A New Derivation of Structural Isomers of Straight Chain Alkanes

Alfred Addo-Yobo

***Abstract*—**Structural isomers are very important due to their different properties. The structural isomers of light weighted straight chain alkanes such as pentane, hexane and butane are easy to derive, as they contain fewer number of carbon atoms. With easy substitution of one or more hydrogen atoms with one or several alkyl groups on specific carbons, different forms of the same compound can be determined. This conventional module of alkyl and hydrogen groups substitution to derive structural isomers, though efficient, may require thorough check up of substituent positions on specific carbons to ensure that, non-permissible structures are not listed. This procedure gets cumbersome when dealing with straight chain alkanes of higher carbon numbers. In this paper, we introduce a new technique by which all possible structural isomers of any straight chain alkane whatsoever can be derived, by a number combination theory as well as introduce three new postulates that validates a compound as being a structural isomer of a particular straight chain alkane or not and eliminates all non-permissible structural isomers from a possible list.

***Keywords*—**Structural isomers, straight chain alkanes, substituent, carbon atoms, new derivation, postulates.

I. Introduction

STRUCTURAL Isomers, being different forms of the same compound as stated in ''Chemistry Unlimited'', Pg. 223, may contain substituents on specific carbons which could be in the form of any alkyl group, whether methyl, ethyl, butyl, etc. However, the new derivation to be discussed is valid for structural isomers containing only methyl groups as substituents. The postulates to be introduced were invented through careful investigation and observation of all structural isomers of few straight chain alkanes and by this, a convenient pattern established.

The postulates can enable anyone spot all permissible structural isomers of any straight chain alkane as well as serve as basis for disqualifying a compound as a structural isomers of a particular straight chain alkane. For any compound to pass as a structural isomer of a particular straight chain alkane, it must not contradict or violate any of the postulates to be introduced.

II. Postulates Of Structural Isomers Of Straight Chain Alkanes

The limit to single locant number structural isomers is n/2 for even carbon number straight chain alkanes and ½ (n-1) for odd carbon number straight chain alkanes where ''n'' is the number of carbon atoms of straight chain alkane.

Alfred Addo-Yobo, Alquad Education, Accra, Ghana. (Email ID alfaddoyobo89@gmail.com)

Structural isomers usually come with certain numbers preceding the substituents which are known as locant numbers as stated in Wumbee Books, pg. 105. The attached numbers which show the position of substituents on a specific carbon atom may appear as single, double, triple or any number of number combinations.

Examples of single locant number structural isomers are 2 methyl pentane, 3 methyl pentane. Double locant number structural isomers could be 2, 3 dimethyl hexane, 3, 4 dimethyl octane or sometimes triple numbers such as 2, 3, 4 trimethyl nonane or 2, 2, 5 trimethyl decane. The first postulate specifically provides restrictions to the number and list of single number locant number structural isomers of any straight chain alkane.

If a compound with a single methyl group as substituent is proposed to be a structural isomer of a particular straight chain alkane, it must not contradict or violate this first postulate in order to pass as a structural isomer of the straight chain alkane under consideration.

Let's take a quick example; In order to list the structural isomers of the straight chain alkane "hexane", it's important to note that there may be present different forms. Since hexane is an even carbon numbered straight chain alkane with a carbon number of 6, according to the first postulate, "if a straight chain alkane contains an even number of carbon atoms, the limit to single number locant numbers is n/2 where "n" is the number of carbon atoms of hexane.

Bearing in mind that this new derivation applies to methyl groups as the only substituents on the structural isomer, the limit to the list of structural isomers of hexane which contain single number locant numbers is $6/2 = 3$.

This means that with methyl groups as the only substituent, the structural isomers of hexane with single number locant numbers are 2 methyl pentane and 3 methyl pentane. Considering an odd carbon numbered straight chain alkane such as "nonane" with a carbon number of nine, the list of structural isomers with single locant numbers will have a limit, according to the first postulate $½ (9 – 1) = 4$. Therefore, the list of single number locant number structural isomers of nonane are 2 methyl octane, 3 methyl octane, 4 methyl octane. If the first postulate of structural isomers is properly understood, it infers that, the compound 7 methyl undecane is not a structural isomer of dodecane. This is because, dodecane

is a straight chain alkane with a carbon number of 12 which is even, thus per the first postulate, the limit to single number locant number of structural isomers is n/2 = 12/2 = 6. Since the limit to the single number locant number is 6, it means 7 methyl undecane is qualified as a structural isomer of dodecane.

NB: For a compound to pass as a structural isomer of a particular straight chain alkane, the sum of carbon numbers of the alkane in the isomer and the substituent must equal the carbon number of straight chain alkane under consideration.

No locant number of a structural isomer must equal to or be greater than the carbon number of the alkane in the isomer.

According to this postulate, no structural isomer should have any of its locant numbers correspond to or greater than the carbon number of alkane in the isomer. For example, the compound 2, 2, 3 trimethyl propane cannot pass as a structural isomer of any straight chain alkane.

This is because, it violates the second postulate. Since, one of the locant numbers, "3" corresponds to the carbon number of the alkane (propane, which has a carbon number of three (3) in the structural isomer. This postulate will disqualify 2, 5 dimethyl pentane as an isomer of heptane because the locant number "5" which corresponds to the carbon number of the alkane (pentane, which has a carbon number of "5" in the isomer.

For structural isomers with only two locant numbers, both numbers must not sum up to the carbon number of the parent straight chain alkane carbon number

Plausible structural isomers of hexane could be 2, 4 dimethyl butane or 3, 3 dimethyl butane. However, the question usually would be, do these compounds pass as structural isomers of the straight chain alkane under consideration?

If any compound violates any of the postulated statements, it fails to pass as a structural isomer of a straight chain alkane. The compounds stated above are 2, 4 dimethyl butane and 3, 3 dimethyl butane do not pass for isomers of hexane because they contain only two locant numbers which sum up the carbon number of straight chain alkane under consideration (hexane) which also has a carbon number of six (6).

This postulate will also disqualify the compounds 3, 4 dimethyl pentane and 2, 5 dimethyl pentane as valid structural isomers of the straight chain alkane, heptane. The reason being that, the above compounds consists of only two locant numbers whose sum equal "7" which is equal to the carbon number of the straight chain alkane under consideration, heptane. As the carbon number of straight chain alkanes increases, it sometimes becomes increasing difficult for many to derive structural isomers. The conventional method of replacing hydrogen atoms with methyl groups on various carbon atoms is excellent but time consuming as carbon number of straight chain alkanes increase.

I invented a new technique for deriving all structural isomers of straight chain alkanes with only methyl groups as substituents. This technique involves laid down procedures which results in the development of several plausible structural isomers and then application of the three postulates earlier discussed to reveal the compounds that pass as structural isomers of particular straight chain alkanes.

III. New Technique For Deriving Structural Isomers Of Straight Chain Alkanes

A characteristic feature of structural isomers is that they consists combination of locant numbers. When these combinations are wrong, the compound does not qualify as a structural isomer.

We shall now discuss a method by which all possible locant numbers of structural isomers can be derived, thereafter, the three postulates introduced above will help eliminate the invalid isomers leaving us only with permissible structural isomers. It must be noted that all discussions are on the premise that methyl groups as the only substituents present in structural isomers.

In a problem where one is to list all structural isomers of a particular straight chain alkane, the carbon number of the straight chain alkane under consideration must be known. We shall employ the straight chain alkane "octane" for our discussions into revealing the new technique for deriving all possible structural isomers of any straight chain alkane. Firstly, it must be known that octane has a carbon number of eight. The next step is to list the number from 2, 3, 4, 5…… n, where "n" is the carbon number of straight chain alkane under consideration. The straight chain alkane under consideration, octane contains eight carbon atoms, meaning that we shall list the numbers 2, 3, 4, 5, 6, 7, 8.

After these numbers are listed, all possible number combinations that sum up to each of the numbers listed with the number "1", excluded from the possible number combinations is noted. The possible locant of structural isomers will thus be each of the listed numbers together with the possible number combinations that sum up to each of the listed numbers.

NB: Two key points must be noted; the number "1" must not be included in the possible number combination of listed numbers and also no single number can appear more than two times in a possible number combination. Let's now take each of the listed numbers (2, 3, 4, 5, 6, 7, 8) and find all possible number combinations that sum up to each of the listed numbers as shown in the table below;

TABLE I
LIST OF NUMBERS

2	
3	
4	(2, 2)
5	(2, 3)
6	(2, 4) , (3, 3)
7	(2, 5) , (3, 4) , (2, 2, 3)
8	(2, 6) , (3, 5) , (4, 4) , (2, 2, 4) , (2, 3, 3)

The above table shows the list of numbers (left) from 2, 3, 4, 5…., n where "n" is the carbon number of straight chain alkane under consideration and the possible number combinations (right) of each of the listed numbers. The numbers on the left and the right hand side of the table above constitute all possible locant numbers of structural isomers of the octane.

As shown in the table above, there are no possible combinations of numbers that sum up to the numbers 2 or 3. This is because, there are no possible combinations of numbers that sum up to 2 or 3 without including the number "1" which must be an exception to all number combinations. The possible combinations that sum up to "3" are (1, 2) and for the number "2", we have (1, 1). The combinations will not pass for possible combinations since they include the number "1" which must be an exception.

The possible number combinations consists of single number, double number as well as triple numbers which represent the locant numbers of the structural isomers of octane. We can now confidently write down the various structural isomers of octane, bearing in mind the only allowable substituents per the technique discussed are methyl groups. The possible structural isomers of octane are; ***2 methyl heptane, 3 methyl heptane, 4 methyl heptane, 5 methyl heptane, 6 methyl heptane, 7 methyl heptane, 8 methyl heptane, 2, 2 dimethyl hexane, 2, 3 dimethyl hexane, 3, 3 dimethyl hexane, 2, 4 dimethyl hexane, 2, 5 dimethyl hexane, 3, 4 dimethyl hexane, 2, 2, 3 trimethyl pentane, 2, 6 dimethyl hexane, 3, 5 dimethyl hexane, 4, 4 dimethyl hexane, 2, 2, 4 trimethyl pentane, 2, 3, 3 trimethyl pentane***. The compounds seen above are possible structural isomers of the straight chain alkane, octane. When you have a number combination consisting of three numbers such as (2, 3, 3), we say a trimethyl and two numbers, a dimethyl and so on.

NB: One must always ensure that the sum of the carbon number of alkane in the isomer and the number of methyl groups as substituents must equal the carbon number of straight chain alkane under consideration. We will now apply the three postulates earlier discussed to rule out the non-permissible structural isomers of octane. We shall apply the first postulate which states that "*the limit to single number locant numbers of structural isomers is n/2 for even carbon numbered straight chain alkanes and ½ (n – 1) for odd carbon numbered alkanes where "n" is the carbon number of straight chain alkane under consideration*" to eliminate the non-permissible structural isomers containing single number locant numbers. Since octane is an even carbon numbered alkane with a carbon number of eight (8), the limit to its single number locant number structural isomers is n/2 = 8/2 = 4. If the limit is 4, then from the list above, the non-permissible structural isomers with single number locant numbers are 5 methyl heptane, 6 methyl heptane, 7 methyl heptane, 8 methyl heptane. Applying the second postulate, we can eliminate 3, 5 dimethyl hexane, 2, 6 dimethyl hexane, 4, 4 dimethyl hexane from the list since these proposed structural isomers consists of only two locant numbers that sum up to the carbon number of the straight chain alkane under consideration. 2, 6 dimethyl hexane even violates the third postulate since one of the locant numbers, "6" corresponds to the carbon number of alkane (hexane) in the isomer. The rest of the proposed structural isomers which consists of three locant numbers, 2, 2, 4 trimethyl pentane, 2, 3, 3 trimethyl pentane and 2, 2, 3 trimethyl pentane do not violate any of the postulates and thus pass as permissible structural isomers of octane. This means that the permissible structural isomers with methyl groups as the only substituents *are **2 methyl heptane, 3 methyl heptane, 4 methyl heptane, 2, 2 dimethyl hexane, 2, 3 dimethyl hexane, 3, 3 dimethyl hexane, 2, 4 dimethyl hexane, 2, 2, 3 trimethyl pentane, 2, 2, 4 trimethyl pentane and 2, 3, 3 trimethyl pentane.***

IV. Capabilities Of The Three Postulates

- Ability to validate a compound with methyl groups as the only substituents as a structural isomer of a particular straight chain alkane.
- Ability to validate a branched chain alkane with methyl groups as the only substituents as an existing compound.

This means that for branched chain straight chain alkanes with methyl groups as the only substituents, the three postulates are capable of validating them as permissible compounds or not. If any such branched chain alkane violates any of three postulates, it's disqualified as a compound. Also, for any compound with methyl groups as the only substituents to qualify as a structural isomer of a particular straight chain alkane, it must not violate any of the three postulates.

V. Summary And Conclusion

Just as there are the rules governing the filling the electrons into orbitals where the electronic configuration of an element could be deemed as wrong when it violates any of the three rules, the Aufbau's rule, Hund's rule of maximum multiplicity and Pauli's exclusion principle. Similarly, the three postulates earlier introduced are proposed to govern structural isomers of straight chain alkanes with methyl groups as the only substituents. These postulates are capable of either passing or disqualifying a compound as a structural isomer of a particular straight chain alkane. If a compound violates any of the rules, it's disqualified as a structural isomer of a straight chain alkane. When structural isomers of a straight chain alkane are to be derived, the carbon number of the straight chain alkane under consideration must be known. Given that the straight chain alkane has a carbon number of "n", a list has to be created from 2, 3, 4, 5…, n where "n" is the carbon number of the straight chain alkane under consideration. Different combination of numbers that sum up to each of the numbers listed must be known. However, the different combination must exclude the number "1". After the different combination of each of the listed numbers is known, structural isomers can be formed with the number combinations as well as the each of the numbers from which the combinations were derived representing the locant numbers (position of the methyl groups on specific carbon atoms). The three postulates earlier introduced will then be employed to sort out the permissible

from the non-permissible structural isomers of a particular straight chain alkane. Any of proposed structural isomer of a particular straight chain alkane that violates any of the three postulates, it's disqualified from being a structural isomer. An added bonus to the capabilities of these three postulates is its ability to tell if a branched chain alkane with methyl groups as the only substituents is a valid existing compound or not. The technique discussed is valid for all straight chain alkanes even for straight chain alkanes with carbon atoms when $n > 20$ where "n" is the carbon number of all straight chain alkanes. The procedure must be adhered to strictly to list the possible number combinations of the listed numbers from 2, 3, 4, 5,…, n where "n" is the carbon number of a particular straight chain alkane. The plausible or possible structural isomers are then listed with the number combinations and then the three postulates are then applied to fish out the permissible structural isomers of straight chain alkane under consideration.

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