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The Full Non-Rigid Group Theory of *cis*-Tetraamminedichlorocobalt(III)

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The non-rigid molecule group theory (NRG), in which the dynamical symmetry operations are defined as physical operations, is a new field of chemistry. In a series of papers Smeyers applied this notion to determine the character table of restricted NRG (r-NRG) of some molecules. For example, Smeyers and Villa computed the r-NRG of the triple equivalent methyl rotation in pyramidal trimethylamine with inversion and proved that the r-NRG of this molecule is a group of order 648, containing two subgroups of order 324 without inversions. In this paper, a simple method is used, by means of which it is possible to calculate character tables for the symmetry group of molecules consisting of a number of XH_3 groups attached to a rigid framework. We have studied the full non-rigid group (f-NRG) of *cis*-tetraamminedichloro-cobalt(III). By separating the type of conjugacy classes of the point group, we construct the full non-rigid group of the molecule. We show that this group has 33 conjugacy classes and therefore 33 irreducible characters. This group has eight non-real valued irreducible characters which computed by inducing the characters of a subgroup of G.

Key Words: Character table, *cis*-Tetraamminedichlorocobalt(III), Full non-rigid group.

INTRODUCTION

The non-rigid molecule group theory (NRG) in which the dynamical symmetry operations are defined as physical operations is a new field of chemistry. Smeyers and Villa in a series of papers[1,2] applied this notation to determine the character table of restricted NRG of some molecules. A molecule is said to be non-rigid if there are several local minima on the potential-energy surface easily attainable by the molecular system *via* a tunneling rearrangement. A non-rigid molecule, which possesses various iso-energetic forms separated by relatively low energy barriers, presents large amplitude movements between various possible configurations. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intermolecular dynamics, which can be studied more easily reporting to group theory.

Finite group theory is the mathematics useful tool. It 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. Numerous applications of group theory to the large amplitude vibration spectroscopy of small organic molecules are appearing in the literature[3-10]. Lomont[10] has proposed two methods for calculating character tables. These are satisfactory for small groups, but both of them require knowledge of the class structure and hence of the group multiplication table and become very unwieldy as soon as the order of the group becomes even moderately large. They are usually quite impracticable for non-rigid molecules, whose symmetry groups may have several thousands of elements. The alternative approach is less mechanical, requiring a certain amount of thought, but it is nevertheless simpler in practice. This involves two steps: (i) the decomposition of the group into classes and (ii) the determination of sets of basis functions for certain representations, whose characters are then determined directly.

The molecular symmetry group theory (MSG) of permutation inversion groups (PI) constructed by permutations and permutation-inversions of identical particles. The MSG group is then formed by all feasible permutations and permutation-inversions[11-13]. In 1963 Longuet-Higgins[11] investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. In many cases, these dynamical symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules and their character tables are not known. It is therefore of some interest and importance to develop simple methods of calculating these character tables, which are needed for classification of wave functions, determination of selection rules and so on. Ashrafi and coauthors, using a computational approach, computed character table of some molecules[14-17]. Stone[13] described a method which is appropriate for molecules with a number of XH_3 groups attached to a rigid framework. However, this method is not appropriate in cases where the framework is linear, as with ethane and dimethylacetylene, but Bunker[12] has shown how to deal with such molecules.

In[1,2], Smeyers and Villa investigated the r-NRG of planer trimethylamine and proved that this is a group of order 324. Furthermore, they showed that this molecule has a pyramidal inversion and so the order of r-NRG of trimethylamine is 648. The full and restricted non-rigid group theory (for r-NRG) built up with physical operations, expressed in terms of internal coordinates that transform one conformation into another iso-energetic one. The r-NRG is then formed by the complete set of physical operations which commute with the given restricted or Hamiltonian operators[18,19].

In this work a simple method is described, by means of which it is possible to calculate character tables for the symmetry group of molecules consisting of a number of XH_3 groups attached to a rigid framework. The motivation for this study is outlined in references[14-17,20-31] and the reader is encouraged to consult these papers for background material as well as basic computational techniques. In this paper,

we investigate the f-NRG of *cis*-tetraamminediclorocobalt(III). It is proved that this is a group of order 324 with 33 conjugacy classes so with 33 irreducible characters. Reference[32] for the standard notation and terminology of character theory is used.

Preliminaries: We now recall some algebraic definitions that will be used in the paper. Suppose that G is a group, the group generated by all elements $x^{-1}y^{-1}xy$ for elements x, y of G is called the derived subgroup of G and denoted by G'. It is a well known fact that the number of linear characters of a finite group G is the order of factor group G modulus its derived subgroup[32].

Let G be a finite group and let N be a normal subgroup of G. We can use the characters of G/N to get some of the characters of G, by a process which is known as lifting. Thus, normal subgroups help us to find characters of G. To see this, we assume that χ is a character of G/N. Define the map $\varphi:G\rightarrow C$, where C is the field of complex numbers, by $\varphi(g)=\chi(gN)$, for $g\in G$. Then φ is a character of G and χ and φ have the same degree. The character φ of G is called the lift of χ to G. It is well known that χ is irreducible if and only if φ is irreducible[32].

Suppose that χ and φ are characters of group G. The scalar product of these characters is denoted by $[\chi,\varphi]$ and defined by $[\chi,\varphi]=\frac{1}{|G|}\sum_{g\in G}\chi(g)\overline{\varphi(g)}$. It is a well known fact that if χ is a character of G and φ is an irreducible character of G and $[\chi, \phi] = 1$ then $\chi - \varphi$ is a character of G. Recall that for a character χ of G, χ is irreducible if and only if $[\chi,\chi] = 1$[32]. If χ and φ are two different irreducible characters of G then we have $[\chi, \varphi] = 0$.

For every element x of group G, the subgroup $C_G(x)=\{y\in G|xy=yx\}$ is called the centralizer of x in G. If G is finite, then $|C_G(x)|=|G|/|Cl_G(x)|$, where $Cl_G(x)$ is the conjugacy class of x in G. Let H be a subgroup of group G and let φ be a character of H. Then φ^G the induced character on G, is given by $\varphi^G(g)=\frac{1}{|H|}\sum_{x\in G}\varphi^{\circ}(xgx^{-1})$, where φ^o is defined by $\varphi^o(h)=\varphi(h)$ if $h\in H$ and $\varphi^o(h) = 0$ if $h \notin H$. It is easy to check that $\varphi^G(1) = \varphi(1)|G|/|H|$. Explicit computation of induced characters is extremely useful for the construction of character tables, despite the fact that φ^G is usually reducible even if φ is irreducible. Given a subgroup H of G and a character φ of H and $g \in G$, an efficient way to compute $\varphi^G(g)$ explicitly is to choose representatives, x_1, x_2, …, x_m for the conjugacy classes of H which contained in $Cl_G(g)$ in G and to use the formula $\varphi^G(g)=|C_G(g)|\Sigma\varphi(x_i)/|C_H(x_i)|$[32].

In this paper we denote a cyclic group of order n by Z_n and a symmetric group on n symbols by S_n. Our notations are standard and adapted mainly from[32]. We apply a useful programming language, namely GAP[33], to find many properties of a group. Using this package we can perform most of our computations.

EXPERIMENTAL

First of all, we consider the point group of each molecule in the rigid state. The point group of *cis*-tetraamminedichlorocobalt (III) is C_{2v}, as shown in Fig. 1. We define the operation $g_1 = (6,8,7)$, $g_2 = (9,10,11)$, $g_3 = (12,13,14)$ and $g_3 = (15,16,17)$ for *cis*-tetraamminedichlorocobalt(III), which are rotations that leave the framework unchanged, in a positive sense, of each NH_3 group. It is assumed that all of these operations are feasible. It is known that every group is union of conjugacy classes. It is easy to check that the conjugacy classes of a group have no common non-identity element, so by characterization of the classes one can construct the group. Using this fact, the full non-rigid group of the molecule has been computed in the next section.

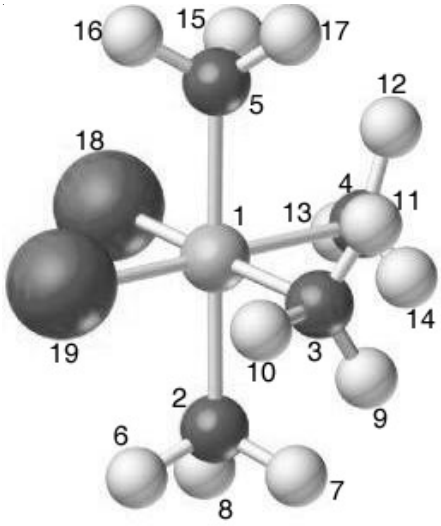

Fig. 1. Structure of *cis*-tetraamminediclorocobalt(III)

RESULTS AND DISCUSSION

In this section we compute all of the conjugacy classes of G by partition the operations that leave the framework of the molecule changed and unchanged. The reflection with respect to the horizontal plane containing molecules 1, 3, 4, 18, 19 is in G. So $h_1 = (2,5)\ (8,15)\ (7,17)\ (6,16)\ (9,10)\ (13,14)$ is an element if G. The reflection with respect to the vertical plan containing molecules 2 and 5, bisecting molecules 18, 19 and 3, 4 is in G. Therefore $h_2 = (19,18)\ (15,17)\ (8,7)\ (3,4)\ (11,12)\ (10,13)\ (9,14)$ is an element of G. It is easy to see that the full non-rigid group of the molecule is generated by $\{g_1, g_2, g_3, g_4, h_1, h_2\}$. At this time we can use the GAP package to compute the conjugacy classes of the group. But in order to investigate the structure of the group we compute these classes by separating the operations.

Let us first consider operations that leave the framework of the molecule unchanged. The operations that rotate different numbers of NH_3 groups must belong to different conjugacy classes. We now consider the four operations that rotate one NH_3 group; it is easy to see that they must belong to the two different classes, since operations involving rotation of the molecular framework will transform g_1 into g_1^{-1} or g_4^{-1} and g_2 into g_2^{-1} or g_3^{-1}, changing the sense of the rotation. Now consider operations that rotate two NH_3 groups. By a simple calculation we have

$Cl_G(g_3g_4) = \{g_3g_4, g_2^{-1}g_4^{-1}, g_1^{-1}g_3^{-1}, g_1g_2\}$
$Cl_G(g_3g_4^{-1}) = \{g_3g_4^{-1}, g_2^{-1}g_4, g_1g_3^{-1}, g_1^{-1}g_2\}$
$Cl_G(g_3^{-1}g_4) = \{g_3^{-1}g_4, g_2g_4^{-1}, g_1^{-1}g_3, g_1g_2^{-1}\}$
$Cl_G(g_3^{-1}g_4^{-1}) = \{g_3^{-1}g_4^{-1}, g_2g_4, g_1g_3, g_1^{-1}g_2^{-1}\}$
$Cl_G(g_2g_3) = \{g_2g_3, g_2^{-1}g_3^{-1}\}$
$Cl_G(g_2g_3^{-1}) = \{g_2g_3^{-1}, g_2^{-1}g_3\}$
$Cl_G(g_1^{-1}g_3) = \{g_1^{-1}g_3, g_1g_3^{-1}\}$
$Cl_G(g_1^{-1}g_3^{-1}) = \{g_1^{-1}g_3^{-1}, g_1g_3\}$.

So we have 8 conjugacy classes with elements that rotate two NH_3 groups. Operations that rotate three NH_3 groups form 8 conjugacy classes because we have

$Cl_G(g_2g_3g_4) = \{g_2g_3g_4, g_2^{-1}g_3^{-1}g_4^{-1}, g_1^{-1}g_2^{-1}g_3^{-1}, g_1g_2g_3\}$
$Cl_G(g_2g_3g_4^{-1}) = \{g_2g_3g_4^{-1}, g_2^{-1}g_3^{-1}g_4, g_1^{-1}g_2g_3, g_1g_2^{-1}g_3^{-1}\}$
$Cl_G(g_2g_3^{-1}g_4) = \{g_2g_3^{-1}g_4, g_2g_3^{-1}g_4^{-1}, g_1^{-1}g_2g_3, g_1g_2^{-1}g_3\}$
$Cl_G(g_2^{-1}g_3g_4) = \{g_2^{-1}g_3g_4, g_2^{-1}g_3g_4^{-1}, g_1^{-1}g_2g_3^{-1}, g_1g_2g_3^{-1}\}$
$Cl_G(g_1^{-1}g_3g_4) = \{g_1^{-1}g_3g_4, g_1^{-1}g_3^{-1}g_4, g_1g_2g_4^{-1}, g_1g_2^{-1}g_4^{-1}\}$
$Cl_G(g_1^{-1}g_3g_4^{-1}) = \{g_1^{-1}g_3g_4^{-1}, g_1^{-1}g_3g_4^{-1}, g_1g_2^{-1}g_4, g_1g_2^{-1}g_4\}$
$Cl_G(g_1^{-1}g_3^{-1}g_4) = \{g_1^{-1}g_3^{-1}g_4, g_1^{-1}g_2^{-1}g_4^{-1}, g_1g_2g_4, g_1g_2g_4\}$
$Cl_G(g_1^{-1}g_2g_4) = \{g_1^{-1}g_2g_4, g_1^{-1}g_2^{-1}g_4, g_1g_3g_4^{-1}, g_1g_3^{-1}g_4^{-1}\}$.

All of operations that rotate four NH_3 groups separate into five conjugacy classes as follows:

$Cl_G(g_1^{-1}g_2g_3g_4) = \{g_1^{-1}g_2g_3g_4, g_1^{-1}g_2^{-1}g_3^{-1}g_4, g_1g_2g_3g_4^{-1}, g_1g_2^{-1}g_3^{-1}g_4^{-1}\}$
$Cl_G(g_1^{-1}g_2g_3g_4^{-1}) = \{g_1^{-1}g_2g_3g_4^{-1}, g_1g_2^{-1}g_3^{-1}g_4\}$
$Cl_G(g_1^{-1}g_2g_3^{-1}g_4) = \{g_1^{-1}g_2g_3^{-1}g_4, g_1^{-1}g_2^{-1}g_3g_4, g_1g_2g_3^{-1}g_4^{-1}, g_1g_2^{-1}g_3g_4^{-1}\}$
$Cl_G(g_1^{-1}g_2g_3^{-1}g_4^{-1}) = \{g_1^{-1}g_2g_3^{-1}g_4^{-1}, g_1^{-1}g_2^{-1}g_3g_4^{-1}, g_1g_2g_3^{-1}g_4^{-1}, g_1g_2^{-1}g_3g_4\}$
$Cl_G(g_1^{-1}g_2^{-1}g_3^{-1}g_4^{-1}) = \{g_1^{-1}g_2^{-1}g_3^{-1}g_4^{-1}, g_1g_2g_3g_4\}$.

The operations that permute the nuclei of the framework are corresponding to the non-identity elements of the C_{2v}. It is known that the point group C_{2v} has four elements and four conjugacy classes which are identity, C_2 and two classes of type σ_v.

The unique C_2 operation of C_{2v} applied to the framework is the permutation (2,5) (3,4) (18,19), but this is not feasible for the molecule as the whole and the protons have to be permuted as well.

Let R_1 = (2,5) (3,4) (6,15) (7,17) (8,16) (9,12) (10,13) (11,14) (18,19). R_1 is the only operation that doesn't rotate any of the NH_3 groups. All of operations that rotate one of the NH_3 groups have form $R_1g_i^j$ or $g_i^jR_1$ such that $i \in \{1,2,3,4\}$ and $j \in \{1,-1\}$. We have

$R_2 = R_1g_1^{-1}$ = (2,5) (3,4) (6,15,7,17,8,16) (9,12) (10,13) (11,14) (18,19)

$R_3 = R_1g_2$ = (2,5) (3,4) (6,15) (7,17) (8,16) (9,12,10,13,11,14) (18,19).

It is easy to check that R_1g_i, g_iR_1 and $g_i^{-1}R_1$ are conjugate with R_2 for $i\in\{1, 4\}$ and are conjugate with R_3 for $i\in\{2, 3\}$. Now consider all of operations that rotate two NH_3 groups. These operations are $R_1g_i^mg_j^n$ or $g_i^mg_j^nR_1$ such that $i,j\in\{1,2,3,4\}$ for $i\neq j$ and $m,n\in\{1,-1\}$. In this case we have

$R_4 = R_1g_1g_2$ = (2,5) (3,4) (6,15,8,16,7,17) (9,12,10,13,11,14) (18,19)

$R_5 = R_1g_1^{-1}g_2$ = (2,5) (3,4) (6,15,7,17,8,16) (9,12,10,13,11,14) (18,19)

The operations $R_1g_i^mg_j^n$ and $g_i^mg_j^nR_1$ for i=1, j=2 or 3 and for i=2 or 3, j=4, are conjugate with R_4 for m=n and are conjugate with R_5 for $m\neq n$. Also these operations are conjugate with R_1 for i=1, j=4 and for i=2, j=3 whenever $m\neq n$. Operations that rotate three NH_3 groups are $R_1g_i^rg_j^sg_k^t$ or $g_i^rg_j^sg_k^tR_1$ such that $i,j,k \in\{1,2,3,4\}$ for distinct i,j,k and $r,s,t\in\{1,-1\}$. These operations are conjugate with R_2 if $i\in\{1,2\}$, $j=i+1$, $k=i+2$, $r=t\neq s$ or $r=s\neq t$. Also these are conjugate with R_3 for $i=1,j\in\{2,3\}$, k=4, $r\neq s=t$ or $r=s\neq t$ and are conjugate with R_4 if $r\neq s=t$ and $r=t\neq s$ and $r=s\neq t$. Finally these operations are conjugate with R_5 for r=s=t.

By considering rotation of all of NH_3 groups we obtain operations $R_1g_h^mg_i^ng_j^rg_k^s$ and $g_h^mg_i^ng_j^rg_k^sR_1$ such that h=1, i=2, j=3, k=4 and $m,n,r,s\in\{1,-1\}$. These are conjugate with R_1 if $m=n\neq r=s$ or $m=r\neq n=s$ and are conjugate with R_2 if $m=r=s\neq n$ or $m=n=s\neq r$ and are conjugate with R_3 for $m\neq n=r=s$ or $m=n=r\neq s$ and are conjugate with R_4 if m=n=r=s and are conjugate with R_5 if $m=s\neq n=r$.

Consequently by considering the operation C_2 and rotations of NH_3 groups (all cases) we obtain five conjugacy classes. At this time we use the GAP package and calculate the size and conjugacy classes of G with representatives as above. But in order to find conjugacy classes of G we may argue as follows. All of the permutations of cycle type 2^9 are conjugate in the group. Thus, we obtain a conjugacy class of length 18 with representative R_1. Similarly R_2, R_3, R_4 and R_5 are not conjugate and length of their conjugacy classes is 18.

Similar methods are applied to other operations of the point group (σ_v) to derive other sets of conjugacy classes of this molecule. In this case put

σ_{v1} = (3,4) (7,8) (9,12) (10,14) (11,13) (16,17) (18,19),

σ_{v2} = (2,5) (6,15) (7,16) (8,17) (10,11) (13,14).

Again in this stage we can consider all operations of the form $\sigma_{vi}g_1^mg_2^ng_3^rg_4^s$, where $i\in\{1,2\}$ and $m,n,r,s\in\{-1,0,1\}$, and obtain all operations that are conjugate with σ_{v1} or σ_{v2} or not. These operations are not conjugate so we can obtain two conjugacy classes of lengths 27 with elements of type 2^7 and 2^6, respectively. Note that R_6 is not conjugate with any of σ_{vi} and R_j, $i\in\{1,2\}$ and $j\in\{1,\ldots,5\}$, where

$R_6 = \sigma_{v2}g_1^{-1}$ = (2,5) (6,15,7,16,8,17) (10,11) (13,14)

The length of class with representative R_6 is 54. Finally we can consider all operations of the form $R_1\sigma_{vi}g_1^mg_2^ng_3^rg_4^s$. It is easy to check that

$R_7 = R_1\sigma_{v2}g_2$ = (3,4) (7,8) (9,12,10,14,11,13) (16,17) (18,19)

Thus we obtained 33 different conjugacy classes of group G. We have summarized our calculations in Table-1.

TABLE-1
REPRESENTATIVES AND SIZES OF THE CONJUGACY CLASSES OF FULL NON-RIGID GROUP OF *cis*-TETRAAMMINEDICLOROCOBALT(III)

No.	Representative	Size	No.	Representative	Size
1	()	1	18	(6,7,8)(12,14,13)(15,17,16)	4
2	(15,16,17)	4	19	(6,7,8)(9,10,11)(15,16,17)	4
3	(12,13,14)	4	20	(6,7,8)(9,10,11)(12,13,14)(15,16,17)	4
4	(12,13,14)(15,16,17)	4	21	(6,7,8)(9,10,11)(12,13,14)(15,17,16)	2
5	(12,13,14)(15,17,16)	4	22	(6,7,8)(9,10,11)(12,14,13)(15,16,17)	4
6	(12,14,13)(15,16,17)	4	23	(6,7,8)(9,10,11)(12,14,13)(15,17,16)	4
7	(12,14,13)(15,17,16)	4	24	(6,7,8)(9,11,10)(12,14,13)(15,17,16)	2
8	(9,10,11)(12,13,14)	2	25	(3,4)(7,8)(9,12)(10,14)(11,13)(16,17)(18,19)	27
9	(9,10,11)(12,13,14)(15,16,17)	4	26	(3,4)(7,8)(9,12,10,14,11,13)(16,17)(18,19)	54
10	(9,10,11)(12,13,14)(15,17,16)	4	27	(2,5)(6,15)(7,16)(8,17)(10,11)(13,14)	27
11	(9,10,11)(12,14,13)	2	28	(2,5)(6,15,7,16,8,17)(10,11)(13,14)	54
12	(9,10,11)(12,14,13)(15,16,17)	4	29	(2,5)(3,4)(6,15)(7,17)(8,16)(9,12)(10,13)(11,14)(18,19)	9
13	(9,11,10)(12,13,14)(15,16,17)	4	30	(2,5)(3,4)(6,15,7,17,8,16)(9,12)(10,13)(11,14)(18,19)	18
14	(6,7,8)(15,16,17)	2	31	(2,5)(3,4)(6,15)(7,17)(8,16)(9,12,10,13,11,14)(18,19)	18
15	(6,7,8)(15,17,16)	2	32	(2,5)(3,4)(6,15,7,17,8,16)(9,12,10,13,11,14)(18,19)	18
16	(6,7,8)(12,13,14)(15,16,17)	4	33	(2,5)(3,4)(6,15,8,16,7,17)(9,12,10,13,11,14)(18,19)	18
17	(6,7,8)(12,13,14)(15,17,16)	4			

By the description in the previous section we have $|G|=\Sigma c_g$ where the sum runs over a set of $g \in G$ using one g from each conjugacy class and c_g is the size of conjugacy class including g. So G has 324 elements.

Now we can use the GAP package and find the character table of G. But in order to find relations between irreducible characters of G we may argue as follows. Since $G/G' \approx Z_2 \times Z_2$, is an abelian group of order 4, we can obtain four linear characters of G, which are irreducible. We denote these irreducible characters by χ_1, χ_2, χ_3 and χ_4.

Now normal subgroups of G are:

$T_1=<(3,4)(7,8)(9,14)(10,13)(11,12)(16,17)(18,19),\ g_4,\ g_1g_4,\ g_1g_2g_3>$

$T_2=<(2,5)(3,4)(6,16,7,15,8,17)(9,13)(10,14)(11,12)(18,19), g_1^{-1}g_4, g_1^{-1}g_2^{-1}g_3g_4>$

$T_3=<(2,5)(6,16)(7,17)(8,15)(10,11)(12,14), g_1g_4, g_3^{-1},\ g_1g_2g_3^{-1}g_4>$

$T_4=<(2,5)(3,4)(6,15)(7,17)(8,16)(9,14,11,13,10,12)(18,19), g_1g_4^{-1},\ g_1g_2^{-1}g_3g_4^{-1}>$

$T_5=<(2,5)(3,4)(6,16,7,15,8,17)(9,14,11,13,10,12)(18,19), g_1g_4^{-1},\ g_1g_2^{-1}g_3g_4^{-1}>$

$T_6=<(2,5)(3,4)(6,17,8,15,7,16)(9,14,11,13,10,12)(18,19), g_1g_4^{-1},\ g_1g_2^{-1}g_3g_4^{-1}>$

$K_1=<g_1g_4,\ g_2^{-1}g_3^{-1}>$

$K_2=<g_1g_4,\ g_2^{-1}g_3>$

$K_3=<g_4^{-1},\ g_1g_4>$

$K_4=<g_1^{-1}g_4,\ g_2^{-1}g_3^{-1}>$

$K_5=<g_1^{-1}g_4,\ g_1g_2^{-1}g_3^{-1}g_4>$

$K_6=<g_1^{-1}g_4,\ g_1^{-1}g_2^{-1}g_3^{-1}g_4^{-1}>$

$K_7=<g_3,\ g_2^{-1}>$

$K_8=<g_1g_2^{-1}g_4,\ g_2^{-1}g_3>$

$K_9=<g_1^{-1}g_2^{-1}g_4^{-1},\ g_2^{-1}g_3>$.

TABLE-2
CHARACTER TABLE OF THE FULL NON-RIGID GROUP OF *cis*-TETRAAMMINEDICLOROCOBALT(III)

	1^{19}	3^1	3^1	3^2	3^2	3^2	3^2	3^2	3^3	3^3	3^2	3^3	3^3	3^2	3^2	3^3	3^3	3^3	3^3	3^4	3^4	3^4	3^4	3^4	2^7	2^46^1	2^6	2^36^1	2^9	2^66^1	2^66^1	2^36^2	2^36^2
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	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	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	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	-1	-1	-1	-1	-1	-1
χ_5	2	-1	2	-1	-1	-1	-1	2	-1	-1	2	-1	-1	2	-1	2	-1	-1	2	2	-1	2	-1	-1	0	0	0	0	-2	1	-2	1	1
χ_6	2	-1	2	-1	-1	-1	-1	2	-1	-1	2	-1	-1	2	-1	2	-1	-1	2	2	-1	2	-1	-1	0	0	0	0	2	-1	2	-1	-1
χ_7	2	-1	2	-1	-1	-1	-1	2	-1	-1	2	-1	-1	-1	2	-1	2	2	-1	-1	2	-1	2	2	0	0	-2	1	0	0	0	0	0
χ_8	2	-1	2	-1	-1	-1	-1	2	-1	-1	2	-1	-1	-1	2	-1	2	2	-1	-1	2	-1	2	2	0	0	2	-1	0	0	0	0	0
χ_9	2	2	-1	-1	-1	-1	-1	2	2	2	-1	-1	-1	2	2	-1	-1	-1	-1	2	2	-1	-1	2	-2	1	0	0	0	0	0	0	0
χ_{10}	2	2	-1	-1	-1	-1	-1	2	2	2	-1	-1	-1	2	2	-1	-1	-1	-1	2	2	-1	-1	2	2	-1	0	0	0	0	0	0	0
χ_{11}	2	-1	-1	-1	2	2	-1	-1	2	-1	2	-1	-1	2	-1	-1	-1	2	-1	-1	2	2	-1	-1	0	0	0	0	-2	1	1	-2	1
χ_{12}	2	-1	-1	-1	2	2	-1	-1	2	-1	2	-1	-1	2	-1	-1	-1	2	-1	-1	2	2	-1	-1	0	0	0	0	2	-1	-1	2	-1
χ_{13}	2	-1	-1	2	-1	-1	2	-1	-1	2	2	-1	-1	2	-1	-1	2	-1	-1	-1	-1	2	-1	2	0	0	0	0	-2	1	1	1	-2
χ_{14}	2	-1	-1	2	-1	-1	2	-1	-1	2	2	-1	-1	2	-1	-1	2	-1	-1	-1	-1	2	-1	2	0	0	0	0	2	-1	-1	-1	2
χ_{15}	2	2	-1	-1	-1	-1	-1	-1	-1	-1	2	2	2	2	2	-1	-1	-1	-1	-1	-1	2	2	-1	0	0	0	0	-2	-2	1	1	1
χ_{16}	2	2	-1	-1	-1	-1	-1	-1	-1	-1	2	2	2	2	2	-1	-1	-1	-1	-1	-1	2	2	-1	0	0	0	0	2	2	-1	-1	-1
χ_{17}	4	-2	-2	1	1	1	1	4	-2	-2	-2	1	1	-2	4	1	-2	-2	1	-2	4	1	-2	4	0	0	0	0	0	0	0	0	0
χ_{18}	4	-2	-2	1	1	1	1	4	-2	-2	-2	1	1	4	-2	-2	1	1	-2	4	-2	-2	1	-2	0	0	0	0	0	0	0	0	0
χ_{19}	4	1	4	1	1	1	1	4	1	1	4	1	1	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	0	0	0	0	0	0	0	0	0
χ_{20}	4	-2	1	1	-2	-2	1	-2	4	-2	-2	1	1	4	-2	1	1	-2	1	-2	4	-2	1	-2	0	0	0	0	0	0	0	0	0
χ_{21}	4	1	-2	1	-2	-2	1	-2	-2	1	4	1	1	-2	-2	1	-2	4	1	1	4	-2	-2	-2	0	0	0	0	0	0	0	0	0
χ_{22}	4	-2	-2	1	1	1	1	-2	1	1	4	-2	-2	-2	4	1	-2	-2	1	1	-2	-2	4	-2	0	0	0	0	0	0	0	0	0
χ_{23}	4	-2	1	-2	1	1	-2	-2	-2	4	-2	1	1	4	-2	1	-2	1	1	-2	-2	-2	1	4	0	0	0	0	0	0	0	0	0
χ_{24}	4	1	-2	-2	1	1	-2	-2	1	-2	4	1	1	-2	-2	1	4	-2	1	1	-2	-2	-2	4	0	0	0	0	0	0	0	0	0
χ_{25}	4	4	1	1	1	1	1	-2	-2	-2	-2	-2	-2	4	4	1	1	1	1	-2	-2	-2	-2	-2	0	0	0	0	0	0	0	0	0
χ_{26}	4	1	-2	A	A	/A	/A	4	1	1	-2	A	/A	-2	-2	1	1	1	1	-2	-2	1	1	-2	0	0	0	0	0	0	0	0	0
χ_{27}	4	1	-2	/A	/A	A	A	4	1	1	-2	/A	A	-2	-2	1	1	1	1	-2	-2	1	1	-2	0	0	0	0	0	0	0	0	0
χ_{28}	4	1	1	A	1	1	/A	-2	-2	1	-2	/A	A	-2	-2	A	1	-2	/A	1	4	1	1	-2	0	0	0	0	0	0	0	0	0
χ_{29}	4	1	1	/A	1	1	A	-2	-2	1	-2	A	/A	-2	-2	/A	1	-2	A	1	4	1	1	-2	0	0	0	0	0	0	0	0	0
χ_{30}	4	-2	1	A	/A	A	/A	-2	1	1	-2	1	1	-2	4	/A	1	1	A	1	-2	1	-2	-2	0	0	0	0	0	0	0	0	0
χ_{31}	4	-2	1	/A	A	/A	A	-2	1	1	-2	1	1	-2	4	A	1	1	/A	1	-2	1	-2	-2	0	0	0	0	0	0	0	0	0
χ_{32}	4	1	1	1	A	/A	1	-2	1	-2	-2	/A	A	-2	-2	/A	-2	1	A	1	-2	1	1	4	0	0	0	0	0	0	0	0	0
χ_{33}	4	1	1	1	/A	A	1	-2	1	-2	-2	A	/A	-2	-2	A	-2	1	/A	1	-2	1	1	4	0	0	0	0	0	0	0	0	0

We can find these normal subgroups using the GAP package. The factor groups of G modulus T_i are non-abelian groups of order 6 and so isomorphic to S_3, the symmetric group on three symbols. Thus we can obtain six irreducible characters of degree 2 of G by lifting irreducible characters of these factor groups. We denote these characters by χ_{16}, χ_{10}, χ_8, χ_6, χ_{14} and χ_{12}. The factor groups of G modulus K_i are isomorphic to $S_3 \times S_3$. Therefore we can obtain nine irreducible characters of degree 4 of G by lifting irreducible characters of these factor groups. We denote these characters by χ_{17}, χ_{22}, χ_{25}, χ_{18}, χ_{20}, χ_{23}, χ_{19}, χ_{24} and χ_{21}. Now put $\chi_5 = \chi_3\,\chi_6$, $\chi_7 = \chi_2\,\chi_8$, $\chi_9 = \chi_2\,\chi_{10}$, $\chi_{11} = \chi_3\,\chi_{12}$, $\chi_{13} = \chi_3\,\chi_{14}$ and $\chi_{15} = \chi_3\,\chi_{16}$. All of these 25 irreducible characters are real valued. It is a well known that g is conjugate to g^{-1} in G if and only if $\chi(g)$ is real for all characters χ of G[32]. Since for every g in the fourth conjugacy class g^{-1} is not in this conjugacy class, so there exist at list one irreducible character χ such that is not real valued. Now we find non-real valued irreducible characters of G. Let

$$N = < g_1^{-1}g_2, g_3g_4, g_1^{-1} >.$$

Then N is an ablelian group of order 27 which is isomorphic to $Z_3 \times Z_3 \times Z_3$ and its character table is well known. Using the irreducible characters of this group we construct irreducible characters of G of degree 4 which is not real valued. Consider below characters as irreducible characters of N

χ = (1,1,1,1,1,1,1,1,1,A,A,A,A,A,A,A,A,A,/A,/A,/A,/A,/A,/A,/A,/A)

ϕ = (1,1,1,1,1,1,1,1,1,/A,/A,/A,/A,/A,/A,/A,/A,/A,A,A,A,A,A,A,A,A,A)

γ = (1,1,1,A,A,A,/A,/A,/A,1,1,1,A,A,A,/A,/A,/A,1,1,1,A,A,A,/A,/A,/A)

ζ = (1,1,1,/A,/A,/A,A,A,A,1,1,1,/A,/A,/A,A,A,A,1,1,1,/A,/A,/A,A,A,A)

δ = (1,1,1,A,A,A,/A,/A,/A,A,A,A,/A,/A,/A,1,1,1,/A,/A,/A,1,1,1,A,A,A)

λ = (1,1,1,/A,/A,/A,A,A,A,/A,/A,/A,A,A,A,1,1,1,A,A,A,1,1,1,/A,/A,/A)

η = (1,1,1,A,A,A,/A,/A,/A,/A,/A,/A,1,1,1,A,A,A,A,A,A,/A,/A,/A,1,1,1)

μ = (1,1,1,/A,/A,/A,A,A,A,A,A,A,1,1,1,/A,/A,/A,/A,/A,/A,A,A,A,1,1,1)

Note that $A = -e^{2\pi i/3} + 2e^{\pi i/3}$ and /A denotes the complex conjugate of A. It is easy to check that χ^G is of degree 12 and $[\chi, \chi_{19}] = 1$ so $\chi - \chi_{19}$ is a character. Further computation yields that $[\chi - \chi_{19}, \chi_{20}] = 1$ so $\chi - \chi_{19} - \chi_{20}$ is also a character of degree 4, but we have $[\chi - \chi_{19} - \chi_{20}, \chi - \chi_{19} - \chi_{20}] = 1$, finally $\chi - \chi_{19} - \chi_{20}$ is an irreducible character of G. We denote this character by χ_{31}. By similarly method we can see that all of $\varphi - \chi_{19} - \chi_{20}$, $\gamma - \chi_{21} - \chi_{25}$, $\zeta - \chi_{21} - \chi_{25}$, $\delta - \chi_{13} - \chi_{14} - \chi_{17}$, $\lambda - \chi_{13} - \chi_{14} - \chi_{17}$, $\eta - \chi_{18} - \chi_{22}$, $\mu - \chi_{18} - \chi_{22}$ are irreducible characters of G of degree 4 which is not real valued. We denote this character by χ_{30}, χ_{26}, χ_{27}, χ_{33}, χ_{32}, χ_{29} and χ_{28}. This completes the character table of G (Table-2).

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