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Perfect Matchings and Hamiltonian Cycles of C_{60}

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Abstract

Let G be a 3-regular connected graph. If we delete a Hamiltonian cycle of G (delete edges but not vertices), then the rest graph is a perfect matching of G. On the contrary, the rest subgraph deleting a perfect matching of G must be Hamiltonian cycle of G provided that it is connected. Consequently, all Hamiltonian cycles of C_{60} are given in this paper by the way of deleting perfect matchings. And then it is shown that the relationship of perfect matchings is obtained by Hamiltonian cycles.

Keywords

Perfect Matchings, C_{60}, Hamiltonian Cycles

C_{60}的完美匹配与Hamilton圈

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摘　要

设G是一个3-正则的连通图。删掉G一个Hamilton圈(删边不删点)后剩下的子图是G的一个完美匹配；反之，删掉G一个完美匹配后剩下的子图只要是连通的，那一定是原图的Hamilton圈。因此本文通过删除完美匹配的方法给出了Buckminsterfullerene (C_{60})的所有Hamilton圈，进而通过Hamilton圈研究了完美匹配之间的关系。

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关键词

完美匹配，C_{60}，Hamilton圈

1. 引言

众所周知，富勒烯(Fullerenes)是由碳一种元素组成，是以球状、椭圆状或管状结构存在的物质。1985年，苏塞克斯大学的Harold Kroto与莱斯大学的James R. Heath，Sean O'Brien，Robert Curl和Richard Smalley合作，在氦气中蒸发碳时产生的烟灰残渣中发现了富勒烯。在产物的质谱中，与60个碳原子或70个碳原子的分子(即现在我们所知的C_{60}或C_{70})对比时，出现了离散峰。研究小组把它们确定为我们现在所熟知的“巴克球”[1]。因为C_{60}的结构与美国建筑师Buckminster Fuller所推广的测地穹顶结构相似，研究者最终给C_{60}取名为“巴克敏斯特富勒烯(Buckminsterfullerene)”，以此来向Buckminster Fuller致敬[2]；选择“烯”结尾是因为C_{60}中碳原子是不饱和的，只与另外三个碳原子相连，而不是正常地与四个碳原子相连。

C_{60}是富勒烯的重要成员，也是其同分异构体中稳定性最强的，因此关于C_{60}的研究很多。Klein等研究得到C_{60}有12,500个Kekulé结构[3]，Vukičević根据C_{60}的对称群I_h群将其所有Kekulé结构分成158等价类，还给出了这158类Kekulé结构的代表元的图示[4]。后来Vukičević等在文献[5]中给出了每个类中Kekulé结构的数目，以及C_{60}的共振6-圈、共振10-圈、共振14-圈和所有共振圈的数目等详细指标，并根据各Kekulé结构的自由度(df)把C_{60}的所有Kekulé结构分成六大类，即df = 5，6，7，8，9，10，给出了每一类中Kekulé结构的个数，而且还表明即使具有相同自由度的Kekulé结构之间C-C单键和C-C双键的模式也存在较大的差异[6]。Schmalz及其同事的研究表明，只有一半的Kekulé结构对C_{60}分子的稳定性有贡献[7] [8]。由此可见，并非所有的Kekulé结构都是平等的，这对于Kekulé结构较多的烃类是非常重要的。

关于C_{60}的Hamilton圈的研究很早便有了一些结果。Barnette猜想所有最大面大小不超过6的3-正则多面体图都是Hamilton图(即存在Hamilton圈) [9]，Goodey也陈述过这一点[10]，只是没有正式提出。Barnettee的这一猜想特别涵盖了富勒烯图，并且多达176个顶点的富勒烯图的Hamilton性已经被验证[11]。František Kardoš证明了Barnette的猜想[12]，因而C_{60}必有Hamilton圈。数学软件Mathematica的图数据库中记录了C_{60}的Hamilton圈的数目为1090，而且给出了C_{60}的其中一个Hamilton圈。本文利用Mathematica软件计算出了C_{60}的所有Hamilton圈，并且研究了Hamilton圈与完美匹配的关系。

2. 符号和预备知识

2.1. 一般图上的准备工作

设G是一个图。G的Hamilton圈是指包含G的每个顶点的圈，以下我们简写为H-圈。G的完美匹配是指覆盖G的所有顶点的不相邻边的集合[13]。图论中的完美匹配就是有机化学中的Kekulé结构。事实上，H-圈是两个特殊完美匹配的不交并。设A，B是两个集合，A和B的对称差定义为$A \oplus B = (A \cup B) \setminus (A \cap B)$；特别地，如果$A \cap B = \varnothing$，则$A \oplus B = A \cup B$，即$A$和$B$的不交并。

本文中我们只考虑 3-正则图中完美匹配与 H-圈之间的联系，那么显然有

命题 1 设 G 是一个 3-正则图，则删掉 G 的一个 H-圈后的图是 G 的一个完美匹配；反之，删掉 G 的一个完美匹配后的图如果是连通的，那一定是 G 的一个 H-圈。

关于完美匹配和 H-圈的关系，通常我们可考虑以下两个问题。

问题 1 哪两个完美匹配作对称差能得到 H-圈，且剩下的完美匹配是哪一个？

问题 2 哪三个完美匹配中的任意两个的不交并刚好是删掉第三个完美匹配后得到的 H-圈？

由命题 1 对以上两个问题换一种等价的问法。

问题 3 删掉哪一个完美匹配后能得到一个 H-圈(该 H-圈是某两个完美匹配的不交并)？

问题 4 是否存在三个完美匹配，删掉其中任意一个得到的 H-圈是另外两个的不交并？

我们起初的想法是让图 G 的所有完美匹配两两作对称差，这样每一对完美匹配都会得到一些圈分支(也可能是一个圈，即连通)，如果是连通的圈分支，那肯定是 H-圈，这刚好是问题 1，2 的答案；但是这样做的话，由于要作 $\binom{12500}{2}$ 次对称差，计算次数会比较多，所以我们可以按照问题 3，4 来做，即从图 G 中直接删掉其完美匹配中的边，如果剩下的子图连通，即为图 G 的 H-圈。我们可以先在一个顶点较少的图上具体看一下这种方法。例如立方体图 Q_3，它的 9 个完美匹配及分别删除这 9 个完美匹配后的子图分别见图 1 和图 2，其中粗边表示匹配边。

我们可以看到，删掉匹配边以后的图中只有 G_4，G_5，G_6，G_7，G_8，G_9 这 6 个是连通的，即 Q_3 的 H-圈的个数为 6，这与 Mathematica 中的结果是相同的。这 6 个 H-圈的每一个都是由两个完美匹配通过不交并唯一确定，详见表 1。

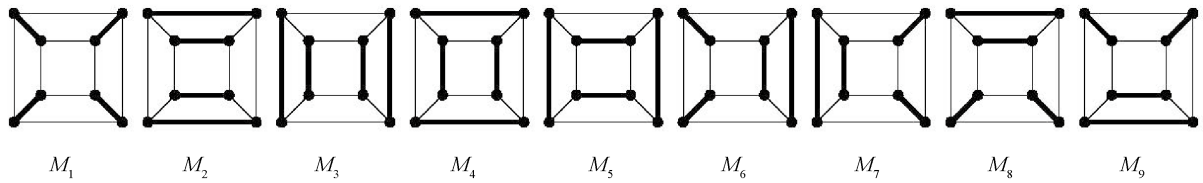


Figure 1. All 9 perfect matchings of Q_3
图 1. Q_3 的所有 9 个完美匹配

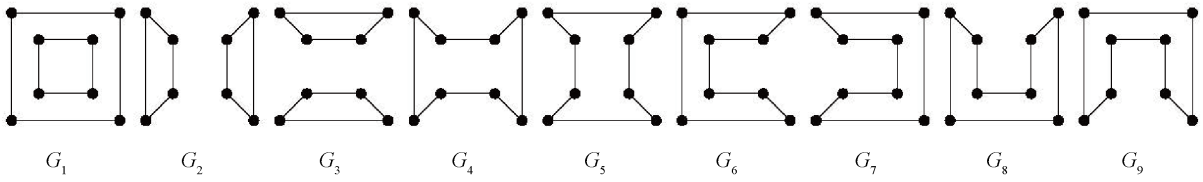


Figure 2. The graphs of deleting each perfect matchings of Q_3
图 2. Q_3 分别删除各完美匹配的子图

Table 1. Representation by perfect matching of 6 H-cycles of Q_3
表 1. Q_3 的 6 个 H-圈的完美匹配表示

H-圈	G_4	G_5	G_6	G_7	G_8	G_9
完美匹配不交并	$M_1 \cup M_5$	$M_1 \cup M_4$	$M_2 \cup M_7$	$M_2 \cup M_6$	$M_3 \cup M_9$	$M_3 \cup M_8$

由表 1 可知，Q_3 的完美匹配中只有问题 1 或问题 3 的答案，并不存在问题 2 或问题 4 的答案；但是由第三节内容可知，C_{60} 中确实存在问题 2 或问题 4 要找的那种完美匹配。

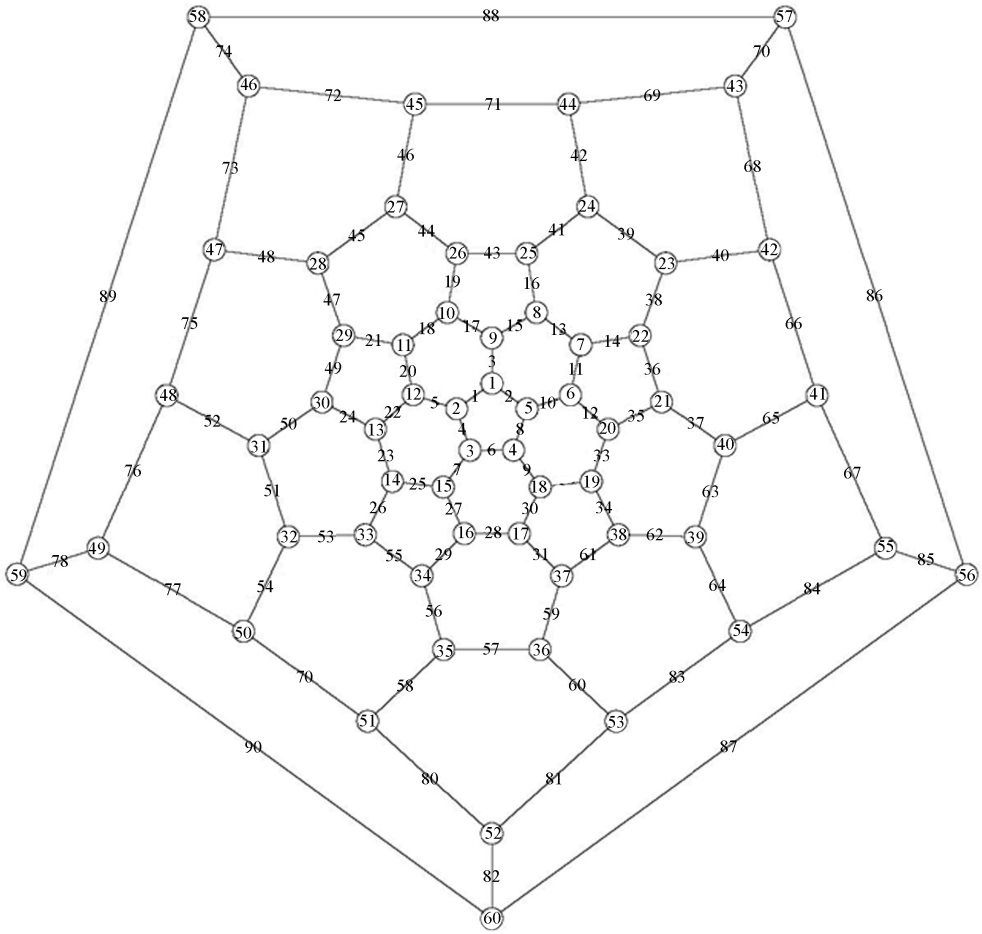


Figure 3. Buckminsterfullerene (C_{60}) and the label of its vertexs and edges
图 3. Buckminsterfullerene (C_{60})及其顶点和边的标号

2.2. C_{60} 上的准备工作

本文是在 C_{60} 中就问题 3 和问题 4 做了回答，计算过程在 Mathematica 11.0 中进行。为此我们需要先对 Mathematica 的程序中用到的符号简单地说明一下。

C_{60} 是一个 3-正则图。设它的顶点标号为{1, 2, …, 60}，边标号为{1, 2, …, 90}，它的画法如图 3 所示，这种标号的顺序是由曾令辉在其学士学位论文中给出的[14]。我们把 C_{60} 的所有点对形式的完美匹配存放在一个数组中，记作 pms，每个完美匹配均是以字典序排序，且按下标或编号 1, 2, …, 12500 来表示各个完美匹配。例如，1 号完美匹配为{{1，2}，{3，4}，{5，6}，{7，8}，{9，10}，{11，12}，{13，14}，{15，16}，{17，18}，{19，20}，{21，22}，{23，24}，{25，26}，{27，28}，{29，30}，{31，32}，{33，34}，{35，36}，{37，38}，{39，40}，{41，42}，{43，44}，{45，46}，{47，48}，{49，50}，{51，52}，{53，54}，{55，56}，{57，58}，{59，60}}。程序中用到的 C_{60} 的边集是以点对形式存放在数组 edges 中。下面是计算的程序代码。

```
Rest[Union[Table[vl = {};DepthFirstScan[Graph[Range[60],
UndirectedEdge @@@ Complement[edges, pms[[i]]]],1,
{"PrevisitVertex" -> (AppendTo[vl, #] &)}];
If[Length[vl] = = 60, {i,Flatten[{Position[pms,
```

```
Sort[Sort /@ Partition[vl,2]]], Position[pms,
Sort[Sort /@ Partition[RotateLeft[vl],2]]]}]},
{}],{i,12500}]]]
Length[%]
```

简单解释一下上面的程序。首先设 vl 是一个变量，从 pms 中取出一个完美匹配，它是点对的形式，算出这个完美匹配在 edges 中的补集，再转换成无向边形式，以这些边为边作一个顶点数为 60 的图，然后从顶点 1 开始，对这个图作“深度优先搜索”，先把顶点 1 放到 vl 中，搜索中找到一个顶点放到 vl 中，再找下一个，直至回到顶点 1 为止；然后判断 vl 的长度，若长度为 60，即 60 个顶点均在 vl 中，那 vl 中的顶点就是一个 Hamilton 圈的所有顶点，再把 v1 中的顶点两个一组进行划分，这样会得到一个完美匹配；然后把 vl 向左轮换一个位置，即第一个位置上顶点放到倒数第一个位置上，第二个位置上的顶点放到第一个位置上，第三个位置上的顶点放到第二个位置上，……，依此类推；轮换以后再两个一组进行划分(轮换和划分操作相当于把 H-圈转了一下)，划分完以后就得到了另一个完美匹配；把后面得到的两个完美匹配进行排序，小的在前，大的在后，最后找到这两个完美匹配在 12500 中的编号，把 vl 长度为 60 时对应的那个完美匹配和后面得到的两个完美匹配以{*，{*，*}}的形式输出；如果 vl 长度不是 60，那么输出一对空的{}；最后对输出结果取并集，去掉空括号就得到了附录中的结果。结果中那种三个一组的完美匹配共有 1090 组(这与 Mathematica 图数据库中的结果一致)，由于考虑篇幅问题，我们把这些结果放在了附录中。

3. 结果分析

3.1. H-圈与完美匹配

现在，我们就 C_{60} 的计算结果对问题 3 作出回答。现在，我们来分析一下 2.2 节中程序输出结果中的 1090 组完美匹配，以第一组{1，{4573，10565}}为例。“1，4573，10565”都是完美匹配的编号，这三个完美匹配意思是，直接把 1 号完美匹配删掉后得到 H-圈，这个 H-圈就是由 4573 号和 10565 号这两个完美匹配的不交并得到。写成{*，{*，*}}这种形式是为了把完美匹配与 H-圈一一对应起来，第一个数字是完美匹配，后面两个是用完美匹配来表示的 H-圈。这样的话问题 3 的答案就有了，即每一组的第一个完美匹配就是问题 3 要找的完美匹配。

我们统计一下这 1090 组数据共有多少个完美匹配。我们把每一组的第一个完美匹配与第二、三个分开，构成两大类，第一类是每组的第一个完美匹配，共 1090 个，第二类是由每组剩下的两个完美匹配构成；可以发现第二类内部有重复元素，互不相同的有 1350 个，当然这里面也包含第一类里面的完美匹配；把这两大类进行对比，重复的有 490 个，那么第二类中互不相同的，且与第一类不重复的就有 860 个。所以那 1090 组数据共涉及到 1950 个互不相同的完美匹配。事实上，第一类就是删掉之后会产生 H-圈的完美匹配，第二类是可以通过不交并构成 H-圈的完美匹配。然而我们只清楚第一类完美匹配的情况，对于第二类完美匹配的情况，以及这两类完美匹配之间的关系我们还不知道，所以需要进一步探索。

3.2. 与 H-圈相关的完美匹配之间的关系

H-圈是一个比较特殊的图论概念，所以我们就想知道与 H-圈有关的完美匹配是否也与其它完美匹配有所不同，或者说它们之间有没有什么特殊的关系。为此，我们以程序计算结果中涉及到的 1950 个完美匹配为顶点构造图，以此来探索一下它们之间的联系。由于这其中有 1090 个完美匹配，每个删掉之后都会产生 H-圈，即两个完美匹配的不交并，所以以那 1090 个完美匹配为出度点，以与之对应的 H-圈中的两个完美匹配为入度点构造有向图。由于删除之后产生 H-圈的完美匹配(1090 个)与构成 H-圈的完美匹配

(1350 个)有重复(490 个)，这些重复的完美匹配在这个有向图中既有出度又有入度，所以这个有向图中只有出度的完美匹配有 600 个，只有入度的完美匹配有 860 个。我们利用 Mathematica 画出了这个有 1950 个有向图，发现它有 290 个连通分支。为给出它的连通分支，我们需要做些准备工作。

我们先把那些删掉之后能得到 H-圈的完美匹配挑出来，并把它们按照 C_{60} 的完美匹配的 158 个等价类进行分类，分类结果见附录 2。分类之后共有 16 个等价类，选取这 16 类的每一类中的编号最小的完美匹配作为代表元，代表元的编号和它所在类中完美匹配的个数见图 4。

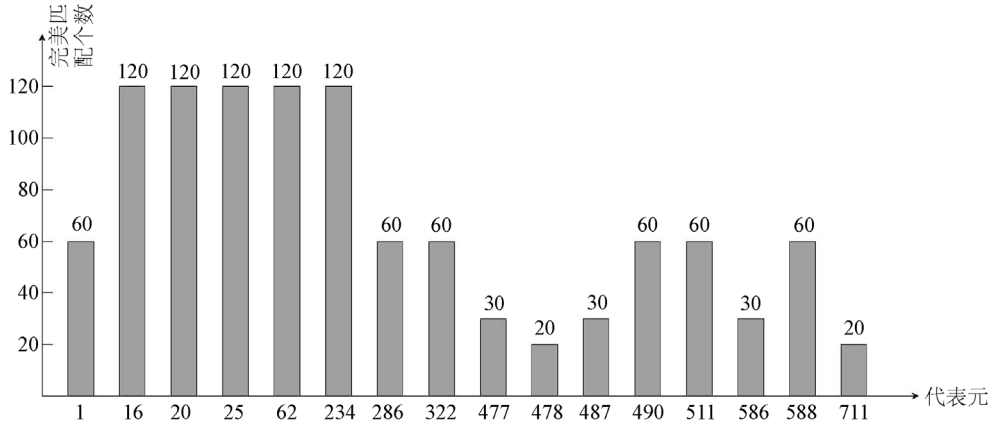


Figure 4. 16 representative perfect matchings and the sizes of their classes
图 4. 16 个代表完美匹配及所在分类的大小

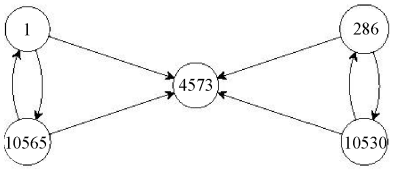
我们在此给出这 16 个完美匹配的边集形式如下。

{1, 6, 10, 13, 17, 20, 23, 27, 30, 33, 36, 39, 43, 45, 49, 51, 55, 57, 61, 63, 66, 69, 72, 75, 77, 80, 83, 85, 88, 90},
{1, 6, 10, 13, 17, 20, 23, 27, 30, 33, 36, 39, 43, 45, 49, 52, 53, 56, 59, 62, 65, 68, 71, 73, 78, 79, 81, 84, 87, 88},
{1, 6, 10, 13, 17, 20, 23, 27, 30, 33, 36, 39, 43, 45, 49, 52, 53, 56, 60, 61, 64, 65, 68, 71, 73, 78, 79, 82, 85, 88},
{1, 6, 10, 13, 17, 20, 23, 27, 30, 33, 36, 39, 43, 46, 47, 50, 53, 56, 60, 61, 63, 66, 69, 73, 76, 79, 82, 84, 86, 89},
{1, 6, 10, 13, 17, 20, 23, 27, 30, 33, 36, 40, 41, 44, 48, 49, 51, 55, 57, 61, 64, 65, 70, 71, 74, 76, 79, 81, 85, 90},
{1, 6, 10, 13, 17, 20, 23, 27, 30, 34, 35, 38, 41, 44, 47, 50, 54, 55, 58, 59, 64, 65, 68, 71, 73, 76, 81, 85, 88, 90},
{1, 6, 10, 13, 17, 20, 23, 27, 31, 32, 35, 38, 42, 43, 45, 49, 51, 55, 57, 62, 65, 68, 72, 75, 77, 80, 83, 85, 88, 90},
{1, 6, 10, 13, 17, 20, 24, 25, 28, 32, 35, 38, 41, 44, 47, 52, 54, 55, 58, 59, 62, 65, 68, 71, 73, 78, 82, 83, 85, 88},
{1, 6, 10, 13, 17, 21, 22, 25, 28, 32, 35, 38, 41, 44, 48, 50, 53, 56, 59, 62, 65, 68, 71, 74, 76, 79, 81, 84, 86, 90},
{1, 6, 10, 13, 17, 21, 22, 25, 28, 32, 35, 38, 41, 44, 48, 50, 53, 56, 60, 61, 63, 66, 69, 72, 76, 79, 82, 84, 86, 89},
{1, 6, 10, 13, 17, 21, 22, 25, 28, 32, 35, 38, 42, 43, 45, 50, 53, 56, 60, 61, 63, 66, 70, 72, 75, 77, 80, 84, 87, 89},
{1, 6, 10, 13, 17, 21, 22, 25, 28, 32, 35, 38, 42, 43, 45, 50, 54, 55, 57, 61, 63, 67, 68, 72, 75, 78, 80, 83, 87, 88},
{1, 6, 10, 13, 17, 21, 22, 25, 29, 30, 33, 36, 39, 43, 45, 50, 53, 58, 60, 61, 63, 66, 69, 72, 75, 77, 82, 84, 86, 89},
{1, 6, 10, 14, 15, 18, 22, 25, 28, 32, 35, 39, 43, 45, 49, 51, 55, 57, 61, 64, 65, 68, 71, 73, 76, 79, 81, 85, 88, 90},
{1, 6, 10, 14, 15, 18, 22, 25, 28, 32, 35, 39, 43, 45, 49, 51, 55, 58, 60, 61, 63, 66, 69, 72, 75, 77, 82, 84, 86, 89},
{1, 6, 10, 14, 15, 18, 22, 25, 29, 30, 34, 35, 39, 43, 46, 48, 49, 52, 53, 58, 59, 63, 66, 69, 74, 77, 81, 84, 86, 90}.

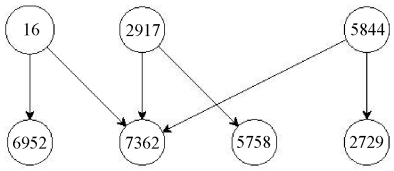
我们把含表 2 中的 16 个代表元的那些连通分支给出来，见图 5；它们是按照 16 个代表元编号的大小顺序排列的。

由图 5 可以看到，三个完美匹配中任意删掉一个都会得到另外两个的不交并的，这种完美匹配只有 30 组，如图 5 中的(k)和(n)，这 30 组分别是

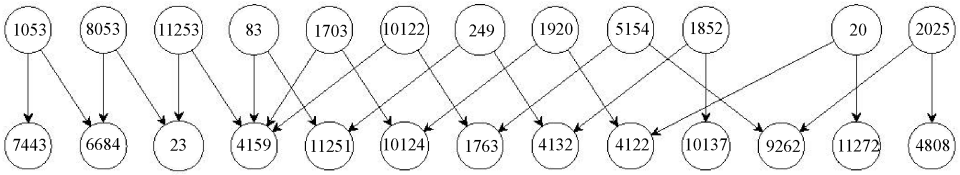
{9869, 4176, 2204}, {4236, 10780, 994}, {6851, 7256, 691}, {5806, 7304, 2974}, {7097, 3210, 5585}, {8696, 1666, 5814}, {4645, 10337, 510}, {10213, 4431, 1260}, {10432, 487, 4633}, {6948, 7149, 477}, {9149, 5552, 1261}, {9058, 1452, 5581}, {10086, 1445, 4555}, {6904, 7350, 513}, {5474, 7733, 3167}, {11107, 4187, 586}, {5436, 7781, 3110}, {5791, 8711, 1678}, {4725, 9621, 1411}, {9563, 4225, 2294}, {7145, 5828, 3020}, {7090, 902, 6829}, {4317, 10510, 697}, {10263, 1226, 4318}, {6748, 7797, 655}, {5674, 9085, 1232}, {7290, 3087, 5558}, {4422, 10492, 823}, {8601, 1426, 5933}, {6689, 7751, 914}.



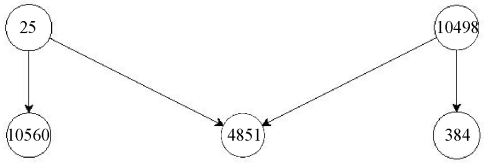
(a)



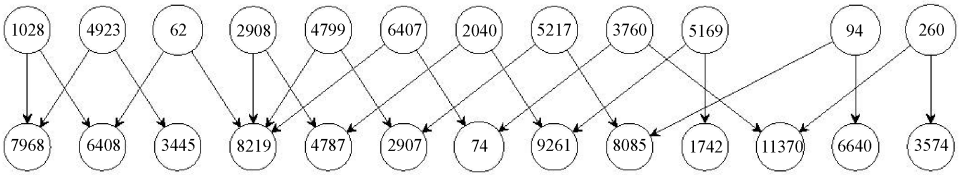
(b)



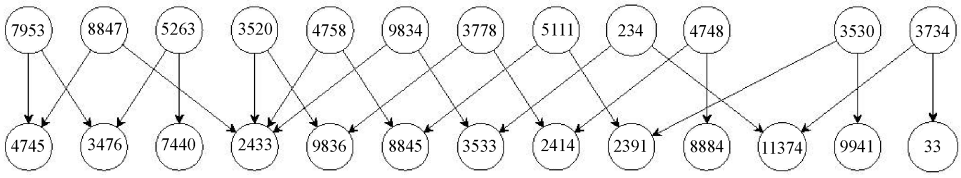
(c)



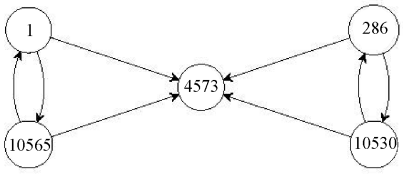
(d)



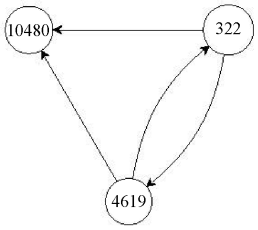
(e)



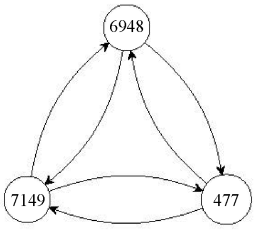
(f)



(g)



(h)



(i)

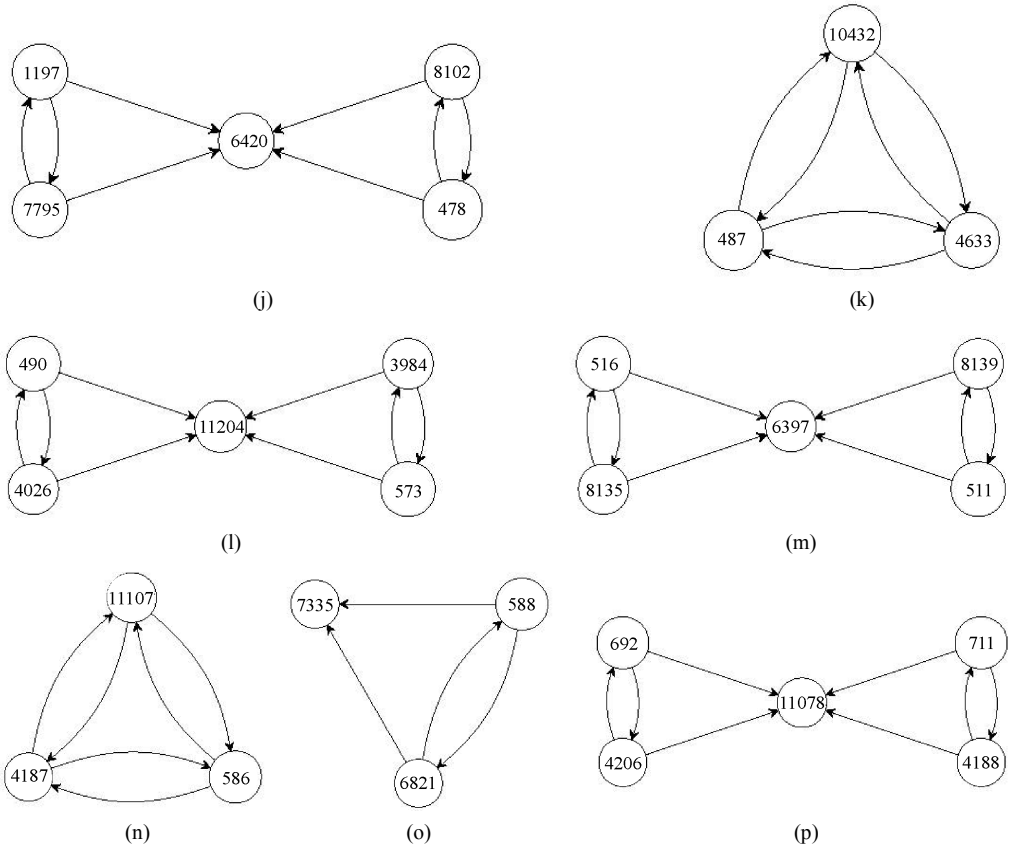


Figure 5. Connected components containing 16 representations
图 5. 包含 16 个代表元的连通分支

这些 30 组特殊的完美匹配，每一组中的任意两个完美匹配作对称差得到的 H-圈都相当于删掉剩下的那个完美匹配得到的 H-圈；反之，删掉任意一个剩下的子图就是另外两个的不交并构成的 H-圈，这就是对问题 4 的回答.我们把同一组的三个完美匹配画到同一个图中，以第一组为例，见图 6。

以上是按照完美匹配同构类进行分类的，也可以按照图同构更加细致的分类，这样分类以后就只剩下(a)，(b)，(c)，(d)，(h)，(i)了。我们对这 6 个连通分支中出度的点进行分析，其它 10 个与这些是图同构的。在分支(a)中，有 4 个完美匹配，删掉任意两个剩下的都是 4573 号完美匹配，而且这 4 个完美匹配来自不同的匹配等价类，分别是 1，286，490，511 所代表的等价类，这 4 个等价类中均有 60 个完美匹配，一个等价类取出两个，就会有 60 个与(a)同构的分支；与(a)同构(图同构)的分支有(j)和(p)，在(j)中同样有 4 个完美匹配，删掉任意两个剩下的都是 6420 号完美匹配，1197 和 8102 属于同一等价类，7795 和 478 属于另一等价类；(p)中有同样的情况，而且 711，4206 与 1197，8102 属于同一等价类，692，4188 与 7795 和 478 属于同一等价类，这两个等价类中均有 20 个完美匹配，一个类中取两个，构成 10 个这样的分支；这样一来，与(a)同构的分支就有 70 个。用类似的方法分析(b)，(c)，(d)，(h)，(i)就得到表 2。

我们再给 860 个在关系图只有入度的完美匹配按 158 个等价类进行分类，共有 11 类，结果见附录 3。关系图中含这些代表元的连通分支参见图 5。类似地，我们从这 11 类中每一类选一个元素作为代表元，除 8086 号完美匹配外的其他代表元在图 5 中均可找到，8086 号完美匹配所在分支与图 5 中的(d)同构，代表元的具体入度数见表 3。由此我们有

命题 2 C_{60} 的每个完美匹配至多包含在 4 个 H-圈中。

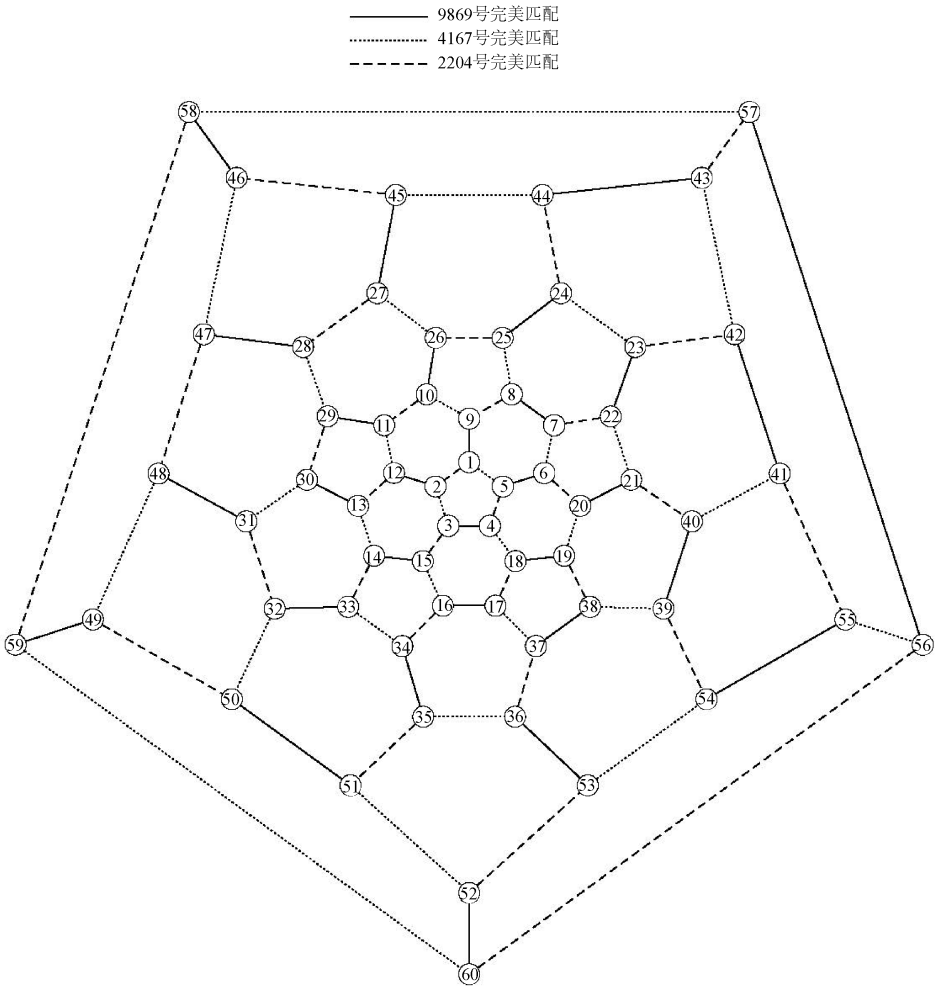


Figure 6. Three special perfect matchings
图 6. 三个特殊的完美匹配匹配

Table 2. The result of components under graph isomorphism
表 2. 连通分支按图同构分类的结果

连通分支	(a)	(b)	(c)	(d)	(h)	(o)
完美匹配数	5	7	25	5	3	3
同构的分支数	70	40	30	60	60	30

Table 3. The sizes of isomorphism classes of perfect matchings with only indegree
表 3. 仅有入度的完美匹配同构类的大小

代表元	23	384	6684	7443	2433	4573	8086	2729	6420	7362	10480
入度	2	1	2	1	4	4	2	1	4	3	2
完美匹配个数	120	120	120	129	30	60	60	120	10	40	60

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附录 1　2.2 中程序的计算结果

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附录 2　问题 3 中的 1090 个完美匹配的编号(分类后的结果)

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附录 3　860 个入度完美匹配的分类

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