Journal of Mathematical Chemistry 20 (1996) 331–349

Extended molecular symmetry groups

Pavel Soldán

J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejškova 3, 182 23 Prague 8, Czech Republic, and
Max-Planck-Institut für Astrophysik, Karl-Schwarzwild-Strasse 1, Postfach 1523, D-85740 Garching, Germany
E-mail: soldan@jh-inst.cas.cz

Received 9 February 1996; revised 16 October 1996

The group theoretical analysis of Longuet–Higgins molecular symmetry groups $G(m,n)$ and $GB(m)$ and their torsional extensions $G^q(m,n)$ and $GB^2(m)$ of molecules consisting of two coaxially rotated parts is presented. The structure of the groups is described in terms of direct and semi-direct products. The groups $G^q(m,n)$ and $GB^2(m)$ are shown to be group extensions of the groups $G(m,n)$ and $GB(m)$, respectively. All irreducible representations of the groups $G(m,n)$, $GB(m)$, and $GB^2(m)$ are derived using standard techniques of the extension or induction. A restriction method is proposed for derivation of irreducible representations of the group $G^q(m,n)$. The class structure of the groups is determined and the character tables are given in the most general case.

1. Introduction

During the past 32 years many papers have been written on the symmetry analysis of molecules consisting of two coaxial rotors using extended permutation-inversion groups [1–22] (see also Table 1). With the exception of ref. [6] these papers have dealt with individual molecules not considering common properties of certain classes of molecules. Nevertheless, in the time of computerization such general consideration of the problem is desirable as it allows to leave the computers most of the tedious work.

Recently [23,24] the author has proposed general symmetry analysis of such systems. This symmetry analysis was concerned with classifications of torsional and rotational states and with the corresponding selection rules of a general molecule consisting of two coaxially rotating parts. It used (but did not present) results of extensive group theoretical analysis of the corresponding permutation-inversion and extended permutation-inversion groups.

The work presented here follows two aims: *to show the relations between the permutation-inversion groups and their extensions and to derive complete sets of ordinary irreducible representations of the above-mentioned symmetry groups.* Up to this time, to author's knowledge, group theoretical analysis of these groups has not

Table 1
Review of fundamental original papers where the extended molecular symmetry groups were used for symmetry analysis.

Authors	Year	Molecule	Original notation	Present notation
Hougen, Bunker [1–5]	1964–1967	2-butine	$G_{36}, G_{36}^{\dagger}$	$GB(3), GB^2(3)$
Bunker and Papoušek [6]	1969	linear molecules	–	–
Papoušek et al. [7]	1971	ethylene	G_{16}, G_{16}^{+}	$GB(2), GB^2(2)$
		nitromethane	G_{12}, G_{12}^{+}	$G(3,2), G^2(3,2)$
Merer and Watson [8]	1973	ethylene	$G_{16}, G_{16}^{(2)}$	$GB(2), GB^2(2)$
Dellepiane, Gussoni and Hougen [9]	1973	XY_2-C≡C-XY_2	$G_4, G_4^{\dagger}$	$GB(1), GB^2(1)$
Yamada, Nakagawa and Kuchitsu [10]	1974	X_2Y_2	D_{2h}^{*}	$GB(1), GB^2(1)$
Hougen [11]; Henry et al. [14]	1980; 1983	ethane	$G_{36}, G_{36}^{\dagger}$	$GB(3), GB^2(3)$
Hougen [12]; Ohashi and Hougen [16]	1981; 1985	hydrazine	$G_{16}, G_{16}^{(2)}$	$GB(2), GB^2(2)$
Hougen and DeKoven [13]	1983	CF_3NO	$C_{3v}, C_{3m,v}$	$G(3,1), G^m(3,1)$
Hougen and Ohashi [15]	1985	HF dimer	$G_4, G_4^{\dagger}$	$GB(1), GB^2(1)$
Hougen [17]	1985	water dimer	$G_{16}, G_{16}^{(2)}$	$GB(2), GB^2(2)$
Ohashi and Hougen [18]	1987	methylamine	G_{12}, G_{12}^{m}	$G(3,2), G^m(3,2)$
Hougen, Meerts and Ozier [19]	1991	H_3C-SiH_3	G_{18}, G_{18}^{m}	$G(3,3), G^m(3,3)$
Hougen, Kleiner and Godefroid [20]	1994	acetaldehyd	C_{3v}, C_{3v}^{m}	$G(3,1), G^m(3,1)$
Soldán [21]	1994	H_5^+	$G_{16}, G_{16}(EM)$	$GB(2), GB^2(2)$
Soldán, Špirko and Kraemer [22,23]	1996	$H_3^+D_2$	G_8, G_8^3	$G(2,2), G^3(2,2)$

been presented on such a general level. Any permutation-inversion group (or its extension) of this type can be treated as a special individual case of the groups presented below and the determination of its irreducible representations is reduced to substitution of a few parameters into simple general formulas. This general approach to the symmetry analysis is similar to the general approach of Balasubramanian to the nuclear spin statistics of weakly bounded complexes [25].

This paper is organised as follows: in section 2 the notation is introduced, and the groups are defined by means of generators and relations using conventions introduced in ref. [23]. In section 3 structures of the groups are described by means of *direct and semi-direct products*. In the case of the Longuet–Higgins molecular symmetry groups, i.e. the permutation-inversion groups [26], the Woodman approach is used [27]. (Thus, the "finest" group structures used here are semi-direct and direct groups products, although some authors [25,28,29] have also used a group wreath product structure [30] for analysis of symmetry groups of complexes which contain identical rotors.) Mutual relations between groups are expressed in terms of *group extensions* [31]. The situation here is similar to the case of electronic double groups, which are expressed as central extensions of the corresponding point groups [32–34]. In the case of identical rotors, extensions are also central. In the case of non-identical rotors, the extensions are not central in general. In section 4 all irreducible representations of these groups are derived using standard techniques of the *extension and induction* [35,36] and one nonstandard method, called here the *restriction*. Section 5 is devoted to class structures and character tables of the groups. In appendix A a short review of the language of group extensions is given. Appendix B is devoted to the restriction method for determination of irreducible representations of certain factor groups.

2. Notation and basic definitions

In this paper, the symbol ":=" will be used for definitions, the commutator and anticommutator of group elements a and b are defined as $[a, b] := aba^{-1}b^{-1}$ and $\{a, b\} := abab$, respectively, and the direct and semi-direct products are denoted by $\otimes$ and $\wedge$, respectively (the latter with the normal subgroup at the first position). By the word "representation" we mean ordinary representations, in general, over the field of complex numbers.

In ref. [23] the presentations of the Longuet–Higgins molecular symmetry groups (permutation-inversion groups [26]) and their torsional extensions [37] are derived for the molecules consisting of two coaxial m-fold and n-fold rotors, and the systematic notation of these groups is also introduced. In the case of *non-identical rotors* the molecular symmetry group is denoted as $G(m, n)$ and its corresponding torsional extension as $G^q(m, n)$, where the parameter q of the extension depends on the fractional representation $\frac{p}{q}$, $\gcd(p, q) = 1$, of a scalar inertia parameter of the internal rotations [13,19,23]. In the case of *identical rotors* ($n = m$) the molecular symmetry group is denoted as $GB(m)$ and its torsional extension as $GB^2(m)$ ($p = 1$ and $q = 2$ in this case). In Table 1 the notation of already used groups of these types is related to the notation proposed in ref. [23] and used here.

The *presentations* of the symmetry groups mentioned above are the following [23]:

DEFINITION 1

The group $G(m, n)$ is generated by elements x, y, and z and relations

$$x^m = y^n = z^2 = [x, y] = \{z, x\} = \{z, y\} = e\,. \tag{1}$$

DEFINITION 2

The group $G^q(m, n)$ is generated by elements X, Y, and Z and relations

$$X^{qm} = Y^{qn} = Z^2 = X^m Y^n = [X, Y] = \{Z, X\} = \{Z, Y\} = E\,. \tag{2}$$

The group $G^q(3,1)$ is known as C^q_{3v} (see e.g. ref. [13]), the group $G^q(3,2)$ is known as G^q_{12} (see e.g. ref. [18]), the group $G^q(3,3)$ is known as G^q_{18} (see e.g. ref. [19]), and the group $G^3(2,2)$ is known as $G^3(8)$ (see e.g. ref. [22]).

DEFINITION 3

The group $GB(m)$ is generated by elements x, y, z, and w and relations

$$x^m = y^m = z^2 = w^2 = [x,y] = \{z,x\} = \{z,y\} = [w,z] = e\,, \tag{3}$$

$$wxw = y\,. \tag{4}$$

DEFINITION 4

The group $GB^2(m)$ is generated by elements X, Y, Z, and W and relations

$$X^{2m} = Y^{2m} = Z^2 = W^2 = X^m Y^m = [X,Y] = \{Z,X\} = \{Z,Y\}$$

$$= [W,Z] = E\,, \tag{5}$$

$$WXW = Y\,. \tag{6}$$

The group $GB^2(1)$ is known as G^2_4 (see e.g. ref. [15]), the group $GB^2(2)$ is the known group G^2_{16} (see e.g. ref. [21]), and the group $GB^2(3)$ is known as G^2_{36} (see e.g. ref. [11]).

The generating elements (in the corresponding order) are called the *canonical generators*. (It is obvious that the canonical generators of $GB(m)$ or $GB^2(m)$ are not algebraically independent, but, as we shall see below, these presentations are very useful.) In the following text we shall suppose that $q \geqslant 2$ and $m \geqslant n$, and the groups defined above are collectively called the *symmetry groups*.

3. Group structure

This section deals with a basic analysis of the symmetry groups. Many theorems presented below are straightforward consequences of presentations of the corresponding groups. Therefore proofs which are obvious or are similar to the ones presented before are omitted. The terminology of group extensions used in this paper is given in Appendix A.

3.1. GROUPS $G(m,n)$ AND $G^q(m,n)$

THEOREM 5

The group $G(m,n)$ possesses the following structure:

$$m = 1\,, \qquad G(1,1) = G(z)\,;$$

$$m = 2 \text{ and } n = 1\,, \quad G(2,1) = G(x) \otimes G(z)\,;$$

$$m \geqslant 3 \text{ and } n = 1\,, \quad G(m,1) = G(x) \wedge G(z)\,;$$

$$m = 2 \text{ and } n = 2\,, \quad G(2,2) = G(x) \otimes G(y) \otimes G(z)\,;$$

$$m \geqslant 3 \text{ and } n \geqslant 2\,, \quad G(m,n) = (G(x) \otimes G(y)) \wedge G(z)\,.$$

Proof

The distinction between the cases of direct and semi-direct products is easily seen from the equation $aza^{-1} = za^{-2}$, where $a = x, y$. □

COROLLARY 6

The order of the group $G(m, n)$ is $2mn$.

Proof

The group structure allows to express unambiguously the elements of $G(m, n)$ in the form $x^k y^l z^j$, $k = 0, 1, \ldots, m-1; l = 0, 1, \ldots, n-1; j = 0, 1$. □

REMARK 1

The group $G(m, 1)$ is the dihedral group D_m [35, p. 22].

EXAMPLE 1

Suppose that $\gcd(m, n) = 1$. In this case we may exclude generators x and y and replace them by $u = xy$. We obtain the presentation of $G(m, n)$ in the form

$$u^{mn} = z^2 = uzuz = e\,. \tag{7}$$

That means that $G(m, n)$ is isomorphic to $G(mn, 1)$, i.e. it is the dihedral group D_{mn}.

PROPOSITION 7

$G(X, Y) \neq G(X) \otimes G(Y)$ in the group $G^q(m, \mathrm{n})$.

Proof

The commutativity between X and Y still holds, but the demand on trivial intersection of $G(X)$ and $G(Y)$ is not satisfied because $E \neq Y^n = X^{-m}$. □

THEOREM 8

The group $G^q(m, n)$ possesses the following structure:

$$\begin{array}{ll} m = 1 \text{ and } q = 2\,, & G^2(1,1) = G(X) \otimes G(Z)\,; \\ m \geqslant 2 \text{ and } n = 1\,, & G^q(m,1) = G(X) \wedge G(Z)\,; \\ n \geqslant 2\,, & G^q(m,n) = G(X,Y) \wedge G(Z)\,. \end{array}$$

EXAMPLE 2

The group $G^q(m, 1)$ is isomorphic to $G(qm, 1)$, i.e. it is the dihedral group D_{qm}.

EXAMPLE 3

Suppose that $\gcd(m, n) = 1$. Then the group $G^q(m, n)$ is isomorphic to $G(qmn, 1)$, i.e. it is the dihedral group D_{qmn}.

Now, let us look at the relation of the groups $G(m, n)$ and $G^q(m, n)$.

THEOREM 9

The group $G^q(m, n)$ is a q-fold cyclic extension of the group $G(m, n)$ by means of the subgroup $G(X^m)$.

Proof

Generators of the group $G(m, n)$ satisfy relations of $G^q(m, n)$ (when the capital letters are substituted by the corresponding small letters). That means that a map φ, $\varphi(A) := a$ for $a = x, y, z$, and the corresponding capital letter A, can be extended to an epimorphism of $G^q(m, n)$ into $G(m, n)$. The kernel of this epimorphism is the group $G(X^m) = G(Y^n)$ which is a cyclic group of order q. It follows that the groups $G^q(m, n)/G(X^m)$ and $G(m, n)$ are isomorphic. □

COROLLARY 10

The order of the group $G^q(m, n)$ is equal to $2qmn$.

Proof

The group structure allows to express unambiguously the elements of $G^q(m, n)$ in the form $X^k Y^l Z^j$, $k = 0, 1, \ldots, qm - 1$; $l = 0, 1, \ldots, n - 1$; $j = 0, 1$. □

COROLLARY 11

If $\gcd(q, m) = 1$ and $\gcd(q, n) = 1$, then $G^q(m, n)$ is a splitting extension of the group $G(m, n)$ and

$$G^q(m,n) = G(X^m) \wedge ((G(X^q) \otimes G(Y^q)) \wedge G(Z))\,. \tag{8}$$

Proof

From the proof of the above theorem, it is obvious that the subgroup $G(X, Y)$ of $G^q(m, n)$ is the q-fold cyclic extension of the subgroup $G(x) \otimes G(y)$ of $G(m, n)$. If $\gcd(q, m) = 1$ and $\gcd(q, n) = 1$, then it follows that $\gcd(q, mn) = 1$. From Schur's theorem [31, p. 201], we conclude that $G(X, Y)$ is a splitting extension of $G(x) \otimes G(y)$, and it is easy to verify that the corresponding image of $G(x) \otimes G(y)$ is the subgroup $G(X^q) \otimes G(Y^q)$. □

COROLLARY 12

If $q = 2$, the $G^q(m,n)$ is a central extension of the group $G(m,n)$.

Proof

Because $X^m Z = Z X^{-m} = Z X^m$, the element X^m belongs to the center of $G^q(m,n)$. □

COROLLARY 13

If $q = 2$ and mn is odd, then

$$G^q(m,n) = G(X^m) \otimes ((G(X^q) \otimes G(Y^q)) \wedge G(z)), \tag{9}$$

where $(G(X^q) \otimes G(Y^q)) \wedge G(z)$ is isomorphic to $G(m,n)$.

Proof

Odd mn implies that m and n are odd. □

EXAMPLE 4

Suppose $q = 3, m = 8$, and $n = 4$. Let us show that we may express the generators X and Y by means of X^8, X^3, and Y^3. We need to find such integers i, j, k, and l that

$$im + jq = 1 \quad \text{and} \quad kn + lq = 1 .$$

In this case we obtain $i = 2, j = -5, k = 1$, and $l = -1$ and

$$X = (X^8)^2 (X^3)^{-5} \quad \text{and} \quad Y = (X^8)^{-1} (Y^3)^{-1} .$$

THEOREM 14

The group $G(qm, qn)$ is a q-fold cyclic extension of the group $G^q(m,n)$.

Proof

Because the relations of the group $G^q(m, n)$ include all relations of the group $G(qm, qn)$, using von Dyck's theorem [38, p. 130], it follows that $G^q(m,n)$ is a factor group of $G(qm, qn)$. Suppose $G(qm, qn)$ is generated by the canonical generators $\tilde{x}$, $\tilde{y}$, and $\tilde{z}$. Then, the kernel of the natural epimorphism of $G(qm, qn)$ to $G^q(m, n)$ is generated by the element $\tilde{x}^m \tilde{y}^n$ of order q. □

2.3. GROUPS $GB(m)$ AND $GB^2(m)$

For the groups $GB(m)$ and $GB^2(m)$ similar theorems are formulated as in the cases of groups $G(m,n)$ and $G^q(m,n)$.

THEOREM 15

The group $GB(m)$ possesses the following structure:

$$m=1, \quad GB(1)=G(z)\otimes G(w)=G(1,1)\otimes G(w);$$

$$m=2, \quad GB(2)=G(x)\otimes G(y)\otimes G(z)\otimes G(w)=G(2,2)\otimes G(w);$$

$$m\geqslant 3, \quad GB(m)=((G(x)\otimes G(y))\wedge(G(z)\otimes G(w))=G(m,m)\wedge G(w).$$

COROLLARY 16

The order of the group $GB(m)$ is $4m^2$.

Proof

The group structure allows to express unambiguously the elements of $GB(m)$ in the form $x^k y^l z^j w^i$, $k=0,1,\ldots,m-1$; $l=0,1,\ldots,n-1$; $j,i=0,1$. □

REMARK 2

In the case of $m\geqslant 3$ the semi-direct product $(G(x)\otimes G(y))\wedge(G(z)\otimes G(w))$ is the wreath product [25,28–30].

THEOREM 17

The group $GB^2(m)$ possesses the following structure:

$$m=1, \quad GB^2(1)=G(X)\otimes G(Z)\otimes G(W)=G^2(m,m)\otimes G(W);$$

$$m\geqslant 2, \quad GB^2(m)=G(X,Y)\wedge(G(Z)\otimes G(W))=G^2(m,m)\wedge G(W).$$

THEOREM 18

The group $GB^2(m)$ is a 2-fold extension of the group $GB(m)$ by means of the subgroup $G(X^m)$.

COROLLARY 19

The order of the group $GB^2(m)$ is $8m^2$.

Proof

The group structure allows one to express unambiguously the elements of $GB^2(m)$ in the form $X^k Y^l Z^j W^i$, $k=0,1,\ldots,qm-1$; $l=0,1,\ldots,n-1$; j, $i=0,1$. □

COROLLARY 20

If m is odd, then

$$GB^2(m)=G(X^m)\otimes((G(X^2)\otimes G(Y^2))\wedge(G(Z)\otimes G(W))), \tag{10}$$

where $((G(X^2) \otimes G(Y^2)) \wedge (G(Z) \otimes G(W)))$ is isomorphic to $GB(m)$.

Proof

The semi-direct product structure and the isomorphism are obvious. Thus, it is sufficient to prove that the second group is also a normal subgroups of $GB^2(m)$. The statement immediately follows from the equation

$$X^m W = WY^m = WX^{-m} = WX^m .$$

□

THEOREM 21

The group $GB(2m)$ is a 2-fold extension of the group $GB^2(m)$.

4. Representations

This section is devoted to derivation of irreducible representations (*irreps*) of the symmetry groups. In the cases of the groups $G(m, n)$, $GB(m)$, and $GB^2(m)$ the complete set of irreps is derived using the *induction* and *extension* techniques [35, pp. 313–365], [36, pp. 132–162]. The completeness of such obtained set of irreps is evident from the discussion provided in ref. [36, pp. 157–162]. (Another way to prove this completeness is to use the fact that the sum of squares of the irrep dimensions over the complete set of irreps is equal to the order of the group [35, p. 186].) In the case of the group $G^q(m, n)$ the irreps are derived using the *restriction* method derived in Appendix B. (In the remainder of this section the word "extension" is used only for extensions of representations of a subgroup to representations of an entire group.)

4.1. GROUP $G(m,n)$

In this subsection the semi-direct product structure $(G(x) \otimes G(y)) \wedge G(z)$ is used for construction of all irreps of the group $G(m, n)$.

Let us denote representations of the group $G(x) \otimes G(y)$ by $\Gamma_{k,l}$ with the conventions $\Gamma_{k,l} = (x) = e^{ik\frac{2\pi}{m}}$ and $\Gamma_{k,l}(y) = e^{il\frac{2\pi}{n}}$, $k = 0, 1, \ldots, m-1$, $l = 0, 1, \ldots, n-1$. Because $\Gamma_{k,l}(zaz) = \Gamma_{k,l}(a^{-1})$, $a = x, y$, the orbit of a representation $\Gamma_{k,l}$ under the action of the group $G(z)$ is formed by this representation itself and the representation $\Gamma_{m-k,n-l}$. Then, the extension of $\Gamma_{k,l}$ exists if and only if $\Gamma_{k,l} = \Gamma_{m-k,n-l}$ [35, p. 353], i.e.,

$$e^{i2k\frac{2\pi}{m}} = e^{i2l\frac{2\pi}{n}} = 1 . \tag{11}$$

This gives only values $k = 0$ for m odd, $k = 0, m/2$ for m even, $l = 0$ for n odd, and $l = 0, n/2$ for n even. From the relation $z^2 = e$ it is obvious that the image of z may be only 1 or -1. Thus, the extended 1-irreps can be distinguished using three symbols. The letters A and B distinguish the values 1 and -1 of the 1-irrep on the generator y, the signs $+$ and $-$ in the superscript of x, and subscripts 1 and 2 of z.

If the extension is impossible, then it means that $\Gamma_{k,l} \neq \Gamma_{m-k,n-l}$. In this case the representation $E_{k,l}$ of $G(m,n)$ induced from $\Gamma_{k,l}$ is irreducible (see Mackay's irreducibility criterion for induced representations in ref. [39, p. 59]).

Now, a review of all irreps of $G(m,n)$ may be given. Let $\mathcal{I}(m,n)$ be the maximal set of double-subscripts of nonequivalent 2-irreps of $G(m,n)$. We distinguish cases of different parity of m and n by means of the ordered pair $(P(m), P(n))$, where $P(k) = o$ if k is odd and $P(k) = e$ if k is even.

In the case (o, o) there are only two 1-irreps: A_1 and A_2, and the set

$$\mathcal{I}(m,n) = \left\{ (s,t); s = 0,1,\ldots,m-1, t = 1,2,\ldots,\frac{n-1}{2} \right\} \cup \left\{ (s,0); s = 1,2,\ldots,\frac{m-1}{2} \right\}$$

contains $(mn-1)/2$ elements.

In the case (e, o) there are four 1-irreps: A_1^+, A_2^+, A_1^- and A_2^-, and the set

$$\mathcal{I}(m,n) = \left\{ (s,t); s = 1,2,\ldots,\frac{m}{2}-1, t = 0,1,\ldots,n-1 \right\} \cup \left\{ (s,t); s = 0,\frac{m}{2}, t = 1,2,\ldots,\frac{n-1}{2} \right\}$$

contains $(mn-2)/2$ elements.

In the case (o, e) there are four 1-irreps: A_1^+, A_2^+, B_1^+, and B_2^+, and the set

$$\mathcal{I}(m,n) = \left\{ (s,t); s = 1,2,\ldots,m-1, t = 0,1,\ldots,\frac{n}{2}-1 \right\} \cup \left\{ (s,t); s = 1,2,\ldots,\frac{m-1}{2}, t = 0,\frac{n}{2} \right\}$$

contains $(mn-2)/2$ elements.

In the case (e, e) there are eight 1-irreps: A_1^+, A_2^+, B_1^+, B_2^+, A_1^-, A_2^-, B_1^-, and B_2^-, and the set

$$\mathcal{I}(m,n) = \left\{ (s,t); s = 1,2,\ldots,\frac{m}{2}-1, t = 0,1,2,\ldots,\frac{n}{2} \right\} \cup \left\{ (s,t); s = 0,\frac{m}{2},\frac{m}{2}+1,\ldots,m-1, t = 1,2,\ldots,\frac{n}{2}-1 \right\}$$

contains $(mn-4)/2$ elements.

The 2-irrep $E_{s,t}$ may adopt by a similarity transformation the following *orthogonal form*:

$$E_{s,t}(x) = \begin{pmatrix} \cos\left(s\frac{2\pi}{m}\right) & -\sin\left(s\frac{2\pi}{m}\right) \\ \sin\left(s\frac{2\pi}{m}\right) & \cos\left(s\frac{2\pi}{m}\right) \end{pmatrix},$$

$$E_{s,t}(y) = \begin{pmatrix} \cos\left(t\frac{2\pi}{n}\right) & -\sin\left(t\frac{2\pi}{n}\right) \\ \sin\left(t\frac{2\pi}{n}\right) & \cos\left(t\frac{2\pi}{n}\right) \end{pmatrix}$$

and

$$E_{s,t}(z) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

EXAMPLE 5

Suppose $m = 4$ and $n = 2$. Then, the group $G(4, 2)$ has eight 1-irreps and

$$\mathcal{I}(4,2) = \{(1,0),(1,1)\}.$$

EXAMPLE 6

Suppose $n = m$. In the case of m odd $G(m, m)$ possesses four 1-irreps and $(m^2 - 1)/2$ 2-irreps. In the case of m even the group possesses eight 1-irreps and $(m^2 - 4)/2$ 2-irreps.

4.2. GROUP $GB(m)$

In this subsection the semi-direct product structure $GB(m) = G(m, m) \wedge G(w)$ is used in order to determine all irreducible representations of the group $GB(m)$.

Because $wxw = y$, it is obvious that only 1-irreps A_1^+, A_2^+, B_1^-, and B_2^- of $G(m, m)$ can be extended to 1-irreps of $GB(m)$. Because $w^2 = e$, it follows that the image of w may be only 1 or -1. Thus, the 1-irreps of $GB(m)$ can be distinguished using three symbols. The letters A and B distinguish the values 1 and -1 on the generator w, the signs $+$ and $-$ in the superscript of x (and also y), and subscripts 1 and 2 of z.

For a 2-irrep $E_{k,l}$ of $G(m, m)$ the condition of possible extension is satisfied in two cases: $l = k$ for $k < \frac{m}{2}$ and $l = m - k$ for $k > \frac{m}{2}$. For $k < \frac{m}{2}$ we obtain two 2-irreps $E_k^{+,+}$ and $E_k^{-,-}$ of $GB(m)$,

$$E_k^{+,+}(w) = \mathrm{diag}(1,1), \tag{12}$$

$$E_k^{-,-}(w) = \mathrm{diag}(-1,-1), \tag{13}$$

and for $k > \frac{m}{2}$ we have

$$E_k^{+,-}(w) = \mathrm{diag}(1,-1), \tag{14}$$

$$\mathrm{E}_k^{-,+}(w) = \mathrm{diag}(-1,1)\,. \tag{15}$$

These results are obtained as solutions of matrix equations which arise from the generating relations of the group using the orthogonal form of 2-irreps of $G(m, m)$. Similarly independent distinction is given by characters

$$\chi(\mathrm{E}_k^{+,+}; w) = 2\,, \tag{16}$$

$$\chi(\mathrm{E}_k^{-,-}; w) = -2\,, \tag{17}$$

$$\chi(\mathrm{E}_k^{+,-}; zw) = 2\,, \tag{18}$$

$$\chi(\mathrm{E}_k^{-,+}; zw) = -2\,. \tag{19}$$

From 2-irreps $E_{k,l}$ of $G(m, m)$, $k \neq l$ and $k + l \neq m$, 4-irreps of $GB(m)$, denoted $G_{k,l}$, are obtained by induction.

Moreover, in the case of m even, by induction the following 2- irreps of $GB(m)$ are obtained: E_1 from A_1^- (or B_1^+) and E_2 from A_2^- (or B_2^+).

Results of this subsection may be summarized as follows:

The case of m odd. The two 1-irreps A_1 and A_2 of $G(m, m)$ are extended into four 1-irreps A_1^+, A_2^+, A_1^-, and A_2^-. The group has $2m - 2$ nonequivalent extended 2-irreps $\mathrm{E}_t^{+,+}$ and $\mathrm{E}_t^{-,-}$, extended from $\mathrm{E}_{t,t}$, and $\mathrm{E}_t^{+,-}$ and $\mathrm{E}_t^{-,+}$, extended from $\mathrm{E}_{m-t,t}$, where $t = 1, 2, \ldots, (m-1)/2$. There are no 2-irreps of $GB(m)$ induced from 1-irreps of $G(m, m)$. And the group possesses $(m-1)^2/2$ 4- irreps $\mathrm{G}_{s,t}$ induced from 2-irreps $\mathrm{E}_{s,t}$ of the group $G(m, m)$. From them, using the equivalence relation $G_{k,l} \sim G_{l,k}$, $\frac{(m-1)^2}{4}$ nonequivalent 4-irreps may be chosen.

The case of m even. The four 1-irreps A_1^+, A_2^+, B_1^-, and B_2^- of $G(m, m)$ are extended into eight 1-irreps A_1^+, A_2^+, A_1^-, A_2^-, B_1^+, B_2^+, B_1^-, and B_2^-. The group has $2m - 4$ nonequivalent extended 2-irreps $\mathrm{E}_t^{+,+}$ and $\mathrm{E}_t^{-,-}$, extended from $\mathrm{E}_{t,t}$, $\mathrm{E}_t^{+,-}$ and $\mathrm{E}_t^{-,+}$, extended from $\mathrm{E}_{t,m-t}$, where $t = 1, 2, \ldots, \frac{m}{2} - 1$. It has two 2-irreps E_1 and E_2 of $GB(m)$ induced from the 1-irreps B_1^+ and B_2^+ of $G(m, m)$ respectively. And the group possesses $m(m-2)/2$ 4-irreps $G_{s,t}$ induced from 2-irreps $\mathrm{E}_{s,t}$ of the group $G(m, m)$. From them, $m(m-2)/4$ nonequivalent 4-irreps may be chosen.

EXAMPLE 7

Suppose $m = 4$. Then the group $GB(4)$ has eight 1-irreps, two induced 2-irreps, four extended 2-irreps, and two 4-irreps.

4.3. GROUP $G^q(m, n)$

In this subsection the factor-group relation $G(qm, qn)/G(\tilde{x}^m\tilde{y}^n) \sim G^q(m, n)$ is used for constructing all irreps of $G^q(m, n)$ by means of the restriction method derived in Appendix B.

The only $G^q(m, n)$-restriction condition for an irrep of the group $G(qm, qn)$ is given by the word $\tilde{x}^m\tilde{y}^n$.

In the case of q odd or q and $m+n$ even, each 1-irrep of $G(qm, qn)$ can be restricted to the group $G^q(m, n)$. In the case of q and m even and n odd, the $\tilde{\mathrm{B}}$ irreps cannot be restricted. In the case of q and n even and m odd, the irreps with the minus sign in the superscript cannot be restricted.

In the case of 2-irreps $\mathrm{E}_{s,t}$ of $G(qm, qn)$, the $G^q(m, n)$-restriction condition is equivalent to the following selection rule:

$$\frac{s+t}{q}2\pi = 0 \bmod 2\pi\,. \tag{20}$$

Thus, the set $\mathcal{I}^q(m, n)$, which parameterizes the nonequivalent 2-irreps of the group $G^q(m, n)$, is the following:

$$\mathcal{I}^q(m,n) = \{(s,t) \in \mathcal{I}(qm,qn); \frac{s+t}{q} \text{ is an integer}\}\,.$$

In the following, summary cases of different parity of q, m, and n are distinguished by the ordered triad $(P(q), P(m), P(n))$. (For irreps of $G^q(m, n)$ the same notation is used as in the case of the group $G(m, n)$. In the case of a possible confusion the irreps of the corresponding groups are distinguished.)

In the case of (o, o, o), there are only two 1-irreps: A_1 and A_2, and the set $\mathcal{I}^q(m,n)$ contains $(qmn-1)/2$ elements.

In the case of (e, o, o), there are four 1-irreps: A_1^+, A_2^+, B_1^-, and B_2^-, and the set $\mathcal{I}^q(m,n)$ contains $(qmn-2)/2$ elements.

In the case of (o, e, o) and (e, e, o), there are four 1-irreps: A_1^+, A_2^+, A_1^-, and A_2^-, and the set $\mathcal{I}^q(m,n)$ contains $(qmn-2)/2$ elements.

In the case of (o, o, e) and (e, o, e), there are four 1-irreps: A_1^+, A_2^+, B_1^+, and B_2^+, and the set $\mathcal{I}^q(m,n)$ contains $(qmn-2)/2$ elements.

In the case of (o, e, e) and (e, e, e), there are eight 1-irreps: A_1^+, A_2^+, B_1^+, B_2^+, A_1^-, A_2^-, B_1^-, and B_2^-, and the set $\mathcal{I}^q(m,n)$ contains $(qmn-4)/2$ elements.

EXAMPLE 8

Suppose $q=3$, $m=4$, and $n=2$. Then, the group $G(12, 6)$ has eight 1-irreps and 34 2-irreps. The group $G^3(4, 2)$ has eight 1- irreps and

$$\mathcal{I} = \{(1,2),(2,1)(3,0),(3,3),(4,2),(5,1),(7,2),(8,1),(10,2),(11,1)\}\,.$$

EXAMPLE 9

Suppose $q=2$ and $n=m$, 2-irreps of $G^2(m, m)$ are determined by the set of parameters

$$\mathcal{I}^2(m,m) = \{(s,t) \in \mathcal{I}(2m,2m); s+t \text{ is even}\}\,.$$

In the case of m odd $G^2(m, m)$ possesses four 1-irreps and $m^2 - 1$ 2-irreps. In the case of m even the group possesses eight 1-irreps and $m^2 - 2$ 2-irreps.

4.4. GROUP $GB^2(m)$

Due to the same semi-direct product structure as in the case of the group $GB(m)$ the extension and induction techniques may be applied to the irreps of the group $G^2(m, m)$ in order to obtain all irreps of the group $GB^2(m)$. (Of course, we have also the possibility to derive all irreps of $GB^2(m)$ using the restriction method applied to the relation $GB(2m)/G(X^m Y^m) \sim GB^2(m)$.)

In the case of m odd, there are eight 1-irreps of $GB^2(m)$ extended from four irreps of $G^2(m, m)$. There is no 2-irreps of $GB^2(m)$ induced from 1-irreps of $G^2(m, m)$. For the extension $2m - 2$ 2-irreps of $G^2(m, m)$ is used, and $4m - 4$ nonequivalent 2-irreps of $GB^2(m)$ is obtained. For the induction $(m - 1)^2$ 2-irreps of $G^2(m, m)$ is used, and $(m - 1)^2/2$ nonequivalent 4-irreps of the group $GB^2(m)$ is obtained.

In the case of m even, there are eight 1-irreps of $GB^2(m)$ extended from four irreps of $G^2(m, m)$ and two nonequivalent 2- irreps of $GB^2(m)$ induced from the other four 1-irreps of $G^2(m, m)$. For the extension $2m - 2$ 2-irreps of $G^2(m, m)$ is used, and $4m - 2$ 2-irreps of $GB^2(m)$ is obtained. For the induction $m^2 - 2m$ irreps of $G^2(m, m)$ is used, and $m(m - 2)/2$ nonequivalent 4-irreps of the group $GB^2(m)$ is obtained.

EXAMPLE 10

Suppose $m = 4$. Then, the group $GB^2(4)$ has eight 1-irreps, 12 extended 2-irreps, 2-induced 2-irreps, and four induced 4-irreps.

5. Character tables

This section is devoted to symbolic character tables of the discussed groups. For this purpose derivation of the conjugacy class structure is shortly described. In general, it should be mentioned that the parities of the integers m, n, and q play a significant role in the class structure of the groups.

The class structure of the group $G(m, n)$ may be simply derived using the conjugacy relations $x^{-1}zx = x^{-2}z$ and $y^{-1}zy = y^{-2}z$.

From the known class structure of $G(m, m)$ the class structure of the group $GB(m)$ may be determined using the relations $wxw = y$ and $y^{-1}x^k y^l wy = x^{k+1}y^{l-1}w$.

Conjugacy classes of the group $G^q(m, n)$ may be derived from the classes of the group $G(qm, qn)$ by means of the corresponding factorization.

Finally, types of conjugacy classes of the group $GB^2(m, m)$ may be determined in the same manner from classes of $G^2(m, m)$ as in the case of the group $GB(m)$ or in the same way from classes of $GB(2m)$ as in the case of the group $G^q(m, n)$.

Table 2
Symbolic character table of the groups $G(m,n)$ in the case of m and n even.

Class	S_e	S_x	S_y	S_{xy}	$S_{k,l}$	S_z	S_y^z	S_x^z	S_{xy}^z
No of elements	1	1	1	1	2	$nm/4$	$nm/4$	$nm/4$	$nm/4$
A_1^+	1	1	1	1	1	1	1	1	1
A_2^+	1	1	1	1	1	-1	-1	-1	-1
B_1^+	1	1	$(-1)^{n/2}$	$(-1)^{n/2}$	$(-1)^l$	1	-1	1	-1
B_2^+	1	1	$(-1)^{n/2}$	$(-1)^{n/2}$	$(-1)^l$	-1	1	-1	1
A_1^-	1	$(-1)^{m/2}$	1	$(-1)^{m/2}$	$(-1)^k$	1	1	-1	-1
A_2^-	1	$(-1)^{m/2}$	1	$(-1)^{m/2}$	$(-1)^k$	-1	-1	1	1
B_1^-	1	$(-1)^{m/2}$	$(-1)^{n/2}$	$(-1)^{(m+n)/2}$	$(-1)^{l+k}$	1	-1	-1	1
B_2^-	1	$(-1)^{m/2}$	$(-1)^{n/2}$	$(-1)^{(m+n)/2}$	$(-1)^{l+k}$	-1	1	1	-1
$E_{s,t}$	2	$(-1)^s 2$	$(-1)^t 2$	$(-1)^{s+t} 2$	$2\cos(\frac{nks+mlt}{nm}2\pi)$	0	0	0	0

The symbolic character tables of the groups $G(m, n)$ and $GB(m)$ are given in the most complicated cases of m and n even in Table 2 and Table 3, respectively. The character tables of the other cases are obtained by omitting the corresponding rows and columns in these tables. The character tables of the extended groups $G^q(m, n)$ and $GB^2(m)$ are obtained from the character tables of the groups $G(qm, qn)$ and $GB(2m)$ using the restriction method (also omitting the corresponding rows and columns in these tables).

Table 3
Symbolic character table of the groups $GB(m)$ in the case of m even.

Class	C_e	C_{xy}	$C_{k,l}$	C^z	C_{xy}^z	$C_{x,y}^z$	C_k^w	C_k^z
No. of elements	1	1	4 (2)	$m^2/4$	$m^2/4$	$m^2/2$	$2m\,(m)$	$2m\,(m)$
A_1^+	1	1	1	1	1	1	1	1
A_2^+	1	1	1	-1	-1	-1	1	-1
A_1^-	1	1	1	1	1	1	-1	-1
A_2^-	1	1	1	-1	-1	-1	-1	1
B_1^+	1	1	$(-1)^{k+l}$	1	1	-1	$(-1)^{k+l}$	$(-1)^{k+l}$
B_2^+	1	1	$(-1)^{k+l}$	-1	-1	1	$(-1)^{k+l}$	$(-1)^{k+l+1}$
B_1^-	1	1	$(-1)^{k+l}$	1	1	-1	$(-1)^{k+l+1}$	$(-1)^{k+l+1}$
B_2^-	1	1	$(-1)^{k+l}$	-1	-1	1	$(-1)^{k+l+1}$	$(-1)^{k+l}$
E_1	2	$(-1)^{m/2}2$	$(-1)^k+(-1)^l$	2	-2	0	0	0
E_2	2	$(-1)^{m/2}2$	$(-1)^k+(-1)^l$	-2	2	0	0	0
$E_i^{+,+}$	2	2	$2\cos\frac{k+l}{m}i2\pi$	0	0	0	$2\cos\frac{k+l}{m}i2\pi$	0
$E_i^{-,-}$	2	2	$2\cos\frac{k+l}{m}i2\pi$	0	0	0	$-2\cos\frac{k+l}{m}i2\pi$	0
$E_i^{+,-}$	2	2	$2\cos\frac{k-l}{m}i2\pi$	0	0	0	0	$2\cos\frac{k-l}{m}i2\pi$
$E_i^{-,+}$	2	2	$2\cos\frac{k-l}{m}i2\pi$	0	0	0	0	$-2\cos\frac{k-l}{m}i2\pi$
$G_{s,t}$	4	$(-1)^{s+t}4$	$2\cos\frac{ks+lt}{m}2\pi$ $+2\cos\frac{kt+ls}{m}2\pi$	0	0	0	0	0

6. Discussion

Finally, let us briefly mention the main questions not solved in this study.

From the point of view of application it is desirable to investigate the following objects concerning the above symmetry groups: *projective representations, electronic spin double groups, and symmetry invariants and covariants.*

Another question arises when one compares the above extended groups with another kind of extended groups – electronic double groups. Several authors [40–42] proposed to use some special projective representations (called spinor representations) of the point groups instead of the ordinary representations of the double groups. Their approach is based on the fact that the electronic double groups are central extensions of the point groups. In this case of the central extension there exists a certain correspondence between projective representations of the corresponding factor groups and the ordinary representations of the extension. The group $GB^2(m)$ is also the central extension of the group $GB(m)$. It seems to be possible, in this case, *to find an analog to the spinor representations following the approach of* [40–42] *modified to the groups* $GB(m)$. The case of groups $G^q(m, n)$ and $G(m, n)$ is rather complicated because, excluding the case of $q = 2$, the extensions are not central. It would be interesting *to investigate relations between projective representations of the group* $G(m, n)$ *and ordinary representation of the group* $G^q(m, n)$.

All above-mentioned problems are proposed for possible further study.

Acknowledgements

This work was supported by the Grant Agency of the Academy of Sciences of the Czech Republic (Grants No. A4040501 and A4040502). This study was completed when the author was visiting the Max-Planck-Institute of Astrophysics during the fall of 1995. He is grateful for hospitality and financial support.

Appendix A. Group extensions

Let us recall the definition of a group homomorphism. Let G and H be groups. A map $\varphi : G \to H$ is a homomorphism if $\varphi(ab) = \varphi(a)\varphi(b)$ for any $a, b \in G$. A homomorphism φ is monomorphic if $\varphi(a) = e_H$ implies $a = e_G$. A homomorphism φ is epimorphic if $\varphi(G) = H$. An isomorphism is a homomorphism which is simultaneously monomorphic and epimorphic.

Let $\ker(\varphi) := \{g \in G \mid \varphi(g) = e_H\}$. Then the *fundamental theorem on homomorphisms* states that the factor group $G/\ker(\varphi)$ is isomorphic to the group $\varphi(G)$ [35, p. 6].

In this paper the following definition of group extensions is used: *A group G is called an extension of a group H by means of its subgroup F if and only if there exists* *an epimorphism* $\varphi : G \to H$ *such that* $ker(\varphi) = F$, i.e. F is a normal subgroup of G and the factor group G/F is isomorphic to the group H [35, p. 23]. (In refs. [31, p. 121] the group G is called the extension of the group F by means of the group H.)

An extension is called a *splitting extension* if there exists a homomorphism $\psi : H \to G$ such that $\varphi\psi$ is the identity map on H. In fact, this property is equivalent to the fact that the group G may be expressed as a semi-direct product $G = F \wedge \tilde{H}$, where $\tilde{H}$ is isomorphic to the group H [31, p. 149], [35, p. 23].

An extension is called a *central extension* if F is a subgroup of the center of the group G [31, p. 145]. A central splitting extension in fact means that the group G is isomorphic to the direct product $F \times H$.

For more theory of group extensions the reader is referred to ref. [31, pp. 121–149].

Appendix B. Restriction method for constructing representations

Let G be a group generated by the set $\mathcal{G} = \{g_1, \ldots, g_k\}$ of generators satisfying the relation $\mathcal{R}_G = \{r_1, \ldots, r_l\}$. (A relation is understood as a word in generators. The group G is then a factor group of the free group generated by these generators over its normal subgroup generated by the relations.) Let H be a group generated also by the set $\mathcal{G}$ of generators satisfying relations $\mathcal{R}_H = \{r_1, \ldots, r_l, r_{l+1}, \ldots, r_{l+m}\}$. In the group G, the words $r_{l+1}, \ldots, r_{l+m}$ are not equal to the identity element. The group H is isomorphic to the factor group G/N, where N is the normal subgroup of G generated by $r_{l+1}, r_{l+2}, \ldots, r_{l+m}$ (see von Dyck's theorem [38, p. 130]).

Let Ψ by a map, $\Psi : \mathcal{G} \to F$, where F is a group. The domain of the map may be extended to all words (in the free group) in the generators by replacing each generator g_i in the word by its image $\Psi(g_i)$. A map defined in this manner determines a homomorphism $K \to F$, where K is a group generated by $\mathcal{G}$ and a set of relations $\mathcal{R}_K$, if and only $\Psi(r) = 1_F$ for all $r \in \mathcal{R}_K$.

Let $\varphi : H \to F$ be a homomorphism. Then, because $\mathcal{R}_G \subset \mathcal{R}_H$, it defines the so-called *expanded* homomorphism $P(\varphi) : G \to F$, which satisfies the following equations $P(\varphi)(r_{l+j}) = 1_F, j = 1, \ldots, m$. Moreover, this homomorphism is the only one because each homomorphism is defined by images of the group generators, and the generators are the same for the groups H and G. In this manner the map P: Hom$(H, F) \to$ Hom(G, F) is defined.

Conversely, if any homomorphism $\psi : G \to F$ satisfies the conditions $\psi(r_{l+j}) = 1_F, j = 1, 2, \ldots, m$, then it defines (one) the so-called *restricted* homomorphism $Q(\psi) : H \to F$ (ψ is called *H-restrictable* and for any homomorphism $\kappa : G \to F$ the elements $\kappa(r_{l+j}), j = 1, 2, \ldots, m$, of F are called *H-restriction conditions*.) Let the set of all H-restrictable homomorphisms $G \to F$ be denoted as Hom$_H(G, F)$. Then, in the same way as above a map Q: Hom$_H(G, F) \to$ Hom(H, F) is defined.

It is easy to prove that for any $\varphi \in \mathrm{Hom}(H, F)$, $Q(P(\varphi)) = \varphi$, and for any $\psi \in \mathrm{Hom}_H(G, F)$, $P(Q(\psi)) = \psi$, i.e. there is a one-to-one correspondence between the set $\mathrm{Hom}(H, F)$ and $\mathrm{Hom}_H(G, F)$.

Particularly, if $F = GL(d, T)$ and $F = GL(d, T)/Z(d, T)$, where d is a non-negative integer and $Z(d, T)$ is the center of the general linear group $GL(d, T)$ over the field T, the word "homomorphism" may be replaced by words "ordinary d-dimensional representation over the field T" and "projective d-dimensional representation over the field T", respectively. Moreover it is obvious that if the representation of H is irreducible, then the corresponding expanded representation of G is also irreducible.

Finally, let us prove the following statement: *Let T be an algebraically closed field of the characteristic 0. If an H-restrictable ordinary representation of the group G over the field T is irreducible, then the corresponding restricted representation of the group H is also irreducible.*

Proof

Let Γ be an H-restrictable irrep of G, χ its character. Let h_i, $i = 1, 2, \ldots, |H|$, be elements of $G/N \equiv H$. Because Γ is H-restrictable, we have $\Gamma(a) = \Gamma(b) =: \Gamma(h_i)$ for $a, b \in h_i$. Because Γ is an irrep of G we have [35, p. 221]

$$\sum_{g \in G} \chi(g)\chi(g^{-1}) = |G| .$$

Then

$$\sum_{i=1}^{|H|} \chi(h_i)\chi(h_i^{-1}) = \frac{1}{|N|}\sum_{i=1}^{|H|} |N|\chi(h_i)\chi(h_i^{-1})$$
$$= \frac{1}{|N|}\sum_{g \in G} \chi(g)\chi(g^{-1}) = \frac{|G|}{|N|} = |H| .$$

Using the irreducibility criterion of characters [35, p. 221] it follows that the corresponding representation of the group H is irreducible. □

That means that there is a one-to-one correspondence between irreps of the group H and H-restrictable irreps of the group G. This correspondence may be used for derivation of all irreps of H from knowledge of the irreps of G by excluding the irreps of G which are not H-restrictable. This approach to the construction of irreps of H from irreps of G is called the *restriction method.*

References

[1] J.T. Hougen, Can. J. Phys. 42 (1964) 1920.
[2] J.T. Hougen, Can. J. PHys. 43 (1965) 935.

[3] P.R. Bunker, J. Chem. Phys. 42 (1965) 2991.
[4] P.R. Bunker and J.T. Hougen, Can. J. Phys. 45 (1967) 3867.
[5] P.R. Bunker, J. Chem. Phys. 47 (1967) 718.
[6] P.R. Bunker and D. Papoušek, J. Mol. Spectrosc. 32 (1969) 419.
[7] D. Papoušek, K. Sarka, V. Špirko and B. Jordanov, Coll. Czech. Chem. Comm. 36 (1971) 890.
[8] A.J. Merer and J.K.G. Watson, J. Mol. Spectrosc. 47 (1973) 499.
[9] G. Dellepiane, M. Gussoni and J.T. Hougen, J. Mol. Spectrosc. 47 (1973) 515.
[10] K. Yamada, T. Nakagawa and K. Kuchitsu, J. Mol. Spectrosc. 51 (1974) 399.
[11] J.T. Hougen, J. Mol. Spectrosc. 82 (1980) 92.
[12] J.T. Hougen, J. Mol. Spectrosc. 89 (1981) 296.
[13] J.T. Hougen and B.M. DeKoven, J. Mol. Spectrosc. 98 (1983) 375.
[14] L. Henry, A. Valentin, W. Lafferty, J.T. Hougen, V. Malathi Devi, P.P. Das and K. Narahari Rao, J. Mol. Spectrosc. 100 (1983) 260.
[15] J.T. Hougen and N. Ohashi, J. Mol. Spectrosc. 109 (1985) 134.
[16] N. Ohashi and J.T. Hougen, J. Mol. Spectrosc. 112 (1985) 384.
[17] J.T. Hougen, J. Mol. Spectrosc. 114 (1985) 395.
[18] N. Ohashi and J.T. Hougen, J. Mol. Spectrosc. 121 (1987) 474.
[19] J.T. Hougen, W.L. Meerts and I. Ozier, J. Mol. Spectrosc. 146 (1991) 8.
[20] J.T. Hougen, I. Kleiner and M. Godefroid, J. Mol. Spectrosc. 163 (1994) 559.
[21] P. Soldán, J. Mol. Spectrosc. 168 (1994) 258.
[22] P. Soldán, V. Špirko and W.P. Kraemer, submitted to J. Mol. Spectrosc.
[23] P. Soldán, J. Mol. Spectrosc. 180 (1996) 249.
[24] P. Soldán: Extended molecular symmetry groups: symmetry analysis of molecules consisting of two coaxial rotors, in: *Advances in Physical Chemistry: Vibration-Rotational Spectroscopy and Molecular Dynamics*, ed. D. Papoušek (World Scientific Publ.), to be published.
[25] K. Balasubramanian, J. Chem. Phys. 95 (1991) 8273.
[26] H.C. Longuet-Higgins, Mol. Phys. 6 (1963) 445.
[27] C.M. Woodman, Mol. Phys. 19 (1970) 753.
[28] K. Balasubramanian, J. Chem. Phys. 72 (1980) 665.
[29] K. Balasubramanian, Theor. Chim. Acta 78 (1990) 31.
[30] A. Kerber, *Lecture Notes in Mathematics*, 240 (Springer, New York, 1971).
[31] A.G. Kurosh, *The Theory of Groups*, Vol. II, 2nd ed. (Chelsea, New York, 1960).
[32] L.L. Boyle and J.R. Walker, Int. J. Quant. Chem. 12, suppl. 1 (1977) 157.
[33] H.P. Fritzer, Physica A114 (1982) 477.
[34] J.H. Bennett and L.L. Boyle, Mol. Phys. 45 (1982) 1279.
[35] C.W. Curtis and L. Reiner, *Representation Theory of Finite Groups and Associative Algebras* (Wiley, New York, London, 1962).
[36] L. Jansen and M. Boon, *Theory of Finite Groups. Application in Physics* (North-Holland, Amsterdam, 1967).
[37] J.T. Hougen, J. Phys. Chem. 90 (1986) 562.
[38] A.G. Kurosh, *The Theory of Groups*, Vol. I, 2nd ed. (Chelsea, New York, 1960).
[39] J.P. Serre, *Linear Representations of Finite groups* (Springer, New York-Heidelberg-Berlin, 1977).
[40] S.L. Altmann, Mol. Phys. 38 (1979) 489.
[41] S.L. Altmann and F. Palacio, Mol. Phys. 38 (1979) 513.
[42] S.L. Altmann and P. Herzig, Mol. Phys. 45 (1982) 585.