cubic ellipsoid nucleus - atomic physics - part 4: intramolecular bonds

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Abstract

According to the ellipsoid model [17], the nuclear structure determines the shape and properties of the atom. In this research we try to connect between the nuclear structure and the bond angles of the atom.
It seems that the positions of the missing protons in the outermost nuclear shell determine the angles of the atomic (intramolecular) bonds, although the forces between the atoms in the molecule can change these angles, in the process of reaching equilibrium.

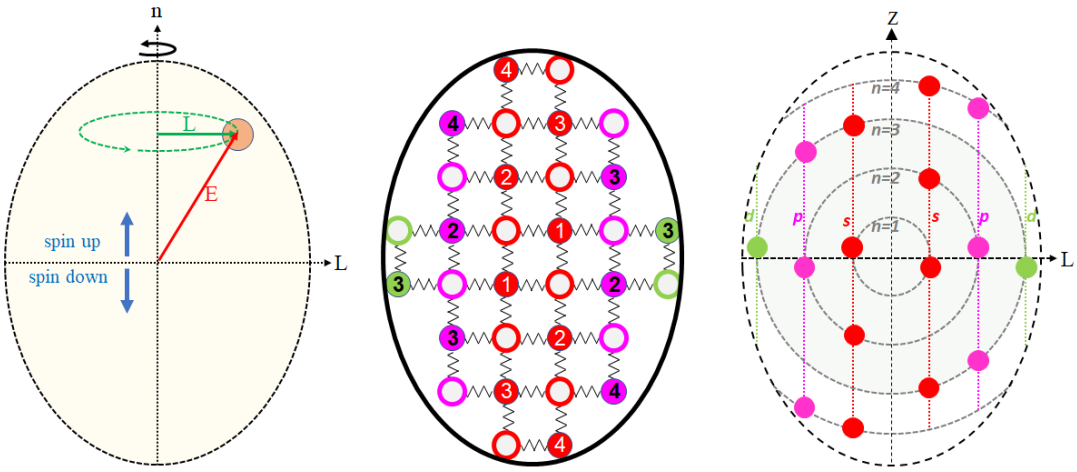
Content

The model at a glance

According to the model these are the shape and properties of the nucleus:

- the nucleus has an ellipsoid shape.
- the nucleon bonds build a cubic system.
- protons are connected to neutrons (**p**-**n**).
- neutrons are connected mainly to protons.
- the protons are populated and organized in shells in the nucleus in analogy to those of the electrons in the atom.
- the energy layers (principal quantum number **n**) grow with the distance from the origin.
- the perpendicular distance from the **z**-axis in the **x**-**y**-plane reflects the angular momentum (**L**, sub-orbitals).
- the upper half of the ellipsoid is referred to as spin-up and the lower part as spin-down.
- the nucleus possibly rotates around its **z**-axis.

The following drawings describe the idea via cross sections in the **x**-**z**-plane of the nucleus.



1: a nucleon in the nucleus *2: the bonds between the nucleons* *3: the energy levels of the nucleus*

1. a nucleon (**circle**) is observed inside the ellipsoid (dashed line) that encloses the nucleons and schematically defines the nuclear surface:
   - the distance from the origin represents its energy **E**.
   - the distance from the **z**-axis depicts it angular momentum **L**.
   - the nucleons in the upper half have spin-up, and in the lower one spin-down.
2. the bonds between the nucleons are shown for visibility as springs.
   - **protons**: full circles of the **s**, **p** and **d** sub-orbitals. **neutrons**: hollow circles.
3. the circles of equal energy states **n** in the ellipsoid.
   - the lines mark the development of the **s**, **p** and **d** sub-orbitals along the **z**-axis.
   - the **s** line crosses all **n** circles from 1 to 4 (**s1** to **s4**).
   - the **p** line begins by **n**=2 and reaches till **n**=4 (**p2** to **p4**).
   - the **d** line begins by **n**=3 and reaches the ellipsoid border, before it reaches the **n**=4 circle, and therefore there are no **d4** states at this stage (only **d3**).

The research

Intramolecular bond vector

Due to the unique pattern of each molecular compound, we assume that the intramolecular bonds are formed by regions of the atom that have a stronger attraction than other regions, and search for such possible regions based on the ellipsoid nuclear model.

From previous studies we postulate the following:

- The structure of the atomic shells corresponds to the nuclear shells.
- Once the outermost nuclear shell is closed, its field does not break through its atomic envelope.
- The chemical attraction is based on the positive electrical attraction that the protons of the outermost nuclear shell exert on the electrons of a neighboring atom.

We conclude that:

- In order to allow chemical bonds, holes in the atomic shell are required, through which the nuclear attraction can act.
- The attraction field is stronger in the plane of the proton orbital, in the direction created from the center of the orbital or of the nucleus to the missing proton.

Bond vector - definition and explanation:

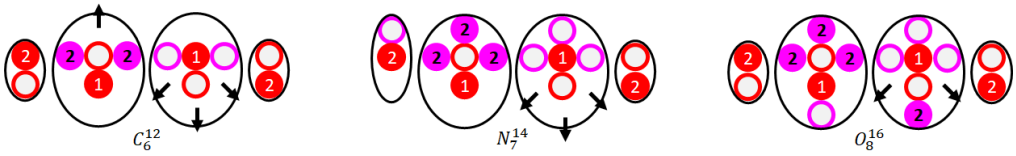
- bond vector: the direction of maximum electric force of the atom.
- the number of bond vectors of an atom equals the number of electrons it is missing to complete its outermost orbital.
- examples: carbon has 4 bond vectors, nitrogen 3 and oxygen 2.

finding the bond vectors

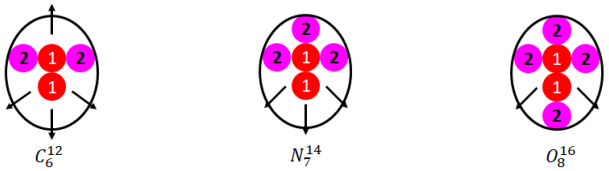
We look for the atomic structure through the structure of the nucleus. We find the nuclear structure that we think is more likely to be the correct one, taking into account:

- the total symmetry of the nucleus.
- the total nuclear spin.
- the angles of the chemical bonds of the element.
- the total nuclear mass, that depends on the number of nuclear bonds.
- in the future we shall check, if the proton configuration is similar to the electron configuration according to Hund's rule. At this stage we mention this, but don't take it into account, while choosing the more probable nuclear configuration.

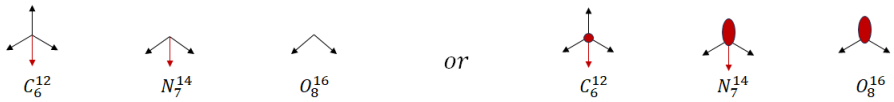
We use the following illustration to describe the nucleus and the bond vectors of the atom.



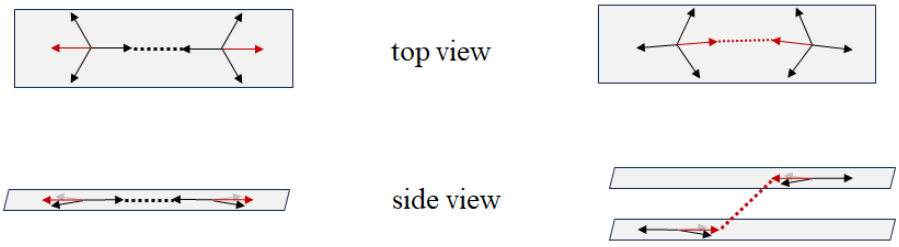
and shorten the above illustration to the following:



or use the following illustrations of the atom:



One bond vector is marked with a different color, to better observe the molecular settings later below. The chemical bonds, no matter of what type (covalent, ionic, metallic), are stronger, when the bond vectors of the atoms involved lie in the same plane and the same direction; the weakest bond occurs, when the planes lie parallel to each other, forcing the bond vectors to be connected in a direction perpendicular to their original direction.
Examples for strong bond vs. weak bond:



strong bond
the vectors lie in the same plane
and are possibly also parallel

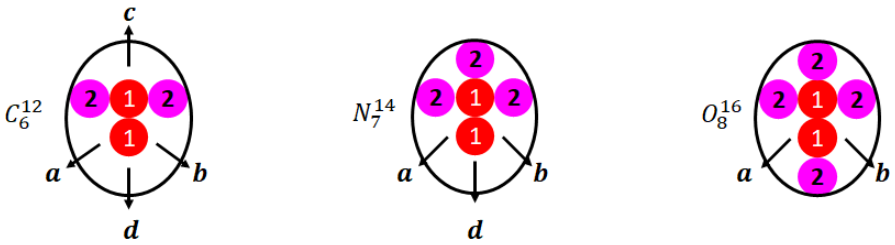
weak bond
the vectors don't lie in the same plane
and are possibly not parallel as well

Calculating the bond angles

After finding the bond vectors we calculate the expected angle between them via the vector product:

$$\cos\alpha = \frac{\boldsymbol{a}\cdot\boldsymbol{b}}{|a|\cdot|b|}$$

We define the vectors **a**, **b**, **c** and **d**, as illustrated here for carbon, nitrogen and oxygen:



The bond vectors are:

	a	**b**	**c**	**d**
x	-1	1	0	0
y	-0.5	-0.5	1.5	-1.5
z	-0.5	-0.5	0.5	-0.5

and the angles between them are thus:

bond vector	**a**	**a**	**a**	**c**
bond vector	**b**	**c**	**d**	**d**
$\cos\alpha$	-0.3	-0.5	0.5	-1.0
α	109.5	121	59	180

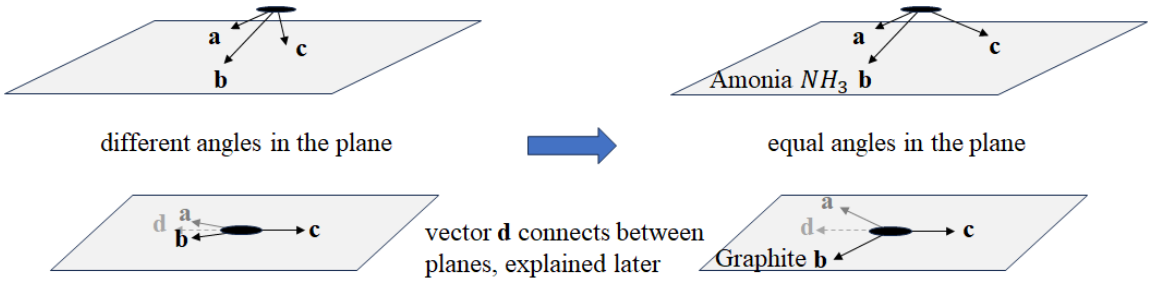
A brief analysis of the table shows the following:

- the water H_2O molecule shall have, according to the model, a bond angle of 109.5°, which is not far from the experimental value of 104.5°, so this strengthen the hypothesis.
- if we sum up the angles, while moving along the vectors $\boldsymbol{a} \rightarrow \boldsymbol{c} \rightarrow \boldsymbol{b} \rightarrow \boldsymbol{a}$ we will get 351.7° and not 360°, which may seem like a contradiction or an error; the reason is, that they don't lie in one plane.

Angles adjustment in the plane

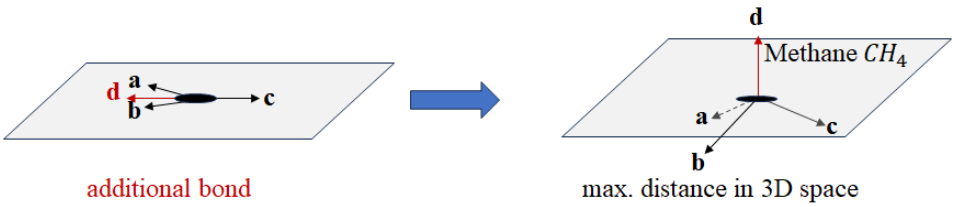
The results for the angles only partially match the experimental data.
For instance for nitrogen in NH_3 the angle between each pair nitrogen-hydrogen bond is about 107° (**a-b**, **a-c**, **b-c** bonds) [10].
The apparent contradiction is eliminated if we assume that the repulsion between all three hydrogen atoms should be the same and that therefore the distances **a-c** and **b-c** increase until they are equal to **a-b** and an equilateral triangle is formed.
A similar situation occurs in graphite, where each carbon atom has three bonds with angles of about 120° between them (**a-b**, **a-c**, **b-c**) [11].
Next illustrations show this for carbon and nitrogen:

Angles adjustment in the plane



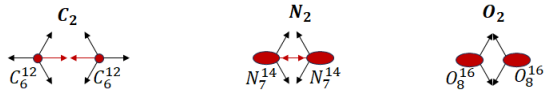
Angles adjustment in the three-dimensional space

Similar to the angle adjustment in the plane, the adjustment takes place in the three-dimensional space.
The adjustment occurs for instance for the methane CH_4, where a carbon atom is connected to four hydrogen atoms; the hydrogen atoms tend to form an equal angle between themselves [12].



The difference between graphite and methane, in this sense, is that in graphite there is no bond vector available for the vector **d** to bound with, so it makes a weak van der Waals bond with a neighboring plane, whereas for methane all carbon bond vectors are equally bound with hydrogen atoms and therefore their distribution in space is with equal distances from each other.

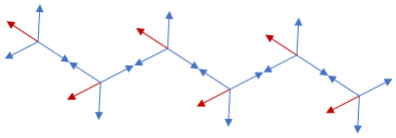
As examples we show the molecules of C_2, N_2 and O_2.
N_2 and O_2 have bond vectors that match each other. In the case of C_2 not all bond vectors are connected, and so additional atoms are expected to bound to it, so the configuration is not expected to be stable.



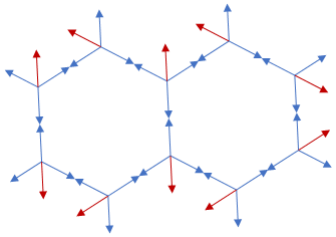
Carbon compounds

The illustrations of the carbon compounds below try to match between the nuclear structure and the atomic and chemical structure.
The angles of the bond vectors are suitable to create the molecules.

Carbon - backbone
In the plane the bond vectors are in about the same direction as their partners, so stronger bonds are expected. Each carbon has two carbon bonds and the other two bond can be with other atoms, like hydrogen for instance, with their bond vector quite parallel and in the same plane, so strong bonds are expected.

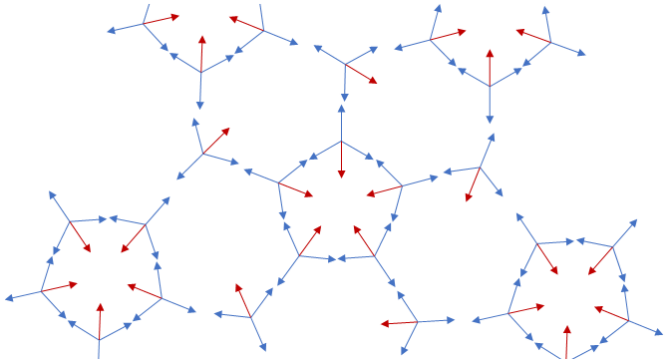


Graphite
In the plane the bond vectors are in about the same direction as their partners, so stronger bonds are expected. Each carbon has one bond vector in the plane, without a partner in its vicinity (marked red); these bond vectors connect between neighboring planes and therefore result in weak (van der Waals) bonds.



Other carbon compounds
In the same manner as for the above examples other carbon compounds like Fullerenes for example can be discussed.

Fullerenes - carbon-60



Discussion of the results and conclusion

The calculation of the bond angles through the positions of missing protons in the nuclear outermost shell seem to deliver good results.
This is not an unequivocal proof of the connection between the cubic ellipsoid nuclear model and the atomic structure, but it is another reinforcement of our hypothesis.

Sources and references

1. *Electronegativity - Wikipedia*
2. *Binding energy - Wikipedia*
3. *Intramolecular force - Wikipedia*
4. *Ionic bonding - Wikipedia*
5. *Covalent bond - Wikipedia*
6. *Metallic bonding - Wikipedia*
7. *Intermolecular force - Wikipedia*
8. *Van Arkel-Ketelaar triangle - Wikipedia*
9. *AP Chemistry Bond Angles and Shapes Flashcards - course-notes*
10. *Ammonia - Wikipedia*
11. *Allotropes of carbon - Wikipedia*
12. *Methane - Wikipedia*
13. *Tetrahedral molecular geometry - Wikipedia*
14. *Diatomic carbon - Wikipedia*
15. *Chemical bonding of water - Wikipedia*
16. *Valence shell electron pair repulsion (VSEPR) theory - Wikipedia*
17. *cubic ellipsoid nucleus - part 1 - the model and its mass formula - Ronen Yavor*
18. *cubic ellipsoid nucleus - atomic physics - part 1 - atomic radius - Ronen Yavor*
19. *cubic ellipsoid nucleus - atomic physics - part 2 - ionization energy - Ronen Yavor*