

The Non-Rigid Group of Tetraamine Platinum(II) as a Wreath Product

M. R. Darafsheh, Y. Farjami,* and A. R. Ashrafi[1]

Department of Mathematics, Statistics and Computer Science, Faculty of Science, University of Tehran, Tehran, Iran

[1]Department of Mathematics, Faculty of Science, University of Kashan, Kashan, Iran

Received November 8, 2004; E-mail: farjami@khayam.ut.ac.ir

A non-rigid molecule group theory (NRG) in which the dynamical symmetry operations are defined as physical operations is a new field of chemistry. Balasubramanian, Smeyers, and Villa in a series of papers applied this notion to determine the character table of restricted NRG (r-NRG) of some molecules. For example, Balasubramanian computed the NRG of the triple equivalent nitro group rotation in 1,3,5-triamino-2,4,6-trinitrobenzene, and proved that the NRG of this molecule is a group of order 48 (see *Chem. Phys. Lett.*, **398**, 15 (2004)). In this work a theoretical method is described for calculating the symmetry group of non-rigid molecules consisting of a number of XY_n ($n = 2, 3, \ldots$) groups attached to a rigid framework. The non-rigid group of the molecule is a wreath product of symmetry group of the rigid frame with the permutation group of the XY_n group. This algebraic structure of NRG helps us to compute the classes and character tables using the ***GAP*** package, even for large groups. We apply this method to find the structure of the non-rigid group of tetraamine platinum(II) with the D_{2d} ordinary point group. It has proved that this is a group of order 5184. The method can be generalized to apply to other non-rigid molecules.

The mathematical tools of group theory have been used extensively to analyze of the symmetry properties of physical systems. Following Y. G. Smeyers[1,2] and K. Balasubramanian,[3,4] the complete set of molecular conversion operations that commute with the nuclear motion operator contains overall rotation operations, describing the molecule rotating as a whole, and intermolecular motion operations, describing molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which we call the Non-Rigid Group (NRG).

Numerous applications of group theory to the large-amplitude vibrational spectroscopy of small organic molecules have appeared in the literature.[3–12] In 1963 Longuet-Higgins[14] investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can easily occur. In many cases, these dynamical 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 to classify wave functions, determine selection rules, and so on. Using a computational approach, Ashrafi and Hamadanian computed character tables of the non-rigid groups of some molecules.[15–17] Balasubramanian, using the wreath product of groups, computed the character table of non-rigid groups for water pentamer and 1,3,5-triamino-2,4,6-trinitrobenzene.[3,4]

The method, as described here, is appropriate for molecules that consist of a number of XY_n groups attached to a rigid framework. An example of such molecules is tetraamine platinum(II) with the D_{2d} ordinary point group, which is considered here in some detail (Fig. 1). Our approach here is as follows. First we specify the algebraic structure of the non-rigid group of this group. With a geometric consideration of dynamic symmetries of the molecules we show that the NRG of the molecule can be specified by the wreath product of some known groups. Then, based on the algebraic structure of the group we apply GAP[18] to compute the character table of NRG of this molecule. The GAP package is useful for computing the character tables, and even the group structure, which merits more attention from the chemical community. The motivation for this study is outlined in Refs. 1, 3, 4, 18–20. Readers are encouraged to consult these papers for background materials and computational techniques. Our notations are standard, and adapted mainly from Refs. 17, 21, and 22.

Structure of the Non-Rigid Group

In this section we first describe some notation, which will be used throughout. Suppose X is a set. The set of all permutations on X, denoted by S_X, is a group, called the symmetric group on X. In the case that $X = \{1, 2, \ldots, n\}$, we denote S_X by S_n or Sym(n).

Let H be a permutation group on X, a subgroup of S_X, and let G be a group. The set of all mappings $X \to G$ is denoted by G^X, i.e., $G^X = \{f | f: X \longrightarrow G\}$. It is clear that $|G^X| = |G|^{|X|}$.

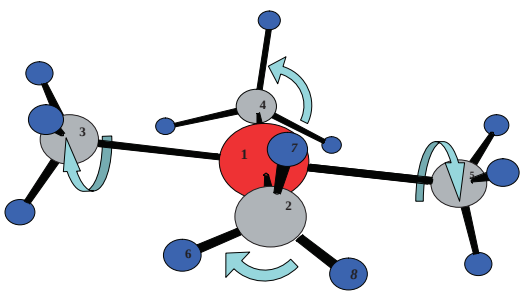

Fig. 1. Structure of tetraamine platinum(II) with D_{2d} ordinary point group symmetry.

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We define $G \sim H = G^X \times H = \{(f; \pi) | f \in G^X, \pi \in H\}$. For $f \in G^X$ and $\pi \in H$, we define $f_\pi \in G^X$ by $f_\pi = f \circ \pi^{-1}$, where "$\circ$" denotes the composition of functions. It is easy to check that the following law of composition:

$$(f; \pi)(f'; \pi') = (ff'_\pi; \pi\pi'), \quad (1)$$

makes $G \sim H$ into a group. This group is called the wreath product of G by H.

In order to characterize the NRG of this molecule, we first note that each dynamic symmetry operation of the molecule, considering the rotations of the NH_3 groups, is composed of two sequential physical symmetry operations. We first have a physical symmetry of the rectangular framework (as we have to map the NH_3 groups on NH_3 groups that are on vertices of the rectangular framework). Such operations are exactly the symmetry operations of a rectangle. It is well-known that such operations form a non-cyclic group of order 4, which is isomorphic to $\boldsymbol{Z_2 \times Z_2}$. After accomplishing the first framework symmetry operation, we have to map each of the four NH_3 group on itself, which forms the symmetric group $\boldsymbol{S_3}$ on three symbols. The number of all such operations is $\boldsymbol{6^4 \times 4 = 5184}$. The composition of such dynamic symmetry elements is described as follows.

Let $\boldsymbol{1}$ denote the platinum atom and use numbers $\boldsymbol{\{2, 3, 4, 5\}}$ to indicate the four nitrogen atoms, and then use $\boldsymbol{6, 7, 8}$ to label the three hydrogen atoms on the $\boldsymbol{2}$ corner. Similarly, let $\boldsymbol{9, 10, 11}$ be the labels of hydrogen atoms on the $\boldsymbol{3}$ corner and so on. Note that the platinum atom is always mapped onto itself. Hence, from a symmetry point of view, the nitrogen atoms on the rectangular rigid frame are mapped on themselves by physical symmetry operations. Due to the position of hydrogen atoms, a mirroring operation through the horizontal plane of the frame is not permitted. This operations form the group $\boldsymbol{\sigma_v(x) \times \sigma_v(y)}$ which is isomorphic to $\boldsymbol{Z_2 \times Z_2}$. We can describe such a configuration with a 3×4 matrix, $[ij]_{3\times4}$, where ij-entry means the i-th hydrogen on the j-th nitrogen corner. The dynamic symmetry operation described above has the form $\boldsymbol{(a_1, a_2, a_3, a_4; \sigma)}$, where $\boldsymbol{\sigma}$ is a symmetry of the rectangle (the first physical operation as above) and, if $\boldsymbol{h:\{1, 2, 3, 4\} \to S_3}$ is a function into the symmetric group $\boldsymbol{S_3}$ of order two with identity element $\boldsymbol{e}$ we write $\boldsymbol{a_1 = h(1)}$, $\boldsymbol{a_2 = h(2)}$, $\boldsymbol{a_3 = h(3)}$, $\boldsymbol{a_4 = h(4)}$. The group $\boldsymbol{G}$ of the symmetries of the molecule acts on the entries of $[ij]_{3\times4}$ as follows. Considering $\boldsymbol{(h;\sigma)}$ and $[ij]$, we first do h on the i-th hydrogen by the rule $\boldsymbol{h}(\sigma(j))(i)$, and then do $\boldsymbol{\sigma}$ on the j-th corner nitrogen to obtain $[\boldsymbol{h}(\sigma(j))(i)\ \sigma(j)]$, which shows the new position of the molecule. This composition rule is the wreath product composition. Therefore, the NRG group $\boldsymbol{G}$ of tetraamine–platinum(II) is isomorphic to $\boldsymbol{S_3 \sim (Z_2 \times Z_2)}$. A similar argument has been given by Balasubramanian.[3,4] From the structure of the wreath product for $\boldsymbol{G}$ we have $|\boldsymbol{G}| = (2 \times 2) \times 6^{(2\times2)} = 5184$; which is consistent with previous results.[15,16] On the other hand, consider the following permutations of the non-rigid group of tetraamine platinum(II):

$$\boldsymbol{x_1} = (2,3,4,5)(6,9,12,15)(7,10,13,16)(8,11,14,17), \quad (2)$$

$$\boldsymbol{x_2} = (2,3,4,5)(6,9,12,15,7,10,13,17,8,11,14,16), \quad (3)$$

$$\boldsymbol{x_3} = (3,5)(7,8)(9,15)(10,17)(11,16)(13,14). \quad (4)$$

Table 1. The Representatives of Conjugacy Classes of the Group $\boldsymbol{G}$

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

Since $\boldsymbol{x_1}$, $\boldsymbol{x_2}$, and $\boldsymbol{x_3}$ are elements of NRG of the molecule, the group generated by these elements is a subgroup of G. However, the command "**Size (Group ($\boldsymbol{x_1, x_2, x_3}$))**" in GAP shows that this subgroup has order 5184, but, $\boldsymbol{G \cong S_3 \sim (Z_2 \times Z_2)}$, and so $\boldsymbol{G}$ has order 5184. This shows that $\boldsymbol{\{x_1, x_2, x_3\}}$ is a generating set for $\boldsymbol{G}$. We now apply GAP to calculate the conjugacy classes and character table of the molecule, (see Tables 1, 2). To do this, we run the following program at the GAP prompt:

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
	11	1a	3a	3b	3c	3d	3e	3f	6a	2a	6b	2b	12a	4a	2c	6c	6d	6e	6f	2d	2e	6g	6h
χ_1		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2		1	1	1	1	1	1	1	1	1	1	1	−1	−1	1	1	1	1	1	1	1	1	1
χ_3		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1
χ_4		1	1	1	1	1	1	1	1	1	1	1	−1	−1	1	1	1	1	1	1	−1	−1	−1
χ_5		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_6		1	1	1	1	1	1	1	1	1	1	1	−1	−1	1	1	1	1	1	1	1	1	1
χ_7		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1
χ_8		1	1	1	1	1	1	1	1	1	1	1	−1	−1	1	1	1	1	1	1	−1	−1	−1
χ_9		2	2	2	2	2	2	2	−2	−2	−2	2	0	0	−2	−2	−2	2	2	2	0	0	0
χ_{10}		2	2	2	2	2	2	2	−2	−2	−2	2	0	0	−2	−2	−2	2	2	2	0	0	0
χ_{11}		2	2	2	2	2	2	2	2	2	2	2	0	0	−2	−2	−2	−2	−2	−2	0	0	0
χ_{12}		2	2	2	2	2	2	2	2	2	2	2	0	0	−2	−2	−2	−2	−2	−2	0	0	0
χ_{13}		2	2	2	2	2	2	2	−2	−2	−2	2	0	0	2	2	2	−2	−2	−2	−2	−2	−2
χ_{14}		2	2	2	2	2	2	2	−2	−2	−2	2	0	0	2	2	2	−2	−2	−2	20	2	2
χ_{15}		4	4	4	4	4	4	4	0	0	0	−4	0	0	0	0	0	0	0	0	0	0	0
χ_{16}		4	4	4	4	4	4	4	0	0	0	−4	0	0	0	0	0	0	0	0	0	0	0
χ_{17}		8	2	−4	5	−1	2	2	−2	4	1	0	0	0	4	1	−2	−2	1	4	0	0	0
χ_{18}		8	2	−4	5	−1	2	2	−2	4	1	0	0	0	4	1	−2	−2	1	4	0	0	0
χ_{19}		8	−4	2	2	−1	5	−4	0	0	0	0	0	0	4	−2	1	0	0	0	−4	2	−1
χ_{20}		8	−4	2	2	−1	5	−4	0	0	0	0	0	0	4	−2	1	0	0	0	−4	2	−1
χ_{21}		8	−4	2	2	−1	5	−4	0	0	0	0	0	0	4	−2	1	0	0	0	4	−2	1
χ_{22}		8	−4	2	2	−1	5	−4	0	0	0	0	0	0	4	−2	1	0	0	0	4	−2	1
χ_{23}		8	−4	2	2	−1	−4	5	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0
χ_{24}		8	−4	2	2	−1	−4	5	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0
χ_{25}		8	−4	2	2	−1	−4	5	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0
χ_{26}		8	−4	2	2	−1	−4	5	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0
χ_{27}		8	5	2	2	−1	−4	−4	1	4	−2	0	−1	2	0	0	0	0	0	0	0	0	0
χ_{28}		8	5	2	2	−1	−4	−4	1	4	−2	0	−1	2	0	0	0	0	0	0	0	0	0
χ_{29}		8	5	2	2	−1	−4	−4	1	4	−2	0	1	−2	0	0	0	0	0	0	0	0	0
χ_{30}		8	5	2	2	−1	−4	−4	1	4	−2	0	1	−2	0	0	0	0	0	0	0	0	0
χ_{31}		8	2	−4	5	−1	2	2	2	−4	−1	0	0	0	−4	−1	2	−2	1	4	0	0	0
χ_{32}		8	2	−4	5	−1	2	2	2	−4	−1	0	0	0	−4	−1	2	−2	1	4	0	0	0
χ_{33}		8	2	−4	5	−1	2	2	−2	4	1	0	0	0	−4	−1	2	2	−1	−4	0	0	0
χ_{34}		8	2	−4	5	−1	2	2	−2	4	1	0	0	0	−4	−1	2	2	−1	−4	0	0	0
χ_{35}		8	2	−4	5	−1	2	2	2	−4	−1	0	0	0	4	1	−2	2	−1	−4	0	0	0
χ_{36}		8	2	−4	5	−1	2	2	2	−4	−1	0	0	0	4	1	−2	2	−1	−4	0	0	0
χ_{37}		16	−8	4	4	−2	10	−8	0	0	0	0	0	0	−8	4	−2	0	0	0	0	0	0
χ_{38}		16	−8	4	4	−2	−8	10	0	0	0	0	0	0	0	0	0	−2	4	−8	0	0	0
χ_{39}		16	10	4	4	−2	−8	−8	−2	−8	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{40}		16	4	1	−8	−2	4	4	0	0	0	0	0	0	0	0	0	0	0	0	−4	−1	2
χ_{41}		16	4	1	−8	−2	4	4	0	0	0	0	0	0	0	0	0	0	0	0	−4	−1	2
χ_{42}		16	4	1	−8	−2	4	4	0	0	0	0	0	0	0	0	0	0	0	0	4	1	−2
χ_{43}		16	4	1	−8	−2	4	4	0	0	0	0	0	0	0	0	0	0	0	0	4	1	−2
χ_{44}		32	−4	−4	−4	5	−4	−4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{45}		32	−4	−4	−4	5	−4	−4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

```
G := Group (x1, x2, x3);
LogTo ("Solution.txt");
T := CharacterTable (G);
U := ConjugacyClasses (G);
Display (T);
LogTo ( );
```

After running our GAP program, the file "**Solution.txt**" will contain the character table and conjugacy classes of the group G.

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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
	4b	12b	4c	2f	6i	2g	6j	6k	6l	6m	6n	6o	6p	6q	6r	2h	4d	4e	12c	4f	6s	6t	2i
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	−1	−1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	1	1	−1	−1	−1	−1
χ_3	−1	−1	−1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
χ_4	−1	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1	1
χ_5	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
χ_6	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	−1	−1	1	1	1	1
χ_7	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1
χ_8	−1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1	−1	−1	−1	−1
χ_9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	−2	2	2	2
χ_{10}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	−2	−2	−2
χ_{11}	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	2	−2	0	0	0	0	0	0
χ_{12}	0	0	0	0	0	0	0	0	0	0	0	0	0	−2	−2	−2	2	0	0	0	0	0	0
χ_{13}	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{14}	−2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{15}	0	0	0	−2	−2	2	2	2	2	2	2	2	2	0	0	0	0	0	0	0	0	0	0
χ_{16}	0	0	0	2	2	−2	−2	−2	−2	−2	−2	−2	−2	0	0	0	0	0	0	0	0	0	0
χ_{17}	0	0	0	−2	1	−6	0	3	−3	−3	−3	0	0	0	0	0	0	0	0	0	0	0	0
χ_{18}	0	0	0	2	−1	6	0	−3	3	3	3	0	0	0	0	0	0	0	0	0	0	0	0
χ_{19}	0	0	0	0	0	−4	2	−1	2	−4	2	−1	2	0	0	0	0	2	−1	0	0	0	0
χ_{20}	0	0	0	0	0	4	−2	1	−2	4	−2	1	−2	0	0	0	0	−2	1	0	0	0	0
χ_{21}	0	0	0	0	0	−4	2	−1	2	−4	2	−1	2	0	0	0	0	2	−1	0	0	0	0
χ_{22}	0	0	0	0	0	4	−2	1	−2	4	−2	1	−2	0	0	0	0	−2	1	0	0	0	0
χ_{23}	0	1	−2	0	0	4	−2	1	−2	−2	4	−2	1	0	0	0	0	0	0	0	−1	2	−4
χ_{24}	0	−1	2	0	0	4	−2	1	−2	−2	4	−2	1	0	0	0	0	0	0	0	1	−2	4
χ_{25}	0	1	−2	0	0	−4	2	−1	2	2	−4	2	−1	0	0	0	0	0	0	0	1	−2	4
χ_{26}	0	−1	2	0	0	−4	2	−1	2	2	−4	2	−1	0	0	0	0	0	0	0	−1	2	−4
χ_{27}	0	0	0	0	0	−4	−1	−1	−4	2	2	2	2	2	−1	−4	0	0	0	0	0	0	0
χ_{28}	0	0	0	0	0	4	1	1	4	−2	−2	−2	−2	−2	1	4	0	0	0	0	0	0	0
χ_{29}	0	0	0	0	0	−4	−1	−1	−4	2	2	2	2	−2	1	4	0	0	0	0	0	0	0
χ_{30}	0	0	0	0	0	4	1	1	4	−2	−2	−2	−2	2	−1	−4	0	0	0	0	0	0	0
χ_{31}	0	0	0	2	−1	−2	−2	1	1	1	−5	−2	4	0	0	0	0	0	0	0	0	0	0
χ_{32}	0	0	0	−2	1	2	2	−1	−1	−1	5	2	−4	0	0	0	0	0	0	0	0	0	0
χ_{33}	0	0	0	−2	1	2	−4	−1	5	−1	−1	2	2	0	0	0	0	0	0	0	0	0	0
χ_{34}	0	0	0	2	−1	−2	4	1	−5	1	1	−2	−2	0	0	0	0	0	0	0	0	0	0
χ_{35}	0	0	0	−2	1	2	2	−1	−1	5	−1	−4	2	0	0	0	0	0	0	0	0	0	0
χ_{36}	0	0	0	2	−1	−2	−2	1	1	−5	1	4	−2	0	0	0	0	0	0	0	0	0	0
χ_{37}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{38}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{39}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{40}	0	0	0	0	0	0	0	0	0	0	0	0	0	−1	2	−4	0	0	0	0	−2	1	4
χ_{41}	0	0	0	0	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0	0	2	−1	−4
χ_{42}	0	0	0	0	0	0	0	0	0	0	0	0	0	−1	2	−4	0	0	0	0	2	−1	−4
χ_{43}	0	0	0	0	0	0	0	0	0	0	0	0	0	1	−2	4	0	0	0	0	−2	1	4
χ_{44}	0	0	0	0	0	−8	−2	1	4	4	4	−2	−2	0	0	0	0	0	0	0	0	0	0
χ_{45}	0	0	0	0	0	8	2	−1	−4	−4	−4	2	2	0	0	0	0	0	0	0	0	0	0

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