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Nonrigid Group Theory of Ammonia Tetramer: $(NH_3)_4$

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Abstract

The character table of the fully nonrigid ammonia tetramer, $(NH_3)_4$, with C_{4h} symmetry is derived for the first time. The group of all feasible permutations is the wreath product $S_4[S_3]$ which consists of 31104 operations divided into 51 conjugacy classes and 51 irreducible representations.

1 Introduction

Although the extent of tunneling would depend on the actual barriers, there is a compelling need to consider the molecular symmetry groups of the nonrigid cluster from semirigid to fully nonrigid limits. Longuet-Higgins [1] has formulated the symmetry groups of nonrigid molecules as permutation-inversion groups by including all feasible permutation of the nuclei under such fluxional or tunneling motions. The fully non-rigid group of $(NH_3)_2$ is computed in [2]. Also we know that the fully non-rigid group of $(NH_3)_3$ with C_{3h} symmetry is isomorphic to the group $S_3[S_3]$ whose character table is computed in [3].

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Up to now, the character table of the fully nonrigid $(NH_3)_4$ with C_{4h} symmetry has not been obtained. Balasubramanian [3-8] has shown that the groups of nonrigid molecules can be expressed as wreath product and generalized wreath product groups. These groups have also been used in a number of chemical applications such as enumeration of isomers [9-12], weakly bound van der Waals, or hydrogen-bonded complexes such as $(NH_3)_2, (H_2O)_2, (H_2O)_5, (C_6H_6)_2$, etc. [1, 13-16], polyhedral structures [17,18], spectroscopy [14-16,19], and cluster [20]. King [17,18] has used the wreath product groups to represent the symmetries of four-dimensional analogues of polyhedra. Thus, apart from the current motivation of calculating the fully nonrigid $(NH_3)_4$, there is considerable interest in wreath product groups of higher order and their character tables. Balasubramanian [5] has applied combinatorial methods without the construction of the character tables for the spin statistics of protonated forms of water cluster. In this study, we have derived the character table of the nonrigid $(NH_3)_4$ in its full nonrigid limit. The resulting group is shown to be the wreath product $S_4[S_3]$, where the group S_n is a permutation group of $n!$ operation, and the square bracket symbol stands for wreath products.

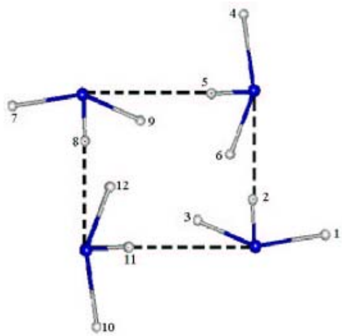

Figure 1: Ammonia tetramer

We show that the fully nonrigid $(NH_3)_4$ with C_{4h} symmetry exhibits a group of 31104 operations divided into 51 conjugacy classes and 51 irreducible representations. The character table of this group helps chemists to compute the Nuclear Spin Statistics and Tunneling Splitting of Ammonia Tetramer.

2 Wreath Product Group $S_4[S_3]$ for Ammonia Tetramer $(NH_3)_4$

Although the theory of wreath product groups and related mathematical details have been described in sufficient details elsewhere [3, 6], we provide the salient points so that this work on $(NH_3)_4$ is sufficiently self contained. Suppose that G is the group of permutations of the nitrogen nuclei in the fully nonrigid limit where they are allowed to exchange and H is the group of permutations of the protons owing to the facile flipping motion. Thus G is the set of $4!$ permutations of four N nuclei, and H is the group

S_3 of protons on each Ammonia molecule that corresponds to the flipping motion which exchanges these protons. In general, the permutation group S_n [21-23] consists of $n!$ permutations of n objects of a set of chosen nuclei, denoted by Ω to represent the rigid framework. Note that the notation S_n that we use here differs from the point group S_n that corresponds to n fold improper axis of rotation. All references to S_n in this work mean the permutation group of $n!$ operations. As the nitrogen atoms get permuted, they carry the protons attached to them, and so induce a permutation of the protons. Consequently, the overall group of $(NH_3)_4$ becomes the wreath product of G with H, denoted by $G[H]$, which becomes $S_4[S_3]$ in this case. The wreath product group $G[H]$ is defined as the set of permutations

$$\{\,(g;\pi)|\pi \quad \text{is a mapping of } \Omega \text{ into } H, g \in G\}$$

and the product of two permutations is defined by

$$(g;\pi)(g^{'};\pi^{'}) = (gg^{'};\pi\pi^{'}_{g})$$

where

$$\pi_g(i) = \pi(g^{-1}i), \forall i \in \Omega$$

$$\pi\pi^{'}(i) = \pi(i)\pi^{'}(i), \forall i \in \Omega$$

An element of $G[H]$ is represented by $(g; h_1, h_2, ..., h_n)$, where $g \in G$ and $h_i \in H$. Thus, the group $G[H]$ contains $|G||H|^n$ elements where n is order of Ω. In the case of $(NH_3)_4$, the order of the full nonrigid permutation group is given by

$$|S_4[S_3]| = 4!(3!)^4 = 31104$$

The group $S_4[S_3]$ is isomorphic with

$$S_4[S_3] = (S_3 \times S_3 \times S_3 \times S_3) \wedge S^{'}_4$$

where the symbols $\times$ and $\wedge$ stand for direct and semidirect product, respectively.

3 Conjugacy Classes

Let $S_n[H]$ be the group under consideration and $(g;\pi)$ be an element of $S_n[H]$. If we adopt the convention to begin each cyclic factor with the least symbol included in the cycle decomposition of g, then we can associate with each cyclic factor $[j; g(j), g^2(j), ..., g^r(j)]$ of g the unique element $\pi\pi_g\pi_{g^2}...\pi_{g^r}(j) = \pi(j)\pi[g^{-1}(j)]...\pi[g^{-r}(j)]$ in H. Let us call this element the cyclic product associated with $[j; g(j), g^2(j), ..., g^r(j)]$ with respect to π. Let the permutation $g \in S_n$ be of the type $T_g = (a_1, a_2, ..., a_n)$ (where a_i denotes cycles of length i). There are a_k cycle products (defined above) associated with the the a_k cycles of length k of g with respect to π. Let $C_1, C_2, ..., C_s$ be the conjugacy classes of H. If exactly a_{ik} of these cycle products belong to C_i, then the $s \times n$ matrix defined below is the cycle type of an element $(g;\pi)$ of the wreath product $T(g;\pi) = a_{ik}(1 \leq i \leq s, 1 \leq k \leq n)$.

Let $P(m)$ denote the number of partitions of the integer m, with the convention that $P(0) = 1$. Let n be partitioned into the ordered s-tuples $(n) = (n_1, n_2, ..., n_s)$ such that $\sum_i n_i = n$. (Recall that s is the number of conjugacy classes of H). Then the number of conjugacy classes of $S_n[H]$ is

$$\sum_{(n)} P(n_1)P(n_2)...P(n_s).$$

For a proof see Kerber [24]. The order of the conjugacy class whose matrix type is (a_{ik}) [25] is given by

$$\frac{|S_n[H]|}{\prod_{i,k} a_{ik}!(k.|H|/|C_i|)^{a_{ik}}}.$$

Therefore, we can compute the conjugacy classes of $S_4[S_3]$ which are shown in Table 1.

No	Class Representation	Order	Symbole
1	Identity of $S_4[S_3]$	1	1a
2	(1,2,3)	8	3a
3	(1,2,3)(4,5,6)	24	3b
4	(1,2,3)(4,5,6)(7,8,9)	32	3c
5	(1,2,3)(4,5,6)(7,8,9)(10,11,12)	16	3d
6	(2,3)	12	2a
7	(2,3)(4,5,6)	72	6a
8	(2,3)(4,5,6)(7,8,9)	144	6b
9	(2,3)(4,5,6)(7,8,9)(10,11,12)	96	6c
10	(2,3)(5,6)	54	2b
11	(2,3)(5,6)(7,8,9)	216	6d
12	(2,3)(5,6)(7,8,9)(10,11,12)	216	6e
13	(2,3)(5,6)(8,9)	108	2c
14	(2,3)(5,6)(8,9)(10,11,12)	216	6f
15	(2,3)(5,6)(8,9)(11,12)	81	2d
16	(1,7)(2,8)(3,9)(4,10)(5,11)(6,12)	108	2e
17	(1,7,2,8,3,9)(4,10)(5,11)(6,12)	432	6g
18	(1,7,2,8,3,9)(4,10,5,11,6,12)	432	6h
19	(1,7)(2,8,3,9)(4,10)(5,11)(6,12)	648	4a
20	(1,7)(2,8,3,9)(4,10,5,11,6,12)	1296	12a
21	(1,7)(2,8,3,9)(4,10)(5,11,6,12)	972	4b
22	(4,10,7)(5,11,8)(6,12,9)	288	3e
23	(1,2,3)(4,10,7)(5,11,8)(6,12,9)	576	3f
24	(4,10,7,5,11,8,6,12,9)	576	9a
25	(1,2,3)(4,10,7,5,11,8,6,12,9)	1152	9b
26	(2,3)(4,10,7)(5,11,8)(6,12,9)	864	6i
27	(2,3)(4,10,7,5,11,8,6,12,9)	1728	18a
28	(4,10,7)(5,11,8,6,12,9)	864	6j
29	(1,2,3)(4,10,7)(5,11,8,6,12,9)	1728	6k
30	(2,3)(4,10,7)(5,11,8,6,12,9)	2592	6l
31	(7,10)(8,11)(9,12)	36	2f
32	(1,2,3)(7,10)(8,11)(9,12)	144	6m
33	(1,2,3)(4,5,6)(7,10)(8,11)(9,12)	144	6n
34	(7,10,8,11,9,12)	72	6o
35	(1,2,3)(7,10,8,11,9,12)	288	6p
36	(1,2,3)(4,5,6)(7,10,8,11,9,12)	288	6q
37	(2,3)(7,10)(8,11)(9,12)	216	2g
38	(2,3)(4,5,6)(7,10)(8,11)(9,12)	432	6r
39	(2,3)(7,10,8,11,9,12)	432	6s
40	(2,3)(4,5,6)(7,10,8,11,9,12)	864	6t
41	(2,3)(5,6)(7,10)(8,11)(9,12)	324	2h
42	(2,3)(5,6)(7,10,8,11,9,12)	648	6u
43	(7,10)(8,11,9,12)	108	4c
44	(1,2,3)(7,10)(8,11,9,12)	432	12b
45	(1,2,3)(4,5,6)(7,10)(8,11,9,12)	432	12c
46	(2,3)(7,10)(8,11,9,12)	648	4d
47	(2,3)(4,5,6)(7,10)(8,11,9,12)	1296	12d
48	(2,3)(5,6)(7,10)(8,11,9,12)	972	4e
49	(1,7,4,10)(2,8,5,11)(3,9,6,12)	1296	4f
50	(1,7,4,10,2,8,5,11,3,9,6,12)	2592	12e
51	(1,7,4,10)(2,8,5,11,3,9,6,12)	3888	8a

Table 1

4 Representation of Wreath Product

Since wreath products are particular types of semidirect products, we may obtain their irreducible representations using MacKey's theory of the semidirect product [26]. Nevertheless, here we follows the procedure outlined by Kerber [24, 27] for wreath products, which is simple and straightforward.
Recall that $H^* = H_1 \times H_2 \times ... \times H_n$, with

$$H \cong H_i = \{(e;\pi) | \pi : \Omega \to \frac{H}{\pi(j)} = 1_H \in H, \forall j \neq i\}.$$

Since H^* is a direct product of the groups $H_1, H_2, ..., H_n$, the irreducible representation of H^* are the outer tensor products

$$F^* = F_1 \# F_2 \# ... \# F_n,$$

where F_i is an irreducible representation of H_i. Formal definitions of outer and inner tensor products can be found in Curtis and Reiner [26]. However, in simple terms, the matrices of outer tensor products can be obtained as the Kronecker products. Symbolically,

$$F^*(e,\pi) = F_1[\pi(1)] \times F_2[\pi(2)] \times ... \times F_n[\pi(n)] = f_{i_1k_1}[\pi(1)] f_{i_2k_2}[\pi(2)] ... f_{i_nk_n}[\pi(n)],$$

if $F(h) = f_{ik}(h)$ for $h \in H$. To obtain the irreducible representations of wreath product groups, first we determine the inertia group $G_{F^*}[H]$, which is defined as

$$G_{F^*}[H] = \{(g;\pi) | F^{*(g;\pi)} \sim F^*\},$$

where $F^{*(g;\pi)}(e;\pi^{'}) = F^*(g;\pi)^{-1}(e;\pi^{'})(g;\pi)$ ($\sim$ denotes equivalence of representations).
The group $G_{F*}[H]$ is by definition the product $H^* G^{'}_{F^*}$, where $G^{'}_{F^*}$ is called the inertia factor of F^* and is defined by

$$G^{'}_{F^*} = \{(g;e^{'}) | F^{*(g;e^{'})} \sim F^*\}.$$

Let $F^1, F^2, ..., F^\gamma$ be a fixed arrangement of γ pairwise nonequivalent representations of H. F^* is said to be of the type $(n) = (n_1, n_2, ..., n_\gamma)$ with respect to this arrangement if n_j is the number of factors F_i of F^* equivalent to F^j. Let S_{n_j} be the subgroup of S_n consisting of the elements permuting exactly the n_j indices of the n_j factors F_j of F^* which are equivalent to F^j. Define $S^{'}_n$ to be $S^{'}_{n_1} \times S^{'}_{n_2} \times ... \times S^{'}_{n_\gamma}$ with

$$S^{'}_{n_j} = \{(g;e^{'}) | g \in S_{n_j}\}.$$

In this setup, Kerber [24] proved that $G^{'}_{F^*} = G^{'} \cap S_{(n)}$.
The representations $\tilde{F}^*$ whose matrices are defined as follows form the representations of $G_{F^*}[H]$:

$$\tilde{F^*}(g;\pi) = f_{i_1k_{g^{-1}(1)}}[\pi(1)] f_{i_2k_{g^{-1}(2)}}[\pi(2)] ... f_{i_nk_{g^{-1}(n)}}[\pi(n)].$$

Alternatively, $\tilde{F^*}(g;\pi)$is found from $F^*(e;\pi)$ by a suitable permutation of the columns of $F^*(e;\pi)$ which is determined by the operation g^{-1} acting on the second index.
Before we proceed to find the irreducible representations of the wreath product group $G[H]$, we need to

know the concept of induced representations. Let G be a group and let K be its normal subgroup. Since K is a normal subgroup, the quotient group G/K is well defined. It is possible to construct the irreducible representations of G from the irreducible representations of K. Let Γ be an irreducible representation of K. Then the irreducible representation of G induced by Γ, denoted by $\Gamma \uparrow G$, is constructed as follows: Let $\sigma \in G/K$ be the coset of the form $\sigma = KS_\sigma$, with $S_\sigma \in G$. Let $k \rightarrow \psi(k)$ be the character of the representation Γ. Then the character $g \rightarrow \chi(g)$ induced by Γ is given by $\chi(g) = \sum_\sigma \chi(S_\sigma g S_\sigma^{-1})$, where the summation is taken over all $\sigma \in G/K$ for which $\sigma g = \sigma$. Note that the dimension of $\Gamma \uparrow G$ is $dim(\Gamma)|G|/|K|$. For an expository survey on induced representation, see Coleman [28] or Curtis and Reiner [26].

Let $F^{'}$ be an irreducible representation of the inertia factor $G^{'}$. Let $\tilde{F^*}$ be determined using the method outlined above. Then the representations induced by the irreducible representations obtained by multiplying $\tilde{F^*}$ and $F^{'}$ are the irreducible representations of the wreath product of G with H. In Kerber's notation, $(\tilde{F^*} \otimes F^{'}) \uparrow G[H]$ are the irreducible representations of $G[H]$.

Note that, since the representation $(\tilde{F^*} \otimes F^{'}) \uparrow G[H]$ is the induced representation of $\tilde{F^*} \otimes F^{'}$ over $G[H]$, the dimension of $(\tilde{F^*} \otimes F^{'}) \uparrow G[H]$ is $dim[(\tilde{F^*} \otimes F^{'}) \uparrow G[H]] = dim(\tilde{F^*} \otimes F^{'})\frac{|G[H]|}{|G_{F^*}[H]|}$. In particular, if $G_{F^*}[H] = G[H]$, then $(\tilde{F^*} \otimes F^{'}) \uparrow G[H] = \tilde{F^*} \otimes F^{'}$.

The representation matrices of the representations of H can be elegantly obtained if H happens be S_m for some m. In this case, to obtain F^*, first one needs to know F. From the partition associated with F, the dimension of F is determined by the Frame-Robinson-Thrall's theorem [29]. The representation matrix is obtained using the representation theory of symmetric groups which can be found in [23]. In this case, a representation F will be denoted by $[P(m)]$, where $P(m)$ is the partition associated with F. The columns of $[P(m)](h), h \in H$, will be labelled by the Young tableaux [23] associated with $P(m)$. F^* is the $n-$fold outer tensor product of copies of F.

Now, we shall illustrate the construction of $\tilde{F^*}$ with a simple example which deserves attention. We derive irreducible representations of $S_2[S_3]$, which is the NMR group of $(NH_3)_2$. First we compute the representations of the basis group $S_3^* \cong S_3 \times S_3$, their types, inertia groups and inertia factors. S_3^* has the following irreducible representations:

$[3]\#[3]$, $[3]\#[2,1]$, $[3]\#[1^3]$, $[2,1]\#[3]$, $[2,1]\#[2,1]$, $[2,1]\#[1^3]$, $[1^3]\#[3]$, $[1^3]\#[2,1]$, $[1^3]\#[1^3]$.

With respect to the arrangement $[3], [2,1], [1^3]$ of the irreducible representations of S_3, the types of these representations are:

$$(2,0,0), (1,1,0), (1,0,1), (1,1,0), (0,2,0), (0,1,1), (1,0,1), (0,1,1), (0,0,2).$$

Hence a complete system of irreducible representations of S_3^* with pairwise different types is

$$\{[3]\#[3], [3]\#[2,1], [3]\#[1^3], [2,1]\#[3], [2,1]\#[2,1], [2,1]\#[1^3], [1^3]\#[3], [1^3]\#[2,1], [1^3]\#[1^3]\}.$$

The corresponding inertia groups are:

$$S_2[S_3], S_3^*, S_3^*, S_2[S_3], S_3^*, S_2[S_3]$$

and the inertia factors are:

$$S_2^{'}, S_1^{'}, S_1^{'}, S_2^{'}, S_1^{'}, S_2^{'}.$$

The irreducible ordinary representations of S_2 are $[2]$ and $[1^2]$, and the only one of S_1 is $[1]$. Thus the irreducible representations of $S_2[S_3]$ are:

$$\widetilde{[3]\#[3]} \otimes [2]^{'} = \widetilde{[3]\#[3]},$$

$$\widetilde{[3]\#[3]} \otimes [1^2]^{'},$$

$$(\widetilde{[3]\#[2,1]} \otimes [1]^{'}) \uparrow S_2[S_3] = [3]\#[2,1] \uparrow S_2[S_3],$$

$$(\widetilde{[3]\#[1]^3} \otimes [1]^{'}) \uparrow S_2[S_3] = [3]\#[1]^3 \uparrow S_2[S_3],$$

$$\widetilde{[2,1]\#[2,1]} \otimes [2]^{'} = \widetilde{[2,1]\#[2,1]},$$

$$\widetilde{[2,1]\#[2,1]} \otimes [1^2]^{'}$$

$$(\widetilde{[2,1]\#[1^3]} \otimes [1]^{'}) \uparrow S_2[S_3] = [2,1]\#[1^3] \uparrow S_2[S_3],$$

$$\widetilde{[1^3]\#[1^3]} \otimes [2]^{'} = \widetilde{[1^3]\#[1^3]},$$

$$\widetilde{[1^3]\#[1^3]} \otimes [1^2]^{'}.$$

Their degrees are $1, 1, 4, 2, 4, 4, 4, 1, 1$ in accordance with

$$1^2 + 1^2 + 4^2 + 2^2 + 4^2 + 4^2 + 4^2 + 1^2 + 1^2 = 72 = |S_2[S_3]|.$$

Next to compute the representing matrices, let us find the matrix of the representation $[2,1]\#[2,1][(12);e^{'}]$ where $[2,1]$ is the irreducible representation corresponding to the partition $(2,1)$ in S_3:

$$[2,1]\#[2,1](e;e^{'}) = \overset{\begin{matrix}\substack{12\\3} & \substack{13\\2}\end{matrix}}{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}} \overset{\begin{matrix}\substack{45\\6} & \substack{46\\5}\end{matrix}}{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}} = \overset{\begin{matrix}\substack{12\\3}\,\substack{45\\6} & \substack{12\\3}\,\substack{46\\5} & \substack{13\\2}\,\substack{45\\6} & \substack{13\\2}\,\substack{46\\5}\end{matrix}}{\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}},$$

which is of the form $f^1_{i_1k_1}(1)f^2_{i_2k_2}(1)$:

$$\widetilde{[2,1]\#[2,1]}[(12);e^{'}] = f^1_{i_1k_{(12)^{-1}(1)}}(1)f^2_{i_2k_{(12)^{-1}(2)}}(1) = f^1_{i_1k_2}(1)f^2_{i_2k_1}(1) = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

Note that each column of $[2,1]\#[2,1](e;e^{'})$ is determined by a pair of Young tableaus. The columns of $[2,\widetilde{1]\#[2},1][(12);e^{'}]$ are determined by the action of g^{-1} on Young tableaus, shown below. Let $T_1(1) = \begin{smallmatrix}12\\3\end{smallmatrix}$, $T_2(1) = \begin{smallmatrix}13\\2\end{smallmatrix}$, $T_1(2) = \begin{smallmatrix}45\\6\end{smallmatrix}$, and $T_2(2) = \begin{smallmatrix}46\\5\end{smallmatrix}$. In general, if $T_i(i)$ is a Young tableaus associated with the partition $p(m)$ which labels a column of $F_i(h), h \in H$, then $g^{-1}T_i(i) = T_i(g^{-1}i)$. In this example, since $g = (12)$,

$$g^{-1}T_1(1) = T_1(2),$$
$$g^{-1}T_2(1) = T_2(2),$$
$$g^{-1}T_1(2) = T_1(1),$$
$$g^{-1}T_2(2) = T_2(1).$$

Thus, the columns of $[2,\widetilde{1]\#[2},1][(12);e^{'}]$ are determined by the pairs $\begin{smallmatrix}45\\6\end{smallmatrix}\ \begin{smallmatrix}12\\3\end{smallmatrix}$, $\begin{smallmatrix}45\\6\end{smallmatrix}\ \begin{smallmatrix}13\\2\end{smallmatrix}$, $\begin{smallmatrix}46\\5\end{smallmatrix}\ \begin{smallmatrix}12\\3\end{smallmatrix}$, and $\begin{smallmatrix}46\\5\end{smallmatrix}\ \begin{smallmatrix}13\\2\end{smallmatrix}$. This is precisely the permutation $(1)(23)(4)$ of $[2,1]\#[2,1](e;e^{'})$. Alternatively, if C_{ji} is the jth column in the ith representation, then a column of the $n-$fold outer tensor product $F^{*}(e;\pi)$ is determined by an unordered $n-$tuple $(C_{j_1 1}, C_{j_2 2}, ..., C_{j_n n})$. The corresponding column of $\tilde{F^{*}}(g;\pi)$ is determined by the action of g^{-1} on this unordered $n-$tuple as shown below:

$$g^{-1}(C_{j_1 1}, C_{j_2 2}, ..., C_{j_n n}) = (C_{j_1 g^{-1}1}, C_{j_2 g^{-1}2}, ..., C_{j_n g^{-1}n}).$$

The character table of $S_2[S_3]$ is shown in Table 2.

	1a	2a	3a	2b	6a	3b	2c	4a	6b
χ_1	1	1	1	1	1	1	1	1	1
χ_2	1	-1	1	1	-1	1	1	-1	1
χ_3	1	1	1	1	1	1	-1	-1	-1
χ_4	1	-1	1	1	-1	1	-1	1	-1
χ_5	2	0	2	-2	0	2	0	0	0
χ_6	4	2	1	0	-1	-2	0	0	0
χ_7	4	-2	1	0	1	-2	0	0	0
χ_8	4	0	-2	0	0	1	-2	0	1
χ_9	4	0	-2	0	0	1	2	0	-1

Table 2

Since the molecule under consideration is $(NH_3)_4$, we can similarly obtain, all the irreducible characters of nonrigid group $(NH_3)_4$, i.e., the irreducible characters of $S_4[S_3]$. Table 3, shows the character table of the nonrigid group of $(NH_3)_4$.

	1a	3a	3b	3c	3d	2a	6a	6b	6c	2b	6d	6e	2c	6f	2d	2e	6g	6h	4a	12a	4b	3e
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	1	1	1	-1	-1	1	1
χ_3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_4	1	1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	1	1	1	-1	-1	1	1
χ_5	2	2	2	2	2	-2	-2	-2	-2	2	2	2	-2	-2	2	2	2	2	-2	-2	2	-1
χ_6	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	-1
χ_7	3	3	3	3	3	-3	-3	-3	-3	3	3	3	-3	-3	3	-1	-1	-1	1	1	-1	0
χ_8	3	3	3	3	3	-3	-3	-3	-3	3	3	3	-3	-3	3	-1	-1	-1	1	1	-1	0
χ_9	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	-1	-1	-1	-1	-1	-1	0
χ_{10}	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	-1	-1	-1	-1	-1	-1	0
χ_{11}	4	4	4	4	4	-2	-2	-2	-2	0	0	0	2	2	-4	0	0	0	0	0	0	1
χ_{12}	4	4	4	4	4	-2	-2	-2	-2	0	0	0	2	2	-4	0	0	0	0	0	0	1
χ_{13}	4	4	4	4	4	2	2	2	2	0	0	0	-2	-2	-4	0	0	0	0	0	0	1
χ_{14}	4	4	4	4	4	2	2	2	2	0	0	0	-2	-2	-4	0	0	0	0	0	0	1
χ_{15}	6	6	6	6	6	0	0	0	0	-2	-2	-2	0	0	6	2	2	2	0	0	-2	0
χ_{16}	6	6	6	6	6	0	0	0	0	-2	-2	-2	0	0	6	2	2	2	0	0	-2	0
χ_{17}	6	6	6	6	6	0	0	0	0	-2	-2	-2	0	0	6	-2	-2	-2	0	0	2	0
χ_{18}	6	6	6	6	6	0	0	0	0	-2	-2	-2	0	0	6	-2	-2	-2	0	0	2	0
χ_{19}	8	5	2	-1	-4	-6	-3	0	3	4	1	-2	-2	1	0	0	0	0	0	0	0	2
χ_{20}	8	5	2	-1	-4	-6	-3	0	3	4	1	-2	-2	1	0	0	0	0	0	0	0	2
χ_{21}	8	5	2	-1	-4	6	3	0	-3	4	1	-2	2	-1	0	0	0	0	0	0	0	2
χ_{22}	8	5	2	-1	-4	6	3	0	-3	4	1	-2	2	-1	0	0	0	0	0	0	0	2
χ_{23}	8	8	8	8	8	-4	-4	-4	-4	0	0	0	4	4	-8	0	0	0	0	0	0	-1
χ_{24}	8	8	8	8	8	4	4	4	4	0	0	0	-4	-4	-8	0	0	0	0	0	0	-1
χ_{25}	16	10	4	-2	-8	-12	-6	0	6	8	2	-4	-4	2	0	0	0	0	0	0	0	-2
χ_{26}	16	10	4	-2	-8	12	6	0	-6	8	2	-4	4	-2	0	0	0	0	0	0	0	-2
χ_{27}	16	-8	4	-2	1	0	0	0	0	0	0	0	0	0	0	4	-2	1	0	0	0	4
χ_{28}	16	-8	4	-2	1	0	0	0	0	0	0	0	0	0	0	4	-2	1	0	0	0	4
χ_{29}	24	15	6	-3	-12	-6	-3	0	3	-4	-1	2	6	-3	0	0	0	0	0	0	0	0
χ_{30}	24	15	6	-3	-12	-6	-3	0	3	-4	-1	2	6	-3	0	0	0	0	0	0	0	0
χ_{31}	24	15	6	-3	-12	6	3	0	-3	-4	-1	2	-6	3	0	0	0	0	0	0	0	0
χ_{32}	24	15	6	-3	-12	6	3	0	-3	-4	-1	2	-6	3	0	0	0	0	0	0	0	0
χ_{33}	24	6	-3	-3	6	12	0	-3	3	4	-2	1	0	0	0	4	1	-2	2	-1	0	0
χ_{34}	24	6	-3	-3	6	-12	0	3	-3	4	-2	1	0	0	0	4	1	-2	-2	1	0	0
χ_{35}	24	6	-3	-3	6	12	0	-3	3	4	-2	1	0	0	0	4	1	-2	2	-1	0	0
χ_{36}	24	6	-3	-3	6	-12	0	3	-3	4	-2	1	0	0	0	4	1	-2	-2	1	0	0
χ_{37}	24	6	-3	-3	6	12	0	-3	3	4	-2	1	0	0	0	-4	-1	2	-2	1	0	0
χ_{38}	24	6	-3	-3	6	-12	0	3	-3	4	-2	1	0	0	0	-4	-1	2	2	-1	0	0
χ_{39}	24	6	-3	-3	6	12	0	-3	3	4	-2	1	0	0	0	-4	-1	2	-2	1	0	0
χ_{40}	24	6	-3	-3	6	-12	0	3	-3	4	-2	1	0	0	0	-4	-1	2	2	-1	0	0
χ_{41}	32	-4	-4	5	-4	-8	4	-2	1	0	0	0	0	0	0	0	0	0	0	0	0	2
χ_{42}	32	-4	-4	5	-4	-8	4	-2	1	0	0	0	0	0	0	0	0	0	0	0	0	2
χ_{43}	32	-4	-4	5	-4	8	-4	2	-1	0	0	0	0	0	0	0	0	0	0	0	0	2
χ_{44}	32	-4	-4	5	-4	8	-4	2	-1	0	0	0	0	0	0	0	0	0	0	0	0	2
χ_{45}	32	-16	8	-4	2	0	0	0	0	0	0	0	0	0	0	8	-4	2	0	0	0	-4
χ_{46}	48	12	-6	-6	12	0	0	0	0	-8	4	-2	0	0	0	0	0	0	0	0	0	0
χ_{47}	48	12	-6	-6	12	0	0	0	0	-8	4	-2	0	0	0	0	0	0	0	0	0	0
χ_{48}	48	-24	12	-6	3	0	0	0	0	0	0	0	0	0	0	-4	2	-1	0	0	0	0
χ_{49}	48	-24	12	-6	3	0	0	0	0	0	0	0	0	0	0	-4	2	-1	0	0	0	0
χ_{50}	64	-8	-8	10	-8	-16	8	-4	2	0	0	0	0	0	0	0	0	0	0	0	0	-2
χ_{51}	64	-8	-8	10	-8	16	-8	4	-2	0	0	0	0	0	0	0	0	0	0	0	0	-2

Table 3

	3f	9a	9b	6i	18a	6j	6k	6l	2f	6m	6n	6o	6p	6q	2g	6r	6s	6t	2h	6u	4c	12b
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	-1	-1	-1	-1	1	1	1	1	1	1	1	-1	-1	-1	-1	1	1	-1	-1
χ_3	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
χ_4	1	1	1	-1	-1	-1	-1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	-1	-1	1	1
χ_5	-1	-1	-1	1	1	1	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_6	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_7	0	0	0	0	0	0	0	0	-1	-1	-1	-1	-1	-1	1	1	1	1	-1	-1	1	1
χ_8	0	0	0	0	0	0	0	0	1	1	1	1	1	1	-1	-1	-1	-1	1	1	-1	-1
χ_9	0	0	0	0	0	0	0	0	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
χ_{10}	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_{11}	1	1	1	1	1	-1	-1	-1	-2	-2	-2	-2	-2	-2	0	0	0	0	2	2	2	2
χ_{12}	1	1	1	1	1	-1	-1	-1	2	2	2	2	2	2	0	0	0	0	-2	-2	-2	-2
χ_{13}	1	1	1	-1	-1	1	1	-1	-2	-2	-2	-2	-2	-2	0	0	0	0	2	2	-2	-2
χ_{14}	1	1	1	-1	-1	1	1	-1	2	2	2	2	2	2	0	0	0	0	-2	-2	2	2
χ_{15}	0	0	0	0	0	0	0	0	2	2	2	2	2	2	0	0	0	0	2	2	0	0
χ_{16}	0	0	0	0	0	0	0	0	-2	-2	-2	-2	-2	-2	0	0	0	0	-2	-2	0	0
χ_{17}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	-2	-2	-2	0	0	2	2
χ_{18}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	2	2	0	0	-2	-2
χ_{19}	-1	2	-1	0	0	-2	1	0	-4	-1	2	-4	-1	2	2	-1	2	-1	0	0	4	1
χ_{20}	-1	2	-1	0	0	-2	1	0	4	1	-2	4	1	-2	-2	1	-2	1	0	0	-4	-1
χ_{21}	-1	2	-1	0	0	2	-1	0	-4	-1	2	-4	-1	2	-2	1	-2	1	0	0	-4	-1
χ_{22}	-1	2	-1	0	0	2	-1	0	4	1	-2	4	1	-2	2	-1	2	-1	0	0	4	1
χ_{23}	-1	-1	-1	-1	-1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{24}	-1	-1	-1	1	1	-1	-1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{25}	1	-2	1	0	0	2	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{26}	1	-2	1	0	0	-2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{27}	-2	-2	1	0	0	0	0	0	8	-4	2	-4	2	-1	0	0	0	0	0	0	0	0
χ_{28}	-2	-2	1	0	0	0	0	0	-8	4	-2	4	-2	1	0	0	0	0	0	0	0	0
χ_{29}	0	0	0	0	0	0	0	0	-4	-1	2	-4	-1	2	-2	1	-2	1	0	0	4	1
χ_{30}	0	0	0	0	0	0	0	0	4	1	-2	4	1	-2	2	-1	2	-1	0	0	-4	-1
χ_{31}	0	0	0	0	0	0	0	0	-4	-1	2	-4	-1	2	2	-1	2	-1	0	0	-4	-1
χ_{32}	0	0	0	0	0	0	0	0	4	1	-2	4	1	-2	-2	1	-2	1	0	0	4	1
χ_{33}	0	0	0	0	0	0	0	0	-6	0	-3	-3	3	0	-2	-2	1	1	-2	1	-4	2
χ_{34}	0	0	0	0	0	0	0	0	-6	0	-3	-3	3	0	2	2	-1	-1	-2	1	4	-2
χ_{35}	0	0	0	0	0	0	0	0	6	0	3	3	-3	0	2	2	-1	-1	2	-1	4	-2
χ_{36}	0	0	0	0	0	0	0	0	6	0	3	3	-3	0	-2	-2	1	1	2	-1	-4	2
χ_{37}	0	0	0	0	0	0	0	0	-2	4	1	-5	1	-2	2	2	-1	-1	2	-1	-4	2
χ_{38}	0	0	0	0	0	0	0	0	-2	4	1	-5	1	-2	-2	-2	1	1	2	-1	4	-2
χ_{39}	0	0	0	0	0	0	0	0	2	-4	-1	5	-1	2	-2	-2	1	1	-2	1	4	-2
χ_{40}	0	0	0	0	0	0	0	0	2	-4	-1	5	-1	2	2	2	-1	-1	-2	1	-4	2
χ_{41}	2	-1	-1	-2	1	0	0	0	-8	-2	4	4	1	-2	4	-2	-2	1	0	0	0	0
χ_{42}	2	-1	-1	-2	1	0	0	0	8	2	-4	-4	-1	2	-4	2	2	-1	0	0	0	0
χ_{43}	2	-1	-1	2	-1	0	0	0	-8	-2	4	4	1	-2	-4	2	2	-1	0	0	0	0
χ_{44}	2	-1	-1	2	-1	0	0	0	8	2	-4	-4	-1	2	4	-2	-2	1	0	0	0	0
χ_{45}	2	2	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{46}	0	0	0	0	0	0	0	0	-4	-4	-4	2	2	2	0	0	0	0	4	-2	0	0
χ_{47}	0	0	0	0	0	0	0	0	4	4	4	-2	-2	-2	0	0	0	0	-4	2	0	0
χ_{48}	0	0	0	0	0	0	0	0	8	-4	2	-4	2	-1	0	0	0	0	0	0	0	0
χ_{49}	0	0	0	0	0	0	0	0	-8	4	-2	4	-2	1	0	0	0	0	0	0	0	0
χ_{50}	-2	1	1	2	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{51}	-2	1	1	-2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Continue of table 3

	12c	4d	12d	4e	4f	12e	8a
χ_1	1	1	1	1	1	1	1
χ_2	-1	1	1	-1	1	1	-1
χ_3	-1	-1	-1	-1	-1	-1	-1
χ_4	1	-1	-1	1	-1	-1	1
χ_5	0	0	0	0	0	0	0
χ_6	0	0	0	0	0	0	0
χ_7	1	-1	-1	1	1	1	-1
χ_8	-1	1	1	-1	-1	-1	1
χ_9	-1	-1	-1	-1	1	1	1
χ_{10}	1	1	1	1	-1	-1	-1
χ_{11}	2	0	0	-2	0	0	0
χ_{12}	-2	0	0	2	0	0	0
χ_{13}	-2	0	0	2	0	0	0
χ_{14}	2	0	0	-2	0	0	0
χ_{15}	0	-2	-2	0	0	0	0
χ_{16}	0	2	2	0	0	0	0
χ_{17}	2	0	0	2	0	0	0
χ_{18}	-2	0	0	-2	0	0	0
χ_{19}	-2	-2	1	0	0	0	0
χ_{20}	2	2	-1	0	0	0	0
χ_{21}	2	-2	1	0	0	0	0
χ_{22}	-2	2	-1	0	0	0	0
χ_{23}	0	0	0	0	0	0	0
χ_{24}	0	0	0	0	0	0	0
χ_{25}	0	0	0	0	0	0	0
χ_{26}	0	0	0	0	0	0	0
χ_{27}	0	0	0	0	2	-1	0
χ_{28}	0	0	0	0	-2	1	0
χ_{29}	-2	2	-1	0	0	0	0
χ_{30}	2	-2	1	0	0	0	0
χ_{31}	2	2	-1	0	0	0	0
χ_{32}	-2	-2	1	0	0	0	0
χ_{33}	-1	0	0	0	0	0	0
χ_{34}	1	0	0	0	0	0	0
χ_{35}	1	0	0	0	0	0	0
χ_{36}	-1	0	0	0	0	0	0
χ_{37}	-1	0	0	0	0	0	0
χ_{38}	1	0	0	0	0	0	0
χ_{39}	1	0	0	0	0	0	0
χ_{40}	-1	0	0	0	0	0	0
χ_{41}	0	0	0	0	0	0	0
χ_{42}	0	0	0	0	0	0	0
χ_{43}	0	0	0	0	0	0	0
χ_{44}	0	0	0	0	0	0	0
χ_{45}	0	0	0	0	0	0	0
χ_{46}	0	0	0	0	0	0	0
χ_{47}	0	0	0	0	0	0	0
χ_{48}	0	0	0	0	-2	1	0
χ_{49}	0	0	0	0	2	-1	0
χ_{50}	0	0	0	0	0	0	0
χ_{51}	0	0	0	0	0	0	0

Continue of table 3

5 Conclusions

The character table for ammonia tetramer has been deduced from:

– the structure of group:

$$S_4[S_3] = (S_3 \times S_3 \times S_3 \times S_3) \wedge S_4^{'}.$$

– the group is divided in 51 classes, the sum of the squares of whose dimensions gives the order of the group:

$$4 \times (1)^2 + 2 \times (2)^2 + 4 \times (3)^2 + 4 \times (4)^2 + 4 \times (6)^2 + 6 \times (8)^2 + 4 \times (16)^2 + 12 \times (24)^2 + 5 \times (32)^2 +$$
$$4 \times (48)^2 + 2 \times (64)^2 = 31104.$$

– the number of elements of these of the 51 classes are; 1, 8, 24, 32, 16, 12, 72, 144, 96, 54, 216, 216, 108, 216, 81, 108, 432, 432, 648, 1296, 972, 288, 576, 576, 1152, 864, 1728, 864, 1728, 2592, 36, 144, 144, 72, 288, 288, 216, 432, 432, 864, 324, 648, 108, 432, 432, 648, 1296, 972, 1296, 2592 and 3888.

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