

Computing the Full Non-Rigid Group of Tetranitrocubane and Octanitrocubane Using Wreath Product

M. R. Darafsheh^{1*}, Y. Farjami² and A. R. Ashrafi³

^{1,2}*Department of Mathematics, Statistics and Computer Science, Faculty of Science,
University of Tehran, Tehran, Iran*

³*Department of Mathematics, Faculty of Science, University of Kashan, Kashan, Iran*
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Abstract

The non-rigid molecule group theory (NRG) in which the dynamical symmetry operations are defined as physical operations is a new field in chemistry. Smeyers in a series of papers applied this notion to determine the character table of restricted NRG (r-NRG) of some molecules. For example, Smeyers and Villa computed the 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 work, a new method is described, by means of which it is possible to calculate the symmetry group of molecules consisting of a number of XO₂ groups attached to a rigid framework. We study the full non-rigid group (f-NRG) of tetranitrocubane and octanitrocubane and prove that these are groups of order 384 and 12288 with 20 and 93 conjugacy classes, respectively. The method can be generalized to apply to other non-rigid molecules.

1. INTRODUCTION

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 [1], 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-

*Author to whom correspondence should be addressed (E-mail: daraf@khayam.ut.ac.ir)

inversions. This way of expressing the non-rigid operations is indeed more descriptive and flexible [2].

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 [3-10, 17, 21-24].

In 1963 Longuet-Higgins [11] investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. 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 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 or XO_2 groups attached to a rigid framework. Examples of such molecules are tetranitrocubane and octanitrocubane, which are considered here in some detail. Previous approaches for computing the f-NRG have been applied to some molecules such as cis-dichloro-diammine platinum(II), trans-dichloro-diammine platinum(II), trimethylamine by Smeyers, Ashrafi in [17, 21-24]. For the linear framework a similar problem has been studied by Bunker [12].

Lomont [15] has given two methods for calculating character tables. These methods are satisfactory for small groups, but both of them require knowledge of the class structure and hence of the group multiplication table and they become very massive 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.

Our approach here is first to specify the algebraic structure of the full non-rigid group of tetranitrocubane and octanitrocubane. With a geometric consideration of dynamic symmetries of the molecules we will show that the f-NRG of both tetranitrocubane and octanitrocubane can be specified by wreath product of some known groups. Then based on

the structure of the group we apply GAP [16] as a useful package for computing the character tables and even the group structure to compute the character table of f-NRG of these molecules. We use [13] and [14] for standard notations and terminologies of character theory.

The successful synthesis of octanitrocubane by Eaton's group [26] and [27] impressed the research area of explosive and highly energetic materials. The subsequent detailed molecular dynamic analysis of octanitrocubane in [25] and [28] motivated the present research. The mathematical motivation for this study is outlined in [17-24] and the reader is encouraged to consult these papers for background material as well as basic computational techniques. It is worth to note that a new type of vibrations (QCTM) has been predicted for octanitrocubane which has been attributed to the rotation of NO_2 group [25]. Hence it will be very important to apply the f-NRG of non-rigid molecules to detect and predict new types of vibrations due to rotations or other types of dynamically symmetric motions. In [25] and [28], the rigid symmetry group of octanitrocubane for an equilibrium state is given, which is a group of order 8. This is because that in the rigid case the substitution, of cubane hydrogen atoms for nitro groups, destroys the 3-fold axes that run along the body diagonals of the O_h frame.

For more theoretical justification and implications of torsional rotation of pairs of oxygen atoms about their respective C-N bonds, the prediction of the physically possible directions of the rotations of the eight NO_2 group and the conformations of the equilibrium states of both tetranitrocubane and octanitrocubane see [25] and [28].

In this paper, the f-NRG of tetranitrocubane and octanitrocubane is investigated (see Figure 1). We prove that these are groups of order 384 and 12288 with 20 and 93 conjugacy classes, respectively. Computations were carried out with the aid of GAP [16] and this was done by characterizing the algebraic structure of f-NRG as the wreath product of known groups. We encourage the reader to consult [25-28] for further information about unusual molecular dynamics and properties of tetranitrocubane and octanitrocubane.

2. Full Non-Rigid Group of Tetranitrocubane and Octanitrocubane

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

Let H be a permutation group on X , a subgroup of S_X , and let G be a group. The set of all mappings $X \longrightarrow G$ is denoted by G^X , i.e. $G^X = \{f \mid f: X \longrightarrow G\}$. It is clear that $|G^X| = |G|^{|X|}$. We put $G \ltimes H = G^X \times H = \{(f; \pi) \mid f \in G^X, \pi \in H\}$. For $f \in G^X$ and $\pi \in H$, we define $f_\pi \in G^X$ by $f_\pi = f \circ \pi^{-1}$, where "o" denotes the composition of functions. It is easy to check that the following law of composition:

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

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

Before going into the details of the computations of tetra- and octa nitrocubane we should mention that we consider the speed of rotations of nitro groups sufficiently high so that the mean time dynamical symmetry of the molecules makes sense. If instead we were to consider all the possible equilibrium states (see [25,28]) of tetra- and octa nitrocubane then we were obliged to consider Z_4 in place of Z_2 resulting very large groups, that is groups of orders at least $4^4 \times 24 = 6144$ and $2 \times 24 \times 4^8 = 3145728$ rather than 384 and 12288, see below.

We begin with tetranitrocubane as is somewhat simpler to describe, discussions for octanitrocubane will be similar. In order to characterize the f -NRG of tetranitrocubane we first note that each dynamic symmetry operation of tetranitrocubane, considering the rotations of NO_2 groups, is composed of two sequential physical operations. We first have a physical symmetry of the tetrahedral framework (as we have to map the NO_2 groups on NO_2 groups which are on vertices of the tetrahedral framework). Such operations are exactly the symmetry operations of a tetrahedral and, as is well-known, such operations form the group T_d of order 24, which as is well known, is isomorphic to S_4 or $\text{Sym}(4)$, the group of permutations on four distinct symbols. After accomplishing the first framework symmetry operation we have to map each of the four NO_2 group on itself which forms the two element group C_2 , also denoted by Z_2 . The number of all such operations is $2^4 \times 24 = 384$. The composition of such dynamic symmetry elements are described as follows.

Let's use numbers $\{1,2,3,4,5,6,7,8\}$ to indicate the carbon atoms and then use 10,11 to label the two oxygen atoms on the 1 corner. Similarly, let 13, 14 be the labels of oxygen atoms on the 2 corner and so on. For tetranitrocubane the 2,3,5,8 have NO_2 attached while for

octanitrocubane all 1-8 carbons have NO_2 . Now from the symmetry point of view the 2,3,5,8 carbons (corners of the tetrahedral framework) are important and the remaining carbons follow the motions of 2,3,5,8 carbons. This means that for computing the f-NRG it is enough to consider the tetrahedron (2,3,5,8) with rotating NO_2 on its corners. We can describe such configuration with a 2×4 matrix $[ij]_{2 \times 4}$ where ij means the i -th oxygen on the j -th carbon corner. Now the dynamic symmetry operation described above has the form $(a_1, a_2, a_3, a_4, \sigma)$, where σ is a symmetry of the tetrahedron (the first physical operation as above) and if $h: \{2,3,5,8\} \longrightarrow \{e, f\}$ is a function into the cyclic group $\{e, f\}$ of order two with identity element e then we write $a_1 = h(2)$, $a_2 = h(3)$, $a_3 = h(5)$, $a_4 = h(8)$. The group V of the symmetries of the molecule tetranitrocubane acts on the eight entries of $[ij]_{2 \times 4}$ as follows. Consider $(h; \sigma)$ and $[ij]$, we first do h on the i -th oxygen by the rule $h(\sigma(j))(i)$, and then we do σ on the j -th corner carbon to obtain $[h(\sigma(j))(i) \sigma(j)]$ which shows the new position of molecule. This composition rule is the wreath product composition. Therefore the f-NRG group V of tetranitrocubane is isomorphic to $Z_2 \wr S_4$. We now apply GAP to obtain the conjugacy classes and character table of the group V , Tables 1, 2. Note that in Table 1 the restrictions of symmetries of the cube to the tetrahedral are written. For example (3,8) stands for the reflection with respect to the plane through the 2,4,5,7 carbon corners, i.e. (1,6)(3,8). Also note that *id* is the identity operation.

We now suppose that U is the f-NRG of octanitrocubane and define four permutations x, y, z and w , as follows:

$$x = (1342)(5786),$$

$$y = (1265)(3487),$$

$$z = (253)(467),$$

$$w = (35)(46).$$

By Figure 1, the point group of the cubane framework is generated by x, y, z and w . In other words, $\langle x, y, z, w \rangle$ has the same structure as O_h . It is a well-known fact that this group has order 48 and is isomorphic to $S_4 \times Z_2$, where Z_2 denotes the cyclic group of order 2. We now assume that $H_2 = \langle x, y, z, w \rangle \cong S_4 \times Z_2$, as a permutation group on $X = \{1, 2, 3, 4, 5, 6, 7, 8\}$ and $G \cong Z_2$, a cyclic group of order 2. We can consider H_2 , as a subgroup of S_8 . In the non-rigid case, the motion of nitro (NO_2) group generates a cyclic group of order 2, which is isomorphic to Z_2 . Therefore, using a similar argument, as above, we can calculate the non-

rigid group of octanitrocubane U as the wreath product of Z_2 by $H_2 = \langle x, y, z, w \rangle \cong S_4 \times Z_2$, that is $U \cong Z_2 \wr (S_4 \times Z_2)$. Simple counting shows that the number of elements of U is $2 \times 24 \times 2^8 = 12288$. Using a GAP program, we compute in Tables 3, 4, the conjugacy classes and character table of U.

Table 1: The Representatives of the Conjugacy Classes of V

No.	Representatives	Size
1	(e, e, e, e; id)	1
2	(e, e, e, e; (3, 8))	12
3	(e, e, e, e; (5, 3, 8))	32
4	(e, e, e, e; (2, 5)(3, 8))	12
5	(e, e, e, e; (2, 5, 3, 8))	48
6	(e, e, e, f; id)	4
7	(e, e, e, f; (3, 8))	12
8	(e, e, e, f; (5, 3))	24
9	(e, e, e, f; (5, 3, 8))	32
10	(e, e, e, f; (2, 5)(3, 8))	24
11	(e, e, e, f; (2, 5, 3))	32
12	(e, e, e, f; (2, 5, 3, 8))	48
13	(e, e, f, f; id)	6
14	(e, e, f, f; (5, 3))	24
15	(e, e, f, f; (2, 5))	12
16	(e, e, f, f; (2, 5, 3))	32
17	(e, e, f, f; (2, 3)(5, 8))	12
18	(e, f, f, f; id)	4
19	(e, f, f, f; (2, 5))	12
20	(f, f, f, f; id)	1

Table 2: The Character Table and Power Map of the Group V

	1a	2a	3a	2b	4a	2c	4b	2d	6a	4c	6b	8a	2e	4d	2f	6c	4e	2g	4f	2h	
	2P	1a	1a	3a	1a	2b	1a	2e	1a	3a	2e	3a	4e	1a	2e	1a	3a	2h	1a	2e	1a
	3P	1a	2a	1a	2b	4a	2c	4b	2d	2g	4c	2c	8a	2e	4d	2f	2h	4e	2g	4f	2h
	5P	1a	2a	3a	2b	4a	2c	4b	2d	6a	4c	6b	8a	2e	4d	2f	6c	4e	2g	4f	2h
	7P	1a	2a	3a	2b	4a	2c	4b	2d	6a	4c	6b	8a	2e	4d	2f	6c	4e	2g	4f	2h
χ_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
χ_3		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
χ_5		2	0	-1	2	0	-2	0	0	1	-2	1	0	2	0	0	-1	2	-2	0	2
χ_6		2	0	-1	2	0	2	0	0	-1	2	-1	0	2	0	0	-1	2	2	0	2
χ_7		3	-1	0	-1	1	-3	1	1	0	1	0	-1	3	-1	-1	0	-1	-3	1	3
χ_8		3	-1	0	-1	1	3	-1	-1	0	-1	0	1	3	-1	-1	0	-1	3	-1	3
χ_9		3	1	0	-1	-1	-3	-1	-1	0	1	0	1	3	1	1	0	-1	-3	-1	3
χ_{10}		3	1	0	-1	-1	3	1	1	0	-1	0	-1	3	1	1	0	-1	3	1	3
χ_{11}		4	-2	1	0	0	-2	2	0	-1	0	1	0	0	0	2	-1	0	2	-2	-4
χ_{12}		4	-2	1	0	0	2	-2	0	1	0	-1	0	0	0	2	-1	0	-2	2	-4
χ_{13}		4	2	1	0	0	-2	-2	0	-1	0	1	0	0	0	-2	-1	0	2	2	-4
χ_{14}		4	2	1	0	0	2	2	0	1	0	-1	0	0	0	-2	-1	0	-2	-2	-4
χ_{15}		6	2	0	2	0	0	0	0	0	0	0	0	-2	-2	2	0	-2	0	0	6
χ_{16}		6	-2	0	2	0	0	0	0	0	0	0	0	-2	2	-2	0	-2	0	0	6
χ_{17}		6	0	0	-2	0	0	-2	2	0	0	0	0	-2	0	0	0	2	0	-2	6
χ_{18}		6	0	0	-2	0	0	2	-2	0	0	0	0	-2	0	0	0	2	0	2	6
χ_{19}		8	0	-1	0	0	-4	0	0	1	0	-1	0	0	0	0	1	0	4	0	-8
χ_{20}		8	0	-1	0	0	4	0	0	-1	0	1	0	0	0	0	1	0	-4	0	-8

Table 3: The Representatives of the non-trivial Conjugacy Classes of U

No.	Representatives	Size
1	(e,f,f,f,f,e,f,f; (2,5)(4,7))	48
2	(e,e,e,f,e,f,f,f; (1,6)(3,8))	48
3	(f,e,f,e,e,f,e,f; id)	6
4	(e,f,f,e,f,f,e,f; (1,6)(2,5)(3,8)(4,7))	192
5	(f,e,e,e,f,e,e; id)	12
6	(f,f,e,f,f,e,f,e; (1,6)(3,8))	48
7	(f,f,f,e,f,e,e,f; (1,6)(3,8))	48
8	(f,f,e,e,e,f,e; (1,6)(2,5)(3,8)(4,7))	192
9	(f,f,e,f,f,f,f,e; id)	4
10	(f,e,e,f,e,e,f,f; (1,6)(2,5)(3,8)(4,7))	64
11	(e,f,e,f,e,e,e; (1,8)(2,4)(3,6)(5,7))	4
12	(f,f,e,e,f,e,e,f; (2,5)(4,7))	192
13	(f,e,f,e,f,e,f,f; (1,8)(2,4)(3,6)(5,7))	12
14	(e,e,f,e,e,f,e,e; id)	96
15	(f,f,f,e,f,e,e,f; (1,8)(2,7)(3,6)(4,5))	96
16	(e,f,f,f,f,f,f,e; id)	48
17	(e,f,e,f,f,f,e; (2,3)(6,7))	48
18	(e,f,e,e,f,e,f,e; (1,8)(2,6)(3,7)(4,5))	192
19	(f,e,e,f,f,f,f,f; (2,3)(6,7))	24
20	(f,f,e,e,e,f,e,f; (1,8)(2,7)(3,6)(4,5))	96
21	(f,e,e,f,e,f,f,e; (1,4)(2,3)(5,8)(6,7))	48
22	(e,f,e,f,e,e,f,f; (1,3)(2,4)(5,7)(6,8))	192
23	(e,e,e,e,f,f,f,f; id)	6
24	(f,f,e,e,e,e,e; (1,2)(3,4)(5,6)(7,8))	48
25	(e,e,f,e,f,e,f,f; (1,8)(2,4)(3,6)(5,7))	96
26	(e,e,f,e,e,f,e,e; (1,6)(3,8))	24
27	(e,f,f,f,e,f,e,e; (1,3)(2,4)(5,7)(6,8))	96
28	(f,e,e,f,e,e,f,f; (1,3)(2,7)(4,5)(6,8))	96
29	(f,f,f,f,f,f,f,f; id)	1
30	(e,f,e,e,e,f,f,f; (2,5)(4,7))	48
31	(f,e,f,f,f,f,e; (2,5)(4,7))	96
32	(e,f,f,e,e,e,f,f; (1,3)(2,4)(5,7)(6,8))	48
33	(f,f,e,e,e,f,e,f; (1,2,6,5)(3,4,8,7))	384
34	(e,e,e,f,f,f,e,f; (1,6)(2,5)(3,8)(4,7))	48
35	(f,e,e,e,e,f,f,f; (1,7,6,4)(2,3,5,8))	384
36	(e,e,e,e,e,f,f; (3,5)(4,6))	48
37	(f,e,f,e,f,e,f,f; id)	24
38	(e,e,e,f,f,e,e,f; (3,5)(4,6))	96
39	(f,f,f,f,e,e,f,f; (3,5)(4,6))	24
40	(e,e,e,f,e,f,f,f; (1,8)(2,7)(3,6)(4,5))	16
41	(f,e,e,e,e,f,e; (1,4,6,7)(2,8,5,3))	384
42	(f,f,e,e,e,e,e; (1,5,6,2)(3,7,8,4))	384
43	(f,e,f,e,e,f,e,f; (1,8)(2,7)(3,6)(4,5))	16
44	(f,f,e,e,e,f,e,e; (1,8)(2,4)(3,6)(5,7))	192
45	(f,f,f,f,e,f,e; id)	12
46	(e,f,f,f,e,e,e; (1,7,6,4)(2,3,5,8))	768

Table 3: (Continued)

No.	Representatives	Size
47	(f,f,e,f,f,f,e,e; (1,6)(3,8))	96
48	(f,e,f,f,e,f,e,f; id)	24
49	(f,e,e,f,f,e,e,e; id)	24
50	(e,f,e,e,e,e,e,e; (3,5)(4,6))	96
51	(e,e,e,e,e,e,e,e; (2,5,3)(4,6,7))	128
52	(e,f,e,e,f,f,f,f; (1,3)(2,4)(5,7)(6,8))	192
53	(e,f,e,f,e,e,e,e; id)	12
54	(e,e,e,f,f,e,f,e; (2,5)(4,7))	48
55	(e,e,e,f,e,f,f,e; (1,6)(3,8))	48
56	(f,f,e,e,f,e,e; (1,6)(2,5)(3,8)(4,7))	96
57	(f,e,e,f,e,f,f,e; id)	2
58	(e,f,e,f,e,f,e,e; (1,4)(5,8))	96
59	(f,e,f,e,e,e,e,e; (1,4)(5,8))	96
60	(e,e,e,e,f,e,f,f; id)	24
61	(f,f,e,f,e,f,f,e; id)	8
62	(f,e,e,e,f,f,f,e; id)	8
63	(e,f,f,f,e,f,e,e; id)	24
64	(e,f,f,e,f,e,f,e; id)	24
65	(f,e,f,e,f,f,e,f; (1,4)(5,8))	96
66	(e,f,e,e,e,e,e,e; id)	8
67	(e,f,e,e,e,f,f,e; (1,3)(2,4)(5,7)(6,8))	192
68	(f,e,f,f,f,e,f,f; (1,4,6)(3,8,5))	256
69	(f,f,f,e,f,e,e,f; (1,6,4)(3,5,8))	256
70	(f,f,f,f,f,f,e,f; id)	8
71	(f,f,e,f,e,e,e,e; (1,4,6)(3,8,5))	256
72	(f,e,f,f,f,e,f,f,e; (1,3,7,8,6,2)(4,5))	512
73	(e,f,e,f,f,f,f,f; (1,7,6)(2,3,8))	128
74	(f,e,e,e,f,e,e,f; (1,8)(2,7)(3,6)(4,5))	64
75	(e,e,f,e,e,e,e,f; (1,3)(2,7)(4,5)(6,8))	96
76	(e,e,e,e,f,e,e,f; (1,6)(3,8))	96
77	(e,f,f,e,f,e,f,e; (1,6)(3,8))	96
78	(f,e,e,f,f,e,e,f; (1,6,7)(2,8,3))	128
79	(f,e,e,f,f,e,e,f; (1,3,7,8,6,2)(4,5))	512
80	(f,f,e,f,f,e,e,f; (1,8)(2,4,3,7,5,6))	512
81	(e,e,e,f,f,f,f,e; (2,3,5)(4,7,6))	128
82	(e,f,e,f,f,e,e,f; (1,8)(2,4,3,7,5,6))	512
83	(e,e,e,e,f,e,e,f; (1,4)(5,8))	24
84	(f,f,e,e,e,e,e,f; (1,8)(2,4)(3,6)(5,7))	192
85	(f,f,e,e,e,f,f,f; (1,2,4,3)(5,6,8,7))	768
86	(e,f,f,e,f,e,f,e; (1,4)(2,3)(5,8)(6,7))	96
87	(e,e,f,f,f,e,e; (1,6)(3,8))	96
88	(f,f,e,f,f,f,f,f; (1,7,6)(2,3,8))	256
89	(e,e,f,e,f,e,e,e; (1,8)(2,4)(3,6)(5,7))	384
90	(f,f,f,f,e,f,f,e; (2,3,5)(4,7,6))	256
91	(f,e,f,e,e,e,f,e; (1,7,6)(2,3,8))	256
92	(e,f,f,e,e,e,e,f; id)	8
93	(e,e,e,e,e,e,e,e; id)	1

Table 4: The Character Table and Power Map of the Group U

	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
2P	1a	4a	2a	1a	4a	1a	2c	1a	2c	1a	2e	1a	2e	1a	2g	1a	2g	1a	2i	1a
3P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
5P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
7P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
11P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
χ_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
χ_3	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
χ_5	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
χ_7	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
χ_9	2	0	2	2	0	2	0	2	0	-2	2	2	0	0	-2	2	0	2	0	2
χ_{10}	2	0	2	2	0	2	0	2	0	-2	2	2	0	0	2	2	0	2	0	2
χ_{11}	2	0	2	2	0	2	0	2	0	2	2	2	0	0	-2	2	0	2	0	2
χ_{12}	2	0	2	2	0	2	0	2	0	2	2	2	0	0	2	2	0	2	0	2
χ_{13}	2	2	2	2	0	2	0	2	0	0	-2	2	0	2	0	-2	0	-2	0	-2
χ_{14}	2	-2	2	2	0	2	0	2	0	0	-2	2	0	-2	0	-2	0	-2	0	-2
χ_{15}	3	-1	-1	3	-1	3	-1	-1	-1	-1	-1	3	1	1	-3	3	-1	3	-1	3
χ_{16}	3	-1	-1	3	-1	3	-1	-1	-1	-1	-1	3	1	1	3	3	1	3	1	3
χ_{17}	3	-1	-1	3	1	3	1	-1	1	1	-1	3	-1	1	-3	3	-1	3	-1	3
χ_{18}	3	-1	-1	3	1	3	1	-1	1	1	-1	3	-1	1	3	3	1	3	1	3
χ_{19}	3	1	-1	3	-1	3	-1	-1	-1	-1	3	1	-1	-3	3	1	3	1	3	1
χ_{20}	3	1	-1	3	-1	3	-1	-1	-1	-1	3	1	-1	3	3	-1	3	-1	3	-1
χ_{21}	3	1	-1	3	1	3	1	-1	1	-1	3	-1	-1	-3	3	-1	3	1	3	1
χ_{22}	3	1	-1	3	1	3	1	-1	1	-1	3	-1	-1	3	3	-1	3	-1	3	-1
χ_{23}	4	0	0	4	0	-4	0	0	0	0	0	4	-2	-2	-2	4	0	4	2	0
χ_{24}	4	0	0	4	0	-4	0	0	0	0	0	4	-2	-2	2	4	0	4	-2	0
χ_{25}	4	0	0	4	0	-4	0	0	0	0	0	4	-2	2	-2	4	0	4	-2	0
χ_{26}	4	0	0	4	0	-4	0	0	0	0	0	4	-2	2	2	4	0	4	2	0
χ_{27}	4	0	0	4	0	-4	0	0	0	0	0	4	2	-2	-2	4	0	4	2	0
χ_{28}	4	0	0	4	0	-4	0	0	0	0	0	4	2	-2	2	4	0	4	-2	0
χ_{29}	4	0	0	4	0	-4	0	0	0	0	0	4	2	2	-2	4	0	4	-2	0
χ_{30}	4	0	0	4	0	-4	0	0	0	0	0	4	2	2	2	4	0	4	2	0
χ_{31}	4	0	4	4	0	4	0	4	0	0	-4	4	0	0	0	-4	0	-4	0	-4
χ_{32}	6	0	2	6	0	6	0	2	0	2	2	6	-2	-2	0	6	0	6	0	-2
χ_{33}	6	0	2	6	0	6	0	2	0	-2	2	6	-2	-2	0	6	0	6	0	-2
χ_{34}	6	0	2	6	0	6	0	2	0	-2	2	6	2	-2	0	6	0	6	0	-2
χ_{35}	6	0	2	6	0	6	0	2	0	2	2	6	2	2	0	6	0	6	0	-2
χ_{36}	6	0	-2	6	0	6	0	-2	0	-2	-2	6	0	0	0	6	-2	6	2	-2
χ_{37}	6	0	-2	6	0	6	0	-2	0	-2	-2	6	0	0	0	6	2	6	2	-2
χ_{38}	6	0	-2	6	0	6	0	-2	0	2	-2	6	0	0	0	6	-2	6	2	-2
χ_{39}	6	0	-2	6	0	6	0	-2	0	2	-2	6	0	0	0	6	2	6	2	-2
χ_{40}	6	-2	-2	6	0	6	2	-2	0	0	2	6	0	2	0	-6	0	-6	0	-2
χ_{41}	6	2	-2	6	0	6	-2	-2	0	0	2	6	0	-2	0	-6	0	-6	0	-2
χ_{42}	6	0	2	6	-2	6	0	2	2	-4	-2	6	0	2	0	-6	0	-6	0	-6
χ_{43}	6	0	2	6	-2	6	0	2	2	4	-2	6	0	-2	0	-6	0	-6	0	-6
χ_{44}	6	0	2	6	2	6	0	2	-2	-4	-2	6	0	-2	0	-6	0	-6	0	2
χ_{45}	6	0	2	6	2	6	0	2	-2	4	-2	6	0	2	0	-6	0	-6	0	2
χ_{46}	8	0	0	8	0	-8	0	0	0	0	0	8	0	-4	0	-8	0	-8	0	0

Table 4: (Continued)

	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i	4i
	2P	1a	4a	2a	1a	4a	1a	2c	1a	2c	1a	2e	1a	2e	1a	2g	1a	2g	1a	2i	1a
	3P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
	5P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
	7P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
	11P	1a	8a	4a	2a	8b	2b	4b	2c	4c	2d	4d	2e	4e	2f	4f	2g	4g	2h	4h	2i
χ_{47}		8	0	0	8	0	-8	0	0	0	0	0	8	0	4	0	-8	0	-8	0	0
χ_{48}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	-4	0	4	0	-4
χ_{49}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	-4	0	4	0	-4
χ_{90}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	-4	0	4	0	-4
χ_{51}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	-4	0	4	0	-4
χ_{52}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	4	0	-4	0	4
χ_{53}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	4	0	-4	0	4
χ_{54}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	4	0	-4	0	4
χ_{55}		8	0	0	-8	0	0	0	0	0	0	0	0	0	0	0	4	0	-4	0	4
χ_{56}		8	0	0	8	0	-8	0	0	0	0	8	0	0	-4	8	0	8	0	0	0
χ_{57}		8	0	0	8	0	-8	0	0	0	0	8	0	0	-4	8	0	8	0	0	0
χ_{58}		8	0	0	8	0	-8	0	0	0	0	8	0	0	4	8	0	8	0	0	0
χ_{59}		8	0	0	8	0	-8	0	0	0	0	8	0	0	4	8	0	8	0	0	0
χ_{60}		12	0	-4	12	0	12	0	4	0	0	-4	0	0	0	0	0	0	0	0	0
χ_{61}		12	0	-4	12	0	12	0	4	0	0	-4	0	0	0	0	0	0	0	0	0
χ_{62}		12	0	-4	12	0	12	0	4	0	0	-4	0	0	0	0	0	0	0	0	0
χ_{63}		12	0	-4	12	0	12	0	4	0	0	-4	0	0	0	0	0	0	0	0	0
χ_{64}		12	0	-4	12	0	12	0	-4	0	0	4	12	0	0	0	-12	0	-12	0	4
χ_{65}		12	0	0	12	0	-12	0	0	0	-4	0	-4	-2	-2	0	0	-2	0	0	4
χ_{66}		12	0	0	12	0	-12	0	0	0	-4	0	-4	-2	-2	0	0	2	0	0	4
χ_{67}		12	0	0	12	0	-12	0	0	0	-4	0	-4	2	2	0	0	-2	0	0	4
χ_{68}		12	0	0	12	0	-12	0	0	0	-4	0	-4	2	2	0	0	2	0	0	4
χ_{69}		12	0	0	12	0	-12	0	0	0	4	0	-4	-2	2	0	0	-2	0	0	4
χ_{70}		12	0	0	12	0	-12	0	0	0	4	0	-4	-2	2	0	0	2	0	0	4
χ_{71}		12	0	0	12	0	-12	0	0	0	4	0	-4	2	-2	0	0	-2	0	0	4
χ_{72}		12	0	0	12	0	-12	0	0	0	4	0	-4	2	-2	0	0	2	0	0	4
χ_{73}		12	0	4	12	0	12	0	-4	0	0	0	-4	0	-4	0	0	0	0	0	0
χ_{74}		12	0	4	12	0	12	0	-4	0	0	0	-4	0	-4	0	0	0	0	0	0
χ_{75}		12	0	4	12	0	12	0	-4	0	0	0	-4	0	4	0	0	0	0	0	0
χ_{76}		12	0	4	12	0	12	0	-4	0	0	0	-4	0	4	0	0	0	0	0	0
χ_{77}		16	0	0	16	0	-16	0	0	0	0	16	0	0	0	0	-16	0	-16	0	0
χ_{78}		16	0	0	-16	0	0	0	0	0	0	0	0	0	0	0	-8	0	8	0	-8
χ_{79}		16	0	0	-16	0	0	0	0	0	0	0	0	0	0	0	-8	0	8	0	-8
χ_{80}		16	0	0	-16	0	0	0	0	0	0	0	0	0	0	0	8	0	-8	0	8
χ_{81}		24	0	0	-16	0	0	0	0	0	0	0	0	0	0	0	8	0	-8	0	8
χ_{82}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	-12	0	12	0	4
χ_{83}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	-12	0	12	0	4
χ_{84}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	-12	0	12	0	4
χ_{85}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	-12	0	12	0	4
χ_{86}		24	0	0	24	0	-24	0	0	0	0	0	-8	0	-4	0	0	0	0	0	-8
χ_{87}		24	0	0	24	0	-24	0	0	0	0	0	-8	0	4	0	0	0	0	0	-8
χ_{88}		24	0	0	24	0	24	0	0	0	0	0	-8	-4	0	0	0	0	0	0	0
χ_{89}		24	0	0	24	0	24	0	0	0	0	0	-8	4	0	0	0	0	0	0	0
χ_{90}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	12	0	-12	0	-4
χ_{91}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	12	0	-12	0	-4
χ_{92}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	12	0	-12	0	-4
χ_{93}		24	0	0	-24	0	0	0	0	0	0	0	0	0	0	0	12	0	-12	0	-4

Table 4: (Continued)

	4i	2j	4j	4k	4l	4m	2k	4n	2l	2m	4o	4p	8c	4q	12a	6a	3a	4r	4s	12b
	2j	1a	2e	2e	2e	2k	1a	2k	1a	1a	2b	2m	4q	2m	6a	3a	3a	2a	2a	6b
	4i	2j	4j	4k	4l	4m	2k	4n	2l	2m	4o	4p	8c	4q	4r	2a	1a	4r	4s	4t
	4i	2j	4j	4k	4l	4m	2k	4n	2l	2m	4o	4p	8c	4q	12a	6a	3a	4r	4s	12b
	4i	2j	4j	4k	4l	4m	2k	4n	2l	2m	4o	4p	8c	4q	12a	6a	3a	4r	4s	12b
	4i	2j	4j	4k	4l	4m	2k	4n	2l	2m	4o	4p	8c	4q	12a	6a	3a	4r	4s	12b
Y1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Y2	-1	1	-1	-1	-1	-1	1	-1	-1	1	1	-1	1	1	-1	1	1	-1	-1	-1
Y3	-1	1	1	1	1	1	1	1	1	1	1	-1	-1	1	-1	1	1	-1	-1	-1
Y4	1	1	-1	-1	-1	-1	1	-1	-1	1	1	1	-1	1	1	1	1	1	1	1
Y5	-1	1	1	-1	1	-1	1	-1	1	1	1	-1	1	1	1	1	1	1	1	-1
Y6	1	1	-1	1	-1	1	1	1	-1	1	1	-1	-1	1	-1	1	1	1	-1	-1
Y7	1	1	1	-1	1	-1	1	-1	1	1	1	-1	1	1	-1	1	1	-1	-1	1
Y8	-1	1	-1	1	-1	1	1	1	-1	1	1	1	1	1	1	1	1	1	1	-1
Y9	-2	2	0	0	0	0	2	0	0	2	2	-2	0	2	1	-1	-1	-2	-2	1
Y10	2	2	0	0	0	0	2	0	0	2	2	-2	0	2	1	-1	-1	-2	-2	-1
Y11	-2	-2	0	0	0	0	2	0	0	2	2	0	2	-1	-1	-1	-1	2	2	1
Y12	2	2	0	0	0	0	2	0	0	2	2	2	0	2	-1	-1	-1	2	2	-1
Y13	0	-2	-2	0	2	0	2	0	-2	2	2	0	0	-2	0	2	2	0	0	0
Y14	0	-2	2	0	-2	0	2	0	2	2	2	0	0	-2	0	2	2	0	0	0
Y15	1	3	1	-1	1	-1	3	-1	1	3	-1	-1	1	-1	0	0	0	3	-1	0
Y16	-1	3	1	1	1	1	3	1	1	3	-1	-1	-1	-1	0	0	0	3	-1	0
Y17	1	3	1	1	1	1	3	1	1	3	-1	1	1	-1	0	0	0	-3	1	0
Y18	-1	3	1	-1	1	-1	3	-1	1	3	-1	1	-1	-1	0	0	0	-3	1	0
Y19	1	3	-1	-1	-1	-1	3	-1	-1	3	-1	1	-1	-1	0	0	0	-3	1	0
Y20	-1	3	-1	1	-1	1	3	1	-1	3	-1	1	1	-1	0	0	0	-3	1	0
Y21	1	3	-1	1	-1	1	3	1	-1	3	-1	-1	-1	-1	0	0	0	3	-1	0
Y22	-1	3	-1	-1	-1	-1	3	-1	-1	3	-1	-1	1	-1	0	0	0	3	-1	0
Y23	0	0	2	0	2	2	0	-2	2	-4	0	0	0	0	1	1	1	4	0	-1
Y24	0	0	2	0	2	-2	0	2	2	-4	0	0	0	0	1	1	1	4	0	1
Y25	0	0	-2	0	-2	2	0	-2	-2	-4	0	0	0	0	-1	1	1	-4	0	-1
Y26	0	0	-2	0	-2	2	0	-2	-4	0	0	0	0	0	-1	1	1	-4	0	1
Y27	0	0	2	0	2	-2	0	2	2	-4	0	0	0	0	-1	1	1	-4	0	-1
Y28	0	0	2	0	2	2	0	-2	2	-4	0	0	0	0	-1	1	1	-4	0	1
Y29	0	0	-2	0	-2	-2	0	2	-2	-4	0	0	0	0	1	1	1	4	0	-1
Y30	0	0	-2	0	-2	2	0	-2	-2	-4	0	0	0	0	1	1	1	4	0	1
Y31	0	-4	0	0	0	0	4	0	0	4	4	0	0	-4	0	-2	-2	0	0	0
Y32	0	-2	-2	0	-2	0	-2	0	-2	6	-2	-2	0	-2	0	0	0	6	2	0
Y33	0	-2	2	0	2	0	-2	0	2	6	-2	2	0	-2	0	0	0	-6	-2	0
Y34	0	-2	-2	0	-2	0	-2	0	-2	6	-2	2	0	-2	0	0	0	-6	-2	0
Y35	0	-2	2	0	2	0	-2	0	2	6	-2	-2	0	-2	0	0	0	6	2	0
Y36	0	-2	0	-2	0	2	-2	2	0	6	2	2	0	2	0	0	0	6	-2	0
Y37	0	-2	0	2	0	-2	-2	-2	0	6	2	2	0	2	0	0	0	6	-2	0
Y38	0	-2	0	2	0	-2	-2	-2	0	6	2	-2	0	2	0	0	0	-6	2	0
Y39	0	-2	0	-2	0	2	-2	2	0	6	2	-2	0	2	0	0	0	-6	2	0
Y40	0	-6	-2	0	2	0	6	0	-2	6	-2	0	0	2	0	0	0	0	0	0
Y41	0	-6	2	0	-2	0	6	0	2	6	-2	0	0	2	0	0	0	0	0	0
Y42	0	2	-2	0	2	0	-2	0	-2	6	-2	0	0	2	0	0	0	0	-4	0
Y43	0	2	2	0	-2	0	-2	0	2	6	-2	0	0	2	0	0	0	0	4	0
Y44	0	2	2	0	-2	0	-2	0	2	6	-2	0	0	2	0	0	0	0	-4	0
Y45	0	2	-2	0	2	0	-2	0	-2	6	-2	0	0	2	0	0	0	0	4	0
Y46	0	0	-4	0	4	0	0	0	-4	-8	0	0	0	0	0	2	2	0	0	0

Table 4: (Continued)

	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	3a	4y	4z	2r	2s	2t	2u	4aa
	3a	2h	2n	1a	2k	2o	1a	1a	4o	1a	2a	6c	3a	2e	1a	1a	1a	1a	1a	1a	2k
	2h	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	4f	2g	4y	4z	2r	2s	2t	2u	4aa	
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa	
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa	
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa	
γ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
γ_2	1	-1	1	1	-1	1	1	-1	-1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	1
γ_3	1	-1	1	1	1	-1	1	-1	1	1	-1	-1	1	1	1	1	1	1	1	1	1
γ_4	1	1	1	1	-1	-1	1	1	-1	-1	-1	1	1	-1	-1	1	-1	1	-1	1	-1
γ_5	1	-1	-1	1	-1	1	1	1	-1	1	1	-1	1	1	-1	-1	1	1	-1	-1	1
γ_6	1	1	-1	1	1	1	1	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	-1
γ_7	1	1	-1	1	-1	-1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	1	-1	-1	-1
γ_8	1	-1	-1	1	1	-1	1	1	1	-1	-1	-1	1	-1	1	-1	-1	1	1	1	-1
γ_9	-1	-2	2	2	0	0	2	-2	0	0	0	0	1	-1	0	0	2	0	2	0	2
γ_{10}	-1	2	-2	2	0	0	2	-2	0	0	0	-1	-1	0	0	-2	0	2	0	0	-2
γ_{11}	-1	-2	-2	2	0	0	2	2	0	0	0	1	-1	0	0	-2	0	2	0	0	-2
γ_{12}	-1	2	2	2	0	0	2	2	0	0	0	0	-1	0	0	2	0	2	0	0	2
γ_{13}	-2	0	0	2	0	0	2	0	0	2	0	0	-2	-2	0	0	-2	-2	0	0	0
γ_{14}	-2	0	0	2	0	0	2	0	0	-2	0	0	-2	2	0	0	2	-2	0	0	0
γ_{15}	0	-3	1	3	-1	1	3	3	1	1	1	0	0	1	-1	-3	1	3	-1	1	1
γ_{16}	0	3	-1	3	1	1	3	3	-1	1	1	0	0	1	1	3	1	3	1	3	-1
γ_{17}	0	-3	-1	3	1	-1	3	-3	-1	1	-1	0	0	1	1	3	1	3	1	3	-1
γ_{18}	0	3	1	3	-1	-1	3	-3	1	1	-1	0	0	1	-1	-3	1	3	-1	1	1
γ_{19}	0	-3	-1	3	-1	1	3	-3	1	-1	1	0	0	-1	-1	3	-1	3	-1	1	-1
γ_{20}	0	3	1	3	1	1	3	-3	-1	-1	1	0	0	-1	1	-3	-1	-3	1	1	1
γ_{21}	0	-3	1	3	1	-1	3	3	-1	-1	-1	0	0	-1	1	-3	-1	3	1	1	1
γ_{22}	0	3	-1	3	-1	-1	3	3	1	-1	-1	0	0	-1	-1	3	-1	3	-1	-1	-1
γ_{23}	1	2	0	0	-2	0	0	-4	0	2	-2	1	1	-2	0	2	-2	0	0	0	0
γ_{24}	1	-2	0	0	2	0	0	-4	0	2	-2	-1	1	-2	0	-2	-2	0	0	0	0
γ_{25}	1	2	0	0	-2	0	0	4	0	-2	-2	1	1	2	0	-2	2	0	0	0	0
γ_{26}	1	-2	0	0	2	0	0	4	0	-2	-2	-1	1	2	0	2	2	0	0	0	0
γ_{27}	1	2	0	0	2	0	0	4	0	2	2	1	1	-2	0	-2	-2	0	0	0	0
γ_{28}	1	-2	0	0	-2	0	0	4	0	2	2	-1	1	-2	0	2	-2	0	0	0	0
γ_{29}	1	2	0	0	2	0	0	-4	0	-2	2	1	1	2	0	2	2	0	0	0	0
γ_{30}	1	-2	0	0	-2	0	0	-4	0	-2	2	-1	1	2	0	-2	2	0	0	0	0
γ_{31}	2	0	0	4	0	0	4	0	0	0	0	0	2	0	0	0	0	-4	0	0	0
γ_{32}	0	0	0	-2	0	2	-2	6	0	-2	-2	0	0	-2	0	0	-2	-2	0	0	0
γ_{33}	0	0	0	-2	0	2	-2	-6	0	2	-2	0	0	2	0	0	2	-2	0	0	0
γ_{34}	0	0	0	-2	0	-2	-2	-6	0	-2	2	0	0	-2	0	0	-2	-2	0	0	0
γ_{35}	0	0	0	-2	0	-2	-2	6	0	2	2	0	0	2	0	0	2	-2	0	0	0
γ_{36}	0	0	0	-2	2	0	-2	6	0	0	0	0	0	0	-2	0	0	-2	-2	-2	0
γ_{37}	0	0	0	-2	-2	0	-2	6	0	0	0	0	0	0	2	0	0	-2	2	0	0
γ_{38}	0	0	0	-2	-2	0	-2	-6	0	0	0	0	0	0	2	0	0	-2	0	0	0
γ_{39}	0	0	0	-2	2	0	-2	-6	0	0	0	0	0	0	-2	0	0	-2	-2	0	0
γ_{40}	0	0	0	6	0	0	6	0	0	2	0	0	0	-2	0	0	-2	-6	0	0	0
γ_{41}	0	0	0	6	0	0	6	0	0	-2	0	0	0	2	0	0	2	0	-6	0	0
γ_{42}	0	0	0	-2	0	0	-2	0	0	2	0	0	0	-2	0	0	-2	2	0	0	0
γ_{43}	0	0	0	-2	0	0	-2	0	0	-2	0	0	0	2	0	0	2	2	0	0	0
γ_{44}	0	0	0	-2	0	0	-2	0	0	-2	0	0	0	2	0	0	2	2	0	0	0
γ_{45}	0	0	0	-2	0	0	-2	0	0	2	0	0	0	-2	0	0	-2	2	0	0	0
γ_{46}	-2	0	0	0	0	0	0	0	0	4	0	0	0	4	0	0	4	0	0	0	0

Table 4: (Continued)

	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa
	3a	2h	2n	1a	2k	2o	1a	1a	4o	1a	2a	6c	3a	2e	2e	1a	1a	1a	1a	2k
	2h	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	4f	2g	4y	4z	2r	2s	2t	2u	4aa
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa
	6b	4t	4u	2n	4v	4w	2o	2p	8d	2q	4x	12c	6c	4y	4z	2r	2s	2t	2u	4aa
χ_{47}	-2	0	0	0	0	0	0	0	0	-4	0	0	-2	-4	0	0	-4	0	0	0
χ_{48}	-2	0	0	-4	0	0	0	0	0	0	0	0	2	0	2	-2	-4	0	-2	0
χ_{49}	-2	0	0	-4	0	0	0	0	0	0	0	0	2	0	2	2	4	0	-2	0
χ_{50}	-2	0	0	-4	0	0	0	0	0	0	0	0	2	0	-2	-2	4	0	2	0
χ_{51}	-2	0	0	-4	0	0	0	0	0	0	0	0	2	0	-2	2	-4	0	2	0
χ_{52}	2	0	0	-4	4	0	0	0	0	0	0	0	-2	0	2	-2	-4	0	2	0
χ_{53}	2	0	0	-4	4	0	0	0	0	0	0	0	-2	0	2	2	4	0	2	0
χ_{54}	2	0	0	-4	-4	0	0	0	0	0	0	0	-2	0	-2	-2	4	0	-2	0
χ_{55}	2	0	0	-4	-4	0	0	0	0	0	0	0	-2	0	-2	2	-4	0	-2	0
χ_{56}	-1	4	0	0	0	0	0	-8	0	0	0	-1	-1	0	0	4	0	0	0	0
χ_{57}	-1	4	0	0	0	0	0	8	0	0	0	-1	-1	0	0	-4	0	0	0	0
χ_{58}	-1	-4	0	0	0	0	0	-8	0	0	0	1	-1	0	0	-4	0	0	0	0
χ_{59}	-1	-4	0	0	0	0	0	8	0	0	0	1	-1	0	0	4	0	0	0	0
χ_{60}	0	0	2	4	2	0	-4	0	0	0	0	0	4	-2	2	-4	0	2	-2	
χ_{61}	0	0	2	4	-2	0	-4	0	0	0	0	0	4	-2	2	4	0	-2	-2	
χ_{62}	0	0	-2	4	-2	0	-4	0	0	0	0	0	0	4	-2	-4	0	-2	2	
χ_{63}	0	0	-2	4	2	0	-4	0	0	0	0	0	0	-4	-2	-2	4	0	2	2
χ_{64}	0	0	0	-4	0	0	-4	0	0	0	0	0	0	0	0	0	4	0	0	0
χ_{65}	0	0	0	0	2	0	0	0	2	2	0	0	0	-2	0	-2	2	-4	0	0
χ_{66}	0	0	0	0	-2	0	0	0	2	2	0	0	0	-2	0	2	-4	0	0	0
χ_{67}	0	0	0	0	2	0	0	0	-2	-2	0	0	2	0	2	-2	-4	0	0	0
χ_{68}	0	0	0	0	-2	0	0	0	-2	-2	0	0	2	0	-2	-2	-4	0	0	0
χ_{69}	0	0	0	0	-2	0	0	0	-2	2	0	0	2	0	-2	-2	-4	0	0	0
χ_{70}	0	0	0	0	2	0	0	0	-2	2	0	0	2	0	2	-2	-4	0	0	0
χ_{71}	0	0	0	0	-2	0	0	0	2	-2	0	0	-2	0	2	2	-4	0	0	0
χ_{72}	0	0	0	0	2	0	0	0	2	-2	0	0	-2	0	-2	2	-4	0	0	0
χ_{73}	0	0	-2	4	-2	0	-4	0	0	-4	0	0	0	-2	2	0	0	2	2	
χ_{74}	0	0	2	4	2	0	-4	0	0	-4	0	0	0	2	-2	0	0	-2	-2	
χ_{75}	0	0	2	4	-2	0	-4	0	0	4	0	0	0	-2	-2	0	0	2	-2	
χ_{76}	0	0	-2	4	2	0	-4	0	0	4	0	0	0	2	2	0	0	-2	2	
χ_{77}	2	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
χ_{78}	2	0	0	-8	0	0	0	0	0	0	0	0	-2	0	0	-4	0	0	0	0
χ_{79}	2	0	0	-8	0	0	0	0	0	0	0	0	-2	0	0	4	0	0	0	0
χ_{80}	-2	0	0	-8	0	0	0	0	0	0	0	0	2	0	0	-4	0	0	0	0
χ_{81}	-2	0	0	-8	0	0	0	0	0	0	0	0	2	0	0	4	0	0	0	0
χ_{82}	0	0	0	4	0	0	0	0	0	0	0	0	0	2	-6	-4	0	-2	0	
χ_{83}	0	0	0	4	0	0	0	0	0	0	0	0	0	2	-6	4	0	-2	0	
χ_{84}	0	0	0	4	0	0	0	0	0	0	0	0	0	-2	-6	4	0	2	0	
χ_{85}	0	0	0	4	0	0	0	0	0	0	0	0	0	-2	6	-4	0	2	0	
χ_{86}	0	0	0	0	0	0	0	0	0	4	0	0	0	4	0	0	-4	8	0	0
χ_{87}	0	0	0	0	0	0	0	0	0	-4	0	0	0	-4	0	0	4	8	0	0
χ_{88}	0	0	0	-8	0	0	8	0	0	4	0	0	0	0	0	0	0	0	0	0
χ_{89}	0	0	0	-8	0	0	8	0	0	0	-4	0	0	0	0	0	0	0	0	0
χ_{90}	0	0	0	4	-4	0	0	0	0	0	0	0	0	2	-2	4	0	2	0	
χ_{91}	0	0	0	4	-4	0	0	0	0	0	0	0	0	2	2	-4	0	2	0	
χ_{92}	0	0	0	4	4	0	0	0	0	0	0	0	0	-2	-2	-4	0	-2	0	
χ_{93}	0	0	0	4	4	0	0	0	0	0	0	0	0	-2	2	4	0	-2	0	

Table 4: (Continued)

	4ab	2v	6d	2w	6e	2x	6f	6g	2y	4ac	4ad	2z	4ae	4af	4ag	4ah	2aa	4ai	2ab	4aj	
	2ka	1a	3a	1a	3a	1a	3a	3a	1a	2k	2k	1a	2e	2i	2j	2k	1a	2k	1a	2e	
	4ab	2v	2w	2w	2x	2x	2v	2y	2y	4ac	4ad	2z	4ae	4af	4ag	4ah	2aa	4ai	2ab	4aj	
	4ab	2v	6d	2w	6e	2x	6f	6g	2y	4ac	4ad	2z	4ae	4af	4ag	4ah	2aa	4ai	2ab	4aj	
	4ab	2v	6d	2w	6e	2x	6f	6g	2y	4ac	4ad	2z	4ae	4af	4ag	4ah	2aa	4ai	2ab	4aj	
	4ab	2v	6d	2w	6e	2x	6f	6g	2y	4ac	4ad	2z	4ae	4af	4ag	4ah	2aa	4ai	2ab	4aj	
Y47	0	0	0	0	0	0	0	2	8	0	0	0	0	0	0	0	0	0	0	-4	0
Y48	0	-6	2	2	-2	-2	0	0	0	2	-2	-2	0	0	0	-2	2	2	2	4	0
Y49	0	6	-2	-2	2	2	0	0	0	-2	2	2	0	0	0	2	-2	-2	-4	0	0
Y50	0	-6	2	2	-2	-2	0	0	0	-2	2	-2	0	0	0	2	2	2	-2	-4	0
Y51	0	6	-2	-2	2	2	0	0	0	2	-2	2	0	0	0	-2	-2	2	4	0	0
Y52	-4	2	0	-6	0	6	2	0	0	2	-2	0	0	0	0	-2	2	-2	4	0	0
Y53	-4	-2	0	6	0	-6	-2	0	0	-2	-2	2	0	0	0	2	-2	2	-4	0	0
Y54	4	2	0	-6	0	6	2	0	0	-2	-2	2	0	0	0	2	2	2	-4	0	0
Y55	4	-2	0	6	0	-6	-2	0	0	2	2	2	0	0	0	-2	-2	-2	4	0	0
Y56	0	-4	1	4	1	4	-1	1	-8	0	0	-4	0	0	0	0	4	0	0	0	0
Y57	0	4	-1	-4	-1	-4	1	1	-8	0	0	4	0	0	0	0	-4	0	0	0	0
Y58	0	4	-1	-4	-1	-4	1	1	-8	0	0	4	0	0	0	0	-4	0	0	0	0
Y59	0	-4	1	4	1	4	-1	1	-8	0	0	-4	0	0	0	0	4	0	0	0	0
Y60	2	-6	0	-6	0	-6	0	0	0	0	2	0	0	0	0	2	0	-4	0	0	0
Y61	-2	-6	0	-6	0	-6	0	0	0	0	2	0	0	0	0	2	0	2	0	4	0
Y62	-2	6	0	6	0	6	0	0	0	0	-2	0	0	0	0	0	-2	0	-4	0	0
Y63	2	6	0	6	0	6	0	0	0	0	0	-2	0	0	0	0	-2	0	4	0	0
Y64	0	0	0	0	0	0	0	0	-12	0	0	0	0	0	0	0	0	0	0	0	0
Y65	2	-6	0	6	0	6	0	0	0	0	2	2	-2	0	0	0	-2	0	2	0	0
Y66	-2	6	0	-6	0	-6	0	0	0	0	-2	2	2	0	0	0	2	0	2	0	0
Y67	2	6	0	-6	0	-6	0	0	0	0	-2	-2	2	0	0	2	0	2	-2	0	0
Y68	-2	-6	0	6	0	6	0	0	0	0	2	-2	-2	0	0	-2	0	-2	0	-2	0
Y69	-2	-6	0	6	0	6	0	0	0	0	2	2	2	0	0	0	-2	0	-2	0	0
Y70	2	6	0	-6	0	-6	0	0	0	0	2	-2	2	-2	0	0	2	0	2	-2	0
Y71	-2	6	0	-6	0	-6	0	0	0	0	-2	-2	-2	0	0	2	0	2	0	2	0
Y72	2	-6	0	6	0	6	0	0	0	0	2	-2	2	0	0	0	-2	0	2	0	0
Y73	-2	-6	0	-6	0	-6	0	0	0	0	2	0	0	0	0	0	2	0	0	0	0
Y74	2	6	0	6	0	6	0	0	0	0	-2	0	0	0	0	0	-2	0	0	0	0
Y75	-2	6	0	6	0	6	0	0	0	0	-2	0	0	0	0	0	-2	0	0	0	0
Y76	2	-6	0	-6	0	-6	0	0	0	0	2	0	0	0	0	0	2	0	0	0	0
Y77	0	0	0	0	0	0	-2	16	0	0	0	0	0	0	0	0	0	0	0	0	0
Y78	0	-12	-2	4	2	-4	0	0	0	0	-4	0	0	0	0	0	4	0	0	0	0
Y79	0	12	2	-4	-2	4	0	0	0	0	4	0	0	0	0	0	-4	0	0	0	0
Y80	0	4	0	-12	0	12	-2	0	0	0	0	-4	0	0	0	0	4	0	0	0	0
Y81	0	-4	0	12	0	12	2	0	0	0	0	4	0	0	0	0	-4	0	0	0	0
Y82	0	6	0	6	0	-6	0	0	0	-2	2	2	0	0	0	2	6	-2	4	0	0
Y83	0	-6	0	-6	0	6	0	0	2	-2	-2	0	0	0	0	-2	-6	2	-4	0	0
Y84	0	6	0	6	0	-6	0	0	2	-2	2	0	0	0	0	-2	6	2	-4	0	0
Y85	0	-6	0	-6	0	6	0	0	-2	-2	-2	0	0	0	0	2	-6	-2	4	0	0
Y86	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	0
Y87	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0
Y88	0	0	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0	0	0	0
Y89	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0
Y90	4	-6	0	-6	0	6	0	0	2	2	6	0	0	0	0	-2	2	-2	-4	0	0
Y91	4	6	0	6	0	-6	0	0	-2	-2	-6	0	0	0	2	-2	2	2	4	0	0
Y92	-4	-6	0	-6	0	6	0	0	-2	-2	6	0	0	0	2	2	2	2	4	0	0
Y93	-4	6	0	6	0	-6	0	0	2	2	-6	0	0	0	0	-2	-2	-2	-4	0	0

Table 4: (Continued)

	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
	3a	3a	1a	1a	1a	2e	2k	2k	2e	3a	2e	1a	2h
	2p	2ac	2ac	2ad	2ae	4ak	4al	4am	4an	2b	4ao	2af	4ap
	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
χ_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
χ_3	-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
χ_5	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
χ_7	-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
χ_9	1	-1	2	2	0	-2	0	0	0	-1	0	0	0
χ_{10}	1	1	-2	-2	0	-2	0	0	0	-1	0	0	0
χ_{11}	-1	1	-2	-2	0	2	0	0	0	-1	0	0	0
χ_{12}	-1	-1	2	2	0	2	0	0	0	-1	0	0	0
χ_{13}	0	0	0	0	0	0	0	0	2	2	2	0	0
χ_{14}	0	0	0	0	0	0	0	0	-2	2	-2	0	0
χ_{15}	0	0	-3	-3	-1	-1	-1	-1	1	0	1	1	-1
χ_{16}	0	0	3	3	1	-1	1	1	1	0	1	1	1
χ_{17}	0	0	3	3	1	1	1	1	1	0	1	-1	-1
χ_{18}	0	0	-3	-3	-1	1	-1	-1	1	0	1	-1	1
χ_{19}	0	0	3	3	-1	1	-1	-1	-1	0	-1	1	1
χ_{20}	0	0	-3	-3	1	1	1	1	-1	0	-1	1	-1
χ_{21}	0	0	-3	-3	1	-1	1	1	-1	0	-1	-1	1
χ_{22}	0	0	3	3	-1	-1	-1	-1	-1	0	-1	-1	-1
χ_{23}	-1	1	-2	-2	0	0	2	2	-2	-1	-2	2	0
χ_{24}	-1	-1	2	2	0	0	-2	-2	-2	-1	-2	2	0
χ_{25}	1	-1	2	2	0	0	2	2	2	-1	2	2	0
χ_{26}	1	1	-2	-2	0	0	-2	-2	2	-1	2	2	0
χ_{27}	1	-1	2	2	0	0	-2	-2	-2	-1	-2	-2	0
χ_{28}	1	1	-2	-2	0	0	2	2	-2	-1	-2	-2	0
χ_{29}	-1	1	-2	-2	0	0	-2	-2	2	-1	2	-2	0
χ_{30}	-1	-1	2	2	0	0	2	2	2	-1	2	-2	0
χ_{31}	0	0	0	0	0	0	0	0	0	-2	0	0	0
χ_{32}	0	0	0	0	0	2	0	0	-2	0	-2	-2	0
χ_{33}	0	0	0	0	0	-2	0	0	2	0	2	-2	0
χ_{34}	0	0	0	0	0	-2	0	0	-2	0	-2	2	0
χ_{35}	0	0	0	0	0	2	0	0	2	0	2	2	0
χ_{36}	0	0	0	0	-2	-2	2	2	0	0	0	0	-2
χ_{37}	0	0	0	0	2	-2	-2	-2	0	0	0	0	2
χ_{38}	0	0	0	0	2	2	-2	-2	0	0	0	0	-2
χ_{39}	0	0	0	0	-2	2	2	2	0	0	0	0	2
χ_{40}	0	0	0	0	0	0	0	0	2	0	2	0	0
χ_{41}	0	0	0	0	0	0	0	0	-2	0	-2	0	0
χ_{42}	0	0	0	0	0	4	0	0	2	0	2	0	0
χ_{43}	0	0	0	0	0	-4	0	0	-2	0	-2	0	0
χ_{44}	0	0	0	0	0	4	0	0	-2	0	-2	0	0
χ_{45}	0	0	0	0	0	-4	0	0	2	0	2	0	0
χ_{46}	0	0	0	0	0	0	0	0	-4	-2	-4	0	0

Table 4: (Continued)

	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
	3a	3a	1a	1a	1a	2e	2k	2k	2e	3a	2e	1a	2h
	2p	2ac	2ac	2ad	2ae	4ak	4al	4am	4an	2b	4ao	2af	4ap
	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
	6h	6i	2ac	2ad	2ae	4ak	4al	4am	4an	6j	4ao	2af	4ap
γ_{47}	0	0	0	0	0	0	0	0	4	-2	4	0	0
γ_{48}	0	0	6	2	2	0	4	0	4	0	-4	0	0
γ_{49}	0	0	-6	-2	2	0	4	0	-4	0	4	0	0
γ_{50}	0	0	6	2	-2	0	-4	0	-4	0	4	0	0
γ_{51}	0	0	-6	-2	-2	0	-4	0	4	0	-4	0	0
γ_{52}	0	-2	-2	2	-2	0	0	0	-4	0	4	0	0
γ_{53}	0	2	2	-2	-2	0	0	0	4	0	-4	0	0
γ_{54}	0	-2	-2	2	2	0	0	0	4	0	-4	0	0
γ_{55}	0	2	2	-2	2	0	0	0	-4	0	4	0	0
γ_{56}	1	-1	-4	-4	0	0	0	0	0	1	0	0	0
γ_{57}	-1	1	4	4	0	0	0	0	0	1	0	0	0
γ_{58}	1	1	4	4	0	0	0	0	0	1	0	0	0
γ_{59}	-1	-1	-4	-4	0	0	0	0	0	1	0	0	0
γ_{60}	0	0	-6	2	2	0	2	-2	0	0	0	0	0
γ_{61}	0	0	-6	2	-2	0	-2	2	0	0	0	0	0
γ_{62}	0	0	6	-2	-2	0	-2	2	0	0	0	0	0
γ_{63}	0	0	6	-2	2	0	2	-2	0	0	0	0	0
γ_{64}	0	0	0	0	0	0	0	0	0	0	0	0	0
γ_{65}	0	0	-6	2	0	0	-2	2	2	0	2	-2	2
γ_{66}	0	0	6	-2	0	0	2	-2	2	0	2	-2	-2
γ_{67}	0	0	6	-2	0	0	-2	2	-2	0	-2	2	2
γ_{68}	0	0	-6	-2	0	0	2	-2	-2	0	-2	2	-2
γ_{69}	0	0	-6	2	0	0	2	-2	-2	0	-2	-2	2
γ_{70}	0	0	6	-2	0	0	-2	2	-2	0	-2	-2	-2
γ_{71}	0	0	6	-2	0	0	2	-2	2	0	2	2	2
γ_{72}	0	0	-6	2	0	0	-2	2	2	0	2	2	-2
γ_{73}	0	0	-6	2	2	0	-2	2	4	0	4	0	0
γ_{74}	0	0	6	-2	-2	0	2	-2	4	0	4	0	0
γ_{75}	0	0	6	-2	-2	0	-2	2	-4	0	-4	0	0
γ_{76}	0	0	-6	2	2	0	2	-2	-4	0	-4	0	0
γ_{77}	0	0	0	0	0	0	0	0	0	2	0	0	0
γ_{78}	0	0	12	4	0	0	0	0	0	0	0	0	0
γ_{79}	0	0	-12	-4	0	0	0	0	0	0	0	0	0
γ_{80}	0	2	-4	4	0	0	0	0	0	0	0	0	0
γ_{81}	0	-2	4	-4	0	0	0	0	0	0	0	0	0
γ_{82}	0	0	-6	-2	2	0	-4	0	4	0	-4	0	0
γ_{83}	0	0	6	2	2	0	-4	0	-4	0	4	0	0
γ_{84}	0	0	-6	-2	-2	0	4	0	-4	0	4	0	0
γ_{85}	0	0	6	2	-2	0	4	0	4	0	-4	0	0
γ_{86}	0	0	0	0	0	0	0	0	4	0	4	0	0
γ_{87}	0	0	0	0	0	0	0	0	-4	0	-4	0	0
γ_{88}	0	0	0	0	0	0	0	0	0	0	0	4	0
γ_{89}	0	0	0	0	0	0	0	0	0	0	0	-4	0
γ_{90}	0	0	6	-6	-2	0	0	0	4	0	-4	0	0
γ_{91}	0	0	-6	6	-2	0	0	0	-4	0	4	0	0
γ_{92}	0	0	6	-6	2	0	0	0	-4	0	4	0	0
γ_{93}	0	0	-6	6	2	0	0	0	4	0	-4	0	0

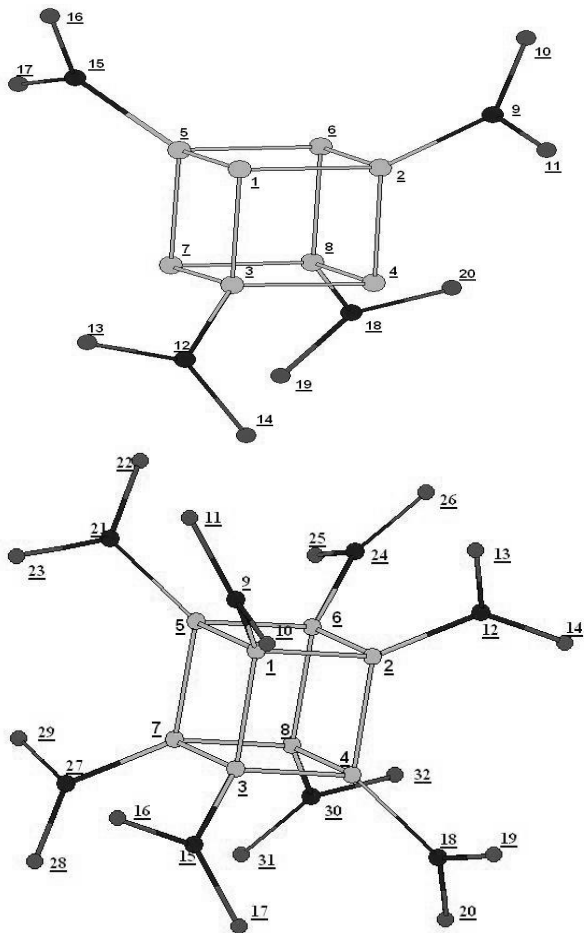


Figure 1: Tetranitrocubane and Octanitrocubane

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