

ORIGINAL ARTICLE

The Full Non-Rigid Group Theory for Triethylborane with C_{3h} Point Group

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ABSTRACT

The full non-rigid molecule group theory in which the dynamical symmetry operations are defined as physical operations is a new field in chemistry. We study the full non-rigid group (f-NRG) of triethylborane with C_{3h} point group and prove that it is a group of order 648 with 88 conjugacy classes. We apply a simple method to compute the character table of this group.

Keywords: triethylborane; non-rigid group; character table; symmetry.

INTRODUCTION

The mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of physical systems and numerous applications to large amplitude vibrational spectroscopy of small organic molecules are appearing in the literature. Group theory is the mathematics of symmetries and plays an important role in the study of molecules, crystals, and clusters in chemistry although applications have usually been restricted to small or moderately sized systems due to computational limitations. To be practical for large systems, finite group theory requires both computer calculation and the advanced computational methods. Group theory for non-rigid molecules is more relevant to large amplitude motion of molecules and its applications appears in the literature [1,5,11,19,23,24,25,26,27].

Lomont [16] has given two methods for calculating character tables. These are satisfactory for small groups, but both of them require knowledge of the class constant 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.

Smeijers and Villa [22] investigate the r-NRG of planar trimethylamine and prove that it is a group of order 324. Also they have proved that this molecule has a pyramidal inversion and so the order of r-NRG of trimethylamine is 648. We may refer to [21,22] for basic properties of non-rigid molecule group and information on NRG and f-NRG.

In a series of paper Ashrafi et al. computed the full non-rigid groups of some molecules such as tetraammine platinum(II) [2], cis- and transdichlorodiammine platinum(II) and trimethylamine [12], tetraammine platinum(II) with C_{2v} and C_{4v} point group [3,20], tetraamine platinum(II) as a wreath product [6], tetra-tertbutyltetrahedrane [7], tetramethylethylene [8], hexamethylbenzene [9] and melamine [4].

Longuet-Higgins [18] 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 of calculating these character tables, which are needed for classification of wave functions, determination of selection rules, and so on.

A flexible molecule may show more than one conformer and the stable structures can lie far away on the potential energy surface (see [10]). So, in this paper, we investigate the f-NRG of triethylborane with C_{3h} point group. Using the chemistry package *Hyperchem* [13] and the group theory package GAP [14], we shall calculate the conjugacy classes and character tables for the full non-rigid point group of $C_6H_{15}B$. Throughout this note, all considered groups are assumed to be finite. Our notation is standard and is taken mainly from [15,17].

THEORETICAL METHOD AND RESULTS

Determination of conjugacy classes

First we consider the point group of triethylborane in the case of non-rigid state and then we shall compute the conjugacy classes of full non-rigid group of this molecule with symmetry group C_{3h} , which is denoted by G. By Figure 1, we have three rotations $\alpha_1=(1,2)$, $\alpha_2=(3,4)$, $\alpha_3=(5,6)$ for three methylene and also three rotations $\beta_1=(7,8,9)$, $\beta_2=(10,11,12)$ and $\beta_3=(13,14,15)$ for three methyl groups. We assume that these operations are all feasible, that barrier to rotation of the methyl group is low. Also, we have a C_3 rotation,

$$\gamma=(1,3,5)(2,4,6)(7,10,13)(8,11,14)(9,12,15),$$

for C_{3h} point groups. The permutations $(\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \gamma)$ generate the group G and a simple GAP program shows that G is groups of order 648 with 88 conjugacy classes. The representative for conjugacy classes of G, H and K are shown in Table 1.

Determination of character table

Utilizing the conjugacy classes of the group G in the last section, the whole irreducible character table of G can be computed directly or by using GAP. The values of the irreducible characters χ_i ($1 \leq i \leq 88$) are illustrated at Table 2.

Table 1
Representative of conjugacy classes of G

No.	Representative	Size	Name
1	0	1	a1
2	(1,2)	3	b1
3	(1,2)(3,4)	3	b2
4	(1,2)(3,4)(5,6)	1	b3
5	(7,8,9)	3	c1
6	(1,2)(7,8,9)	3	f1
7	(3,4)(7,8,9)	3	f2
8	(1,2)(3,4)(7,8,9)	3	f3
9	(5,6)(7,8,9)	3	f4
10	(1,2)(5,6)(7,8,9)	3	f5
11	(3,4)(5,6)(7,8,9)	3	f6
12	(1,2)(3,4)(5,6)(7,8,9)	3	f7
13	(7,9,8)	3	c2
14	(1,2)(7,9,8)	3	f8
15	(3,4)(7,9,8)	3	f9
16	(1,2)(3,4)(7,9,8)	3	f10
17	(5,6)(7,9,8)	3	f11
18	(1,2)(5,6)(7,9,8)	3	f12
19	(3,4)(5,6)(7,9,8)	3	f13
20	(1,2)(3,4)(5,6)(7,9,8)	3	f14

Aghaei and Taghi

21	(7,8,9)(10,11,12)	3	c3
22	(1,2)(7,8,9)(10,11,12)	3	f15
23	(3,4)(7,8,9)(10,11,12)	3	f16
24	(1,2)(3,4)(7,8,9)(10,11,12)	3	f17
25	(5,6)(7,8,9)(10,11,12)	3	f18
26	(1,2)(5,6)(7,8,9)(10,11,12)	3	f19
27	(3,4)(5,6)(7,8,9)(10,11,12)	3	f20
28	(1,2)(3,4)(5,6)(7,8,9)(10,11,12)	3	f21
29	(7,9,8)(10,11,12)	3	c4
30	(1,2)(7,9,8)(10,11,12)	3	f22
31	(3,4)(7,9,8)(10,11,12)	3	f23
32	(1,2)(3,4)(7,9,8)(10,11,12)	3	f24
33	(5,6)(7,9,8)(10,11,12)	3	f25
34	(1,2)(5,6)(7,9,8)(10,11,12)	3	f26
35	(3,4)(5,6)(7,9,8)(10,11,12)	3	f27
36	(1,2)(3,4)(5,6)(7,9,8)(10,11,12)	3	f28
37	(7,8,9)(10,12,11)	3	c5
38	(1,2)(7,8,9)(10,12,11)	3	f29
39	(3,4)(7,8,9)(10,12,11)	3	f30
40	(1,2)(3,4)(7,8,9)(10,12,11)	3	f31
41	(5,6)(7,8,9)(10,12,11)	3	f32
42	(1,2)(5,6)(7,8,9)(10,12,11)	3	f33
43	(3,4)(5,6)(7,8,9)(10,12,11)	3	f34
44	(1,2)(3,4)(5,6)(7,8,9)(10,12,11)	3	f35

Table 1. (Continued)

No.	Representative	Size	Name
45	(7,9,8)(10,12,11)	3	c6
46	(1,2)(7,9,8)(10,12,11)	3	f36
47	(3,4)(7,9,8)(10,12,11)	3	f37
48	(1,2)(3,4)(7,9,8)(10,12,11)	3	f38
49	(5,6)(7,9,8)(10,12,11)	3	f39
50	(1,2)(5,6)(7,9,8)(10,12,11)	3	f40

51	(3,4)(5,6)(7,9,8)(10,12,11)	3	f41
52	(1,2)(3,4)(5,6)(7,9,8)(10,12,11)	3	f42
53	(7,8,9)(10,11,12)(13,14,15)	1	c7
54	(1,2)(7,8,9)(10,11,12)(13,14,15)	3	f43
55	(1,2)(3,4)(7,8,9)(10,11,12)(13,14,15)	3	f44
56	(1,2)(3,4)(5,6)(7,8,9)(10,11,12)(13,14,15)	1	f45
57	(7,9,8)(10,11,12)(13,14,15)	3	c8
58	(1,2)(7,9,8)(10,11,12)(13,14,15)	3	f46
59	(3,4)(7,9,8)(10,11,12)(13,14,15)	3	f47
60	(1,2)(3,4)(7,9,8)(10,11,12)(13,14,15)	3	f48
61	(5,6)(7,9,8)(10,11,12)(13,14,15)	3	f49
62	(1,2)(5,6)(7,9,8)(10,11,12)(13,14,15)	3	f50
63	(3,4)(5,6)(7,9,8)(10,11,12)(13,14,15)	3	f51
64	(1,2)(3,4)(5,6)(7,9,8)(10,11,12)(13,14,15)	3	f52
65	(7,9,8)(10,12,11)(13,14,15)	3	c9
66	(1,2)(7,9,8)(10,12,11)(13,14,15)	3	f53
67	(3,4)(7,9,8)(10,12,11)(13,14,15)	3	f54
68	(1,2)(3,4)(7,9,8)(10,12,11)(13,14,15)	3	f55
69	(5,6)(7,9,8)(10,12,11)(13,14,15)	3	f56
70	(1,2)(5,6)(7,9,8)(10,12,11)(13,14,15)	3	f57
71	(3,4)(5,6)(7,9,8)(10,12,11)(13,14,15)	3	f58
72	(1,2)(3,4)(5,6)(7,9,8)(10,12,11)(13,14,15)	3	f59
73	(7,9,8)(10,12,11)(13,15,14)	1	c10
74	(1,2)(7,9,8)(10,12,11)(13,15,14)	3	f60
75	(1,2)(3,4)(7,9,8)(10,12,11)(13,15,14)	3	f61
76	(1,2)(3,4)(5,6)(7,9,8)(10,12,11)(13,15,14)	1	f62
77	(1,3,5)(2,4,6)(7,10,13)(8,11,14)(9,12,15)	36	c11
78	(1,3,5,2,4,6)(7,10,13)(8,11,14)(9,12,15)	36	f63
79	(1,3,5)(2,4,6)(7,10,13,8,11,14,9,12,15)	36	i1
80	(1,3,5,2,4,6)(7,10,13,8,11,14,9,12,15)	36	r1
81	(1,3,5)(2,4,6)(7,10,13,9,12,15,8,11,14)	36	i2
82	(1,3,5,2,4,6)(7,10,13,9,12,15,8,11,14)	36	r2
83	(1,5,3)(2,6,4)(7,13,10)(8,14,11)(9,15,12)	36	c12

84	$(1,5,3,2,6,4)(7,13,10)(8,14,11)(9,15,12)$	36	f64
85	$(1,5,3)(2,6,4)(7,13,10,8,14,11,9,15,12)$	36	i3
86	$(1,5,3,2,6,4)(7,13,10,8,14,11,9,15,12)$	36	r3
87	$(1,5,3)(2,6,4)(7,13,10,9,15,12,8,14,11)$	36	i4
88	$(1,5,3,2,6,4)(7,13,10,9,15,12,8,14,11)$	36	r4

Table 2
Character table of the group G

	a1	b1	c1	f1	c2	f2	c3	f3	f4	f5	c4	f6	f7	f8	c5	f9	f10	f11	f12	f13	f14	c7	f15	f16	f17	c8	f18	f19	
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	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^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	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	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	1	1	1	1		
χ^7	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a	a			
χ^8	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d	d			
χ^9	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a			
χ^{10}	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d			
χ^{11}	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a			
χ^{12}	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d			
χ^{13}	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a			
χ^{14}	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d			
χ^{15}	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a			
χ^{16}	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d			
χ^{17}	1	1	1	1	1	1	1	1	1	1	d	d	d	d	d	d	d	d	d	d	d	d	a	a	a	a			
χ^{18}	1	1	1	1	1	1	1	1	1	1	a	a	a	a	a	a	a	a	a	a	a	a	a	d	d	d			
χ^{19}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	3	-1	-1	3	-1	-1	3	-1	-1	-1	3	-1	-1		
χ^{20}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	3	-1	-1	3	-1	-1	3	-1	-1	-1	3	-1	-1		
χ^{21}	3	3	3	3	3	f	f	f	f	c	c	c	c	c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
χ^{22}	3	3	3	3	3	c	c	c	c	f	f	f	f	f	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
χ^{23}	3	3	3	3	3	f	f	f	f	c	c	c	c	c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
χ^{24}	3	3	3	3	3	c	c	c	c	f	f	f	f	f	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
χ^{25}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	f	-d	-d	-d	f	-d	-d	-d	c	-a	-a	-a	-a		
χ^{26}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	c	-a	-a	-a	c	-a	-a	-a	c	-a	-a	f	-d	-d	
χ^{27}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	-h	-h	-h	-h	k	k	k	g	g	g	g	-k	-k		
χ^{28}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	-k	-k	-k	-k	h	h	h	-g	-g	-g	-g	-h	-h		
χ^{29}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	k	k	k	k	g	g	g	-h	-h	-h	-h	h	h		
χ^{30}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	h	h	h	h	-g	-g	-g	-g	-h	-h	h	h			
χ^{31}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	g	g	g	g	-h	-h	-h	-h	k	k	k	g	-g		
χ^{32}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	-g	-g	-g	-g	k	k	k	h	h	h	g	g	g		
χ^{33}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	f	-d	-d	-d	f	-d	-d	-d	c	-a	-a	-a	-a		
χ^{34}	3	-1	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	c	-a	-a	-a	c	-a	-a	-a	f	-d	-d	-d	-d		
χ^{35}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	-h	-h	-h	-h	k	k	k	g	g	g	-k	-k	-k		
χ^{36}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	-k	-k	-k	-k	h	h	h	-g	-g	-g	-h	-h	-h		
χ^{37}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	k	k	k	k	g	g	g	-h	-h	-h	h	h	h		
χ^{38}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	h	h	h	h	-g	-g	-g	-g	-k	-k	-k	k	k		
χ^{39}	3	3	f	f	c	c	0	0	0	0	0	0	0	0	g	g	g	g	-h	-h	-h	-h	k	k	k	g	-g		
χ^{40}	3	3	c	c	f	f	0	0	0	0	0	0	0	0	-g	-g	-g	-g	k	k	k	h	h	h	g	g	g		
χ^{41}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	-h	-d	o	-d	k	-a	j	-a	g	-1	-l	-1	-k	-a	n

χ^{42}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	-k	-a	n	-a	h	-d	-i	-d	-g	-1	-m	-1	-h	-d	o
χ^{43}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	k	-a	j	-a	g	-1	-l	-1	-h	-d	o	-d	h	-d	-i
χ^{44}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	h	-d	-i	-d	-g	-1	-m	-1	-k	-a	n	-a	k	-a	j

Table 2. (Continued)

	f20	c9	f21	f22	f23	c10	f24	f25	f26	c11	i1	i2	c12	i3	i4	b2	b3	f27	f28	f29	f30	f31	f32	f33	f34	f35	f36	f37	f38	
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	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	-1		
χ^3	1	1	1	1	1	1	1	1	d	d	d	a	a	a	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^4	1	1	1	1	1	1	1	1	a	a	a	d	d	d	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^5	1	1	1	1	1	1	1	1	d	d	d	a	a	a	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^6	1	1	1	1	1	1	1	1	a	a	a	d	d	d	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^7	a	a	a	a	a	a	a	a	1	d	a	1	d	a	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^8	d	d	d	d	d	d	d	d	1	a	d	1	a	d	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^9	a	a	a	a	a	a	a	a	1	d	a	1	d	a	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{10}	d	d	d	d	d	d	d	d	1	a	d	1	a	d	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{11}	a	a	a	a	a	a	a	a	a	d	a	1	a	1	d	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^{12}	d	d	d	d	d	d	d	d	d	a	d	1	d	1	a	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^{13}	a	a	a	a	a	a	a	a	a	d	a	1	a	1	d	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{14}	d	d	d	d	d	d	d	d	d	a	d	1	d	1	a	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{15}	a	a	a	a	a	a	a	a	a	a	1	d	d	a	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^{16}	d	d	d	d	d	d	d	d	d	1	a	a	d	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
χ^{17}	a	a	a	a	a	a	a	a	a	1	d	d	a	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{18}	d	d	d	d	d	d	d	d	d	1	a	a	d	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
χ^{19}	-1	3	-1	-1	-1	3	-1	-1	-1	0	0	0	0	0	0	0	-3	1	-3	1	-3	1	1	-3	1	1	1	1	1	
χ^{20}	-1	3	-1	-1	-1	3	-1	-1	-1	0	0	0	0	0	0	0	0	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1	
χ^{21}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	-3	-3	-3	-3	-f	-f	-f	-c	-c	-c	-c		
χ^{22}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	-3	-3	-3	-3	-c	-c	-c	-c	-f	-f	-f		
χ^{23}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	3	3	3	3	3	f	f	f	c	c	c	c		
χ^{24}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	3	3	3	3	c	c	c	f	f	f	f		
χ^{25}	-a	c	-a	-a	c	-a	-a	-a	0	0	0	0	0	0	0	-3	1	-3	1	-3	1	1	1	-3	1	1	1	1	1	
χ^{26}	-d	f	-d	-d	f	-d	-d	-d	0	0	0	0	0	0	0	-3	1	-3	1	-3	1	1	1	-3	1	1	1	1	1	
χ^{27}	-k	-g	-g	-g	h	h	h	h	0	0	0	0	0	0	0	3	3	f	f	c	c	0	0	0	0	0	0	0	0	
χ^{28}	-h	g	g	g	g	k	k	k	k	0	0	0	0	0	0	0	3	3	c	c	f	f	0	0	0	0	0	0	0	0

χ^{29}	h	-k	-k	-k	-k	-g	-g	-g	0	0	0	0	0	0	0	3	3	f	f	c	c	0	0	0	0	0	0	0	
χ^{30}	k	-h	-h	-h	-h	g	g	g	0	0	0	0	0	0	0	3	3	c	c	f	f	0	0	0	0	0	0	0	
χ^{31}	-g	h	h	h	h	-k	-k	-k	0	0	0	0	0	0	0	3	3	f	f	c	c	0	0	0	0	0	0	0	
χ^{32}	g	k	k	k	k	-h	-h	-h	0	0	0	0	0	0	0	3	3	c	c	f	f	0	0	0	0	0	0	0	
χ^{33}	-a	c	-a	-a	-a	c	-a	-a	0	0	0	0	0	0	0	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1		
χ^{34}	-d	f	-d	-d	-d	f	-d	-d	0	0	0	0	0	0	0	3	-1	3	-1	3	-1	-1	-1	3	-1	-1	-1		
χ^{35}	-k	-g	-g	-g	-g	h	h	h	h	0	0	0	0	0	0	-3	-3	-f	-f	-c	-c	0	0	0	0	0	0	0	
χ^{36}	-h	g	g	g	g	k	k	k	k	0	0	0	0	0	0	-3	-3	-c	-c	-f	-f	0	0	0	0	0	0	0	
χ^{37}	h	-k	-k	-k	-k	-g	-g	-g	0	0	0	0	0	0	0	-3	-3	-f	-f	-c	-c	0	0	0	0	0	0	0	
χ^{38}	k	-h	-h	-h	-h	g	g	g	g	0	0	0	0	0	0	-3	-3	-c	-c	-f	-f	0	0	0	0	0	0	0	
χ^{39}	-g	h	h	h	h	-k	-k	-k	0	0	0	0	0	0	0	-3	-3	-f	-f	-c	-c	0	0	0	0	0	0	0	
χ^{40}	g	k	k	k	k	-h	-h	-h	0	0	0	0	0	0	0	-3	-3	-c	-c	-f	-f	0	0	0	0	0	0	0	
χ^{41}	-a	-g	-1	-m	-1	h	-d	-i	-d	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-2	-b	-e	0	-2	-e	-b
χ^{42}	-d	g	-1	-l	-1	k	-a	j	-a	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-2	-e	-b	0	-2	-b	-e
χ^{43}	-d	-k	-a	n	-a	-g	-1	-m	-1	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-2	-b	-e	0	-2	-e	-b
χ^{44}	-a	-h	-d	o	-d	g	-1	-l	-1	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-2	-e	-b	0	-2	-b	-e

Table 2. (Continued)

	f39	f40	f41	f42	f43	f44	f45	f46	f47	f48	f49	f50	f51	f52	f53	f54	f55	f56	f57	f58	f59	f60	f61	f62	f63	r1	r2	f64	r3	r4
χ^1	-g	1	l	1	h	d	-o	d	-k	a	-j	a	g	1	m	1	-h	d	i	d	k	a	-n	a	0	0	0	0	0	
χ^2	g	1	m	1	k	a	-n	a	-h	d	i	d	-g	1	l	1	-k	a	-j	a	h	d	-o	d	0	0	0	0	0	
χ^3	-h	-d	o	-d	k	-a	j	-a	g	-1	-l	-1	-k	-a	n	-a	-g	-1	-m	-1	h	-d	-i	-d	0	0	0	0	0	
χ^4	-k	-a	n	-a	h	-d	-i	-d	-g	-1	-m	-1	-h	-d	o	-d	g	-1	-l	-1	k	-a	j	-a	0	0	0	0	0	
χ^5	k	-a	j	-a	g	-1	-l	-1	-h	-d	o	-d	h	-d	-i	-d	-k	-a	n	-a	-g	-1	-m	-1	0	0	0	0	0	
χ^6	h	-d	-i	-d	-g	-1	-m	-1	-k	-a	n	-a	k	-a	j	-a	-h	-d	o	-d	g	-1	-l	-1	0	0	0	0	0	
χ^7	g	-1	-l	-1	-h	-d	o	-d	k	-a	j	-a	-g	-1	-m	-1	h	-d	-i	-d	-k	-a	n	-a	0	0	0	0	0	
χ^8	-g	-1	-m	-1	-k	-a	n	-a	h	-d	-i	-d	g	-1	-l	-1	k	-a	j	-a	-h	-d	o	-d	0	0	0	0	0	
χ^9	0	-2	-b	-e	0	-2	-b	-e	0	-2	-b	-e	0	-2	-e	-b	0	-2	-e	-b	0	-2	-e	-b	0	0	0	0	0	
χ^{10}	0	-2	-e	-b	0	-2	-e	-b	0	-2	-e	-b	0	-2	-b	-e	0	-2	-b	-e	0	-2	-b	-e	0	0	0	0	0	
χ^{11}	0	2	b	e	0	2	b	e	0	2	b	e	0	2	e	b	0	2	e	b	0	2	e	b	0	0	0	0	0	
χ^{12}	0	2	e	b	0	2	e	b	0	2	e	b	0	2	b	e	0	2	b	e	0	2	b	e	0	0	0	0	0	
χ^{13}	0	-e	-2	-b	0	-e	-2	-b	0	-e	-2	-b	0	-b	-2	-e	0	-b	-2	-e	0	-b	-2	-e	0	0	0	0	0	
χ^{14}	0	-b	-2	-e	0	-b	-2	-e	0	-b	-2	-e	0	-e	-2	-b	0	-e	-2	-b	0	-e	-2	-b	0	0	0	0	0	

Table 2. (Continued)

	a1	b1	c1	f1	c2	f2	c3	f3	c4	f6	f7	f8	c5	f9	f10	f11	c6	f12	f13	f14	c7	f15	f16	f17	c8	f18	f19		
χ^{45}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	g	-1	-l	-1	-h	-d	o	-d	k	-a	j	-a	-g	-1	-m
χ^{46}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	-g	-1	-m	-1	-k	-a	n	-a	h	-d	-i	-d	g	-1	-l
χ^{47}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	-h	-d	o	-d	k	-a	j	-a	g	-1	-l	-1	-k	-a	n
χ^{48}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	-k	-a	n	-a	h	-d	-i	-d	-g	-1	-m	-1	-h	-d	o
χ^{49}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	k	-a	j	-a	g	-1	-l	-1	-h	-d	o	-d	h	-d	i
χ^{50}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	h	-d	-i	-d	-g	-1	-m	-1	-k	-a	n	-a	k	-a	j
χ^{51}	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b	g	-1	-l	-1	-h	-d	o	-d	k	-a	j	-a	-g	-1	-m
χ^{52}	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e	-g	-1	-m	-1	-k	-a	n	-a	h	-d	-i	-d	g	-1	-l
χ^{53}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	2	b	e	0	2	b	e	0	2	e				
χ^{54}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	2	e	b	0	2	e	b	0	2	b				
χ^{55}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	2	b	e	0	2	b	e	0	2	b				
χ^{56}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	2	e	b	0	2	e	b	0	2	b				
χ^{57}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	e	2	b	0	e	2	b	0	e	2	b	0	b	2
χ^{58}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	b	2	e	0	b	2	e	0	b	2	e	0	e	2
χ^{59}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	e	2	b	0	e	2	b	0	e	2	b	0	b	2
χ^{60}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	b	2	e	0	b	2	e	0	b	2	e	0	e	2
χ^{61}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	b	e	2	0	b	e	2	0	b	e	2	0	e	b
χ^{62}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	e	b	2	0	e	b	2	0	e	b	2	0	b	e
χ^{63}	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a	0	b	e	2	0	b	e	2	0	b	e	2	0	e	b
χ^{64}	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d	0	e	b	2	0	e	b	2	0	e	b	2	0	b	e
χ^{65}	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e	-h	-d	-d	o	k	-a	-a	j	g	-1	-1	-l	-k	-a	-a
χ^{66}	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b	-k	-a	-a	n	h	-d	-d	-i	-g	-1	-1	-m	-h	-d	-d
χ^{67}	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e	-h	-d	-d	o	k	-a	-a	j	g	-1	-1	-l	-k	-a	-a
χ^{68}	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b	-k	-a	-a	n	h	-d	-d	-i	-g	-1	-1	-m	-h	-d	-d
χ^{69}	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e	g	-1	-1	-l	-h	-d	-d	-o	k	-a	-a	j	-g	-1	-1
χ^{70}	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b	-g	-1	-1	-m	-k	-a	-a	n	h	-d	-d	-i	g	-1	-1
χ^{71}	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e	g	-1	-1	-l	-h	-d	-d	-o	k	-a	-a	j	-g	-1	-1
χ^{72}	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b	-g	-1	-1	-m	-k	-a	-a	n	h	-d	-d	-i	g	-1	-1

χ^{73} 3 -1 f -d c -a 0 e 2 b 0 b 2 e k -a -a j g -1 -1 -l -h -d -d o h -d -d
 χ^{74} 3 -1 c -a f -d 0 b 2 e 0 e 2 b h -d -d -i -g -1 -1 -m -k -a -a n k -a -a
 χ^{75} 3 -1 f -d c -a 0 e 2 b 0 b 2 e k -a -a j g -1 -1 -l -h -d -d o h -d -d
 χ^{76} 3 -1 c -a f -d 0 b 2 e 0 e 2 b h -d -d -i -g -1 -1 -m -k -a -a n k -a -a
 χ^{77} 3 -1 f -d c -a 0 b e 2 0 e b 2 -h o -d -d k j -a -a g -l -1 -1 -k n -a
 χ^{78} 3 -1 c -a f -d 0 e b 2 0 b e 2 -k n -a -a h -i -d -d -g -m -1 -1 -h o -d
 χ^{79} 3 -1 f -d c -a 0 b e 2 0 e b 2 -h o -d -d k j -a -a g -l -1 -1 -k n -a
 χ^{80} 3 -1 c -a f -d 0 e b 2 0 b e 2 -k n -a -a h -i -d -d -g -m -1 -1 -h o -d
 χ^{81} 3 -1 f -d c -a 0 b e 2 0 e b 2 g -l -1 -1 -h o -d -d k j -a -a -g -m -1
 χ^{82} 3 -1 c -a f -d 0 e b 2 0 b e 2 -g -m -1 -1 -k n -a -a h -i -d -d g -l -1
 χ^{83} 3 -1 f -d c -a 0 b e 2 0 e b 2 g -l -1 -1 -h o -d -d k j -a -a -g -m -1
 χ^{84} 3 -1 c -a f -d 0 e b 2 0 b e 2 -g -m -1 -1 -k n -a -a h -i -d -d g -l -1
 χ^{85} 3 -1 f -d c -a 0 b e 2 0 e b 2 k j -a -a g -l -1 -1 -h o -d -d h -i -d
 χ^{86} 3 -1 c -a f -d 0 e b 2 0 b e 2 h -i -d -d -g -m -1 -1 -k n -a -a k j -a
 χ^{87} 3 -1 f -d c -a 0 b e 2 0 e b 2 k j -a -a g -l -1 -1 -h o -d -d h -i -d
 χ^{88} 3 -1 c -a f -d 0 e b 2 0 b e 2 h -i -d -d -g -m -1 -1 -k n -a -a k j -a

Table 2. (Continued)

	f20	c9	f21	f22	f23	c10	f24	f25	f26	c11	i1	i2	c12	i3	i4	b2	b3	f27	f28	f29	f30	f31	f32	f33	f34	f35	f36	f37	f38
χ^{45}	-1	h	-d	-i	-d	-k	-a	n	-a	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-2	-b	-e	0	-2	-e	-b
χ^{46}	-1	k	-a	j	-a	-h	-d	o	-d	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-2	-e	-b	0	-2	-b	-e
χ^{47}	-a	-g	-1	-m	-1	h	-d	-i	-d	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b
χ^{48}	-d	g	-1	-l	-1	k	-a	j	-a	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e
χ^{49}	-d	-k	-a	n	-a	-g	-1	-m	-1	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b
χ^{50}	-a	-h	-d	o	-d	g	-1	-l	-1	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e
χ^{51}	-1	h	-d	-i	-d	-k	-a	n	-a	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	2	b	e	0	2	e	b
χ^{52}	-1	k	-a	j	-a	-h	-d	o	-d	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	2	e	b	0	2	b	e
χ^{53}	b	0	2	e	b	0	2	e	b	0	0	0	0	0	0	-3	1	-3	1	-3	1	-f	d	d	-c	a	a	a	a
χ^{54}	e	0	2	b	e	0	2	b	e	0	0	0	0	0	0	-3	1	-3	1	-3	1	-c	a	a	a	-f	d	d	d
χ^{55}	b	0	2	e	b	0	2	e	b	0	0	0	0	0	0	3	-1	3	-1	3	-1	f	-d	-d	c	-a	-a	-a	-a
χ^{56}	e	0	2	b	e	0	2	b	e	0	0	0	0	0	0	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d
χ^{57}	e	0	b	2	e	0	b	2	e	0	0	0	0	0	0	-3	1	-3	1	-3	1	-f	d	d	d	-c	a	a	a
χ^{58}	b	0	e	2	b	0	e	2	b	0	0	0	0	0	0	-3	1	-3	1	-3	1	-c	a	a	a	-f	d	d	d

χ^{59}	e	0	b	2	e	0	b	2	e	0	0	0	0	0	0	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a
χ^{60}	b	0	e	2	b	0	e	2	b	0	0	0	0	0	0	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d
χ^{61}	2	0	e	b	2	0	e	b	2	0	0	0	0	0	0	-3	1	-3	1	-3	1	-f	d	d	d	-c	a	a	a
χ^{62}	2	0	b	e	2	0	b	e	2	0	0	0	0	0	0	-3	1	-3	1	-3	1	-c	a	a	a	-f	d	d	d
χ^{63}	2	0	e	b	2	0	e	b	2	0	0	0	0	0	0	3	-1	3	-1	3	-1	f	-d	-d	-d	c	-a	-a	-a
χ^{64}	2	0	b	e	2	0	b	e	2	0	0	0	0	0	0	3	-1	3	-1	3	-1	c	-a	-a	-a	f	-d	-d	-d
χ^{65}	n	-g	-1	-1	-m	h	-d	-d	-i	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-e	-2	-b	0	-b	-2	-e
χ^{66}	o	g	-1	-1	-l	k	-a	-a	j	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-b	-2	-e	0	-e	-2	-b
χ^{67}	n	-g	-1	-1	-m	h	-d	-d	-i	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e
χ^{68}	o	g	-1	-1	-l	k	-a	-a	j	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b
χ^{69}	-m	h	-d	-d	-i	-k	-a	-a	n	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-e	-2	-b	0	-b	-2	-e
χ^{70}	-l	k	-a	-a	j	-h	-d	-d	o	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-b	-2	-e	0	-e	-2	-b
χ^{71}	-m	h	-d	-d	-i	-k	-a	-a	n	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e
χ^{72}	-l	k	-a	-a	j	-h	-d	-d	o	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b
χ^{73}	-i	-k	-a	-a	n	-g	-1	-1	-m	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-e	-2	-b	0	-b	-2	-e
χ^{74}	j	-h	-d	-d	o	g	-1	-1	-l	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-b	-2	-e	0	-e	-2	-b
χ^{75}	-i	-k	-a	-a	n	-g	-1	-1	-m	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	e	2	b	0	b	2	e
χ^{76}	j	-h	-d	-d	o	g	-1	-1	-l	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	b	2	e	0	e	2	b
χ^{77}	-a	-g	-m	-1	-1	h	-i	-d	-d	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-b	-e	-2	0	-e	-b	-2
χ^{78}	-d	g	-l	-1	-1	k	j	-a	-a	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-e	-b	-2	0	-b	-e	-2
χ^{79}	-a	-g	-m	-1	-1	h	-i	-d	-d	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	b	e	2	0	e	b	2
χ^{80}	-d	g	-l	-1	-1	k	j	-a	-a	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	e	b	2	0	b	e	2
χ^{81}	-1	h	-i	-d	-d	-k	n	-a	-a	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-b	-e	-2	0	-e	-b	-2
χ^{82}	-1	k	j	-a	-a	-h	o	-d	-d	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-e	-b	-2	0	-b	-e	-2
χ^{83}	-1	h	-i	-d	-d	-k	n	-a	-a	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	b	e	2	0	e	b	2
χ^{84}	-1	k	j	-a	-a	-h	o	-d	-d	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	e	b	2	0	b	e	2
χ^{85}	-d	-k	n	-a	-a	-g	-m	-1	-1	0	0	0	0	0	0	-3	1	-f	d	-c	a	0	-b	-e	-2	0	-e	-b	-2
χ^{86}	-a	-h	o	-d	-d	g	-l	-1	-1	0	0	0	0	0	0	-3	1	-c	a	-f	d	0	-e	-b	-2	0	-b	-e	-2
χ^{87}	-d	-k	n	-a	-a	-g	-m	-1	-1	0	0	0	0	0	0	3	-1	f	-d	c	-a	0	b	e	2	0	e	b	2
χ^{88}	-a	-h	o	-d	-d	g	-l	-1	-1	0	0	0	0	0	0	3	-1	c	-a	f	-d	0	e	b	2	0	b	e	2

Table 2. (Continued)

f39 f40 f41 f42 f43 f44 f45 f46 f47 f48 f49 f50 f51 f52 f53 f54 f55 f56 f57 f58 f59 f60 f61 f62 f63 r1 r2 f64 r3 r4

χ^{45}	-g	1	l	1	h	d	-o	d	-k	a	-j	a	g	1	m	1	-h	d	i	d	k	a	-n	a	0	0	0	0	0	0
χ^{46}	g	1	m	1	k	a	-n	a	-h	d	i	d	-g	1	l	1	-k	a	-j	a	h	d	-o	d	0	0	0	0	0	0
χ^{47}	-h	-d	o	-d	k	-a	j	-a	g	-1	-l	-1	-k	-a	n	-a	-g	-1	-m	-1	h	-d	-i	-d	0	0	0	0	0	0
χ^{48}	-k	-a	n	-a	h	-d	-i	-d	-g	-1	-m	-1	-h	-d	o	-d	g	-1	-l	-1	k	-a	j	-a	0	0	0	0	0	0
χ^{49}	k	-a	j	-a	g	-1	-l	-1	-h	-d	o	-d	h	-d	-i	-d	-k	-a	n	-a	-g	-1	-m	-1	0	0	0	0	0	0
χ^{50}	h	-d	-i	-d	-g	-1	-m	-1	-k	-a	n	-a	k	-a	j	-a	-h	-d	o	-d	g	-1	-l	-1	0	0	0	0	0	0
χ^{51}	g	-1	-l	-1	-h	-d	o	-d	k	-a	j	-a	-g	-1	-m	-1	h	-d	-i	-d	-k	-a	n	-a	0	0	0	0	0	0
χ^{52}	-g	-1	-m	-1	-k	-a	n	-a	h	-d	-i	-d	g	-1	-l	-1	k	-a	j	-a	-h	-d	o	-d	0	0	0	0	0	0
χ^{53}	0	-2	-b	-e	0	-2	-b	-e	0	-2	-b	-e	0	-2	-e	-b	0	-2	-e	-b	0	-2	-e	-b	0	0	0	0	0	0
χ^{54}	0	-2	-e	-b	0	-2	-e	-b	0	-2	-e	-b	0	-2	-b	-e	0	-2	-b	-e	0	-2	-b	-e	0	0	0	0	0	0
χ^{55}	0	2	b	e	0	2	b	e	0	2	b	e	0	2	e	b	0	2	e	b	0	2	e	b	0	0	0	0	0	0
χ^{56}	0	2	e	b	0	2	e	b	0	2	e	b	0	2	b	e	0	2	b	e	0	2	b	e	0	0	0	0	0	0
χ^{57}	0	-e	-2	-b	0	-e	-2	-b	0	-e	-2	-b	0	-b	-2	-e	0	-b	-2	-e	0	-b	-2	-e	0	0	0	0	0	0
χ^{58}	0	-b	-2	-e	0	-b	-2	-e	0	-b	-2	-e	0	-e	-2	-b	0	-e	-2	-b	0	-e	-2	-b	0	0	0	0	0	0
χ^{59}	0	e	2	b	0	e	2	b	0	e	2	b	0	b	2	e	0	b	2	e	0	b	2	e	0	0	0	0	0	0
χ^{60}	0	b	2	e	0	b	2	e	0	b	2	e	0	e	2	b	0	e	2	b	0	e	2	b	0	0	0	0	0	0
χ^{61}	0	-b	-e	-2	0	-b	-e	-2	0	-b	-e	-2	0	-e	-b	-2	0	-e	-b	-2	0	-e	-b	-2	0	0	0	0	0	0
χ^{62}	0	-e	-b	-2	0	-e	-b	-2	0	-e	-b	-2	0	-b	-e	-2	0	-b	-e	-2	0	-b	-e	-2	0	0	0	0	0	0
χ^{63}	0	b	e	2	0	b	e	2	0	b	e	2	0	e	b	2	0	e	b	2	0	e	b	2	0	0	0	0	0	0
χ^{64}	0	e	b	2	0	e	b	2	0	e	b	2	0	b	e	2	0	b	e	2	0	b	e	2	0	0	0	0	0	0
χ^{65}	h	d	d	-o	-k	a	a	-j	-g	1	1	l	k	a	a	-n	g	1	1	m	-h	d	d	i	0	0	0	0	0	0
χ^{66}	k	a	a	-n	-h	d	d	i	g	1	1	m	h	d	d	-o	-g	1	1	l	-k	a	a	-j	0	0	0	0	0	0
χ^{67}	-h	-d	-d	o	k	-a	-a	j	g	-1	-1	-l	-k	-a	-a	n	-g	-1	-1	-m	h	-d	-d	-i	0	0	0	0	0	0
χ^{68}	-k	-a	-a	n	h	-d	-d	-i	-g	-1	-1	-m	-h	-d	-d	o	g	-1	-1	-l	k	-a	-a	j	0	0	0	0	0	0
χ^{69}	-g	1	1	l	h	d	d	-o	-k	a	a	-j	g	1	1	m	-h	d	d	i	k	a	a	-n	0	0	0	0	0	0
χ^{70}	g	1	1	m	k	a	a	-n	-h	d	d	i	-g	1	1	l	-k	a	a	-j	h	d	d	-o	0	0	0	0	0	0
χ^{71}	g	-1	-1	-l	-h	-d	-d	o	k	-a	-a	j	-g	-1	-1	-m	h	-d	-d	-i	-k	-a	-a	n	0	0	0	0	0	0
χ^{72}	-g	-1	-1	-m	-k	-a	-a	n	h	-d	-d	-i	g	-1	-1	-l	k	-a	-a	j	-h	-d	-d	o	0	0	0	0	0	0
χ^{73}	-k	a	a	-j	-g	1	1	l	h	d	d	-o	-h	d	d	i	k	a	a	-n	g	1	1	m	0	0	0	0	0	0
χ^{74}	-h	d	d	i	g	1	1	m	k	a	a	-n	-k	a	a	-j	h	d	d	-o	-g	1	1	l	0	0	0	0	0	0
χ^{75}	k	-a	-a	j	g	-1	-1	-l	-h	-d	-d	o	h	-d	-d	-i	-k	-a	-a	n	-g	-1	-1	-m	0	0	0	0	0	0
χ^{76}	h	-d	-d	-i	-g	-1	-1	-m	-k	-a	-a	n	k	-a	-a	j	-h	-d	-d	o	g	-1	-1	-l	0	0	0	0	0	0

χ^{77}	h	-o	d	d	-k	-j	a	a	-g	l	1	1	k	-n	a	a	g	m	1	1	-h	i	d	d	0	0	0	0	0	0	0
χ^{78}	k	-n	a	a	-h	i	d	d	g	m	1	1	h	-o	d	d	-g	l	1	1	-k	-j	a	a	0	0	0	0	0	0	0
χ^{79}	-h	o	-d	-d	k	j	-a	-a	g	-l	-1	-1	-k	n	-a	-a	-g	-m	-1	-1	h	-i	-d	-d	0	0	0	0	0	0	0
χ^{80}	-k	n	-a	-a	h	-i	-d	-d	-g	-m	-1	-1	-h	o	-d	-d	g	-l	-1	-1	k	j	-a	-a	0	0	0	0	0	0	0
χ^{81}	-g	l	1	1	h	-o	d	d	-k	-j	a	a	g	m	1	1	-h	i	d	d	k	-n	a	a	0	0	0	0	0	0	0
χ^{82}	g	m	1	1	k	-n	a	a	-h	i	d	d	-g	l	1	1	-k	-j	a	a	h	-o	d	d	0	0	0	0	0	0	0
χ^{83}	g	-l	-1	-1	-h	o	-d	-d	k	j	-a	-a	-g	-m	-1	-1	h	-i	-d	-d	-k	n	-a	-a	0	0	0	0	0	0	0
χ^{84}	-g	-m	-1	-1	-k	n	-a	-a	h	-i	-d	-d	g	-l	-1	-1	k	j	-a	-a	-h	o	-d	-d	0	0	0	0	0	0	0
χ^{85}	-k	-j	a	a	-g	l	1	1	h	-o	d	d	-h	i	d	d	k	-n	a	a	g	m	1	1	0	0	0	0	0	0	0
χ^{86}	-h	i	d	d	g	m	1	1	k	-n	a	a	-k	-j	a	a	h	-o	d	d	-g	l	1	1	0	0	0	0	0	0	0
χ^{87}	k	j	-a	-a	g	-l	-1	-1	-h	o	-d	-d	h	-i	-d	-d	-k	n	-a	-a	-g	-m	-1	-1	0	0	0	0	0	0	0
χ^{88}	h	-i	-d	-d	-g	-m	-1	-1	-k	n	-a	-a	k	j	-a	-a	-h	o	-d	-d	g	-l	-1	-1	0	0	0	0	0	0	0

Table caption

$$\alpha = \frac{1}{2} + \frac{\sqrt{3}}{2} \hat{i}, \hat{i} = \sqrt{-1},$$

$$a = \alpha, b = 2\alpha, c = 3\alpha, d = \alpha^2, e = 2\alpha^2, f = 3\alpha^2, g = \alpha - \alpha^2,$$

$$h = 2\alpha + \alpha^2, i = 2\alpha - \alpha^2, j = \alpha - 2\alpha^2, k = \alpha + 2\alpha^2, l = 3\alpha + \alpha^2,$$

$$m = \alpha + 3\alpha^2, n = 3\alpha + 2\alpha^2, o = 2\alpha + 3\alpha^2$$

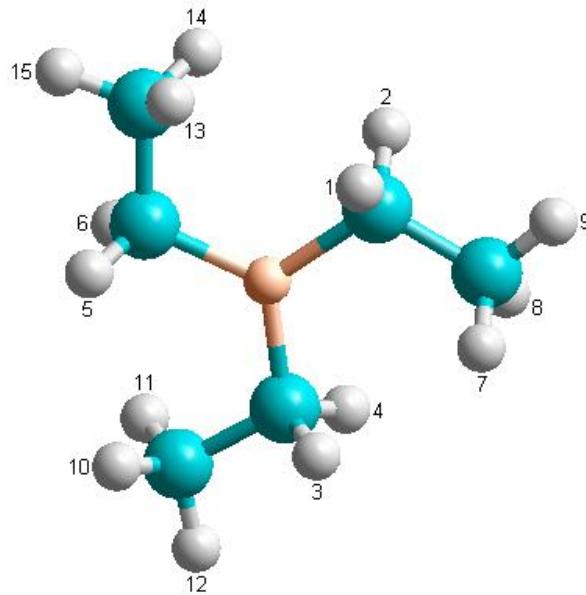


Fig. 1. The structures of triethylborane with C_{3h} symmetry

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REFERENCES

1. S. L. Altmann, (1977). *Induced Representation in Crystal & Molecules*, Academic Press, London.
2. A. R. Ashrafi, M. Hamadanian. (2003). *Croat. Chem. Acta*, 76, 299.
3. A. R. Ashrafi, M. Hamadanian,(2004). *J. Appl. Math. & Computing*, 14, 289.
4. A. R. Ashrafi, M. Hamadanian (2005). *J. Iran. Chem. Soc.*, 2, 135.
5. P. R. Bunker.(1964). *Mol. Phys.*, 8, 81
6. M. R. Darafsheh, Y. Farjami and A. R. Ashrafi. (2005). *Bull. Chem. Soc. Jpn.*, 78, 996.
7. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh. (2005). *Int. J. Quantum Chem.*, 105, 485.
8. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh. (2005). *Acta Chim. Slov.*, 52, 282.
9. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh.(2006). *Chem. Phys. Lett.*, 421, 566.
10. M. F. Erben, R. Boese, C O. Della Ve'dova, H. Oberhammer, and H. Willner.(2006). *J. Org. Chem.*, 71, 616.
11. G. S. Ezra.(1982). *Symmetry Properties of Molecules*, Lecture Notes in Chemistry 28, Springer.
12. M. Hamadanian, A. R. Ashrafi, (2003). *Croat. Chem. Acta*, 76.
13. Hyperchem, Version 8.0.7 (2009) (<http://www.hyper.com/>)
14. The GAP Group.(2008). GAP-Groups, Algorithms, and Programming, Version 4.4.12 (<http://www.gap-system.org/>).
15. I. M. Isaacs. (1978). *Character Theory of Finite Groups*, Academic Press.
16. J. S. Lomont, (1959). *Applications of Finite Groups*, Academic Press, New York
17. G. James, M. Liebeck, (1993). *Representations and Characters of Groups*, Cambridge University Press.
18. H. C. Longuet-Higgins,(1963). *Mol. Phys.* 6, 445.
19. J. Maruani, J. Serre (eds),(1983). *Symmetries and Properties of Non-rigid Molecules*, Elsevier, Amsterdam.
20. G. Moghani, A. Ashrafi, M. Hamadanian, (2005). *J. Zhejiang Univ. Sci.*, 6, 222.
21. Y. G. Smeyers, (1991). *Adv. Quantum Chem.*, 24, 1.
22. Y. G. Smeyers, (1995).Structure and dynamics of non-rigid molecular systems, Kluwar Adademic, Dordrecht, 121-151
23. Y. G. Smeyers, M. L. Senent, V. Botella, D. C. Moule,(1993). *J. Chem. Phys.* 98, 2754.
24. Y. G. Smeyers, M. Villa,(2000). *J. Math. Chem.* 28(4), 377.
25. Y. G. Smeyers, M. Villa, M. L. Senent, (1998). *J. Mol. Spectrosc.*, 232.
26. A. Van der Avoird,(1993). *J. Chem. Phys.*,98, 5327.
27. A. Vivier-Bunge, V. H. Uct, Y. G. Smeyers. (1998). *J. Chem. Phys.*, 109, 2279.