Best lower and upper bounds for the Randić index R_{-1} of chemical trees*

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(Received December 30, 2003)

Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. Clark and Moon gave the lower and upper bounds for the Randić index R_{-1} of all trees, and posed the problem to determine better bounds. In this paper we give the best possible lower and upper bounds for R_{-1} among all chemical trees, i.e., trees with maximum degree at most 4. Some (but not all) of the corresponding tree structures are also determined.

1 Introduction

In 1975 Randić [13] proposed the following two important topological indices

$$R_{-1}(G) = \sum_{uv \in E} (d_G(u)d_G(v))^{-1} \quad and \quad R_{-\frac{1}{2}}(G) = \sum_{uv \in E} (d_G(u)d_G(v))^{-\frac{1}{2}}$$

in his research on molecular structures. In the above formula the graph $G = (V, E)$ corresponds to a certain molecule, the vertices correspond to the atoms and the edges correspond to the chemical bonds between atoms. The index $R_{-\frac{1}{2}}$ is called *Randić index*. Afterwards, researchers generalized Randić index by replacing $-\frac{1}{2}$ by a real number α, and called the new index *general Randić index*. Studies on the extremum of Randić index and general Randić index attracted much attention from chemists and mathematicians, see $[1-12, 15]$.

It is know to all that many molecules such as alkane have molecular graphs with no cycles. In chemical graph theory [14] acyclic molecular graphs with no vertices of degree greater than 4 are usually referred to as *chemical trees*. So, researches on chemical trees are of much

*Supported by the National Science Foundation of China.

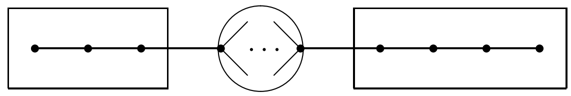


Figure 1: a 2-leaf and a 3-leaf

importance. Bollobás and Erdős [1] gave a sharp lower bound for $R_{-\frac{1}{2}}$ of general trees. Yu [15] gave a sharp upper bound for $R_{-\frac{1}{2}}$ of general trees. Based on the two results for general trees, Caporossi et al [2] got a sharp lower bound for Randić index $R_{-\frac{1}{2}}$ of chemical trees. Gutman et al [8] got both bounds for $R_{-\frac{1}{2}}$ of chemical trees.

Clark and Moon [4] are interested in the Randić index R_{-1}. They obtained a sharp lower bound and an upper bound for general trees, but the upper bound is not sharp. Recently, Rautenbach [12] gave an upper bound for R_{-1} of trees with maximum degree 3, but his proof is very complicated. In this paper we give sharp bounds for R_{-1} of chemical trees. At the same time a simple proof of Rautenbach's theorem is presented.

2 Some notations and known results

Theorem 2.1 *[4] For a tree T with $n \geq 2$ vertices,*

$$1 \leq R_{-1}(G) \leq \frac{5n+8}{18},$$

with the former equality if and only if G is a star.

Theorem 2.2 *[12] Let T be a tree with n vertices and with maximum degree 3. Then*

$$R_{-1}(T) \leq \begin{cases} 0 & if\ n=1, \\ 1 & if\ n=2, \\ \frac{1}{4}n+\frac{1}{4} & if\ 3 \leq n \leq 9, \\ \frac{7}{27}n+\frac{5}{27} & if\ n \geq 10\ and\ n \equiv 1\ mod\ 3, \\ \frac{7}{27}n+\frac{19}{108} & if\ n \geq 11\ and\ n \equiv 2\ mod\ 3, \\ \frac{7}{27}n+\frac{1}{6} & if\ n \geq 12\ and\ n \equiv 0\ mod\ 3. \end{cases}$$

For a graph $G=(V,E)$, we denote the number of vertices (or order) by n, and for any vertex $v \in V$ we denote its degree by $d(v)$. For a vertex of degree 1, we call it a *leaf*. If there are k vertices of degree 2 between a leaf to the first vertex with degree larger than 2, we call this structure a *k-leaf*, see Figure 1. Let $x_{ij}, 1 \leq i \leq j \leq 4$ be the number of edges of a tree T, connecting a vertex of degree i with a vertex of degree j. Denote the number of vertices of degree $i, 1 \leq i \leq 4$ by n_i. Throughout this paper, we only discuss the Randić index R_{-1}.

3 Chemical trees with minimum value of R_{-1}

From Theorem 2.1 we know that the values for R_{-1} of stars reach the minimum. However, when $n > 5$ the stars never belong to chemical trees. So we must reconsider the minimum for $n > 5$. In the following we give the chemical trees with minimum values for R_{-1} by a linear programming.

Theorem 3.1 *Let T be a chemical tree of order n. Then*

$$R_{-1}(T) \geq \begin{cases} 1 & if\ n \leq 5, \\ \frac{11}{8} & if\ n = 6, \\ \frac{3}{2} & if\ n = 7, \\ 2 & if\ n = 10, \\ \frac{9n}{48} + \frac{1}{16} & other \end{cases}$$

Proof. From the basic relations of degrees and edges, we have the following group of linear equations:

$$\begin{cases} x_{12} + x_{13} + x_{14} = n_1 \\ x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2 \\ x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \\ x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4 \\ n_1 + n_2 + n_3 + n_4 = n \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1) \end{cases} \qquad (*)$$

we can assume that $n_1, n_2, n_3, n_4, x_{14}, x_{44}$ are unknown and solve the group of linear equations since the number of equations is 6, i.e.,

$$\begin{cases} n_1 = \frac{2n+2}{3} - \frac{1}{3}x_{12} - \frac{2}{3}x_{22} - \frac{4}{9}x_{23} - \frac{1}{9}x_{13} - \frac{1}{3}x_{24} - \frac{2}{9}x_{33} - \frac{1}{9}x_{34} \\ n_2 = \frac{1}{2}x_{12} + x_{22} + \frac{1}{2}x_{23} + \frac{1}{2}x_{24} \\ n_3 = \frac{1}{3}x_{13} + \frac{1}{3}x_{23} + \frac{2}{3}x_{33} + \frac{1}{3}x_{34} \\ n_4 = \frac{n-2}{3} - \frac{1}{6}x_{12} - \frac{1}{2}x_{22} - \frac{7}{18}x_{23} - \frac{2}{9}x_{13} - \frac{1}{6}x_{24} - \frac{4}{9}x_{33} - \frac{2}{9}x_{34} \\ x_{14} = \frac{n+2}{3} - \frac{4}{3}x_{12} - \frac{10}{9}x_{13} - \frac{2}{3}x_{22} - \frac{4}{9}x_{23} - \frac{1}{3}x_{24} - \frac{2}{9}x_{33} - \frac{1}{9}x_{34} \\ x_{44} = \frac{n-5}{3} + \frac{1}{3}x_{12} + \frac{1}{9}x_{13} - \frac{1}{3}x_{22} - \frac{5}{9}x_{23} - \frac{2}{3}x_{24} - \frac{7}{9}x_{33} - \frac{8}{9}x_{34} \end{cases}$$

By substituting the solutions x_{14} and x_{44} into $R_{-1}(T)$, we get

$$R_{-1}(T) = \frac{1}{2}x_{12} + \frac{1}{3}x_{13} + \frac{1}{4}(x_{14} + x_{22}) + \frac{1}{6}x_{23} + \frac{1}{8}x_{24} + \frac{1}{9}x_{33} + \frac{1}{12}x_{34} + \frac{1}{16}x_{44} \qquad (3.1)$$

$$= \frac{3n}{16} + \frac{1}{16} + \frac{27}{144}x_{12} + \frac{9}{144}x_{13} + \frac{9}{144}x_{22} + \frac{3}{144}x_{23} + \frac{1}{144}x_{33}. \qquad (3.2)$$

So in fact we only need to consider the following formula:

$$f(T) = 27x_{12} + 9x_{13} + 9x_{22} + 3x_{23} + x_{33}$$

From the above formula we can easily see that $f(T)$ reaches its minimum if T is a tree such that $x_{12}, x_{13}, x_{22}, x_{23}, x_{33}$ are all zero. One simple way to make them all zero is to seek a tree with vertices of degrees 1 and 4. We know that only when $n \equiv 2\ mod\ 3, n \geq 5$ there exist such trees. So, it is clear that when $n \equiv 2\ mod\ 3, n \geq 5$, $f(T)$ reaches its minimum

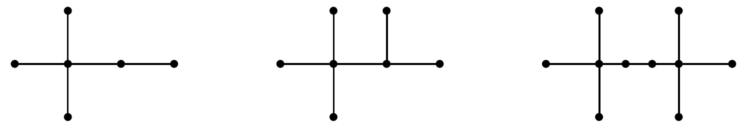


Figure 2: minimum trees for $n = 6, 7, 10$

0. For the case $n \equiv 0 \ mod \ 3, n \geq 8$, we can find a tree with $x_{12}, x_{13}, x_{22}, x_{23}, x_{33}$ all zero by two steps. The first step chooses a tree of order $n-1$ with vertices of degrees 1 and 4 and subdivides once one of the edges that connect two vertices of degree 4. For the case $n \equiv 1 \ mod \ 3, n \geq 11$, we first choose a tree of order $n-2$ with vertices of degrees 1 and 4 and subdivides once two of the edges that connect two vertices of degree 4, respectively. By doing so, it only produces edges with two endpoints of degrees 2 and 4 while contributes zero to $f(T)$. So what left for us are the cases for $n = 6, 7, 10$ since stars reach the minimum when $n \leq 5$. When $n = 6$, there is no tree with $x_{12}, x_{13}, x_{22}, x_{23}, x_{33}$ all zero, and so $R_{-1}(T)$ reaches its minimum if and only if T is the tree as shown in Figure 2 [a]. When $n = 7$ there is no tree with $x_{12}, x_{13}, x_{22}, x_{23}, x_{33}$ all zero either, and so the best case is that there is a tree with $x_{13} = 2$ and others equal to zero (see Figure 2 [b]). At last we consider the case for $n = 10$. If the tree has no vertices of degree 4, then it must has at least two leaves connected with vertices of degrees 2 or 3; if the tree has only one vertex of degree 4, then it has at least one leaf connected with a vertex of degree 2 or two leaves connected with a vertex of degree 3; but if the tree has two vertices of degree 4, we can let $x_{22} = 1$, while others are equal to zero. So the tree in Figure 2 [c] reaches the minimum when $n = 10$. ∎

4 Chemical trees with maximum value of R_{-1}

The upper bound in Theorem 2.1 is not sharp, and the authors asked for better bounds. Unfortunately, there is no further results for general trees, but for chemical trees there exist sharp upper bounds. In this section we not only show the bounds, but also give the structures of some chemical trees with the maximum values for R_{-1}.

Theorem 4.1 *Let T be a chemical tree of order $n > 6$, then*

$$R_{-1}(T) \leq Max\{F_1(n), F_2(n), F_3(n)\},$$

where

$$i)\ F_1(n) = \begin{cases} \frac{3n+1}{16} + \frac{1}{144}\frac{31n+53}{3} & if\ n = 1\ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}(\frac{31n+22}{3} + 9) & if\ n = 2\ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}(\frac{31n-9}{3} + 18) & if\ n = 0\ mod\ 3, \end{cases}$$

ii) $F_2(n) = \frac{3n+1}{16} + \frac{1}{144} \cdot max\{11n - N_4 - 2k + 10, k = 0, 1, 2\}$, *where N_4 is the minimal integer*

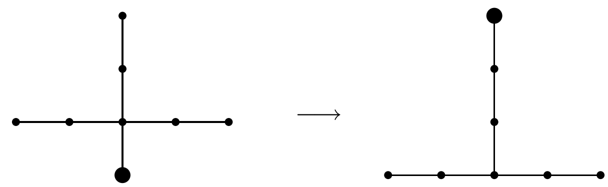


Figure 3: Transfer operation A

solution of n_4 *in the following group of equations:*

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \le 2n_4 + 2 \end{cases}$$

and

iii) $F_3(n) = \frac{3n+1}{16} + \frac{1}{144} \cdot max\{4n + 19N_1 + 5k + 4, k = 0, 1, 2\}$ *where* N_1 *is the maximal integer solution of* n_1 *in the following group of equations:*

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \ge 2n_4 + 2 \\ n_4 \ge 1 \end{cases}$$

Proof. Just like the proof of Theorem 3.1, here we try to make $f(T)$ reach its maximum. At first let's see three transfer operations of chemical trees under which the value $f(T)$ increases.

Transfer operation A. Move each leaf connected with a vertex of degree 3 or 4 to a leaf connected with a vertex of degree 2 (See Figure 3).

Transfer operation B. Move successive vertices of degree 2 between two vertices of degrees 3 or 4 to any leaf (See Figure 4).

Transfer operation C. Choose any two vertices of degree 2 not connected with leaves from the k-leaves, then connect them one by one to any vertex of degree 2 not connected with a leaf and connected with a vertex of degree 3 or 4(See Figure 5).

For any chemical tree, after completely doing the above transfer operations, it must be changed into the structure shown in Figure 6. Here we should note that trees with this structure have $n_2 - n_1 \le 2$. So we only need to seek trees with the maximum value for R_{-1} among the trees in Figure 6. We distinguish it by two cases.

Case I. $n_4 = 0$.

In this case we have

$$\begin{cases} n_1 + 3n_3 = 2(n_1 + n_3 - 1) \\ n_1 + n_2 + n_3 = n \\ n_1 - n_2 \le 2 \end{cases}$$

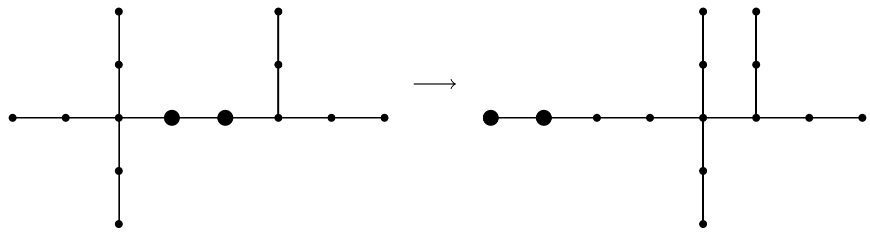


Figure 4: Transfer operation B

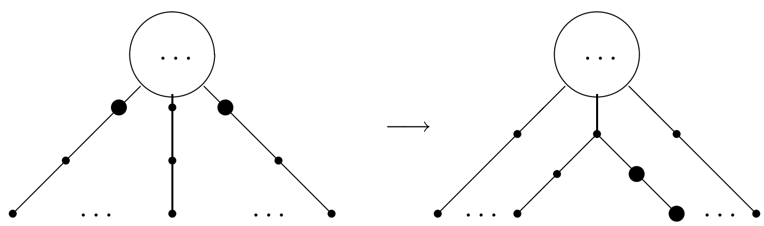


Figure 5: Transfer operation C

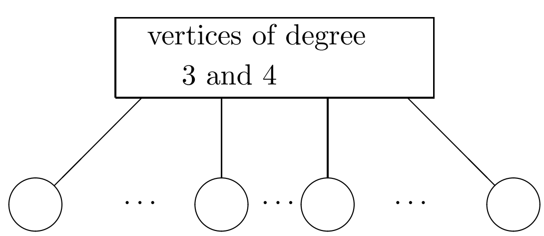
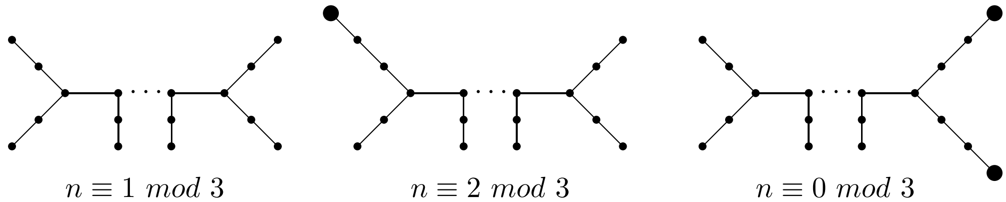


Figure 6: the circle means 2-leaves or 1-leaves



$n \equiv 1 \ mod\ 3$ $\qquad$ $n \equiv 2 \ mod\ 3$ $\qquad$ $n \equiv 0 \ mod\ 3$

Figure 7: The trees in Case I

We can easily solve the group of linear equations, and get that

$$\begin{cases} n_1 = \frac{n+2}{3}, & n_2 = \frac{n+2}{3}, & n_3 = \frac{n-4}{3} & if \ \ n \equiv 1 \ mod\ 3 \\ n_1 = \frac{n+1}{3}, & n_2 = \frac{n+4}{3}, & n_3 = \frac{n-5}{3} & if \ \ n \equiv 2 \ mod\ 3 \\ n_1 = \frac{n}{3}, & n_2 = \frac{n+6}{3}, & n_3 = \frac{n-6}{3} & if \ \ n \equiv 0 \ mod\ 3 \end{cases}$$

From $(*)$ we have

$$\begin{cases} x_{12} = \frac{n+2}{3}, & x_{22} = 0 & x_{13} = 0 & x_{23} = \frac{n+2}{3}, & x_{33} = \frac{n-7}{3} & if \ \ n \equiv 1 \ mod\ 3 \\ x_{12} = \frac{n+1}{3}, & x_{22} = 1 & x_{13} = 0 & x_{23} = \frac{n+1}{3}, & x_{33} = \frac{n-8}{3} & if \ \ n \equiv 2 \ mod\ 3 \\ x_{12} = \frac{n}{3}, & x_{22} = 2 & x_{13} = 0 & x_{23} = \frac{n}{3}, & x_{33} = \frac{n-9}{3} & if \ \ n \equiv 0 \ mod\ 3 \end{cases}$$

By taking the above results into the (3.2), we have

$$R_{-1}(T) = \begin{cases} \frac{3n+1}{16} + \frac{1}{144}\frac{31n+53}{3} & if \ n = 1 \ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}(\frac{31n+22}{3} + 9) & if \ n = 2 \ mod\ 3, \\ \frac{3n+1}{16} + \frac{1}{144}(\frac{31n-9}{3} + 18) & if \ n = 0 \ mod\ 3, \end{cases}$$

Case II. $n_4 \neq 0$.

For the reason to make $f(T)$ as large as possible, the trees must have enough k-leaves connected with vertices of degree 3, so that x_{23} can be larger.

a) If $n_3 \leq 2n_4 + 2$, the trees with each vertex of degree 3 connected with two k-leaves and one vertex of degree 4 must have the maximum $f(T)$ since only in these trees x_{23} contributes the most to the sum $f(T)$. For these trees we have

$$f(T) = 27n_1 + 6n_3 + 9(n_1 - n_2)$$

and

$$n_1 + 3n_3 + 4n_4 = 2(n_1 + n_3 + n_4 - 1) \quad (4.1)$$

$$n_1 + n_2 + n_3 + n_4 = n \quad (4.2)$$

$$n_1 - n_2 \leq 2 \quad (4.3)$$

$$n_3 \leq 2n_4 + 2. \quad (4.4)$$

Let $n_2 - n_1 = k$, we get $3n_1 - n_4 - 2 = n - k$ by (4.1) and (4.2). By taking it into $f(T)$, we have

$$f(T) = 11n - n_4 - 2k + 10.$$

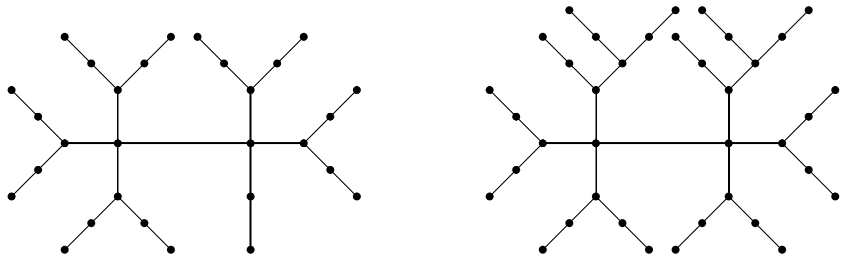


Figure 8: a tree of Case II a), and a tree of Case II b)

In order to make $f(T)$ reach the maximum, we must choose the smallest n_4, denoted by N_4. In finding N_4, we should note that from (4.4), $2n_4+2$ must close to n_3 so that N_4 can be smaller.

b) When $n_3 > 2n_4 + 2$, the trees whose paths between two vertices of degree 4 composed of all vertices of degree 4 must have the maximum $f(T)$, because these trees have the largest x_{23}. The $2n_4 + 2$ vertices of degree 3 contribute 2 to x_{23}, and the left $(n_3 - 2n_4 - 2)$ vertices of degree 3 contribute 1 to x_{33} and x_{23} respectively, and so we have

$$f(T) = 27n_1 + 6(2n_4 + 2) + 4(n_3 - 2n_4 - 2) + 9(n_2 - n_1)$$

and

$$n_1 + 3n_3 + 4n_4 = 2(n_1 + n_3 + n_4 - 1) \tag{4.5}$$
$$n_1 + n_2 + n_3 + n_4 = n \tag{4.6}$$
$$n_1 - n_2 \leq 2 \tag{4.7}$$
$$n_3 > 2n_4 + 2 \tag{4.8}$$
$$n_4 > 0. \tag{4.9}$$

Here we let $n_2 - n_1 = k$, and then (4.6) changes into $n_3 + n_4 = n - k - 2n_1$. By taking it into $f(T)$, we have

$$f(T) = 4n + 19n_1 + 5k + 4.$$

In order to make $f(T)$ reach the maximum, we must choose the largest n_1, denoted by N_1. From (4.5) and (4.6) we have $3n_1 = n - k + n_4 + 2$. So, in order to make n_1 larger, we must let n_4 be larger. While from (4.9) we should let $2n_4 + 2$ close to n_3 in finding N_1.

We know that $R_{-1}(T)$ reaches its maximum if and only if $f(T)$ reaches its maximum. The above proof contains all possible cases for the maximum of $R_{-1}(T)$. So the maximum must be one of the cases above, and the theorem is thus proved. ∎

When $3 \leq n \leq 6$ the trees have at most 2 edges connected with a vertex of degree 1 and a vertex of degree 2, and so the trees with maximum value of R_{-1} must be a path.

Example 4.2 Let's determine the maximum for R_{-1} of chemical trees with 55 vertices by using the results of Theorem 4.1.

Since $55 \equiv 1 \ mod\ 3$, we have

$$F_1(55) = \frac{3 \times 55 + 1}{16} + \frac{1}{144}\frac{31 \times 55 + 53}{3} = \frac{2080}{144}.$$

By solving the two groups of linear equations:

$$\begin{cases} n_1 + 3n_3 + 4n_4 = 2(n_1 + n_3 + n_4 - 1) \\ n_1 + n_2 + n_3 + n_4 = 55 \\ n_1 - n_2 \leq 2 \\ n_3 \leq 2n_4 + 2 \end{cases}$$

and

$$\begin{cases} n_1 + 3n_3 + 4n_4 = 2(n_1 + n_3 + n_4 - 1) \\ n_1 + n_2 + n_3 + n_4 = 55 \\ n_1 - n_2 \leq 2 \\ n_3 > 2n_4 + 2 \\ n_4 > 0, \end{cases}$$

respectively, we get that $N_4 = \begin{cases} 6, & n_2 - n_1 = 0 \\ 4, & n_2 - n_1 = 1 \\ 5, & n_2 - n_1 = 2 \end{cases}$ and $n_1 = \begin{cases} 20, & n_2 - n_1 = 0 \\ 19, & n_2 - n_1 = 1 \\ 19, & n_2 - n_1 = 2. \end{cases}$

So,

$$F_2(55) = \frac{3 \times 55 + 1}{16} + \frac{1}{144} \times (11 \times 55 - 6 + 10)(\ or\ (11 \times 55 - 4 - 2 \times 1)) = \frac{2103}{144}$$

and

$$F_3(55) = \frac{3 \times 55 + 1}{16} + \frac{1}{144} \times (4 \times 55 + 19 \times 20 + 4) = \frac{2098}{144}.$$

Thus, the maximum value for R_{-1} of chemical trees with 55 vertices is $\frac{2103}{144}$.

5 A simple proof of Theorem 2.2

Proof. When the maximum degree of T is 3, we can still get that

$$R_{-1}(T) = \frac{9n}{48} + \frac{1}{16} + \frac{27}{144}x_{12} + \frac{9}{144}x_{13} + \frac{9}{144}x_{22} + \frac{3}{144}x_{23} + \frac{1}{144}x_{33}.$$

We only need to consider

$$f(T) = 27x_{12} + 9x_{13} + 9x_{22} + 3x_{23} + x_{33}.$$

By the three transfer operations, we can determine that the trees with the maximum values of R_{-1} must have the structure shown in Figure 6, but the vertices in the circle of Figure 6 must be of degree 3. We can easily find that it is the same with **Case 1**. Three extremal trees corresponding to different $n > 6$ are given in Figure 7.

When $3 \leq n \leq 6$, x_{12} is at most 2, and so the path of order n reaches the maximum. We can easily get that the value for R_{-1} of the path is $\frac{n+1}{4}$. So, the proof of Theorem 2.2 is complete. ∎

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