Short communication

The Combinatorial Isomer Enumeration of 1, 3, 5-trimethylbenzene by Fujita's Topological Index

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Abstract

The unmatured full non-rigid group of 1,3,5-trimethylbenzene is isomorphic to the wreath product of the cyclic group of order three and the symmetric group of order six on three letters (see *Int. J. Quantum Chem*. **2007**, *107*, 340 and *Bull. Chem. Soc. Jpn*. **2008**, *81*, 279). In this paper the unit subduced cycle index table introduced by S. Fujita of the full non-rigid group 1,3,5-trimethylbenzene of order 162 are successfully derived for the first time.

Keywords: Non-rigid molecule group, Unit subduced cycle index, 1,3,5-trimethylbenzene.

1. Introduction

Chemically, for any non-rigid molecules, there are one or more contortional large amplitude vibrations, such as inversion or internal rotation, which lead to tunneling splitting. Because of this deformability, such molecules exhibit some remarkable properties of intermolecular dynamics, which can be surveyed more easily by resorting to Group theory. A complete set of molecular conversion operations that commute with the nuclear motion operator includes total rotation operations, describing the molecule rotating as a whole and the non-rigid tunneling motion operations that depict molecular moieties moving with respect to the rest of the molecule. Such a set forms a group called the full non-rigid group (f-NRG).[1–3]

In 1960's, Longuet-Higgins[3] investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur effortlessly. The method described here is appropriate for molecules consisting of a number of CH_3 groups attached to a rigid framework.[3–10]

Through the present study, we intend to probe the unite subduced cycle indices for the f-NRG 1,3,5-trimethylbenzene as are presented introduced by S. Fujita.[11–18]

The motivations for this study, utilizing GAP[19] are the authors previous works on the chemical molecules.[20–25]

2. Experimental

In this section, in respect to Fujita's symbols, we describe some notations that will be kept thoroughly in this paper.

Let G be an arbitrary finite group and $h_1, h_2, \in G$, we say h_1 and h_2 are Q-conjugate, denoted by $h_2 \sim_Q h_2$, if we can find any $t \in G$ such that $t^{-1} \langle h_1 \rangle t = \langle h_2 \rangle$. Obviously, this Q-conjugacy is an equivalence relation on group G and it generates equivalence classes that are called dominant classes. Therefore G is partitioned into the dominant classes as follows: $G = K_1 + K_2 + \cdots + K_s$. Now assume that an action P of G on a set X and a subgroup H of G are given. So by considering the set X consisting of all the H's, right cosets,and the partition of G induced by these cosets; $G = \oplus_i^m Hg_i$, we have an action of G on X and a permutation representation signified by $G(/H)$ correspondingly. If G_i and G_j be any subgroups of an arbitrary finite group G, a subduced representation denoted $G(/G_i) \downarrow G_j$ is known as a subgroup of the coset representation $G(/G_i)$ that contains only the elements associated with the elements in G_j.[11–14]

The table of marks of a finite group G is a square matrix $M(G) = (m_{ik})_{\substack{1 \le k \le r \\ 1 \le i \le r}}$ where m_{ik} is the number of right cosets of G_k in G which remain fixed under right multiplication by the elements of G_i.[26]

Let G_i and G_j be two subgroups of an arbitrary finite group G. A unit subduced cycle index (USCI) is delineated as $Z(G(/G_i) \downarrow G_j, s_d) = \prod_{g \in \Omega} s_{dg}^{(ij)}$ where Ω is a transversal set for the double coset decompositions concerning G_i and G_j for $i,j = 1,2,3, \cdots, s$ and $s_{dg}^{(ij)} = |G_i|/|g^{-1}G_i g \cap G_j|$, the reader is recommended to consult the ref. 11–18 and 24.

If K and H are groups and H acts on the set Γ, then the wreath product of K by H, denoted by $K_{wr}\,H$ is identified with $K^\Gamma : H$ is semi direct product K^Γ by H such that $K^\Gamma = \{f \mid f : \Gamma \to K\}$.[8–10, 25]

Suppose that H is a cyclic subgroup of order n of a finite group G. Then the maturity discriminant of H, denoted by $m(H)$, is an integer number delineated by $|N_G(H)$:

Table 1: The unit subduced cycle indices for the f-NRG of TMB (i.e. $Z(G(/G_i)\downarrow G_{j,}\, s_d)$) fo i, j = 1 to 34

USCI	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8	G_9	G_{10}	G_{11}	G_{12}	G_{13}	G_{14}	G_{15}	G_{16}	G_{17}
$G(/G_1)$	s_1^{162}	s_2^{81}	s_3^{54}	s_3^{54}	s_3^{54}	s_3^{54}	s_3^{54}	s_3^{54}	s_6^{27}	s_6^{27}	s_6^{27}	s_6^{27}	s_6^{27}	s_6^{27}	s_9^{18}	ss_9^{18}	s_9^{18}
$G(/G_2)$	s_1^{81}	$s_2^{36}s_1^9$	s_3^{27}	s_3^{27}	s_3^{27}	s_3^{27}	s_3^{27}	s_3^{27}	$s_6^9s_3^9$	$s_6^{12}s_3^3$	$s_6^{12}s_3^3$	$s_6^{12}s_3^3$	$s_3^{12}s_3^3$	$s_6^9s_3^9$	s_9^9	s_9^9	s_9^9
$G(/G_3)$	s_1^{54}	s_2^{27}	s_1^{54}	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	s_6^9	s_6^9	s_6^9	s_6^9	s_2^{27}	s_6^9	s_3^{18}	s_3^{18}	s_9^6
$G(/G_4)$	s_1^{54}	s_2^{27}	s_3^{18}	$s_3^{12}s_1^{18}$	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	s_6^9	$s_9^6s_2^9$	s_6^9	s_6^9	s_6^9	s_6^9	s_9^6	$s_9^4s_3^6$	s_9^6
$G(/G_5)$	s_1^{54}	s_2^{27}	s_3^{18}	s_3^{18}	$s_3^{12}s_1^{18}$	s_3^{18}	s_3^{18}	s_3^{18}	$s_6^6s_2^9$	s_6^9	s_6^9	s_6^9	s_6^9	s_6^9	s_3^{18}	s_9^6	$s_9^4s_1^6$
$G(/G_6)$	s_1^{54}	s_2^{27}	s_3^{18}	s_3^{18}	s_3^{18}	$s_3^{12}s_1^{18}$	s_3^{18}	s_3^{18}	s_6^9	s_6^9	s_6^9	$s_9^6s_2^9$	s_6^9	s_6^9	s_9^6	$s_9^4s_3^6$	$s_9^4s_3^6$
$G(/G_7)$	s_1^{54}	s_2^{27}	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	$s_3^{12}s_1^{18}$	s_3^{18}	s_6^9	s_6^9	$s_6^6s_2^9$	s_6^9	s_6^9	s_6^9	s_9^6	$s_9^4s_3^6$	$s_9^2s_3^1$
$G(/G_8)$	s_1^{54}	s_2^{27}	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	s_3^{18}	$s_3^{16}s_1^6$	s_6^9	s_6^9	s_6^9	s_6^9	s_6^9	$s_6^8s_2^3$	s_9^6	s_9^6	s_9^6
$G(/G_9)$	s_1^{27}	$s_2^9s_1^9$	s_3^9	s_3^9	$s_3^6s_1^9$	s_3^9	s_3^9	s_3^9	$s_6^3s_1^9$	$s_6^3s_3^3$	$s_6^3s_3^3$	$s_6^3s_3^3$	$s_6^3s_3^3$	s_3^9	s_3^9	s_9^3	$s_9^2s_3^3$
$G(/G_{10})$	s_1^{27}	$s_2^{12}s_1^3$	s_3^9	$s_3^6s_1^9$	s_3^9	s_3^9	s_3^9	s_3^9	$s_6^3s_3^3$	$s_6^3s_2^3s_1^3$	$s_6^4s_3$	$s_6^4s_3$	$s_6^4s_3^1$	$s_6^3s_3^3$	s_9^3	$s_9^2s_3^3$	s_9^3
$G(/G_{11})$	s_1^{27}	$s_2^{12}s_1^3$	s_3^9	s_3^9	s_3^9	s_3^9	$s_3^6s_1^9$	s_3^9	$s_6^3s_3^3$	$s_6^4s_3$	$s_6^3s_2^3s_1^3$	$s_6^4s_3$	$s_6^4s_3^1$	$s_6^3s_3^3$	s_9^3	$s_9^2s_3^3$	$s_9s_3^6$
$G(/G_{12})$	s_1^{27}	$s_2^{12}s_1^3$	s_3^9	s_3^9	s_3^9	$s_3^6s_1^9$	s_3^9	s_3^9	$s_6^3s_3^3$	$s_6^4s_3$	$s_6^4s_3$	$s_6^3s_2^3s_1^3$	$s_6^4s_3^1$	$s_6^3s_3^3$	s_9^3	$s_9^2s_3^3$	$s_9^2s_3^3$
$G(/G_{13})$	s_1^{27}	$s_2^{12}s_1^3$	s_1^{27}	s_3^9	s_3^9	s_3^9	s_3^9	s_3^9	$s_6^3s_3^3$	$s_6^4s_3$	$s_6^4s_3$	$s_6^4s_3$	$s_2^{12}s_1^3$	$s_6^3s_3^3$	s_3^9	s_3^9	s_9^3
$G(/G_{14})$	s_1^{27}	$s_2^9s_1^9$	s_3^9	s_3^9	s_3^9	s_3^9	s_3^9	$s_3^8s_1^3$	s_3^9	$s_6^3s_3^3$	$s_6^3s_3^3$	$s_6^3s_3^3$	$s_6^3s_3^3$	$s_6s_3^6s_1^3$	s_9^3	s_9^3	s_9^3
$G(/G_{15})$	s_1^{18}	s_2^9	s_1^{18}	s_3^6	s_1^{18}	s_3^6	s_3^9	s_3^6	s_2^9	s_6^3	s_6^3	s_6^3	s_2^9	s_6^3	s_1^{18}	s_3^6	s_3^6
$G(/G_{16})$	s_1^{18}	s_2^9	s_1^{18}	$s_3^4s_1^6$	s_3^6	$s_3^4s_1^6$	$s_3^4s_1^6$	s_3^6	s_6^3	$s_6^2s_2^3$	$s_6^2s_2^3$	$s_6^2s_2^3$	s_2^9	s_6^3	s_3^6	$s_3^4s_1^6$	s_3^6
$G(/G_{17})$	s_1^{18}	s_2^9	s_3^6	s_3^6	$s_3^4s_1^6$	$s_3^4s_1^6$	$s_3^2s_1^{12}$	s_3^6	$s_6^2s_2^3$	s_6^3	$s_6s_2^6$	$s_6^2s_2^3$	s_6^3	s_6^3	s_3^6	s_3^6	$s_3^4s_1^6$
$G(/G_{18})$	s_1^{18}	s_2^9	s_3^6	$s_3^2s_1^{12}$	$s_3^4s_1^6$	s_3^6	$s_3^4s_1^6$	s_3^6	$s_6^2s_2^3$	$s_6s_2^6$	$s_6^2s_2^3$	s_6^3	s_6^3	s_6^3	s_3^6	s_3^6	s_3^6
$G(/G_{19})$	s_1^{18}	s_2^9	s_1^{18}	s_3^6	s_3^6	s_3^6	s_3^6	$s_3^4s_1^6$	s_6^3	s_6^3	s_6^3	s_6^3	s_2^9	$s_6^2s_2^3$	s_3^6	s_3^6	s_9^2
$G(/G_{20})$	s_1^{18}	s_2^9	s_3^6	$s_3^4s_1^6$	$s_3^4s_1^6$	$s_3^2s_1^{12}$	s_3^6	s_3^6	$s_6^2s_2^3$	$s_2^6s_2^3$	s_6^3	$s_6s_2^6$	s_6^3	s_6^3	s_3^6	s_3^6	s_3^6
$G(/G_{21})$	s_1^{18}	s_2^9	s_1^{18}	s_3^6	s_3^6	s_3^6	s_3^6	s_3^6	s_6^3	s_6^3	s_6^3	s_6^3	s_2^9	s_6^3	s_3^6	s_9^2	s_9^2
$G(/G_{22})$	s_1^9	$s_2^3s_1^3$	s_3^3	$s_3^2s_1^3$	$s_3^2s_1^3$	$s_3s_1^6$	s_3^3	s_3^3	$s_6s_1^3$	$s_6s_1^3$	s_6s_3	$s_3s_2^3$	s_6s_3	s_3^3	s_3^3	s_3^3	s_3^3
$G(/G_{23})$	s_1^9	$s_2^3s_1^3$	s_1^9	s_3^3	s_1^9	s_3^3	s_3^3	s_3^3	$s_2^3s_1^3$	s_6s_3	s_6s_3	s_6s_3	$s_2^3s_1^3$	s_3^3	s_1^9	s_3^3	s_3^3
$G(/G_{24})$	s_1^9	$s_2^3s_1^3$	s_3^3	s_3^3	$s_3^2s_1^3$	$s_3^2s_1^3$	$s_3s_1^6$	s_3^3	$s_6s_1^3$	s_6s_3	$s_3s_2^3$	$s_6s_1^3$	s_6s_3	s_3^3	s_3^3	s_3^3	$s_3^2s_1^3$
$G(/G_{25})$	s_1^9	$s_2^3s_1^3$	s_3^3	$s_3s_1^6$	$s_3^2s_1^3$	s_3^3	$s_3^2s_1^3$	s_3^3	$s_6s_1^3$	$s_3s_2^3$	$s_6s_1^3$	s_6s_3	s_6s_3	s_3^3	s_3^3	s_3^3	s_3^3
$G(/G_{26})$	s_1^9	$s_2^4s_1$	s_1^9	$s_3^2s_1^3$	s_3^3	$s_3^2s_1^3$	$s_3^2s_1^3$	s_3^3	s_6s_3	$s_6s_2s_1$	$s_6s_2s_1$	$s_6s_2s_1$	$s_2^4s_1$	s_6s_3	s_3^3	$s_3^2s_1^3$	s_3^3
$G(/G_{27})$	s_1^9	$s_3^2s_1^3$	s_1^9	s_3^3	s_3^3	s_3^3	s_3^3	$s_2^3s_1^3$	s_3^3	s_6s_3	s_6s_3	s_6s_3	$s_2^3s_1^3$	$s_3^2s_2s_1$	s_3^3	s_3^3	s_9
$G(/G_{28})$	s_1^6	s_2^3	s_1^6	s_1^6	s_1^6	s_1^6	s_1^6	s_3^2	s_2^3	s_2^3	s_2^3	s_2^3	s_2^3	s_6	s_1^6	s_1^6	s_1^6
$G(/G_{29})$	s_1^6	s_2^3	s_1^6	s_3^2	s_1^6	s_3^2	s_3^2	s_1^6	s_2^3	s_6	s_6	s_6	s_2^3	s_2^3	s_1^6	s_3^2	s_3^2
$G(/G_{30})$	s_1^6	s_2^3	s_1^6	s_3^2	s_1^6	s_3^2	s_3^2	s_3^2	s_2^3	s_6	s_6	s_6	s_2^3	s_6	s_1^6	s_3^2	s_3^2
$G(/G_{31})$	s_1^3	s_1^3	s_1^3	s_3	s_1^3	s_3	s_3	s_1^3	s_1^3	s_3	s_3	s_3	s_1^3	s_1^3	s_1^3	s_1^3	s_1^3
$G(/G_{32})$	s_1^3	s_2s_1	s_1^3	s_1^3	s_1^3	s_1^3	s_1^3	s_3	s_2s_1	s_2s_1	s_2s_1	s_2s_1	s_2s_1	s_3	s_1^3	s_1^3	s_1^3
$G(/G_{33})$	s_1^2	s_2	s_1^2	s_1^2	s_1^2	s_1^2	s_1^2	s_1^2	s_2	s_2	s_2	s_2	s_2	s_2	s_1^2	s_1^2	s_1^2
$G(/G_{34})$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1

$C_G(H)|$ in addition, the dominant class of $K \cap H$ in $N_G(H)$ is the union of $t = \varphi(n)/m(H)$ conjugacy classes of G where φ is Euler function, i.e. the maturity of G is clearly defined by examining how a dominant class corresponding to H contains conjugacy classes. If $t = \varphi(n)/m(H) = 1$, the group G should be matured, but if $m(H) \leq \varphi(n)$ or $t > 2$, the group G is an unmatured concerning subgroup H.[13–17]

Theorem: The wreath products of the matured finite groups are again a matured group, but the wreath products of some finite groups with at least one unmatured group should be an unmatured group.[25]

3. Results and Discussion

According to the above Theorem and ref. 27, the f-NRG 1,3,5-trimethylbenzene (TMB) is an unmatured group isomorphic to $C_{3\,wr}\,S_3$ of order 162, see Figure 1.

In order to compute the mark table $M_{34\times 34}$ and then the set SSG_X of TMB with the symmetry $X = C_{3\,wr}\,S_3$, run the program below in the GAP prompt as follows:

```
LogTo("1,3,5-trimethylbenzene.txt");
 c3:=CyclicGroup(IsPermGroup,(3));
```

Table 1 (continued)

USCI	G_{18}	G_{19}	G_{20}	G_{21}	G_{22}	G_{23}	G_{24}	G_{25}	G_{26}	G_{27}	G_{28}	G_{29}	G_{30}	G_{31}	G_{32}	G_{33}	G_{34}
$G(/G_1)$	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_9^{18}	s_{27}^6	s_{27}^6	s_{27}^6	s_{54}^3	s_{54}^3	s_{81}^2	s_{162}
$G(/G_2)$	s_9^9	s_9^9	s_9^9	s_9^9	$s_{18}^3s_9^3$	$s_{18}^3s_9^3$	$s_{18}^3s_9^3$	$s_{18}^3s_9^3$	$s_{18}^4s_9$	$s_{18}^3s_9^3$	s_{27}^3	s_{27}^3	s_{27}^3	s_{27}^3	$s_{54}s_{27}$	s_{81}	s_{81}
$G(/G_3)$	s_3^{18}	s_3^{18}	s_9^6	s_3^{18}	s_{18}^3	s_6^9	s_{18}^3	s_{18}^3	s_6^9	s_6^9	s_9^6	s_9^6	s_9^6	s_{18}^3	s_{18}^3	s_{27}^2	s_{54}
$G(/G_4)$	s_9^6	s_9^6	$s_9^4s_3^6$	s_9^6	$s_{18}^2s_6^3$	s_{18}^3	s_{18}^3	$s_{18}s_6^6$	$s_{18}^2s_6^3$	s_{18}^3	s_9^6	s_{27}^2	s_{27}^2	s_{54}	s_{18}^3	s_{27}^2	s_{54}
$G(/G_5)$	s_9^6	s_9^6	$s_9^4s_3^6$	s_9^6	$s_{18}^2s_6^3$	s_6^9	$s_{18}^2s_6^3$	$s_{18}^2s_6^3$	s_{18}^3	s_{18}^3	s_9^6	s_9^6	s_9^6	s_{18}^3	s_{18}^3	s_{27}^2	s_{54}
$G(/G_6)$	s_9^6	s_9^6	$s_9^2s_3^{12}$	s_9^6	$s_{18}s_6^6$	s_{18}^3	$s_{18}^2s_6^3$	s_{18}^3	$s_{18}^2s_6^3$	s_{18}^3	s_9^6	s_{27}^2	s_{27}^2	s_{54}	s_{18}^3	s_{27}^2	s_{54}
$G(/G_7)$	s_9^6	s_9^6	s_9^6	s_6^9	s_{18}^3	s_{18}^3	$s_{18}s_6^6$	$s_{18}^2s_6^3$	$s_{18}^2s_6^3$	s_{18}^3	s_9^6	s_{27}^2	s_{27}^2	s_{54}	s_{18}^3	s_{27}^2	s_{54}
$G(/G_8)$	$s_9^4s_3^6$	$s_9^4s_3^6$	s_9^6	s_9^6	s_{18}^3	s_{18}^3	s_{18}^3	s_{18}^3	s_{18}^3	$s_9^2s_6^3$	s_{27}^2	s_9^6	s_{27}^2	s_{18}^3	s_{54}	s_{27}^2	s_{54}
$G(/G_9)$	s_9^3	s_9^3	$s_9^2s_3^3$	s_9^3	$s_{18}s_3^3$	$s_6^3s_3^3$	$s_{18}s_3^3$	$s_6^3s_3^3$	$s_{18}s_9$	s_9^3	s_9^3	s_9^3	s_9^3	s_9^3	$s_{18}s_9$	s_{27}	s_{27}
$G(/G_{10})$	s_9^3	s_9^3	$s_9^2s_3^3$	s_9^3	$s_{18}s_3^3$	$s_{18}s_9$	$s_{18}s_9$	$s_{18}s_9$	$s_{18}s_6s_3$	$s_{18}s_9$	s_9^3	s_{27}	s_{27}	s_{27}	$s_{18}s_9$	s_{27}	s_{27}
$G(/G_{11})$	s_9^3	s_9^3	s_9^3	s_9^3	$s_{18}s_9$	$s_{18}s_9$	$s_{18}s_3^3$	$s_{18}s_3^3$	$s_{18}s_6s_3$	$s_{18}s_9$	s_9^3	s_{27}	s_{27}	s_{27}	$s_{18}s_9$	s_{27}	s_{27}
$G(/G_{12})$	s_9^3	s_9^3	$s_9s_3^6$	s_9^3	$s_9s_6^3$	$s_{18}s_9$	$s_{18}s_3^3$	$s_{18}s_9$	$s_{18}s_6s_3$	$s_{18}s_9$	s_9^3	s_{27}	s_{27}	s_{27}	$s_{18}s_9$	s_{27}	s_{27}
$G(/G_{13})$	s_3^9	s_3^9	s_9^3	s_3^9	$s_{18}s_9$	$s_6^3s_3^3$	$s_{18}s_9$	$s_{18}s_9$	$s_6^4s_3$	$s_6^3s_3^3$	s_9^3	s_9^3	s_9^3	s_9^3	$s_{18}s_9$	s_{27}	s_{27}
$G(/G_{14})$	$s_9^2s_3^2$	$s_9^2s_3^3$	s_9^3	s_9^3	s_9^3	s_9^3	s_9^3	s_9^3	$s_{18}s_9$	$s_9^2s_6s_3$	s_{27}	s_9^3	s_{27}	s_9^3	s_{27}	s_{27}	s_{27}
$G(/G_{15})$	s_3^6	s_3^6	s_3^6	s_3^6	s_6^3	s_2^9	s_6^3	s_6^3	s_6^3	s_6^3	s_3^6	s_3^6	s_3^6	s_6^3	s_6^3	s_9^2	s_{18}
$G(/G_{16})$	s_3^6	s_3^6	s_3^6	s_3^6	s_6^3	s_6^3	s_6^3	s_6^3	$s_6^2s_2^3$	s_6^3	s_3^6	s_9^2	s_9^2	s_{18}	s_6^3	s_9^2	s_{18}
$G(/G_{17})$	s_9^2	s_9^2	s_3^6	s_9^2	s_6^3	$s_6s_2^3$	$s_6s_2^3$	s_6^3	s_6^3	s_{18}	s_3^6	s_9^2	s_9^2	s_{18}	s_6^3	s_9^2	s_{18}
$G(/G_{18})$	s_9^2	s_9^2	s_3^6	s_9^2	s_{18}	$s_6^2s_3^2$	$s_3^4s_2^3$	$s_6^2s_3^2$	s_6^3	s_{18}	s_9^2	s_3^6	s_9^2	s_6^3	s_{18}	s_9^2	s_{18}
$G(/G_{19})$	$s_3^4s_1^6$	$s_3^4s_1^6$	s_9^2	s_3^6	$s_6^2s_2^3$	s_3^6	$s_6^2s_3^2$	s_{18}	s_6^3	$s_6^2s_2^3$	s_9^2	s_3^6	s_9^2	s_6^3	s_{18}	s_9^2	s_{18}
$G(/G_{20})$	s_9^2	s_9^2	$s_3^4s_1^6$	s_9^2	s_{18}	$s_6^2s_3^2$	s_{18}	$s_6^2s_3^2$	s_6^3	s_{18}	s_3^6	s_9^2	s_9^2	s_{18}	s_6^3	s_9^2	s_{18}
$G(/G_{21})$	s_3^6	s_3^6	s_9^2	$s_3^5s_1^3$	$s_6^2s_2^3$	s_6^3	s_6^3	s_{18}	s_6^3	s_6^3	s_9^2	s_9^2	$s_9s_3^3$	s_{18}	s_{18}	s_9^2	s_{18}
$G(/G_{22})$	s_9	s_9	$s_3^2s_1^3$	s_9	$s_6s_1^3$	s_3^3	s_9	s_6s_3	s_6s_3	s_9	s_3^3	s_3^3	s_3^3	s_9	s_6s_3	s_9	s_9
$G(/G_{23})$	s_3^3	s_3^3	s_3^3	s_3^3	s_6s_3	$s_2^3s_1^3$	s_6s_3	s_6s_3	s_6s_3	s_3^3	s_3^3	s_3^3	s_3^3	s_3^3	s_6s_3	s_9	s_9
$G(/G_{24})$	s_9	s_9^1	s_3^3	s_9	s_6s_3	$s_2^3s_1^3$	s_6s_3	s_6s_3	s_6s_3	s_9	s_3^3	s_9	s_9	s_9	s_6s_3	s_9	s_9
$G(/G_{25})$	s_9	s_9	s_3^3	s_9	s_6s_3	s_6s_3	s_3^3	$s_6s_1^3$	s_6s_3	s_9	s_3^3	s_9	s_9	s_9	s_6s_3	s_9	s_9
$G(/G_{26})$	s_3^3	s_3^3	s_3^3	s_3^3	s_6s_3	s_6s_3	s_3^3	s_6s_3	$s_6s_2s_1$	s_6s_3	s_3^3	s_9	s_9	s_9	s_6s_3	s_9	s_9
$G(/G_{27})$	$s_2^3s_1^3$	$s_2^3s_1^3$	s_9^1	s_3^3	s_9	s_3^3	s_9	s_9	s_6s_3	$s_3^2s_2s_1$	s_9	s_3^3	s_9	s_3^3	s_9	s_9	s_9
$G(/G_{28})$	s_3^2	s_3^2	s_1^6	s_3^2	s_2^3	s_2^3	s_2^3	s_2^3	s_2^3	s_6	s_6	s_2^3	s_2^3	s_6	s_2^3	s_6	s_6
$G(/G_{29})$	s_1^6	s_1^6	s_3^2	s_3^2	s_2^3	s_2^3	s_6	s_6	s_6	s_2^3	s_2^3	s_2^3	s_2^3	s_2^3	s_6	s_3^2	s_6
$G(/G_{30})$	s_3^2	s_3^2	s_3^2	$s_3s_1^3$	s_2^3	s_2^3	s_6	s_6	s_6	s_6	s_2^3	s_2^3	s_2^3	s_6	s_6	s_3	s_6
$G(/G_{31})$	s_1^3	s_1^3	s_3^1	s_3	s_3	s_1^3	s_3	s_3	s_3	s_1^3	s_3	s_1^3	s_3	s_1^3	s_3	s_3	s_3
$G(/G_{32})$	s_3^1	s_3^1	s_1^3	s_3	s_2s_1	s_2s_1	s_2s_1	s_2s_1	s_2s_1	s_3	s_1^3	s_3	s_3	s_3	s_2s_1	s_3	s_3
$G(/G_{33})$	s_1^2	s_1^2	s_1^2	s_1^2	s_2	s_2	s_2	s_2^1	s_2	s_2	s_2	s_1^2	s_1^2	s_2	s_2	s_2	s_2
$G(/G_{34})$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1

```
s3:=SymmetricGroup(IsPermGroup,(3));
 X:=WreathProduct(c3,s3);
Order(X);
IsPermGroup(X);
 s:=ConjugacyClassesSubgroups(X);
  Sort("s");
  M:=TableOfMarks(X);
   Display(s);
    LogTo( );
     Print("1,3,5-trimethylbenzene.txt", "|n");
```

Afterwards, it can be seen that the non-redundant set of subgroups of *X* with size 34 consists of the following elements required to calculate all the Fujita's topological indices (i.e. USCIs) as collected in Table 1:

$G_1 = Id$, $G_2 = \langle(4,7)(5,8)(6,9)\rangle$, $G_3 = \langle(1,2,3)(4,5,6)(7,8,9)\rangle$,
$G_4 = \langle(4,5,6)(7,8,9)\rangle$, $G_5 = \langle(4,5,6)(7,9,8)\rangle$, $G_6 = \langle(7,8,9)\rangle$,
$G_7 = \langle(1,2,3)(4,5,6)(7,9,8)\rangle$, $G_8 = \langle(1,4,7)(2,5,8)(3,6,9)\rangle$,
$G_9 = \langle(4,5,6)(7,9,8),(4,7)(5,8)(6,9)\rangle$, $G_{10} = \langle(4,5,6)(7,8,9),(4,7)(5,8)(6,9)\rangle$,
$G_{11} = \langle(4,7)(5,8)(6,9),(1,3,2)(4,5,6)(7,8,9)\rangle$, $G_{12} = \langle(7,8,9),(1,4)(2,5)(3,6)\rangle$,
$G_{13} = \langle(4,7)(5,8)(6,9),(1,2,3)(4,5,6)(7,8,9)\rangle$,
$G_{14} = \langle(1,4,7)(2,5,8)(3,6,9),(4,7)(5,8)(6,9)\rangle$,
$G_{15} = \langle(4,5,6)(7,9,8),(1,2,3)(4,5,6)(7,8,9)\rangle$, $G_{16} = \langle(7,8,9),(1,2,3)(4,5,6)\rangle$,
$G_{17} = \langle(7,8,9),(1,2,3)(4,6,5)\rangle$, $G_{18} = \langle(4,5,6)(7,8,9),(1,2,3)(7,8,9)\rangle$,
$G_{19} = \langle(1,2,3)(4,5,6)(7,8,9),(1,4,7)(2,5,8)(3,6,9)\rangle$, $G_{20} = \langle(7,8,9),(4,5,6)\rangle$,
$G_{21} = \langle(1,2,3)(4,5,6)(7,8,9),(1,4,7,2,5,8,3,6,9)\rangle$,
$G_{22} = \langle(7,8,9),(4,5,6),(4,7)(5,8)(6,9)\rangle$,
$G_{23} = \langle(4,5,6)(7,9,8),(4,7)(5,8)(6,9),(1,2,3)(4,5,6)(7,8,9)\rangle$,
$G_{24} = \langle(7,8,9),(1,2,3)(4,6,5),(1,4)(2,5)(3,6)\rangle$,
$G_{25} = \langle(4,5,6)(7,8,9),(1,2,3)(7,8,9),(1,4)(2,5)(3,6)\rangle$,
$G_{26} = \langle(7,8,9),(1,2,3)(4,5,6),(1,4)(2,5)(3,6)\rangle$,
$G_{27} = \langle(1,2,3)(4,5,6)(7,8,9),(1,4,7)(2,5,8)(3,6,9),(4,7)(5,8)(6,9)\rangle$,
$G_{28} = \langle(7,8,9),(4,5,6),(1,2,3)\rangle$,
$G_{29} = \langle(4,5,6)(7,9,8),(1,2,3)(4,5,6)(7,8,9),(1,4,7)(2,5,8)(3,6,9)\rangle$,
$G_{30} = \langle(4,5,6)(7,9,8),(1,2,3)(4,5,6)(7,8,9),(1,4,7,2,5,8,3,6,9)\rangle$,
$G_{31} = \langle(4,5,6)(7,9,8),(1,2,3)(4,5,6)(7,8,9),(1,4,7)(2,5,8)(3,6,9),(4,7)(5,8)(6,9)\rangle$,
$G_{32} = \langle(7,8,9),(4,5,6),(4,7)(5,8)(6,9),(1,2,3)\rangle$,
$G_{33} = \langle(7,8,9),(4,5,6),(1,2,3),(1,4,7)(2,5,8)(3,6,9)\rangle$, $G_{34} = X$.

Now, we utilize GAP to calculate all the USCIs of *X* for TMB. As a matter of fact, for instance, to calculate the column no. 26 in Table 1 (i.e. for G_{26} of order 18) equivalently for i = 1 to 34, $Z(G(G_i) \downarrow G_{26}, s_d)$, the following program is operated in GAP system as well:

```
G26=GroupWithGenerators((7,8,9),(1,2,3)(4,5,6),(1,4)
(2,5)(3,6));
 M26:=TableOfMarks(G26);
  Inv:=(M26)^-1;
   S26:=ConjugacyClassesSubgroups(G26);
    Sort(s26);
   A:=[[18,0,0,0,0,0,0,0,0,0,0,0],[9,9,0,0,0,0,0,0,
   0,0,0,0],[6,0,6,0,0,0,0,0,0,0,0,0],[6,0,0,6,0,0,0,0
   ,0,0,0,0],[6,0,0,0,6,0,0,0,0,0,0,0],[6,0,0,0,0,6,0,
   0,0,0,0,0],[3,3,3,0,0,0,3,0,0,0,0,0],[3,3,0,3,0,0,0
   ,3,0,0,0,0],[3,3,0,0,3,0,0,0,3,0,0,0],[3,3,0,0,0,3,
   0,0,0,3,0,0],[2,0,2,2,2,2,0,0,0,0,2,0],[1,1,1,1,1,1
   ,1,1,1,1,1,1]];
 Column26:=A*(Inv);
  Print("Column26", "|n");
```

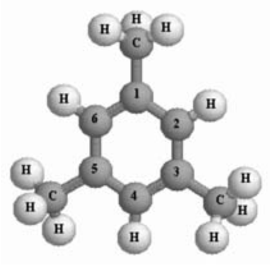

Figure 1: Structure of 1,3,5-trimethylbenzene

4. Conclusions

By applying similar and above calculation for other columns, we are able to calculate Fujita's combinatorial enumeration USCI table of 1,3,5-trimethylbenzene stored in Table 1 which would also be valuable in other applications such as in the context of chemical applications of graph theory and aromatic compounds.[1–18, 28]

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Povzetek

Nezrela, popolnoma nerigidna grupa 1,3,5-trimetilbenzena je izomorfna s spletnim produktom ciklične grupe tretjega reda in simetrične grupe šestega reda na treh črkah (gl. *Int. J. Quantum Chem*. **2007**, *107*, 340 and *Bull. Chem. Soc. Jpn*. **2008**, *81*, 279).V tem prispevku prvič uspešno izpeljemo tabelo enotnih zmanjšanih cikličnih indeksov (ki jo je vpeljal S. Fujita) za popolnoma nerigidno grupo 1,3,5-trimetilbenzena reda 162.