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The K value enumeration of hydrocarbons alkanes, alkenes and alkynes

E.M.R. KIREMIRE

Department of Chemistry, University of Namibia,
Private Bag 13301 , Windhoek (Namibia).

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ABSTRACT

Isomerism is a powerful concept in chemistry. The use of the K value greatly simplifies the sketching of structural isomers in hydrocarbons. The calculation of the K value has been demonstrated. The number of isomers and K values of selected hydrocarbons have been tabulated. The K value complements the octet rule. It is hoped that the use of K value will greatly enhance the teaching of structural isomerism and molecular geometry in organic compounds at undergraduate level.

Key words: k value, hydrocarbons, alkanes, alkenes and alkynes.

INTRODUCTION

Isomerism in alkanes has attracted the attention of many researchers for about 150 years[1]. It is exhibited in all the alkanes starting with butane, C_4H_{10} which has 2 isomers. Pentane, C_5H_{12} has 3 and C_6H_{14} has 5 while C_7H_{16} has 9 isomers. As the number of carbon atoms increases more and more, the number of isomers increases almost expnentially[1-4]. For instance $C_{10}H_{22}$ has 75, $C_{11}H_{24}$(159), $C_{13}H_{28}$(802), $C_{15}H_{32}$(4,347), $C_{17}H_{36}$(24,894) and $C_{20}H_{42}$(366,319). There is no simple formula of generating the number of isomers as the number of carbon atoms increases.

The number of isomers of hydrocarbons

The number of isomers have been determined by using sophisticated mathematical generating functions[1-5].

An example of a generating function in an algebraic form is[3]:

$$C(z) = 1z+1z^3+1z^4+2z^5+2z^6+6z^7+ 9z^8+20z^9+37z^{10}+ 86z^{11}+181z^{12}+422z^{13}+ \dots$$

$$B(z) = 0z+1z^2+0z^3+ 1z^4+1z^{5+\ 3\ z}7+9z^8+15z^9+38z^{10} +73z^{11}+174z^{12}+380z^{13}+ \dots.$$

$$F(z) = C(z) + B(z) = 1z + 1 z^2 + 1z^3 + 2z^4 +3z^5 + 5z^6 + 9z^7 + 18z^8 + 35z^9 + 75z^{10} + 159z^{11}+ 802 z^{13}+ ..$$

The number of isomers of the alkane series correspond to the coefficients of the formula series.

This work has been extended to include the number of isomers for alkene and alkyne series[1-2]. These have been given in Table 2 for the series C_1 to C_{20}.

Ideally, the number of alkane isomers of given molecular formula can be deduced from sketching all the possible isomers guided by the valence principle. This can readily be done for C_4H_{10} to C_6H_{14}. However from C_7H_{16} upwards, the exercise becomes more and more difficult.

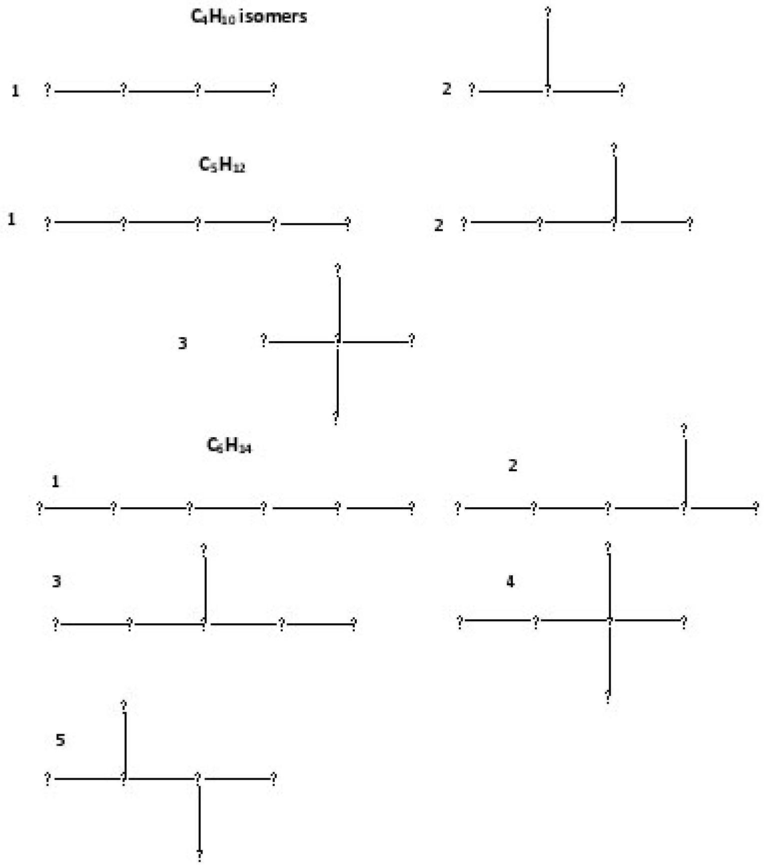

Fig. 1: Isomers of C_4H_{10} , C_5H_{12}, and C_6H_{14}

Table 1: The number of isomers (NI)[1-2] and K-values of selected series of hydrocarbons

C_nH_m	MF m =2	NI	K	MF m = 4	NI	K	MF m = 6	NI	K
n =1				CH_4	1	0			
2	C_2H_2	1	3	C_2H_4	1	2	C_2H_6	1	1
3	C_3H_2	0	5	C_3H_4	2	4	C_3H_6	2	3
4	C_4H_2	1	7	C_4H_4	2	6	C_4H_6	4	5
5	C_5H_2	0	9	C_5H_4	4	8	C_5H_6	6	7
6	C_6H_2	1	11	C_6H_4	5	10	C_6H_6	15	9
	m= 8			m = 10			m =12		
3	C_3H_8	1	2						
4	C_4H_8	3	4	C_4H_{10}	2	3			
5	C_5H_8	9	6	C_5H_{10}	5	5	C_5H_{12}	3	4
6	C_6H_8	22	8	C_6H_{10}	23	7	C_6H_{12}	13	6
	m=14								
6	C_6H_{14}	5	5						

MF = Molecular formula, NI = Number of Isomers.

Application of k formula to hydrocarbons

The use of K formula has been found to be of great assistance in constructing molecular geometries which obey the octet rule and/or the eighteen electron rule[6-7]. The K formula is given by K = ½ (E-V),

where K is the number of bonds linking the atoms that obey the octet rule, E is the sum of octet electrons surrounding the isolated atoms that obey the octet rule and V is the sum of the valence electrons contributed by all the atoms in a molecular formula in question. This is illustrated by the following examples.

Calculation of the k values

Each of the 4 carbon atoms obey the octet rule. Hence the sum of octet electrons will be E= 4x8 =32. The sum of the valence electrons V = 4x4+1x10 = 26. Therefore the K value will be given by K = ½ (32-26) =3. Thus all the skeletal C atoms of isomers of C_4H_{10} will be joined by 3 bonds. A similar calculation for C_5H_{12} gives a K value of 4 while C_6H_{14} and C_7H_{16} have K values of 5 and 6 respectively. The geometries of the corresponding isomers are given in Figures 1 and 2. The simple calculation is easily extended to alkenes and alkynes. For instance, C_2H_4 , K = ½ (16-12) =2 and K for C_2H_2 is given by K = ½ (16-10) =3. Thus, C_2H_4 has a double bond while C_2H_2 has a triple bond. Tables 1 and 2 show the number of isomers (NI)[1-2] and the calculated K-values of a limited selected series of hydrocarbons.

Sketching the isomers

The sketching the isomers of a given molecular formula is easily done by using the corresponding K value. This has been illustrated for the alkanes C_4H_{10} to C_7H_{16} given in Figures 1 and 2. This has been extended to cover other hydrocarbons systems with isomers both acyclic and cyclic ones for C_3H_4, C_4H_4 , and C_5H_6 taken as examples. The selected sketched isomers are given in Figures 3-5.

Table 2: The number of isomers(NI) 1-2 and the K values of alkanes, alkenes and alkynes for the hydrocarbons systems C_1 -C_{20}

	Alkanes			Alkenes			Alkynes		
n	C_nH_{2n+2}	K	NI	C_nH_{2n}	K	NI	C_nH_{2n-2}	K	NI
1	CH_4	0	1	CH_2			C		
2	C_2H_6	1	1	C_2H_4	2	1	C_2H_2	3	1
3	C_3H_8	2	1	C_3H_6	3	1	C_3H_4	4	2
4	C_4H_{10}	3	2	C_4H_8	4	3	C_4H_6	5	4
5	C_5H_{12}	4	3	C_5H_{10}	5	5	C_5H_8	6	9
6	C_6H_{14}	5	5	C_6H_{12}	6	13	C_6H_{10}	7	23
7	C_7H_{16}	6	9	C_7H_{14}	7	27	C_7H_{12}	8	58
8	C_8H_{18}	7	18	C_8H_{16}	8	66	C_8H_{14}	9	152
9	C_9H_{20}	8	35	C_9H_{18}	9	153	C_9H_{16}	10	400
10	$C_{10}H_{22}$	9	75	$C_{10}H_{20}$	10	377	$C_{10}H_{18}$	11	1072
11	$C_{11}H_{24}$	10	159	$C_{11}H_{22}$	11	914	$C_{11}H_{20}$	12	2876
12	$C_{12}H_{26}$	11	355	$C_{12}H_{24}$	12	2281	$C_{12}H_{22}$	13	7783
13	$C_{13}H_{28}$	12	802	$C_{13}H_{26}$	13	5690	$C_{13}H_{24}$	14	21099
14	$C_{14}H_{30}$	13	1858	$C_{14}H_{28}$	14	14397	$C_{14}H_{26}$	15	57447
15	$C_{15}H_{32}$	14	4347	$C_{15}H_{30}$	15	36564	$C_{15}H_{28}$	16	156686
16	$C_{16}H_{34}$	15	10359	$C_{16}H_{32}$	16	93650	$C_{16}H_{30}$	17	428438
17	$C_{17}H_{36}$	16	24894	$C_{17}H_{34}$	17	240916	$C_{17}H_{32}$	18	1173253
18	$C_{18}H_{38}$	17	60523	$C_{18}H_{36}$	18	623338	$C_{18}H_{34}$	19	3218346
19	$C_{19}H_{40}$	18	148284	$C_{19}H_{38}$	19	1619346	$C_{19}H_{36}$	20	8839226
20	$C_{20}H_{42}$	19	366319	$C_{20}H_{40}$	20	4224993	$C_{20}H_{38}$	21	24307593

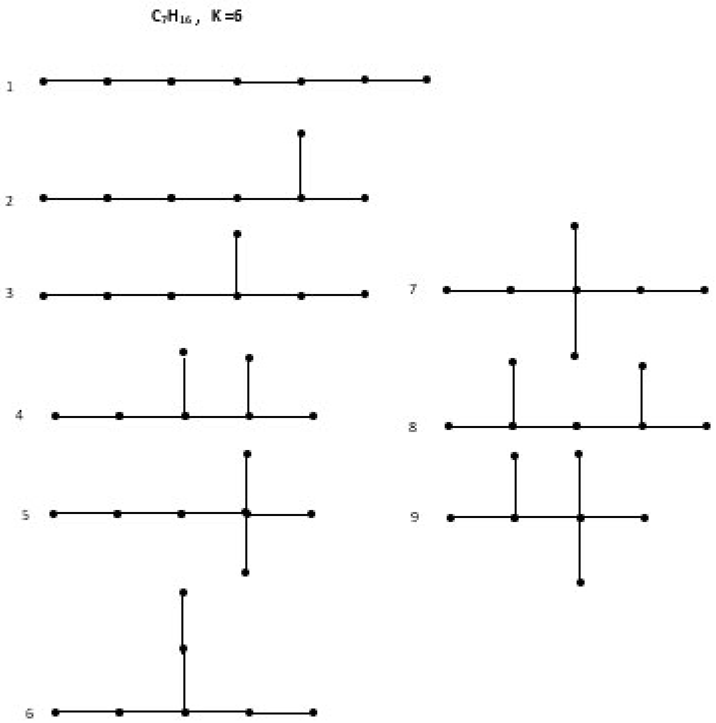

Fig. 2: Isomers of C_7H_{16}

Isomers of C_3H_4

The possible isomers of C_3H_4 (K = 4, NI = 2) formula are shown in Figure 3.

As can be seen, the number of acyclic isomers of C_3H_4 are 2. However, there is one more isomer which is cyclic. It should be emphasized that Tables 1 and 2 gives only the number of acyclic isomers[1-2].

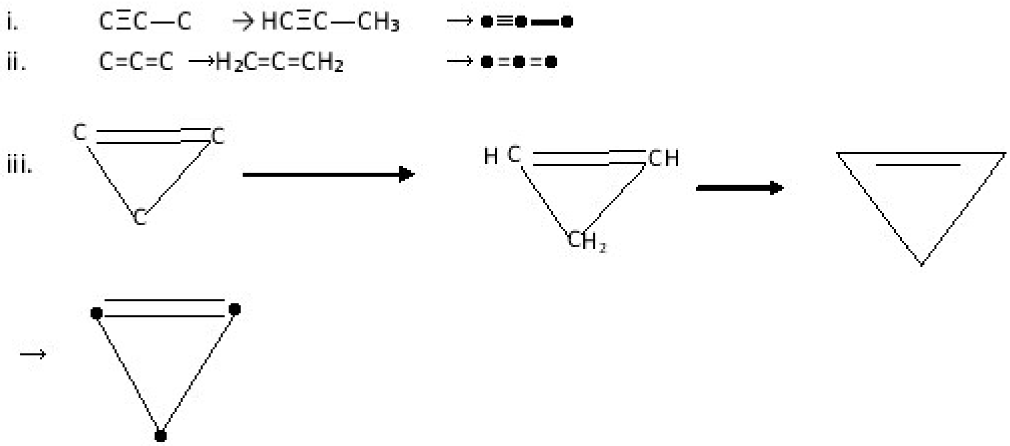

Fig. 3: Isomers of C_3H_4

Isomers of C_4H_4

The second example is C_4H_4 (K = 6, NI =2). The selected possible isomers are shown in Figure 4.

In this example, two ways of sketching the isomers have been shown in such a way as to emphasize the significance of using the K value. In addition to the 2 isomers as predicted from the Formula Periodic Table[1], there are more cyclic ones that can be drawn as indicated in Figure 4.

Isomers of C_5H_6 , K = 7

The C_5H_6 has 6 acyclic isomers[1] and a K value of 7. The selected isomers of C_5H_6 are shown in Figure 5.

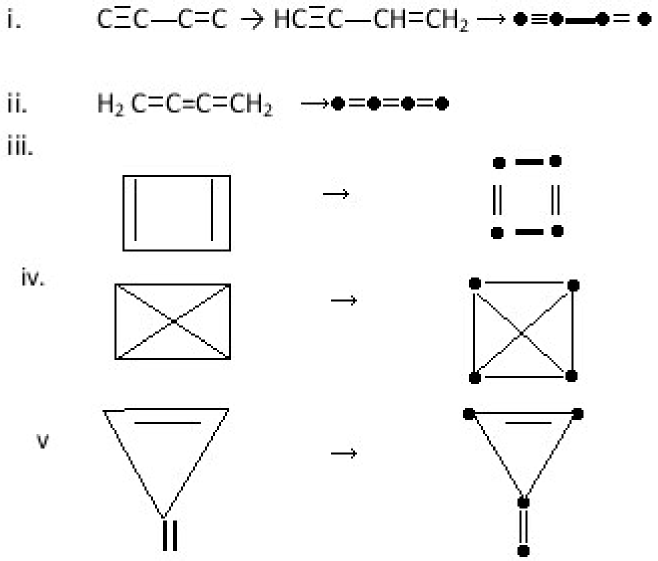

Fig. 4: Selected isomers of C_4H_4

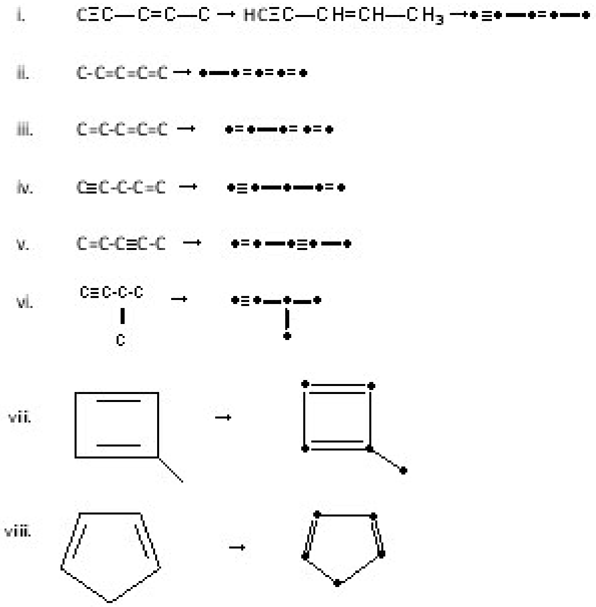

Fig. 5: Selected isomers of C_5H_6

CONCLUSION

The use of K value greatly simplifies the construction of isomers of a given molecular formula of a hydrocarbon. The method is readily extended to other organic compounds with other common elements such as O, N and S. It is hoped that by popularizing the use of K value, the teaching and understanding of structural isomerism and molecular geometry particularly at undergraduate level will immensely be enhanced.

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