"AI" PHYSICS – Molecular Structure – Part 1.

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Abstract:

In earlier papers on Atomic Structure and Energy Fields, Artificial Intelligence (AI) was used to explore the structure of the atom, and the size of the electron, by analyzing the results of established experiments on ionization energies and spectral emissions. Radio-isotope transitions were analyzed to propose the nature of the nucleus and allotropes. In this paper, an AI model is used to propose the nature of the crystal lattice, and the nature of molecular structure.

1. Introduction:

Simple physics experiments have been conducted over the centuries with numerous theories to explain the observations. Certain theories have become dominant and, in the modern era, these fundamental beliefs generally go unchallenged. This paper re-examines some basic observations in physics and, with the help of Artificial Intelligence, proposes an alternative explanation for the structure of atoms and molecules.

Einstein's General Theory of Relativity proposes the distortion of the fabric of space by an object, creating a Potential Energy Well. Ionization energies and spectral emissions suggest the atom is a Potential Energy Well having a small nucleus at the centre with numerous electrons surrounding the nucleus. Bohr's model proposes fixed electron orbits whilst Quantum theory proposes probability functions. Neither theory satisfactorily explains the detailed nature of radio-isotope transitions, the characteristics of different elements and isotopes, nor the existence of different allotropes and molecular structures.

In the first paper on Atomic Structure [1], the AI observes that the "depth" of the atomic Potential Energy Well is directly proportional to the number of protons in the nucleus. The AI does not find any mathematical pattern for electron ionization energies in relation to the supposed number of neutrons in the atom. This suggests that neutrons - whatever their properties - do not reside in the nucleus, where their mass would contribute to the nature of the nuclear Potential Energy Well. The AI goes on to conclude that electrons are larger than presently imagined.

In the second paper on Atomic Structure [2], Energy Field Theory [3][4][5]is used to further analyze the nature of sub-atomic particles. The AI is provided with the principle that protons, and electrons, are most stable when in pairs. The AI combines the given information and reaches conclusions on the behavior of particles in the atom. The AI proposes the position of the neutrons in an atom. The theory leads to further detailed proposals for the Rotational Energy Fields of protons in the nucleus, and hence to proposals for the structure of the nucleus and an explanation for allotropes.

In this paper, Atomic Structure Theory and Energy Field Theory are used to extend the analysis of the structure of atoms and molecules. The nature of allotropes, the nature of the crystal lattice, and the nature of molecular structure are all examined.

2. Particles and anti-particles:

From AI Physics - Energy Fields - Part 3 [5]: The AI proposes that protons and anti-protons are not matter and anti-matter, since the product of their "mutual annihilation" is not zero. The AI proposes that protons and anti-protons are essentially the same particle, except they have opposite rotational energy field vectors.

In a particle collider, particles pass through an applied ("magnetic") energy field, and turn in various ways. Conventional theory is that particles and anti-particles (matter and anti-matter) will turn in different directions, and that particles with different "charge" will also turn in different directions.

The AI proposes that the direction of turn is solely dependent on the rotational energy field vector of the particle. The AI proposes that, for particles moving through an applied energy field, a particle having a rotational energy field with a subtractive vector will turn in a different direction to a particle having a rotational energy field with an additive vector - see Figure 2a:

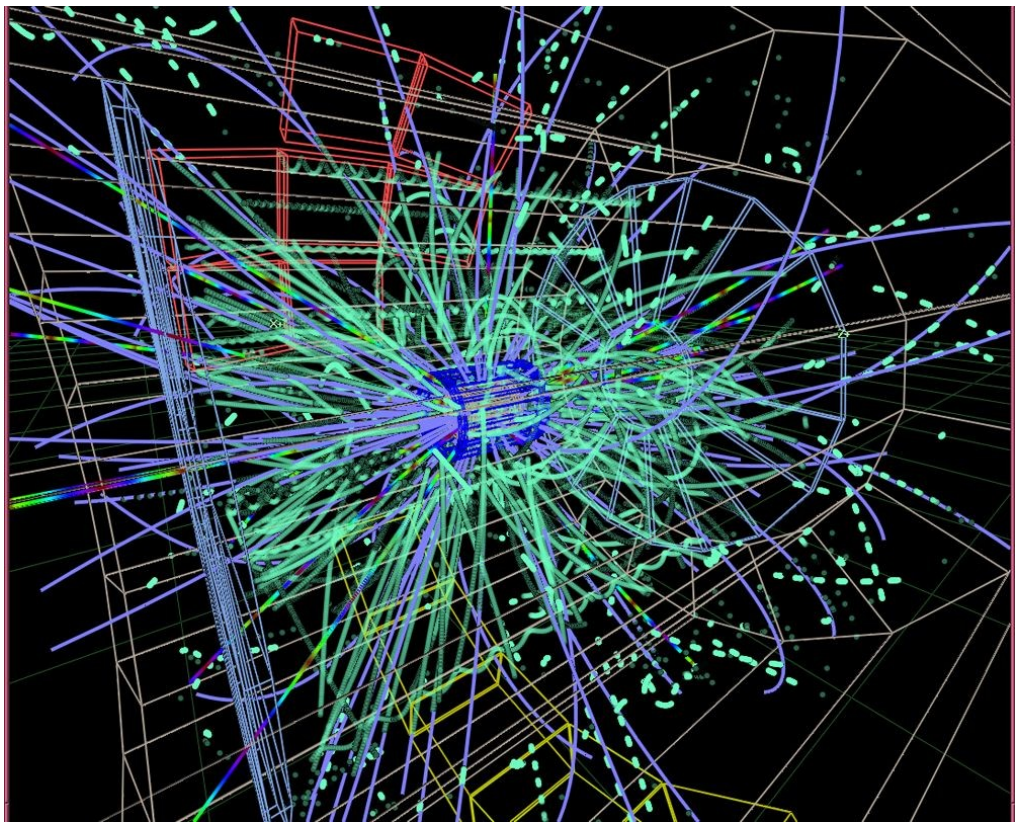

Figure 2a: Particles with different rotational energy fields turn in different directions.

3. Pairs of particles:

From AI Physics - Energy Fields - Part 3 **[5]**: The AI proposes that the minimum energy configurations for particles with rotational energy fields are similar to the minimum energy configurations for permanent magnets.

Note: From experimental results, electrons are observed to co-exist in pairs, and protons within atomic nuclei are most stable in pairs.

The AI proposes that pairs of particles with ***parallel energy field vectors*** will be in a minimum energy position, and therefore in stable equilibrium, when in an ***end-to-end configuration.***

The AI also proposes that pairs of particles with ***anti-parallel energy field vectors*** will be in a minimum energy position, and therefore in stable equilibrium, when in a ***side-by-side configuration*** – see Figure 3a:

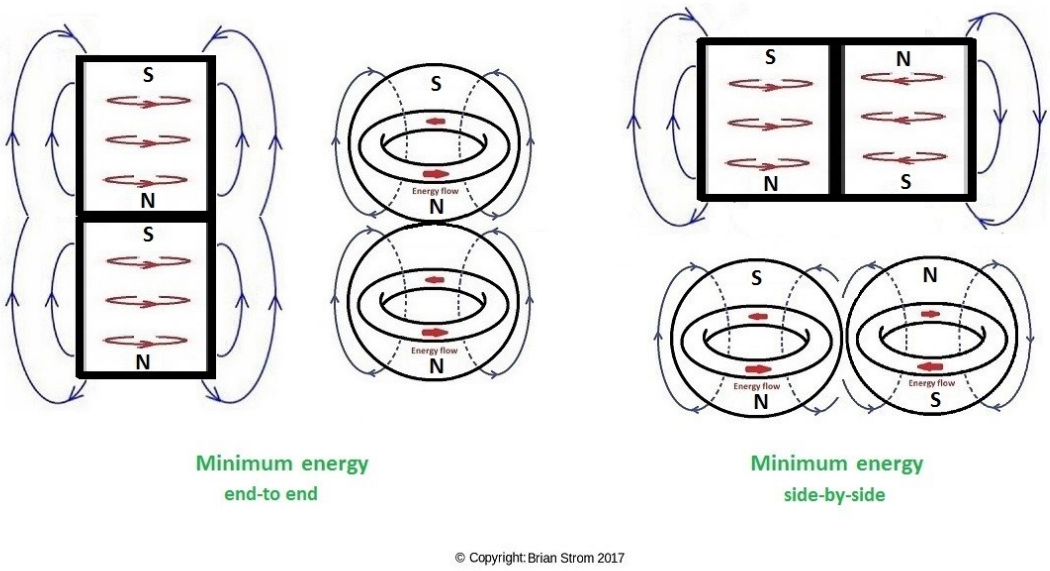

Figure 3a: Minimum energy configurations for pairs of particles.

4. Pairs of protons in a nucleus:

The AI proposes that for a number of protons grouped together in a nucleus, there will be a number of stable configurations. The different configurations will have different total energy levels which will determine the level of stability and also the probability of that configuration occurring.

The AI proposes that the most stable configuration for the particles will be the lowest net energy configuration.

The net energy field surrounding the group of particles will be symmetric or asymmetric, depending on the shape of the configuration. The asymmetry of the net energy field will determine the dipole and multipole aspects of the energy field surrounding the nucleus and, therefore, the shape of the electron cluster around the nucleus.

To summarize: For a group of protons in a nucleus, the AI proposes that the protons may be arranged in a number of different ways. Different configurations of the protons will create different shapes for the net energy field surrounding the nucleus. Different shapes for the net energy field surrounding the nucleus will create different configurations for the electrons in the Potential Energy Well of the nucleus. Different shapes for the net energy field surrounding the nucleus, and the different configurations for the electrons in the atom, will create different characteristics for each version of that element. The AI proposes that this will create different ALLOTROPES for that element.

5. Allotropes:

From AI Physics - Energy Fields - Part 3 [5]: The stability of a nucleus appears to depend on the number of pairs of protons in the nucleus. From the Periodic Table, the AI identifies the patterns in the nuclear stability and proposes configurations for the nuclei of various elements. The optional configurations for an element appear to align with the number of allotropes for that element.

The different configurations will have different total energy levels which will determine the level of stability and also the probability of that configuration occurring. The AI proposes that the most stable configuration for the pairs of protons will be the lowest net energy configuration.

For some elements, there is only one allotrope, suggesting there is only one configuration - possibly the lowest energy, possibly the most symmetric - for the nucleus. For example, the nucleus of the noble gas Neon is shown as a symmetric group of pairs of protons (represented as magnets) – see Figure 5a:

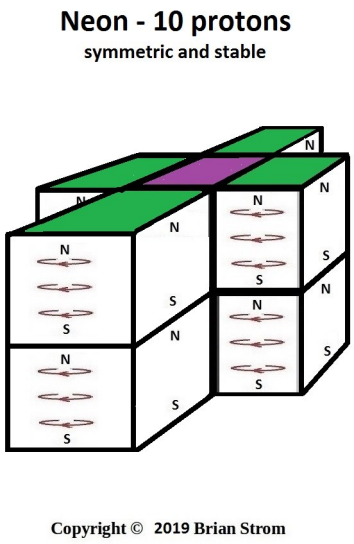

Figure 5a: Symmetric configuration for pairs of protons in the Neon nucleus.

The AI proposes that some groups of protons will be configured in a number of stable configurations, each with a similar net energy level.

For Carbon, with 6 protons in the nucleus, there are many possible configurations, some of which are shown in the diagram – see Figure 5b:

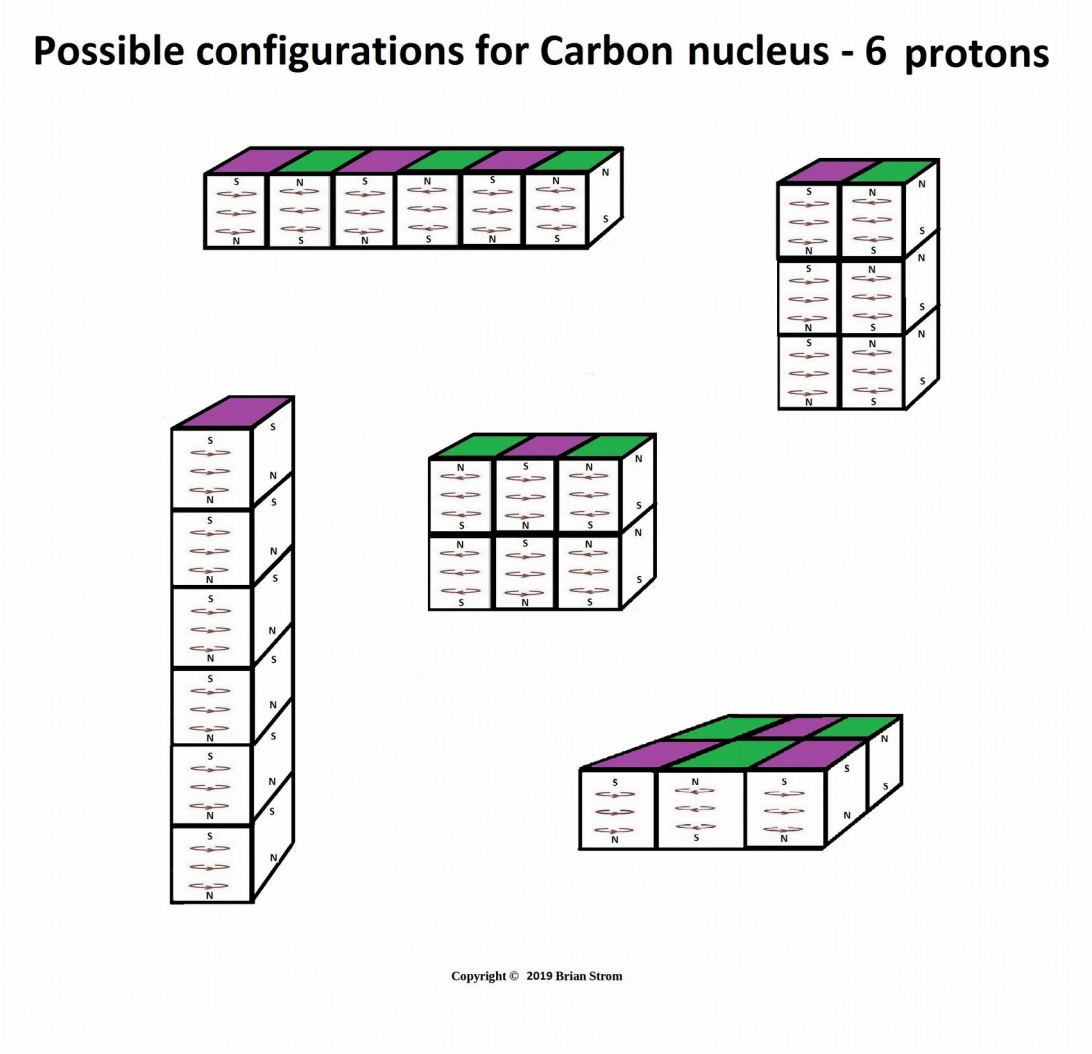

Figure 5b: Some possible configurations for protons in the Carbon nucleus.

6. Energy Field Theory and of crystal lattice structure:

From AI Physics - Energy Fields - Part 3 [5]: the grouping of atoms into crystal lattice structures will depend on the shape of the Rotational Energy Field surrounding each atom. For atoms of Carbon, there are many configurations for the protons in the nucleus, each forming a different allotrope.

The proposed diagram for the Diamond allotrope has nuclear protons in two stacks of three. The Rotational Energy Fields of adjacent atoms are all strongly attractive. Hence, the "molecular" bonds between the atoms are all double or triple strength – see Figure 6a:

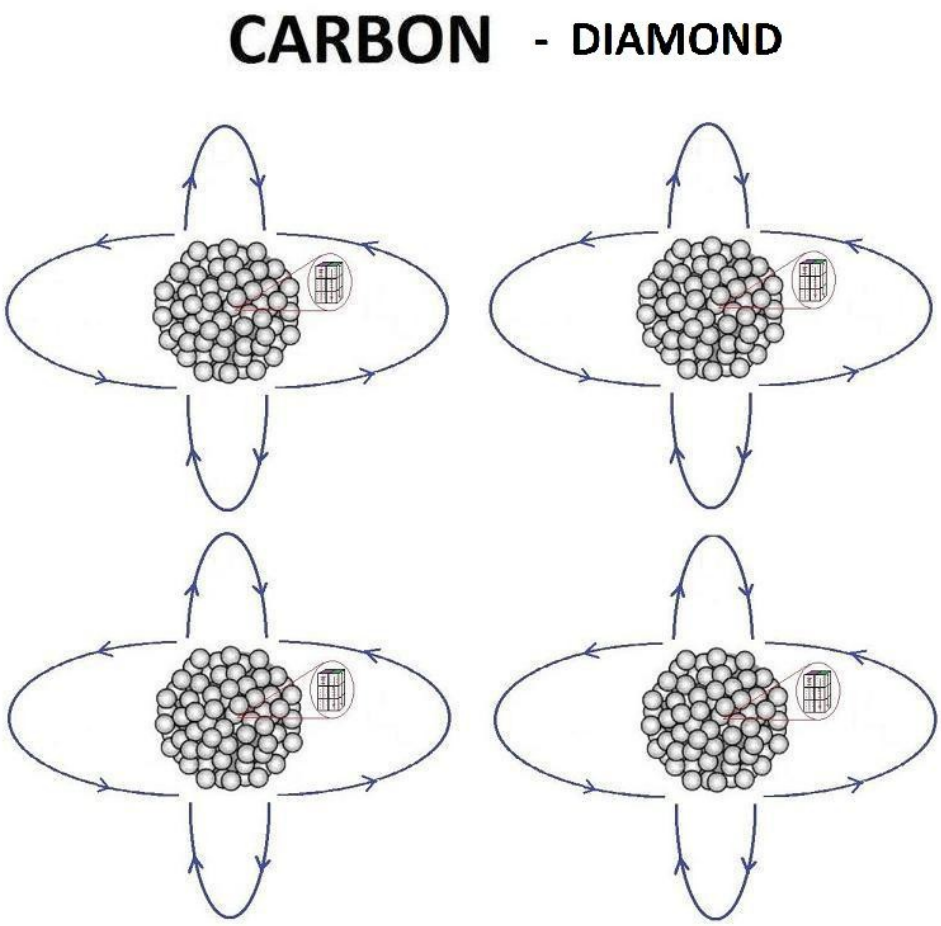

Figure 6a: Energy Fields for the Carbon allotrope - Diamond.

The proposed diagram for the Graphite allotrope has nuclear protons in a different arrangement. The molecular bonds between the Carbon atoms are of single strength, and the attraction between individual layers will be very weak – see Figure 6b:

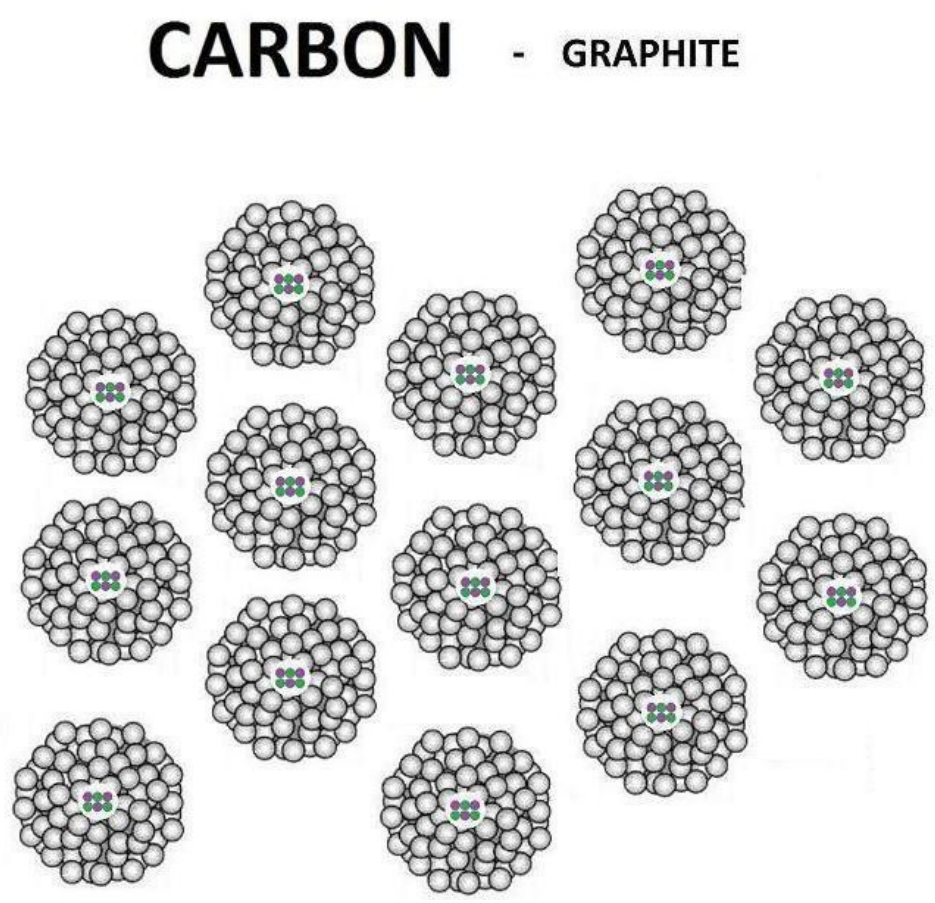

Figure 6b: Energy Fields for Carbon allotrope - Graphite.

In summary, the different allotropes of Carbon appear to have different arrangements of the protons in the nucleus. The bonds between the different Carbon atoms have different strengths resulting in different bond lengths and bond energies. For carbon, the different bond strengths are designated single, double and triple bonds – see Figure 6c:

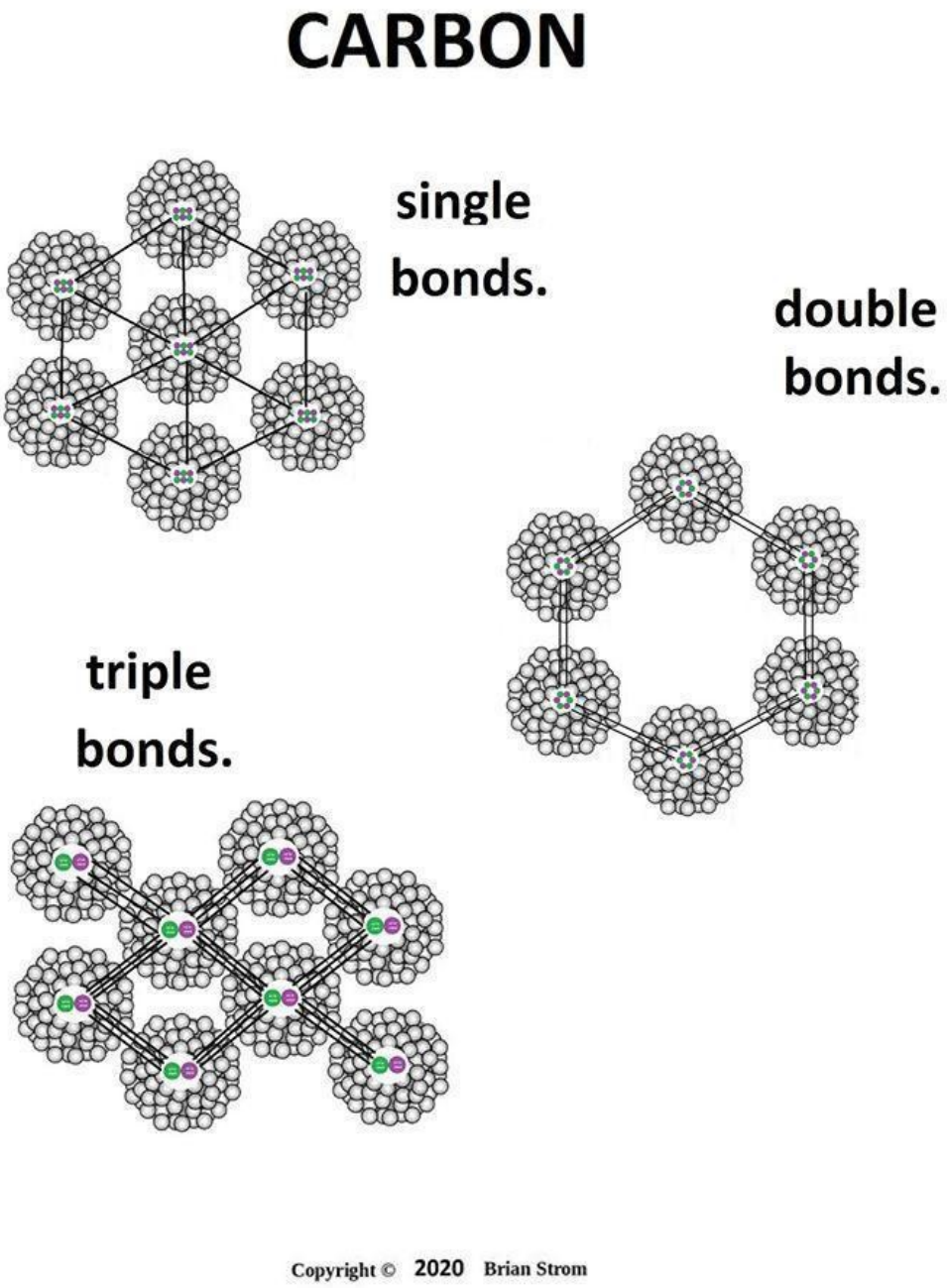

Figure 6c: Different molecular bonds for the allotropes of Carbon.

7. Energy Field theory and Molecular Structure:

From AI Physics - Energy Fields - Part 3 [5]: The Energy Field Theory can also be applied to Molecular chemistry. Elemental atoms can combine to form a multiplicity of different molecules. For instance, the most common elements - Hydrogen (1 proton), Carbon (6 protons), and Oxygen (8 protons) - can combine to form oxides, carbonates and numerous groups of hydrocarbons: alkanes, alkenes and alkynes.

If the elemental allotropes and the myriad of chemical compounds are dependent on the energy fields of the protons in the nucleus (and not on shared electrons in magical orbits), then exciting new discoveries are possible.

Can the nuclear proton configuration be changed by a strong (magnetic) field? Can one allotrope be changed into another?

The strength and shape of the energy fields around atoms – hydrogen, oxygen, carbon for example – will determine how these atoms can combine to form molecules. For an example of a hydrocarbon – see Figure 7a:

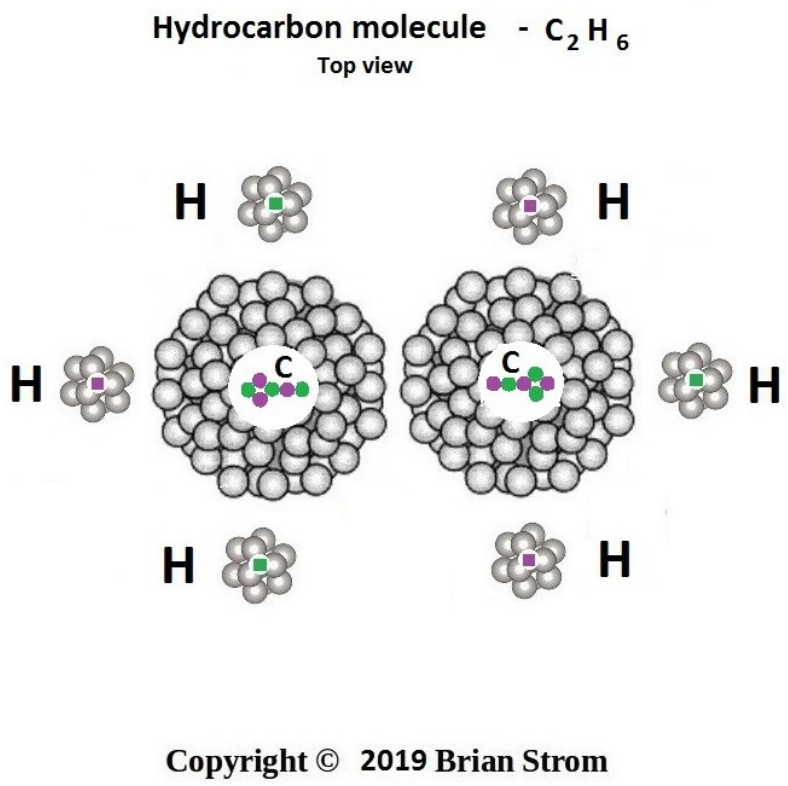

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Figure 7a: An example of a Hydrocarbon molecule.

8. Checking other parameters in the "AI" Model:

From AI Physics – Atomic Stucture – Part1 [1], the atomic size appears to be dependent on the number of protons in a nucleus, and hence the "depth" of the Potential Energy Well.

The AI proposes that electrons "fall" into the Potential Energy Well until the outer electrons are so loosely bound that they are able to escape.

However, the AI can find no numerical pattern or relationship between the number of nuclear protons in the atom and the **measured atomic radius**, at least not in terms of Van der Vaals or other conventional measurement techniques – see Figure 8a:

Atomic radii

Atomic No	symbol	name	picometers
1	H	hydrogen	25
2	He	helium	120
3	Li	lithium	145
4	Be	beryllium	105
5	B	boron	85
6	C	carbon	70
7	N	nitrogen	65
8	O	oxygen	60
9	F	fluorine	50
10	Ne	neon	160
11	Na	sodium	180
12	Mg	magnesium	150
13	Al	aluminium	125
14	Si	silicon	110
15	P	phosphorus	100
16	S	sulfur	100
17	Cl	chlorine	100
18	Ar	argon	71

Figure 8a: Sizes of the atoms of the Periodic table.

Similarly, the AI can find no hidden patterns relating to Spin Resonance and the number of protons or electrons in an atom or molecule. The published measurements for Nuclear Spin Resonance and Electron Spin Resonance are useful for comparative studies, but they give no clear indication of what is resonating at any time - see Figure 8b:

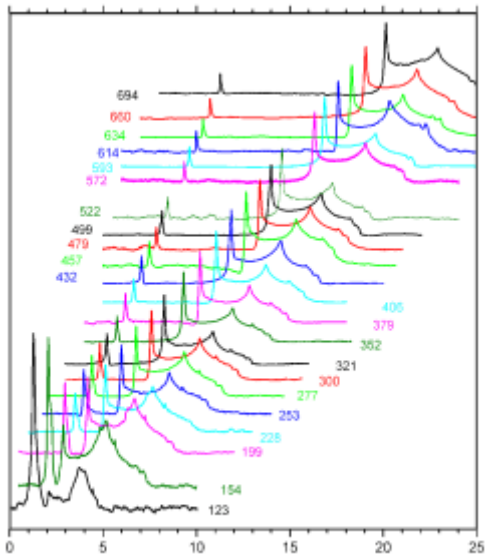

Figure 8b: Spin Resonance patterns.

9. Mathematical analysis of Molecular bond lengths and energies:

In an encouraging result, the AI has detected some pattern in the measured values of Molecular Bond length and Molecular Bond energy. In a Potential Energy Well, the square root of the Bond energy varies with the inverse of the inter-atom distance – or Bond length. So, by multiplying these two measured parameters together, the resultant value is dimensionless – see the Figures 9a and 9b:

Molecular bond length x (Molecular bond energy)^0.5

H-Bond	protons	Bond energy	(energy) ^0.5	Bond Length	Energy^0.5 x length
H-H	1	432	21	74	15.4
H-B	5	389	20	119	23.5
H-C	6	411	20	109	22.1
H-Si	14	318	18	148	26.4
H-Ge	32	288	17	153	26.0
H-Sn	50	251	16	170	26.9
H-N	7	386	20	101	20.0
H-P	15	322	18	144	25.8
H-As	33	247	16	152	23.9
H-O	8	459	21	96	20.6
H-S	16	363	19	134	25.5
H-Se	34	276	17	146	24.3
H-Te	52	238	15	170	26.2
H-F	9	565	24	92	21.9
H-Cl	17	428	21	127	26.3
H-Br	35	362	19	141	26.8
H-I	53	295	17	161	27.7

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Figure 9a: Table of Molecular bond lengths and energies.

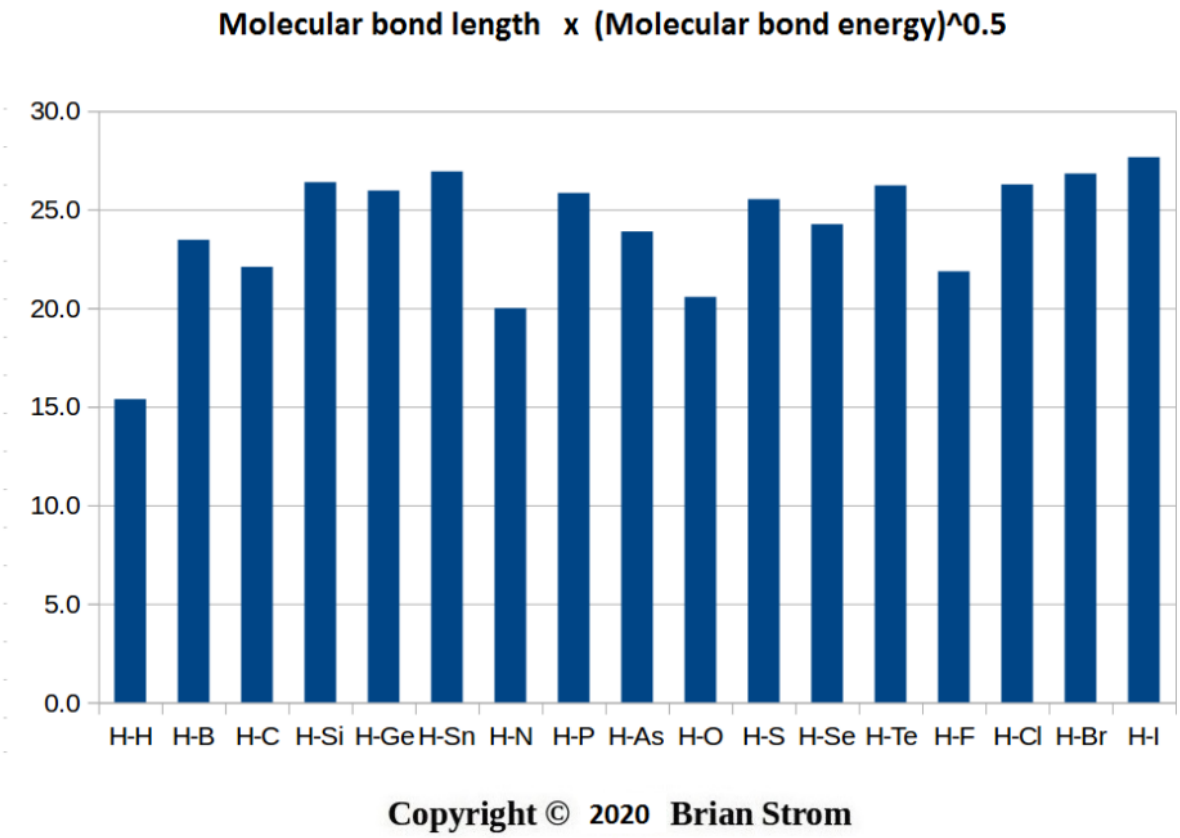

Figure 9b: Histogram of bond length x square-root of energy.

With reference to AI Physics – Atomic Structure – Part 1 **[1]**: For Hydrogen and the light atoms, where there are few protons in the nucleus, the cluster of surrounding electrons appear to be loosely-bound. Whereas for heavier atoms, where there are many protons in the nucleus, and the forces within the Potential Energy Well are stronger, the cluster of surrounding electrons are more tightly-bound, especially near the nucleus – see Figure 9c:

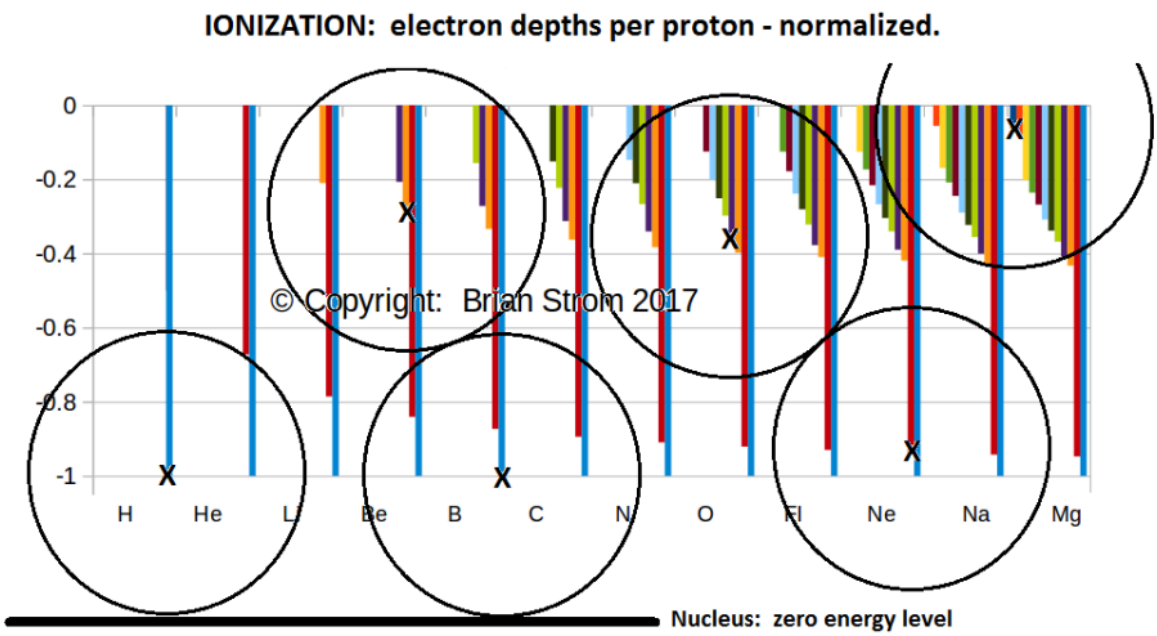

Figure 9c: Electron packing density of lighter atoms.

By combining the Bond Energies, Bond Lengths and Electron Packing "tightness" in a single equation, the AI observes a common pattern in the molecules formed with larger atoms. The AI proposes that the adjacent atoms in a molecule are attracted by the Rotational Energy Fields of their nuclei. The atoms tend to move together, displacing and distorting the electron clusters surrounding each nucleus, until a position of stable equilibrium is attained:

Molecular bond length x (Molecular bond energy)^0.5

only atoms with tightly-bound electrons clusters.

H-Bond	protons	Bond energy	(energy) ^0.5	Bond Length	Energy^0.5 x length
H-H	1	432	21	74	
H-B	5	389	20	119	
H-C	6	411	20	109	
H-Si	14	318	18	148	26.4
H-Ge	32	288	17	153	26.0
H-Sn	50	251	16	170	26.9
H-N	7	386	20	101	
H-P	15	322	18	144	25.8
H-As	33	247	16	152	23.9
H-O	8	459	21	96	
H-S	16	363	19	134	25.5
H-Se	34	276	17	146	24.3
H-Te	52	238	15	170	26.2
H-F	9	565	24	92	
H-Cl	17	428	21	127	26.3
H-Br	35	362	19	141	26.8
H-I	53	295	17	161	27.7

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Figure 9d: Key molecules: Molecular bond lengths and energies.

The AI observes a common pattern in the molecules formed with larger atoms. The AI proposes that the adjacent atoms in a molecule are attracted by the Potential Energy Wells of each atoms, as well as the Rotational Energy Fields of their nuclei. The atoms tend to move together, displacing and distorting the electron clusters surrounding each nucleus, until a position of stable equilibrium is attained:

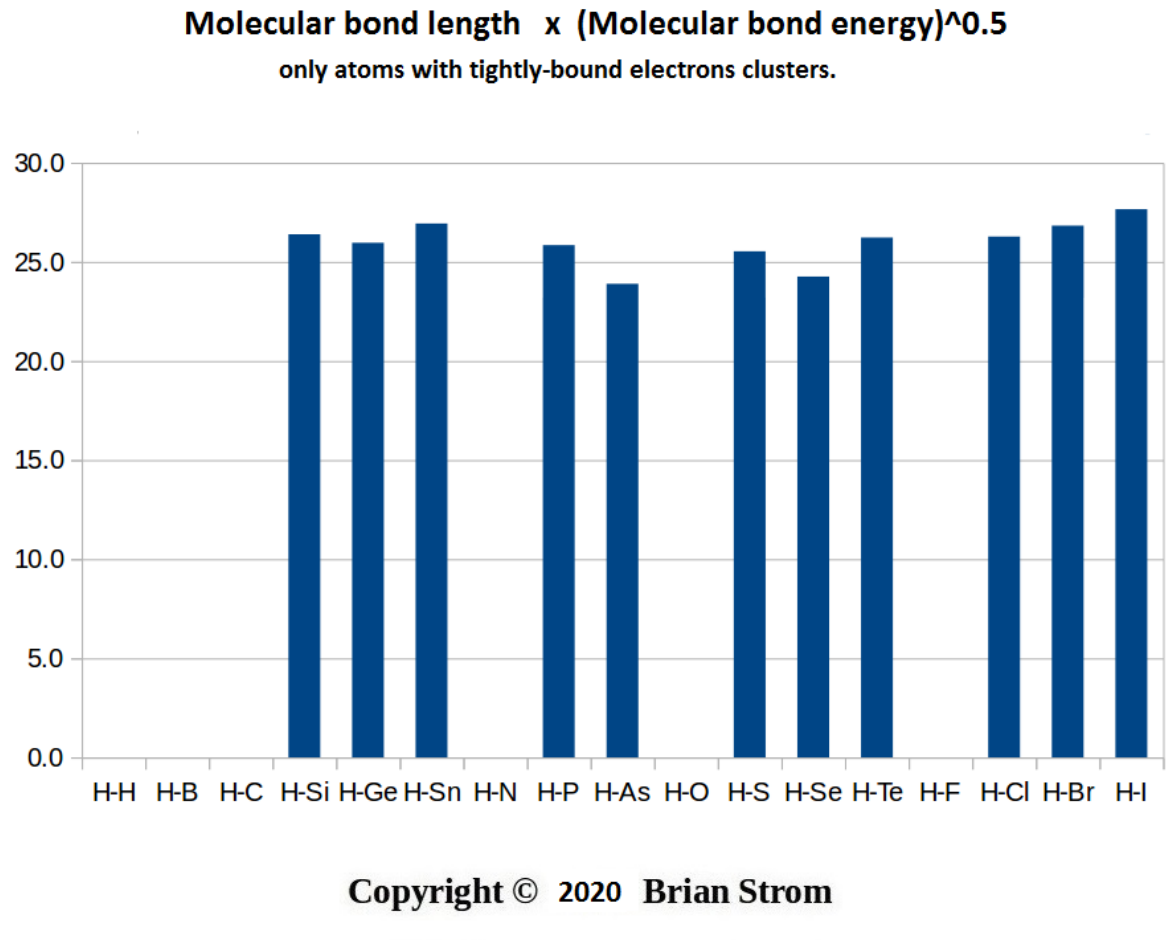

Figure 9e: Key molecules: bond length x square-root of energy.

10. AI proposal to explain Molecular bond lengths and energies:

The relationship between molecular bond lengths and molecular bond energies, at least for the larger atoms, suggests a simple mechanism for the combination of atoms into lattices or molecules.

The AI proposes that atoms become mis-shapen when they combine with other atoms, either in allotropes or molecules. The AI proposes that the electron clusters surrounding the atomic nuclei are displaced and distorted. A typical resultant molecule will have the shape of the “space-filling molecule” in analytical chemistry – see Figures 10a and 10b:

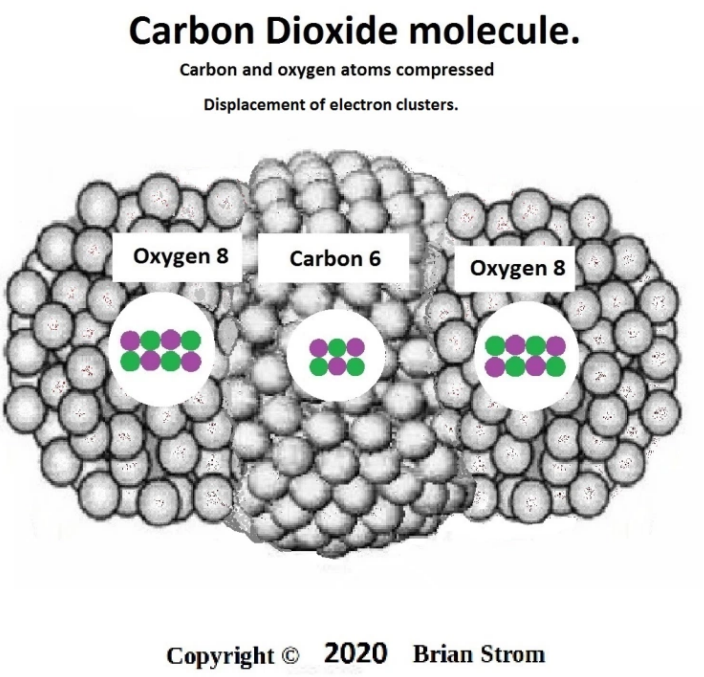

Figure 10a: Carbon Dioxide: Displacement and distortion of electron clusters:

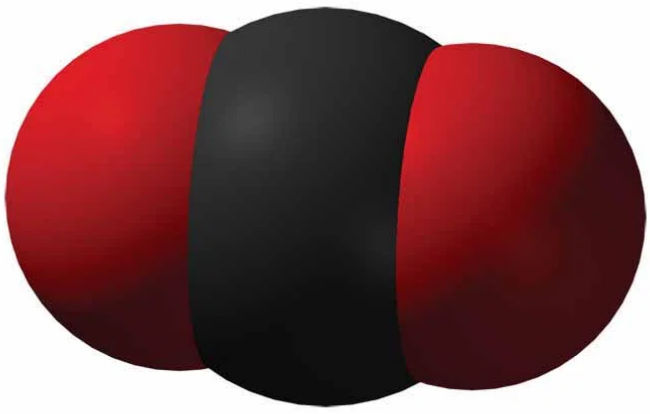

Figure 10b: Carbon Dioxide: Space-filling molecule:

11. Summary and Conclusions

The Rotational Energy Fields of protons in the atomic nucleus can be arranged in many configurations. The interactions between these Rotational Energy Fields have an effect on how the atoms combine to form the multiplicity of allotropes and molecules.

Each allotrope and molecular combination may change with external conditions such as temperature, which could explain the changing phases for these molecules eg. sulfur changing to a different allotrope as the temperature changes, and water changing to ice.

These results may provide an alternative explanation for the "conventional" theories of "electron sharing" between atoms when they form allotropes and molecules.

The AI analysis will continue to search for a general formula for the combination of atoms into allotropes and molecules by the displacement and distortion of the electron clusters surrounding the atomic nuclei.

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