

# 两类图族的 Merrifield-Simmons 指标的最大值\*

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**摘要:** 图族  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  分别是由圈  $C_k$ , 路  $P_k$  和轮  $W_k$  的每个顶点  $v_i (i = 1, 2, \dots, k)$  (轮的中心顶点除外) 分别顶点粘接圈  $C_{s_i} (i = 1, 2, \dots, k)$  而得到的图; 通过对图族  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  的 Merrifield-Simmons 指标进行研究, 刻画出了这两类图族的 Merrifield-Simmons 指标 (在顶点数一定时) 取得最大值的图分别是  $Q(C_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$  和  $Q(W_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$ 。

**关键词:** 独立集; 匹配; Merrifield-Simmons 指标

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## The Largest Merrifield-Simmons Index of Two Graphs of $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$ and $Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$

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**Abstract:** Let graphs  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  be obtained from  $C_k, P_k, W_k$ , with every vertex  $v_i (i = 1, 2, \dots, k)$  (The center vertex of  $W_k$  can not be contained) attached one cycle  $C_{s_i} (i = 1, 2, \dots, k)$ , respectively. The highest bounds of Merrifield-Simmons indexes of  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  graphs are determined. The two graphs  $Q(C_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$  and  $Q(W_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$  which have the largest Merrifield-Simmons index of those graphs are characterized, respectively.

**Key words:** independent set; matchings set; Merrifield-Simmons index

设图  $G = (V, E)$  是简单的连通图, 并且  $V(G)$  是它的顶点集和  $E(G)$  是它的边集。对一个图  $G$  的任意两个顶点  $u$  和  $v$ , 如果它们不相邻, 则称它们是相互独立的。一个顶点集  $V(G)$  的子集  $I$ , 如果它的任意两个顶点都相互独立, 则称它是图  $G$  的一个独立集。用  $i(G)$  表示图  $G$  的独立集的个数, 在化学中  $i(G)$  也被称为 Merrifield-Simmons 指标, 此指标与化学分子的许多物理、化学性质密切相关, 如分子的熔点、沸点等; 对该指标的研究成果很多, 参见文献 [1-8]。

设  $C_k, P_k$  和  $W_k$  分别表示顶点数分别为  $k, k, k+1$  的圈, 路和轮。则用  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  表示图族圈粘接圈是由圈  $C_k$  的每个顶点  $v_i (i = 1, 2, \dots, k)$  分别点粘接圈  $C_{s_i} (i = 1, 2, \dots, k)$  而得到的图; 用  $Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  表示图族路粘接圈是由路  $P_k$  的每个顶点  $v_i (i = 1, 2, \dots, k)$  分别点粘接圈  $C_{s_i} (i = 1, 2, \dots, k)$  而得到的图; 用  $Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  表示图族轮粘接圈是由轮  $W_k$  的每个顶

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点  $v_i (i = 1, 2, \dots, k)$  (除中心顶点外) 分别点粘接圈  $C_{s_i} (i = 1, 2, \dots, k)$  而得到的图。本文通过对图族  $Q(C_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}), Q(W_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  的 Merrifield-Simmons 指标进行研究, 刻画出了这两类图族的 Merrifield-Simmons 指标在顶点数一定时, 取得最大值的图分别是  $Q(C_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)}), Q(W_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$ 。在本文中未给出的专业术语、记号可参见文献 [9]。

### 1 预备引理

**引理 1**<sup>[9]</sup> 设图  $G_1$  和  $G_2$  是图  $G$  的两个分支, 则  $i(G) = i(G_1)i(G_2)$ 。

**引理 2**<sup>[9]</sup> 设图  $G$  是简单图且任意的  $v \in V(G)$ , 则有  $i(G) = i(G-v) + i(G-N_G[v])$ , 其中  $N_G[v]$  是  $v$  的闭邻集。

**引理 3**<sup>[1]</sup> 设  $\alpha = \frac{1+\sqrt{5}}{2}$  和  $\beta = \frac{1-\sqrt{5}}{2}$ , 并且  $F_n$  和  $L_n$  分别是 Fibonacci 数列和 Lucas 数, 则

$$F_n = \frac{\alpha^n - \beta^n}{\sqrt{5}}, L_n = \alpha^n + \beta^n,$$

$$F_n F_m = \frac{1}{5}(L_{n+m} - (-1)^n L_{m-n})$$

**引理 4**<sup>[3]</sup> 设图  $Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})$  是图族路粘接圈, 在顶点数取定值时, 则有  $i(Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k})) \leq i(Q(P_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)}))$ , 等式成立当且仅当,  $Q(P_k; C_{s_1}, C_{s_2}, \dots, C_{s_k}) \cong Q(P_k; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_k-4(k-1)})$ 。

### 2 主要结论

**定理 1** 假设  $s_1, s_2, \dots, s_k$  都是正整数且满足  $2 \leq s_1 \leq s_2 \leq \dots \leq s_k$ , 在顶点数取定值时, 则有:  $i(P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_k}) \geq i(P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_k-3(k-1)})$ , 等式成立当且仅当,  $P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_k} \cong P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_k-3(k-1)}$ 。

**证明** (归纳法) 假设  $n$  是路并图  $P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_k}$  的分支数, 那么当  $n = 2$  时, 由引理 1, 引理 2 和引理 3 得到

$$i(P_{s_1} \cup P_{s_2}) = F_{s_1+2} F_{s_2+2} = \frac{1}{5}(L_{s_1+s_2+4} - (-1)^{s_1} L_{s_2-s_1});$$

$$i(P_3 \cup P_{s_1+s_2-3}) = F_5 F_{s_1+s_2-1} =$$

$$\frac{1}{5}(L_{s_1+s_2+4} + L_{s_1+s_2-6});$$

$$i(P_{s_1} \cup P_{s_2}) - i(P_3 \cup P_{s_1+s_2-3}) =$$

$$\frac{1}{5}(-L_{s_1+s_2-6} - (-1)^{s_1} L_{s_2-s_1}) \leq 0$$

等号成立当且仅当,  $s_1 = 3$ 。所以当  $n = 2$  时, 结论成立。假设当  $n = k$  时, 结论成立。即  $i(P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_k}) \leq i(P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_k-3(k-1)})$ , 那么当  $n = k + 1$  时, 由归纳假设, 我们得到

$$i(P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_{k+1}}) = F_{s_1+2} F_{s_2+2} \dots F_{s_k+2} F_{s_{k+1}+2} \leq 5^{k-1} F_{s_1+s_2+\dots+s_k-3k+5} F_{s_{k+1}+2} = 5^{k-2}(L_{s_1+s_2+\dots+s_{k+1}-3k+7} - (-1)^{s_{k+1}} L_{s_1+s_2+\dots+s_k-s_{k+1}-3k+3});$$

$$i(P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_k+s_{k+1}-3k}) = 5^{k-1} F_5 F_{s_1+s_2+\dots+s_{k+1}-3k+2} = 5^{k-2}(L_{s_1+s_2+\dots+s_{k+1}-3k+7} - L_{s_1+s_2+\dots+s_k-s_{k+1}-3k-3})$$

所以

$$i(P_{s_1} \cup P_{s_2} \cup \dots \cup P_{s_{k+1}}) - i(P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_{k+1}-3k}) \leq 5^{k-2}(-L_{s_1+s_2+\dots+s_{k+1}-3k-3} - (-1)^{s_{k+1}} L_{s_1+s_2+\dots+s_k-s_{k+1}-3k+3}) \leq 0$$

等式成立当且仅当,  $s_{k+1} = 3$ 。

由上面两个证明过程可知, 当  $n$  取遍所有大于 2 的自然数时, 结论都成立。

**定理 2** 假设  $s_1, s_2, \dots, s_n$  都是正整数且满足  $s_i \geq 3 (i = 1, 2, \dots, n)$ , 在顶点数取定值时, 则有

$$i(Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n})) \leq i(Q(C_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-4(n-1)}))$$

并且等式成立当且仅当

$$Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n}) \cong$$

$$Q(C_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-4(n-1)})$$

**证明** 由引理 4 和定理 1, 我们得到

$$i(Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n})) = i(Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n}) - v) + i(Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n}) - N_G[v]) \leq i(T_{4, (n-2)}) F_{s_1+s_2+\dots+s_{n-1}-4(n-2)+1} F_{s_n+1} + i(T_{4, (n-3)}) F_5 F_{s_1+s_2+\dots+s_{n-1}-4(n-2)-1} F_{s_n+1} + i(T_{4, (n-4)}) F_{s_2+s_3+\dots+s_{n-2}-4(n-4)+1} F_{s_1+1} F_{s_{n-1}+1} F_{s_{n-1}} + i(T_{4, (n-5)}) F_5 F_{s_2+s_3+\dots+s_{n-2}-4(n-4)-1} F_{s_1+1} F_{s_{n-1}+1} F_{s_{n-1}} = i(T_{4, (n-4)}) (35 F_{s_1+s_2+\dots+s_{n-1}-4n+9} F_{s_n+1} + 25 F_{s_1+s_2+\dots+s_{n-1}-4n+7} F_{s_n+1} + F_{s_2+s_3+\dots+s_{n-2}-4n+17} F_{s_1+1} F_{s_{n-1}+1} F_{s_{n-1}}) + i(T_{4, (n-5)}) (50 F_{s_1+s_2+\dots+s_{n-1}-4n+9} F_{s_n+1} + 50 F_{s_1+s_2+\dots+s_{n-1}-4n+7} F_{s_n+1} + 5 F_{s_2+s_3+\dots+s_{n-2}-4n+15} F_{s_1+1} F_{s_{n-1}+1} F_{s_{n-1}}) =$$

$$\frac{1}{25} \left\{ i(T_{4,(n-4)}) [175L_{s_1+s_2+\dots+s_n-4n+10} + (-1)^{s_n} 175L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+8} + 125L_{s_1+s_2+\dots+s_n-4n+8} + (-1)^{s_n} 125L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+6} + L_{s_1+s_2+\dots+s_n-4n+18} + (-1)^{s_n} L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+20} + (-1)^{s_{n-1}} L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+16} + (-1)^{s_1} L_{s_2+s_3+\dots+s_n-s_1-4n+16} + (-1)^{s_1+s_n} L_{s_2+s_3+\dots+s_{n-1}-s_1-s_n-4n+18} + (-1)^{s_1+s_{n-1}} L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+14} + (-1)^{s_{n-1}+s_n} L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+18} + (-1)^{s_1+s_{n-1}+s_n} L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+16} ] + i(T_{4,(n-5)}) [250L_{s_1+s_2+\dots+s_n-4n+10} + (-1)^{s_n} 250L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+8} + 250L_{s_1+s_2+\dots+s_n-4n+8} + (-1)^{s_n} 250L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+6} + 5L_{s_1+s_2+\dots+s_n-4n+16} + (-1)^{s_n} 5L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+18} + (-1)^{s_{n-1}} 5L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+14} + (-1)^{s_1} 5L_{s_2+s_3+\dots+s_n-s_1-4n+14} + (-1)^{s_1+s_n} 5L_{s_2+s_3+\dots+s_{n-1}-s_1-s_n-4n+16} + (-1)^{s_1+s_{n-1}} 5L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+12} + (-1)^{s_{n-1}+s_n} 5L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+16} + (-1)^{s_1+s_{n-1}+s_n} 3L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+14} ] \right\}$$

同理得到

$$i(Q(C_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-4(n-1)})) = i(T_{4,(n-1)}) F_{s_1+s_2+\dots+s_n-4n+5} + i(T_{4,(n-3)}) F_5 F_5 F_{s_1+s_2+\dots+s_n-4n+3} = \frac{1}{5} i(T_{4,(n-4)}) [45L_{s_1+s_2+\dots+s_n-4n+10} - 45L_{s_1+s_2+\dots+s_n-4n} + 25L_{s_1+s_2+\dots+s_n-4n+8} - 25L_{s_1+s_2+\dots+s_n-4n-2}] + i(T_{4,(n-5)}) [70L_{s_1+s_2+\dots+s_n-4n+10} - 70L_{s_1+s_2+\dots+s_n-4n} + 50L_{s_1+s_2+\dots+s_n-4n+8} - 50L_{s_1+s_2+\dots+s_n-4n-2}]$$

因此

$$i(Q(C_n; C_{s_1}, C_{s_2}, \dots, C_{s_n})) - i(Q(C_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-3(n-1)})) \leq \frac{1}{25} i(T_{4,(n-4)}) [-50L_{s_1+s_2+\dots+s_n-4n+10} + 225L_{s_1+s_2+\dots+s_n-4n} + 125L_{s_1+s_2+\dots+s_n-4n-2} + 5L_{s_1+s_2+\dots+s_n-4n+18} + (-1)^{s_n} 175L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+8} + (-1)^{s_n} 125L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+6} + (-1)^{s_n} L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+20} + (-1)^{s_{n-1}} L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+18} + (-1)^{s_1} L_{s_2+s_3+\dots+s_n-s_1-4n+16} + (-1)^{s_1+s_n} L_{s_2+s_3+\dots+s_{n-1}-s_1-s_n-4n+18} +$$

$$(-1)^{s_1+s_{n-1}} L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+14} + (-1)^{s_{n-1}+s_n} L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+18} + (-1)^{s_1+s_{n-1}+s_n} L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+14}] + i(T_{4,(n-5)}) [-100L_{s_1+s_2+\dots+s_n-4n+10} + 5L_{s_1+s_2+\dots+s_n-4n+16} + 350L_{s_1+s_2+\dots+s_n-4n} + 250L_{s_1+s_2+\dots+s_n-4n-2} + (-1)^{s_n} 250(L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+8} + L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+6} + (-1)^{s_n} 5L_{s_1+s_2+\dots+s_{n-1}-s_n-4n+18} + (-1)^{s_{n-1}} 5L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+14} + (-1)^{s_1} 5L_{s_2+s_3+\dots+s_n-s_1-4n+14} + (-1)^{s_1+s_n} 5L_{s_2+s_3+\dots+s_{n-1}-s_1-s_n-4n+16} + (-1)^{s_1+s_{n-1}} 5L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}+s_n-4n+12} + (-1)^{s_{n-1}+s_n} 5L_{s_1+s_2+\dots+s_{n-2}-s_{n-1}+s_n-4n+16} + (-1)^{s_1+s_{n-1}+s_n} 5L_{s_2+s_3+\dots+s_{n-2}-s_1-s_{n-1}-s_n-4n+14}] \leq \frac{1}{25} i(T_{4,(n-4)}) (L_{s_2+s_3+\dots+s_{n-2}-4n+30} - L_{s_2+s_3+\dots+s_{n-2}-4n+24} - 51L_{s_2+s_3+\dots+s_{n-2}-4n+22} - L_{s_2+s_3+\dots+s_{n-2}-4n+20} + 2L_{s_2+s_3+\dots+s_{n-2}-4n+14} + 50L_{s_2+s_3+\dots+s_{n-2}-4n+12} - L_{s_2+s_3+\dots+s_{n-2}-4n+2}) + i(T_{4,(n-5)}) (5L_{s_2+s_3+\dots+s_{n-2}-4n+28} - 105L_{s_2+s_3+\dots+s_{n-2}-4n+22} - 10L_{s_2+s_3+\dots+s_{n-2}-4n+18} + 110L_{s_2+s_3+\dots+s_{n-2}-4n+12} + 5L_{s_2+s_3+\dots+s_{n-2}-4n+8} - 5L_{s_2+s_3+\dots+s_{n-2}-4n+2})] = \frac{1}{25} i(T_{4,(n-4)}) \cdot (-55L_{s_2+s_3+\dots+s_{n-2}-4n+17} - 37L_{s_2+s_3+\dots+s_{n-2}-4n+16} + 2L_{s_2+s_3+\dots+s_{n-2}-4n+14} + 50L_{s_2+s_3+\dots+s_{n-2}-4n+12} - L_{s_2+s_3+\dots+s_{n-2}-4n+2} + i(T_{4,(n-5)}) (-130L_{s_2+s_3+\dots+s_{n-2}-4n+17} - 90L_{s_2+s_3+\dots+s_{n-2}-4n+16} + 110L_{s_2+s_3+\dots+s_{n-2}-4n+12} + 5L_{s_2+s_3+\dots+s_{n-2}-4n+8} - 5L_{s_2+s_3+\dots+s_{n-2}-4n+2})] \leq 0$$

并且等式成立当且仅当  $Q(C_n; C_3, C_3, \dots, C_3, C_{s_1+s_2+\dots+s_n-3(n-1)}) \cong Q(C_n; C_3, C_3, \dots, C_3, C_{s_1}, C_{s_2}, \dots, C_{s_n}) \cong Q(C_n; C_3, C_3, \dots, C_3, C_{s_1+s_2+\dots+s_n-3(n-1)})$ .

在证明过程中, 用到的符号标记  $T_{4,k} = Q(P_k; C_4, C_4, \dots, C_4)$  ( $k = 1, 2, \dots, n$ ), 因此结论成立.

**定理 3** 假设  $s_1, s_2, \dots, s_n$  都是正整数且满足  $s_i \geq 3$  ( $i = 1, 2, \dots, n$ ), 在顶点数为定值时, 则有

$$i(Q(W_n; C_{s_1}, C_{s_2}, \dots, C_{s_n})) \leq i(Q(W_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-4(n-1)}))$$

并且等式成立当且仅当

$$Q(W_n; C_{s_1}, C_{s_2}, \dots, C_{s_n}) \cong Q(W_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n-4(n-1)})$$

**证明** 由引理 2、定理 1 和定理 2, 可以得到

$$i(Q(W_n; C_{s_1}, C_{s_2}, \dots, C_{s_n})) \leq i(Q(C_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n+4(n-1)})) + i(P_3 \cup P_3 \cup \dots \cup P_3 \cup P_{s_1+s_2+\dots+s_n-4n+1}) =$$

$$i(Q(W_n; C_4, C_4, \dots, C_4, C_{s_1+s_2+\dots+s_n+4(n-1)}))$$

所以定理 3 成立。

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