

The Full Non-Rigid Group Theory for the bipyramidal Geometry of Pentamethylphosphorus

M. Dabirian and A. Iranmanesh *

Department of Mathematics, Tarbiat Modarres University
P.O.Box: 14115-137, Tehran, Iran
iranmana@modares.ac.ir

(Received May 2, 2004)

Abstract

A simple method is described for calculation of character tables of the symmetry groups of molecules consisting of a number methyl groups attached to a rigid framework. For the full non-rigid group (f-NRG) of the bipyramidal geometry pentamethylphosphorus, with C_{3h} symmetry, we prove that it is a group of order 1458 with 90 conjugacy classes. The character tables of this group are calculated.

1. Introduction

The non-rigid molecule group theory (NRG) in which the dynamical symmetry operations are defined as physical operations is a new field of chemistry. Some authors in a series of papers applied this theory to determine the character table of restricted NRG of some molecules [1-7].

A molecule undergoing such large amplitude movements, between various possible configurations, is known as a non-rigid molecule. Because of this deformability, the non-rigid molecules exhibit some

* Author for correspondence

interesting properties of intramolecular dynamics, which can be studied more easily resorting to Group Theory [2; p.5].

The complete set of molecular conversion operations will contain overall rotation operations, describing the molecule rotating as a whole, and intramolecular motion operations, describing molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which we call the full non-rigid group (f-NRG).

Group theory for non-rigid molecules is becoming more and more relevant, and numerous applications to large amplitude vibrational spectroscopy of small organic molecules are appearing in the literature [8-16].

In [17] Longuet-Higgins investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. 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 for calculating these character tables. These character tables are needed for classification of wave functions, of selection rules, etc. [18,19].

The method as described here is appropriate for molecules which consist of a number of XH_3 groups attached to a rigid framework. An example of such a molecule is bipyramidal geometry pentamethylphosphorus which is considered here in some detail. The method is not appropriate in the case where the framework is linear, as in ethane. However, Bunker [20] has shown how to deal with such molecules. In computing the character table of this molecule, we use [21,22], for the standard notation and terminology on character theory.

Lomont [23] has given two methods for calculating character tables. These are satisfactory for small groups, but both of them require a knowledge of the class structure and hence the group multiplication table. These become inaccessible as soon as the order of the group becomes moderately large. For a non-

rigid molecule whose symmetry group has several thousands of elements, they are usually quite impracticable.

The alternative approach is less mechanical and is simpler in practice. It involves two steps: decomposition of the group into classes, and determination of sets of basis functions for certain representations whose characters are then determined.

2. Theory

Throughout the present paper, the concepts of direct and semi-direct products will be used. For this purpose, let us consider two groups, I and G , which have no element in common except for the identity.

If I and G are such that any element I_s commutes with any element G_r :

$$I_s G_r = G_r I_s$$

their product forms a group S which is the direct product of I and G :

$$I \times G = S$$

On the other hand, if I and G do not commute in detail but rather:

$$I G_r = G_r I$$

for all $G_r \in G$, then the group forms a set which is called the semi-direct product of I and G , and is expressed as:

$$I \wedge G = S$$

where the invariant subgroup I with respect to G is written on left side [2; p.15].

Bipyramidal geometry pentamethylphosphorus occurs in its preferred conformation with five equivalent methyl groups in "staggered" configuration (see figure 1) [24].

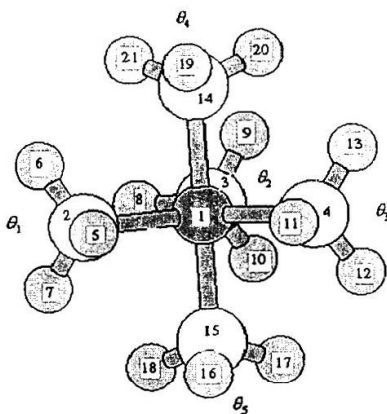


Figure 1

At first glance, the bipyramidal geometry of pentamethylphosphorus presents a type of large amplitude internal motion: the five rotations of the methyl groups. The variables which describe the five methyl rotations are θ_1 , θ_2 , θ_3 , θ_4 and θ_5 , while the five rotation axes are the being the P-CH₃ bonds.

The existence of the five equivalent methyl groups implies the existence of 243 isoenergetic conformations, described by five equivalent C_3 non-rigid subgroups. Notice that even when the methyl groups are distorted because of environmental effects, the C_3 symmetry has to be respected since the hydrogen atoms are indistinguishable [25]:

$$\begin{aligned}
 C'_{3_1} &= [\hat{E} + \hat{C}_{3_1} + \hat{C}_{3_1}^2], \\
 C'_{3_2} &= [\hat{E} + \hat{C}_{3_2} + \hat{C}_{3_2}^2], \\
 C'_{3_3} &= [\hat{E} + \hat{C}_{3_3} + \hat{C}_{3_3}^2], \\
 C'_{3_4} &= [\hat{E} + \hat{C}_{3_4} + \hat{C}_{3_4}^2], \\
 C'_{3_5} &= [\hat{E} + \hat{C}_{3_5} + \hat{C}_{3_5}^2].
 \end{aligned} \tag{1}$$

The direct product of these five subgroups contains 243 dynamical symmetry operations:

$$G_{243} = C'_{3_1} \times C'_{3_2} \times C'_{3_3} \times C'_{3_4} \times C'_{3_5}, \tag{2}$$

which describe 243 potential energy wells on the potential energy hypersurface.

In order to establish the remaining transformation operations let us consider the bipyramidal geometry of pentamethylphosphorus in an arbitrary conformation in which $\theta_1 \neq \theta_2 \neq \theta_3 \neq \theta_4 \neq \theta_5$. Since the three equatorial methyl-groups are equivalent, the rotation angles may be interchanged by a 3-fold rotation without any energy variation,

$$\begin{aligned}
 \hat{W} f(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5) &\equiv f(\theta_3, \theta_1, \theta_2, \theta_4, \theta_5), \\
 \hat{W}^2 f(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5) &\equiv f(\theta_2, \theta_3, \theta_1, \theta_4, \theta_5)
 \end{aligned} \tag{3}$$

or by binary exchange (reflection) which induces an inversion of the rotation sense:

$$\hat{V} f(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5) = f(\theta_1, \theta_3, \theta_2, \theta_4, \theta_5), \quad (4)$$

being

$$W^I = [E + \hat{W} + \hat{W}^2],$$

$$V^I = [E + \hat{V}], \quad (5)$$

The semidirect product of these two subgroups forms another subgroup isomorphic to the C_{3h} symmetry point group:

$$G_6 = [W^I \wedge V^I] \sim C_{3h}, \quad (6)$$

which is the symmetry group of the bipyramidal geometry of pentamethylphosphorus, skeleton with unstructured methyl groups.

As a result, the complete f-NRG of the bipyramidal geometry of pentamethylphosphorus may be written as

$$G_{1458} = [W^I \wedge V^I] \wedge [C_3^I \times C_3^I \times C_3^I \times C_3^I \times C_3^I] \quad (7)$$

which is group of order 1458.

3. Determination of the conjugacy classes and the character table

We consider the point group of the bipyramidal geometry of pentamethylphosphorus in the case of a rigid framework. We consider the full non-rigid group G (f-NRG) of this molecule each equilibrium conformation of which has an ordinary point-group symmetry C_{3h} .

Since G is a permutation group, every two elements of this group with different cycle structure belong to different conjugacy classes. Using figure 1, we give the cycle structure of the representatives of the conjugacy classes of G in Table 1. In this table, cc stands for conjugacy classes, n is their number, and a permutation $\underbrace{(r_1, \dots, r_a)}_{b\text{-number}} \dots \underbrace{(l_1, \dots, l_a)}_{d\text{-number}} \dots (s_1, \dots, s_c)$ is denoted by $a^b \cdot c^d$ for $a, b, c, d \in N$.

Table 1

cc	1	3	3 ²	3 ³	3 ⁴	3 ⁵	3 ⁶	3.9	3 ² .9	3 ³ .9	2 ⁷	3 ² .6 ² .2	2 ⁴ .6	3 ² .6.2 ⁴
n	1	3	9	14	18	12	6	2	9	7	1	4	2	2

We need the generators of G . For this purpose, we doing the following procedure:

Let us first consider the operations which leave the framework of the molecule unchanged. In this case, each methyl group can be left alone or rotated through 120° in either direction which commute with another equivalent methyl group;

We first obtain the following permutations:

h_1, h_2 : The permutations obtained from the above rule (h_1 obtained when the methyl group left alone and h_2 obtained when the methyl group rotated through 120° in either direction) when the element of symmetry σ_h passes through the atoms: 11,4,8,3,2,5,1.

r_1, r_2, r_3 : The permutations obtained from the above rule (r_1 obtained when the methyl group left alone, r_2 obtained when the methyl group rotated through 120° in left direction and r_3 obtained when the methyl group rotated through 120° in right direction) when the element of symmetry C_{3h} passes through the atoms: 14,15,1.

Therefore, we can write these relations as follows:

$$\begin{aligned} r_1 &:= (21,19,20)(18,16,17)(2,3,4)(5,8,11)(6,9,12)(7,10,13); \\ r_2 &:= (21,19,20)(18,16,17)(2,3,4)(5,9,13,7,8,12,6,10,11); \\ r_3 &:= (21,19,20)(18,16,17)(2,3,4)(5,10,12,6,8,13,7,9,11); \\ h_1 &:= (14,15)(19,16)(20,17)(21,18)(6,7)(13,12)(9,10); \\ h_2 &:= (14,15)(19,18,21,17,20,16)(6,7)(13,12)(9,10); \end{aligned}$$

By using the program GAP [26], we can see that the permutation h_1, h_2, r_1, r_2, r_3 are generators of G (any permutation in G can be written as a product of some r_i and h_j for $1 \leq i \leq 3$ and $1 \leq j \leq 2$). That is, $G = \langle h_1, h_2, r_1, r_2, r_3 \rangle$. Hence G is a group of order 1458 and has 90 conjugacy classes which are listed in Table 2.

We now calculate the character table of G by the following details in the environment of GAP:

```
gap> G = < h1, h2, r1, r2, r3 >;
gap> cc:= ConjugacyClasse(G);
gap> n:=List(cc, x->Size(x));
gap> tb:=CharacterTable(G);
gap> Display(tb);
```

The character table of G is listed in Table 3.

Table 2: The representatives of conjugacy classes of the group G

No.	Representatives	Size
1	Identity	1
2	(5, 6, 7)(8, 9, 10)(11, 12, 13)	2
3	(2, 3, 4)(5, 8, 11)(6, 9, 12)(7, 10, 13)(16, 17, 18)(19, 20, 21)	9
4	(2, 4, 3)(5, 11, 8)(6, 12, 9)(7, 13, 10)(16, 18, 17)(19, 21, 20)	9
5	(8, 10, 9)(11, 12, 13)	6
6	(11, 13, 12)	6
7	(5, 6, 7)(8, 9, 10)	6
8	(5, 7, 6)(8, 10, 9)(11, 12, 13)	6
9	(2, 3, 4)(5, 8, 11, 7, 10, 13, 6, 9, 12)(16, 17, 18)(19, 20, 21)	18
10	(2, 4, 3)(5, 11, 10, 7, 13, 9, 6, 12, 8)(16, 18, 17)(19, 21, 20)	18
11	(16, 18, 17)(19, 20, 21)	2
12	(5, 6, 7)(8, 9, 10)(11, 12, 13)(16, 18, 17)(19, 20, 21)	2
13	(5, 7, 6)(8, 10, 9)(11, 13, 12)(16, 18, 17)(19, 20, 21)	2
14	(2, 3, 4)(5, 8, 11)(6, 9, 12)(7, 10, 13)(19, 21, 20)	18
15	(2, 4, 3)(5, 11, 8)(6, 12, 9)(7, 13, 10)(16, 17, 18)	18
16	(8, 10, 9)(11, 12, 13)(16, 18, 17)(19, 20, 21)	6
17	(8, 9, 10)(11, 13, 12)(16, 18, 17)(19, 20, 21)	6
18	(11, 13, 12)(16, 18, 17)(19, 20, 21)	6
19	(5, 6, 7)(8, 9, 10)(16, 18, 17)(19, 20, 21)	6
20	(5, 7, 6)(8, 10, 9)(11, 12, 13)(16, 18, 17)(19, 20, 21)	6
21	(2, 3, 4)(5, 8, 11, 7, 10, 13, 6, 9, 12)(19, 21, 20)	18
22	(2, 4, 3)(5, 11, 10, 7, 13, 9, 6, 12, 8)(16, 17, 18)	18
23	(11, 12, 13)(16, 18, 17)(19, 20, 21)	6
24	(5, 6, 7)(8, 9, 10)(11, 13, 12)(16, 18, 17)(19, 20, 21)	6
25	(5, 7, 6)(8, 10, 9)(16, 18, 17)(19, 20, 21)	6
26	(2, 3, 4)(5, 8, 11, 6, 9, 12, 7, 10, 13)(19, 21, 20)	18
27	(2, 4, 3)(5, 11, 9, 6, 12, 10, 7, 13, 8)(16, 17, 18)	18
28	(6, 7)(9, 10)(12, 13)(14, 15)(16, 19)(17, 20)(18, 21)	81
29	(2, 3, 4)(5, 8, 11)(6, 10, 12, 7, 9, 13)(14, 15)(16, 20, 18, 19, 17, 21)	81
30	(2, 4, 3)(5, 11, 8)(6, 13, 9, 7, 12, 10)(14, 15)(16, 21, 17, 19, 18, 20)	81
31	(19, 20, 21)	2
32	(5, 6, 7)(8, 9, 10)(11, 12, 13)(19, 20, 21)	2
33	(5, 7, 6)(8, 10, 9)(11, 13, 12)(19, 20, 21)	2
34	(2, 3, 4)(5, 8, 11)(6, 9, 12)(7, 10, 13)(16, 17, 18)(19, 21, 20)	18
35	(2, 4, 3)(5, 11, 8)(6, 12, 9)(7, 13, 10)(16, 18, 17)	18
36	(8, 10, 9)(11, 12, 13)(19, 20, 21)	6
37	(8, 9, 10)(11, 13, 12)(19, 20, 21)	6
38	(11, 13, 12)(19, 20, 21)	6
39	(5, 6, 7)(8, 9, 10)(19, 20, 21)	6
40	(5, 7, 6)(8, 10, 9)(11, 12, 13)(19, 20, 21)	6
41	(2, 3, 4)(5, 8, 11, 7, 10, 13, 6, 9, 12)(16, 17, 18)(19, 21, 20)	18
42	(2, 4, 3)(5, 11, 10, 7, 13, 9, 6, 12, 8)(16, 18, 17)	18
43	(11, 12, 13)(19, 20, 21)	6
44	(5, 6, 7)(8, 9, 10)(11, 13, 12)(19, 20, 21)	6
45	(5, 7, 6)(8, 10, 9)(19, 20, 21)	6
45	(2, 3, 4)(5, 8, 11, 6, 9, 12, 7, 10, 13)(16, 17, 18)(19, 21, 20)	18
47	(2, 4, 3)(5, 11, 9, 6, 12, 10, 7, 13, 8)(16, 18, 17)	18

Table 2 (continued)

No.	Representatives	Size
48	(16,18,17)(19,21,20)	1
49	(5,6,7)(8,9,10)(11,12,13)(16,18,17)(19,21,20)	2
50	(2,3,4)(5,8,11)(6,9,12)(7,10,13)	9
51	(2,4,3)(5,11,8)(6,12,9)(7,13,10)(16,17,18)(19,20,21)	9
52	(8,10,9)(11,12,13)(16,18,17)(19,21,20)	6
53	(11,13,12)(16,18,17)(19,21,20)	6
54	(5,6,7)(8,9,10)(16,18,17)(19,21,20)	6
55	(5,7,6)(8,10,9)(11,12,13)(16,18,17)(19,21,20)	6
56	(2,3,4)(5,8,11,7,10,13,6,9,12)	18
57	(2,4,3)(5,11,10,7,13,9,6,12,8)(16,17,18)(19,20,21)	18
58	(6,7)(9,10)(12,13)(14,15)(16,19,17,20,18,21)	81
59	(2,3,4)(5,8,11)(6,10,12,7,9,13)(14,15)(16,20)(17,21)(18,19)	81
60	(2,4,3)(5,11,8)(6,13,9,7,12,10)(14,15)(16,21,18,20,17,19)	81
61	(19,21,20)	2
62	(5,6,7)(8,9,10)(11,12,13)(19,21,20)	2
63	(5,7,6)(8,10,9)(11,13,12)(19,21,20)	2
64	(2,3,4)(5,8,11)(6,9,12)(7,10,13)(16,17,18)	18
65	(2,4,3)(5,11,8)(6,12,9)(7,13,10)(16,18,17)(19,20,21)	18
66	(8,10,9)(11,12,13)(19,21,20)	6
67	(8,9,10)(11,13,12)(19,21,20)	6
68	(11,13,12)(19,21,20)	6
69	(5,6,7)(8,9,10)(19,21,20)	6
70	(5,7,6)(8,10,9)(11,12,13)(19,21,20)	6
71	(2,3,4)(5,8,11,7,10,13,6,9,12)(16,17,18)	18
72	(2,4,3)(5,11,10,7,13,9,6,12,8)(16,18,17)(19,20,21)	18
73	(11,12,13)(19,21,20)	6
74	(5,6,7)(8,9,10)(11,13,12)(19,21,20)	6
75	(5,7,6)(8,10,9)(19,21,20)	6
76	(2,3,4)(5,8,11,6,9,12,7,10,13)(16,17,18)	18
77	(2,4,3)(5,11,9,6,12,10,7,13,8)(16,18,17)(19,20,21)	18
78	(16,17,18)(19,20,21)	1
79	(5,6,7)(8,9,10)(11,12,13)(16,17,18)(19,20,21)	2
80	(2,3,4)(5,8,11)(6,9,12)(7,10,13)(16,18,17)(19,21,20)	9
81	(2,4,3)(5,11,8)(6,12,9)(7,13,10)	9
82	(8,10,9)(11,12,13)(16,17,18)(19,20,21)	6
83	(11,13,12)(16,17,18)(19,20,21)	6
84	(5,6,7)(8,9,10)(16,17,18)(19,20,21)	6
85	(5,7,6)(8,10,9)(11,12,13)(16,17,18)(19,20,21)	6
86	(2,3,4)(5,8,11,7,10,13,6,9,12)(16,18,17)(19,21,20)	18
87	(2,4,3)(5,11,10,7,13,9,6,12,8)	18
88	(6,7)(9,10)(12,13)(14,15)(16,19,18,21,17,20)	81
89	(2,3,4)(5,8,11)(6,10,12,7,9,13)(14,15)(16,20,17,21,18,19)	81
90	(2,4,3)(5,11,8)(6,13,9,7,12,10)(14,15)(16,21)(17,19)(18,20)	81

Table 3-A: Character Table of G

$$A = (-1+i\sqrt{3})/2, B = (-1+i\sqrt{3}), C = (-3+3i\sqrt{3}), D = (3-3i\sqrt{3})/2$$

$$IA = \bar{A}, IB = \bar{B}, IC = \bar{C}, ID = \bar{D}$$

	1a	3a	3b	3c	3d	3e	3f	3g	9a	9b	3h	3i	3j	3k	3l	3m	3n	3o	3p	3q	9c
x1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x3	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x4	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x5	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x6	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x9	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x10	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x11	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x12	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x13	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x14	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x15	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x16	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x17	1	1	A/A	A/A	1	1	1	1	A/A	A/A	1	1	1	1	1	1	1	1	1	1	A/A
x18	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x19	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x20	2	2	2	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x21	2	2	2	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x22	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
x23	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x24	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x25	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x26	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x27	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x28	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x29	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x30	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x31	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x32	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x33	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x34	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x35	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x36	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x37	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x38	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x39	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x40	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x41	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x42	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x43	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x44	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x45	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x46	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x47	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x48	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x49	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x50	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x51	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x52	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x53	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x54	2	2	B/B	B/B	2	2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x55	6	6	0	0	0	-3	0	0	0	0	0	6	6	6	0	0	-3	-3	0	0	0
x56	6	6	0	0	0	-3	0	0	0	0	0	6	6	6	0	0	-3	-3	0	0	0
x57	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x58	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x59	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x60	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x61	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x62	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x63	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x64	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x65	6	6	-3	0	0	0	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	0	0
x66	6	6	0	0	0	-3	0	0	0	0	0	-3	-3	0	0	6	-3	0	0	0	0

Table 3-A (Continued)

x67	6	6	0	0	-3	0	0	0	0	0	6	6	6	0	0	-3	-3	0	0	0	0	0	0
x68	6	6	0	0	0	-3	0	0	0	0	0	6	6	6	0	0	-3	-3	0	0	0	0	0
x69	6	-3	0	0	0	-3	3	0	0	0	0	-3	6	-3	0	0	0	0	0	-3	3	0	0
x70	6	-3	0	0	0	-3	3	0	0	0	0	-3	6	-3	0	0	0	0	0	0	-3	3	0
x71	6	-3	0	0	0	0	3	0	-3	0	0	0	-3	6	-3	0	0	0	0	-3	3	0	0
x72	6	-3	0	0	0	0	3	0	-3	0	0	0	-3	6	-3	0	0	0	0	-3	3	0	0
x73	6	-3	0	0	0	0	0	-3	3	0	0	0	-3	6	-3	0	0	0	0	0	3	0	-3
x74	6	-3	0	0	0	0	0	-3	3	0	0	0	-3	6	-3	0	0	0	0	0	3	0	-3
x75	6	-3	0	0	0	0	3	0	-3	0	0	0	-3	6	0	0	0	0	0	0	0	-3	3
x76	6	-3	0	0	0	0	3	0	-3	0	0	0	-3	6	0	0	0	0	0	0	0	-3	3
x77	6	-3	0	0	0	0	0	-3	3	0	0	0	-3	6	0	0	0	0	0	-3	3	0	0
x78	6	-3	0	0	0	0	0	-3	3	0	0	0	-3	6	0	0	0	0	0	0	0	-3	3
x79	6	-3	0	0	0	0	-3	3	0	0	0	0	-3	6	0	0	0	0	0	0	0	0	-3
x80	6	-3	0	0	0	0	-3	3	0	0	0	0	-3	6	0	0	0	0	0	0	0	0	-3
x81	6	-3	0	0	0	0	3	0	-3	0	0	0	6	-3	-3	0	0	0	0	0	3	0	-3
x82	6	-3	0	0	0	0	3	0	-3	0	0	0	6	-3	-3	0	0	0	0	0	3	0	-3
x83	6	-3	0	0	0	0	0	-3	3	0	0	0	6	-3	-3	0	0	0	0	0	3	0	-3
x84	6	-3	0	0	0	0	0	-3	3	0	0	0	6	-3	-3	0	0	0	0	0	0	0	-3
x85	6	-3	0	0	0	0	-3	3	0	0	0	0	6	-3	-3	0	0	0	0	0	-3	3	0
x86	6	-3	0	0	0	0	-3	3	0	0	0	0	6	-3	-3	0	0	0	0	0	-3	3	0
x87	6	6	0	0	-3	0	0	0	0	0	-3	-3	-3	0	0	-3	6	0	0	0	0	0	0
x88	6	6	0	0	-3	0	0	0	0	0	-3	-3	-3	0	0	-3	6	0	0	0	0	0	0
x89	6	6	0	0	-3	0	0	0	0	0	-3	-3	-3	0	0	-3	6	0	0	0	0	0	0
x90	6	6	0	0	-3	0	0	0	0	0	-3	-3	-3	0	0	6	-3	0	0	0	0	0	0

Table 3-B: Character Table of G

	9d	3r	3s	3t	9e	9f	2a	6a	6b	3u	3v	3w	3x	3y	3z	3aa	3ab	3ac
x1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x2	1	1	1	1	1	-1	-1	-1	-1	1	1	1	1	1	1	1	1	1
x3	/A	1	1	1	A	/A	1	/A	/A	1	1	1	1	/A	/A	1	1	1
x4	/A	1	1	1	A	-1	-A	-1	-A	1	1	1	1	/A	/A	1	1	1
x5	A	1	1	1	/A	A	-1	/A	-A	1	1	1	1	/A	A	1	1	1
x6	A	1	1	1	1	1	1	1	1	A	A	A	A	A	A	A	A	A
x7	1	1	1	1	1	1	1	1	1	A	A	A	A	A	A	A	A	A
x8	1	1	1	1	1	-1	-1	-1	-1	A	A	A	A	A	A	A	A	A
x9	/A	1	1	1	A	/A	-1	-A	/A	A	A	A	/A	1	A	A	A	A
x10	/A	1	1	1	A	/A	-1	-A	/A	A	A	A	/A	1	A	A	A	A
x11	A	1	1	1	/A	A	1	/A	A	A	A	A	1	/A	A	A	A	A
x12	A	1	1	1	/A	A	-1	-A	A	A	A	A	1	/A	A	A	A	A
x13	1	1	1	1	1	1	1	1	1	/A	/A	/A	/A	/A	/A	/A	/A	/A
x14	1	1	1	1	1	-1	-1	-1	-1	/A	/A	/A	/A	/A	/A	/A	/A	/A
x15	/A	1	1	1	A	/A	1	A	/A	/A	1	A	/A	A	/A	/A	/A	/A
x16	/A	1	1	1	A	/A	-1	-A	/A	/A	1	A	/A	A	/A	/A	/A	/A
x17	A	1	1	1	/A	A	1	/A	A	/A	/A	A	1	/A	/A	/A	/A	/A
x18	A	1	1	1	/A	A	-1	-A	-A	/A	/A	A	1	/A	/A	/A	/A	/A
x19	-1	-1	-1	-1	-1	0	0	0	0	2	2	2	2	2	2	2	2	2
x20	-1	-1	-1	-1	-1	0	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1
x21	-1	2	2	2	2	2	2	2	2	0	0	0	0	-1	-1	-1	-1	-1
x22	-1	-1	-1	-1	-1	-1	0	0	0	0	0	0	0	-1	-1	-1	-1	-1
x23	-A	-1	-1	-1	-A	-A	0	0	0	B	B	B	B	/B	2	B	B	B
x24	-A	-1	-1	-1	-A	-A	0	0	0	B	B	B	B	/B	2	B	B	B
x25	-1	-1	-1	-1	-1	0	0	0	0	B	B	B	B	/B	2	B	B	B
x26	-A	-1	-1	-1	-A	-A	0	0	0	B	B	B	B	/B	2	B	B	B
x27	-A	-1	-1	-1	-A	-A	0	0	0	B	B	B	B	/B	2	B	B	B
x28	-1	-1	-1	-1	-1	-1	0	0	0	B	B	B	B	/B	2	B	B	B
x29	-A	-1	-1	-1	-A	-A	0	0	0	B	B	B	B	/B	2	B	B	B
x30	-A	-1	-1	-1	-A	-A	0	0	0	2	2	2	2	/B	2	2	2	2
x31	/B	-1	-1	-1	-A	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x32	B	-1	-1	-1	/A	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x33	B	-1	-1	-1	/A	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x34	/B	-1	-1	-1	-A	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x35	B	-1	-1	-1	/A	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x36	2	-1	-1	-1	-1	-1	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A
x37	/B	-1	-1	-1	-A	-A	0	0	0	-1	-1	-1	-1	-1	-A	-1	-1	-1
x38	B	-1	-1	-1	/A	-A	0	0	0	-1	-1	-1	-1	-1	-A	-1	-1	-1
x39	-1	2			2	0	0	0	0	-A	-A	-A	-A	-1	-A	-1	B	B

Table3-C (Continued)

x84	-/d	0	0	0	-/d	/d	0	0	/C	/d	0	0	0	0	/d	-/d	0
x85	0	0	0	/d	0	-/d	0	0	/C	/d	0	0	0	0	/d	-/d	0
x86	0	0	0	0	0	0	0	0	/C	/d	0	0	0	0	0	0	0
x87	0	0	0	0	0	0	0	0	/C	0	0	0	0	0	0	0	0
x88	0	0	0	0	0	0	0	0	/C	/C	0	0	0	/d	0	0	0
x89	0	0	0	0	0	0	0	0	/C	0	0	0	0	0	0	0	0
x90	0	0	0	0	0	0	0	0	/C	/C	0	0	0	/d	0	0	0

Table3-D: Character Table of G

	91	6c	6d	6e	3ap	3aq	3ar	3as	3at	3au	3av	3aw	3ax	3ay	9m	9n	3az
x1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x2	1	-1	-1	-1	1	1	1	1	1	1	1	1	1	1	1	1	1
x3	/A	1	-A	/A	1	1	1	1	A	/A	1	1	1	1	A	/A	1
x4	/A	-1	-A	/A	1	1	1	1	A	/A	1	1	1	1	A	/A	1
x5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
x6	A	-1	/A	-A	1	1	1	1	/A	A	1	1	1	1	/A	A	1
x7	A	A	A	A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x8	A	-A	-A	-A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x9	A	1	-A	/A	1	1	1	1	A	/A	1	1	1	1	A	/A	1
x10	-A	-1	-A	/A	-1	-1	-1	-1	A	/A	1	1	1	1	A	/A	1
x11	/A	A	-1	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x12	/A	-A	-1	-A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x13	/A	/A	/A	/A	A	A	A	A	A	A	A	A	A	A	A	A	A
x14	/A	/A	-A	/A	A	A	A	A	A	A	A	A	A	A	A	A	A
x15	A	/A	1	A	A	A	A	A	A	A	A	A	A	A	A	A	A
x16	A	-A	-A	-1	-A	A	A	A	A	1	A	A	A	A	A	1	A
x17	1	1	1	1	A	A	A	A	1	/A	A	A	A	A	1	/A	A
x18	-1	1	-A	-A	A	A	A	A	1	/A	A	A	A	A	1	/A	A
x19	0	0	0	0	0	2	2	2	2	2	2	-1	-1	-1	-1	-1	-1
x20	-1	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x21	-1	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x22	2	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
x23	-1	0	0	0	/B	/B	/B	/B	2	/B	/B	/B	/B	/B	-1	-1	-1
x24	-A	0	0	0	/B	/B	/B	/B	2	/B	/B	/B	/B	/B	-A	-A	-A
x25	-A	0	0	0	/B	/B	/B	/B	2	/B	/B	/B	/B	/B	-A	-A	-A
x26	-A	0	0	0	B	B	B	B	2	/B	B	B	B	B	-A	-A	-A
x27	-1	0	0	0	B	B	B	B	2	/B	B	B	B	B	-1	-1	-1
x28	-A	0	0	0	B	B	B	B	2	/B	B	B	B	B	-A	-A	-A
x29	-A	0	0	0	2	2	2	2	B	/B	2	2	2	2	-1	-1	-1
x30	-1	0	0	0	2	2	2	2	/B	B	2	2	2	2	-1	-1	-1
x31	-A	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x32	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x33	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x34	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x35	-1	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x36	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x37	-A	0	0	0	-1	-1	-1	-1	-A	-A	-1	-1	-1	-1	-1	-1	-1
x38	-A	0	0	0	-1	-1	-1	-1	-A	-A	-1	-1	-1	-1	-1	-1	-1
x39	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x40	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x41	B	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x42	-A	0	0	0	-A	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A
x43	-B	0	0	0	-1	-1	-1	-1	-A	-A	-1	-1	-1	-1	-1	-1	-1
x44	/A	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x45	-1	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x46	B	0	0	0	-1	-1	-1	-1	-A	-A	-1	-1	-1	-1	-1	-1	-1
x47	/B	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x48	2	0	0	0	-A	-A	-1	-1	-A	-A	-A	-A	-A	-A	-1	-1	-1
x49	-A	0	0	0	-1	-1	-1	-1	-A	-A	-1	-1	-1	-1	-1	-1	-1
x50	-1	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x51	-A	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x52	/B	0	0	0	0	0	0	0	-A	-1	-1	-1	-1	-1	-1	-1	-1
x53	2	0	0	0	C	-A	-A	-A	-1	-A	-1	-1	-1	-1	-1	-1	-1
x54	0	0	0	0	-A	-A	-A	-1	-A	-A	-A	-A	-A	-A	-A	-A	-A
x55	0	0	0	0	6	6	6	6	0	0	-3	-3	0	0	0	0	0
x56	0	0	0	0	-3	6	6	-3	0	0	0	0	0	0	3	0	3

Table3-D (Continued)

x57	0	0	0	0	-3	6	-3	0	0	0	0	-3	3	0	0	0	0	0
x58	0	0	0	0	-3	6	-3	0	0	0	0	-3	3	0	0	0	0	-3
x59	0	0	0	0	-3	-3	6	0	0	0	0	-3	-3	0	0	0	0	-3
x60	0	0	0	0	-3	-3	6	0	0	0	0	-3	0	0	0	0	0	3
x61	0	0	0	0	-3	-3	6	0	0	0	0	3	0	-3	0	0	0	0
x62	0	0	0	0	6	-3	-3	0	0	0	0	3	0	0	0	0	0	3
x63	0	0	0	0	6	-3	-3	0	0	0	0	0	0	-3	3	0	0	0
x64	0	0	0	0	6	-3	-3	0	0	0	0	-3	3	0	0	0	0	-3
x65	0	0	0	0	-3	-3	-3	0	0	-3	6	0	0	0	0	0	0	0
x66	0	0	0	0	-3	-3	-3	0	0	-3	-3	0	0	0	0	0	0	0
x67	0	0	0	0	/C	/C	/C	0	0	/D	/D	0	0	0	0	0	0	0
x68	0	0	0	0	/C	/C	/C	0	0	/D	/D	0	0	0	0	0	0	0
x69	0	0	0	0	/D	/C	/D	0	0	0	0	0	0	/D	/D	0	0	-D
x70	0	0	0	0	0	D	C	D	0	0	0	0	0	0	0	0	0	0
x71	0	0	0	0	/D	/C	/D	0	0	0	0	0	0	/D	/D	0	0	0
x72	0	0	0	0	0	D	C	D	0	0	0	0	0	0	0	0	0	0
x73	0	0	0	0	/D	/C	/D	0	0	0	0	0	0	-D	0	0	0	/D
x74	0	0	0	0	0	D	C	D	0	0	0	0	0	0	0	0	0	D
x75	0	0	0	0	/D	/D	/C	0	0	0	0	0	0	/D	/D	0	0	/D
x76	0	0	0	0	0	D	D	C	0	0	0	0	0	-D	0	0	0	D
x77	0	0	0	0	/D	/D	/C	0	0	0	0	0	0	/D	0	0	0	-D
x78	0	0	0	0	0	D	C	D	0	0	0	0	0	-D	0	0	0	0
x79	0	0	0	0	/D	/D	/C	0	0	0	0	0	0	/D	0	0	0	0
x80	0	0	0	0	0	D	D	C	0	0	0	0	0	-D	0	0	0	0
x81	0	0	0	0	/C	/D	/D	0	0	0	0	0	0	/D	0	0	0	-D
x82	0	0	0	0	0	D	C	D	0	0	0	0	0	0	0	0	0	0
x83	0	0	0	0	/C	/D	/D	0	0	0	0	0	0	/D	0	0	0	0
x84	0	0	0	0	0	C	D	D	0	0	0	0	0	D	-D	0	0	0
x85	0	0	0	0	/C	/D	/D	0	0	0	0	0	0	/D	-D	0	0	/D
x86	0	0	0	0	0	C	D	D	0	0	0	0	0	-D	0	0	0	0
x87	0	0	0	0	/D	/D	/D	0	0	/D	/C	0	0	0	0	0	0	0
x88	0	0	0	0	0	D	C	D	0	0	0	0	0	0	0	0	0	0
x89	0	0	0	0	/D	/D	/D	0	0	0	/D	0	0	0	0	0	0	0
x90	0	0	0	0	0	D	D	D	0	0	C	0	0	0	0	0	0	0

Table3-E: Character Table of G

	3ba	3bb	9a	9p	3bc	3bd	3be	3bf	3bg	3bh	3bi	3bj	9q	9r	6f	6g	6h
x1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
x2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	-1
x3	1	1	A	/A	1	1	A	/A	1	1	1	1	A	/A	-1	-A	-A
x4	1	1	A	/A	1	1	A	/A	1	1	1	1	A	/A	1	A	-A
x5	1	1	/A	A	1	1	/A	A	1	1	1	1	/A	A	1	/A	A
x6	1	1	/A	A	1	1	/A	A	1	1	1	1	/A	A	-1	/A	-A
x7	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x8	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A	/A
x9	/A	/A	1	A	/A	/A	1	A	/A	/A	/A	1	A	/A	1	A	-A
x10	/A	/A	1	A	/A	/A	1	A	/A	/A	/A	1	A	/A	1	A	-A
x11	/A	/A	A	1	/A	/A	A	1	/A	/A	/A	A	1	/A	A	1	-A
x12	/A	/A	A	1	/A	/A	A	1	/A	/A	/A	A	1	/A	A	-1	-A
x13	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A
x14	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A
x15	A	A	A	A	A	A	A	1	A	A	A	A	A	/A	1	-A	-A
x16	A	A	A	/A	1	A	A	/A	1	A	A	A	A	A	1	-A	-A
x17	A	A	A	1	/A	A	A	1	/A	A	A	A	A	1	/A	A	1
x18	A	A	A	1	/A	A	A	1	/A	A	A	A	A	1	/A	A	-1
x19	-1	-1	-1	-1	2	2	2	2	2	-1	-1	-1	-1	-1	0	0	0
x20	-1	-1	-1	-1	2	2	2	2	2	-1	-1	-1	-1	-1	0	0	0
x21	2	2	2	2	2	2	2	2	2	2	-1	-1	-1	-1	0	0	0
x22	-1	-1	-1	-1	2	2	2	2	2	2	2	2	2	2	0	0	0
x23	-A	-A	-1	-A	/B	/B	2	B	/B	-A	-A	-A	-1	-A	0	0	0
x24	-A	-A	-1	-A	/B	/B	B	2	/B	-A	-A	-A	-1	-A	0	0	0
x25	-A	-A	-A	-A	/B	/B	/B	2	/B	-A	-A	-A	-A	-A	0	0	0
x26	-A	-A	-A	-A	/B	/B	B	2	/B	-A	-A	-A	-1	0	0	0	0
x27	-A	-A	-1	-A	B	B	B	2	/B	B	-A	-A	-1	0	0	0	0
x28	-A	-A	-A	-A	B	B	B	B	B	-A	-A	-A	-A	0	0	0	0
x29	-1	-1	-A	-A	2	2	2	B	/B	2	-1	-1	-1	-A	0	0	0
x30	-1	-1	-A	-A	2	2	2	B	/B	2	-1	-1	-1	-A	0	0	0

4. Conclusions

The present character table for bipyramidal geometry pentamethylphosphorus has been deduced from:

- the structure of group:

$$G_{1458} = [W^I \wedge V^I] \wedge [C_{3v}^I \times C_{3v}^I \times C_{3v}^I \times C_{3v}^I \times C_{3v}^I]$$

- the division of group in 90 conjugacy classes, the sum of squares of the dimensions of which gives the order of the group:

$$18 \times (1)^2 + 36 \times (4)^2 + 36 \times (6)^2 = 1458$$

- the composition of the 90 conjugacy classes in;

1, 2, 9, 9, 6, 6, 6, 6, 18, 18, 2, 2, 2, 18, 18, 6, 6, 6, 6, 6, 6, 18, 18, 6, 6, 6, 18, 18, 81, 81, 81, 2, 2, 2, 18, 18, 6, 6, 6, 6, 18, 18, 6, 6, 6, 18, 18, 1, 2, 9, 9, 6, 6, 6, 6, 18, 18, 81, 81, 81, 2, 2, 2, 18, 18, 6, 6, 6, 6, 6, 18, 18, 6, 6, 6, 18, 18, 1, 2, 9, 9, 6, 6, 6, 6, 18, 18, 81, 81, and 81 elements.

The potential energy function for rotation of five methyl groups may now be described by a 243-fold well potential energy hypersurface. As a result, the spectrum of the bipyramidal geometry of pentamethylphosphorus is expected to possess 243 substates.

The 5-coordinated Phosphorus compounds such as PCl_5 and PF_5 have been reported in the literature [27], and the preparation of $P(CH_3)_5$ (RN 113848-99-0) seems to be described in [28]. The compound is mentioned in [29,30]. See as well work on as $P(CH_3)_5$ in [31].

Acknowledgement : to express their gratitude to Professor I. Yavari for many useful discussions.

References

- [1] Y. G. Smeyers and M. Villa, *J. Math. Chem.* 28(4) (2000) 377-388.
- [2] Y. G. Smeyers, *Adv. Quantum Chem.* 24 (1992) 1-77.
- [3] Y. G. Smeyers, in: *Structure and Dynamics of Non- Rigid Molecular Systems*, Y. G. Smeyers (ed), Kluwer Academic, Dordrecht. 1995, 121-151.
- [4] A. R. Ashrafi and M. Hamadani, to appear in *Croat. Chem. Acta* (2003).
- [5] M. Hamadani and A. R. Ashrafi, to appear in *Croat. Chem. Acta* (2003).
- [6] A. R. Ashrafi, to appear in *Korean J. Comput. Appl. Math.*
- [7] M. Hamadani and A. R. Ashrafi, *IJMMS.*, 42 (2003) 2701-2706.
- [8] P. R. Bunker, *Mol. Phys.*, 8 (1964) 81.
- [9] J. Serre, *Intl. J. Quantum Chem.*, S 2 (1968) 107.
- [10] S. L. Altmann, " *Induced Representation in Crystal & Molecules*", Academic Press, London, 1977.
- [11] G. S. Ezra, " *Symmetry Properties of Molecules*", *Lecture Note in Chemistry* 28, Springer, 1982.
- [12] J. Maruani and J. Serre (eds), " *Symmetries and Properties of Non-Rigid Molecules*", Elsevier, Amsterdam, 1983.
- [13] Y. G. Smeyers, M. L. Senent, V. Botella and D. C. Moule, *J. Chem. Phys.*, 98 (1993) 2754.
- [14] A. Van der Avoird, *J. Chem. Phys.*, 98 (1993) 5327.
- [15] Y. G. Smeyers, M. Villa and M. L. Senent, *J. Mol. Spect.*, 191 (1998) 232.
- [16] A. Viver-Bung, V. H. Uet and Y. G. Smeyers, *J. Chem. Phys.*, 109 (1998) 2279.
- [17] H. C. Longuet-Higgins, *Mol. Phys.* 6 (1963) 445.
- [18] P. R. Bunker, *Molecular Symmetry in Spectroscopy*, NRC Research Prss, 1998
- [19] I. M. Isaacs, *Character Theory of Finite Groups*, Academic Press, 1978.
- [20] G. James and M. Liebeck. *Representation and Characiers of Goups*, Cambridge University Press, 1993.

- [21] J. S. Lomont, *Applications of Finite Groups*, Academic Press Inc., New York, 1959.
- [22] D. R. Lide and D. E. Man, *J. Chem. Phys.* 28 (1958) 572
- [23] Y. G. Smeyers and M. Villa, *Chem. Phys. Lett.* 235 (1995) 576.
- [24] M. Schonert et al., *GAP, Groups, Algorithms and Programming*, Lehrstuhl De für Mathematik, RWTH, Aachen, 1992.
- [25] A. J. Stone, *J. Chem. Phys.*, 41 (1964) 1568-1579.
- [26] J. T. Hougen, *J. Mol. Spec.*, 82 (1980) 92.
- [27] A. Earnshaw and N. N. Greenwood, *Chemistry of Elements*, Elsevier Science, 1997.
- [28] R. Bartsch et al., *Journal of Fluorine Chemistry* (1987), 36 (1), 107-117.
- [29] E. Chamorro, P. Fuentealba and A. Savin, *J. Comp. Chem.*, 24(4) (2003) 496-504.
- [30] Stéphane Noury, Bernard Silvi, and Ronald J. Gillespie, *Inorganic Chemistry*, 41(8) (2002) 2164-2172.
- [31] Tim M. Greene et al., *Organometallics*, 17(24) (1998) 5287 – 5293.