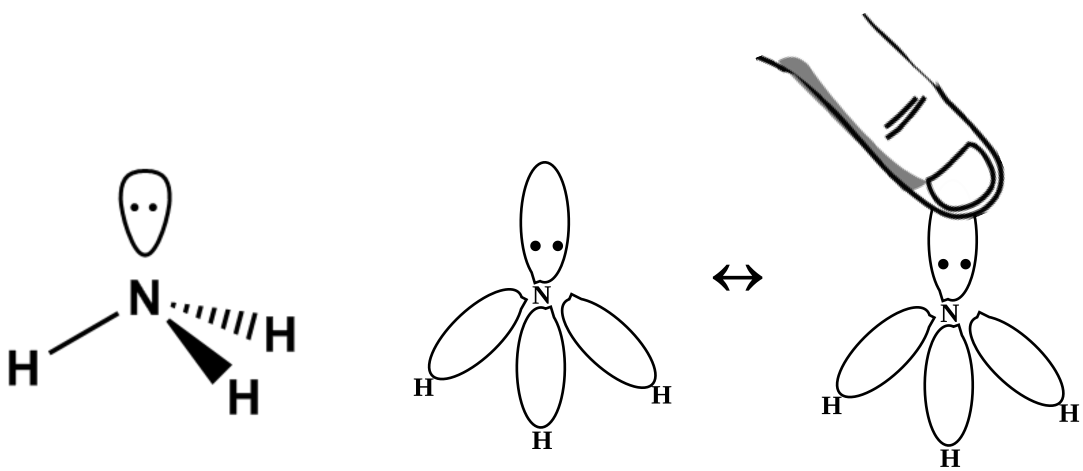


Figure 4. Left: Representation of ammonia based on Lewis structure and principles of VSEPR theory. Using the Thumb Rule- Middle: Electron geometry of ammonia (Tetrahedral). Right: Molecular geometry of ammonia (Trigonal pyramidal).

The thumb rules clearly facilitate discrimination between electron and molecular geometries. This is particularly true when the central atom possesses one or more lone pairs. The use of the thumb to conceal the lone pair when transitioning from electron to molecular geometry helps the student focus on bonding pairs and the atoms in the molecule. Conversely, application of rule 5 when transition from molecular geometry to electron geometry, reveals the lone pair and "all regions of electron density", permitting the electron geometry to be accurately recognized.

Using a few more examples, we demonstrate the application of the thumb rule to facilitate the transition from electron to molecular geometry and vice versa.

Beryllium Chloride: Central atom, Beryllium; Two bonding pairs and no lone pairs

Figure 5. Beryllium Chloride. Rule 2 of the Thumb rule suggests identical electron (Left) and molecular (right) geometries

Water: Central atom, Oxygen; Two bonding pairs and two lone pairs

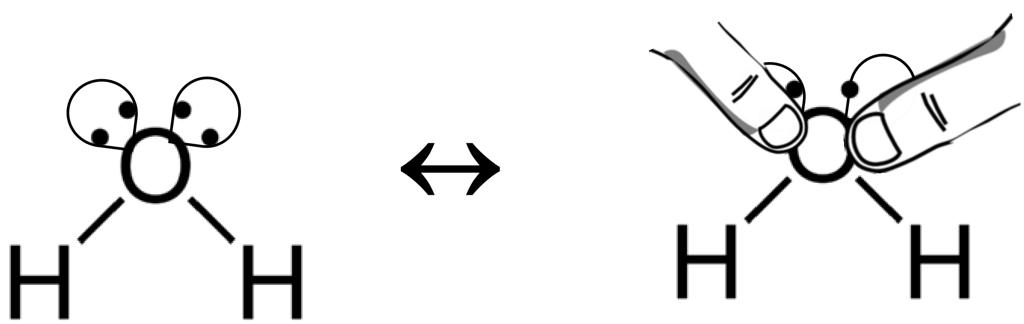


Figure 6. Transition between the electron (left; tetrahedral) and molecular (right; bent) geometry of water facilitated by application of the Thumb rule

Additional Exercises

Sulfur dioxide: Central Atom Sulfur; Two bonding pairs and one lone pair

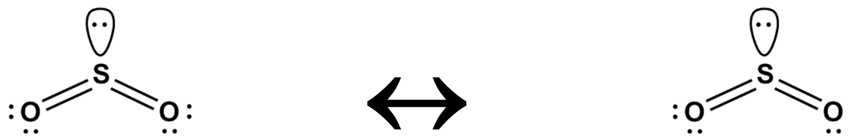


Figure 7. Apply thumb rule to transition between the electron (left) and molecular (right) geometry of sulfur dioxide

Sulfur tetrafluoride: Central atom, Sulfur; Four bonding pairs and one lone pair

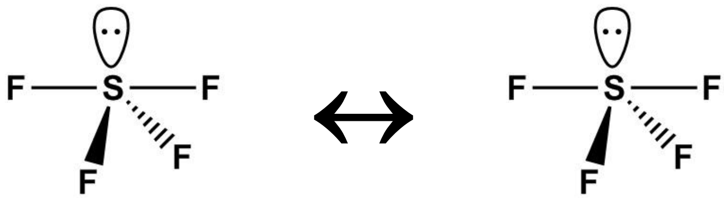


Figure 8. Apply the thumb rule to transition between the electron (left) and molecular (right) geometry of sulfur tetrafluoride

CONCLUSION

The Thumb rule tool helps the beginner student easily recognize the difference between molecular and electron geometries. This tool is especially effective when there are lone pairs present on the central atom, resulting in a difference between the electron and molecular geometries.

We submit that the application of the thumb rule to transition between the said geometries can be a fun exercise. It can also be applied in a team-learning format in addition to the individual student. It requires no additional material and is therefore widely accessible among all socio-economic backgrounds. It facilitates learning of a very important concept in general chemistry and beyond: The shape of a molecule.

In conclusion, sometimes, the eager learner must ask a friend to lend a few thumbs!

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