Multicolour models of natural embedding for SU($2 \leqslant m \leqslant 4$) $\times \mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ NMR spin symmetry: Determinacy of nuclear spin weights for (1,12)-car-^{11}B-boranes *,**

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The *inherent (in)determinacy* implicit in the SU($m \geqslant 3$) $\times \mathcal{S}_n{\downarrow}\mathcal{G}$ natural embedding aspects of (NMR) spin symmetry of clusters is investigated, as part of a multicolour modelling scheme, where the SU2-branching level meets the initial $n(\mathcal{S}_n) = /\mathcal{G}/$ condition. We focus on correlative mappings derived from $[\lambda]_{\mathrm{SA}}$ (self-associate) irreps for natural group embeddings and compare these with certain Yamanouchi–Gel'fand chain properties of $\mathcal{S}_{10}$. Mathematical decompositions of $\mathbf{M}^{\lambda}$ simple $\mathcal{S}_n$-modules with ($2 \leqslant p \leqslant 4$)-branchings of $\lambda \trianglerighteq \lambda_{\mathrm{SA}}$ (for $\lambda \vdash n$ partitions of n) provide the initial insight into the monocluster spin (NP) physics of $[^2\mathrm{H}]_{10}$, $[^{11}\mathrm{B}]_{10}$ ($\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$), as aspects of (1,12)-$(\mathrm{HC})_2(\mathrm{H}^{11}\mathrm{B})_{10}$ or $(\mathrm{HC})_2(^2\mathrm{H}^{11}\mathrm{B})_{10}$ carborane cage isotopomers. The questions raised are significant for their impact on CNP nuclear spin weighting of ro-vibrational spectra. The methods used are those of combinatorics-via-group actions, as physical $\mathcal{S}_n$-encodings applied to nuclear spin algebras.

1. Introduction

The study of specific cage-cluster isotopomers, in regard to the impact of nuclear spin statistical weights on, e.g., ro-vibrational properties, is intimately linked to the question of the *abstract-space* NMR spin symmetry implicit in their $[A]_n^{(I_i)}$ clusters. The latter arises directly [2] from the automorphic intra-cluster spin coupling $\{J_{ij}\}$ hierarchy, within the zeroth order Hamiltonian of $[A,\ldots,X]_n$ NMR spin systems. These well-established aspects, with the use of $\Gamma(\mathcal{S}_n \otimes \mathcal{S}_n{\downarrow}\mathcal{S}_n)$ inner products derived from the corresponding monocluster NMR symmetries, follow directly from the work of Corio [9] and Balasubramanian [2,3]. In extending these concepts to higher identical spin-($I_i \geqslant 1$) sets of $[A]_n$ cage-clusters, both physical and mathematical modelling techniques are necessary [21–23,27]. The former treats the invariance over $\mathfrak{C}_i$, $\{\chi_i\}^M(\mathcal{S}_n{\downarrow}\mathcal{G})$ (for M, the outer-SO(2) weight), of such n-fold spin (site-based

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automorphic symmetry) sets, where their full nuclear permutational (NP) properties are based on the $p \leqslant 3(4)$ (maximal part) model $\lambda \vdash n$ mathematical partitions which encompass all $m \leqslant p$ branching [19,20] of $\lambda \vdash n$. These SU(m) $\times$ $\mathcal{S}_n$ dual group properties are essential features of the $[^2\mathrm{H}]_{10}$ and $[^{11}\mathrm{B}]_{10}$ NMR subsystems, whose determinacy is seen to lie *beyond* the realms of Cayley's $n(\mathcal{S}_n) \equiv /\mathcal{G}/$ theorem [8,28]. Whilst the latter criterion is a necessary condition, by itself it is *not a sufficient condition* to guarantee determinacy in SU($m \geqslant 3$) $\times$ $\mathcal{S}_n{\downarrow}\mathcal{G}$ spin algebras. This preamble highlights the reasons underlying our specific interest in the determinacy of natural group-embeddings inherent in such multispin cluster problems.

First, we define and rationalise the nature of the abstract finite group $\mathcal{G}$ (based on automorphic encapped (decapped) polyhedra) and its embedding into specific branching levels of $\mathcal{S}_n$-permutational spin symmetry. This is defined by the SU($m \leqslant p$) $\times$ $\mathcal{S}_n$ direct product group and derived via $\mathbf{M}^\lambda$ $\mathcal{S}_n$-modules [19,22]. Decompositions of the latter constitute the purely mathematical $[A]_n$ modelling aspects, whereas the nature of the embedding is determined by the physical p-adic multicolour permutational site-modelling of invariance under some specific $\{\mathcal{C}_i\}(\mathcal{G})$ cycle set. Here it is natural to focus first on cage-type spin *monoclusters* of identical spin-I_i nuclei in order to derive an initial $\{[\lambda] \rightarrow \Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}$ correlative mapping. Thence, suitable $\Gamma(((\mathcal{S}_n{\downarrow}\mathcal{G}) \times (\mathcal{S}_n{\downarrow}\mathcal{G})){\downarrow}(\mathcal{S}_n{\downarrow}\mathcal{G}))$ inner product formation yields a full description of the (CNP or NMR) spin symmetry.

To obtain meaningful results from such modelling, it is essential that the embedding in the initial process is one associated with a determinable invariance algebra. This introduces a further requirement beyond Cayley's theorem, for the system invariants to be *determinable* at the maximal SU(m) branching level of physical interest; Sullivan and Siddall III in their work on Casimir invariants of SU($m \geqslant 6$) $\times$ $\mathcal{S}_6{\downarrow}\mathcal{O}$ embedded spin algebras [20] stress this point. The absence of degeneracy between distinct elements of the physical model is important here. SU(m) branching is defined within the $\mathbf{M}^\lambda$ simple $\mathcal{S}_n$-modules ($\equiv$:λ: in numeric examples), with forms contributing to the $\{|I(M = 0)\rangle\}$ aspects are of especial importance. With the exception of $0(3) \supset \cdots \supset \mathcal{G}$ chains for 3-space finite groups appropriate to optical spectra [1,7,11], the nature of SU($m \geqslant 3$) $\times$ $\mathcal{S}_n{\downarrow}\mathcal{G}$ group embeddings *for spin algebras* represent a somewhat neglected area of physics.

The present work starts from a consideration of the $[^1\mathrm{H}]_{10}$ cage cluster, whose abstract space spin symmetry corresponds directly to the criterion denoted by Cayley's ($n(\mathcal{S}_n)$ index $\equiv /\mathcal{G}/$) theorem [8,28], and, hence, is not in doubt for SU(2) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ natural embedding. Utilising, for SU($m \geqslant 3$) branchings, the above $\mathcal{S}_n$-modules and the p-adic spin invariance set models yield the form of the $\{[\lambda] \rightarrow \Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}$ mappings. These afford much insight into the (determinable) SU($m \geqslant 3$) $\times$ $\mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings.

Much of the subsequent discussion focusses on the $[^2\mathrm{H}]_{10}$ and $[^{11}\mathrm{B}]_{10}$ cage clusters and their irreps associated with higher branching levels of $\mathcal{S}_n{\downarrow}\mathcal{G}$ spin symmetry embeddings, respectively, for $p \leqslant 3,4$ (part) $\lambda \vdash n$ partitions. This article extends work on nuclear spin weightings of isotopomeric cage clusters, as set out elsewhere [21–23,27]. Since much of the discussion given in the latter is concerned with combinatorics-via-group actions [12–14,19] and p-adic multi-colour ($\lambda \vdash n$) modelling [21,22], the symbolism and notation are taken as established, and the reader is referred to them for clarification of other aspects of the modelling techniques invoked. Suffice it to recall that only the SU(2) $\times$ $\mathcal{S}_n$ algebras and their specific $\mathcal{S}_n$-modules are simply reducible in terms of their decomposition over $\{[\lambda]\}(\mathcal{S}_n\colon\ p \leqslant 2)$ sets, yielding unit (or null) $\Lambda_{\lambda\lambda'}$ (Kostka) reduction coefficients.

From an explicit knowledge of the Kostka coefficient sets for $m \geqslant 3$ dual algebras, introduced in [21,22], the hierarchical recursive difference mappings for the $\{[\lambda] \rightarrow \Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}$ correlative properties follow directly from a generalised SU($m \geqslant 3$)$\times$$\mathcal{S}_n$ extension (given in [21,22]) to Corio's initial SU(2) approach [9]. To clarify the distinct nature of NMR spin algebras we make one further general (NMR) point. While an automorphism may exist between an abstract space spin symmetry and one of the finite groups, the groups involved here are strictly rotational subgroups [2,3] – $\mathcal{J}$, $\mathcal{O}$, or their subgroups, as a result of the inversion–reflection operation of 3-space *not being a permissible* operation under abstract NMR spin symmetry or under NP, CNP.

Rather general criteria are sought for ascertaining the validity of the determinacy of a $\mathcal{S}_n{\downarrow}\mathcal{G}$ group embedding, exhibited by the component $[A]_n$ spin clusters inherent in a specific isotopomer. In $\lambda \vdash n$ partitional terms, these represent direct extensions of concepts introduced and discussed analytically in [20] for a definitive case. Our viewpoint is one based on combinatorics [3,6,12–14,18,19,21–23,27] applied to physics.

The article is arranged as follows: in section 2, we briefly summarise the mathematical modelling methods employed; by contrast, section 3 sets out the nature of the p-adic *physical* modelling of the $[A]_{10}$ spin clusters, as subcomponents under the natural embedding of $\mathcal{D}_5$ into the full spin algebra for (total ^{1}H or ^{2}H) $[AX]_{10}[M]_2$ NMR spin systems of (1,12)-di^{12}C-car(^{11}B)borane. The correlative mappings associated with $\mathcal{S}_n{\downarrow}\mathcal{G}$ group embeddings follow directly in section 4. The difficult question of determinacy vs. indeterminacy of natural $\mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings under higher-m SU(m) $[A]_{10}^{(I_i)}$ spin clusters is discussed in section 5.

2. Mathematical modelling from $\mathbf{M}^{\lambda} \equiv {:}\lambda{:}$, for λ a ($\lambda \vdash n$)-partition: Specific simple $\mathcal{S}_n$-module decompositions for $p \leqslant 4$ part $\lambda \trianglerighteq \lambda_{\mathrm{SA}}$ [19]

The standard definition [19] of such simple modules derived from the $\{\xi^{[\lambda]}_{(\ldots)}\}$ Young permutational-character sets [12–14,18] associated with all $\mathcal{S}_n$ groups. The weakly branched aspects of these $\mathcal{S}_n$-modules correspond to the dominant $\lambda \vdash n$ (parts of n) p-adic tuples [12–14,18], whose numerical $\lambda \vdash n$ forms will be written here as, e.g., $:n-r, r-r', r':$, rather than as superscripts of the $\mathbf{M}^{\lambda}$ form for $\mathcal{S}_n$-modules. These and their associated Kostka reduction coefficients have been derived in a general weak-branching $:n-r, r-r', r':$ ($\mathcal{S}_n$) context, as tabulated in [22].

Here, we restrict discussion to the intermediate branching level with its specific Kostka coefficient set $\{\Lambda_{\lambda\lambda'}\}$ under $\trianglerighteq$ dominance ordering [12–14,18,19,22] of the basis $\mathcal{L}^{\dagger} \equiv \{[\lambda]\} \equiv \{[n], \ldots, [n-2, 11]; [n-3, 3], \ldots; \ldots\}$ for reductive mapping, where the ; delineate the $n-\mu$ to $n-\mu'$ change of the leading integer part in such sequences. Hence, from the Sagan algorithmic form of Young's rule, equation (2.22.2) of [19], one has

$$\mathbf{M}^{\lambda} \equiv \bigoplus_{\lambda'} \Lambda_{\lambda\lambda'}[\lambda'], \tag{1}$$

where $\Lambda_{\lambda\lambda'}$ (the multiplicity of $[\lambda']$ in $\mathbf{M}^{\lambda}$) is equal to $\mathrm{sst}^{\lambda'}(\lambda)$, the number of semi-standard tableaux of shape λ' and content λ. Hence, the reductive decompositions are

$$\begin{pmatrix} :622: \\ :6211: \\ :61^4: \end{pmatrix} = \begin{pmatrix} 1,2,3,1;\ 2,2,-;\ 1,1,1,-,- \\ 1,3,4,3;\ 3,4,\ 1;\ 1,2,1,\ 1,- \\ 1,4,6,6;\ 4,8,\ 4;\ 1,3,2,\ 3,\ 1 \end{pmatrix} \mathcal{L}, \tag{2}$$

whereas at the next principal level of $:n-r,\ldots:$, one has

$$\begin{pmatrix} :541: \\ :532: \\ :5311: \\ :5221: \\ :52111: \end{pmatrix} = \begin{pmatrix} 1,2,2,1;\ 2,\ 1,-;\ 2,1,-,-,-;\ 1,1,-,-,-,- \\ 1,2,3,1;\ 3,\ 2,-;\ 2,2,\ 1,-,-;\ 1,1,\ 1,-,-,- \\ 1,3,4,3;\ 4,\ 4,\ 1;\ 3,4,\ 1,\ 1,-;\ 1,2,\ 1,\ 1,-,- \\ 1,3,5,3;\ 5,\ 6,\ 1;\ 3,5,\ 3,\ 2,-;\ 1,2,\ 2,\ 1,\ 1,- \\ 1,4,7,6;\ 7,11,\ 4;\ 4,9,\ 5,\ 6,\ 1;\ 1,3,\ 3,\ 3,\ 2,\ 1 \end{pmatrix} \mathcal{L} \tag{3}$$

from this general combinatorial algorithm based on the third form of Young's rule. It is stressed that the decomposition of $\mathbf{M}^{\lambda}$ modules and the expansion of Schur functions (over a complete $\mathcal{S}_n$ $\{[\lambda]\}$-basis) are essentially equivalent (isometric) processes [19].

The remaining subset of $\mathcal{S}_n$ modules may be shown to yield $\{\Lambda_{\lambda[\lambda']}\}$ Kostka sets:

$$\begin{pmatrix} :442: \\ :4411: \\ :433: \\ :4321: \end{pmatrix}$$
$$= \begin{pmatrix} 1,2,3,1;\ 3,2,-;\ 3,2,1,-,-;\ 1^*,2,1,-,-,-;\ 1,-,-,- \\ 1,3,4,3;\ 4,4,\ 1;\ 4,4,1,\ 1,-;\ 2^*,4,1,\ 1,-,-;\ 1,\ 1,-,- \\ 1,2,4,1;\ 3,3,-;\ 3,3,1,-,-;\ 2^*,3,1,-,-,-;\ 1,-,\ 1,- \\ 1,3,5,3;\ 6,6,\ 1;\ 5,7,3,\ 2,-;\ 2^*,5,4,\ 2,\ 1,-;\ 2,\ 1,\ 1,\ 1 \end{pmatrix} \mathcal{L}, \tag{4}$$

where the $*$-starred coefficients are from specific intermediate branchings, rather than general forms within the high-n weak branching limit of [22]; we note that the last module component of each of these subsets is a self-associate form. Naturally, the initial $[\lambda'] = [n]$ and final $[\lambda'] = [\lambda]$ reduction coefficients $\forall \lambda \vdash n$ are identically unity [19].

3. p-adic models of physical invariance for SU($m \geqslant 2$) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ natural embeddings

Here one considers the automorphic group properties of a suitably labelled truncated polyhedra over the $\mathfrak{C}^\dagger$ unit cycle operator set $\{E, (5)\mathcal{C}_2, (2)\mathcal{C}_5, (2)\mathcal{C}_5\}$ for the $[A]_{10}$ spin cluster to derive the following spin-site M-weight invariance mappings:

$$\begin{pmatrix} :91: \\ :82: \\ :73: \\ :64: \\ :55: \end{pmatrix} \to \begin{pmatrix} \{10,0,0,0\} \\ \{45,5,0,0\} \\ \{120,0,0,0\} \\ \{210,10,0,0\} \\ \{252,0,2,2\} \end{pmatrix} \mathfrak{C}(\mathcal{S}_{10}{\downarrow}\mathcal{D}_5) \tag{5}$$

and

$$\begin{pmatrix} :811: \\ :721: \\ :631: \\ :622: \end{pmatrix} \to \begin{pmatrix} \{90,0,0,0\} \\ \{360,0,0,0\} \\ \{840,0,0,0\} \\ \{1260,20,0,0\} \end{pmatrix} \mathfrak{C}, \tag{6}$$

$$\begin{pmatrix} :541: \\ :532: \\ :442: \\ :433: \end{pmatrix} \to \begin{pmatrix} \{1260,0,0,0\} \\ \{2520,0,0,0\}^{\#\#} \\ \{3150,30,0,0\} \\ \{4200,0,0,0\} \end{pmatrix} \mathfrak{C}. \tag{7}$$

Figure 1 provides an illustration of the M-weight multi-colour problem for $\mathbf{M}^\lambda$ models with, e.g., $\lambda \equiv$:55: and $\lambda \equiv$:433:.

In contrast, for ($p \leqslant 4$)-adic models derived from $[^{11}\mathrm{B}]_{10}$ spin clusters, the invariance algebra for models involving $p = 4$ $\lambda \vdash n$ partitions take the forms

$$\begin{pmatrix} :7111: \\ :6211: \\ :5311: \end{pmatrix} \to \begin{pmatrix} \{720,0,0,0\} \\ \{2520,0,0,0\}^{\#\#} \\ \{5040,0,0,0\} \end{pmatrix} \mathfrak{C}, \tag{8}$$

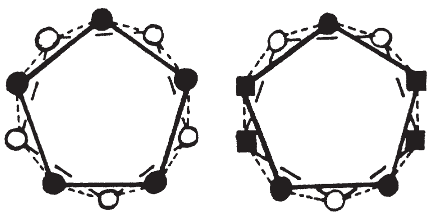

Figure 1. Examples of components (as M-weight spin site decapped icosahedral figures) contributing to the automorphic multicolour $\mathbf{M}^\lambda$ modules, respectively, for :55: ($p \leqslant 2$: $\mathcal{S}_{10}$) and (on the right) :433: ($p \leqslant 3$: $\mathcal{S}_{10}$). The $\mathcal{C}_5$ 5-fold axes at the incentres of the pentagons are perpendicular to the diagram, whilst lone (potential) $\mathcal{C}_2$ axis lies in E $\leftrightarrow$ W direction in the space between the pentagons.

$$\begin{pmatrix} :5221: \\ :4411: \\ :4321:_{\mathrm{SA}} \\ :4222: \end{pmatrix} \rightarrow \begin{pmatrix} \{7560,0,0,0\} \\ \{6300,0,0,0\} \\ \{12600,0,0,0\} \\ \{37800,60,0,0\} \end{pmatrix} \mathfrak{C}, \tag{9}$$

where the χ_{E} first entries are now monomials.

Immediately, one observes that there is just one pair of degenerate model entities. This implies that a physical basis for total independence over the SU($m \geqslant 4$) set, or specifically between the :532: and :6211: ($\lambda \vdash n$) $\mathbf{M}^{\lambda}s$, is lacking; we denote this by ## markings in equations (7) and (8). However, these are not explicitly concerned with the $\{|IM = 0\rangle\}$ components constituting system invariants; thus, they may be regarded as weak accidental degeneracies. Also, on noting conceptual parallels to the SU($m > 6$) $\times$ $\mathcal{S}_6$ case discussed in [20] (and the position of self-associate forms), we make one further point. Since all SU(7) p-adic model ($\lambda \vdash n$) entities of [20] lie not only beyond the corresponding self-associate $\lambda \vdash n$ form, but outside the range of the actual $\mathcal{S}_6$ irrep algebra, clearly the information content in *that case* is not defined. The case of SU(7) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ naturally embedded spin algebra for $[^{10}\mathrm{B}]_{10}$ is also beyond λ_{SA} and so it is not ameniable to any specific determinacy tests *beyond* those given for SU(4) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$. Hence, its isotopomeric forms are not discussed here. The SU(4) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ case examined here is interesting precisely because it is less clear-cut in its determinacy properties than the NMR system investigated by Sullivan and Siddall III [20]. Further aspects of the structure of Hilbert spin spaces in terms of sets (subsets) of p-adic ($\lambda \vdash n$) parts of n, as used in table 2, has been given in some related 1991 work of ours [21].

4. Natural embeddings SU($m \geqslant 3$) $\times$ $\mathcal{S}_n{\downarrow}\mathcal{G}$ and their $\{[\lambda] \rightarrow \Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}$ correlative mappings

Three initial points are make here. First, we note that nuclear spin-labelled cage structures exhibit a special condition when the order of the embedded (abstract space) finite group corresponds to the symmetric group index, n. Hence Cayley's theorem [8,28] applies and, in addition for this specific $[A]_{10}(\mathcal{S}_{10}{\downarrow}\mathcal{D}_5)$ model embedded symmetry, the axes of the automorphic rotational subgroup operations components of the spin cluster are non-coincident to the vertix spin-site labelling of the underlying residual (de-capped $\mathcal{J}$) cage structure. This allows one to demonstrate the existence of a geometric algebraic concept which parallels [25] Cayley's theorem for SU2-branched spin algebras. In such cases, the corresponding embedded spin-symmetry invariance properties take on an exclusively combinatorial form. Analogous properties for other cage-cluster spin systems have been observed [22,23,25,27] for certain specific high-n fold $\mathcal{O}$ or $\mathcal{J}$ related polyhedral models.

As a second point, the CNP [5,17] or total isotopomer nuclear spin symmetry is seen to arise directly from suitable inner direct products, e.g., for (1,12)-car^{11}B-borane:

$$\Gamma_{\text{total: (spin)}} = \big(\Gamma\big(\mathrm{SU}(2) \times \mathcal{S}_{10}{\downarrow}\mathcal{D}_5\big) \otimes \Gamma\big(\mathrm{SU}(4) \times \mathcal{S}_{10}{\downarrow}\mathcal{D}_5\big)\big) \otimes \Gamma(\mathcal{S}_2). \tag{10}$$

Table 1
The correlative mappings associated with the $\mathcal{S}_{10}\downarrow\mathcal{D}_5$ natural embedding.

$[\lambda]$	$\mathbb{Z}(\mathcal{S}_n)$				$\{[\lambda] \to \Gamma(\mathcal{S}_{10}\downarrow\mathcal{D}_5)\}$	Coefficients over
	$\chi^{[\lambda]}_{1^n}$	χ'	χ''	χ'''	$\ldots\chi$	(A_1, A_2, E_1, E_2)
[91]	9	7	5	3	$\ldots -1$	0, 1, 2, 2
[82]	35	21	11	5	0	6, 1, 7, 7
[811]	36	20	8	0	1	2, 6, 7, 7
[73]	75	35	15	7	0	5, 10, 15, 15
[721]	160	64	16	0	0	16, 16, 32, 32
$[71^3]$	84	28	0	-8	-1	10, 6, 17, 17
[64]	90	34	14	6	0	14, 3, 18, 18
[631]	315	91	19	3	0	29, 34, 63, 63
[622]	225	55	5	3	0	30, 15, 45, 45
[6211]	350	70	-10	-10	0	30, 40, 70, 70
$[61^4]$	126	14	-14	-6	1	16, 10, 25, 25
[55]	42	14	6	2	0	0, 10, 8, 8
[541]	288	64	16	0	0	28, 28, 58, 58
[532]	450	70	10	6	0	40, 50, 90, 90
[5311]	567	63	-9	-9	0	65, 50, 113, 113
[5221]	525	35	-15	7	0	50, 55, 105, 105
$[52111]^{\#}$	448	0	-32	0	0	44, 44, 90, 90
$\ldots[51^5] = [1^{10}] \otimes [61^4]$						
[442]	252	28	8	0	0	36, 16, 50, 50
[4411]	300	20	0	-8	0	20, 40, 60, 60
[433]	210	14	6	2	0	11, 31, 42, 42
$[4321]^{\#}$	768	0	0	0	0	81, 71, 154, 154
$\ldots[4222] = [1^{10}] \otimes [4411]$						
$[3322] = [1^{10}] \otimes [442]$						

Such total spin irreps correspond to the 'non-magnetically equivalent' $[AP]_{10}[X]_2$ NMR spin system of the (1,12)-$[^1\mathrm{H}^{11}\mathrm{B}]_{10}[^{12}\mathrm{CH}]_2$ isotopomer; here, it is necessary that the higher branched SU(4) $\times$ $\mathcal{S}_{10}\downarrow\mathcal{D}_5$ embedded spin algebra is determinable; otherwise, equation (10) would be undefined. Discrimination between $[\lambda]^{(2:11)}$ components in a $\mathcal{S}_2$-plethysmic view of $[\lambda] \otimes [\lambda]$ is now possible, via recent work on domino tableaux [6].

The detailed spin symmetry enumerations of individual component monoclusters (to within determinacy considerations) yield the tabulated results for the SU(2), SU(3) and SU(4) branching levels set out in table 1, where the $\mathcal{S}_{10}$ p-adic models have been mapped onto the natural embedded group symmetry $\mathcal{S}_{10}\downarrow\mathcal{D}_5$ irreps. Here we utilise the recursive hierarchical approach [22], based on the λ p-tuplar component structures of table 2, as $\mathcal{S}_n$-modules decomposable under Sagan's algorithmic variant [19] of Young's rule. This has been demonstrated over the dominant $\mathcal{S}_n$ space in earlier discussions [22]. The derived $\mathrm{sst}^{\lambda'}(\lambda)$ of (2)–(4) utilise the fitting of seminormal contents (λ) into specific Young tableau λ'-shapes as a method of enumerations.

Table 2

The ($p \leqslant 3$)-tuples yielding the set of monomials defining the SU(3) $\times$ $\mathcal{S}_{10}$ spin algebra. Treating these ($\lambda \vdash n$) parts of n as ($\mathbf{M}^\lambda$) modules with inherent Kostka reduction coefficients allows the full $\{:\lambda: \rightarrow \{[\lambda'']\}\}$ decompositions to be derived directly as set out in the text.

Subdimen. $:M \geqslant 0$ of $\lvert IM(\cdot)\rangle$:		p-part $\lambda \vdash n$ $\mathbf{M}^\lambda$ modules of set			
1	10	:10:			
10		:91:			
55	8	:82:	$:9-1:$		
210		:73:		:811:	
615	6	:64:	$:8-2:$	:721:	
1452		:55:		:631:	:712:
2850	4	:4, 6:	$:7-3:$	:541:, :622:	
4740		:3, 7:		:532:	:451:, :613:
6765	2	:2, 8:	$:6-4:$	:442:	:523:, :361:
8350		:1, 9:		:433:	:514:, :352:, :271:
8953	0	:10:	$:5-5:$	:181:, :262:	:343:, :424:

$59049 = 3^{10}$: total space dimensionality ($-10 \leqslant M \leqslant 10$).

On considering the natural embedded spin symmetry aspects, it is useful to distinguish between the physical $\mathbf{M}^\lambda$ (p-tuplar) model components occurring in the $(\lambda \vdash n) \trianglerighteq$ (prior) λ_{SA} dominant sector, with those found in the other sector. On balance, the evidence available would suggest the SU(3) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ spin algebra retains determinacy, in accord with the original criterion for the SU2-branching level. Thereafter, it is helpful to compare the mapping derived from the initial and final self-associate $(\lambda \vdash n)_{\mathrm{SA}}$ forms here, with the known self-associacy derived over irrep subsets for the corresponding Yamanouchi chain, $\mathcal{S}_{10} \supset \mathcal{S}_9 \supset \mathcal{S}_8 \supset \cdots \supset \mathcal{S}_2$, e.g., in the initial subduction stages

$$\begin{aligned}[4321]_{\mathrm{SA}} &\rightarrow \big\{[432] \oplus [4311] \oplus [4221] \oplus [3321]\big\}_{\mathrm{SA}}(\mathcal{S}_9) \\ &\rightarrow \big\{2[431] \oplus 2[422] \oplus 2[4211]_{\mathrm{SA}} \oplus 2[332]_{\mathrm{SA}} \oplus 2[3311] \\ &\qquad \oplus 2[3221]\big\}_{\mathrm{SA}}(\mathcal{S}_8). \end{aligned} \tag{11}$$

Over the full hierarchy, such processes constitute the origin of democratic $\mathcal{S}_n$-invariants under the dual group. A correspondence is observed to Levy-Leblond's democratic invariants [10,15,16], deduced from eigenvalue QM formalisms and $6j$-coefficients.

What one finds for the natural embedding is a contrasting behaviour between (11), or the SU(m) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ initial λ_{SA}, and the final SU(4) $\times$ $\mathcal{S}_{10}{\downarrow}\mathcal{D}_5$ $(\lambda \vdash n) \equiv$:4321:, with the $[\lambda]_{\mathrm{SA}}$ irrep $\equiv$ [4321] failing to map onto an overall SA-subduced subset. Any prediction of overall self-associacy under this subduced abstract group would require completely bijective maps, which finally yield

$$[\lambda]_{\mathrm{SA}} \rightarrow \big\{\mu(\mathcal{A}_1 + \mathcal{A}_2) + \mu'(\mathcal{E}_1 + \mathcal{E}_2)\big\}_{\mathrm{SA}}(\mathcal{S}_{10}{\downarrow}\mathcal{D}_5). \tag{12}$$

Behaviour departing from this strongly calls into question the SU(4)$\times\mathcal{S}_{10}\downarrow\mathcal{D}_5$ algebra's complete determinacy; the underlying cause for indeterminacy may be attributed to the observed weak degeneracy in the p-adic physical model in the ($\lambda \vdash n$) pre-SA dominant sector. Since the initial SA–SU(6) irrep retains self-associacy on subduction, our inference on degeneracy-induced indeterminacy at (or above) the SU($m \geqslant 4$)$\times\mathcal{S}_{10}\downarrow\mathcal{D}_5$ branching aspects appears valid. The present (weak) indeterminacy for $[^{11}\mathrm{B}]_{10}$ spin clusters is still in strong contrast to the absolute indeterminacy represented by the natural embedding SU(7) $\times$ $\mathcal{S}_6$ discussed in the work of Sullivan and Siddall III [20].

The physical importance of (8) lies in the way this *total-spin* irrep *constrains* a product with Γ(vib.) under the molecular symmetry group [5,17] to

$$\Gamma(\mathrm{spin, CNP}) \otimes \Gamma(\mathrm{m.vib.}) \equiv \mathcal{A}_i, \quad \text{with } i = 2(1),$$

as $I_l = n/2$ (integer) spins. To retain u, g for molecular symmetry conventions, inversion (as in [5]) should be interposed in the product irrep.

The explicit evaluation of (8) for the specific isotopomers, $\{[^1\mathrm{H}^{11}\mathrm{B}]_{10}[^{12}\mathrm{C}^1\mathrm{H}]_2; [^2\mathrm{H}^{11}\mathrm{B}]_{10}[^{12}\mathrm{C}^1\mathrm{H}]_2\}$, to give the CNP spin irreps as an inner product enumeration is not given, in view of the partial indeterminate nature of SU(4) $\times$ $\mathcal{S}_{10}\downarrow\mathcal{D}_5$. In any case, the physical insight on the determinacy aspects comes from the individual $[A]_{10}$ NMR monoclusters. The extensive work of Balasubramanian [3,4] on cage-clusters and fullerenes should be consulted for further aspects of rovibrational nuclear spin weights.

5. Conclusions

The specific criteria for independance of information content of such p-adic models is taken as the lack of any degeneracy involving a $\{|IM = 0\rangle\}$-contributing p-adic component, i.e., *prior* to λ_{SA} self-associate partition in the branching sequence.

Whilst the weak degeneracy observed above has no effect on the SU2, SU(3) $\times$ $\mathcal{S}_{10}$ branching level behaviour of the $[^1\mathrm{H}]_{10}$ or the $[^2\mathrm{H}]_{10}$ spin clusters with their simple $/\mathcal{G}/ = 10$ determinacy, the $[^{11}\mathrm{B}]_{10}$ spin system exhibits the (partial) physical indeterminacy reported above, as confirmed by [4411] being a multiple of [73].

Our purpose in presenting this form of discrete mathematical modelling is to stress its value when correctly interpreted. The results above underline the need to examine symmetry-embedding problems in some detail, even when the primary SU(2)-branching level of the subduced dual spin algebras is covered by Cayley's criterion; thus a case can be made for examining all the intermediate SU(m)-branched direct product algebras contributing to the pre-self-associate sector, since the $n \equiv /\mathcal{G}/$ condition alone *is not a sufficient condition* for full determinacy in SU($m \geqslant 3$) $\times$ $\mathcal{S}_n\downarrow\mathcal{G}$ group natural embeddings.

Finally, the existence of an equivalent quasi-geometrical formalism to Cayley's theorem has been demonstrated elsewhere [23,25,27]. Both lead to sets of specialised exclusively-combinatorial forms for spin invariance hierarchy under the SU2-level embedded spin symmetry inherent in nuclear spin vertex-labelled cages of t-polyhedra, as seen with other cage-isotopomers [23–27]. Recent work [24–26] has shown how the geometric (Voronoi) dual figures can serve to define these combinatorial geometric algebras. Naturally, the invariance properties for the *regular* automorphic polyhedral bicolour models come from a $\{\chi_i\}^M(\mathcal{S}_n\downarrow\mathcal{G})$ hierarchy of $\{M_i\}^{(M)}$ (inner/outer) SO(2)-weight sets, evaluated over $I \geqslant M \geqslant 0$.

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