

Computing the Dominant Subgroups of the Full Non-rigid Group of Hexamethylethane

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Abstract: Rercently, the full non-rigid (f-NRG) group of hexamethylethane has been introduced by Darafsheh and et al (J. Chem. Phy.). The f-NRG of hexamethethane is isomorphic to the semidirect product of six copies of the cyclic group of order 3 by the dihedral group of order 12 (with order 8748). The dominant subgroups of finite group has been proposed by S. Fujita who applied his results in this area of research to enumerate isomers of molecules. In this paper, via GAP program all the dominant subgroups of the above molecule are computed.

Keywords: Full non-rigid group, Symmetry, Dominant subgroup, hexamethethane.

1. Introduction

The enumeration of chemical compounds has been accomplished by various methods but the Pólya-Redfield theorem has been a standard method for combinatorial enumerations of graphs and chemical compounds. A dominant class is defined as a disjoint union of conjugacy classes that corresponds to the same cyclic subgroup, which is selected as a representative of conjugate cyclic subgroups.

Let G be a finite group and $h_1, h_2 \in G$. We say h_1, h_2 are Q-conjugate if there exists $t \in G$ such that $t^{-1} \langle h_1 \rangle t = \langle h_2 \rangle$. It is easy to see that 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: $G = K_1 + K_2 + \dots + K_s$ in which K_i corresponds to the cyclic (dominant) subgroup G_i selected from a non-redundant set of cyclic subgroups of G denoted by SCSG [8-12].

A molecule is said to be non-rigid if there are several local minima on the potential energy surface easily surmountable by the molecular system via a tunneling rearrangement. A non-rigid molecule typically possesses several potential valleys separated by relatively low energy barriers, and thus exhibits large amplitude tunneling dynamics among various potential minima. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intramolecular dynamics, spectroscopy, dynamical NMR and so all of which can be interpreted resorting to group theory.

Group theory is one of the most powerful mathematical tools in quantum

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chemistry and spectroscopy. It can predict, interpret and simplify complex theory and data. Group theory is the best formal method to describe the symmetry concept of molecular structures. Group theory for non-rigid molecules is becoming increasingly relevant and its numerous applications to large amplitude vibrational spectroscopy of small organic molecules are in the literature [1-7, 14-17].

The complete set of the molecular conversion operations that commute with the nuclear motion operator will contain overall rotation operations that describe the molecule rotating as a whole, and intramolecular motion operations that describe molecular moieties moving with respect to the rest of the molecule. Together these operations form a group which is called the full non-rigid molecule group (f-NRG) by Smeyers [21, 22]. The notation we use is standard and the reader may consult references [8-12, 18-20].

In this paper, We prove with the aid of GAP [13] that the unmaturated group for hexamethylethane [5] has ninth nine idominant subgroups.

2. Results and Discussion

In this section we first describe some notation which will be kept throughout. A permutation representation P of a finite group G is obtained when the group G acts on a finite set $X = \{x_1, x_2, \dots, x_t\}$ from the right, which means that we are given a mapping $P: X \times G \rightarrow X$ via $(x, g) \rightarrow xg$ such that the following holds: $(xg)g' = x(gg')$ and $x1 = x$, for each $g, g' \in G$ and $x \in X$. Now let us assume that we are given an action P of G on X and a subgroup H of G . We consider the set of its right cosets H_{g_i} and the corresponding partition of G into these cosets: $G = H_{g_1} + H_{g_2} + \dots + H_{g_m}$. If we multiply the cosets from the right by a group element g these cosets are permuted, in fact we obtain an action of G on the set X of cosets and correspondingly a permutation representation which we denote by $G/(H)$, following Fujita's notation.

We recall from the theory of group actions that the sets $xG = \{xg \mid g \in G\}$, the orbits, form a set partition of X , and that the action is called transitive, if there is exactly one such orbit. Shinsaku Fujita has introduced the notations SSGG and SCSGG [10-12]. A group contained in the SCSGG is called a dominant subgroup. Any action of G on X induces the set partition of X into its orbits, i.e. into transitive permutation representations. Moreover it can easily be seen that a complete set of pairwise inequivalent transitive permutation representations is formed by the set $\{G/(G_1), \dots, G/(G_r)\}$. If M is a normal subgroup of G and K is another subgroup of G such that $M \cap K = \{e\}$ and $G = MN = \langle M, N \rangle \cong N \times M$, then G is called a semi direct product of N by M which is denoted by $N \wedge M$. To denote the consecutive classes of elements of order n , for example if an element g has order n , then its class is denoted by nx , where x runs over the letters a, b , etc.

It is described in [5] that the f-NRG of hexamethylethane is isomorphic to the semidirect product of six copies of the cyclic group of order 3 by the dihedral group of order 12 (with order 8748) as follows:

We have a physical symmetry of the hexamethylethane framework which

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consist of two carbon atoms, which are denoted by “a” and “b” in Figure 1. In the event that free rotation around the C_a-C_b bond 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 D₃, the dihedral group of order 3, for this framework or a group with 6 operations, and it is isomorphic to S₃, the symmetric group on 3 letters. When one includes the inversion operation, this becomes a group of 12 operations denoted by G₁₂, which is isomorphic to the dihedral group of order 12. 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/mole. In this case, the symmetry group of the hexamethylethane is $36 \wedge G_{12}$, or equivalently $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$ (see Fig. 1). Furthermore it has been proved that the symmetry group of the hexamethylethane is an unmaturated group.

The computations of the symmetry properties of molecules were carried out with the aid of GAP SYSTEM [13], a group theory software package which is free and extendable. We run the following program at the GAP prompt to compute C_{174×174} the character table of Hex = $(Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3 \times Z_3) \wedge G_{12}$ and the set SCSG as follows:

“A GAP Program for the full non-rigid group of Hexamethylethane”

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LogTo("Hexamethylethane.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);μ:=(7,10,13,16,19,22)(8,11,14,17,20,23)(9,12,15,18,21,24);
λ:=(7,22)(10,19)(13,16)(8,23)(11,20)(14,17)(9,24)(12,21)(15,18);
Hex:=GroupWithGenerators(α,β,γ,δ,ε,φ,μ,λ);
Char:=CharacterTable(Hex);
Order(Hex);
IsPermGroup(Hex);
s:=ConjugacyClassesSubgroups(Hex);
Sort("s");M:=TableOfMarks(Hex);
W:=List(ConjugacyClassesSubgroups(Hex),x->Elements(x));
Len:=Length(W); y:=[];for i in [1..Len]do
if IsCyclic(W[i][1])then Add(y,H[i][1]);
fi;od;Display(Char);
Display(s);Display(y);Print("y", "\n");
Print("Char", "\n");
Print("W", "\n");LogTo();
Print("Hexamethylethane.txt", "\n");

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After running the program, we can compute that SCSG of Hex has exactly 99 elements (i.e. G_i) with corresponding dominant class K_i for 1 ≤ i ≤ 99 which are collected in Table 1, see :

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Table 1: G_i in non-redundant set of cyclic subgroups of Hex and its corresponding dominant class K_i for $1 \leq i \leq 99$.

i	G_i	K_i
1	id	1a
2	$\langle (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$3a \cup 3b$
3	$\langle (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$3c \cup 3e$
4	$\langle (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) \rangle$	3d
5	$\langle (7, 9, 8)(22, 23, 24) \rangle$	$3f \cup 3l$
6	$\langle (7, 8, 9) \rangle$	$3g \cup 3n$
7	$\langle (7, 8, 9)(22, 23, 24) \rangle$	$3h \cup 3m$
8	$\langle (10, 11, 12)(22, 23, 24) \rangle$	3i
9	$\langle (10, 11, 12)(22, 23, 24) \rangle$	$3j \cup 3k$
10	$\langle (7, 8, 9)(10, 11, 12)(22, 23, 24) \rangle$	$3o \cup 3ad$
11	$\langle (7, 9, 8)(10, 11, 12)(22, 23, 24) \rangle$	$3p \cup 3af$
12	$\langle (7, 9, 8)(10, 11, 12)(19, 20, 21) \rangle$	$3q \cup 3ae$
13	$\langle (7, 8, 9)(10, 11, 12)(22, 23, 24) \rangle$	$3r \cup 3ai$
14	$\langle (10, 11, 12)(19, 20, 21) \rangle$	$3s \cup 3ah$
15	$\langle (7, 9, 8)(10, 11, 12)(19, 20, 21)(22, 23, 24) \rangle$	$3t \cup 3ag$
16	$\langle (10, 12, 11)(19, 20, 21) \rangle$	3u
17	$\langle (7, 8, 9)(10, 12, 11)(19, 20, 21) \rangle$	$3v \cup 3aa$
18	$\langle (7, 9, 8)(10, 12, 11)(19, 20, 21) \rangle$	$3w \cup 3x$
19	$\langle (7, 8, 9)(10, 12, 11)(19, 20, 21)(22, 23, 24) \rangle$	$3y \cup 3ac$
20	$\langle (7, 9, 8)(10, 12, 11)(19, 20, 21)(22, 23, 24) \rangle$	3z
21	$\langle (7, 8, 9)(10, 12, 11)(19, 20, 21)(22, 23, 24) \rangle$	3ab
22	$\langle (7, 8, 9)(13, 14, 15)(19, 20, 21) \rangle$	$3aj \cup 3bq$
23	$\langle (7, 9, 8)(13, 14, 15)(19, 20, 21) \rangle$	$3ak \cup 3ay$
24	$\langle (7, 8, 9)(10, 11, 12)(19, 20, 21) \rangle$	$3al \cup 3bs$
25	$\langle (7, 9, 8)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3am \cup 3bj$
26	$\langle (7, 8, 9)(10, 11, 12)(19, 20, 21)(22, 23, 24) \rangle$	$3an \cup 3br$
27	$\langle (7, 9, 8)(10, 11, 12)(19, 20, 21)(22, 23, 24) \rangle$	$3ao \cup 3bc$
28	$\langle (10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3ap \cup 3bx$
29	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3aq \cup 3bz$
30	$\langle (7, 9, 8)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3ar \cup 3by$
31	$\langle (10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3at \cup 3bw$
32	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3au \cup 3bv$
33	$\langle (7, 9, 8)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	3av
34	$\langle (10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3aw \cup 3bu$
35	$\langle (7, 8, 9)(10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3ax \cup 3bt$
36	$\langle (7, 9, 8)(10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3az \cup 3bi$
37	$\langle (7, 8, 9)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3ba \cup 3bb$
38	$\langle (7, 9, 8)(13, 14, 15)(19, 21, 20)(22, 23, 24) \rangle$	$3bd \cup 3bp$
39	$\langle (7, 8, 9)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	$3be \cup 3bo$
40	$\langle (7, 9, 8)(13, 14, 15)(19, 20, 21)(22, 23, 24) \rangle$	3bf
41	$\langle (10, 11, 12)(13, 14, 15)(19, 21, 20)(22, 23, 24) \rangle$	$3bg \cup 3bh$
42	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(19, 21, 20)(22, 23, 24) \rangle$	3bk
43	$\langle (10, 12, 11)(13, 14, 15)(19, 21, 20)(22, 23, 24) \rangle$	$3bl \cup 3bm$
44	$\langle (7, 8, 9)(10, 12, 11)(13, 14, 15)(19, 21, 20)(22, 23, 24) \rangle$	$3bn \cup 3as$
45	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24) \rangle$	$3ca \cup 3cm$

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Table 1 (Continued)

i	G_i	K_i
46	< (7, 9, 8)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24) >	3cb ∪ 3cl
47	< (7, 9, 8)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 24, 23) >	3cc ∪ 3ch
48	< (7, 8, 9)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 24, 23) >	3cd ∪ 3cj
49	< (7, 9, 8)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 24, 23) >	3ce
50	< (7, 8, 9)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 21, 20)(22, 23, 24) >	3cf ∪ 3ck
51	< (7, 9, 8)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 21, 20)(22, 23, 24) >	3cg
52	< (7, 9, 8)(10, 11, 12)(13, 15, 14)(16, 17, 18)(19, 21, 20)(22, 23, 24) >	3ci
53	< (7, 8, 9)(10, 11, 12)(13, 14, 15)(19, 21, 20)(22, 23, 24) >	3cn
54	< (7, 9, 8)(10, 11, 12)(13, 14, 15)(19, 21, 20)(22, 23, 24) >	9a ∪ 9b
55	< (7, 13, 19)(8, 14, 20)(9, 15, 21)(10, 16, 22)(11, 17, 23)(12, 18, 24) >	9c ∪ 9e
56	< (7, 9, 8)(13, 14, 15)(19, 21, 20)(22, 23, 24) >	9d
57	< (7, 9, 8)(10, 12, 11)(16, 17, 18)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6a
58	< (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	18a ∪ 18b
59	< (7, 8, 9)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	2a
60	< (7, 9, 8)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6b ∪ 6c
61	< (7, 9, 8)(10, 11, 12)(13, 15, 14)(16, 17, 18)(19, 21, 20)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6d ∪ 6f
62	< (7, 10, 13, 16, 19, 22)(8, 11, 14, 17, 20, 23)(9, 12, 15, 18, 21, 24) >	6e
63	< (7, 8, 9), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6g ∪ 6j
64	< (7, 9, 8)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6h ∪ 6i
65	< (13, 14, 15)(22, 23, 24), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	2b
66	< (7, 8, 9)(10, 11, 12)(13, 14, 15)(22, 23, 24), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6k ∪ 6l
67	< (7, 9, 8)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6m ∪ 6p
68	< (7, 8, 9)(10, 11, 12)(16, 17, 18)(19, 20, 21), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6n ∪ 6r
69	< (7, 9, 8)(10, 12, 11)(16, 17, 18)(19, 20, 21), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6o ∪ 6q
70	< (7, 8, 9)(10, 12, 11)(13, 15, 14)(16, 17, 18)(19, 21, 20)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6s ∪ 6ab
71	< (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6t ∪ 6aa
72	< (7, 8, 9)(16, 17, 18), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6u ∪ 6ae
73	< (7, 9, 8)(16, 17, 18), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6v ∪ 6ag
74	< (7, 8, 9)(10, 11, 12)(13, 15, 14)(16, 17, 18)(19, 20, 21)(22, 24, 23), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) >	6w ∪ 6af
75	< (7, 9, 8)(10, 11, 12)(16, 17, 18)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) >	6x

Table 1 (Continued)

i	G_i	K_i
76	$\langle (7, 8, 9)(10, 12, 11)(16, 17, 18)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6y \cup 6ad$
77	$\langle (7, 9, 8)(10, 12, 11)(13, 14, 15)(22, 23, 24), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) \rangle$	$6z \cup 6ac$
78	$\langle (10, 12, 11)(13, 14, 15)(19, 21, 20)(22, 23, 24), (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$6ah \cup 6aw$
79	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$6ai$
80	$\langle (7, 8, 9)(10, 12, 11)(13, 14, 15)(16, 17, 18)(19, 21, 20)(22, 23, 24), (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$6aj \cup 6ay$
81	$\langle (10, 11, 12)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6ak \cup 6as$
82	$\langle (7, 8, 9)(10, 11, 12), (7, 10)(8, 11)(9, 12)(13, 22)(14, 23)(15, 24)(16, 19)(17, 20)(18, 21) \rangle$	$6al \cup 6ax$
83	$\langle (10, 11, 12)(19, 20, 21), (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$6am \cup 6an$
84	$\langle (10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24), (7, 16)(8, 17)(9, 18)(10, 19)(11, 20)(12, 21)(13, 22)(14, 23)(15, 24) \rangle$	$6ao \cup 6bb$
85	$\langle (7, 9, 8)(13, 14, 15)(19, 20, 21), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6ap \cup 6av$
86	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6aq \cup 6ba$
87	$\langle (7, 9, 8)(10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6ar$
88	$\langle (10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6at$
89	$\langle (7, 9, 8)(10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6au \cup 6az$
90	$\langle (7, 8, 9)(10, 12, 11)(13, 14, 15)(19, 20, 21)(22, 24, 23), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$2c$
91	$\langle (7, 9, 8)(10, 11, 12)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6bc \cup 6bd$
92	$\langle (7, 8, 9)(10, 11, 12)(16, 17, 18)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6be \cup 6bh$
93	$\langle (7, 8, 9)(10, 11, 12)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6bf \cup 6bj$
94	$\langle (7, 8, 9)(13, 14, 15)(19, 20, 21), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6bg \cup 6bi$
95	$\langle (10, 11, 12)(13, 14, 15)(19, 20, 21)(22, 23, 24), (10, 22)(11, 23)(12, 24)(13, 19)(14, 20)(15, 21) \rangle$	$6bk \cup 6bq$
96	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (7, 13, 19, 8, 14, 20, 9, 15, 21)(10, 16, 23, 11, 17, 24, 12, 18, 22) \rangle$	$6bl$
97	$\langle (7, 9, 8)(10, 11, 12)(13, 15, 14)(16, 17, 18)(19, 21, 20)(22, 23, 24), (7, 13, 19, 9, 15, 21, 8, 14, 20)(10, 16, 23, 11, 17, 24, 12, 18, 22) \rangle$	$6bm \cup 6bs$
98	$\langle (7, 8, 9)(13, 14, 15)(19, 20, 21), (7, 13, 19, 8, 14, 20, 9, 15, 21)(10, 16, 22)(11, 17, 23)(12, 18, 24) \rangle$	$6bn \cup 6bp$
99	$\langle (7, 8, 9)(10, 11, 12)(13, 14, 15)(16, 17, 18)(19, 20, 21)(22, 23, 24), (7, 10, 13, 16, 19, 22, 8, 11, 14, 17, 20, 23, 9, 12, 15, 18, 21, 24) \rangle$	$6bo \cup 6br$

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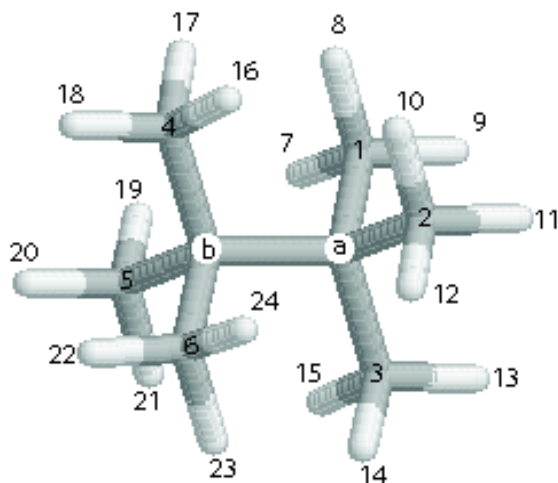


Figure 1 The Structure of Hexamethylethane.

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