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# On Non-Rigid Group Theory For Some Molecules

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## Abstract

Non-rigid molecule group theory (NRG) in which dynamical symmetry operations are defined as physical operations is a new field of chemistry. Smeyers and Villa computed the restricted NRG (r-NRG) of the triple equivalent methyl rotation in pyramidal trimethylamine with inversion and proved that the r-NRG of this molecule is a group of order 648, containing two subgroups of order 324 without inversions (see *J. Math. Chem.* 28 (4)(2000) 377-388).

In this paper, we introduce the Computer Algebra System GAP for solving some problems in Computational Chemistry. We reprove the results of the mentioned paper of Smeyers and Villa by Computer Algebra System GAP. Finally, we apply GAP to find the character table of full non-rigid group(f-NRG) of tetraamine platinum (II) with the point-group symmetry $C_{4v}$.

## INTRODUCTION

GAP stands for Groups, Algorithms and Programming. The name was chosen to reflect the aim of the system, which is a group theoretical software for solving computational problems in group theory. The last years have seen a rapid spread of interest in the understanding, design and even implementation of group theoretical algorithms. These are gradually becoming accepted both as standard tools for a working group theoretician, like certain methods of proof, and as worthwhile objects of study, like connections between notions expressed in theorems. GAP was started as an attempt to meet this interest. This software was constructed by GAP's team in Aachen [1].

GAP is a free and extensible software package for computation in discrete abstract algebra. The term extensible means that you can write your own programs in the GAP language, and use them in just the same way as the programs which form part of the system (the "library").

Development of GAP began at Lehrstuhl D fur Mathematik, RWTH-Aachen, under the leadership of Professor Joachim Neubuser in 1985. Version 2.4 was released in 1988 and version 3.1 in 1992. The final full release of GAP 3, version 3.4, was made in 1994. In 1997, Professor Neubuser retired, and overall coordination of GAP development, now very much an international effort, was transferred to St Andrews. A complete internal redesign and almost complete rewrite of the system, which was already in progress in Aachen, was completed and following five, increasingly usable, beta-test releases, version 4.1, released July 1999, was the first version of the rewritten system to be released without any restriction for general use. Version 4.2 followed in spring 2000, version GAP 4.3 in May 2002 and, GAP 4.4 is being released in March 2004. More information on the motivation and development of GAP to date, can be found on GAP web page that you find on http://www.gap-system.org.

The method described in this paper appears to be quite general, and can be extended to solve several problems in computational chemistry. GAP contains a large library of groups, named small group library. The Small Group Library contains all groups of order up to 2000, except for 1024, up to isomorphism. The function SmallGroup(n,i) returns the $i^{th}$ group of order n in the catalogue. Also, the functions NrSmallGroups(n) and AllSmallGroups(n) return the number of groups of order n and the list of all groups of order n, respectively. It is possible to work with the catalogue of groups of small order just using the functions described above. However, the catalogue is rather large even though the groups are stored in a very compact description.

The mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of physical systems. The symmetry properties of rigid molecules are well known and so it is natural to investigate non-rigid molecules. Following Y.G. Smeyers [2], the non-rigid molecule group (NRG) will be strictly defined as the complete set of the molecular conversion operations, which commute with a given nuclear Hamiltonian operator, limited to large amplitude motions. In addition, these molecular conversation operations will be expressed in terms of physical operations, such as rotations, internal rotations, inversions, similarly as in the Altmann's theory, rather than in terms of permutations and permutations-inversions. This way of expressing the non-rigid operations is indeed more descriptive and flexible [3].

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 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 have appeared in the literature [4-11].

In 1963 Longuet-Higgins [12], 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 to calculate these character tables, which are needed for classification of wave functions, determination of selection rules, and so on.

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 tetraamine platinum (II), which is considered here in some detail. It is not appropriate in cases where the framework is linear, as in ethane, but Bunker [13] has shown how to deal with such molecules. To compute the character table of this molecule we use [14,15] for the standard notation and terminology on character theory.

Lomont [16], 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 of the group multiplication table and they become very unwieldy as soon as the order of the group becomes even moderately large. For non-rigid molecules, whose symmetry groups may have several thousand elements, they are usually quite impracticable. We show that in such a case GAP is a useful package for computing the character table and even the group structure.

The alternative approach is less mechanical, requiring a certain amount of thought, but it is nevertheless simpler in practice. This involves two steps: first, by the decomposition of the group into classes and second, by the determination of sets of basis functions for certain representations, the characters are then determined.

Let G be a group and 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 $G = HN = \{xy \mid x \in H, y \in N\}$, then we say that G is a semidirect product of H by N

denoted by H∧N. It is a well-known fact that every semidirect product of H by N, completely determines by a homomorphism $\alpha$: H $\longrightarrow$ Aut(N), where Aut(N) denotes the full automorphism group of N(for details see [15]). We now suppose that $G_{648}$ is the r-NRG of trimethylamine. In [17] Smeyers and Villa investigated the r-NRG of planar trimethylamine and proved that this is a group of order 324. They showed that this molecule has a pyramidal inversion and so the order of the r-NRG of trimethylamine is 648. Moreover, $G_{648} = [U^I \wedge W^I] \wedge I^I \wedge [C^I_{3_1} \times C^I_{3_2} \times C^I_{3_3}] \times V^I$, in which for groups A and B, A ∧ B denotes the semidirect product of A and B, A × B denotes the direct product of A and B and $U^I$, $W^I$, $I^I$, $C^I_{3_1}$, $C^I_{3_2}$, $C^I_{3_3}$ and $V^I$ are subgroups of $G_{648}$ defined as follows:

$$U^I = [\hat{E} + \hat{U}],\ W^I = [\hat{E} + \hat{W} + \hat{W}^2],\ I^I = [\hat{E} + \hat{I}],$$
$$V^I = [\hat{E} + \hat{V}],\ C^I_{3_j} = [\hat{E} + \hat{C}_{3_j} + \hat{C}_{3_j}{}^2];\ j = 1,2,3.$$

For basic properties of non-rigid molecule group and information on r-NRG and f-NRG the reader is referred to [2,18].

In [19] Stone described a method which is appropriate for molecules with a number of $XH_3$ groups attached to a rigid framework. It is not appropriate in cases where the framework is linear, as in ethane and dimethylacetylene.

In [20, 21], the present author investigated the f-NRG of tetraamine platinum(II) with the symmetry group $C_{2v}$ and the f-NRG of *cis*- and *trans*-dichloro-diammine platinum(II). In this paper, using the mathematical software GAP, we calculate the f-NRG of tetraamine platinum(II) with the $C_{4v}$ point group and prove that it is a group of order 5184 with 45 conjugacy classes. Also, we compute the character table of this group. Our notation is standard and taken mainly from [2,14,15].

## EXPERIMENTAL

In order to deduce the character table of a group, we have to know first the number of classes, as well as the number of elements in each class. As it is well known, the number of classes gives the number of irreducible representations. For every element x of a group T, the subgroup $C_T(x) = \{y \in T \mid xy = yx\}$ is called the centralizer of x in T. Moreover, $Z(G) = \cap C_T(x)$, when x varies on G, is called the centre of G and G is called centreless if $|Z(G)| = 1$.

If T is finite, then by a well-known theorem in group theory $|C_T(x)| = |T|/|Cl_T(x)|$, in which $Cl_T(x)$ is the conjugacy class of x in T [14]. Also, $|C_T(x)|$ and $|Cl_T(x)|$ are called the centraliser order and conjugacy length of x in the group T, respectively. To simplify our argument we denote by na, nb, nc, ... the different conjugacy classes of elements of order n in the group T.

For a given group, G, Exp(G) denotes the least positive integer for which every element of G to the power of this integer is the identity element of G. If $|G| = p^n a$, where p is a prime number and a is an integer which is not divisible by p, then by a well known theorem on finite groups, G has a subgroup of order $p^n$, which is called the Sylow p-subgroup of G. Smeyers and Villa [17] determined the character table for the triple equivalent methyl rotation and pyramidal inversion in trimethylamine. Using GAP-SYSTEM we first present another approach to calculate these character tables and then we compute the character table of tetraamine platinum (II) with the point-group symmetry $C_{4v}$. We will see that the later is a group of order 5184 with 45 irreducible characters.

## RESULTS AND DISCUSSION

In this section we first present a new method to compute the character table of the triple equivalent methyl rotation and pyramidal inversion in trimethylamine. As we mentioned before, $G_{648} = [U^I \wedge W^I] \wedge I^I \wedge [C_{3_1}^I \times C_{3_2}^I \times C_{3_3}^I] \times V^I$. By a well-known fact in finite groups, if $G = H \times K$ then every conjugacy class of G is the product of a conjugacy class of H and a conjugacy class of K. A similar fact is true for the irreducible characters of G. Thus it is enough to compute the character tables of the group $G_{324} = [U^I \wedge W^I] \wedge I^I \wedge [C_3 \times C_3 \times C_3]$. To do this we note that by equations (2) and (6) of [17] $G_{324}$ is a centreless group of exponent 18. Also, by these equations $G_{324}$ has a normal Sylow 3-subgroup. Using these facts and the Small Group Library of GAP, we write a GAP-program, as follows:

```
gap> X:=[];
gap> n:=NrSmallGroups(324);
gap> for i in [1,2..n] do
gap> a:=SmallGroup(324,i);
gap> b:=SylowSubgroup(a,3);
gap> e := Size(Centre(a));
gap>  if IsNormal(a,b)=true and IsAbelian(a)=false and
        Exponent(a)=18 and e=1  then Add(X,i);fi;
gap> od;
```

In this program the command "NrSmallGroups(324)" computes the number of non-isomorphic groups of order 324. Also, we can see that the output of this program will be the set X = {36,37,39,40,41,118,119,120,123,125}. This shows that there are only ten groups of order 324 which are a semidirect product of a group of order 12 and an elementary abelian group of order 27. The arrays of $G_{324}$ must be integral. Using this fact, we write another GAP-program, as follows:

```
gap> X = [36,37,39,40,41,118,119,120,123,125];
gap> for i in x do
gap> a:=SmallGroup(324,i);
gap> b:=CharacterTable(a);
gap> t:=Irr(b);
gap> n:=Size(t);
gap> y:=[];
gap> for j in [1,2..n] do
gap> y:=Union(y,t[j]);
gap> od;
gap> if IsSubset(Integers,y)=true then Print(i,"\n");fi;
gap> od;
```

The output of this program is 39 and so there is a unique group of order 324 which satisfies the conditions of Smeyers and Villa [17]. Thus $G_{324}$ = SmallGroup(324,39), according to the notation of GAP. Now we can see that the command "Display(CharacterTable(SmallGroup(324,39)))" computes the full character table of $G_{324}$.

Next we compute the character table of f-NRG of tetraamineplatinum (II) with point group symmetry $C_{4v}$. Firstly, we consider the point group of tetraamineplatinum (II) in the case of 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 $C_{4v}$.

Using Figure 1, we define three permutations x, y and z, as follows:

x = (2,3,4,5)(6,9,12,15,7,10,13,16,8,11,14,17),
y = (2,3,4,5)(6,9,12,15,7,10,13,17,8,11,14,16),
z = (4,3)(2,5)(6,15)(7,17)(8,16)(12,9)(13,11)(14,10).

In fact in this figure we label the central Platinum atom by number 1, four nitrogen atoms by 2, 3, 4 and 5, and, hydrogen atoms by 6, ... ,17. Thus (2,6,7,8), (3,9,10,11), (4,12,13,14) and (5,15,16,17) label the four $XH_3$-bonds of the molecule. Set A = {x, y, z}. We claim that A is a generating set for G. Since $G_{324} = [U^I \wedge W^I] \wedge I^I \wedge [C^I_{3_1} \times C^I_{3_2} \times C^I_{3_3}]$, we can choose a set X containing 6 permutations of {1,...,17} such that two of them generate the subgroup $[U^I \wedge W^I]$, one of them generates $I^I$ and other permutations generate $C^I_{3_1} \times C^I_{3_2} \times C^I_{3_3}$. We now write a simple program in GAP-language to find the order of G.

```
gap> G:=Group(X);
gap> H:=Group(x,y,z);
gap> P:=Elements(G);
gap> Q:= Elements(H);
gap> IsEqualSet(P,Q);
gap> Size(G);
```

The output of the program is "true" and 5184, which denotes H = G and the order of G is 5184. Now we find a representative for all of the conjugacy classes of the group G. To do this, we consider the following GAP-program:

```
gap> E := [] ;
gap>F:= [];
gap> n:= NrConjugacyClasses(G);
gap> t:= ConjugacyClasses(G);
gap> for i in [1,2..n] do
gap> v:= Representative(t[i]);
gap> w:= Size(t[i]);
gap> Add(E,v);
gap> Add(F,w);
gap>od;
```

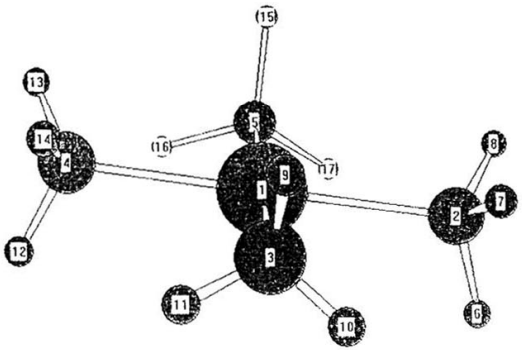


**Figure 1:** The structure of tetraaminoplatinum (II) with the $C_{4v}$ symmetry group

The output of this program is n = 45, which shows that G has exactly 45 conjugacy classes and so 45 irreducible characters. Also, the set E is a representative set for the conjugacy classes of G and the set F contains the class lengths of the group G. We note that in the command "t:=ConjugacyClasses(G)" the classes are computed by random search. In Table 1 we summarise the output of this program.

For computing the character table of G, we run the simple GAP-program:

```
gap> d:=CharacterTable(G);
gap> Display(d);
```

Table 2 contains the output of the above program. If we need the sum of some of irreducible characters of the group, say the $a_1^{th}$, $a_2^{th}$,..., $a_r^{th}$ irreducible characters of G, we can do this by running the following program:

```
gap> t:=CharacterTable(G);
gap> R:=[ a1,..., ar];
gap> J:=[];
gap> for i in R do
gap> g:= Irr(t)[i];
gap> Add(J,g);
gap> od;
gap> Sum(J);
```

## CONCLUDING REMARKS

We can use this method for computing with small groups. When the order of the group is large, the command "CharacterTable(G)" is interrupted. In this situation, one can find a normal subgroup N of G and then compute the character table of G/N. Then lifting the irreducible characters of G/N to the group G, one can determine some of the irreducible characters of G. This method is usually very useful for completing the character table of the group, see [19,20].

On the other hand, there is a well-known method for computing the irreducible characters of a finite group with a subgroup of index 2 [14]. Using the mentioned functions in GAP SYSTEM and the method of subgroups of index 2, one can find a new fast method to compute the character table of groups of order greater than 2000, when the group has a subgroup of index 2.

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**Table 1**: The Representatives of Conjugacy Classes of the Group G

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

**Table 2:** The Character Table and Power Map of the Group G

| | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 6a | 2a | 6b | 2b | 12a | 4a | 2c | 6c | 6d | 6e | 6f | 2d | 2e | 6g | 6h |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2p | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 3a | 1a | 3c | 1a | 6a | 2a | 1a | 3c | 3e | 3f | 3c | 1a | 1a | 3e | 3e |
| 3p | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 2a | 2a | 2a | 2b | 4a | 4a | 2c | 2c | 2c | 2d | 2d | 2d | 2e | 2b | 2e |
| 5p | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 6a | 2a | 6b | 2b | 12a | 4a | 2c | 6c | 6d | 6e | 6f | 2d | 2e | 6g | 6h |
| 7p | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 6a | 2a | 6b | 2b | 12a | 4a | 2c | 6c | 6d | 6e | 6f | 2d | 2e | 6g | 6h |
| 11p | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 6a | 2a | 6b | 2b | 12a | 4a | 2c | 6c | 6d | 6e | 6f | 2d | 2e | 6g | 6h |
| $\chi_1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_2$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_3$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 |
| $\chi_4$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 |
| $\chi_5$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_6$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_7$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 |
| $\chi_8$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 |
| $\chi_9$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | -2 | -2 | -2 | 2 | 0 | 0 | -2 | -2 | -2 | 2 | 2 | 2 | 0 | 0 | 0 |
| $\chi_{10}$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | -2 | -2 | -2 | 2 | 0 | 0 | -2 | -2 | -2 | 2 | 2 | 2 | 0 | 0 | 0 |
| $\chi_{11}$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 0 | 0 | -2 | -2 | -2 | -2 | -2 | -2 | 0 | 0 | 0 |
| $\chi_{12}$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 0 | 0 | -2 | -2 | -2 | -2 | -2 | -2 | 0 | 0 | 0 |
| $\chi_{13}$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | -2 | -2 | -2 | 2 | 0 | 0 | 2 | 2 | 2 | -2 | -2 | -2 | -2 | -2 | -2 |
| $\chi_{14}$ | 2 | 2 | 2 | 2 | 2 | 2 | 2 | -2 | -2 | -2 | 2 | 0 | 0 | 2 | 2 | 2 | -2 | -2 | -2 | 20 | 2 | 2 |
| $\chi_{15}$ | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 0 | 0 | 0 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{16}$ | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 0 | 0 | 0 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{17}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | -2 | 4 | 1 | 0 | 0 | 0 | 4 | 1 | -2 | -2 | 1 | 4 | 0 | 0 | 0 |
| $\chi_{18}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | -2 | 4 | 1 | 0 | 0 | 0 | 4 | 1 | -2 | -2 | 1 | 4 | 0 | 0 | 0 |
| $\chi_{19}$ | 8 | -4 | 2 | 2 | -1 | 5 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | 0 | 0 | 0 | -4 | 2 | -1 |
| $\chi_{20}$ | 8 | -4 | 2 | 2 | -1 | 5 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | 0 | 0 | 0 | -4 | 2 | -1 |
| $\chi_{21}$ | 8 | -4 | 2 | 2 | -1 | 5 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | 0 | 0 | 0 | 4 | -2 | 1 |
| $\chi_{22}$ | 8 | -4 | 2 | 2 | -1 | 5 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | 0 | 0 | 0 | 4 | -2 | 1 |
| $\chi_{23}$ | 8 | -4 | 2 | 2 | -1 | -4 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 |
| $\chi_{24}$ | 8 | -4 | 2 | 2 | -1 | -4 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 |
| $\chi_{25}$ | 8 | -4 | 2 | 2 | -1 | -4 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 |
| $\chi_{26}$ | 8 | -4 | 2 | 2 | -1 | -4 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 |
| $\chi_{27}$ | 8 | 5 | 2 | 2 | -1 | -4 | -4 | 1 | 4 | -2 | 0 | -1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{28}$ | 8 | 5 | 2 | 2 | -1 | -4 | -4 | 1 | 4 | -2 | 0 | -1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{29}$ | 8 | 5 | 2 | 2 | -1 | -4 | -4 | 1 | 4 | -2 | 0 | 1 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{30}$ | 8 | 5 | 2 | 2 | -1 | -4 | -4 | 1 | 4 | -2 | 0 | 1 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{31}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | 2 | -4 | -1 | 0 | 0 | 0 | -4 | -1 | 2 | -2 | 1 | 4 | 0 | 0 | 0 |
| $\chi_{32}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | 2 | -4 | -1 | 0 | 0 | 0 | -4 | -1 | 2 | -2 | 1 | 4 | 0 | 0 | 0 |
| $\chi_{33}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | -2 | 4 | 1 | 0 | 0 | 0 | -4 | -1 | 2 | 2 | -1 | -4 | 0 | 0 | 0 |
| $\chi_{34}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | -2 | 4 | 1 | 0 | 0 | 0 | -4 | -1 | 2 | 2 | -1 | -4 | 0 | 0 | 0 |
| $\chi_{35}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | 2 | -4 | -1 | 0 | 0 | 0 | 4 | 1 | -2 | 2 | -1 | -4 | 0 | 0 | 0 |
| $\chi_{36}$ | 8 | 2 | -4 | 5 | -1 | 2 | 2 | 2 | -4 | -1 | 0 | 0 | 0 | 4 | 1 | -2 | 2 | -1 | -4 | 0 | 0 | 0 |
| $\chi_{37}$ | 16 | -8 | 4 | 4 | -2 | 10 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | -8 | 4 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{38}$ | 16 | -8 | 4 | 4 | -2 | -8 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 4 | -8 | 0 | 0 | 0 |
| $\chi_{39}$ | 16 | 10 | 4 | 4 | -2 | -8 | -8 | -2 | -8 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{40}$ | 16 | 4 | 1 | -8 | -2 | 4 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -1 | 2 |
| $\chi_{41}$ | 16 | 4 | 1 | -8 | -2 | 4 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -1 | 2 |
| $\chi_{42}$ | 16 | 4 | 1 | -8 | -2 | 4 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 1 | -2 |
| $\chi_{43}$ | 16 | 4 | 1 | -8 | -2 | 4 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 1 | -2 |
| $\chi_{44}$ | 32 | -4 | -4 | -4 | 5 | -4 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{45}$ | 32 | -4 | -4 | -4 | 5 | -4 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**Table 2:** (Continued)

| | 4b | 12b | 4c | 2f | 6i | 2g | 6j | 6k | 6l | 6m | 6n | 6o | 6p | 6q | 6r | 2h | 4d | 4e | 12c | 4f | 6s | 6t | 2i |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 2b | 6e | 2d | 1a | 3c | 1a | 3a | 3d | 3c | 3c | 3c | 3e | 3f | 3b | 3a | 1a | 2b | 2c | 6d | 2b | 3f | 3b | 1a |
| | 4b | 4c | 4c | 2f | 2f | 2g | 2g | 2g | 2g | 2g | 2g | 2g | 2g | 2h | 2h | 2h | 4d | 4e | 4e | 4f | 2i | 2i | 2i |
| | 4b | 12b | 4c | 2f | 6i | 2g | 6j | 6k | 6l | 6m | 6n | 6o | 6p | 6q | 6r | 2h | 4d | 4e | 12c | 4f | 6s | 6t | 2i |
| | 4b | 12b | 4c | 2f | 6i | 2g | 6j | 6k | 6l | 6m | 6n | 6o | 6p | 6q | 6r | 2h | 4d | 4e | 12c | 4f | 6s | 6t | 2i |
| $\chi_1$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_2$ | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | -1 | -1 | -1 | -1 |
| $\chi_3$ | -1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| $\chi_4$ | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 |
| $\chi_5$ | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| $\chi_6$ | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_7$ | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\chi_8$ | -1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 |
| $\chi_9$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 2 | 2 | 2 | 2 |
| $\chi_{10}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -2 | -2 | -2 | -2 |
| $\chi_{11}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 2 | 2 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{12}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -2 | -2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{13}$ | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{14}$ | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{15}$ | 0 | 0 | 0 | -2 | -2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{16}$ | 0 | 0 | 0 | 2 | 2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{17}$ | 0 | 0 | 0 | -2 | 1 | -6 | 0 | 3 | -3 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{18}$ | 0 | 0 | 0 | 2 | -1 | 6 | 0 | -3 | 3 | 3 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{19}$ | 0 | 0 | 0 | 0 | 0 | -4 | 2 | -1 | 2 | -4 | 2 | -1 | 2 | 0 | 0 | 0 | 0 | 2 | -1 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{20}$ | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | -2 | 4 | -2 | 1 | -2 | 0 | 0 | 0 | 0 | -2 | 1 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{21}$ | 0 | 0 | 0 | 0 | 0 | -4 | 2 | -1 | 2 | -4 | 2 | -1 | 2 | 0 | 0 | 0 | 0 | 2 | -1 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{22}$ | 0 | 0 | 0 | 0 | 0 | 4 | -2 | 1 | -2 | 4 | -2 | 1 | -2 | 0 | 0 | 0 | 0 | -2 | 1 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{23}$ | 0 | 1 | -2 | 0 | 0 | 4 | -2 | 1 | -2 | -2 | 4 | -2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 2 | -4 | |
| $\chi_{24}$ | 0 | -1 | 2 | 0 | 0 | 4 | -2 | 1 | -2 | -2 | 4 | -2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | |
| $\chi_{25}$ | 0 | 1 | -2 | 0 | 0 | -4 | 2 | -1 | 2 | 2 | -4 | 2 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | |
| $\chi_{26}$ | 0 | -1 | 2 | 0 | 0 | -4 | 2 | -1 | 2 | 2 | -4 | 2 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 2 | -4 | |
| $\chi_{27}$ | 0 | 0 | 0 | 0 | 0 | -4 | -1 | -1 | -4 | 2 | 2 | 2 | 2 | 2 | -1 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{28}$ | 0 | 0 | 0 | 0 | 0 | 4 | 1 | 1 | 4 | -2 | -2 | -2 | -2 | -2 | 1 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{29}$ | 0 | 0 | 0 | 0 | 0 | -4 | -1 | -1 | -4 | 2 | 2 | 2 | 2 | -2 | 1 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{30}$ | 0 | 0 | 0 | 0 | 0 | 4 | 1 | 1 | 4 | -2 | -2 | -2 | -2 | 2 | -1 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{31}$ | 0 | 0 | 0 | 2 | -1 | -2 | -2 | 1 | 1 | 1 | -5 | -2 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{32}$ | 0 | 0 | 0 | -2 | 1 | 2 | 2 | -1 | -1 | -1 | 5 | 2 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{33}$ | 0 | 0 | 0 | -2 | 1 | 2 | -4 | -1 | 5 | -1 | -1 | 2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{34}$ | 0 | 0 | 0 | 2 | -1 | -2 | 4 | 1 | -5 | 1 | 1 | -2 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{35}$ | 0 | 0 | 0 | -2 | 1 | 2 | 2 | -1 | -1 | 5 | -1 | -4 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{36}$ | 0 | 0 | 0 | 2 | -1 | -2 | -2 | 1 | 1 | -5 | 1 | 4 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{37}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{38}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{39}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{40}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 2 | -4 | 0 | 0 | 0 | 0 | -2 | 1 | 4 |
| $\chi_{41}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 | 0 | 2 | -1 | -4 |
| $\chi_{42}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 2 | -4 | 0 | 0 | 0 | 0 | 2 | -1 | -4 |
| $\chi_{43}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -2 | 4 | 0 | 0 | 0 | 0 | -2 | 1 | 4 |
| $\chi_{44}$ | 0 | 0 | 0 | 0 | 0 | -8 | -2 | 1 | 4 | 4 | 4 | -2 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\chi_{45}$ | 0 | 0 | 0 | 0 | 0 | 8 | 2 | -1 | -4 | -4 | -4 | 2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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