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Full Non-Rigid Group Theory for Hexamethylethane

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The non-rigid molecule group theory in which the dynamical symmetry operations are defined as physical operations is applied to deduce the character table of the full non-rigid molecule group (f-NRG) of hexamethylethane. The f-NRG of this molecule is seen to be isomorphic to the group $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$ of order 8748 which has 174 conjugacy classes. Here $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$ denotes the semi direct product of the direct products of 6 copies of the cyclic group Z_3 by the dihedral group of order 12. Using some results in finite group theory and GAP system, we find the complex character table of this group.

Key Words: Character table, Hexamethylethane, Full non-rigid group, Semidirect product.

INTRODUCTION

A non-rigid molecule is a molecular system which presents large vibrational modes. This kind of motion appears whenever the molecule possesses various isoenergetic forms seperated by relatively low energy barrier. In such cases, intra-molecular transformations occur. Following Smeyers the complete set of molecular conversion operations which commute with the nuclear motion operator contains overall rotation operations, describing the molecule rotating as a whole, and the non-rigid tunneling motion operations, describing molecular moieties moving with respect to the rest of the molecule[1,2]. Such a set forms a group, which is called the full non-rigid group (f-NRG). Numerous applications of the group theory for the non-rigid molecules to large amplitude vibrational spectroscopy of small molecules have appeared in the literatures[3-9].

Longuet-Higgins investigated the symmetry groups of non-rigid molecules where changes from one conformation to another can occur easily[10]. In many cases these symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules and their character tables are not known. It is therefore of some interest and importance to develop simple methods of calculating these character tables, which are needed for classification of wave functions, determination of selection

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rules and so on. The method which is described here is appropriate for molecules which have a number of XO_2 or XH_3 groups attached to a rigid framework. An example of such molecules is hexamethylethane which is considered here in some detail.

In this paper, we show that the symmetry of the Fig. 1 leads to a permutation group of order 8748 with 174 conjugacy classes and 174 irreducible characters for the symmetry group of hexamethylethane. As seen in Fig. 1, the molecule has two branches "a" and "b". We need to specify feasible symmetries of the molecule. Our approach here is first to specify the algebraic structure of the full non-rigid group of hexamethylethane. With a geometric consideration of dynamic symmetries of the molecule we will show that the f-NRG of hexamethylethane can be specified by a set of permutations. Then based on the structure of the group we apply GAP[11] as a useful computer package to compute the character table of the f-NRG of this molecule.

Alperin and Bell[12] notations were used for the standard notations and terminology of character theory. The motivation for this study is outlined in Refeerences[13-33] and the reader is encouraged to consult these papers for background material and basic computational techniques. Computations are carried out with the aid of GAP and this was done by characterizing the algebraic structure of the f-NRG as the semidirect products of known groups.

EXPERIMENTAL

In this section we describe some notation which used in the paper. Suppose G and H are groups and $f:G \to H$ is a function such that $f(xy) = f(x)f(y)$. f is called a homomorphism from G into H. If f is one to one, we call f monomorphism. We now assume that N be a subgroup of G. N is called a normal subgroup of G, if for any $g \in G$ and $x \in N$, $g^{-1}xg \in N$. Moreover, if H is another subgroup of G such that $H \cap N = \{e\}$ and $G = HN = \{xy|\ x \in H, y \in N\}$, then we say that G is a semidirect product of N by H denoted by $N \wedge H$. Let us make some observations about semidirect product. Since $G = NH$, each $x \in G$ can be written uniquely as $x = nh$ for some $n \in N$ and $h \in H$. Fix element h in H, since N is normal in G, conjugation by h maps N to H, consequently we can define a map φ_h: $N \to N$ by $\varphi_h(n) = hnh^{-1}$ for $n \in N$. It is easy to show that φ_h is an automorphism of N and also that $\varphi_{ho}\ \varphi_h = \varphi_{hj}$ for any $j \in H$. Therefore, we have constructed a homomorphism φ: $H \to Aut(N)$, where $\varphi(h) = \varphi_h$, we call φ conjugation homomorphism of the semidirect product G and write $G = N \wedge_\varphi H$. We can see that if the homomorphism φ: $H \to Aut(N)$ defined above is trivial, then semidirect product reduces to the direct product of $N \times H$.

It is a well-known fact that the homomorphism φ completely determines the semi-direct product. Furthermore, if H is cyclic and φ and ψ are monomorphism from H into Aut(N) such that $\varphi(H)$ and $\psi(H)$ are conjugate in Aut(N), then the semi-direct products $N \wedge_\varphi H$ and $N \wedge_\psi H$ are isomorphic[12].

RESULTS AND DISCUSSION

Before going into the details of the computations of hexamethylethane, it is mentioned that we consider the speed of rotations of methyl groups sufficiently high so that the mean time dynamical symmetry of the molecules makes sense. In order to characterize the f-NRG of hexamethylethane it is noted that each dynamic symmetry operation of this molecule, considering the rotations of CH_3 groups, is composed of two sequential physical operations. First we have a physical symmetry of the hexamethylethane framework which consists of two carbon atoms, which are denoted by "a" and "b" in Fig. 1. In the event that free rotation around the C_a-C_b bound is not favorable due to steric crowding, the group of the 8 carbon atoms of the molecule would correspond to a rigid group of the framework. The rotational subgroup is D_3, the dihedral group of order 6 for this framework or a group with 6 operations and it is isomorphic to S_3, the symmetric group on 3 letters. When one includes the inversion operation, this becomes a group of 12 operations denoted by G_{12}, which is isomorphic to the dihedral group of order 12.

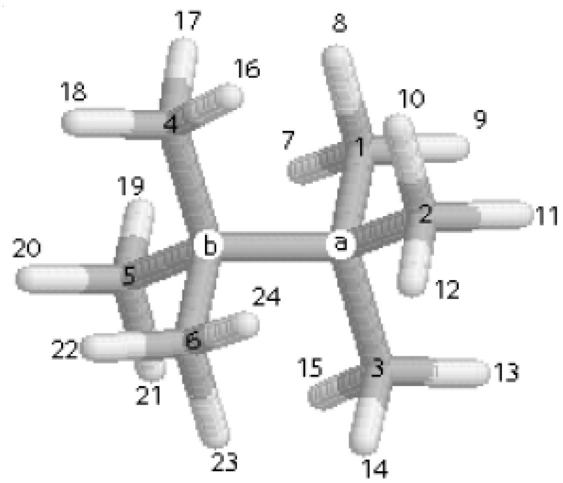

Fig. 1. Structure of hexamethylethane

We may also call this correlated motion or the groups do not rotate freely. The protons of the methyl group will still be allowed to rotate freely since the barrier for that is less than a few kcal/mol. In this case, the symmetry group of the hexamethylethane is $3^6 \wedge G_{12}$, or equivalently $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$.

The computations of the symmetry properties of the molecule are carried out using GAP which is group theoretical software for solving computational problems in computational group theory. The following program was run at the GAP prompt to compute all representatives of the conjugacy classes, Table-1 and irreducible characters, of the f-NRG of hexamethylethane, *i.e.*, $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$.

TABLE-1
REPRESENTATIVES OF THE CONJUGACY CLASSES OF THE GROUP ($Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3$) ^ G_{12}, THE NON-RIGID GROUP OF HEXAMETHYLETHANE CONTAINING 8748 OPERATIONS

No.	Representatives	Size	No.	Representatives	Size
1	( )	1	59	(4,6,5)(7,9,8)(13,14,15)(16,17,18)	6
2	(1,2,3)	6	60	(1,2,3)(4,6,5)(7,9,8)(13,14,15)(16,17,18)	12
3	(1,3,2)	6	61	(1,3,2)(4,6,5)(7,9,8)(13,14,15)(16,17,18)	12
4	(1,2,3)(4,5,6)	6	62	(1,2,3)(7,9,8)(13,14,15)(16,18,17)	6
5	(1,3,2)(4,5,6)	12	63	(1,3,2)(7,9,8)(13,14,15)(16,18,17)	12
6	(1,3,2)(4,6,5)	6	64	(4,5,6)(7,9,8)(13,14,15)(16,18,17)	6
7	(4,5,6)(16,17,18)	6	65	(1,2,3)(4,5,6)(7,9,8)(13,14,15)(16,18,17)	12
8	(1,2,3)(4,5,6)(16,17,18)	6	66	(1,3,2)(4,5,6)(7,9,8)(13,14,15)(16,18,17)	12
9	(1,3,2)(4,5,6)(16,17,18)	6	67	(4,6,5)(7,9,8)(13,14,15)(16,18,17)^	12
10	(4,6,5)(16,17,18)	12	68	(1,2,3)(4,6,5)(7,9,8)(13,14,15)(16,18,17)	12
11	(1,2,3)(4,6,5)(16,17,18)	12	69	(1,3,2)(4,6,5)(7,9,8)(13,14,15)(16,18,17)	12
12	(1,3,2)(4,6,5)(16,17,18)	12	70	(1,3,2)(7,9,8)(13,15,14)	2
13	(4,6,5)(16,18,17)	6	71	(1,3,2)(4,5,6)(7,9,8)(13,15,14)	6
14	(1,2,3)(4,6,5)(16,18,17)	6	72	(1,3,2)(4,6,5)(7,9,8)(13,15,14)	6
15	(1,3,2)(4,6,5)(16,18,17)	6	73	(1,2,3)(4,5,6)(7,9,8)(13,15,14)(16,17,18)	6
16	(7,8,9)(16,17,18)	3	74	(1,3,2)(4,5,6)(7,9,8)(13,15,14)(16,17,18)	6
17	(1,2,3)(7,8,9)(16,17,18)	12	75	(1,2,3)(4,6,5)(7,9,8)(13,15,14)(16,17,18)	12
18	(1,3,2)(7,8,9)(16,17,18)	12	76	(1,3,2)(4,6,5)(7,9,8)(13,15,14)(16,17,18)	12
19	(1,2,3)(4,5,6)(7,8,9)(16,17,18)	6	77	(4,6,5)(7,9,8)(13,15,14)(16,18,17)	3
20	(1,3,2)(4,5,6)(7,8,9)(16,17,18)	12	78	(1,2,3)(4,6,5)(7,9,8)(13,15,14)(16,18,17)	6
21	(1,3,2)(4,6,5)(7,8,9)(16,17,18)	6	79	(1,3,2)(4,6,5)(7,9,8)(13,15,14)(16,18,17)	6
22	(7,8,9)(16,18,17)	6	80	(1,2,3)(4,5,6)(7,8,9)(10,11,12)(13,14,15)(16,17,18)	1
23	(1,2,3)(7,8,9)(16,18,17)	12	81	(1,3,2)(4,5,6)(7,8,9)(10,11,12)(13,14,15)(16,17,18)	6
24	(1,3,2)(7,8,9)(16,18,17)	12	82	(1,3,2)(4,6,5)(7,8,9)(10,11,12)(13,14,15)(16,17,18)	6
25	(4,5,6)(7,8,9)(16,18,17)	12	83	(1,2,3)(4,6,5)(7,8,9)(10,11,12)(13,14,15)(16,18,17)	6
26	(1,2,3)(4,5,6)(7,8,9)(16,18,17)	12	84	(1,3,2)(4,6,5)(7,8,9)(10,11,12)(13,14,15)(16,18,17)	6
27	(1,3,2)(4,5,6)(7,8,9)(16,18,17)	12	85	(1,2,3)(4,5,6)(7,9,8)(10,11,12)(13,14,15)(16,18,17)	3
28	(4,6,5)(7,8,9)(16,18,17)	12	86	(1,3,2)(4,5,6)(7,9,8)(10,11,12)(13,14,15)(16,18,17)	12
29	(1,2,3)(4,6,5)(7,8,9)(16,18,17)	12	87	(1,3,2)(4,6,5)(7,9,8)(10,11,12)(13,14,15)(16,18,17)	6
30	(1,3,2)(4,6,5)(7,8,9)(16,18,17)	12	88	(1,3,2)(4,5,6)(7,9,8)(10,11,12)(13,15,14)(16,17,18)	2
31	(7,9,8)(16,18,17)	3	89	(1,3,2)(4,6,5)(7,9,8)(10,11,12)(13,15,14)(16,17,18)	6
32	(1,2,3)(7,9,8)(16,18,17)	12	90	(1,2,3)(4,6,5)(7,9,8)(10,11,12)(13,15,14)(16,18,17)	3
33	(1,3,2)(7,9,8)(16,18,17)	12	91	(1,3,2)(4,6,5)(7,9,8)(10,11,12)(13,15,14)(16,18,17)	6
34	(1,2,3)(4,5,6)(7,9,8)(16,18,17)	6	92	(1,3,2)(4,6,5)(7,9,8)(10,12,11)(13,15,14)(16,18,17)	1
35	(1,3,2)(4,5,6)(7,9,8)(16,18,17)	12	93	(1,7,13)(2,8,14)(3,9,15)(4,10,16)(5,11,17)(6,12,18)	162
36	(1,3,2)(4,6,5)(7,9,8)(16,18,17)	6	94	(1,7,13,2,8,14,3,9,15)(4,10,16)(5,11,17)(6,12,18)	324
37	(1,2,3)(7,8,9)(13,14,15)	2	95	(1,7,13,3,9,15,2,8,14)(4,10,16)(5,11,17)(6,12,18)	324
38	(1,3,2)(7,8,9)(13,14,15)	6	96	(1,7,13,2,8,14,3,9,15)(4,10,16,5,11,17,6,12,18)	162
39	(1,2,3)(4,5,6)(7,8,9)(13,14,15)	6	97	(1,7,13,3,9,15,2,8,14)(4,10,16,5,11,17,6,12,18)	324
40	(1,3,2)(4,5,6)(7,8,9)(13,14,15)	12	98	(1,7,13,3,9,15,2,8,14)(4,10,16,6,12,18,5,11,17)	162
41	(1,2,3)(4,6,5)(7,8,9)(13,14,15)	6	99	(1,4,7,10,13,16)(2,5,8,11,14,17)(3,6,9,12,15,18)	486
42	(1,3,2)(4,6,5)(7,8,9)(13,14,15)	12	100	(1,4,7,10,13,16,2,5,8,11,14,17,3,6,9,12,15,18)	486
43	(4,5,6)(7,8,9)(13,14,15)(16,17,18)	3	101	(1,4,7,10,13,16,3,6,9,12,15,18,2,5,8,11,14,17)	486
44	(1,2,3)(4,5,6)(7,8,9)(13,14,15)(16,17,18)	6	102	(1,10)(2,11)(3,12)(4,13)(5,14)(6,15)(7,16)(8,17)(9,18)	27
45	(1,3,2)(4,5,6)(7,8,9)(13,14,15)(16,17,18)	6	103	(1,10,2,11,3,12)(4,13)(5,14)(6,15)(7,16)(8,17)(9,18)	81
46	(4,6,5)(7,8,9)(13,14,15)(16,17,18)	12	104	(1,10,3,12,2,11)(4,13)(5,14)(6,15)(7,16)(8,17)(9,18)	81
47	(1,2,3)(4,6,5)(7,8,9)(13,14,15)(16,17,18)	12	105	(1,10,2,11,3,12)(4,13,5,14,6,15)(7,16)(8,17)(9,18)	81
48	(1,3,2)(4,6,5)(7,8,9)(13,14,15)(16,17,18)	12	106	(1,10,3,12,2,11)(4,13,5,14,6,15)(7,16)(8,17)(9,18)	162
49	(4,6,5)(7,8,9)(13,14,15)(16,18,17)	6	107	(1,10,3,12,2,11)(4,13,6,15,5,14)(7,16)(8,17)(9,18)	81
50	(1,2,3)(4,6,5)(7,8,9)(13,14,15)(16,18,17)	6	108	(1,10,2,11,3,12)(4,13,5,14,6,15)(7,17,8,18,9,16)	27
51	(1,3,2)(4,6,5)(7,8,9)(13,14,15)(16,18,17)	6	109	(1,10,3,12,2,11)(4,13,5,14,6,15)(7,17,8,18,9,16)	81
52	(1,3,2)(7,9,8)(13,14,15)	6	110	(1,10,3,12,2,11)(4,13,6,15,5,14)(7,17,8,18,9,16)	81
53	(1,3,2)(4,5,6)(7,9,8)(13,14,15)	6	111	(1,10,3,12,2,11)(4,13,6,15,5,14)(7,18,9,17,8,16)	27
54	(1,3,2)(4,6,5)(7,9,8)(13,14,15)	6	112	(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)	27
55	(1,2,3)(7,9,8)(13,14,15)(16,17,18)	6	113	(1,2,3)(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)	54
56	(1,3,2)(7,9,8)(13,14,15)(16,17,18)	12	114	(1,3,2)(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)	54
57	(1,2,3)(4,5,6)(7,9,8)(13,14,15)(16,17,18)	12	115	(4,16,5,17,6,18)(7,13)(8,14)(9,15)	54
58	(1,3,2)(4,5,6)(7,9,8)(13,14,15)(16,17,18)	12	116	(1,2,3)(4,16,5,17,6,18)(7,13)(8,14)(9,15)	54
117	(1,3,2)(4,16,5,17,6,18)(7,13)(8,14)(9,15)	54	146	(1,3,2)(4,16,6,18,5,17)(7,13,8,14,9,15)(10,11,12)	54
118	(4,16,6,18,5,17)(7,13)(8,14)(9,15)	54	147	(1,3,2)(4,16)(5,17)(6,18)(7,13,9,15,8,14)(10,11,12)	54

119	(1,2,3)(4,16,6,18,5,17)(7,13)(8,14)(9,15)	54	148	(1,3,2)(4,16,5,17,6,18)(7,13,9,15,8,14)(10,11,12)	54
120	(1,3,2)(4,16,6,18,5,17)(7,13)(8,14)(9,15)	54	149	(1,2,3)(4,16,6,18,5,17)(7,13,9,15,8,14)(10,11,12)	27
121	(1,2,3)(4,16)(5,17)(6,18)(7,13,8,14,9,15)	54	150	(1,3,2)(4,16,6,18,5,17)(7,13,9,15,8,14)(10,11,12)	54
122	(1,3,2)(4,16)(5,17)(6,18)(7,13,8,14,9,15)	54	151	(1,3,2)(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)(10,12,11)	27
123	(4,16,5,17,6,18)(7,13,8,14,9,15)	27	152	(1,3,2)(4,16,5,17,6,18)(7,13)(8,14)(9,15)(10,12,11)	54
124	(1,2,3)(4,16,5,17,6,18)(7,13,8,14,9,15)	54	153	(1,3,2)(4,16,6,18,5,17)(7,13)(8,14)(9,15)(10,12,11)	54
125	(1,3,2)(4,16,5,17,6,18)(7,13,8,14,9,15)	54	154	(1,3,2)(4,16,5,17,6,18)(7,13,8,14,9,15)(10,12,11)	27
126	(4,16,6,18,5,17)(7,13,8,14,9,15)	54	155	(1,3,2)(4,16,6,18,5,17)(7,13,8,14,9,15)(10,12,11)	54
127	(1,2,3)(4,16,6,18,5,17)(7,13,8,14,9,15)	54	156	(1,3,2)(4,16,6,18,5,17)(7,13,9,15,8,14)(10,12,11)	27
128	(1,3,2)(4,16,6,18,5,17)(7,13,8,14,9,15)	54	157	(1,4)(2,5)(3,6)(7,16)(8,17)(9,18)(10,13)(11,14)(12,15)	81
129	(1,2,3)(4,16)(5,17)(6,18)(7,13,9,15,8,14)	54	158	(1,4,2,5,3,6)(7,16)(8,17)(9,18)(10,13)(11,14)(12,15)	162
130	(1,3,2)(4,16)(5,17)(6,18)(7,13,9,15,8,14)	54	159	(1,4,3,6,2,5)(7,16)(8,17)(9,18)(10,13)(11,14)(12,15)	162
131	(1,2,3)(4,16,5,17,6,18)(7,13,9,15,8,14)	54	160	(1,4)(2,5)(3,6)(7,17,8,18,9,16)(10,13)(11,14)(12,15)	81
132	(1,3,2)(4,16,5,17,6,18)(7,13,9,15,8,14)	54	161	(1,4,2,5,3,6)(7,17,8,18,9,16)(10,13)(11,14)(12,15)	162
133	(4,16,6,18,5,17)(7,13,9,15,8,14)	27	162	(1,4,3,6,2,5)(7,17,8,18,9,16)(10,13)(11,14)(12,15)	162
134	(1,2,3)(4,16,6,18,5,17)(7,13,9,15,8,14)	54	163	(1,4)(2,5)(3,6)(7,18,9,17,8,16)(10,13)(11,14)(12,15)	81
135	(1,3,2)(4,16,6,18,5,17)(7,13,9,15,8,14)	54	164	(1,4,2,5,3,6)(7,18,9,17,8,16)(10,13)(11,14)(12,15)	162
136	1,2,3)(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)(10,11,12)	27	165	(1,4,3,6,2,5)(7,18,9,17,8,16)(10,13)(11,14)(12,15)	162
137	1,3,2)(4,16)(5,17)(6,18)(7,13)(8,14)(9,15)(10,11,12)	54	166	(1,4,2,5,3,6)(7,16)(8,17)(9,18)(10,14,11,15,12,13)	81
138	1,2,3)(4,16,5,17,6,18)(7,13)(8,14)(9,15)(10,11,12)	54	167	(1,4,3,6,2,5)(7,16)(8,17)(9,18)(10,14,11,15,12,13)	162
139	1,3,2)(4,16,5,17,6,18)(7,13)(8,14)(9,15)(10,11,12)	54	168	(1,4,2,5,3,6)(7,17,8,18,9,16)(10,14,11,15,12,13)	81
140	1,2,3)(4,16,6,18,5,17)(7,13)(8,14)(9,15)(10,11,12)	54	169	(1,4,3,6,2,5)(7,17,8,18,9,16)(10,14,11,15,12,13)	162
141	1,3,2)(4,16,6,18,5,17)(7,13)(8,14)(9,15)(10,11,12)	54	170	(1,4,2,5,3,6)(7,18,9,17,8,16)(10,14,11,15,12,13)	81
142	1,3,2)(4,16)(5,17)(6,18)(7,13,8,14,9,15)(10,11,12)	54	171	(1,4,3,6,2,5)(7,18,9,17,8,16)(10,14,11,15,12,13)	162
143	(1,2,3)(4,16,5,17,6,18)(7,13,8,14,9,15)(10,11,12)	27	172	1,4,3,6,2,5)(7,16)(8,17)(9,18)(10,15,12,14,11,13)	81
144	(1,3,2)(4,16,5,17,6,18)(7,13,8,14,9,15)(10,11,12)	54	173	(1,4,3,6,2,5)(7,17,8,18,9,16)(10,15,12,14,11,13)	81
145	(1,2,3)(4,16,6,18,5,17)(7,13,8,14,9,15)(10,11,12)	54	174	(1,4,3,6,2,5)(7,18,9,17,8,16)(10,15,12,14,11,13)	81

```
LogTo("gcharactertable.txt");
α:=(7,8,9);
β:=(10,11,12);
γ:=(13,14,15);
δ:=(16,17,18);
ε:=(19,20,21);
φ:=(22,23,24);
Hex:=GroupWithGenerators([α,β,γ,δ,ε,φ,(1,2,3,4,5,6),(2,6)(3,5)]);
Order(Hex);
Char:=Character table (Hex);
Con:=List(ConjugacyClassess(Char),x->Elements(x));
SizesConjugacyClasses(Char);
Display(Char);
Display(Con);
Print("Char", "\n");
LogTo( );
```

Assume C is the character table of the f-NRG of hexamethylethane, by the above GAP program C is a 174×174 matrix, consists of 174 irreducible characters and 174 conjugacy classes, since it is very large in size, it is deposited as a supplementary material to this letter. In the supplementary Table-2, $A = (-1 - i\sqrt{3})/2$, $B = -1 - i\sqrt{3}$, $C = (-3 - i\sqrt{3}\ )/2$, $D = -i\sqrt{3}$, $E = (-3 - 3i\sqrt{3})/2$, $F = (9 - i\sqrt{3})/2$, $G = -3 - i\sqrt{3}$, $H = -2i\sqrt{3}$, $I = (-3 - 5i\sqrt{3})/2$, $J = -3 - 2i\sqrt{3}$, $K = -3 - 3i\sqrt{3}$, $L = -2 - 2i\sqrt{3}$, $M = -6 + 2i\sqrt{3}$, $N = 4i\sqrt{3}$ and $O = -6 + 6i\sqrt{3}$. Furthermore, $i = \sqrt{-1}$ and /X denotes the complex conjugate of X.

The maturated and unmaturated groups were introduced by Fujita who applied the results in this area of research to enumerate isomers of molecules[9]. Let G be a finite group and $h_1, h_2 \in G$. Then h_1, h_2 are Q-conjugate if there exists $t \in G$ such that $t^{-1} <h_1> t = <h_2>$. The Q-conjugacy is an equivalence relation on G and generates equivalence classes which are called dominant classes, *i.e*. the group G is partitioned into dominant classes as follows: $G = K_1 + K_2 + \ldots + K_s$ in which K_i corresponds to the cyclic (dominant) subgroup G_i selected from a non-redundant set of cyclic subgroups of G. set $t_i = m(G_i)/\phi(|G_i|)$ where $m(G_i) = |N_G(G_i)|/|C_G(G_i)|$ (called the maturity discriminant), ϕ is the Euler function and finally $N_G(G_i)$ and $C_G(G_i)$ denote the normalizer and centralizer of G_i in G, respectively for i = 1, …, s. Now, if for each i, $t_i = 1$ then K_i is exactly a conjugacy class and G is called a maturated group. But if $t_i > 1$ then K_i is a union of t_i-conjugacy classes of G, hence G is called an unmaturated group. By the following theorem, we prove that the f-NRG of hexamethylethane is an umaturated group.

Theorem: (i) The direct product of the maturated groups is a maturated group. But the direct product of at least one unmaturated group is an unmaturated group. (ii) The semidirect product of the maturated groups is a maturated group. But the semi direct product of at least one unmaturated group is an unmaturated group[34].

Since the dihedral group G_{12} is a maturated group with all integer-valued irreducible characters; but Z_3 is an unmaturated group (*i.e*., there is a row-reduction and a column-reduction in the character table of Z_3) then by (i) in the above theorem $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3)$ is an unmaturated group. Therefore, by (ii) in the above theorem the f-NRG of hexamethylethane, *i.e.* $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$ should be an unmaturated group. All integer-valued reducible characters, the markaracter table and the Q-conjugacy character table for the f-NRG of hexamethylethane will be considered in our future work.

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