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# extended aromatic C48N12 Azafullerene 

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# Nuclear Spin Statistics of extended aromatic $\mathrm{C}_{48} \mathbf{N}_{12}$ Azafullerene 

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We have presented the nuclear spin statistics of the novel extended aromatic $\mathrm{C}_{48} \mathrm{~N}_{12}$ azafullerene. The nuclear spin multiplets and statistical weights of ${ }^{14} \mathrm{~N}$ spin-1 bosons are provided. In addition we have also provided the ${ }^{13} \mathrm{C}$ nuclear spin species and spin statistical weights of ${ }^{13} \mathrm{C}_{48} \mathrm{~N}_{12}$. The spin statistical weights and spin species show that the presence of ${ }^{14} \mathrm{~N}$ nuclei in the aromatic fullerene can provide unique experimental opportunity to investigate the nuclear spin species.

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## 1. Introduction

As can be seen from the previous paper [1], hereafter to be referred to as I, there is considerable experimental and theoretical interest in novel extended heterofullerene clusters such as $\mathrm{C}_{48} \mathrm{~N}_{12}$ [2-10]. The presence of ${ }^{14} \mathrm{~N}$ nuclei in this cluster can provide opportunity to investigate the spin statistics, as ${ }^{14} \mathrm{~N}$ nuclei are spin- 1 particles. The extended aromatic heterofullerenes have provided new platform to investigate the concept of aromaticity [11,12]. Graph theory and group theory have become particularly useful to study and classify the electronic and spectroscopic properties of fullerenes [1217]. Manaa and others [6-9] have recently studied $\mathrm{C}_{48} \mathrm{~N}_{12}$ and other analogs of extended aromatic fullerenes. They $[6,7]$ have shown that a new isomer of $\mathrm{C}_{48} \mathrm{~N}_{12}$ is $13.1 \mathrm{kcal} / \mathrm{mole}$ energetically more stable than the previously reported isomer by Stafström et al. [3].

In this letter we have considered the nuclear spin species and spin statistical weights of $\mathrm{C}_{48} \mathrm{~N}_{12}$ since ${ }^{14} \mathrm{~N}$ exhibits three nuclear spin orientations, and thus provides interesting experimental opportunity for the investigation of nuclear spin species and statistical weights. This is particularly so since $\mathrm{C}_{48} \mathrm{~N}_{12}$ is very stable and thus generation and spectroscopic characterization of laser-vaporized and cooled $\mathrm{C}_{48} \mathrm{~N}_{12}$ is imminent. From a group theoretical stand point it is quite challenging to enumerate the spin species of $\mathrm{C}_{48} \mathrm{~N}_{12}$, and we have also considered the nuclear spin species of ${ }^{13} \mathrm{C}_{48} \mathrm{~N}_{12}$.

## II. Group Theoretical Analysis of Nuclear Spin Species

Figures 1 of the previous paper I shows two different perspectives of the $\mathrm{C}_{48} \mathrm{~N}_{12}$ isomer. The isomer has an improper $\mathrm{S}_{6}$ axis that passes through the center of cup and cap of the structure as shown on Fig. 1 of the current paper. The overall point group is $S_{6}$, and it is isomorphic to the $\mathrm{C}_{3 \mathrm{~h}}$ symmetry. In order to enumerate the nuclear spin species, it is necessary to seek the effect of the operations generated by $S_{6}$ as permutations of the nuclei. Since we have two kinds of nuclei, namely, C and N , the permutations are partitioned according to their chemical identities. Since the $S_{6}$ group or $C_{3 h}$ has a single generator, namely, the $\mathrm{s}_{6}$ operation, all the operations form conjugacy classes by themselves, and the group is abelian. However, it is traditional to treat the representations that have complex characters in pairs so that we have 2 pseudo two-dimensional representations. The effect of each operation as a permutation can be characterized by its
orbit structure. For example the $c_{3}$ operation generates a permutation of nitrogen nuclei that contains 4 cycles of length 3 , which we denote by $\mathrm{s}_{3}{ }^{4}$, where the superscript is the number of orbits and the suffix is the length of the orbit. Likewise, the inversion operation, $i$, generates 6 cycles of length 2 among the nitrogen nuclei which we characterize by $\mathrm{s}_{2}{ }^{6}$. In this way, we have obtained all permutation representations for the nitrogen and carbon nuclei. It is interesting that the $\mathrm{S}_{6}$ group's character table is generated by powers of $\exp (2 \pi i / 6)$ as it is a cyclic group.

The generation of the nuclear spin species of $\mathrm{C}_{48} \mathrm{~N}_{12}$ involves the construction of the polynomials, which yield the generating functions for the spin- $1{ }^{14} \mathrm{~N}$ nuclear spin functions. The present author [18-20] has formulated operator-based methods, which effectively become the generalized Pólya's theorem [21,22] to all irreducible representations of a group. This was proposed earlier by Williamson [23] and Merris [24] with a single group action and the present author provided a physical interpretation and generalized the technique to multiple group actions. A special case of this operator for the alternating representation was used by King [25-26] to construct chiral isomers with ligand partitions. In the most general case of a group $G$, let us suppose a symmetry operator $\mathrm{T}_{\mathrm{G}}{ }^{\chi}$ is constructed as

$$
T_{G}^{\chi}=\frac{1}{|G|} \sum_{g \varepsilon G} \chi(g) P(g)
$$

where $\chi(\mathrm{g})$ be the character value of $g \varepsilon \mathrm{G}$ for an irreducible representation $\Gamma$ in the group $G$, and $P(g)$ is a permutation operator for $g$. A weighted permutation operator is obtained by introducing a weight $r$ for each kind of color in a set R with D being the set of nitrogen nuclei in $\mathrm{C}_{48} \mathrm{~N}_{12}$. Since the naturally occurring ${ }^{14} \mathrm{~N}$ nucleus is a spin-1 particle, it has three different orientations, and each of those three orientations can be envisaged as a distinct color. Then a nuclear spin function for all 12 nitrogen nuclei can be thought of as a coloring or simply a $\operatorname{map} f$ from the set D to the set R . In combinatorial terms, the weight of a nuclear spin function $f$ from $D$ to $R$ is given by

$$
W(f)=\prod_{i=1}^{n} w(f(i))
$$

We can define a permutational operator for each weight W , and denote it by $\mathrm{P}_{\mathrm{W}}(\mathrm{g})$. In the most general form of matrix representations of $\mathrm{P}_{\mathrm{w}}(\mathrm{g})$, the tensor version of the projection operator for all irreducible representations in the group would simply use the above matrix operators for each representation. As a special case, a more convenient character version is obtained by considering the trace of $\mathrm{P}_{\mathrm{w}}(\mathrm{g})$ given by

$$
\operatorname{Tr}\left(P_{w}(g)\right)=\sum_{f}^{(g)} W(f)
$$

where the sum is over all f for which $\mathrm{gf}=\mathrm{f}$, and thus

$$
\begin{aligned}
& T_{G}^{W, \chi}=\frac{1}{|G|} \sum_{g \varepsilon G} \chi(g) P_{W}(g) \\
& \operatorname{Tr} T_{G}^{W, \chi}=\frac{1}{|G|} \sum_{g \varepsilon G} \chi(g) \operatorname{Tr}\left[P_{W}(g)\right]=\frac{1}{|G|} \sum_{g \varepsilon G} \chi(g) \sum_{f}^{(g)} W(f)
\end{aligned}
$$

It can be shown that this amounts to replacement of every $\mathrm{s}_{\mathrm{k}}$ in the generalized character cycle index $(\mathrm{GCCI}) \mathrm{P}_{\mathrm{G}}{ }^{\chi}$ for every irreducible representation as defined below:

$$
P_{G}^{\chi}=\frac{1}{|G|} \sum_{g \varepsilon G} \chi(g) s_{1}^{b_{1}} s_{2}^{b_{2}} \ldots . . s_{n}^{b_{n}}
$$

where the sum is over all elements of the group, and $s_{1}^{b_{1}} s_{2}^{b_{2}} \ldots . . s_{n}^{b_{n}}$ is the cyclic polynomial representation if $g$ in $G$ generates $b_{1}$ cycles of length $1, b_{2}$ cycles of length $2, \ldots . b_{n}$ cycles of length $n$ when $g$ acts on the set of elements $D$. We carry out a trinomial replacement of every $s_{k}$ in the above expression for the nitrogen nuclear spins since each nucleus has 3 possible spin orientations. Let $\lambda_{1}, \lambda_{2}$, and $\lambda_{3}$ be three distinct weights for the three nuclear spin projections. The trinomial function is computed by replacing every $\mathrm{s}_{\mathrm{k}}$ in the above GCCI by $\lambda_{1}^{k}+\lambda_{2}^{k}+\lambda_{3}^{k}$. That is,

$$
G F^{\chi}=P_{G}^{\chi}\left(s_{k} \rightarrow \sum_{i} \lambda_{i}^{k}\right)
$$

The GF thus obtained above provides for generating functions for the ${ }^{14} \mathrm{~N}$ nuclear spin functions that transform according to the irreducible representation $\Gamma$ whose character is $\chi$. In general, multinomial expansions are constructed in terms of ordered partitions of $n$, denoted by, [ $n$ ] into p parts (composition of the integer n into p parts) where $\mathrm{p}=3$ for the ${ }^{14} \mathrm{~N}$ nuclei such that $n_{1} \geq 0, n_{2} \geq 0, \ldots . ., n_{p} \geq 0, \quad \sum_{i=1}^{p} n_{i}=n$.

A multinomial expansion in $\lambda$ 's is defined as

$$
\left(\lambda_{1}+\lambda_{2}+\ldots . \lambda_{p}\right)^{n}=\sum_{[\lambda]}\left(\begin{array}{ccccc} 
& n & \\
& n_{2} & \cdot & . & n_{p}
\end{array}\right) \lambda_{1}^{n_{1}} \lambda_{2}^{n_{2}} \ldots \lambda_{p}^{n p}
$$

where $\left(\right.$|  | $n$ |  |  |  |
| :--- | :--- | :--- | :--- | :--- |
| $n_{1}$ | $n_{2}$ | . | . |  |
| $n_{p}$ |  |  |  |  |$)$ are the multinomial coefficients and the sum is over all such ordered partitions. The multinomial coefficients are computed as

$$
\left( n_{p} .\right)=\frac{n!}{n_{1}!n_{2}!\ldots . . . n_{p}!}
$$

As we have shown above, the various terms in the GF have all ordered partitions of $n$ into various parts given by their Young's diagrams. The terms in the complete generating function that are combinatorially equivalent such as the terms $\lambda_{1}^{8} \lambda_{2}^{2} \lambda_{3}^{2}$, $\lambda_{1}^{2} \lambda_{2}^{8} \lambda_{3}^{2}, \lambda_{1}^{2} \lambda_{2}^{2} \lambda_{3}^{8}$, etc., all have equal coefficients in the multinomial expansion. The unique terms of the multinomial $\mathrm{GF}^{\chi}$, s are the Young diagrams of partitions n into various parts.

When these representations are multiplied by the corresponding character values, we obtain the GCCI for the particular set of nuclei and the irreducible representation. To illustrate, consider the ${ }^{14} \mathrm{~N}$ nuclei of $\mathrm{C}_{48} \mathrm{~N}_{12}$ and the $\mathrm{E}_{\mathrm{u}}$ representation. The GCCI polynomial is constructed for this case as

$$
P_{S_{6}}^{E_{u}}=\frac{1}{6}\left[2 s_{1}^{12}-2 s_{3}^{4}-2 s_{2}^{6}+2 s_{6}^{2}\right]
$$

If we replace every $\mathrm{s}_{\mathrm{k}}$ by $\sum_{i=1}^{3} \lambda_{i}^{k}$ in the above expression, we obtain,

$$
\begin{aligned}
& P_{S_{6}}^{E_{u}}=\frac{1}{6}\left[2\left(\lambda_{1}+\lambda_{2}+\lambda_{3}\right)^{12}-2\left(\lambda_{1}+\lambda_{2}+\lambda_{3}\right)^{4}\right. \\
& \left.-2\left(\lambda_{1}+\lambda_{2}+\lambda_{3}\right)^{6}+2\left(\lambda_{1}^{6}+\lambda_{2}^{6}+\lambda_{3}^{6}\right)^{2}\right]
\end{aligned}
$$

The above expression can be simplified and the coefficients of the various terms can be collected together. It can be seen that the powers of the above trinomial are partitions of integer 12 into 3 parts and the coefficients of the terms $\lambda_{1}^{8} \lambda_{2}^{2} \lambda_{3}^{2}, \lambda_{1}^{2} \lambda_{2}^{8} \lambda_{3}^{2}, \lambda_{1}^{2} \lambda_{2}^{2} \lambda_{3}^{8}$, etc are equivalent. Thus we construct a table of young diagrams for partitioning 12 into 3 parts, and the corresponding coefficients for each irreducible representation of the $\mathrm{S}_{6}$ group as obtained from the above generating functions. Table 1 shows these combinatorial numbers together with the Young diagrams for the spin- $1{ }^{14} \mathrm{~N}$ nuclei. As can be seen from Table 1, the Young diagrams of 12 for ${ }^{14} \mathrm{~N}$ bosons can have at most 3 rows. This is a natural combinatorial consequence of the trinomial generating functions, but it also follows from the fact that spin- 1 particles can have at most 3 rows due to three possible spin projections for ${ }^{14} \mathrm{~N}$.

The coefficients in Table 1 can be sorted according to the total $\mathrm{M}_{\mathrm{F}}$ values for each of the spin functions. When the resulting spin functions are sorted according to their $\mathrm{M}_{\mathrm{F}}$ values they span nuclear spin multiplets with $\mathrm{M}_{\mathrm{F}}$ values varying from $-\mathrm{I},-\mathrm{I}+1,-$ $\mathrm{I}+2, \ldots . .0, \ldots . \mathrm{I}-1, \mathrm{I}$ for a general integer I. The nuclear spin functions are thus grouped according to their spin multiplicities and are shown in Table 2 for the ${ }^{14} \mathrm{~N}$ nuclear spin functions as well as ${ }^{13} \mathrm{C}$ spin functions of $\mathrm{C}_{48} \mathrm{~N}_{12}$. The naturally occurring cluster of $\mathrm{C}_{48} \mathrm{~N}_{12}$ would have the nuclear spin species shown in Table 2 for the nitrogens for the $\mathrm{S}_{6}$ symmetry isomers.

We have also considered the labeled carbon isomers corresponding to ${ }^{13} \mathrm{C}_{48} \mathrm{~N}_{12}$. Since there are $2^{48}$ nuclear spin functions for the ${ }^{13} \mathrm{C}$ nuclei the combinatorics is more involved for the carbon nuclei. A similar procedure was used to sort out the coefficients in the combinatorial generating functions, and the results of the ${ }^{13} \mathrm{C}$ nuclear spin species are shown in Table 2. As can be seen from Table 2, the number of nuclear spin multiplets for the ${ }^{13} \mathrm{C}$ nuclei becomes astronomical due to the presence of $48{ }^{13} \mathrm{C}$ nuclei.

An interesting aspect of table 2 is the difference in the spin populations of the $u$ and $g$ parities. For example, the spin multiplet with the multiplicity of 47 has $8 A_{u}$ and $7 \mathrm{~A}_{g}$ representations. Likewise the multiplet with $2 \mathrm{I}+1=45$ has a frequency of 184 for $\mathrm{A}_{\mathrm{g}}$ and 176 for $\mathrm{A}_{\mathrm{u}}$ for the carbon species. The nitrogen species, which can be probed in their natural isotopic abundance, also exhibit appreciable differences in the g and u parties. It remains to be seen if these parity differences that we have predicted for $\mathrm{C}_{48} \mathrm{~N}_{12}$ can be observed experimentally. Table 3 shows the actual nuclear spin statistical weights as obtained by summing the spin multiplicity times the frequencies and then stipulating the antisymmetrization of the total wave function as required by the Pauli principle.

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Table 1 Generating Functions for the Gel'fand states of ${ }^{14} \mathrm{~N}$ bosonic Statistics of $\mathrm{C}_{48} \mathrm{~N}_{12}$



Table $2{ }^{14} \mathrm{~N}$ Nuclear Spin Species and ${ }^{13} \mathrm{C}$ species of $\mathrm{C}_{48} \mathrm{~N}_{12}$ in the $\mathrm{S}_{6}$ group

| IR | Spin species |
| :---: | :---: |
| $\begin{aligned} & \mathrm{A}_{\mathrm{g}-} \\ & { }^{4} \end{aligned}$ | ${ }^{1} \mathrm{Ag}_{\mathrm{g}}(733){ }^{3} \mathrm{~A}_{\mathrm{g}}(1862)$ ${ }^{5}{ }^{5} \mathrm{Ag}_{\mathrm{g}}(2520)$${ }^{7} \mathrm{Ag}(2480){ }^{9}{ }^{9} \mathrm{Ag}_{\mathrm{g}}(2028){ }^{11}{ }^{11} \mathrm{Ag}_{\mathrm{g}}(1348){ }^{13} \mathrm{Ag}(786)$ |
| $\begin{gathered} { }_{14}{ }_{14} \mathrm{~N} \end{gathered}$ | ${ }^{1} \mathrm{~A}_{\mathrm{u}}(684)$ ${ }^{15} \mathrm{~A}_{\mathrm{u}}(372){ }^{3} \mathrm{~A}_{\mathrm{u}}(1904){ }^{17} \mathrm{~A}_{\mathrm{u}}(140){ }^{5}{ }^{19} \mathrm{~A}_{\mathrm{u}}(2478){ }^{7} \mathrm{~A}_{\mathrm{u}}(48){ }^{21} \mathrm{~A}_{\mathrm{u}}(2510)$ $\mathrm{A}_{\mathrm{u}}(10){ }^{9}{ }^{23} \mathrm{~A}_{\mathrm{u}}(2)$ |
| ${ }_{14}^{\mathrm{E}_{\mathrm{g}}} \mathrm{N}$ | $\begin{aligned} & { }^{1} \mathrm{E}_{\mathrm{g}}(1444){ }^{3} \mathrm{E}_{\mathrm{g}}(3724){ }^{5} \mathrm{E}_{\mathrm{g}}(5056){ }^{7} \mathrm{E}_{\mathrm{g}}(4944){ }^{9} \mathrm{E}_{\mathrm{g}}(4056){ }^{11} \mathrm{E}_{\mathrm{g}}(2708){ }^{13} \mathrm{E}_{\mathrm{g}}(1560) \\ & { }^{15} \mathrm{E}_{\mathrm{g}}(730){ }^{17} \mathrm{E}_{\mathrm{g}}(298){ }^{19} \mathrm{E}_{\mathrm{g}}(88){ }^{21} \mathrm{E}_{\mathrm{g}}(24){ }^{23} \mathrm{E}_{\mathrm{g}}(4) \end{aligned}$ |
| $\begin{aligned} & { }^{{ }^{14} \mathrm{~N}} \mathrm{~N} \end{aligned}$ | ${ }^{1} \mathrm{E}_{\mathrm{u}}(1352)$ ${ }^{3} \mathrm{E}_{\mathrm{u}}(744){ }^{17}(3808){ }^{17} \mathrm{E}_{\mathrm{u}}(284){ }^{5}{ }^{5} \mathrm{E}_{\mathrm{u}}(4972) \mathrm{E}_{\mathrm{u}}(92){ }^{21} \mathrm{E}_{\mathrm{u}}(5004){ }^{21} \mathrm{E}_{\mathrm{u}}(20){ }^{93}{ }^{9} \mathrm{E}_{\mathrm{u}}(4)$ |
| $\begin{gathered} \mathrm{A}_{\mathrm{g}} \\ { }^{13} \mathrm{C} \end{gathered}$ | $\begin{aligned} & { }^{1} \mathrm{~A}_{\mathrm{g}}(5372453585209){ }^{3}{ }^{3} \mathrm{~A}_{\mathrm{g}}(5157469105649) \\ & { }^{7} \mathrm{~A}_{\mathrm{g}}{ }^{5} \mathrm{~A}_{\mathrm{g}}(4562129145985) \\ & { }^{13}(371689397921){ }^{9} \mathrm{Ag}_{\mathrm{g}}(2787132751545) \\ & { }^{11} \mathrm{~A}_{\mathrm{g}}(1921493832433) \\ & \mathrm{Ag}_{\mathrm{g}}(1216158903809){ }^{15} \mathrm{Ag}_{\mathrm{g}}(705256097105){ }^{17} \mathrm{~A}_{\mathrm{g}}(373660791206) \\ & { }^{19} \mathrm{Ag}_{\mathrm{g}}(180062531033){ }^{21}{ }^{21} \mathrm{Ag}_{\mathrm{g}}(78239344577){ }^{23} \mathrm{~A}_{\mathrm{g}}(30007224569) \\ & { }^{25} \mathrm{Ag}_{\mathrm{g}}(9463961813){ }^{27} \mathrm{~A}_{\mathrm{g}}(2675740328){ }^{29} \mathrm{Ag}_{\mathrm{g}}(810608440) \\ & { }^{31} \mathrm{~A}_{\mathrm{g}}(216624690){ }^{33} \mathrm{~A}_{\mathrm{g}}(50621758){ }^{35} \mathrm{Ag}_{\mathrm{g}}(10225880){ }^{37} \mathrm{~A}_{\mathrm{g}}(1760248){ }^{39} \mathrm{~A}_{\mathrm{g}}(252908) \\ & { }^{41} \mathrm{Ag}_{\mathrm{g}}(29588){ }^{43} \mathrm{~A}_{\mathrm{g}}(2696){ }^{45} \mathrm{Ag}_{\mathrm{g}}(184){ }^{47} \mathrm{Ag}_{\mathrm{g}}(7){ }^{49} \mathrm{Ag}_{\mathrm{g}}(1) \end{aligned}$ |
| $\begin{aligned} & \mathrm{A}_{\mathrm{u}} \\ & { }^{13} \mathrm{C} \end{aligned}$ | ${ }^{1} \mathrm{~A}_{\mathrm{u}}(5372452683777){ }^{3} \mathrm{Au}(5157469105649){ }^{5} \mathrm{Au}(4562128313937)$ ${ }^{7} \mathrm{Au}(3716892397921)$ ${ }^{9}{ }^{9} \mathrm{~A}_{\mathrm{u}}(2787132097793){ }^{11} \mathrm{Au}(1921493832433)$ ${ }^{13} \mathrm{Au}(1216158467937)$ ${ }^{15} \mathrm{Au}(705256097105)$ ${ }^{17} \mathrm{Au}(2675754496) \mathrm{A}_{\mathrm{u}}(9463916929.0)$ ${ }^{27} \mathrm{Au}(180062531033){ }^{29} \mathrm{Au}(810594272){ }^{23} \mathrm{Au}(216628232){ }^{25} \mathrm{~A}_{\mathrm{u}}(373660546049)$ ${ }^{35} \mathrm{Au}(10226560){ }^{37} \mathrm{Au}(1759568){ }^{39} \mathrm{Au}(253000){ }^{31} \mathrm{Au}(30007224569){ }^{41} \mathrm{Au}(29496){ }^{43} \mathrm{Au}(50618216)$ ${ }^{45} \mathrm{Au}(176){ }^{47} \mathrm{Au}(8)$ |
| $\begin{aligned} & \mathrm{E}_{\mathrm{g}} \\ & { }^{13} \mathrm{C} \end{aligned}$ | ${ }^{1} \mathrm{E}_{\mathrm{g}}(10747054641125){ }^{3} \mathrm{Eg}(10317085694945){ }^{5} \mathrm{Eg}(9126405775617)$ <br> ${ }^{7} \operatorname{Eg}(7435932268049){ }^{9} \operatorname{Eg}(5576412986737){ }^{11} \operatorname{Eg}(3845135148513)$ <br> ${ }^{13} \operatorname{Eg}(2434465283201){ }^{15} \operatorname{Eg}(1412659677857){ }^{17} \operatorname{Eg}(749469066059)$ <br> ${ }^{19} \operatorname{Eg}(362272541345){ }^{21} \operatorname{Eg}(158626172801){ }^{23} \operatorname{Eg}(62161932785)$ <br> ${ }^{25} \operatorname{Eg}(21075405425){ }^{27} \operatorname{Eg}(5384249809){ }^{29} \operatorname{Eg}(1621217440)$ <br> ${ }^{31} \operatorname{Eg}(433248820){ }^{33} \operatorname{Eg}(101243516){ }^{35} \operatorname{Eg}(20451888)$ <br> ${ }^{37} \operatorname{Eg}(3520368){ }^{39} \operatorname{Eg}(505816){ }^{41} \operatorname{Eg}(59192){ }^{43} \operatorname{Eg}(5376){ }^{45} \operatorname{Eg}(368){ }^{47} \mathrm{Eg}_{\mathrm{g}}(16)$ |
| $\begin{aligned} & { }^{{ }^{13}}{ }_{\mathrm{u}} \mathrm{C} \end{aligned}$ |  |

Table 3 Nuclear Spin Statistical Weights of the rovibronic levels of $\mathrm{C}_{48} \mathrm{~N}_{12}$.

| IR | Nuclear Spin Statistical Weights |
| :--- | :--- |
| $\mathrm{A}_{\mathrm{g}}$ | 88725 |
| $\mathrm{~A}_{\mathrm{u}}$ | 88476 |
| $\mathrm{E}_{\mathrm{g}}$ | 177360 |
| $\mathrm{E}_{\mathrm{u}}$ | 176880 |

## Figure Captions

Fig. 1 The triphenylene structure fused with five-membered heterocycles containing Nitrogens is the cup and cap of the $\mathrm{C}_{48} \mathrm{~N}_{12}$ structure. The $\mathrm{S}_{6}$ axis passes through the center of the hexagons forming the cup and cap.


Fig 1 Balasubramanian


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