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Non-Rigid Group Theory for 2,3-Dimethylbutane

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Abstract

In this paper, we consider 2,3-dimethylbutane and find the structure of the full non-rigid group (f-NRG) of this molecule to be isomorphic to the group $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ of order 162 with 54 conjugacy classes and hence 54 irreducible characters. Here $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ denotes the semi direct product of four copies of the cyclic group Z_3 by cyclic group Z_2 of order 2. Then we use the GAP software package and find the complex character table of this group.

1. Introduction

A non-rigid molecule is a molecular system which presents large vibrational modes. This kind of motion appears whenever the molecule possesses various isoenergetic forms seperated by relatively low energy barrier. In such cases, intramolecular transformations occur. The group theory for non-rigid molecules finds numerous applications ranging from the rovibronic spectroscopy of molecules exhibiting large amplitude motions, chemical reactions, dynamic stereochemistry to weakly-bound van der Waals complexes. [1-8]

The molecular symmetry group for non-rigid molecules, where changes from one conformation to another can occur easily, is first defined by Longuet-Higgins[9] although

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there have been earlier works that suggested the need for such a framework. In many cases, these symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules, and their character tables are not known. It is therefore of some interest and importance to develop simple methods of calculating these character tables, which are needed for classification of wavefunctions, determination of selection rules, and so on.

Bunker and Papoušek extended the definition of the molecular symmetry group to linear molecules using an extended molecular symmetry.[10] The operations of the molecular symmetry group and the three-dimensional rotation group are used together to treat the symmetry properties of molecules in electric and magnetic fields by Watson.[11]

The complete set of molecular conversion operations which commute with the nuclear motion operator contains overall rotation operations, describing the molecule rotating as a whole, and the non-rigid tunneling motion operations, describing molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which is called the full non-rigid group (f-NRG).[12]

Our approach here is first to specify the algebraic structure of the full non-rigid group of 2,3-dimethylbutane. Non-rigidity of methyl derivatives is due to torsion of methyl groups assuming that the barrier to rotation of the methyl groups is low. With a geometric consideration of dynamic symmetries of the molecule we will show the f-NRG of the molecule is $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$ with order 162, where Z_3 and Z_2 are the cyclic groups of order 3 and 2 respectively, then we compute the character table of this group using GAP,[13] a useful package to compute the character tables and even the group structure. This method is appropriate for molecules which consist of a number of XH_3 or XO_2 groups attached to a rigid framework. The motivation for this study is outlined in [14-29] and the reader is encouraged to consult these papers for background material as well as a computational techniques. The notation we use is standard and the reader may consult [30-31].

2. Results and discussion

In order to characterize the f-NRG of this molecule, we first note that each dynamic symmetry operation of the molecule, considering the rotations of CH_3 groups, is composed of two sequential physical operations. We first have a physical symmetry of the framework with a carbon atom at each corner (as we have to map CH_3 groups to CH_3 groups which are on vertices of the framework). Such operations are exactly the symmetry operations of the framework and it is easy to see that there are only two operations which form the cyclic group of order 2 and is denoted by Z_2. After accomplishing the first framework symmetry operation, we have to map each of the four CH_3 group to itself, which forms the rotations on three symbols and is a group isomorphic to Z_3. The number of all such operations is $3^4 \times 2 = 162$. The composition of such dynamic symmetry elements is described as follows.

Let's use numbers {1, 2, 3, 4, 5, 6} to indicate the carbon atoms and use numbers {7, 8, 9} to label the three hydrogen atoms on the 1 corner. Similarly, let {10, 11, 12} be the labels of hydrogen atoms on the 3 corner and so on, see figure I. Now the symmetry of order 2 of the framework in terms of permutations is:

$$\sigma = (1,4)(2,5)(3,6)(7,13)(8,14)(9,15)(10,16)(11,17)(12,18)(19,20).$$

The group of symmetries of each CH_3 group in terms of a generating system is:

$$H = < (7, 8, 9) > \cong Z_3$$

$$K = < (13, 14, 15) > \cong Z_3$$

$$P = < (10, 11, 12) > \cong Z_3$$

$$Q = < (16, 17, 18) > \cong Z_3$$

Since we do not need the effect of σ on the carbon atoms, we consider its effect on the hydrogen atoms, i.e. $\sigma' = (7,13)(8,14)(9,15)(10,16)(11,17)(12,18)$. Therefore the f-NRG of this molecule in terms of generators is $G = < \theta_1, \theta_2, \theta_3, \theta_4, \sigma' >$ where $\theta_1 = (7, 8, 9)$, $\theta_2 = (13, 14, 15)$, $\theta_3 = (10, 11, 12)$, $\theta_4 = (16, 17, 18)$. Here we remark that σ' interchanges H with K, and P with Q. Now we apply GAP to compute the conjugacy classes and character table of the f-NRG of this molecule. Representatives of the conjugacy classes of the group G is tabulated in Table 1 and the character table is tabulated in Table 2. In Table 2, $A = e^{i\pi/3}$, $B = 2.e^{i\pi/3}$, $C = e^{-i\pi/3}$ and $D = 2.e^{-i\pi/3}$, where $i = \sqrt{-1}$. Our GAP program is the following:

X_1 := (7, 8, 9);
X_2 := (10, 11, 12);
X_3 := (13, 14, 15);
X_4 := (16, 17, 18);
Y := (7,13)(8,14)(9,15)(10,16)(11,17)(12,18);
G := Group(X_1,X_2,X_3,X_4,Y);
T := CharacterTable(G);
S := ConjugacyClasses(T);
Display(T);
SizesConjugacyClasses(T);

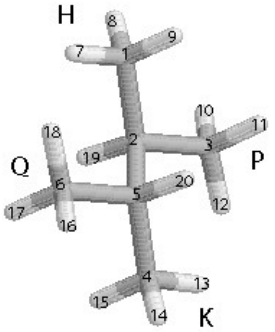

Figure 1. The structure of 2,3-dimethylbutane with full non-rigid group isomorphic to the group $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$.

3. Conclusions

We have developed the group theory and character table of the non-rigid 2,3-dimethylbutane as a group $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$ which consists of 162 operations divided into 54 conjugacy classes and irreducible representations. The derived character tables would also be valuable in other applications such as in the context of chemical applications of graph theory [32] and aromatic compounds [33]. In the case of chemical applications of graph theory, applications can range from enumeration f isomers to the automorphism groups of chemical graphs.

Table 1. The representatives of the conjugacy classes of G

No.	Representatives	Size	No.	Representatives	Size
1	()	1	28	(7,8,9)(13,15,14)	2
2	(16,17,18)	2	29	(7,8,9)(13,15,14)(16,17,18)	2
3	(16,18,17)	2	30	(7,8,9)(13,15,14)(16,18,17)	2
4	(13,14,15)	2	31	(7,8,9)(10,11,12)(13,14,15)(16,17,18)	1
5	(13,14,15)(16,17,18)	2	32	(7,8,9)(10,11,12)(13,14,15)(16,18,17)	2
6	(13,14,15)(16,18,17)	2	33	(7,8,9)(10,11,12)(13,15,14)	2
7	(13,15,14)	2	34	(7,8,9)(10,11,12)(13,15,14)(16,17,18)	2
8	(13,15,14)(16,17,18)	2	35	(7,8,9)(10,11,12)(13,15,14)(16,18,17)	2
9	(13,15,14)(16,18,17)	2	36	(7,8,9)(10,12,11)(13,14,15)(16,18,17)	1
10	(10,11,12)(16,17,18)	1	37	(7,8,9)(10,12,11)(13,15,14)	2
11	(10,11,12)(16,18,17)	2	38	(7,8,9)(10,12,11)(13,15,14)(16,17,18)	2
12	(10,11,12)(13,14,15)	2	39	(7,8,9)(10,12,11)(13,15,14)(16,18,17)	2
13	(10,11,12)(13,14,15)(16,17,18)	2	40	(7,9,8)(13,15,14)	1
14	(10,11,12)(13,14,15)(16,18,17)	2	41	(7,9,8)(13,15,14)(16,17,18)	2
15	(10,11,12)(13,15,14)	2	42	(7,9,8)(13,15,14)(16,18,17)	2
16	(10,11,12)(13,15,14)(16,17,18)	2	43	(7,9,8)(10,11,12)(13,15,14)(16,17,18)	1
17	(10,11,12)(13,15,14)(16,18,17)	2	44	(7,9,8)(10,11,12)(13,15,14)(16,18,17)	2
18	(10,12,11)(16,18,17)	1	45	(7,9,8)(10,12,11)(13,15,14)(16,18,17)	1
19	(10,12,11)(13,14,15)	2	46	(7,13)(8,14)(9,15)(10,16)(11,17)(12,18)	9
20	(10,12,11)(13,14,15)(16,17,18)	2	47	(7,13)(8,14)(9,15)(10,16,11,17,12,18)	9
21	(10,12,11)(13,14,15)(16,18,17)	2	48	(7,13)(8,14)(9,15)(10,16,12,18,11,17)	9
22	(10,12,11)(13,15,14)	2	49	(7,13,8,14,9,15)(10,16)(11,17)(12,18)	9
23	(10,12,11)(13,15,14)(16,17,18)	2	50	(7,13,8,14,9,15)(10,16,11,17,12,18)	9
24	(10,12,11)(13,15,14)(16,18,17)	2	51	(7,13,8,14,9,15)(10,16,12,18,11,17)	9
25	(7,8,9)(13,14,15)	1	52	(7,13,9,15,8,14)(10,16)(11,17)(12,18)	9
26	(7,8,9)(13,14,15)(16,17,18)	2	53	(7,13,9,15,8,14)(10,16,11,17,12,18)	9
27	(7,8,9)(13,14,15)(16,18,17)	2	54	(7,13,9,15,8,14)(10,16,12,18,11,17)	9

Table 2. The character table of the group G

	1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	3l	3m	3n	3o	3p	3q	3r	3s	3t	3u	3v	3w	3x	3y	3z
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	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	1	1	1	1
χ_3	1	1	1	A	A	A	C	C	C	1	1	A	A	A	C	C	C	1	A	A	A	C	C	C	C	C	C
χ_4	1	1	1	C	C	C	A	A	A	1	1	C	C	C	A	A	A	1	C	C	C	A	A	A	A	A	A
χ_5	1	1	1	A	A	A	C	C	C	1	1	A	A	A	C	C	C	1	A	A	A	C	C	C	C	C	C
χ_6	1	1	1	C	C	C	A	A	A	1	1	C	C	C	A	A	A	1	C	C	C	A	A	A	A	A	A
χ_7	1	A	C	1	A	C	1	A	C	C	1	A	C	1	A	C	1	A	C	1	A	C	1	A	1	A	C
χ_8	1	C	A	1	C	A	1	C	A	A	1	C	A	1	C	A	1	C	A	1	C	A	1	C	1	C	A
χ_9	1	A	C	1	A	C	1	A	C	C	1	A	C	1	A	C	1	A	C	1	A	C	1	A	1	A	C
χ_{10}	1	C	A	1	C	A	1	C	A	A	1	C	A	1	C	A	1	C	A	1	C	A	1	C	1	C	A
χ_{11}	1	A	C	A	C	1	C	1	A	C	1	C	1	A	1	A	C	A	1	A	C	A	C	1	C	1	A
χ_{12}	1	C	A	C	A	1	A	1	C	A	1	A	1	C	1	C	A	C	1	C	A	C	A	1	A	1	C
χ_{13}	1	A	C	A	C	1	C	1	A	C	1	C	1	A	1	A	C	A	1	A	C	A	C	1	C	1	A
χ_{14}	1	C	A	C	A	1	A	1	C	A	1	A	1	C	1	C	A	C	1	C	A	C	A	1	A	1	C
χ_{15}	1	A	C	C	1	A	A	C	1	C	1	1	A	C	C	1	A	A	A	C	1	1	A	C	A	C	1
χ_{16}	1	C	A	A	1	C	C	A	1	A	1	1	C	A	A	1	C	C	C	A	1	1	C	A	C	A	1
χ_{17}	1	A	C	C	1	A	A	C	1	C	1	1	A	C	C	1	A	A	A	C	1	1	A	C	A	C	1
χ_{18}	1	C	A	A	1	C	C	A	1	A	1	1	C	A	A	1	C	C	C	A	1	1	C	A	C	A	1
χ_{19}	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	2	-1	-1	2	-1	-1	2	2	-1	-1
χ_{20}	2	2	2	-1	-1	-1	-1	-1	-1	2	2	-1	-1	-1	-1	-1	-1	2	-1	-1	-1	-1	-1	-1	2	2	2
χ_{21}	2	-1	-1	-1	-1	2	-1	2	-1	2	-1	2	-1	-1	-1	-1	2	2	-1	2	-1	2	-1	-1	2	-1	-1
χ_{22}	2	-1	-1	-1	2	-1	-1	-1	2	2	-1	-1	-1	2	2	-1	-1	2	2	-1	-1	-1	2	-1	2	-1	-1
χ_{23}	2	-1	-1	B	-C	-C	D	-A	-A	2	-1	-C	B	-C	-A	D	-A	2	-C	-C	B	-A	-A	D	D	-A	-A
χ_{24}	2	-1	-1	D	-A	-A	B	-C	-C	2	-1	-A	D	-A	-C	B	-C	2	-A	-A	D	-C	-C	B	B	-C	-C
χ_{25}	2	-C	-A	B	-A	-1	D	-1	-C	D	-1	-A	2	-C	-1	B	-A	B	-1	-C	D	-C	-A	2	D	-1	-C
χ_{26}	2	-A	-C	D	-C	-1	B	-1	-A	B	-1	-C	2	-A	-1	D	-C	D	-1	-A	B	-A	-C	2	B	-1	-A
χ_{27}	2	-C	-A	D	-1	-C	B	-A	-1	D	-1	-1	B	-A	-A	2	-C	B	-C	-A	2	-1	-C	D	B	-A	-1
χ_{28}	2	-A	-C	B	-1	-A	D	-C	-1	B	-1	-1	D	-C	-C	2	-A	D	-A	-C	2	-1	-A	B	D	-C	-1
χ_{29}	2	-C	-A	2	-C	-A	2	-C	-A	D	-1	-C	D	-1	-C	D	-1	B	-A	-1	B	-A	-1	B	2	-C	-A
χ_{30}	2	-A	-C	2	-A	-C	2	-A	-C	B	-1	-A	B	-1	-A	B	-1	D	-C	-1	D	-C	-1	D	2	-A	-C
χ_{31}	2	2	2	-C	-C	-C	-A	-A	-A	2	-1	-C	-C	-C	-A	-A	-A	2	-C	-C	-C	-A	-A	-A	D	D	D
χ_{32}	2	2	2	-A	-A	-A	-C	-C	-C	2	-1	-A	-A	-A	-C	-C	-C	2	-A	-A	-A	-C	-C	-C	B	B	B
χ_{33}	2	B	D	-C	-A	-1	-A	-1	-C	D	2	-A	-1	-C	-1	-C	-A	B	-1	-C	-A	-C	-A	-1	D	2	B
χ_{34}	2	D	B	-A	-C	-1	-A	-1	-A	B	2	-C	-1	-A	-1	-A	-C	D	-1	-A	-C	-A	-C	-1	B	2	D
χ_{35}	2	B	D	-A	-1	-C	-C	-A	-1	D	2	-1	-C	-A	-A	-1	-C	B	-C	-A	-1	-1	-C	-A	B	D	2
χ_{36}	2	D	B	-C	-1	-A	-A	-C	-1	B	2	-1	-A	-C	-C	-1	-A	D	-A	-C	-1	-1	-A	-C	D	B	2

Table 2. (Continued)

	1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	3l	3m	3n	3o	3p	3q	3r	3s	3t	3u	3v	3w	3x	3y	3z
χ_{37}	2	B	D	-1	-C	-A	-1	-C	-A	D	2	-C	-A	-1	-C	-A	-1	B	-A	-1	-C	-A	-1	-C	2	B	D
χ_{38}	2	D	B	-1	-A	-C	-1	-A	-C	B	2	-A	-C	-1	-A	-C	-1	D	-C	-1	-A	-C	-1	-A	2	D	B
χ_{39}	2	-1	-1	-C	-C	B	-A	D	-A	2	2	B	-C	-C	-A	-A	D	2	-C	B	-C	D	-A	-A	D	-A	-A
χ_{40}	2	-1	-1	-A	-A	D	-C	B	-C	2	2	D	-A	-A	-C	-C	B	2	-A	D	-A	B	-C	-C	B	-C	-C
χ_{41}	2	-1	-1	-A	B	-C	-A	-A	D	2	-1	-C	-C	B	D	-A	-A	2	B	-C	-C	-A	D	-A	D	-A	-A
χ_{42}	2	-1	-1	-C	D	-A	-C	-C	B	2	-1	-A	-A	D	B	-C	-C	2	D	-A	-A	-C	B	-C	B	-C	-C
χ_{43}	2	-C	-A	-1	-C	D	-1	B	-A	D	-1	B	-A	-1	-C	-A	2	B	-A	2	-C	D	-1	-C	2	-C	-A
χ_{44}	2	-A	-C	-1	-A	B	-1	D	-C	B	-1	D	-C	-1	-A	-C	2	D	-C	2	-A	B	-1	-A	2	-A	-C
χ_{45}	2	-C	-A	-1	B	-A	-1	-C	D	D	-1	-C	-A	2	B	-A	-1	B	D	-1	-C	-A	2	-C	2	-C	-A
χ_{46}	2	-A	-C	-1	D	-C	-1	-A	B	B	-1	-A	-C	2	D	-C	-1	D	B	-1	-A	-C	2	-A	2	-A	-C
χ_{47}	2	-C	-A	-C	-A	2	-A	2	-C	D	-1	D	-1	-C	-1	-C	D	B	-1	B	-A	B	-A	-1	D	-1	-C
χ_{48}	2	-A	-C	-A	-C	2	-C	2	-A	B	-1	B	-1	-A	-1	-A	B	D	-1	D	-C	D	-C	-1	B	-1	-A
χ_{49}	2	-C	-A	-C	D	-1	-A	-1	B	D	-1	-A	-1	B	2	-C	-A	B	2	-C	-A	-C	D	-1	D	-1	-C
χ_{50}	2	-A	-C	-A	B	-1	-C	-1	D	B	-1	-C	-1	D	2	-A	-C	D	2	-A	-C	-A	B	-1	B	-1	-A
χ_{51}	2	-C	-A	-A	-1	B	-C	D	-1	D	-1	2	-C	-A	-A	-1	B	B	-C	D	-1	2	-C	-A	B	-A	-1
χ_{52}	2	-A	-C	-C	-1	D	-A	B	-1	B	-1	2	-A	-C	-C	-1	D	D	-A	B	-1	2	-A	-C	D	-C	-1
χ_{53}	2	-C	-A	-A	2	-C	-C	-A	2	D	-1	-1	-C	D	D	-1	-C	B	B	-A	-1	-1	B	-A	B	-A	-1
χ_{54}	2	-A	-C	-C	2	-A	-A	-C	2	B	-1	-1	-A	B	B	-1	-A	D	D	-C	-1	-1	D	-C	D	-C	-1

	3aa	3ab	3ac	3ad	3ae	3af	3ag	3ah	3ai	3aj	3ak	3al	3am	3an	3ao	3ap	3aq	3ar	2a	6a	6b	6c	6d	6e	6f	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	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	-1	-1	-1	-1
χ_3	1	1	1	C	C	1	1	1	C	1	1	1	A	A	A	A	A	A	-1	-1	-1	-A	-A	-A	-C	-C	-C
χ_4	1	1	1	A	A	1	1	1	A	1	1	1	C	C	C	C	C	C	-1	-1	-1	-C	-C	-C	-A	-A	-A
χ_5	1	1	1	C	C	1	1	1	C	1	1	1	A	A	A	A	A	A	1	1	1	A	A	A	C	C	C
χ_6	1	1	1	A	A	1	1	1	A	1	1	1	C	C	C	C	C	C	1	1	1	C	C	C	A	A	A
χ_7	1	A	C	C	1	A	C	1	A	C	1	A	1	A	C	C	1	A	-1	-A	-C	-1	-A	-C	-1	-A	-C
χ_8	1	C	A	A	1	C	A	1	C	A	1	C	1	C	A	A	1	C	-1	-C	-A	-1	-C	-A	-1	-C	-A
χ_9	1	A	C	C	1	A	C	1	A	C	1	A	1	A	C	C	1	A	1	A	C	1	A	C	1	A	C
χ_{10}	1	C	A	A	1	C	A	1	C	A	1	C	1	C	A	A	1	C	1	C	A	1	C	A	1	C	A
χ_{11}	1	A	C	A	C	A	C	1	1	C	1	A	A	C	1	1	A	C	-1	-A	-C	-A	-C	-1	-C	-1	-A
χ_{12}	1	C	A	C	A	C	A	1	1	A	1	C	C	A	1	1	C	A	-1	-C	-A	-C	-A	-1	-A	-1	-C
χ_{13}	1	A	C	A	C	A	C	1	1	C	1	A	A	C	1	1	A	C	1	A	C	A	C	1	C	1	A
χ_{14}	1	C	A	C	A	C	A	1	1	A	1	C	C	A	1	1	C	A	1	C	A	C	A	1	A	1	C
χ_{15}	1	A	C	1	A	A	C	1	C	C	1	A	C	1	A	A	C	1	-1	-A	-C	-C	-1	-A	-A	-C	-1
χ_{16}	1	C	A	1	C	C	A	1	A	A	1	C	A	1	C	C	A	1	-1	-C	-A	-A	-1	-C	-C	-A	-1
χ_{17}	1	A	C	1	A	A	C	1	C	C	1	A	C	1	A	A	C	1	1	A	C	C	1	A	A	C	1

Table 2. (Continued)

	3aa	3ab	3ac	3ad	3ae	3af	3ag	3ah	3ai	3aj	3ak	3al	3am	3an	3ao	3ap	3aq	3ar	2a	6a	6b	6c	6d	6e	6f	6g	6h
χ_{18}	1	C	A	1	C	C	A	1	A	A	1	C	A	1	C	C	A	1	1	C	A	A	1	C	C	A	1
χ_{19}	2	-1	-1	2	-1	-1	2	-1	2	-1	-1	2	2	-1	-1	2	-1	2	0	0	0	0	0	0	0	0	0
χ_{20}	-1	-1	-1	2	2	-1	-1	-1	2	-1	-1	-1	2	2	2	2	2	2	0	0	0	0	0	0	0	0	0
χ_{21}	-1	-1	2	2	-1	2	-1	-1	2	-1	2	-1	2	-1	-1	2	-1	2	0	0	0	0	0	0	0	0	0
χ_{22}	-1	2	-1	2	-1	-1	-1	2	2	2	-1	-1	2	-1	-1	2	-1	2	0	0	0	0	0	0	0	0	0
χ_{23}	2	-1	-1	D	-A	-1	2	-1	D	-1	-1	2	B	-C	-C	B	-C	B	0	0	0	0	0	0	0	0	0
χ_{24}	2	-1	-1	B	-C	-1	2	-1	B	-1	-1	2	D	-A	-A	D	-A	D	0	0	0	0	0	0	0	0	0
χ_{25}	2	-C	-A	B	-A	-C	D	-1	2	-A	-1	B	B	-A	-1	2	-C	D	0	0	0	0	0	0	0	0	0
χ_{26}	2	-A	-C	D	-C	-A	B	-1	2	-C	-1	D	D	-C	-1	2	-A	B	0	0	0	0	0	0	0	0	0
χ_{27}	2	-C	-A	2	-C	-C	D	-1	D	-A	-1	B	D	-1	-C	B	-A	2	0	0	0	0	0	0	0	0	0
χ_{28}	2	-A	-C	2	-A	-A	B	-1	B	-C	-1	D	B	-1	-A	D	-C	2	0	0	0	0	0	0	0	0	0
χ_{29}	2	-C	-A	D	-1	-C	D	-1	B	-A	-1	B	2	-C	-A	D	-1	B	0	0	0	0	0	0	0	0	0
χ_{30}	2	-A	-C	B	-1	-A	B	-1	D	-C	-1	D	2	-A	-C	B	-1	D	0	0	0	0	0	0	0	0	0
χ_{31}	-1	-1	-1	D	D	-1	-1	-1	D	-1	-1	-1	B	B	B	B	B	B	0	0	0	0	0	0	0	0	0
χ_{32}	-1	-1	-1	B	B	-1	-1	-1	B	-1	-1	-1	D	D	D	D	D	D	0	0	0	0	0	0	0	0	0
χ_{33}	-1	-C	-A	B	D	-C	-C	-1	2	-A	-1	-C	B	D	2	2	B	D	0	0	0	0	0	0	0	0	0
χ_{34}	-1	-A	-C	D	B	-A	-A	-1	2	-C	-1	-A	D	B	2	2	D	B	0	0	0	0	0	0	0	0	0
χ_{35}	-1	-C	-A	2	B	-C	-A	-1	D	-A	-1	-C	D	2	B	B	D	2	0	0	0	0	0	0	0	0	0
χ_{36}	-1	-A	-C	2	D	-A	-C	-1	B	-C	-1	-A	B	2	D	D	B	2	0	0	0	0	0	0	0	0	0
χ_{37}	-1	-C	-A	D	2	-C	-A	-1	B	-A	-1	-C	2	B	D	D	2	B	0	0	0	0	0	0	0	0	0
χ_{38}	-1	-A	-C	B	2	-A	-C	-1	D	-C	-1	-A	2	D	B	B	2	D	0	0	0	0	0	0	0	0	0
χ_{39}	-1	-1	2	D	-A	2	-1	-1	D	-1	2	-1	B	-C	-C	B	-C	B	0	0	0	0	0	0	0	0	0
χ_{40}	-1	-1	2	B	-C	2	-1	-1	B	-1	2	-1	D	-A	-A	D	-A	D	0	0	0	0	0	0	0	0	0
χ_{41}	-1	2	-1	D	-A	-1	-1	2	D	2	-1	-1	B	-C	-C	B	-C	B	0	0	0	0	0	0	0	0	0
χ_{42}	-1	2	-1	B	-C	-1	-1	2	B	2	-1	-1	D	-A	-A	D	-A	D	0	0	0	0	0	0	0	0	0
χ_{43}	-1	-C	D	D	-1	B	-A	-1	B	-A	2	-C	2	-C	-A	D	-1	B	0	0	0	0	0	0	0	0	0
χ_{44}	-1	-A	B	B	-1	D	-C	-1	D	-C	2	-A	2	-A	-C	B	-1	D	0	0	0	0	0	0	0	0	0
χ_{45}	-1	B	-A	D	-1	-C	-A	2	B	D	-1	-C	2	-C	-A	D	-1	B	0	0	0	0	0	0	0	0	0
χ_{46}	-1	D	-C	B	-1	-A	-C	2	D	B	-1	-A	2	-A	-C	B	-1	D	0	0	0	0	0	0	0	0	0
χ_{47}	-1	-C	D	B	-A	B	-A	-1	2	-A	2	-C	B	-A	-1	2	-C	D	0	0	0	0	0	0	0	0	0
χ_{48}	-1	-A	B	D	-C	D	-C	-1	2	-C	2	-A	D	-C	-1	2	-A	B	0	0	0	0	0	0	0	0	0
χ_{49}	-1	B	-A	B	-A	-C	-A	2	2	D	-1	-C	B	-A	-1	2	-C	D	0	0	0	0	0	0	0	0	0
χ_{50}	-1	D	-C	D	-C	-A	-C	2	2	B	-1	-A	D	-C	-1	2	-A	B	0	0	0	0	0	0	0	0	0
χ_{51}	-1	-C	D	2	-C	B	-A	-1	D	-A	2	-C	D	-1	-C	B	-A	2	0	0	0	0	0	0	0	0	0
χ_{52}	-1	-A	B	2	-A	D	-C	-1	B	-C	2	-A	B	-1	-A	D	-C	2	0	0	0	0	0	0	0	0	0
χ_{53}	-1	B	-A	2	-C	-C	-A	2	D	D	-1	-C	D	-1	-C	B	-A	2	0	0	0	0	0	0	0	0	0
χ_{54}	-1	D	-C	2	-A	-A	-C	2	B	B	-1	-A	B	-1	-A	D	-C	2	0	0	0	0	0	0	0	0	0

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