

**Determinable partitional modelling of Cayleyan**  
 **$SU(m \leq n/2) \times \mathcal{S}_n \downarrow \mathcal{G}$  NMR spin symmetries of**  
**isotopomeric cage-clusters:**  
**Specific  $\mathcal{S}_{n \geq 12} \supset \dots \supset \mathcal{D}_3$  group chains,**  
**for  $\mathcal{S}_n$ -modules in high- $n$  weak-branching limit**

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The use over certain modestly branched  $(\lambda \vdash n)$  partitional models of Young's  $\mathcal{S}_n$ -module decomposition algorithm in the high- $n$  limit is considered for  $SU(m) \times \mathcal{S}_n (\downarrow \mathcal{G})$  nuclear spin algebras associated with both NMR and ro-vibrational (R-V) aspects of specific cluster isotopomers. This approach allows additional dual-group projective mapping over simple Hilbert spaces to be derived from the natural embedding of higher finite groups in specific  $\mathcal{S}_n$  groups, for either the original simply-reducible (SR)  $SU(2)$ -, or various related higher non-SR  $SU(m) \times \mathcal{S}_n$ , forms. The work arises from earlier interests in the NMR spin symmetry of the  $[^{11}\text{B} \text{ } ^1\text{H}]_{12}^{2-}$  borohydride anions and the nature of analogous ro-vibrational (R-V) spin statistical problems for higher  $n \geq 12$ -fold clusters. Here, the role of the scalar invariants is shown to be critical in determining the spin algebras of isotopomeric clusters within Cayley's theorem for some particular depth of  $SU(m)$  branching in the  $SU(m) \times \mathcal{S}_n$  dual-group algebra. Certain additional quasi-geometric models for the full  $\lambda (\geq \lambda_{\text{SA}})$  (self-associate) dominant-sector set of  $(\lambda \vdash n)$  partitions-of- $n$  are discussed, in the context of specific determinacy of natural  $\mathcal{S}_n \supset \mathcal{G}$  group embeddings at a given branching level.

## 1. Introduction

Physical insight into the nature of  $n$ -fold identical spin many-body problems of NMR [1–5] owes much to the early work of Corio [1], Jones [2] and, from its further realisation under an automorphic group which may be related to the purely rotational symmetry operations [5], to that of Balasubramanian [6] in the 1980s. These concepts apply to “rigid” molecules, which on NMR time-scales are rapidly tumbling in a fluid medium.

The Biedenharn and Louck [7] viewpoint of (boson) mapping arising from dual-group projective operators over a carrier space and other mathematical studies of scalar invariants [4] and Cayley algebras [8] allow various extensions to these

ideas; in addition once  $n \geq 6$ -fold spin cluster problems are considered, the concept of induced (subduced) representations [9] and the body of generalised mathematical work on the  $\mathcal{GL}(n, \mathbb{C})$  and  $S_n$  groups [9–11] play an essential role. The contrasting nonrigid multi-cluster NMR problem was originally treated by Longuet-Higgins [12] in 1963, prior to it being perceived as an aspect of semi-direct product symmetry [13], or more generally as a generalised wreath-product spin symmetry [14]. Applications in both NMR and ro-vibrational (R-V) statistical spectra have been discussed by Balasubramanian [15]. For the purposes of the present paper, we shall not dwell on the case of non-rigid NMR forms, beyond noting its close association with representations of the symmetric groups [11a, b].

The work reported here arises from the projective aspects of  $(\lambda \vdash n)$  partitions-of- $n$ , with quasi-geometric parallels within their  $S_n \downarrow \mathcal{G}$  models. It has some similarity to ideas developed by Coxeter, and referred to by him as polytopes [16]. Our present models are  $S_n$ -modules which are amenable to  $S_n$ -algorithmic decomposition [10]. This is determined by the level of their  $SU(p)$  ( $p \leq m$ ) branching. They are also  $(\lambda \vdash n)$  partitional models of  $SU(m) \times S_n \downarrow \mathcal{G}$  subduced spin algebras for general  $[A]_n$ ,  $[AX]_n^{(I)}$  specific isotopomeric clusters. Hence, the irrep structure of each monocluster originates from a set of model  $(\lambda \vdash n) \equiv \{:\lambda:\}$  partitions [10] over the  $M$ -weights of  $\{|IM\rangle\}$ .

Indeed for NMR, it has been established [17] that the  $p \leq m$   $SU(p)$  branched partitions of all possible orderings over the full  $SU(m)$  fields constitute a complete set, defining the bases of all identical  $n$ -fold  $I_i$ -type spin clusters. Use of the (inner) direct product formalisms extends these results from (theoretical) monoclusters to all  $[AX \dots]_n$ -type NMR systems [18].

Since the implicit recoupling of spins considered in the context of rovibrational (R-V) spin statistics has analogous origins, the conceptual ideas given here likewise apply to the study of many cluster R-V spectroscopic ‘weight’ problems.

The advent of pulse-NMR [19] has led one to consider the symmetry aspects [5,20,21] inherent in such formalisms and how extended projective mapping [22] ideas apply over augmented spin spaces. The most notable feature here is the need to retain the  $\nu$ -recoupling labelling in describing the  $\mathbb{H}_\nu$  carrier subspaces [22] from which arise the full set of  $\{D^k(\tilde{U}) \times \tilde{\Gamma}^{(\lambda)}(\nu)\}$  ( $SU(2) \times S_n$ ) irreps. For more general  $I_i$  isotopomeric clusters, some initial insight into the simple Hilbert space aspects is an essential pre-requisite. We shall focus here on extending a recent discussion of the identical-H(D) 12-fold  $^{11}\text{B}$ -borohydride ions [23] to the (10, 11, 12) trideutero, the (1, 2, 3, 10, 11, 12) or the (4, 5, 6, 7, 8, 9) hexadeutero [ $^{11}\text{B}_{12}\text{H}_{12-nn}\text{D}_{nn}$ ] $^{2-}$  and related isotopomeric molecular forms, in respect of the novel  $[A]_n^{(I)}$  monocluster aspects. The recursive inner product aspects required to define the full NMR system, or R-V cluster species, is too extensive and well-known a topic to give here in any detail. For any present purposes, we stress general conceptual aspects of the modelling from  $(\lambda \vdash n)$  partitions. In particular, two aspects of dual group mapping are focussed on for their importance in typical models of the specific  $S_n \supset \mathcal{G}$  natural embeddings to which Cayley’s theorem applies [24,25].

## 2. Origins of low- $m$ branched higher- $n$ ( $\lambda \vdash n$ ) model limit for module decomposition

The use of ( $\lambda \vdash n$ ) partitions-of- $n$  in modelling higher dual unitary spin algebras and in demonstrating the completeness of the hierarchy of all reordered forms (over full  $SU(m)$  fields) has been given in our 1990 work [17]. Subsequently, we have examined the value of the higher- $n$  limit of  $S_n$ -module decomposition of such modest  $SU(m)$  branched (numeric) models, using the algorithmic techniques of enumeration of the associated Kostka coefficients [26,27] presented by Sagan [10]. Such discussions of Young's rule are based on fitting semi-normal contents to Young box tableaux shapes. Provided the branching of interest is of a low/modest form, the consequence of such enumerative techniques generates some limiting set of Kostka  $\{\Lambda_{\lambda[\lambda']}\}$  coefficients, once a certain (high) value of  $n$  is reached, i.e. without any further variation in the  $\{\Lambda_{\lambda[\lambda']}\}$  set with incremental- $n$ , for the specific  $m$ -branching. Here, the ' $m$ ' corresponds to a value of  $(2I_i + 1)$  and ' $n$ ' to the  $[A]_n$  spin cluster size, respectively.

Given its combinatorial derivation, it would be surprising if there were not a limiting form for the  $\{\Lambda_{\lambda[\lambda']}\}$  set. In addition, certain standard requirements apply: e.g., the initial  $\Lambda_{\lambda[n]}$  and final  $\Lambda_{\lambda[\lambda'=\lambda]}$  components of the set are necessarily unity, or

$$\Lambda_{\lambda[n]} = \Lambda_{\lambda[\lambda]} = 1. \tag{1}$$

To demonstrate the general limits we shall consider the  $SU(3)$  and  $SU(4)$  branchings for  $\lambda \equiv :n - 4, 22:$  and  $\lambda \equiv :n - 4, 211:$ , in contrast to the  $SU(6)$  branching  $:n - 5, 1^5:$  under  $:\lambda: \equiv (\lambda \vdash n)$   $S_n$ -module decomposition. The ' $n$ ' of the partitions considered here will be taken as some values typical of spin clusters associated with borohydride ions or fullerene clusters: viz.  $n = 6$  (8) in the lower range, or  $n = (10)$  12 (14) and  $n = 20$  (24) in the higher region.

For our first two example of  $S_n$ -modules – initially with  $n = 6$  (8, 12) – it may be demonstrated that

$$\begin{aligned} :\lambda: = :n - 4, 22: &\rightarrow \{[n], 2[n - 1, 1], 3[n - 2, 2], [n - 2, 11]; \\ &a[n - 3, 3], 2[n - 3, 21], -, [n - 4, 22]\} \end{aligned} \tag{2a}$$

and

$$\begin{aligned} :\lambda': = :n - 4, 211: &\rightarrow \{[n], 3[n - 1, 1], 4[n - 2, 2]3[n - 2, 11]; \\ &b[n - 3, 3], 4[n - 3, 21], [n - 3, 1^3]; \dots [n - 4, 22], [n - 4, 211]\}, \end{aligned} \tag{3a}$$

within which the numeric ' $a$ ' and ' $b$ ' values for these  $S_6$ -modules are non-maximal (or subset(s) of  $\Lambda$ s) with ' $a$ ' = 1 and ' $b$ ' = 2, compared to those for higher  $S_n$ -mod-

ules. Naturally, only a restricted subset  $\{\cdot, \cdot, [n - 4, 22]\}$  of irreps occurs and these are late in-dominance-sequence irreps, and so frequently associated with *unit* Kostka coefficients.

In contrast with the higher  $n = 12$  case, one finds now ‘ $a$ ’ = 2 and ‘ $b$ ’ = 3 in their respective decompositions; these *now correspond* to the high- $n$  limit. In consequence, the module(s) decompose into

$$:n - 4, 22: \rightarrow \{[n], 2[n - 1, 1], 3[n - 2, 2], [n - 2, 11];$$

$$2[n - 3, 3], 2[n - 3, 21], -; [n - 4, 4], 2[n - 4, 31], [n - 4, 22]\}, \tag{2b}$$

$$:n - 4, 211: \rightarrow \{[n], 3[n - 1, 1]4[n - 2, 2], 3[n - 2, 11];$$

$$3[n - 3, 3], 4[n - 3, 21], [n - 3, 1^3];$$

$$[n - 4, 4], 2[n - 4, 31], [n - 4, 22], [n - 4, 211]\}. \tag{3b}$$

On considering the  $\lambda = :n - 5, 1^5:$  module as an aspect of  $SU(6)$  branching – utilising a more compact notation – one finds that

$$:n - 5, 1^5:(\mathcal{S}_7) = \{1, 5, 10, 10; \underline{9}, 20, 10; -, \underline{11}, 10, 15, 5; -, -, 5, 4, 1\} \mathcal{L}, \tag{4a}$$

$$:\lambda:(\mathcal{S}_8) = \{1, 5, 10, 10; 10, 20, 10; \underline{4}, 15, 10, 15, 5; 5, 6, 5, 4, 1\} \mathcal{L}, \tag{4b}$$

where  $\mathcal{L}^\dagger$  is the *unit* (standard dominance ( $\geq$  ordered) set of  $S_n$ -irreps and now the non-maximal coefficients of a *subset* are shown underlined. The final limiting set of Kostka coefficients (for  $12 \leq n \leq 20, \dots$ ) for  $:\lambda = :n - 5, 1^5:$  spans

$$:\lambda:(\mathcal{S}_{n \geq 12}) = \{1, 5, 10, 10; 10, 20, 10; 5, 15, 10, 15, 5; 1, 4, 5, 6, 5, 1\} \mathcal{L}, \tag{4c}$$

where we have used the  $Z(\mathcal{S}_{12})$  characters established by Ziauddin [28] in the mid-1930s. In all of the above examples, the  $S_n$ -algorithm adopted within the conventions of ref. [10] may be realised [26,27] simply as

$$\Lambda_{\lambda[\lambda]} = i, \text{ final; from } \sum_i \oplus (\text{shape } \lambda'; \text{ semi-normal contents } \lambda). \tag{5}$$

There is a possible alternative method which derives the Kostka coefficients from the  $\xi^{\lambda:}(\mathcal{C})$  Young permutational characters, by working back from the least dominant  $:1^n:$  properties and noting that the  $\{\Lambda_{\lambda[\lambda]}\}$  associated with the  $:1^n:$  module are identical to the  $Z(\mathcal{S}_n)$  principal characters of a specific symmetric group. The upper-left skew-triangular form of the  $\xi^{\lambda:}(\mathcal{C}(\mathcal{S}_n))$  sets was given in ref. [27] for  $6 \leq n \leq 8 S_n$  groups. Also, the form of the Kostka coefficients within this projective formalism follows directly from the definition [10] of a  $S_n$ -module:

$$\Lambda_{\lambda^{[\lambda]}} = \{ \xi_{i=1}^{:\lambda} \times \chi_{i=1}^{[\lambda]} + \sum_{i=2} g_i \xi_i^{:\lambda} \chi_i^{[\lambda]} \} // \mathcal{G} / . \tag{6}$$

This approach starting from the least-dominant sector is complementary to the earlier one for model  $S_n$ -module decompositions. The value of such modelling [23,29] and of all these results for spin (cage) clusters arises from combining these theoretical aspects with certain projective invariance properties for  $:\lambda:$  models under the isomorphic rotational symmetry  $S_n \downarrow \mathcal{G}$ . This implies the  $S_n \supset \mathcal{G}$  embedding is a natural one, which is determinate up to and including the specific  $SU(m)$  branch depth being investigated.

**3. Realisation of  $\{[\lambda](S_n) \rightarrow \Gamma\}$  correlative mappings for general  $SU(m \geq 3)$  branchings**

From the established Kostka coefficient and the determinable  $\{\chi_i(\mathcal{C})\}(S_n \downarrow \mathcal{G})$  properties of the  $:\lambda:$  models under the automorphic spin symmetry, one has a direct pathway to establishing the  $[\lambda]$  symmetry correlated to the irreps of some naturally embedded finite group. The method of calculation follows the difference scheme from the most significant  $\{[n], [n - 1, 1], \dots\}$  ( $\geq [\lambda_{SA}]$ ) sector of the hierarchy, using the Kostka terms in sequential calculations, as a straightforward extension to the method given by Corio [1] in discussing the (simply reducible  $\Lambda_{\lambda^{[\lambda]}} = 1$ )  $SU(2)$  dual group invariance properties, as for the bi-partite irreps:

$$[n - r, r] \equiv :n - r, r: - :n - r + 1, r - 1:, \quad \forall 1 \leq r < n/2 . \tag{8}$$

The form of calculation which follows from the recursive use of

$$[\lambda] = [n - r, r - r', r'] = : \lambda : - \sum_{\lambda' \preceq \lambda} \Lambda_{\lambda^{[\lambda]}[\lambda']} \tag{9}$$

is given in some detail in earlier work [26,29], and in the context of model  $:\lambda:(S_{12})$  modules in two recent papers [23]; it is rather too lengthy to include here in any detail, but may be found in the appendices to ref. [23b]. It suffices to point out that the recursive sequence of difference calculations starts from the least branched  $S_n$ -modules, and proceeds by evaluating all members of the  $\{[n - r, r], [n - r - 1, r, 1], [n - r - 2, r, 2], \dots, [n - r - 2, r, 1, 1], [n - r - 3, r, 2, 1], \dots\}$  hierarchies, since the higher branching aspects in any one  $SU(m) \times S_n$  algebra, e.g.,  $[\lambda] = [n - 4, 2, 2]$  or  $[n - 5, 3, 1, 1]$ , do not occur in either of the *lower-r*  $:\lambda: = :n - r - 1, r, 1:$ , or,  $:n - r - 2, r, 1, 1:$   $S_n$ -modules. The power of the approach will be appreciated by noting that it gives the following representative examples of  $\{[\lambda] \rightarrow \Gamma\}(S_{12})$  mappings from the  $[^{11}B]_{12}$  monocluster:

$$[6, 6] \rightarrow \{10, 10, 14, 2, 2\} \mathcal{V}(S_{12} \downarrow A_5 \equiv \mathcal{I}) , \tag{10}$$

$$[6, 51] \rightarrow \{16, 75, 97, 59, 59\} \mathcal{V}^\dagger, \tag{11}$$

$$[6, 42] \rightarrow \{55, 197, 234, 122, 122\} \mathcal{V}^\dagger, \tag{12}$$

$$[6, 411] \rightarrow \{42, 206, 246, 164, 164\} \mathcal{V}^\dagger, \tag{13}$$

$$[6, 33] \rightarrow \{21, 114, 123, 93, 93\} \mathcal{V}^\dagger, \tag{14}$$

together with the self-associate irreps:

$$[6, 21^4] \rightarrow \{41, 138, 185, 97, 97\} \mathcal{V}^\dagger, \tag{15}$$

$$[4^2, 2^2] \rightarrow \{65, 174, 245, 109, 109\} \mathcal{V}^\dagger. \tag{16}$$

Finally, for modules beyond the self-associate (SA) form(s), no new information has been contributed; the corresponding irreps are already defined by the associate  $[\lambda]/[\lambda']$  pair relationship(s):

$$[\lambda'] \text{ (post SA)} = [\lambda] \otimes [1^n], \quad \forall n \text{ of } S_n. \tag{17}$$

**4. Higher  $[A]_n^{I_i}$  clusters: Complete  $\{|IM\rangle\}$  sets over (re-ordered)  $\{:\lambda:\}$  ( $m \leq 4$ , branched) sets**

For the modest  $n$ -fold  $[A]^{(I_i)}$  spin cluster, the methods developed in ref. [17] may be extended to  $SU(4, 6) \times S_n$  algebras; as examples, using a unit vector  $\mathcal{W}$  over all  $\{(\lambda \vdash n)\}$  forms within

$$\mathcal{W}^\dagger \equiv \{ :n:, :n-1, 1:, :n-2, 2:, :n-2, 11:, \dots \}. \tag{18}$$

Hence, the complete  $\{|IM\rangle\}$  under  $SU(3, 4) \times S_6$ , for the  $[A]_6$  clusters with  $I_i = 1$  and  $3/2$  are given, respectively, as

$$\{|IM\rangle\} = \begin{pmatrix} 1 \\ -, 1 \\ -, 1, 1 \\ -, -, -1, 1 \\ -, -, 2, -, -, 1 \\ -, 1, -, -, -, 2 \\ 1, -, -, 1, 1, -, 1 \end{pmatrix} \mathcal{W} \tag{19}$$

and

$$\{|IM\rangle\} = \left( \begin{array}{l} 1 \\ -, 1 \\ -, 1, 1 \\ -, 1, -, 1, 1 \\ -, -, 2, -, 1, 1 \\ -, 1, -, 1, -, 3 \\ 1, -, 1, 1, 1, 1, 1 \\ -, 1, -, 1, -, 4, -, -, 1 \\ -, 1, 2, -, -, 2, 1, 1, 1 \\ -, -, -, 2, 2, 2, -, -, 2 \end{array} \right) \mathfrak{W}. \tag{20}$$

Here the sets shown span  $0 \leq M \leq I = \sum_i I_i$ , and the last subset of each corresponds to the scalar invariant  $(\lambda \vdash n)$   $p$ -tuples, associated with  $M = 0$  for the cluster under  $SU(m) \times S_n(\downarrow \mathcal{G})$  algebra.

Hence, we have defined the underlying bases for  $[H]_6$ ,  $[^2D]_6$ ,  $[^{11}B]_6$  and  $[^{11}B']_6$  6-fold monoclusters inherent in the (1, 2, 3; 10, 11, 12), or (4, 5, 6, 7, 8, 9), hexadeutero  $^{11}B$ -borohydride ions. Similarly, the  $[^2D]_9$  and  $[^{11}B]_9$  monoclusters of the specific (1, 2, 3) trihydroborodeuteride ion under  $\Gamma([H^{11}B]_3) \otimes \Gamma([^2D^{11}B]_9)$  follow from the corresponding  $I = 1$ , or  $3/2$ , 9-fold monocluster bases and the SR reducible bases of the  $[H]_n$  clusters. These bases are set out in Tables 1 and 2.

Table 1

The hierarchy of  $\lambda$  ( $p \leq 3$ ) tuplar models defining the 9-fold identical  $I_i = 1$  NMR cluster problem. These  $\lambda$  models and those of Table 2 are analogues to the  $S_6 \downarrow \mathcal{O}$  and  $S_{12} \downarrow \mathcal{A}_5 \equiv \mathcal{I}$  models discussed, respectively, in earlier work [26, 23].

$M$	Dimension	$\lambda, p = 2$	over $p = 3$	$\lambda, p = 3$ , reordered
9	1	:9:		
	9	:81:		
7	45	:72:	:8-1:	
	156	:63:		:711:
5	414	:54:	:7-2:	:621:
	882	:45:		:531:, :612:
3	1554	:36:	:6-3:	:522:, :441:
	2304	:27:		:432:, :351:, :513:
1	2907	:18:	:5-4:	:423:, :342:, :261:
0	3067	: - 9:	:333:	:414:, :252:, :171:

$\{M\}$ , total: 19 683

Table 2

The hierarchy of  $p = 2, 3, 4$  simple, simple re-ordered  $\lambda$  models, together with the  $p = 2, 3$  forms over expanded 3, 4 part fields, which taken together serve to define the 9-fold identical  $I_i = 3/2$  (e.g.:  $^{11}\text{B}$ ) spin cluster system.

Outer $M$ : space	Dimen. of $M$	$\lambda, p = 2$	$\lambda, p = 2,$ $p = 3, 4$	over fields	$\lambda, p = 3$	over $p = 4$	$\lambda, p = 4,$ reordered
27/2	1	:9:					
	9	:81:					
21/2	45	:72:	:8-1:				
	165	:63:		:8-1:	:711:		
	486	:54:	:7-2:		:621:	:71-:	
	1206	:45:		:7-2:	:531:	:7-11; :62-1:	
15/2	2598	:36:	:6-3:		:441; :522:	:53-1:	:6111:
	4950	:27:			:432; :513; :351:		:5211:
	8461	:18:	:5-4:		:423; :342; :261:	:44-1; :6-21; :61-2:	:4311; :5121:
9/2	13051	: -9:		:6-3:	:333:	:52-2; :35-1; :6-12:	:4221; :5112:
	17847	: -81:	:4-5:		:243; :324; :162:	:5-31; :26-1:	:3411:
	23607	: -72:		: -8-1:	:234; :315; :153:	:43-2:	:3321; :4131:
3/2	27876	: -63:	:3-6:	:5-4:	:225; :144:	:5-22:	:2511; :4212:
	30770	: -54:		: -7-2:	:216; :135:	:17-1; :34-2:	:3312; :3231;
						:25-2;	:1611;
						:5-13; :4-41:	:2421; :4122:
						:42-3:	:3222; :2331;
						:16-2; : -711:	:3141; :1521:
						:33-3; :4-32:	:2412; :4113:
						:4-23; :24-3:	:2322; :3213;
						:41-4; :3-51:	:3132; :1512:
						: -621;	:1431; :2231:

$\{M\}_T : 262\ 144$



**5.  $(\lambda \vdash n)$  model invariance properties over  $\{\chi_i\}(\mathcal{C})$ , for invariant forms:**  
 $S_n \leq S_{14}$

Recognition of scalar invariants, for their importance in yielding a focus to the determinacy questions associated with subduced finite group  $SU(m) \times S_n \downarrow \mathcal{G}$  spin algebras, may be found in the recent literature [29], as well as in the earlier work of Sullivan and Siddall-III [4]. Their discussion of the role of Casimir invariants (in terms of unitary algebras) in respect of the  $S_6 \downarrow \mathcal{O}$  representations is pertinent here. The invariance and subduced group representational properties of some typical scalar invariants [30], in the form of  $(\lambda \vdash n)$  model forms as numerical  $:\lambda:$   $p$ -tuples, are inherent in  $n$ -fold spin clusters, once an automorphic finite  $S_n \downarrow \mathcal{G}$  group is considered in the NMR spin symmetry. Whilst our focus is necessarily on determinable irreps under natural embedded algebras such as  $S_n \supset \mathcal{G}$ , with the finite group representing the hierarchical structure within the intra-cluster coupling, some appreciation of the wider origins of indeterminacy in various  $SU(m) \times S_n \downarrow \mathcal{G}$  spin algebras is essential.

First, indeterminacies arising from  $\mathcal{G}$  finite group order under circumstances where the classic Cayley theorem criteria [24,25]

$$n \equiv /G/ \tag{21}$$

in fact *does not apply* are designated as ‘indeterminacies of the first kind’. The Sullivan and Siddall-III discourse [4] demonstrates that in addition to some higher  $SU(m)$  branching, a limit to (21)-Cayleyan determinacy exists, i.e., even in cases where the initial  $SU(2, 3) \times S_n \downarrow \mathcal{G}$  algebra is determinable under the condition (21), or is otherwise determinable. Such higher  $m$ -branching induced indeterminacies will be referred to as ‘indeterminacies of the second kind’. Their origins may be traced back (in part) to degeneracies which arise whenever the scalar invariant form(s) exhibit a non-distinct invariance set,  $\{\chi_i(\mathcal{C})\}(S_n \downarrow \mathcal{G})$ , from that of some preceding  $SU(m - i)$  subset, between  $\{:\lambda:\}$  component sets.

Naturally, any form of indeterminacy is simply a reflection of the mis-match between the model forms and the nature or extent of operators under the distinct group symmetries. The case actually discussed in ref. [4] is seen as an absolute indeterminacy, in the sense that the  $SU(m)$  branching level is not attainable under the  $S_6$  group.

In the following illustrations, drawn from  $SU(m) \times S_n \downarrow \mathcal{G}$  models corresponding to scalar invariant modelling of specific  $SU(m)$  branching under  $S_6 \leq S_n \leq S_{14}$ ,  $S_{20}$  are often caused by a weak accidental-degeneracy induced indeterminacy. For such phenomena, it is only necessary to consider the  $:\lambda:$  ( $\geq : \lambda_{SA}:$  ( $S_n$ ) component  $\lambda \vdash n$  aspects, as the least dominant sector has its own natural (and allowed) non-simply reducible properties.

Hence, it is appropriate to set out the  $\lambda_{SA}$  self-associate forms for  $S_n$  groups, as

$$\lambda_{SA} = \{321; 4211; \{54, 333\}; \{52111, 4321\}; \} \tag{22}$$

for  $n = 6$  (8);  $n = 9$  (10), respectively. For  $n = 12$  (14), one has the more extended  $\lambda_{SA}$  sets:

$$\lambda_{SA} = \{621^4, 5321^2, \text{ and } 4422\}(\mathcal{S}_{12}); \{721^5, 6321^3, \text{ and } 542211\}(\mathcal{S}_{14}). \quad (23)$$

The extended  $\lambda_{SA}$  set for  $\mathcal{S}_{20}$  has been given previously [31].

Returning to the scalar invariant components of  $\{\lambda \vdash n\} \equiv \{:\lambda:\}(\mathcal{S}_n : n = 6(9))$ , we note their embedded symmetry invariance properties:

$$\begin{aligned} \{\chi_i\}(:33:) &\equiv \{20, 2, 4, 0, 0\}\mathcal{C}(\mathcal{S}_6 \downarrow \mathcal{O}) \rightarrow \{2, 2, 2, 2, 2\}\mathcal{F} \rightarrow \{4, 4, 6\}\mathcal{F}'(\mathcal{S}_6 \downarrow \mathcal{D}_3), \\ \{\chi_i\}(:222:) &\equiv \{90, 0, 6, 0, 6\}\mathcal{C} \rightarrow \{6, 3, 9, 9, 12\}\mathcal{F} \rightarrow \{18, 18, 30\}\mathcal{F}', \end{aligned} \quad (24)$$

which may be contrasted with that for the embedded  $\mathcal{S}_9$  group,

$$\{\chi_i\}(:333:) \equiv \{1680, 6, 6\}\mathcal{C}(\mathcal{S}_9 \downarrow \mathcal{G}_3) \rightarrow \{564, 558\}\mathcal{F}''(\mathcal{S}_9 \downarrow \mathcal{G}_3). \quad (25)$$

For the  $\mathcal{S}_{10} \downarrow \mathcal{D}_5$  embedding, one finds that the spin-site invariance properties are

$$\begin{aligned} \{\chi_i\}(:4411:) &\equiv \{6300, 0, 0, 0\}\mathcal{C} \rightarrow \{630, 630, 1260, 1260\}\mathcal{F}'(\mathcal{S}_{10} \downarrow \mathcal{D}_5), \\ \{\chi_i\}(:3322:) &\equiv \{25\ 200, 0, 0, 0\}\mathcal{C} \rightarrow \{2520, 2520, 5040, 5040\}\mathcal{F}' \end{aligned} \quad (26)$$

for  $\lambda \vdash n$   $\mathcal{S}_{10}$  models. Under  $\mathcal{S}_{12} \downarrow \mathcal{A}_5 \equiv \mathcal{I}$ , the invariance set from mapping onto icosahedral automorphic NMR spin symmetry takes the form

$$\begin{aligned} \{\chi_i\}(:4422:) &\equiv \{207\ 900, 180, 0, 0, 0\}\mathcal{C}(\mathcal{S}_{12} \downarrow \mathcal{A}_5) \\ &\rightarrow \{3510, 13860, 17370, 10350, 10350\}\mathcal{F}'(\mathcal{S}_{12} \downarrow \mathcal{A}_5 \equiv \mathcal{I}), \\ \{\chi_i\}(:3333:) &\equiv \{369\ 600, (4! = 24), 0, 0, 0\}\mathcal{C} \\ &\rightarrow \{6168, 24648, 30792, 18480, 18480\}\mathcal{F}'. \end{aligned} \quad (27)$$

Finally for the totally encapped octahedron<sup>1</sup>, the  $\mathcal{S}_{14} \downarrow \mathcal{O}$  scalar invariant forms are of interest within the specific enumerations  $\binom{4}{2} \binom{2}{1} = 12$  under the  $C_3$  operation and  $\binom{6}{3} \binom{2}{1} = 40$  under  $C_2$ . Here the final :11: sites are on the implied rotational  $C_4$  axes, so that the invariant  $\lambda \vdash n$  forms over the class algebra yield

$$\begin{aligned} \{\chi_i\}(:6611:)(\mathcal{S}_{14} \downarrow \mathcal{O}) &\equiv \{168168, 12, 40, 0, 0\}\mathcal{C} \\ &\rightarrow \{7016, 7016, 14020, 21016, 21016\}\mathcal{F}'(\mathcal{S}_{14} \downarrow \mathcal{O}), \end{aligned} \quad (28)$$

$$\begin{aligned} \{\chi_i\}(:442211:) &\equiv \{37\ 837\ 800, 0, 360, 0, 0\}\mathcal{C} \\ &\equiv \{1576\ 620, 1576\ 620, 3153\ 240, 4729\ 680, 4729\ 680\}\mathcal{F}', \end{aligned} \quad (29)$$

<sup>1</sup> See footnote 2.

$$\begin{aligned} \{\chi_i\}(:333311:) &\equiv \{67\ 267\ 200, (4! = 24), 0, 0, 0\} \\ &\rightarrow \{2\ 802\ 808, 2\ 802\ 808, 5\ 605\ 592, 8\ 408\ 400, 8\ 408\ 400\} \end{aligned} \quad (30)$$

for  $SU(4)(6)$  branchings. It is noted that the automorphic encapping process ensures the distinctness of the invariance sets and hence the determinacy associated with these group embeddings for the type of systems discussed by Quong et al. [32].

### 6. Cayleyan determinacy of $S_n \supset \mathcal{G}$ for $[A]_n$ spin clusters: A quasi-geometric view

The  $[A]_n, n = 20, 24$ , spin clusters under the  $S_{20} \downarrow \mathcal{I}$  and  $S_{24} \downarrow \mathcal{O}$  algebras exhibit additional points of interest, in that their isomorphic rotational symmetry is associated with a cage polyhedral structure, as found for  $S_{12} \downarrow \mathcal{I}$  and  $S_{12} \downarrow \mathcal{I} \downarrow \mathcal{D}_3$  above. For both the  $S_{24} \downarrow \mathcal{O}$  and  $S_{12} \downarrow \mathcal{D}_3$  isomorphic symmetries, one notes that the Cayley criteria apply [25], as  $n = 24 \equiv /S_{24} \downarrow \mathcal{O}/$  and  $n = 6 \equiv /S_{12}(\downarrow \mathcal{I}) \downarrow \mathcal{D}_3/$ ; this yields a geometric lemma analogous to the well-established algebraic criterium. This takes the form [24,29],

“that for all spin clusters to which Cayley’s theorem applies, the  $C_l$  axes corresponding to the isomorphic rotational symmetry operators under the embedded algebra will be found to non-coincident with *any* of the model spin sites”. (31)

The more general low  $n$ -fold clusters, for which the Cayley criteria does not apply, need to be examined for the presence of indeterminacy. This may be done either, by searching for degeneracies in their  $p$ -tuplar ( $\lambda \vdash n$ ) model invariance sets, or alternatively, by examining the nature of their implied correlative mappings:

$$[\lambda_{SA}](S_n) \rightarrow \{i', j', k', \dots\} \mathcal{P}(S_n \downarrow \mathcal{G}). \quad (32)$$

A determinable set of irreps to that level of branching would imply that the resultant set of subduced irreps should retain the original self-associacy property. Cases of spin cluster involving indeterminacy of the second kind, for  $SU(m \geq 3)$  and further branching, have been demonstrated [29, 32, b] for  $(S_8 \downarrow \mathcal{O})$  or its subgroups. In addition, an examination of  $S_9 \downarrow C_3$   $p$ -tuples implies that over the invariance set *in this system also* there are degeneracies present, which involve model  $SU(4, 5) : \lambda$ : scalar invariants.

Whilst investigation of further ‘indeterminacies of the second kind’ are called

<sup>2</sup> Multifaceted cappings are referred as an ‘encapping’ [33].

## Appendix

For convenience of the reader, a brief glossary of special symbols is given below:

$\mathcal{G}$	a finite group; $S_n \downarrow \mathcal{G}$ , finite group subduction (restricted to the $\mathcal{G}$ group algebra), $\equiv S_n \supset \mathcal{G}$ , i.e. an embedding of a finite group into a specific $S_n$ group.
$(\lambda \vdash n)$	a (model) partition of $n$ (into $p$ parts within the $SU(p)$ level of branching).
$\equiv : \lambda$ :	a $p$ -tuple numerical realisation onto $S_n$ , or on a regular polyhedral $S_n \downarrow \mathcal{G}$ fig.
$m, n$	“reserved” integers, associated with $SU(m \leq n/2) \times S_n$ dual group algebras.
$Z(S_n)$	the characters of a specific ( $n$ -index) symmetric group.
$\lambda_{SA}$	self-associate form – the # hatch symbol is used to identify $[\lambda_{SA}]$ forms.
$\lambda$	in general a Young tableau or $(\lambda \vdash n)(S_n)$ partition, as above.
$(\geq$	standard dominance ordering of $\lambda \vdash n$ forms: i.e., $\{[n], [n-1, 1], \cdot, [\lambda_{SA}], \cdot, [1^n]\}$ .
$/\mathcal{G}/$	cardinality (order) of a group, as in $\sum_{[\lambda]} m_{[\lambda]} \chi_{1^n}^{[\lambda]} \equiv \sum_i g_i(\mathcal{C})$ , for $S_n$ groups = $n!$ , where $m_{[\lambda]}$ is the multiplicity of $[\lambda]$ and $g_i$ the cycle(class) order.
$S_n$ -module	a mathematical structure for which, $\sum_i g_i \xi_i^{\lambda}(\mathcal{C})(S_n) = /S_n/$ ; it is decomposable over a set $\{[\lambda']\}$ involving a set of $\{\Lambda_{\lambda[\lambda']}\}$ Kostka coefficients.
$\xi_i^{\lambda}(\mathcal{C})$	the permutational character for $: \lambda$ : form over the $S_n$ cycle set.
$\{\Lambda_{\lambda[\lambda']}\}$	the set of Kostka coefficients of a $S_n$ -module decomposition- underlined numbers belong to a <i>subset</i> of the high- $n$ limit decompositions.
$\rightarrow$	a mapping onto, or a 1 : 1 correlation.
$\{D^k(\tilde{U}) \times \tilde{\Gamma}^{[\lambda]}(v)\}$	Liouville space irrep set over the dual group $SU(m) \times S_n$ carrier space.

for, it suffices to note here that neither in the  $\mathcal{S}_{12} \downarrow \mathcal{I}$  cases, nor in the (en)capped<sup>2</sup>  $\mathcal{S}_{14} \downarrow \mathcal{O}$ , which corresponds to the tentative borohydride structure proposed by Quong et al. [32a], is there any evidence for such indeterminacy, i.e. up to the  $SU(6)$  branching level. Indeed in the latter case, we have noted that the presence of the inclusion structure serves to lift the degeneracy previously found to be associated with simple cubes as polyhedral NMR symmetry forms. Likewise, truncation of a cube to yield a (8, 3, 3)-polyhedral form within rotational subgroups isomorphism serves a similar purpose for the  $[A]_{24}$  NMR monocenter. Indeed, this exhibits Cayleyan [25] noncoincidence of the  $C_3$  isomorphic rotational operators to *any* of the model spin sites [24,29].

## 7. Some mapping aspects derived from symmetry axes of cage polyhedra [34,35]

A somewhat selective overview follows on the nature of  $\mathcal{S}_{12} \supset (\mathcal{S}_6 \downarrow \mathcal{O}) \supset \mathcal{S}_6 \downarrow \mathcal{D}_3 \otimes \mathcal{S}_6 \downarrow \mathcal{D}_3$ , or the analogous  $\mathcal{S}_{20} \supset \dots \supset \mathcal{S}_9 \downarrow \mathcal{D}_3 \otimes \mathcal{S}_9 \downarrow \mathcal{D}_3$  chain of spin symmetries, for isotopomeric cage geometries, beyond the scalar invariant model aspects discussed earlier in section 5.

### 7.1. CASE OF $\mathcal{S}_{12} \supset \mathcal{S}_6 \downarrow \mathcal{D}_3$

First, one enumerates combinatorially the  $:\lambda:(SU(m) \times \mathcal{S}_6 \downarrow \mathcal{D}_3)$  model. Over the full standard ( $\geq$  dominance order, this becomes

$$\{\chi_i\} \begin{pmatrix} :6: \\ :51: \\ :42: \\ :411: \\ :33: \end{pmatrix} \equiv \begin{pmatrix} 1, & 1 \\ 6, & 0, & 0 \\ 15, & 0, & 3 \\ 30, & 0, & 0 \\ 20, & 2, & 0 \end{pmatrix} \not\rightarrow \begin{pmatrix} 1, \\ 1, & 1, & 2 \\ 4, & 1, & 5 \\ 5, & 5, & 10 \\ 4, & 4, & 6 \end{pmatrix} \mathcal{V}(\mathcal{S}_6 \downarrow \mathcal{D}_3) \quad (33)$$

and

$$\{\chi_i\} \begin{pmatrix} :321: \\ :3111: \\ :222: \\ :2211: \\ :21^4: \end{pmatrix} \equiv \begin{pmatrix} 60, & 0, & 0 \\ 120, & 0, & 0 \\ 90, & 0, & 6 \\ 180, & 0, & 0 \\ 360, & 0, & 0 \end{pmatrix} \not\rightarrow \begin{pmatrix} 10, & 10, & 20 \\ 20, & 20, & 40 \\ 18, & 12, & 30 \\ 30, & 30, & 60 \\ 60, & 60, & 120 \end{pmatrix} \mathcal{V}, \quad (34)$$

from which it follows that the chain process  $\mathcal{S}_6 \downarrow \mathcal{O} \supset \mathcal{S}_6 \downarrow \mathcal{D}_3$  correspond to the correlative mapping

$$\begin{pmatrix} [6] \\ [51] \\ [42] \\ [411] \\ [33] \end{pmatrix} \rightarrow \begin{pmatrix} 1, \\ -, -, 1 \\ 1, -, 1, -, 2 \\ -, 1, -, 2, 1 \\ -, 2, -, 1, - \end{pmatrix} \mathbb{V}(S_6 \downarrow \mathcal{O}) \rightarrow \begin{pmatrix} 1, \\ -, 1, 2 \\ 3, -, 3 \\ 1, 3, 3 \\ -, 3, 1 \end{pmatrix} \mathbb{V}(S_6 \downarrow \mathcal{D}_3) \quad (35)$$

and

$$\begin{pmatrix} [321] \# \\ [31^3] \\ [222] \\ [2^2 1^2] \\ [21^4] \end{pmatrix} \rightarrow \begin{pmatrix} -, -, 2, 2, 2 \\ 1, -, -, 1, 2 \\ 2, -, -, -, 1 \\ -, 1, 1, 2, - \\ -, -, 1, -, 1 \end{pmatrix} \mathbb{V}(S_6 \downarrow \mathcal{O}) \rightarrow \begin{pmatrix} 2, 2, 6 \\ 3, 1, 3 \\ 3, -, 1 \\ -, 3, 3 \\ 1, -, 2 \end{pmatrix} \mathbb{V}(S_6 \downarrow \mathcal{D}_3), \quad (36)$$

where the # hatch marking denotes a self-associate irrep; the subsequent sets derived from these  $\lambda_{SA}$  should retain an overall set self-associacy, as seen over the  $S_6 \supset \mathcal{O} \supset \mathcal{D}_3$  chain of natural group embeddings.

On account of the lack of degeneracies over all these  $:\lambda: \equiv (\lambda \vdash n)$  models for all the accessible  $SU(m)$  branching, it may reasonably be held that the inner product spin algebras for the (1, 2, 3; 10, 11, 12) hexadeutero- (or the (4, 5, 6, 7, 8, 9) hexa-deutero-) 12-fold  $^{11}\text{B}$  borohydrides are determinable algebras governed by

$$\Gamma_T = (\Gamma^{I_i=1/2} \otimes \Gamma^{I_i=1})(S_6 \downarrow \mathcal{D}_3) \otimes (\Gamma^{I_i=3/2} \otimes \Gamma^{I_i=3/2})(S_6 \downarrow \mathcal{D}_3). \quad (37)$$

They are associated with the specific component invariance terms:

$$\begin{aligned} \{\chi_i\} &= \{64, 4, 8\} \mathcal{C}, & \text{for } I_i = 1/2, \\ &= \{729, 9, 27\} \mathcal{C}, & \text{for } I_i = 1, \\ &= \{4096, 16, 64\} \mathcal{C}, & \text{for } I_i = 3/2, \end{aligned} \quad (38)$$

from which the sub-total invariance set associated with  $(\Gamma \otimes \Gamma^{I_i=1})(S_6 \downarrow \mathcal{D}_3)$  and the analogous  $(\Gamma' \otimes \Gamma'')^{I_i=3/2}(S_6 \downarrow \mathcal{D}_3)$  direct product components become, respectively,

$$\begin{aligned} \{\chi_i\} &= \{46\ 656, 36, 216\} \mathcal{C}, \\ \{\chi'_i\} &= \{16\ 777\ 216, 256, 4096\} \mathcal{C}(S_6 \downarrow \mathcal{D}_3). \end{aligned} \quad (39)$$

In consequence, the total invariance and irrep sets clearly span the sets

$$\begin{aligned} \{\chi_i\}(\otimes)(S_6 \downarrow \mathcal{D}_3) &= \{782\ 757\ 789\ 696, 9216, 884\ 736\} \mathcal{C}, \quad \text{or} \\ \Gamma(\otimes)(S_6 \downarrow \mathcal{D}_3) &= \{130\ 459\ 192\ 320, 130\ 459\ 192\ 320, 260\ 919\ 260\ 160\} \mathbb{V} \end{aligned} \quad (40)$$

The detailed development of the component Latin square  $\{\chi_i\}(\otimes)$  invariance algebra over the individual (outer-)  $M$  subspaces is too extensive a topic to develop here.

A general point of interest is seen in the quasi-geometric viewpoint which applies to systems for which the Cayley criteria holds – such as  $/D_3/ = 6 = n$  of  $S_6$ . Analysis now gives a contrasting physical insight, i.e. compared to the nature of the earlier isomorphism to a simple octahedral form of regular (3, 3, 3, 3) polyhedra [34], in which the  $C_3$ ,  $C_4$  and one  $C_2$  axis necessarily must pass through one, or other, pair of spin-sites associated with realising the component  $(\lambda \vdash n)(SU(m))$  models.

## 7.2. BRIEF COMMENTS ON $S_{12} \supset S_3 \otimes S_9 \downarrow C_3$ NMR SPIN SYSTEMS

Analogous full treatments of the cage form of  $[AX]_9[A'X']_3$  bicluster NMR system from the recognition of the underlying automorphic structural invariance aspects:

$$\begin{pmatrix} :9: \\ :81: \\ :72: \\ :63: \\ :54: \end{pmatrix} \rightarrow \begin{pmatrix} 1, & 1 \\ 9, & 0 \\ 36, & 0 \\ 84, & 6 \\ 126, & 0 \end{pmatrix} \not\subseteq, \quad (41)$$

yield

$$\begin{pmatrix} [9] \\ [81] \\ [72] \\ [63] \\ [54] \end{pmatrix} \rightarrow \begin{pmatrix} 1, & 1 \\ 8 & -1 \\ 27, & 0 \\ 48, & 6 \\ 42, & 6 \end{pmatrix} \not\subseteq \rightarrow \begin{pmatrix} 1, & \\ 2, & 3 \\ 9, & 9 \\ 18, & 15 \\ 10, & 16 \end{pmatrix} \not\subseteq (S_9 \downarrow C_3). \quad (42)$$

As noted, the more generally branched models may not be determinable in their higher dual group (unitary) aspects. This is a direct consequence of accidental degeneracy amongst the scalar invariant component  $(\lambda \vdash n)$  forms, :3321: and :32<sup>2</sup>1<sup>2</sup>: of  $SU(4)$  and  $SU(5)$ . By implication the spin algebra associated with these higher branchings are indeterminate. There would also appear to be a weaker degeneracy, involving 4-tuple :6111:, but the latter does not act as a system  $M = 0$  scalar invariant.

On comparing the difference in the order of the  $D_3$  and  $\mathcal{O}$  automorphic rotational symmetry groups, the former  $SU(5)$  result is comparable to the Sullivan and Siddall-III  $SU(m > 6) \times S_6$  NMR symmetry observation [4], in which the branching is not accessible under the low  $/(S_n \downarrow)G/$  group cardinality.

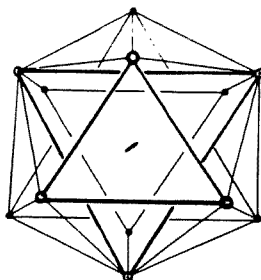


Fig. 1. Diagram illustrating the dispositions about the  $C_3$  (spin-site non-coincident) axis of  $S_{12} \supset S_{12} \downarrow \mathcal{I} \supset S_6 \downarrow \mathcal{D}_3 \otimes S_6 \downarrow \mathcal{D}_3 \supset \mathcal{D}_3$ , the NMR spin group, a subgroup of  $\mathcal{D}_{3d}$ , the molecular symmetry group for (1, 2, 3:10, 11, 12) like substituted (or (4, 5, 6, 7, 8, 9) like-substituted) 12-cage borohydride isotopomer ions. Note that one pair of larger triangles, *within the geometric solid*, have been included to stress the  $C_3$  symmetry about this rotational axis. These  $S_{12} \supset \dots \supset \mathcal{D}_3$  group chain NMR spin symmetries are the simplest known forms (beyond the trivial  $\mathcal{D}_3$  symmetry) and the mid-face centred axis is an element typical of a Voronoi polyhedra, as discussed in a recent related work [35].

### 7.3. ON THE $S_{20} \supset (S_9 \downarrow \mathcal{D}_3) \otimes (S_9 \downarrow \mathcal{D}_3)$ CAGE-CLUSTER SYSTEMS

Whilst this higher cage-cluster system does not correspond to a spin system to which Cayley's theorem criteria applies, it still exhibits more promise for the absence of degeneracy than the preceding  $S_9 \downarrow C_3$  case, largely on the basis of its encapped-like structure. This opens up the promise of further insight into isotopomeric spin cage-cluster forms corresponding to certain higher regular polyhedra [33], in addition to the fullerene isotopomer cages discussed in refs. [24,29].

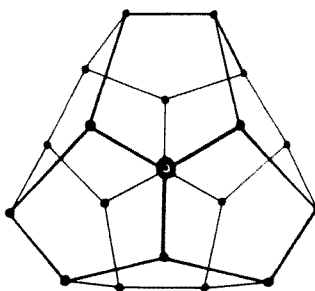


Fig. 2. Projective illustration of the rotational dispositions about the 1, 20  $C_3$  (spin-site co-incident) axis of the  $\mathcal{D}_3$  (nuclear spin subgroup) isotopomers of the  $\mathcal{D}_{3d}$  cage molecules, 1, 20-disubstituted dodecahedrane, or (2, 3, 4:17, 18, 19) (or 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16) substituted dodecahedrane. The former corresponds to  $S_{20} \supset S_{18} \supset S_9 \downarrow \mathcal{D}_3 \otimes S_9 \downarrow \mathcal{D}_3 \supset \mathcal{D}_3$ , whereas the latter involves  $S_{20} \supset S_{12} \downarrow \mathcal{D}_3 \otimes S_6 \downarrow \mathcal{D}_3$  spin symmetries. The ten nuclear spin sites on the anterior faces are shown in heavier relief compared to those of the posterior faces. Sites 1 and 20 are on the symmetry axis at the centre of this projection.



## 8. Concluding remarks

The role of the isomorphic symmetry properties of regular polyhedra, as defined by the regular geometric solids vertex indices [34], is of special value in the physical understanding of  $p$ -tuple  $(\lambda \vdash n)$  modelling of spin algebras on account of the automorphic nature of NMR and its nuclear spin group. Further, the value of Biedenharn and Louck ideas on mapping [7] in the context of NMR is enhanced by an appreciation of scalar invariants [30]. The nature of  $v$ -recoupling is especially valuable in the study of the explicit structure [22] of  $SU2 \times S_n$  Liouville carrier space, where the recoupling term(s), in one or other form, are explicit labels necessary for the retention of simple reducibility properties. The additional  $n - 2$  scalar invariant terms are an important part of the symmetry aspects of NMR. They point to the existence of the  $\{D^k(\bar{U}) \times \bar{\Gamma}^{[\lambda]}(v)\}$  irrep sets, as part of the mapping over the  $\{\mathbb{H}_v\}$  carrier subspaces [22] with various practical aspects of utility in spin dynamics [19–21]. The ideas presented here are necessary for the use of such augmented spaces over a wider range of spin systems.

The contrasting ro-vibration spin weight aspects of cage-clusters have become more important in recent chemical physics research, following extensive work on fullerene and other cage isotopomers [29]. Furthermore, some recent chemical interest in encapped molecular geometric structures [33] suggests that the underlying associated invariants and  $:\lambda:(S_n)$  models as  $S_n$ -modules are of importance and largely determine the nature of the corresponding  $SU(m) \times S_n(\downarrow \mathcal{G})$  subduced spin algebras. Included in this topic is the determinacy-question for natural embedding of finite groups in a specific  $S_n$  group. Our most recent work has demonstrated how ideas concerning determinacy may be generalised [35] by recalling the properties of Voronoi polyhedra.

For certain specific determinable  $S_n \supset \mathcal{G}$  embedding associated with cage isotopomeric NMR spin clusters, the geometric analogues given as alternatives to Cayley's algebraic theorem are especially appropriate [35]. They deserve to be more widely known for their  $\lambda \vdash n$  model properties (see above), which provided the original motivation of this presentation.

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$v$	a generalised recoupling label, subsumes <i>both</i> $(k_1 - k_n)$ fields and any $n - 2$ invariants.
$\mathbb{H}, \tilde{\mathbb{H}}, \{\tilde{\mathbb{H}}_v\}$	(respectively) the Hilbert (Liouville) carrier spaces, subspaces.
$\otimes, \oplus$	in group theory, direct product and direct sum, respectively.
$\forall$	'for all' symbol.
$[\lambda']$ (prior to $\lambda$ )	the incremental irrep label over a $S_n$ -module decomposition.
$\mathfrak{W}$	Gothic $W$ , symbol refers to a unit set of $:\lambda$ : in dominance order as a vector.

The slashed (crossed)  $\cancel{\mathcal{L}}$  and  $\cancel{\mathcal{C}}$ , Gothic (El, Cee) symbols, respectively, refer to the *unit* set of group irreps and the standard set of class or cycle operators of a group. All other symbols are standard mathematical-text symbols.

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