match no. 30 pp. 189-201 1994

THE COPOSITIVE PROPERTY OF A TYPE OF CUBIC FORMS AND AN APPLICATION IN THE COMPARISON OF S,T–ISOMERS*

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(received: January 1994)

ABSTRACT.

Let $\sum_{i,j,k=1}^{n} a_{i,j,k}x_ix_jx_k$ be a cubic form and the coefficients have the symmetric properties that

$$a_{i,j,k} = a_{n-i+1,n-k+1,n-j+1},$$
$$a_{i,j,k} = a_{j,k,i} = a_{k,i,j}.$$

Then the copositive property of the cubic form

$$\sum_{i,j,k=1}^{n} a_{i,j,k}x_ix_jx_k - \sum_{i,j,k=1}^{n} a_{i,j,k}x_{n-i+1}x_jx_k$$

is studied and an application in the comparison of S,T-isomers is also presented.

I. The Copositive Property.

Let $f(x_1, x_2, \cdots, x_n) = \sum_{i,j,k=1}^{n} \beta_{i,j,k}x_ix_jx_k$ be a real cubic form with n variables. If for any $x_1 \geq 0, x_2 \geq 0, \cdots, x_n \geq 0$ we have that $f(x_1, x_2, \cdots, x_n) \geq 0$, then we

*Supported by ECFC .

call $f(x_1, x_2, \cdots, x_n)$ copositive. if moreover $f(x_1, x_2, \cdots, x_n) = 0$ if and only if $x_1 = x_2 = \cdots = x_n = 0$, then we call $f(x_1, x_2, \cdots, x_n)$ positive.

The copositive property of a quadratic form has been studied and used extensively. However, the same property of a cubic form has received much less attention. In the present paper we will study the copositive property for a type of cubic forms and an application in chemistry for the comparison of the numbers of Kekulé structures of S and T isomers.

Let $\sum_{i,j,k=1}^{n} a_{i,j,k} x_i x_j x_k$ be a cubic form and the coefficients have the symmetric properties that

$$(*) \qquad a_{i,j,k} = a_{n-i+1,n-k+1,n-j+1}$$

and

$$(**) \qquad a_{i,j,k} = a_{j,k,i} = a_{k,i,j}.$$

Denote by $D(x_1, x_2, \cdots, x_n)$ the difference

$$\sum_{i,j,k=1}^{n} a_{i,j,k} x_i x_j x_k - \sum_{i,j,k=1}^{n} a_{i,j,k} x_{n-i+1} x_j x_k.$$

Then $D(x_1, x_2, \cdots, x_n)$ is again a cubic form. In this section we will give a sufficient condition for $D(x_1, x_2, \cdots, x_n)$ to be copositive.

It is easily seen that

$$\begin{aligned} D(x_1, x_2, \cdots, x_n) &= \sum_{i=1}^{n} (x_i - x_{n-i+1}) \sum_{j,k=1}^{n} a_{i,j,k} x_j x_k \\ &= \sum_{i=1}^{[\frac{n}{2}]} (x_i - x_{n-i+1}) \sum_{j \le k}^{n} b_{i,j,k} x_j x_k, \end{aligned}$$

where

$$(***) \qquad b_{i,j,k} = \begin{cases} a_{i,j,k} - a_{n-i+1,j,k} & for \quad j = k \\ a_{i,j,k} - a_{n-i+1,j,k} + a_{i,k,j} - a_{n-i+1,k,j} & for \quad j < k. \end{cases}$$

We introduce the following linear transformation

$$\begin{cases} x_i = \frac{1}{2}(y_i + y_{n-i+1}) & \\ x_{n-i+1} = \frac{1}{2}(y_{n-i+1} - y_i) & for \quad 1 \le i \le [\frac{n}{2}] \\ x_{[\frac{n}{2}]+1} = y_{[\frac{n}{2}]+1} & for \quad n \ \ odd. \end{cases}$$

The inverse transformation is as follows

$$\begin{cases} y_i = x_i - x_{n-i+1} & \\ y_{n-i+1} = x_i + x_{n-i+1} & for \quad 1 \le i \le [\frac{n}{2}] \\ x_{[\frac{n}{2}]+1} = x_{[\frac{n}{2}]+1} & for \quad n \ \ odd. \end{cases}$$

Then, we obtain that

$$D(x_1, x_2, \cdots, x_n) = F(y_1, y_2, \cdots, y_n) = \sum_{i=1}^{[\frac{n}{2}]} y_i \sum_{j \le k}^{n} c_{i,j,k} y_j y_k,$$

where $c_{i,j,k}$ is determined by the following way.

Obviously, the four coefficients $c_{i,j,k}$, $c_{i,j,n-k+1}$, $c_{i,k,n-j+1}$ and $c_{i,n-k+1,n-j+1}$ of $y_j y_k, y_j y_{n-k+1}, y_k y_{n-j+1}$ and $y_{n-k+1} y_{n-j+1}$ are completely determined by the four coefficients $b_{i,j,k}$, $b_{i,j,n-k+1}$, $b_{i,k,n-j+1}$ and $b_{i,n-k+1,n-j+1}$ of $x_j x_k$, $x_j x_{n-k+1}$, $x_k x_{n-j+1}$ and $x_{n-k+1} x_{n-j+1}$. We can always assume that $j \le k \le [\frac{n}{2}]$ if n is even and $j \le k \le [\frac{n}{2}] + 1$ if n is odd. We distinguish the following cases.

Case 1. n is even.

Subcase 1.1. $j = k$.

The three coefficients $c_{i,j,j}$, $c_{i,j,n-j+1}$ and $c_{i,n-j+1,n-j+1}$ of $y_j y_j, y_j y_{n-j+1}$ and $y_{n-j+1} y_{n-j+1}$ are determined by the three coefficients $b_{i,j,j}$, $b_{i,j,n-j+1}$ and $b_{i,n-j+1,n-j+1}$ of $x_j x_j, x_j x_{n-j+1}$ and $x_{n-j+1} x_{n-j+1}$.

Since

$$x_j x_j = \frac{1}{4}(y_j + y_{n-j+1})(y_j + y_{n-j+1})$$
$$x_j x_{n-j+1} = \frac{1}{4}(y_j + y_{n-j+1})(y_{n-j+1} - y_j)$$

and

$$x_{n-j+1} x_{n-j+1} = \frac{1}{4}(y_{n-j+1} - y_j)(y_{n-j+1} - y_j),$$

so we have

$$c_{i,j,j} = \frac{1}{4}(b_{i,j,j} - b_{i,j,n-j+1} + b_{i,n-j+1,n-j+1}),$$
$$c_{i,j,n-j+1} = \frac{1}{4}(2b_{i,j,j} - 2b_{i,n-j+1,n-j+1})$$

and

$$c_{i,n-j+1,n-j+1} = \frac{1}{4}(b_{i,j,j} + b_{i,j,n-j+1} + b_{i,n-j+1,n-j+1}).$$

Subcase 1.2. $j < k$.

The four coefficients $c_{i,j,k}$, $c_{i,j,n-k+1}$, $c_{i,k,n-j+1}$ and $c_{i,n-k+1,n-j+1}$ of $y_j y_k$, $y_j y_{n-k+1}$, $y_k y_{n-j+1}$ and $y_{n-k+1}\ y_{n-j+1}$ are determined by the four coefficients $b_{i,j,k}$, $b_{i,j,n-k+1}$, $b_{i,k,n-j+1}$ and $b_{i,n-k+1,n-j+1}$ of $x_j x_k, x_j x_{n-k+1}$, $x_k x_{n-j+1}$ and $x_{n-k+1} x_{n-j+1}$.
Since

$$x_j x_k = \frac{1}{4}(y_j + y_{n-j+1})(y_k + y_{n-k+1})$$
$$x_j x_{n-k+1} = \frac{1}{4}(y_j + y_{n-j+1})(y_{n-k+1} - y_k)$$
$$x_k x_{n-j+1} = \frac{1}{4}(y_k + y_{n-k+1})(y_{n-j+1} - y_j)$$

and

$$x_{n-k+1} x_{n-j+1} = \frac{1}{4}(y_{n-k+1} - y_k)(y_{n-j+1} - y_j),$$

so we have

$$c_{i,j,k} = \frac{1}{4}(b_{i,j,k} - b_{i,j,n-k+1} - b_{i,k,n-j+1} + b_{i,n-k+1,n-j+1}),$$
$$c_{i,j,n-k+1} = \frac{1}{4}(b_{i,j,k} + b_{i,j,n-k+1} - b_{i,k,n-j+1} - b_{i,n-k+1,n-j+1}),$$
$$c_{i,k,n-j+1} = \frac{1}{4}(b_{i,j,k} - b_{i,j,n-k+1} + b_{i,k,n-j+1} - b_{i,n-k+1,n-j+1}),$$

and

$$c_{i,n-k+1,n-j+1} = \frac{1}{4}(b_{i,j,k} + b_{i,j,n-k+1} + b_{i,k,n-j+1} + b_{i,n-k+1,n-j+1}).$$

Case 2. n is odd.

Subcase 2.1. $j = k \leq [\frac{n}{2}]$

The same as Subcase 1.1.

Subcase 2.2. $j < k \leq [\frac{n}{2}]$

The same as Subcase 1.2.

Subcase 2.3. $j < k = [\frac{n}{2}] + 1$

The two coefficients $c_{i,j,k}$ and $c_{i,k,n-j+1}$ of $y_j y_k$ and $y_k y_{n-j+1}$ are determined by the two coefficients $b_{i,j,k}$ and $b_{i,k,n-j+1}$ of $x_j x_k$ and $x_k x_{n-j+1}$.
Since

$$x_j x_k = \frac{1}{2}(y_j + y_{n-j+1}) y_k$$

and

$$x_k x_{n-j+1} = \frac{1}{2} y_k (y_{n-j+1} - y_j),$$

so we have

$$c_{i,j,k} = \frac{1}{2}(b_{i,j,k} - b_{i,k,n-j+1})$$

and

$$c_{i,k,n-j+1} = \frac{1}{2}(b_{i,j,k} + b_{i,k,n-j+1}).$$

Subcase 2.4. $j = k = [\frac{n}{2}] + 1$**.**

Clearly, we have $c_{i,j,k} = b_{i,j,k}$.

By substituting $(***)$ and the property $(*)$ into the expressions of $c_{i,j,k}$, $c_{i,j,n-k+1}$, $c_{i,k,n-j+1}$ and $c_{i,n-k+1,n-j+1}$, we obtain the following.
(A).n is even.
(A).1. $j = k$.

$$c_{i,j,j} = 0, \qquad c_{i,n-j+1,n-j+1} = 0$$

and

$$c_{i,j,n-j+1} = \frac{1}{4}(b_{i,j,j} - b_{i,n-j+1,n-j+1}).$$

Again by $(***)$ and the property $(*)$ we can get that

$$b_{i,j,n-j+1} = 0 \qquad and \qquad b_{i,j,j} = -b_{i,n-j+1,n-j+1}.$$

Therefore,

$$c_{i,j,n-j+1} = \frac{1}{2}(b_{i,j,n-j+1} - b_{i,n-j+1,n-j+1}).$$

(A).2. $j < k$.

$$c_{i,j,k} = 0, \qquad c_{i,n-k+1,n-j+1} = 0$$

and

$$\begin{aligned} c_{i,j,n-k+1} &= \frac{1}{2}(b_{i,j,n-k+1} - b_{i,n-k+1,n-j+1}), \\ c_{i,k,n-j+1} &= \frac{1}{2}(b_{i,k,n-j+1} - b_{i,n-k+1,n-j+1}) \\ &= \frac{1}{2}(b_{i,k,n-j+1} - b_{i,n-j+1,n-k+1}). \end{aligned}$$

(B). n is odd.

(B).1. $j = k \leq [\frac{n}{2}]$.

The same as (A).1.

(B).2. $j < k \leq [\frac{n}{2}]$.

The same as (A).2.

(B).3. $j < k = [\frac{n}{2}] + 1$.

$$c_{i,j,k} = \frac{1}{2}(b_{i,j,k} - b_{i,k,n-j+1}) \quad and \quad c_{i,k,n-j+1} = 0.$$

(B).4. $j = k = [\frac{n}{2}] + 1$.

$c_{i,j,k} = 0$.

To sum up the above cases, we obtain a general expression for $c_{i,j,k}$ as follows

$$c_{i,j,k} = \begin{cases} \frac{1}{2}(b_{i,j,k} - b_{i,k,n-j+1}) & for \quad j \leq [\frac{n}{2}] < k \quad and \quad for \quad j < k = [\frac{n}{2}] + 1 \\ & if \quad n \quad is \quad odd, \\ 0 & for \quad [\frac{n}{2}] < j \leq k \quad and \quad j \leq k \leq [\frac{n}{2}], \\ & and \quad for \quad [\frac{n}{2}] + 1 \leq j \leq k \quad if \quad n \quad is \quad odd. \end{cases}$$

Now we can simply write $F(y_1, y_2, \cdots, y_n)$ as

$$\sum_{i=1}^{[\frac{n}{2}]} \sum_{j=1}^{[\frac{n}{2}]} \sum_{k=[\frac{n}{2}]+1}^{n} c_{i,j,k} y_i y_j y_k,$$

i.e.,

$$\sum_{k=[\frac{n}{2}]+1}^{n} y_k \sum_{i=1}^{[\frac{n}{2}]} \sum_{j=1}^{[\frac{n}{2}]} c_{i,j,k} y_i y_j.$$

By the property (**) we can see that $c_{i,j,k} = c_{j,i,k}$ for each $k = [\frac{n}{2}]+1, \cdots, n$. Hence if we denote $g_k(y_1, y_2, \cdots, y_{[\frac{n}{2}]})$ by

$$\sum_{i=1}^{[\frac{n}{2}]} \sum_{j=1}^{[\frac{n}{2}]} c_{i,j,k} y_i y_j \qquad \textit{for each} \quad k = [\frac{n}{2}] + 1, \cdots, n,$$

then $g_k(y_1, y_2, \cdots, y_{[\frac{n}{2}]})$ is a quadratic form and

$$D(x_1, x_2, \cdots, x_n) = \sum_{k=[\frac{n}{2}]+1}^{n} y_k g_k(y_1, y_2, \cdots, y_{[\frac{n}{2}]}),$$

where for each k the coefficient matrix M_k is given as follows

$$M_k = (c_{i,j,k})_{[\frac{n}{2}]\times[\frac{n}{2}]},$$

in which

$$\begin{aligned} c_{i,j,k} &= \frac{1}{2}(b_{i,j,k} - b_{i,k,n-j+1}) \\ &= \frac{1}{2}(a_{i,j,k} - a_{n-i+1,j,k} + a_{i,k,j} - a_{n-i+1,k,j} \\ &\quad - a_{i,k,n-j+1} + a_{n-i+1,k,n-j+1} - a_{i,n-j+1,k} \\ &\quad + a_{n-i+1,n-j+1,k}). \end{aligned}$$

Now we give our main result of this section.

THEOREM 1. *If for each $k = [\frac{n}{2}] + 1, \cdots, n$ the matrix M_k is copositive, then so is the cubic form $D(x_1, x_2, \cdots, x_n)$.*

Proof. For any $x_1 \geq 0, x_2 \geq 0, \cdots, x_n \geq 0$ we know from the inverse transformation that $y_k \geq 0$ for each $k = [\frac{n}{2}] + 1, \cdots, n$. Since the matrix M_k is copositive for each $k = [\frac{n}{2}] + 1, \cdots, n$, so the corresponding quadratic form $g_k(y_1, y_2, \cdots, y_{[\frac{n}{2}]}) \geq 0$ and therefore $D(x_1, x_2, \cdots, x_n)$ is copositive.

II. An Application in Chemistry.

Isomers, which may be constructed from several subunits $A, B, \cdots$ by linking them in a different manner, are called topologically related, usually, they are denoted by S and T, respectively. There are several ways in which pairs of topologically related isomers may be constructed, each one is called a topological model or type. Many types of S and T isomers were introduced by Polansky et. al., see [3]. Polansky and Zander [1, 13] discussed the topological effect on the molecular orbital (TEMO) of topologically related isomers. The comparisons of the numbers of Kekulé structures and the characteristic polynomials of S and T isomers will indicate that the TEMO has or does not have inversions. In this section we will consider the comparison of the numbers of Kekulé structures of a new type of S and T isomers. From [7] and the references therein, we know that the π-electron energy (E) of hydrocarbon C_nH_s has the following approximate relation

$$E = [0.201n - 0.049s + 0.043K(0.795)^{n-s}]E(benzene),$$

and the Dewar resonance energy (RE) can be well reproduced by

$$RE = 114.3 \ln K \qquad [kJmol^{-1}],$$

where K is the number of Kekulé structures. Therefore, generally speaking, the larger the number of Kekulé structures of a benzenoid hydrocarbon is, the higher its resonance energy and Dewar energy should be. So, our comparisons should lead to the energy comparisons of the corresponding isomers.

The new type of S and T isomers of benzenoid systems is shown in Figure 1.

For terminology and notation not defined here, we refer the readers to [7, 13, 14].

Let B be a benzenoid system, C be a cut segment and M be a Kekulé structure of B. Denote by $M(C)$ the number of M-double bonds intersected by C.

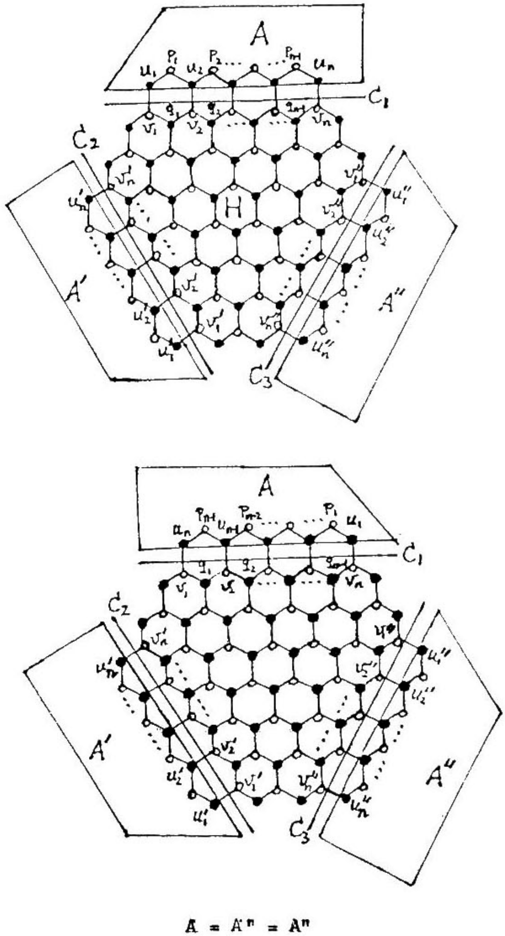
LEMMA 1 [14]. *For any two Kekulé structures M and M' of B, we have $M(C) = M'(C)$.*

LEMMA 2. *Let M be a Kekulé structure of the S or T isomer, and the three cut segments C_1, C_2 and C_3 be as shown in Figure 1. Then we have*

$$M(C_1) = M(C_2) = M(C_3).$$

S:

T:



$A = A' = A''$

(Figure 1)

Proof. By the symmetric property of S or T and Lemma 1, this lemma follows immediately.

LEMMA 3 [14]. *Let B be a benzenoid system with a Kekulé structure M and B' be a sub-system of B. Let d be the difference of the number of peaks and the number of valleys of B'. For a normal color of B with black and white, denote by r the difference of the number of black vertices and the number of white vertices of all the M-double bonds, each having precisely one vertex in B'. Then we have that $d = r$.*

LEMMA 4. *For any Kekulé structure M of the S or T isomer, we have $M(C_1) = M(C_2) = M(C_3) = 1$, where C_1, C_2 and C_3 are the cut segments shown in Figure 1.*

Proof. By Lemma 2, we can assume that

$$M(C_1) = M(C_2) = M(C_3) = k.$$

Since 3 is the difference of the number of peaks and the number of valleys of H, from the color given in Figure 1 and Lemma 3 we know that $3k = 3$. Thus, $k = 1$.

Denote by $a_{i,j,k}$ the number of Kekulé structures of $H \setminus \{v_i, v'_j, v"_k\}$, where H is given in Figure 1. Then by the symmetric property of H, we obtain the following lemma.

LEMMA 5.

$$(i) \qquad a_{i,j,k} = a_{j,k,i};$$
$$(ii) \qquad a_{i,j,k} = a_{k,i,j};$$
$$(iii) \qquad a_{i,j,k} = a_{n-i+1,n-k+1,n-j+1};$$
$$(iv) \qquad a_{i,1,n} = a_{1,n,i} = a_{n,i,1} = 0;$$
$$(v) \qquad a_{i,1,n-1} = a_{i,2,n}.$$

Proof. The first two equalities can be obtained by turning H respectively in a clockwise and counter-clockwise manner. The third one can be obtained by reflecting H with respect to the vertical line that bisects H. The remaining two equalities can be obtained by successive matching of the vertices of valence one.

The number of Kekulé structures of a benzenoid system B will be denoted by $K(B)$, as usual. For simplicity, we will use x_i to denote $K(A \setminus \{u_i\})$, where u_i is a vertex of A , see Figure 1.

Since $A = A' = A"$ in the S and T isomers, by Lemma 4 we know that

$$K(S) = \sum_{i,j,k=1}^{n} a_{i,j,k} x_i x_j x_k \qquad \textit{and}$$

$$K(T) = \sum_{i,j,k=1}^{n} a_{i,j,k} x_{n-i+1} x_j x_k .$$

Denote by D the difference $K(S) - K(T)$. Then from Lemma 5 we know that the cubic forms $K(S), K(T)$ and D satisfy the conditions of Theorem 1 in Section 1.

THEOREM 2. *If for each $k = [\frac{n}{2}] + 1, \cdots, n$ the matrix M_k, defined from $a_{i,j,k}$ here, is copositive, then the number of Kekulé structures of the isomer S is not less than that of the corresponding isomer T, i.e., $K(S) \geq K(T)$.*

For general n we have not proved that each M_k here is copositive. Anyway, for $n = 3, 4, 5$ and 6 we will check that it is really so. In the following, $a_{i,j,k}$ are obtained by a result of [15], i.e., the number of Kekulé structures of a benzenoid system is equal to the square root of the absolute value of the determinant of its adjacency matrix. By using a computer, we obtain the following.

The case $n = 3$.

Since $[\frac{n}{2}] = 1$, we have the two matrices M_2 and M_3 of order 1 as follows $M_2 = [1]$ and $M_3 = [4]$, which are copositive. Thus, for $n = 3$, we have that $K(S) \geq K(T)$.

The case $n = 4$.

Since $[\frac{n}{2}] = 2$, we have the two matrices M_3 and M_4 of order 2 as follows

$$M_3 = M_4 = \begin{bmatrix} 20 & 10 \\ 10 & 5 \end{bmatrix}$$

It is easily seen that they are copositive and hence $K(S) \geq K(T)$ for $n = 4$.

The case $n = 5$.

Since $[\frac{n}{2}] = 2$, we have the three matrices M_3, M_4 and M_5 of order 2 as follows

$$M_3 = \begin{bmatrix} 1568 & 1568 \\ 1568 & 1568 \end{bmatrix}$$

$$M_4 = \begin{bmatrix} 1470 & 1470 \\ 1470 & 1470 \end{bmatrix}$$

$$M_5 = \begin{bmatrix} 980 & 980 \\ 980 & 980 \end{bmatrix},$$

which are copositive. Thus we have that $K(S) \geq K(T)$ for $n = 5$.

The case $n = 6$.

Since $[\frac{n}{2}] = 3$, we have the three matrices M_4,M_5 andM_6 of order 3 as follows

$$M_4 = \begin{bmatrix} 582,120 & 873,180 & 415,800 \\ 873,180 & 1,309,770 & 632,770 \\ 415,800 & 623,700 & 297,000 \end{bmatrix},$$

$$M_5 = \begin{bmatrix} 465,696 & 698,544 & 332,640 \\ 698,544 & 1,047,816 & 498,960 \\ 332,640 & 498,960 & 237,600 \end{bmatrix},$$

$$M_6 = \begin{bmatrix} 232,848 & 349,272 & 166,320 \\ 349,272 & 523,908 & 249,480 \\ 166,320 & 249,480 & 118,800 \end{bmatrix}.$$

By directly calculating, we know that the ranks of the three matrices are all equal to 1. Therefore, they are copositive and hence $K(S) \geq K(T)$ for $n = 6$.

An interesting observation is that all these matrices for $n = 3, 4, 5$ and 6 are of rank 1. We propose the following conjecture to end this paper: For $n \geq 3$ and each $k = [\frac{n}{2}] + 1, \cdots, n$ the matrix M_k, defined from $a_{i,j,k}$ in this section, is of rank 1. This will imply that $K(S) \geq K(T)$ for all $n \geq 3$.

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