Periodic Systems of Molecular States from the Boson Group Dynamics of $SO(3) \times SU(2)_s$

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An overview of the principles of group-dynamic periodic systems is given. The process by which atomic and molecular multiplets are obtained is then described, and reference is made to the support provided by the data. Atomic and molecular periodic systems consist of these multiplets situated in coordinates with axes which are the chemical angular-momentum quantum number l (or L) and the principal quantum number n (or n summed over all atoms). The periodic system for atoms serves as a template for the systems for molecules, and only one additional quantum number is needed for the molecular systems. Equivalence classes of substitutable multiplets are then defined and their numbers given. The structures of the resulting molecular periodic systems are shown as plots of the number of substitutable multiplets located at given quantum-number coordinates. Wall charts are available from R.A.H. or G.V.Zh.

1. INTRODUCTION

1.1. Periodic Systems. The purpose of constructing periodic systems of molecules is to make pertinent knowledge of experienced chemists available to the scientific community in a graphic manner. They are a small-molecule alternative to the large-molecule graph-theoretical classification schemes developed by organic and pharmaceutical chemists.[1]

1.2. Group-Dynamic Periodic Systems. In atomic and molecular spectroscopy, multiplets of single-electron states can be combined to obtain multiplets for many-electron states by using quantum vector addition (Clebsch−Gordan coefficients). The group-theoretical parallel to this procedure is to consider the single-electron states as basis vectors of the multiplets and to obtain the basis vectors of the many-electron multiplets by using seniority vectors and ladder operators.

In fundamental-particle group dynamics, quarks are combined to explain the existence of mesons and baryons (together known as hadrons). Considering multiplets with three or more quarks (or antiquarks) as basis vectors, multiplets of hadron basis vectors can be obtained by using the same techniques.[2,3] The diagrams often used to illustrate the process are actually periodic systems of quarks and hadrons.[4]

In previous papers, we showed how to use group theory to combine multiplets of atoms to create multiplets of molecules formed from two, three, or more atoms.[5−7] The individual atoms are basis vectors in their space, and there are also basis vectors in the space for N-atomic molecules. The theory is supported by extensive graphical studies of data, found in critical tables, for diatomic and triatomic molecules.[8]

2. ATOMIC AND MOLECULAR MULTIPLETS[7]

The group-theoretical description of the periodic system of atoms[7,9] presupposes that different chemical elements p are vectors formed by the use of the creation operator b_p^+

$$|p\rangle = b_p^+|0\rangle \qquad (1)$$

where $|0\rangle$ is the vacuum state. These vectors form an orthonormal set in the linear space $H(1)$ of the chemical elements

$$\langle p|q\rangle = \langle 0|b_p b_q^+|0\rangle = \delta_{pq} \qquad (2)$$

The description also assumes that there exists a group, G, of equivalent transformations of chemical elements one into another, and that a linear representation of G and of its algebra are given for $H(1)$. Group chains allow chemical elements to be associated into different classes and subclasses called multiplets. Multiplets, and elements in multiplets, can be enumerated by quantum numbers which are introduced to mark vectors of the space $H(1)$.

N-atomic molecules are taken to be vectors

$$|p_1 p_2 ... p_N\rangle = b_{p_1}^+ b_{p_2}^+ ... b_{p_N}^+|0\rangle \qquad (3)$$

For example, the vector $|CO\rangle = b_C^+ b_O^+|0\rangle$ represents the molecule carbon monoxide. The basis of the linear space $H(N)$ consists of orthonormal vectors, each formed from one or more terms (in linear combination) like eq 3. The description treats molecules as many-body bosonic systems. The computation of the vectors in any multiplet requires the use of Clebsch−Gordan coefficients or of chemical seniority vectors and ladder operators (using the symbolic mathematics program *GTPS*). The ladder operators are expressed in terms of bosonic creation and annihilation operators b_p^+ and b_q,
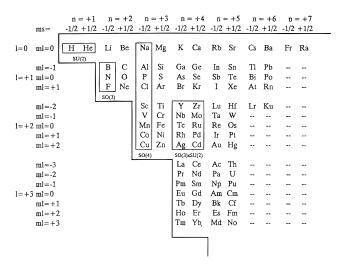
Figure 1. Schematic of the periodic system of atoms for the symmetry wherein $SO(3) \times SU(2)_s$ is in a subgroup chain of $SO(4,2) \times S(2)_s$. Typical multiplets are shown. The symbols *ms* and *ml* mean m_s and m_l.

where *p* and *q* denote any atoms, defined by

$$[b_p^+, b_q^+] = 0, \quad [b_p, b_q] = 0, \quad [b_p, b_q^+] = \delta_{pq} \qquad (4)$$

To compute the orthogonal multiplets, symbolic-manipulation programs were used to obtain seniority vectors, and then ladder operators were used again. The space $H(N)$ is thus reduced with respect to the group G and every subspace gives a molecular multiplet.

3. DESCRIPTION OF THE PERIODIC SYSTEMS

3.1. Chemical Quantum Numbers and Periodic Systems of Atoms. Chemical quantum numbers pertain to atoms and molecules and not to electron orbitals within them. The numbers which define multiplets in the case of $SO(3) \times SU(2)_s$ symmetry are *n, l* (for atoms) or *L* (for molecules), and *s* or *S*. It is assumed that all atomic state vectors exist for $n \leq 7$ and $l \leq 3$, i.e., all real atoms are included along with most, but not all, states up to $Z = 200$. The atomic periodic system consists only of multiplets with chemical spin $s = 1/2$, with one and only one doublet for each allowed pair of *n* and *l* (Figure 1). The first multiplet for a given *n* occurs at $l = n - 1$.

3.2. Substitutability of Multiplets. Any two atomic multiplets are said to be substitutable (to belong to the same equivalence class) if the atomic symbols come from different periods; for instance {B, C, N, O, F, Ne} and {Al, Si, P, S, Cl, Ar} are substitutable. For sets of molecular multiplets to be substitutable, they must contain basis vectors of substitutable atomic multiplets and must contain the same number of similar molecular multiplets. The second restriction allows multiplets derived from the chemical seniority vectors |BBB> and |AlAlAl> to be substitutable but causes those with |BBAl> and |BAlGa> not to be.

There are 76 different diatomic equivalence classes. The basis vectors, in terms of specific molecular formulas, have been determined for all the states of one (in many cases, more than one) multiplet in each of these equivalence classes. There exist 954 equivalence classes for triatomic multiplets. The number of multiplets in each class is obtained combinatorially.
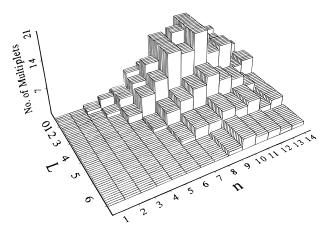

Figure 2. Schematic of the periodic system for singlet diatomic-molecular states in $SO(3) \times SU(2)_s$ symmetry.
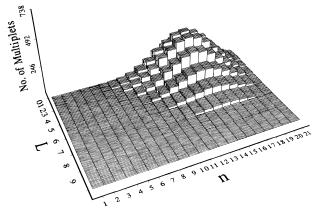

Figure 3. Schematic for the periodic system of quartet triatomic-molecular states in $SO(3) \times SU(2)_s$ symmetry.

3.3. Diatomic Systems. The diatomic molecular-state periodic system for $SO(3) \times SU(2)_s$ consists of roughly equal numbers of triplet and singlet (Figure 2) chemical-spin multiplets. Thus, the multiplicity is the only new quantum number introduced in the transition from atomic to molecular-state systems, and so the dimensionality of the systems does not increase further as N increases. The first multiplets for a given *n* occur at $L = n - 2$. The position with the largest number of multiplets (21) is $(n,L) = (10,2)$.

The system of singlets is similar to that of the triplets. Two wall charts showing the multiplets and basis vectors for both triplet and singlet systems are available from R.A.H. and G.V.Zh.

3.4. Triatomic Systems. The diagrams for the triatomic systems of $SO(3) \times SU(2)_s$ are constructed in the same manner. There are quartet and doublet chemical spin states. In Figure 3, the first quartet multiplets for a given *n* occur along the line $L = n - 3$; the number of multiplets along that line is relatively small, and thus the boundary is difficult to see. The number of doublets is approximately twice the number of quartets, and their distribution is shown on one wall chart.

4. DISCUSSION

This paper presents periodic systems of diatomic and triatomic molecular states in $SO(3) \times SU(2)_s$ group-dynamic symmetries. These complete periodic systems require only one quantum number more than does the periodic system of the elements, and the latter serves as a template for the former.

A parallel construction of periodic systems for diatomic and triatomic molecular states has been effected for symmetry $SO(2,1)$ for later publication. The really significant achievement which these periodic systems represent is the formulation of visual molecular classification schemes from symmetry first principles, i.e., from the group dynamics which is appropriate to boson statistics. This formulation gives them the same sort of solid footing which is characteristic of the standard quark model.

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