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Periodic Systems of Molecules from Group Theory

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(Received

Abstract.

Atoms are indistinguishable particles which can be transformed one into another by the elements of a group G ,¹ which corresponds to the internal symmetry of their periodic system. We construct a molecular periodic system using G and bosonic creation operators. The vectors $|\hat{i}\rangle = b^+_{\hat{i}}|0\rangle$ correspond to various atoms where $|0\rangle$ is the vacuum state vector, and b^+_i is the creation operator for atom i . The annihilation operator is b_i ; boson symmetry requires $[b_i, b_j] = b^+_i b^+_j] = 0$, $[b_i, b^+_i] = 1$. State vectors $|ijk\dots\rangle$ correspond to molecules. They can be recast as a direct sum of irreducible representations whose vectors are (often) linear combinations of individual molecular states. The one-particle operator P_1 of the Lie algebra of G is $\sum_{i,j} P_1(i;j) b^+_i b_j$. We have tested our systems by plotting a variety of tabulated experimental data along principle axes for atomic and for diatomic and triatomic molecular multiplets.

1. Zhuvikin, G.V., Hefferlin, R., Vestnik Leningradskovo Universiteta No. 16, Pg. 10, 1983.

Part 1. Introduction

This study extends the group theoretical concepts applied to the periodic system of atoms, outlined by A. I. Fet, to that of molecules. Bosonic symmetry is required in accordance with the previous work completed by R. Hefferlin and G.V. Zhuvikin. This paper results from their previous work along with the development of a computer program which computes symmetry multiplets, thus bypassing the tedious algebraic work of hand producing multiplets for the study of particular symmetries.

Part 2. Theory

The set of atoms, designated as A throughout the paper, is assumed to be a noncompact set of indistinguishable particles. We assume that this set of atoms possesses an internal symmetry for which there exists symmetry groups corresponding to particular subsets of A . If we suppose B is one of these particular subsets of A , then there is a symmetry group, call it G , corresponding to this internal symmetry of B . The elements (atoms) of B are defined to be linearly independent basis vectors for some Hilbert space L_{γ} . See figure 1. More precisely, we define an isomorphism between the atoms in B and the basis vectors in L_{γ} . Now if we define γ as a homomorphism from G to $GL(L_{\gamma})$, where $GL(L_{\gamma})$ is the group of all injective linear transformations from L_{γ} to L_{γ} , then γ is a representation of G and L_{γ} is a representation space¹ of G . See figure 2. Thus, any representation matrix M_g in $GL(L_{\gamma})$, corresponding to the operator g in G , operating any vector $|a\rangle$ in L_{γ} , converts $|a\rangle$ into some other vector $|b\rangle$ in L_{γ} with the property that any element g of G operating on any element (atom) a in B converts a into some other element (atom) b in B . In effect, the elements of G change one atom into another atom in exactly the same way that ladder operators change one state vector into some other state vector. In this sense, all atoms are theorized to be excited states of some abstract particle.

Similarly, N-atomic molecules are assumed to be indistinguishable N-tuples in the direct product $M = \prod_{i=1}^N A_i$. This set M is clearly also a noncompact set for which there exist symmetry groups corresponding to the internal symmetry of the N-atomic molecules under study, i.e., for particular subsets of M . If we suppose that C is one of these particular

subsets of M , then the N -tuples of C are defined to be linearly independent basis vectors for some Hilbert space L_N . Again, we define a homomorphism from G to $GL(L_N)$ so that L_N is a representation space of G . In an analogous fashion to the atomic case, any representation matrix M_g in $GL(L_N)$, corresponding to the operator g in G , operating any vector $|a_1, a_2, a_3, \dots, a_N\rangle$ in L_N , converts $|a_1, a_2, a_3, \dots, a_N\rangle$ into some other vector $|b_1, b_2, b_3, \dots, b_N\rangle$ in L_N with the property that any element g of G operating on any element (N-atomic molecule) $(a_1, a_2, a_3, \dots, a_N)$ in B converts $(a_1, a_2, a_3, \dots, a_N)$ into some other element (N-atomic molecule) $(b_1, b_2, b_3, \dots, b_N)$ in B . The representation space L_N is not in general an irreducible representation space of G . Thus, this vector space can be decomposed into a direct sum of irreducible subspaces L_{N_i} for i in some indexing set² I .

Section 2.1. The symmetry groups, and their subgroups

The groups acting on the particular subsets of A are known as special unitary groups and/or special orthogonal groups. See table 1. Of particular interest to the theory are the groups $SO(4,2)$ and $SU(2)$. The symmetry group $SO(4,2)$ consists of all orthogonal transformations with determinant 1 in the pseudo-Euclidian space $(x_1, x_2, x_3, x_4, x_5, x_6)$. This group has two chains of subgroups. See figure 3. However, for the scope of this paper we will concern ourselves only with the chain: $SO(4,2) > SO(4) > SO(3) > SO(2)$. The matrix operators corresponding to the subgroup $SO(4) < SO(4,2)$ consist of all orthogonal transformations with determinant 1 in the subspace (x_1, x_2, x_3, x_4) of $(x_1, x_2, x_3, x_4, x_5, x_6)$ while keeping the subspace (x_5, x_6) constant³. It can be shown that the decomposition of the representation space of $SO(4)$ generates irreducible subspaces (i.e. multiplets), each of which correspond to some unique element in the index set $\{1,2,3,\dots\}$. See figure 4. We associate this index set with the set of chemical principle quantum states $n = 1, 2, 3, \dots$ and denote the multiplet corresponding to some state n as $\{n\}$. In short, the chemical principle quantum ground state $n = 1$ corresponds to the multiplet $\{1\}$ of $SO(4)$, the chemical principle quantum state $n = 2$ corresponds to the multiplet $\{2\}$, and so on.

Continuing in this fashion, we obtain the subgroup $SO(3)$ from the chain $SO(3) < SO(4) < SO(4,2)$. The matrix operators corresponding to this subgroup consists of all orthogonal transformations with determinant 1 in the subspace (x_1, x_2, x_3) while keeping the coordinates in the subspace (x_4, x_5, x_6) constant. The decomposition of the representation

space of SO(3) generates submultiplets of $\{n\}$, that is, each set of multiplets in SO(3) corresponds to a particular chemical principle quantum number n and each multiplet in each set corresponds to a particular chemical angular momentum l_n . See figure 5. We denote these multiplets as $\{n;l\}$. Continuing down the chain, the multiplets of the representation space of SO(2), are distinguished by different values of chemical magnetic quantum numbers m , where m takes on the values $-l, -l+1, \dots, 0, \dots, l-1, l$.

So far, we have demonstrated the existence of three different indices (or quantum numbers) for which we can distinguish multiplets of A in SO(4,2) symmetry, that is, the multiplets of SO(2) are denoted $\{n;l;m\}$. (Note: since A and the representation Hilbert space L_1 are isomorphic, we will often speak of A as if it were the representation space L_1) However, it can be shown that two atoms correspond to each particular multiplet $\{n;l;m\}$. Thus there is not a one to one correspondence between the multiplets generated by SO(4,2) and the set of atoms. Now, the well known unitary group SU(2) produces doublets which we denote as corresponding to chemical spin μ ($\mu = +1/2$ or $\mu = -1/2$). Thus, by forming the direct product SO(4,2)xSU(2), we see that the unitary group SU(2) effectively distinguishes between the two atoms corresponding to some particular multiplet $\{n;l;m\}$ by producing the multiplets $\{n;l;m;+1/2\}$ and $\{n;l;m;-1/2\}$. As a result, there is a one to one correspondence between the multiplets of SO(4,2)xSU(2) and the set of atoms A .

As is evident, this particular chain of subgroups of SO(4,2)xSU(2) produces four different quantum numbers:

$$\begin{aligned} n &= 1, 2, 3, \dots; \\ l &= 0, 1, 2, 3, \dots, n-1; \\ m &= -l, -l+1, \dots, 0, \dots, l-1, l; \\ \mu &= +1/2, -1/2; \end{aligned}$$

where each vector, representing the elements of SO(4,2)xSU(2), corresponds to a particular multiplet⁴ $\{n;l;m;\mu\}$ in SO(2)xSU(2) and conversely, each multiplet in SO(2)xSU(2) corresponds to a particular vector. See figure 6.

Section 2.2. Application of the group SO(4,2)xSU(2) and its subgroups to periodic systems of molecules.

Let $V = \{v_1, v_2, v_3, \dots\}$ be some subset of A . Then, in accordance with the general method, the set of basis vectors spanning L_1 is defined as $\{|v_1\rangle, |v_2\rangle, |v_3\rangle, \dots\}$ where

the basis vector $|v_i\rangle$ corresponds to the atom v_i in V , for some i in $\{1,2,3,\dots\}$. The creation operator $b_{v_i}^+$ is defined as the operator which, when operating on the vacuum state $|0\rangle$, produces the vector $|v_i\rangle$ corresponding to the atom v_i . That is:

$$b_{v_i}^+|0\rangle = |v_i\rangle$$

The annihilation operator b_{v_i} is defined as the operator which, when operating on the atomic state $|v_i\rangle$ produces the vacuum state $|0\rangle$. That is:

$$b_{v_i}|v_i\rangle = |0\rangle.$$

When the annihilation operator operates on the vacuum state, the result is the scalar zero. Notice that since every vector has a one to one correspondence to some particular multiplet $\{n;l;m;\mu\}$, the vector $|v_i\rangle$ can be equivalently denoted $|n;l;m;\mu\rangle$. In fact, since one need not be restricted to one particular periodic system, the most precise way to denote any vector is to denote it using its corresponding quantum numbers. However, in order to simplify many of the equations, we will usually use v and $|v\rangle$, instead of $\{n;l;m;\mu\}$ and $|nlm\mu\rangle$ to denote atoms and atomic vectors respectively.

Since observations in nature have demonstrated that a molecule may have any number of identical atoms, it seems natural that bosonic symmetry is required. Thus, we obtain the following commutators:

$$\begin{aligned} [b_v^+, b_w^+] &= 0 \\ [b_v, b_w] &= 0 \\ [b_v, b_w^+] &= \delta_{v,w} \end{aligned}$$

for any v, w in V . It can easily be shown that these commutation relations imply that

$$\langle v|v\rangle = 1 \quad \text{for any } v \text{ in } V.$$

Thus, all atomic basis vectors are naturally normalized.

To generalize the discussion from atoms to N-atomic molecules, let $\{ (a_1 a_2 a_3 \dots a_N), (b_1 b_2 b_3 \dots b_N), (c_1 c_2 c_3 \dots c_N), \dots \}$ be a set of N-atomic molecules. Then the corresponding set of basis vectors spanning L_N is $\{|a_1 a_2 a_3 \dots a_N\rangle, |b_1 b_2 b_3 \dots b_N\rangle, |c_1 c_2 c_3 \dots c_N\rangle, \dots\}$. The creation and annihilation operators are defined as in the atomic case. However, the creation of any state vector, say $|a_1 a_2 a_3 \dots a_N\rangle$, is defined as:

$$b_{a_1}^+ b_{a_2}^+ b_{a_3}^+ \dots b_{a_N}^+ |0\rangle = |a_1 a_2 a_3 \dots a_N\rangle.$$

Now, we require that these basis vectors be normalized. Thus for N-atomic molecules, a normalized basis vector is:

$$1/\text{Sqrt}[\langle a_1 a_2 a_3 \dots a_N | a_1 a_2 a_3 \dots a_N \rangle] b^+ a_1 b^+ a_2 b^+ a_3 \dots b^+ a_N | 0 \rangle$$

Analogous to the atomic case, it can be shown that repeated application of the commutation relations produces:

$$\langle a_1 a_2 a_3 \dots a_N | a_1 a_2 a_3 \dots a_N \rangle = \prod_{i=1}^m C(S_i)! ,$$

where m is the number of distinct atoms and $C(S_i)$ is cardinality of the i th set of homonuclear atoms, S_i , belonging to the N -atomic molecule $a_1 a_2 a_3 \dots a_N$. For example, suppose that from the atoms x, y, z , we construct the the 6-atomic basis vector $xxxxyyz$. Then the norm of $xxxxyyz$ is just:

$$\langle xxxxyyz | xxxxyyz \rangle = \prod_{i=1}^3 C(S_i)! = C(\{x, x, x\})! C(\{y, y\})! C(\{z\})! = 3! 2! 1! = 12.$$

Section 2.3. Description of the representation space operators of the subgroups of SO(4,2) and SU(2)

Every subgroup G of SO(4,2) has generators of G which correspond to the group representation matrix generators in $GL(L_N)$, call them $\Gamma_z, \Gamma_+, \Gamma_-$. We associate these generators with ladder operators. In addition, bosonic symmetry requires that these ladder satisfy the following commutation relations:

$$[\Gamma_z, \Gamma_+] = \Gamma_+$$

$$[\Gamma_z, \Gamma_-] = -\Gamma_-$$

$$[\Gamma_+, \Gamma_-] = 2\Gamma_z$$

It can be shown that for SO(4)xSU(2) these representation matrix ladder operators take the form:

$$A_z = \sum_{n,l,m,\mu} [(l+m+1)(l-m+1)(n-l)(n+l+1) / (2l+3)(2l+1)]^{1/2} b^+_{n,l+1,m,\mu} b_{n,l,m,\mu} + \sum_{n,l,m,\mu} [(l+m)(l-m)(n-l)(n+l) / (2l+1)(2l-1)]^{1/2} b^+_{n,l-1,m,\mu} b_{n,l,m,\mu}$$

$$A_+ = \sum_{n,l,m,\mu} [(l-m)(l-m-1)(n-l)(n+l) / (2l+1)(2l-1)]^{1/2} b^+_{n,l-1,m+1,\mu} b_{n,l,m,\mu} + \sum_{n,l,m,\mu} [(l+m+1)(l+m+2)(n-l-1)(n+l+1) / (2l+3)(2l+1)]^{1/2} b^+_{n,l+1,m+1,\mu} b_{n,l,m,\mu}$$

$$A_- = - \sum_{n,l,m,\mu} [(l+m)(l+m-1)(n+l)(n-l) / (2l+1)(2l-1)]^{1/2} b^+_{n,l-1,m-1,\mu} b_{n,l,m,\mu} + \sum_{n,l,m,\mu} [(l-m+1)(l-m+2)(n-l-1)(n+l+1) / (2l+3)(2l+1)]^{1/2} b^+_{n,l+1,m-1,\mu} b_{n,l,m,\mu}$$

The representation space generators of SO(3) have the form:

$$M_z = \sum_{n,l,m,\mu} m b_{n,l,m,\mu}^+ b_{n,l,m,\mu}$$

$$M_+ = \sum_{n,l,m,\mu} [(l+m+1)(l-m)]^{1/2} b_{n,l,m+1,\mu}^+ b_{n,l,m,\mu}$$

$$M_- = \sum_{n,l,m,\mu} [(l-m+1)(l+m)]^{1/2} b_{n,l,m-1,\mu}^+ b_{n,l,m,\mu}$$

Analogously, the representation space of the group SU(2) has generators:

$$S_z = \sum_{n,l,m,\mu} m b_{n,l,m,\mu}^+ b_{n,l,m,\mu}$$

$$S_+ = \sum_{n,l,m,\mu} [(1/2 + \mu + 1)(3/2 - \mu)]^{1/2} b_{n,l,m+1,\mu}^+ b_{n,l,m,\mu}$$

$$S_- = \sum_{n,l,m,\mu} [(1/2 - \mu + 1)(3/2 + \mu)]^{1/2} b_{n,l,m-1,\mu}^+ b_{n,l,m,\mu}$$

Thus for atoms, $S_+ |n, l, m, \mu\rangle$ will produce $|n, l, m, \mu+1\rangle$ and $M_+ |n, l, m, \mu\rangle$ will produce $|n, l, m+1, \mu\rangle$, where we have normalized both results. As a specific example, suppose we choose to operate on the diatomic vector $|HHe\rangle$ with the operator S_+ , then we obtain (after normalizing) the vector $1/\sqrt{2} |HeHe\rangle$.

Section 2.4. Description of the decomposition of the representation space L_N into a direct sum of irreducible subspaces of L_N

We define a seniority vector as a vector in L_N such that either the raising ladder operator operating on the vector produces the zero result or the lowering ladder operator operating on the seniority vector produces the zero result. In some sense, a seniority vector is analogous to a generating element in a group under one of the operators M_+, M_-, S_+, S_- , etc. This follows since repeated function composition on the seniority vector will generate the smallest possible multiplet containing it. Another way of saying the same thing is that the multiplet generated by the seniority vector is an irreducible subspace of L_N . Turning to the specific symmetry SO(3)xSU(2), we construct irreducible multiplets (that is, irreducible subspaces of L_N) of state vectors by repeated use of the ladder operators M_+, M_- and S_+ or S_- on some seniority state vector in L_N . This is all done with the goal of finding the irreducible

multiplet decomposition of the Hilbert representation space L_N . The process of repeated ladder operation on the seniority vector may produce mixed states and, in fact, this is usually the case. These mixed states are, by definition, linear combinations of the basis state vectors of L_N (take $|ab\rangle + |bc\rangle$ in L_2 for example). Thus, to find all irreducible multiplets one must not only find the multiplets generated by each basis state, but also the multiplets generated by the vectors orthogonal to the generated mixed state vectors.

For example, in $SO(3) \times SU(2)$ we select the subset $\{B, C, N, O, F, Ne\} \times \{B, C, N, O, F, Ne\}$ of $A \times A$. The ortho-normalized basis vectors spanning L_2 are defined to be $1/\sqrt{2} |BB\rangle, |BC\rangle, |BN\rangle, \dots, |NeF\rangle, 1/\sqrt{2} |NeNe\rangle$. Note: to simplify notation we will denote specific vectors like $1/\sqrt{2} |BB\rangle$ as just $1/\sqrt{2} BB$ and so on, instead of using traditional dirac notation. (Reference to figure 7 throughout the rest of this paragraph will be helpful.) Now if we select $1/\sqrt{2} BB$ as the seniority vector, then one readily forms an irreducible multiplet by using the raising operators M_+ and S_+ repeatedly on $1/\sqrt{2} BB$. This multiplet, which has spin multiplicity $S = 3$ and angular momentum $L = 2$, is denoted using spectroscopic notation as 3D . Now, that there exists mixed states in the 3D multiplet. Thus, the 3D multiplet does not span all of L_2 . By finding the vector orthogonal to $1/\sqrt{3} (BF + NN)$, namely $1/\sqrt{6} (2BF - NN)$, we can form a new irreducible multiplet. This new irreducible multiplet again has spin multiplicity $S = 3$. However, the angular momentum L has changed from 2 to 0. Thus, this multiplet is denoted as 3S . Consequently, we see that the process of finding a vector orthogonal to some mixed state vector and generating its resulting multiplet effectively raises or lowers the angular momentum L . However, this process is not analogous to some new raising or lowering operator for L , since it allows one to skip integral steps of L (example given: the previous case).

In completely the same way, we construct the 1P multiplet from the vector orthogonal to $1/\sqrt{2} (BO + CN)$, namely: $1/\sqrt{2} (BO - CN)$. Notice that the three multiplets all contain mutually orthogonal vectors with respect to like quantum numbers μ and m . Thus, we have exhausted the different possibilities of orthogonal mixed state vectors, and thus we have exhausted the different possibilities of irreducible multiplets. Now, since we know that in general L_N can be expressed as a direct sum of irreducible subspaces, we must have $L_2 = {}^3S + {}^1P + {}^3D$.

Section 2.5. Expectation values for observables

For atoms, the expectation value of any single particle observable P is given by:

$$\langle P \rangle = \langle v | P | v \rangle$$

where P may be the single particle operator defined as:

$$P = P_1 = \sum_i P(i;n) b_i^\dagger b_n$$

N-Atomic molecules are analogous. That is, the expectation value of any observable P is given by:

$$\langle P \rangle = \langle a_1 a_2 a_3 \dots a_N | P | a_1 a_2 a_3 \dots a_N \rangle / \langle a_1 a_2 a_3 \dots a_N | a_1 a_2 a_3 \dots a_N \rangle$$

Notice that since N-atomic molecular state vectors are not naturally normalized, we must worry about normalization. Now, for the N-atomic case we need not restrict ourselves to single particle operators like was required for the atomic case. The analogous definition for a two particle operator is:

$$P_2 = \sum_{i \geq j} \sum_{n \geq p} P(i,j;n,p) b_i^\dagger b_j^\dagger b_n b_p$$

And a three particle operator takes the form:

$$P_3 = \sum_{i \geq j \geq k} \sum_{n \geq p \geq r} P(i,j,k;n,p,r) b_i^\dagger b_j^\dagger b_k^\dagger b_n b_p b_r$$

In general, given an N-atomic molecular vector, N-particle operators exist and follow the same pattern.

If we take the case of triatomic molecules, then we may employ single-, double-, or triple-particle operators to find expectation values. Supposing a vector of the form $|xyz\rangle$, then a three particle operator trivially gives:

$$\langle xyz | P_3 | xyz \rangle = \langle xyz | P_3 | xyz \rangle.$$

A two particle operator gives the diatomic identity:

$$\langle xyz | P_2 | xyz \rangle = \langle xy | P_2 | xy \rangle + \langle xz | P_2 | xz \rangle + \langle yz | P_2 | yz \rangle.$$

And a single particle operator gives the atomic identity:

$$\langle xyz | P_1 | xyz \rangle = \langle x | P_1 | x \rangle + \langle y | P_1 | y \rangle + \langle z | P_1 | z \rangle.$$

This pattern can be extended to N-atomic molecules as well. In fact, for a single particle operation on an N-atomic vector we get:

$$\begin{aligned} \langle a_1 a_2 a_3 \dots a_N | P_1 | a_1 a_2 a_3 \dots a_N \rangle &= \langle a_1 | P_1 | a_1 \rangle + \langle a_2 | P_1 | a_2 \rangle + \\ &+ \langle a_3 | P_1 | a_3 \rangle + \dots + \langle a_N | P_1 | a_N \rangle \end{aligned}$$

The extent to which any particle operator other than an N-atomic particle operator operating on an N-atomic vector has any practical physical significance in predicting data for various N-

atomic molecules is unknown at the present time. A study of various plots involving different particle operators will indicate the degree of usefulness of these nontrivial identities.

However, there does exist a theoretical importance to the identities. Notice that,

$$\langle a_1 | P_1 | a_1 \rangle = \langle a_1 a_1 a_1 \dots a_1 | P_1 | a_1 a_1 a_1 \dots a_1 \rangle,$$

$$\langle a_2 | P_1 | a_2 \rangle = \langle a_2 a_2 a_2 \dots a_2 | P_1 | a_2 a_2 a_2 \dots a_2 \rangle$$

and so on. Thus, it follows that the expectation value of the original N-atomic state vector, can be rewritten completely in terms of homonuclear expectation values:

$$\begin{aligned} \langle a_1 a_2 a_3 \dots a_N | P_1 | a_1 a_2 a_3 \dots a_N \rangle = & \\ & \langle a_1 a_1 a_1 \dots a_1 | P_1 | a_1 a_1 a_1 \dots a_1 \rangle + \\ & + \langle a_2 a_2 a_2 \dots a_2 | P_1 | a_2 a_2 a_2 \dots a_2 \rangle + \\ & + \langle a_3 a_3 a_3 \dots a_3 | P_1 | a_3 a_3 a_3 \dots a_3 \rangle + \\ & + \dots + \\ & + \langle a_N a_N a_N \dots a_N | P_1 | a_N a_N a_N \dots a_N \rangle \end{aligned}$$

This is of great theoretical as well as practical interest since we see that one can employ this homonuclear identity to reduce a problem involving heteronuclear expectation values to sums of only homonuclear expectation values. Graphs using this homonuclear approximation have been plotted with good results (see parts 3 and 4).

Section 2.6. Computer program which produces symmetry multiplets and expectation values.

The process of hand producing multiplets and expectation values becomes very tedious for diatomic and higher order molecules. Consequently, a computer program has been constructed to provide multiplets and expectation values for certain symmetries. In particular, given a seniority vector in SO(3)xSU(2) symmetry, the program will produce the irreducible multiplet which contains the seniority vector. While the program is still in the developmental stage, it has nevertheless produced some nice results. Specifically, the appendix contains a listing of the diatomic multiplets in SO(3)xSU(2) symmetry that the program has generated. Notice that for a specific chemical angular momentum b, all triplet multiplets formed with $I = b \times b$ are seen to be isomorphic. This is particularly nice since with the construction of one triplet multiplet with $I = b \times b$, all other triplet multiplets with $I = b \times b$, can be formed by just a renaming process. The same result holds true for all singlet multiplets as well.

Part 3. Results for ionization potentials

Expectation values of ionization potentials for the P atoms of row 2 (B, C, N, O, F, Ne) have been plotted in figure 8. The expectation value for each state was calculated using a single particle operator. The number on each block represents the number of electrons which the molecule, or atom in this case, possesses. The trend for this plot is clear--ionization potentials increase with both μ and m .

The expectation values for the states belonging to the triplet D multiplet for diatomics formed from the same set of atoms have been plotted in figure 9. Again, a single particle operator was used to formulate the expectation values. Unfortunately, it is not clear whether the ionization potentials decrease or increase with μ and m . It does appear, however, that the data seems not to contradict the atomic case. Figure 10 corresponds to this same multiplet, however, using various homonuclear identities, the formulas for the expectation values have been recast into a sum involving only homonuclear terms. This has the effect of smoothing the surface of the graph. For purposes of interpolation, we have assumed that the ionization potential of B_2 was 8 eV for the white and light shaded areas and we have assumed that the ionization potential for NeNe is 16 eV for the white and medium shaded areas. Notice that the ionization potentials increase with μ and m as it did in the atomic case. In addition, the level curves of the surface seem parallel to isoelectronic sequences. Least-squares analysis will demonstrate whether this appearance is indeed the case.

The expectation values for the states belonging to the singlet P multiplet for diatomics have been plotted on figure 11. The assumptions made on this plot correspond to the assumptions made in figure 10. Notice that the ionization potentials increase with m . Since this multiplet is a singlet, we can have no graphical information about μ , however the variation of ionization potentials with m is in agreement with figures 8 and 9.

The expectation values for the states belonging to the triplet S multiplet for diatomics have been plotted in figure 12. The assumptions made for the singlet P and the triplet D plots hold for this graph as well. Notice that the ionization potentials increase with μ in agreement with the Diatomic triplet D and the atomic doublet P plot. Thus the same general trend for the ionization potentials is found to be consistent with all the graphs plotted for ionization potentials

Part 4. Results for Heat of atomization

The expectation values for ΔH_a of the states belonging to the triplet D multiplet for diatomic molecules formed from the P atoms of row 2 have been plotted in figure 14. A single particle operator was used to formulate the expectation values. Notice that ΔH_a first increases with μ and m , but then later decrease with μ and m . Again, to a first approximation, the level curves of of the surface seem to be parallel to isoelectronic sequences. Figure 15 is a plot of ΔH_a for this same triplet D multiplet, however the expectation value formulation has been recasted so as to involve only homonuclear terms. The effect is that the surface is smoother than the previous case. Notice that the same trends are visible for this plot as was for the previous case.

The expectation values of ΔH_a for the states belonging to the singlet P multiplet for diatomics formed from the same set of atoms have been plotted on figure 16. Notice that ΔH_a decreases with m . Referring back to figures 14 and 15, one sees that, for the same range of quantum numbers, the trend of ΔH_a for the singlet P multiplet agrees with the trend found in the triplet D multiplet (that is figures 14 and 15). The corresponding plot involving only homonuclear terms in the expectation value is found in figure 17. This plot contains a minimum which is inconsistant with both figures 14 and 15. Further investigation as to why this inconsistency occurs should be undertaken.

The expectation values of ΔH_a for the state belonging to the triplet S multiplet of diatomic molecules formed from the same set of atoms have been plotted on figures 18 and 19. Figure 18 has been plotted using the original formulation of the expectation values of the states. Figure 19, however has been plotted by using homonuclear identities. Notice that ΔH_a decreases with μ for both plots; this is in agreement with figures 14 and 15.

For triatomics, we have plotted the molecules formed from this same set of P atoms from row 2. In figure 20, notice that while a good portion of the data for the quartet F multiplet is missing, the data available does seem to agree with the general trend for ΔH_a . Notice also that, to a first approximation, the level curves of this plot seem to lie along the isoelectronic sequences. As in the other cases, least squares analysis will determine whether this is truly the case or not.

The doublet D multiplet also seems to support this general trend for ΔH_a . Figure 21 is a plot of ΔH_a for the doublet D multiplet.

Figure 22 is a plot of ΔH_a for the P multiplet of triatomic molecules formed from the same

P atoms of row 2. From the available data, one can not draw any conclusion about the trend in figure 22 for the quartet P multiplet. However, the plot does not appear to contradict the general trend for ΔH_a . Thus, we conclude that the same general trend for the heat of atomization is found or is consistent in nearly all of the graphs plotted.

Conclusion

This paper considers only vectors corresponding to like quantum numbers n and l . However, "off diagonal" multiplets do exist which contain vectors corresponding to mixed quantum numbers n and l . Thus, a complete listing for diatomics should be done. This is currently being accomplished via the computer program and the results appear encouraging. Both diatomic and triatomic molecules are also being heavily investigated, though triatomics will take considerably more time due to the intensity of the calculations involved and the lack of experimental data. In addition, a bridge between the general theory outlined in this paper and that of quantum mechanics needs to be done to more fully demonstrate the theory's promise.

Clearly, the trends visible in ionization potential and heat of atomization for up to triatomic molecules from the P atoms of row 2 suggest that significant trends might be global. However, this set of graphs is very small compared to the number of multiplets that exist for even a diatomic periodic system in $SO(3) \times SU(2)$ symmetry. As a result of the increase in calculation efficiency which the computer program brings to the development of the study, many more graphs will be able to be produced in an effort to conclusively demonstrate that these and other trends are in fact general.

**APPENDIX: Incomplete listing of diatomic multiplets in $SO(3) \times SU(2)$
symmetry produced by computer program**

3S ; $n = 1 \times 1$; $l = 0 \times 0$

$m = 0$

$\mu = -1$ $\sqrt{1/2}$ (1 HH)
 $\mu = 0$ $\sqrt{1/1}$ (1 HHe)
 $\mu = +1$ $\sqrt{1/2}$ (1 HeHe)

3S ; $n = 2 \times 2$; $l = 0 \times 0$

$m = 0$

$\mu = -1$ $\sqrt{1/2}$ (1 LiLi)
 $\mu = 0$ $\sqrt{1/1}$ (1 LiBe)
 $\mu = +1$ $\sqrt{1/2}$ (1 BeBe)

3S ; $n = 2 \times 2$; $l = 1 \times 1$

$m = 0$

$\mu = -1$ $\sqrt{1/6}$ (2 BF + -1 NN)
 $\mu = 0$ $\sqrt{1/3}$ (1 BNe + 1 CF + -1 NO)
 $\mu = +1$ $\sqrt{1/6}$ (2 CNe + -1 OO)

1P ; $n = 2 \times 2$; $l = 1 \times 1$

$m = -1$

$\mu = 0$ $\sqrt{1/2}$ (1 BO + -1 CN)

$m = 0$

$\mu = 0$ $\sqrt{1/2}$ (-1 BNe + 0 NO + 1 CF)

$m = +1$

$\mu = 0$ $\sqrt{1/2}$ (-1 NNe + 1 OF)

$3D$; $n = 2 \times 2$; $l = 1 \times 1$

$m = -2$

$\mu = -1$ $\sqrt{1/2}$ (1 BB)

$\mu = 0$ $\sqrt{1/1}$ (1 BC)

$\mu = +1$ $\sqrt{1/2}$ (1 CC)

$m = -1$

$\mu = -1$ $\sqrt{1/1}$ (1 BN)

$\mu = 0$ $\sqrt{1/2}$ (1 BO + 1 CN)

$\mu = +1$ $\sqrt{1/1}$ (1 CO)

$m = 0$

$\mu = -1$ $\sqrt{1/3}$ (1 BF + 1 NN)

$\mu = 0$ $\sqrt{1/6}$ (1 BNe + 1 CF + 2 NO)

$\mu = +1$ $\sqrt{1/3}$ (1 CNe + 1 OO)

$m = +1$

$\mu = -1$ $\sqrt{1/1}$ (1 NF)

$\mu = 0$ $\sqrt{1/2}$ (1 NNe + 1 OF)

$\mu = +1$ $\sqrt{1/1}$ (1 ONe)

$m = +2$

$\mu = -1$ $\sqrt{1/2}$ (1 FF)

$\mu = 0$ $\sqrt{1/1}$ (1 FNe)

$\mu = +1$ $\sqrt{1/2}$ (1 NeNe)

$3S$; $n = 3 \times 3$; $l = 0 \times 0$

$m = 0$

$\mu = -1$ $\sqrt{1/2}$ (1 NaNa)

$\mu = 0$ $\sqrt{1/1}$ (1 NaMg)

$\mu = +1$ $\sqrt{1/2}$ (1 MgMg)

$3S$; $n = 3 \times 3$; $l = 1 \times 1$

$m = 0$

$\mu = -1$ $\sqrt{1/6}$ (2 AlCl + -1 PP)

$$\mu = 0 \quad \text{sqrt}[1/3] \quad (1 \text{ AIAr} + 1 \text{ SiCI} + -1 \text{ PS})$$

$$\mu = +1 \quad \text{sqrt}[1/6] \quad (2 \text{ SiAr} + -1 \text{ SS})$$

1P ; n = 3 x 3; l = 1 x 1

$$m = -1$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (-1 \text{ AIS} + 1 \text{ SiP})$$

$$m = 0$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (-1 \text{ AIAr} + 0 \text{ PS} + 1 \text{ SiCI})$$

$$m = +1$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (-1 \text{ PAr} + 1 \text{ SCI})$$

3D ; n = 3 x 3; l = 1 x 1

$$m = -2$$

$$\mu = -1 \quad \text{sqrt}[1/2] \quad (1 \text{ AIAI})$$

$$\mu = 0 \quad \text{sqrt}[1/1] \quad (1 \text{ AISi})$$

$$\mu = +1 \quad \text{sqrt}[1/2] \quad (1 \text{ SiSi})$$

$$m = -1$$

$$\mu = -1 \quad \text{sqrt}[1/1] \quad (1 \text{ AIP})$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (1 \text{ AIS} + 1 \text{ SiP})$$

$$\mu = +1 \quad \text{sqrt}[1/1] \quad (1 \text{ SIS})$$

$$m = 0$$

$$\mu = -1 \quad \text{sqrt}[1/3] \quad (1 \text{ AICI} + 1 \text{ PP})$$

$$\mu = 0 \quad \text{sqrt}[1/6] \quad (1 \text{ AIAr} + 1 \text{ SiCI} + 2 \text{ PS})$$

$$\mu = +1 \quad \text{sqrt}[1/3] \quad (1 \text{ SiAr} + 1 \text{ SS})$$

$$m = +1$$

$$\mu = -1 \quad \text{sqrt}[1/1] \quad (1 \text{ PCI})$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (1 \text{ PAr} + 1 \text{ SCI})$$

$$\mu = +1 \quad \text{sqrt}[1/1] \quad (1 \text{ SAr})$$

$$m = +2$$

$$\mu = -1 \quad \text{sqrt}[1/2] \quad (1 \text{ CICI})$$

$$\mu = 0 \quad \text{sqrt}[1/1] \quad (1 \text{ CIAr})$$

$$\mu = +1 \quad \text{sqrt}[1/2] \quad (1 \text{ ArAr})$$

3S ; $n = 3 \times 3$; $l = 2 \times 2$

$m = 0$

$$\mu = -1 \quad \text{sqrt}[1/10] \quad (-2 \text{ ScCu} + 2 \text{ VCo} + -1 \text{ MnMn})$$

$$\mu = 0 \quad \text{sqrt}[1/5] \quad (-1 \text{ ScZn} + -1 \text{ TiCu} + 1 \text{ VNi} + 1 \text{ CrCo} + -1 \text{ MnFe})$$

$$\mu = +1 \quad \text{sqrt}[1/10] \quad (-2 \text{ TiZn} + 2 \text{ CrNi} + -1 \text{ FeFe})$$

3D ; $n = 3 \times 3$; $l = 2 \times 2$

$m = -2$

$$\mu = -1 \quad \text{sqrt}[1/168] \quad (-4 \text{ sqrt}[6] \text{ ScMn} + 6 \text{ VV})$$

$$\mu = 0 \quad \text{sqrt}[1/42] \quad (-2 \text{ sqrt}[3] \text{ ScFe} + -2 \text{ sqrt}[3] \text{ TiMn} + \\ + 3 \text{ sqrt}[2] \text{ VCr})$$

$$\mu = +1 \quad \text{sqrt}[1/42] \quad (-2 \text{ sqrt}[6] \text{ TiFe} + 3 \text{ CrCr})$$

$m = -1$

$$\mu = -1 \quad \text{sqrt}[1/42] \quad (-6 \text{ ScCo} + 1 \text{ sqrt}[6] \text{ VMn})$$

$$\mu = 0 \quad \text{sqrt}[1/42] \quad (-3 \text{ sqrt}[2] \text{ ScNi} + -3 \text{ sqrt}[2] \text{ TiCo} + 1 \text{ sqrt}[3] \text{ VFe} \\ + 1 \text{ sqrt}[3] \text{ CrMn})$$

$$\mu = +1 \quad \text{sqrt}[1/42] \quad (-6 \text{ TiNi} + 1 \text{ sqrt}[6] \text{ CrFe})$$

$m = 0$

$$\mu = -1 \quad \text{sqrt}[1/7] \quad (-2 \text{ ScCu} + -1 \text{ VCo} + 1 \text{ MnMn})$$

$$\mu = 0 \quad \text{sqrt}[1/14] \quad (-2 \text{ ScZn} + -2 \text{ TiCu} + -1 \text{ VNi} + -1 \text{ CrCo} + 2 \text{ MnFe})$$

$$\mu = +1 \quad \text{sqrt}[1/7] \quad (-2 \text{ TiZn} + -1 \text{ CrNi} + 1 \text{ FeFe})$$

$m = +1$

$$\mu = -1 \quad \text{sqrt}[1/42] \quad (-6 \text{ VCu} + 1 \text{ sqrt}[6] \text{ MnCo})$$

$$\mu = 0 \quad \text{sqrt}[1/42] \quad (-3 \text{ sqrt}[2] \text{ VZn} + -3 \text{ sqrt}[2] \text{ CrCu} + 1 \text{ sqrt}[3] \text{ MnNi} \\ + 1 \text{ sqrt}[3] \text{ FeCo})$$

$$\mu = +1 \quad \text{sqrt}[1/42] \quad (-6 \text{ CrZn} + 1 \text{ sqrt}[6] \text{ FeNi})$$

$m = +2$

$$\mu = -1 \quad \text{sqrt}[1/42] \quad (-2 \text{ sqrt}[6] \text{ MnCu} + 3 \text{ CoCo})$$

$$\mu = 0 \quad \text{sqrt}[1/42] \quad (-2 \text{ sqrt}[3] \text{ MnZn} + -2 \text{ sqrt}[3] \text{ FeCu} +$$

+ 3 sqrt[2] CoNi)

$\mu = +1$ sqrt[1/42] (-2 sqrt[6] FeZn + 3 NiNi)

1F ; n = 3 x 3; l = 2 x 2

m = -3

$\mu = 0$ sqrt[1/2] (-1 ScCr + 1 TiV)

m = -2

$\mu = 0$ sqrt[1/12] (-1 sqrt[6] ScFe + 0 VCr + 1 sqrt[6] TiMn)

m = -1

$\mu = 0$ sqrt[1/30] (-3 ScNi + -1 sqrt[6] VFe + 3 TiCo +
+ 1 sqrt[6] CrMn)

m = 0

$\mu = 0$ sqrt[1/360] (-6 ScZn + -12 VNi + 0 MnFe + 6 TiCu + 12 CrCo)

m = +1

$\mu = 0$ sqrt[1/30] (-3 VZn + -1 sqrt[6] MnNi + 3 CrCu +
+ 1 sqrt[6] FeCo)

m = +2

$\mu = 0$ sqrt[1/300] (-5 sqrt[6] MnZn + 0 CoNi + 5 sqrt[6] FeCu)

m = +3

$\mu = 0$ sqrt[1/2] (-1 CoZn + 1 NiCu)

3G ; n = 3 x 3; l = 2 x 2

m = -4

$\mu = -1$ sqrt[1/2] (1 ScSc)

$\mu = 0$ sqrt[1/1] (1 ScT)

$\mu = +1$ sqrt[1/2] (1 TiTi)

m = -3

$\mu = -1$ sqrt[1/1] (1 ScV)

$\mu = 0$ sqrt[1/2] (1 ScCr + 1 TiV)

$\mu = +1$ sqrt[1/1] (1 TiCr)

m = -2

$\mu = -1$ sqrt[1/14] (1 sqrt[6] ScMn + 2 VV)

$\mu = 0$ $\sqrt{1/14}$ (1 $\sqrt{3}$ ScFe + 1 $\sqrt{3}$ TiMn + 2 $\sqrt{2}$ VCr)
 $\mu = +1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ TiFe + 2 CrCr)

m = -1

$\mu = -1$ $\sqrt{1/7}$ (1 ScCo + 1 $\sqrt{6}$ VMn)
 $\mu = 0$ $\sqrt{1/28}$ (1 $\sqrt{2}$ ScNi + 1 $\sqrt{2}$ TiCo + 2 $\sqrt{3}$ VFe +
 + 2 $\sqrt{3}$ CrMn)
 $\mu = +1$ $\sqrt{1/7}$ (1 TiNi + 1 $\sqrt{6}$ CrFe)

m = 0

$\mu = -1$ $\sqrt{1/35}$ (1 ScCu + 4 VCo + 3 MnMn)
 $\mu = 0$ $\sqrt{1/70}$ (1 ScZn + 1 TiCu + 4 VNi + 4 CrCo + 6 MnFe)
 $\mu = +1$ $\sqrt{1/35}$ (1 TiZn + 4 CrNi + 3 FeFe)

m = +1

$\mu = -1$ $\sqrt{1/7}$ (1 VCu + 1 $\sqrt{6}$ MnCo)
 $\mu = 0$ $\sqrt{1/28}$ (1 $\sqrt{2}$ VZn + 1 $\sqrt{2}$ CrCu + 2 $\sqrt{3}$ MnNi +
 + 2 $\sqrt{3}$ FeCo)
 $\mu = +1$ $\sqrt{1/7}$ (1 CrZn + 1 $\sqrt{6}$ FeNi)

m = +2

$\mu = -1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ MnCu + 2 CoCo)
 $\mu = 0$ $\sqrt{1/14}$ (1 $\sqrt{3}$ MnZn + 1 $\sqrt{3}$ FeCu + 2 $\sqrt{2}$ CoNi)
 $\mu = +1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ FeZn + 2 NiNi)

m = +3

$\mu = -1$ $\sqrt{1/1}$ (1 CoCu)
 $\mu = 0$ $\sqrt{1/2}$ (1 CoZn + 1 NiCu)
 $\mu = +1$ $\sqrt{1/1}$ (1 NiZn)

m = +4

$\mu = -1$ $\sqrt{1/2}$ (1 CuCu)
 $\mu = 0$ $\sqrt{1/1}$ (1 CuZn)
 $\mu = +1$ $\sqrt{1/2}$ (1 ZnZn)

3S ; $n = 4 \times 4$; $l = 0 \times 0$

$m = 0$

$\mu = -1$ $\sqrt{1/2}$ (1 KK)
 $\mu = 0$ $\sqrt{1/1}$ (1 KCa)
 $\mu = +1$ $\sqrt{1/2}$ (1 CaCa)

3D ; $n = 4 \times 4$; $l = 1 \times 1$

$m = -2$

$\mu = -1$ $\sqrt{1/2}$ (1 GaGa)
 $\mu = 0$ $\sqrt{1/1}$ (1 GaGe)
 $\mu = +1$ $\sqrt{1/2}$ (1 GeGe)

$m = -1$

$\mu = -1$ $\sqrt{1/1}$ (1 GaAs)
 $\mu = 0$ $\sqrt{1/2}$ (1 GaSe + 1 GeAs)
 $\mu = +1$ $\sqrt{1/1}$ (1 GeSe)

$m = 0$

$\mu = -1$ $\sqrt{1/3}$ (1 GaBr + 1 AsAs)
 $\mu = 0$ $\sqrt{1/6}$ (1 GaKr + 1 GeBr + 2 AsSe)
 $\mu = +1$ $\sqrt{1/3}$ (1 GeKr + 1 SeSe)

$m = +1$

$\mu = -1$ $\sqrt{1/1}$ (1 AsBr)
 $\mu = 0$ $\sqrt{1/2}$ (1 AsKr + 1 SeBr)
 $\mu = +1$ $\sqrt{1/1}$ (1 SeKr)

$m = +2$

$\mu = -1$ $\sqrt{1/2}$ (1 BrBr)
 $\mu = 0$ $\sqrt{1/1}$ (1 BrKr)
 $\mu = +1$ $\sqrt{1/2}$ (1 KrKr)

3G ; $n = 4 \times 4$; $l = 2 \times 2$

$m = -4$

$\mu = -1$ $\sqrt{1/2}$ (1 YY)
 $\mu = 0$ $\sqrt{1/1}$ (1 YZr)

$\mu = +1$ $\sqrt{1/2}$ (1 ZrZr)

$m = -3$

$\mu = -1$ $\sqrt{1/1}$ (1 YNb)

$\mu = 0$ $\sqrt{1/2}$ (1 YMo + 1 ZrNb)

$\mu = +1$ $\sqrt{1/1}$ (1 ZrMo)

$m = -2$

$\mu = -1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ YTc + 2 NbNb)

$\mu = 0$ $\sqrt{1/14}$ (1 $\sqrt{3}$ YRu + 1 $\sqrt{3}$ ZrTc + 2 $\sqrt{2}$ NbMo)

$\mu = +1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ ZrRu + 2 MoMo)

$m = -1$

$\mu = -1$ $\sqrt{1/7}$ (1 YRh + 1 $\sqrt{6}$ NbTc)

$\mu = 0$ $\sqrt{1/28}$ (1 $\sqrt{2}$ YPd + 1 $\sqrt{2}$ ZrRh + 2 $\sqrt{3}$ NbRu +
 + 2 $\sqrt{3}$ MoTc)

$\mu = +1$ $\sqrt{1/7}$ (1 ZrPd + 1 $\sqrt{6}$ MoRu)

$m = 0$

$\mu = -1$ $\sqrt{1/35}$ (1 YAg + 4 NbRh + 3 TcTc)

$\mu = 0$ $\sqrt{1/70}$ (1 YCd + 1 ZrAg + 4 NbPd + 4 MoRh + 6 TcRu)

$\mu = +1$ $\sqrt{1/35}$ (1 ZrCd + 4 MoPd + 3 RuRu)

$m = +1$

$\mu = -1$ $\sqrt{1/7}$ (1 NbAg + 1 $\sqrt{6}$ TcRh)

$\mu = 0$ $\sqrt{1/28}$ (1 $\sqrt{2}$ NbCd + 1 $\sqrt{2}$ MoAg + 2 $\sqrt{3}$ TcPd
 + 2 $\sqrt{3}$ RuRh)

$\mu = +1$ $\sqrt{1/7}$ (1 MoCd + 1 $\sqrt{6}$ RuPd)

$m = +2$

$\mu = -1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ TcAg + 2 RhRh)

$\mu = 0$ $\sqrt{1/14}$ (1 $\sqrt{3}$ TcCd + 1 $\sqrt{3}$ RuAg + 2 $\sqrt{2}$ RhPd)

$\mu = +1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ RuCd + 2 PdPd)

$m = +3$

$\mu = -1$ $\sqrt{1/1}$ (1 RhAg)

$\mu = 0$ $\sqrt{1/2}$ (1 RhCd + 1 PdAg)

$\mu = +1$ $\sqrt{1/1}$ (1 PdCd)

$$m = +4$$

$$\mu = -1 \quad \text{sqrt}[1/2] \quad (1 \text{ AgAg})$$

$$\mu = 0 \quad \text{sqrt}[1/1] \quad (1 \text{ AgCd})$$

$$\mu = +1 \quad \text{sqrt}[1/2] \quad (1 \text{ CdCd})$$

$$3I; n = 4 \times 4; l = 3 \times 3$$

$$m = -6$$

$$\mu = -1 \quad \text{sqrt}[1/2] \quad (1 \text{ LaLa})$$

$$\mu = 0 \quad \text{sqrt}[1/1] \quad (1 \text{ LaCe})$$

$$\mu = +1 \quad \text{sqrt}[1/2] \quad (1 \text{ CeCe})$$

$$m = -5$$

$$\mu = -1 \quad \text{sqrt}[1/1] \quad (1 \text{ LaPr})$$

$$\mu = 0 \quad \text{sqrt}[1/2] \quad (1 \text{ LaNd} + 1 \text{ CePr})$$

$$\mu = +1 \quad \text{sqrt}[1/1] \quad (1 \text{ CeNd})$$

$$m = -4$$

$$\mu = -1 \quad \text{sqrt}[1/11] \quad (1 \text{ sqrt}[5] \text{ LaPm} + 1 \text{ sqrt}[3] \text{ PrPr})$$

$$\mu = 0 \quad \text{sqrt}[1/22] \quad (1 \text{ sqrt}[5] \text{ LaSm} + 1 \text{ sqrt}[5] \text{ CePm} + \\ + 2 \text{ sqrt}[3] \text{ PrNd})$$

$$\mu = +1 \quad \text{sqrt}[1/11] \quad (1 \text{ sqrt}[5] \text{ CeSm} + 1 \text{ sqrt}[3] \text{ NdNd})$$

$$m = -3$$

$$\mu = -1 \quad \text{sqrt}[1/22] \quad (2 \text{ LaEu} + 3 \text{ sqrt}[2] \text{ PrPm})$$

$$\mu = 0 \quad \text{sqrt}[1/22] \quad (1 \text{ sqrt}[2] \text{ LaGd} + 1 \text{ sqrt}[2] \text{ CeEu} + 3 \text{ PrSm} + \\ + 3 \text{ NdPm})$$

$$\mu = +1 \quad \text{sqrt}[1/22] \quad (2 \text{ CeGd} + 3 \text{ sqrt}[2] \text{ NdSm})$$

$$m = -2$$

$$\mu = -1 \quad \text{sqrt}[1/198] \quad (2 \text{ sqrt}[3] \text{ LaTb} + 4 \text{ sqrt}[6] \text{ PrEu} + \\ + 3 \text{ sqrt}[5] \text{ PmPm})$$

$$\mu = 0 \quad \text{sqrt}[1/198] \quad (1 \text{ sqrt}[6] \text{ LaDy} + 1 \text{ sqrt}[6] \text{ CeTb} + \\ + 4 \text{ sqrt}[3] \text{ PrGd} + 4 \text{ sqrt}[3] \text{ NdEu} + 3 \text{ sqrt}[10] \text{ PmSm})$$

$$\mu = +1 \quad \text{sqrt}[1/198] \quad (2 \text{ sqrt}[3] \text{ CeDy} + 4 \text{ sqrt}[6] \text{ NdGd} + \\ + 3 \text{ sqrt}[5] \text{ SmSm})$$

$m = -1$

$\mu = -1$ $\sqrt{1/1980}$ (1 $\sqrt{30}$ LaHo + 15 $\sqrt{2}$ PrTb +
+ 10 $\sqrt{15}$ PmEu)

$\mu = 0$ $\sqrt{1/1980}$ (1 $\sqrt{15}$ LaEr + 1 $\sqrt{15}$ CeHo + 15 PrDy +
+ 15 NdTb + 5 $\sqrt{30}$ PmGd + 5 $\sqrt{30}$ SmEu)

$\mu = +1$ $\sqrt{1/1980}$ (1 $\sqrt{30}$ CeEr + 15 $\sqrt{2}$ NdDy +
+ 10 $\sqrt{15}$ SmGd)

$m = 0$

$\mu = -1$ $\sqrt{1/462}$ (1 LaTm + 6 PrHo + 15 PmTb + 10 EuEu)

$\mu = 0$ $\sqrt{1/924}$ (1 LaYb + 1 CeTm + 6 PrEr + 6 NdHo + 15 PmDy +
+ 15 SmTb + 20 EuGd)

$\mu = +1$ $\sqrt{1/462}$ (1 CeYb + 6 NdEr + 15 SmDy + 10 GdGd)

$m = +1$

$\mu = -1$ $\sqrt{1/396}$ (1 $\sqrt{6}$ PrTm + 3 $\sqrt{10}$ PmHo +
+ 10 $\sqrt{3}$ EuTb)

$\mu = 0$ $\sqrt{1/396}$ (1 $\sqrt{3}$ PrYb + 1 $\sqrt{3}$ NdTm +
+ 3 $\sqrt{5}$ PmEr + 3 $\sqrt{5}$ SmHo + 5 $\sqrt{6}$ EuDy +
+ 5 $\sqrt{6}$ GdTb)

$\mu = +1$ $\sqrt{1/396}$ (1 $\sqrt{6}$ NdYb + 3 $\sqrt{10}$ SmEr +
+ 10 $\sqrt{3}$ GdDy)

$m = +2$

$\mu = -1$ $\sqrt{1/990}$ (2 $\sqrt{15}$ PmTm + 4 $\sqrt{30}$ EuHo + 15 TbTb)

$\mu = 0$ $\sqrt{1/990}$ (1 $\sqrt{30}$ PmYb + 1 $\sqrt{30}$ SmTm +
+ 4 $\sqrt{15}$ EuEr + 4 $\sqrt{15}$ GdHo + 15 $\sqrt{2}$ TbDy)

$\mu = +1$ $\sqrt{1/990}$ (2 $\sqrt{15}$ SmYb + 4 $\sqrt{30}$ GdEr + 15 DyDy)

$m = +3$

$\mu = -1$ $\sqrt{1/22}$ (2 EuTm + 3 $\sqrt{2}$ TbHo)

$\mu = 0$ $\sqrt{1/22}$ (1 $\sqrt{2}$ EuYb + 1 $\sqrt{2}$ GdTm + 3 TbEr +
+ 3 DyHo)

$\mu = +1$ $\sqrt{1/22}$ (2 GdYb + 3 $\sqrt{2}$ DyEr)

$m = +4$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/165] (5 \text{ sqrt}[3] \text{ TbTm} + 3 \text{ sqrt}[5] \text{ HoHo}) \\ \mu = 0 & \quad \text{sqrt}[1/330] (5 \text{ sqrt}[3] \text{ TbYb} + 5 \text{ sqrt}[3] \text{ DyTm} + \\ & \quad + 6 \text{ sqrt}[5] \text{ HoEr}) \\ \mu = +1 & \quad \text{sqrt}[1/165] (5 \text{ sqrt}[3] \text{ DyYb} + 3 \text{ sqrt}[5] \text{ ErEr})\end{aligned}$$

$m = +5$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/1] (1 \text{ HoTm}) \\ \mu = 0 & \quad \text{sqrt}[1/2] (1 \text{ HoYb} + 1 \text{ ErTm}) \\ \mu = +1 & \quad \text{sqrt}[1/1] (1 \text{ ErYb})\end{aligned}$$

$m = +6$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/2] (1 \text{ TmTm}) \\ \mu = 0 & \quad \text{sqrt}[1/1] (1 \text{ TmYb}) \\ \mu = +1 & \quad \text{sqrt}[1/2] (1 \text{ YbYb})\end{aligned}$$

$3S$; $n = 5 \times 5$; $l = 0 \times 0$

$m = 0$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/2] (1 \text{ RbRb}) \\ \mu = 0 & \quad \text{sqrt}[1/1] (1 \text{ RbSr}) \\ \mu = +1 & \quad \text{sqrt}[1/2] (1 \text{ SrSr})\end{aligned}$$

$3D$; $n = 5 \times 5$; $l = 1 \times 1$

$m = -2$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/2] (1 \text{ InIn}) \\ \mu = 0 & \quad \text{sqrt}[1/1] (1 \text{ InSn}) \\ \mu = +1 & \quad \text{sqrt}[1/2] (1 \text{ SnSn})\end{aligned}$$

$m = -1$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/1] (1 \text{ InSb}) \\ \mu = 0 & \quad \text{sqrt}[1/2] (1 \text{ InTe} + 1 \text{ SnSb}) \\ \mu = +1 & \quad \text{sqrt}[1/1] (1 \text{ SnTe})\end{aligned}$$

$m = 0$

$$\begin{aligned}\mu = -1 & \quad \text{sqrt}[1/3] (1 \text{ InI} + 1 \text{ SbSb}) \\ \mu = 0 & \quad \text{sqrt}[1/6] (1 \text{ InXe} + 1 \text{ SnI} + 2 \text{ SbTe})\end{aligned}$$

$$\begin{aligned}
& \mu = +1 \quad \text{sqrt}[1/3] (1 \text{ SnXe} + 1 \text{ TeTe}) \\
m = +1 & \\
& \mu = -1 \quad \text{sqrt}[1/1] (1 \text{ Sbl}) \\
& \mu = 0 \quad \text{sqrt}[1/2] (1 \text{ SbXe} + 1 \text{ Tel}) \\
& \mu = +1 \quad \text{sqrt}[1/1] (1 \text{ TeXe}) \\
m = +2 & \\
& \mu = -1 \quad \text{sqrt}[1/2] (1 \text{ l l}) \\
& \mu = 0 \quad \text{sqrt}[1/1] (1 \text{ l Xe}) \\
& \mu = +1 \quad \text{sqrt}[1/2] (1 \text{ XeXe})
\end{aligned}$$

3G ; $n = 5 \times 5$; $l = 2 \times 2$

$$\begin{aligned}
m = -4 & \\
& \mu = -1 \quad \text{sqrt}[1/2] (1 \text{ LuLu}) \\
& \mu = 0 \quad \text{sqrt}[1/1] (1 \text{ LuHf}) \\
& \mu = +1 \quad \text{sqrt}[1/2] (1 \text{ HfHf}) \\
m = -3 & \\
& \mu = -1 \quad \text{sqrt}[1/1] (1 \text{ LuTa}) \\
& \mu = 0 \quad \text{sqrt}[1/2] (1 \text{ LuW} + 1 \text{ HfTa}) \\
& \mu = +1 \quad \text{sqrt}[1/1] (1 \text{ HfW}) \\
m = -2 & \\
& \mu = -1 \quad \text{sqrt}[1/14] (1 \text{ sqrt}[6] \text{ LuRe} + 2 \text{ TaTa}) \\
& \mu = 0 \quad \text{sqrt}[1/14] (1 \text{ sqrt}[3] \text{ LuOs} + 1 \text{ sqrt}[3] \text{ HfRe} + 2 \text{ sqrt}[2] \text{ TaW}) \\
& \mu = +1 \quad \text{sqrt}[1/14] (1 \text{ sqrt}[6] \text{ HfOs} + 2 \text{ WW}) \\
m = -1 & \\
& \mu = -1 \quad \text{sqrt}[1/7] (1 \text{ LuIr} + 1 \text{ sqrt}[6] \text{ TaRe}) \\
& \mu = 0 \quad \text{sqrt}[1/28] (1 \text{ sqrt}[2] \text{ LuPt} + 1 \text{ sqrt}[2] \text{ HfIr} + 2 \text{ sqrt}[3] \text{ TaOs} + \\
& \quad + 2 \text{ sqrt}[3] \text{ WRe}) \\
& \mu = +1 \quad \text{sqrt}[1/7] (1 \text{ HfPt} + 1 \text{ sqrt}[6] \text{ WOs}) \\
m = 0 & \\
& \mu = -1 \quad \text{sqrt}[1/35] (1 \text{ LuAu} + 4 \text{ Talr} + 3 \text{ ReRe}) \\
& \mu = 0 \quad \text{sqrt}[1/70] (1 \text{ LuHg} + 1 \text{ HfAu} + 4 \text{ TaPt} + 4 \text{ Wlr} + 6 \text{ ReOs}) \\
& \mu = +1 \quad \text{sqrt}[1/35] (1 \text{ HfHg} + 4 \text{ WPt} + 3 \text{ OsOs})
\end{aligned}$$

$m = +1$

$\mu = -1$ $\sqrt{1/7}$ (1 TaAu + 1 $\sqrt{6}$ ReIr)

$\mu = 0$ $\sqrt{1/28}$ (1 $\sqrt{2}$ TaHg + 1 $\sqrt{2}$ WAu + 2 $\sqrt{3}$ RePt
+ 2 $\sqrt{3}$ OsIr)

$\mu = +1$ $\sqrt{1/7}$ (1 WHg + 1 $\sqrt{6}$ OsPt)

$m = +2$

$\mu = -1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ ReAu + 2 IrIr)

$\mu = 0$ $\sqrt{1/14}$ (1 $\sqrt{3}$ ReHg + 1 $\sqrt{3}$ OsAu + 2 $\sqrt{2}$ IrPt)

$\mu = +1$ $\sqrt{1/14}$ (1 $\sqrt{6}$ OsHg + 2 PtPt)

$m = +3$

$\mu = -1$ $\sqrt{1/1}$ (1 IrAu)

$\mu = 0$ $\sqrt{1/2}$ (1 IrHg + 1 PtAu)

$\mu = +1$ $\sqrt{1/1}$ (1 PtHg)

$m = +4$

$\mu = -1$ $\sqrt{1/2}$ (1 AuAu)

$\mu = 0$ $\sqrt{1/1}$ (1 AuHg)

$\mu = +1$ $\sqrt{1/2}$ (1 HgHg)

3I ; $n = 5 \times 5$; $l = 3 \times 3$

$m = -6$

$\mu = -1$ $\sqrt{1/2}$ (1 AcAc)

$\mu = 0$ $\sqrt{1/1}$ (1 AcTh)

$\mu = +1$ $\sqrt{1/2}$ (1 ThTh)

$m = -5$

$\mu = -1$ $\sqrt{1/1}$ (1 AcPa)

$\mu = 0$ $\sqrt{1/2}$ (1 AcU + 1 ThPa)

$\mu = +1$ $\sqrt{1/1}$ (1 ThU)

$m = -4$

$\mu = -1$ $\sqrt{1/11}$ (1 $\sqrt{5}$ AcNp + 1 $\sqrt{3}$ PaPa)

$\mu = 0$ $\sqrt{1/22}$ (1 $\sqrt{5}$ AcPu + 1 $\sqrt{5}$ ThNp + 2 $\sqrt{3}$ PaU)

$\mu = +1$ $\sqrt{1/11}$ (1 $\sqrt{5}$ ThPu + 1 $\sqrt{3}$ UU)

$m = -3$

$$\mu = -1 \quad \sqrt{1/22} (2 \text{ AcAm} + 3 \sqrt{2} \text{ PaNp})$$

$$\mu = 0 \quad \sqrt{1/22} (1 \sqrt{2} \text{ AcCm} + 1 \sqrt{2} \text{ ThAm} + 3 \text{ PaPu} + 3 \text{ UNp})$$

$$\mu = +1 \quad \sqrt{1/22} (2 \text{ ThCm} + 3 \sqrt{2} \text{ UPu})$$

$m = -2$

$$\mu = -1 \quad \sqrt{1/198} (2 \sqrt{3} \text{ AcBk} + 4 \sqrt{6} \text{ PaAm} + 3 \sqrt{5} \text{ NpNp})$$

$$\mu = 0 \quad \sqrt{1/198} (1 \sqrt{6} \text{ AcCf} + 1 \sqrt{6} \text{ ThBk} + 4 \sqrt{3} \text{ PaCm} + 4 \sqrt{3} \text{ UAm} + 3 \sqrt{10} \text{ NpPu})$$

$$\mu = +1 \quad \sqrt{1/198} (2 \sqrt{3} \text{ ThCf} + 4 \sqrt{6} \text{ UCm} + 3 \sqrt{5} \text{ PuPu})$$

$m = -1$

$$\mu = -1 \quad \sqrt{1/1980} (1 \sqrt{30} \text{ AcEs} + 15 \sqrt{2} \text{ PaBk} + 10 \sqrt{15} \text{ NpAm})$$

$$\mu = 0 \quad \sqrt{1/1980} (1 \sqrt{15} \text{ AcFm} + 1 \sqrt{15} \text{ ThEs} + 15 \text{ PaCf} + 15 \text{ UBk} + 5 \sqrt{30} \text{ NpCm} + 5 \sqrt{30} \text{ PuAm})$$

$$\mu = +1 \quad \sqrt{1/1980} (1 \sqrt{30} \text{ ThFm} + 15 \sqrt{2} \text{ UCf} + 10 \sqrt{15} \text{ PuCm})$$

$m = 0$

$$\mu = -1 \quad \sqrt{1/462} (1 \text{ AcMd} + 6 \text{ PaEs} + 15 \text{ NpBk} + 10 \text{ AmAm})$$

$$\mu = 0 \quad \sqrt{1/924} (1 \text{ AcNo} + 1 \text{ ThMd} + 6 \text{ PaFm} + 6 \text{ UEs} + 15 \text{ NpCf} + 15 \text{ PuBk} + 20 \text{ AmCm})$$

$$\mu = +1 \quad \sqrt{1/462} (1 \text{ ThNo} + 6 \text{ UFm} + 15 \text{ PuCf} + 10 \text{ CmCm})$$

$m = +1$

$$\mu = -1 \quad \sqrt{1/396} (1 \sqrt{6} \text{ PaMd} + 3 \sqrt{10} \text{ NpEs} + 10 \sqrt{3} \text{ AmBk})$$

$$\mu = 0 \quad \sqrt{1/396} (1 \sqrt{3} \text{ PaNo} + 1 \sqrt{3} \text{ UMd} + 3 \sqrt{5} \text{ NpFm} + 3 \sqrt{5} \text{ PuEs} + 5 \sqrt{6} \text{ AmCf} + 5 \sqrt{6} \text{ CmBk})$$

$$\mu = +1 \quad \sqrt{1/396} (1 \sqrt{6} \text{ UNo} + 3 \sqrt{10} \text{ PuFm} + 10 \sqrt{3} \text{ CmCf})$$

$m = +2$

$$\mu = -1 \quad \sqrt{1/990} (2 \sqrt{15} \text{ NpMd} + 4 \sqrt{30} \text{ AmEs} + 15 \text{ BkBk})$$

$$\mu = 0 \quad \sqrt{1/990} (1 \sqrt{30} \text{ NpNo} + 1 \sqrt{30} \text{ PuMd} + \\ + 4 \sqrt{15} \text{ AmFm} + 4 \sqrt{15} \text{ CmEs} + 15 \sqrt{2} \text{ BkCf})$$

$$\mu = +1 \quad \sqrt{1/990} (2 \sqrt{15} \text{ PuNo} + 4 \sqrt{30} \text{ CmFm} + 15 \text{ CfCf})$$

$m = +3$

$$\mu = -1 \quad \sqrt{1/22} (2 \text{ AmMd} + 3 \sqrt{2} \text{ BkEs})$$

$$\mu = 0 \quad \sqrt{1/22} (1 \sqrt{2} \text{ AmNo} + 1 \sqrt{2} \text{ CmMd} + 3 \text{ BkFm} + \\ + 3 \text{ CfEs})$$

$$\mu = +1 \quad \sqrt{1/22} (2 \text{ CmNo} + 3 \sqrt{2} \text{ CfFm})$$

$m = +4$

$$\mu = -1 \quad \sqrt{1/165} (5 \sqrt{3} \text{ BkMd} + 3 \sqrt{5} \text{ EsEs})$$

$$\mu = 0 \quad \sqrt{1/330} (5 \sqrt{3} \text{ BkNo} + 5 \sqrt{3} \text{ CfMd} + \\ + 6 \sqrt{5} \text{ EsFm})$$

$$\mu = +1 \quad \sqrt{1/165} (5 \sqrt{3} \text{ CfNo} + 3 \sqrt{5} \text{ FmFm})$$

$m = +5$

$$\mu = -1 \quad \sqrt{1/1} (1 \text{ EsMd})$$

$$\mu = 0 \quad \sqrt{1/2} (1 \text{ EsNo} + 1 \text{ FmMd})$$

$$\mu = +1 \quad \sqrt{1/1} (1 \text{ FmNo})$$

$m = +6$

$$\mu = -1 \quad \sqrt{1/2} (1 \text{ MdMd})$$

$$\mu = 0 \quad \sqrt{1/1} (1 \text{ MdNo})$$

$$\mu = +1 \quad \sqrt{1/2} (1 \text{ NoNo})$$

${}^3\mathbf{s} ; n = 6 \times 6 ; l = 0 \times 0$

$m = 0$

$$\mu = -1 \quad \sqrt{1/2} (1 \text{ CsCs})$$

$$\mu = 0 \quad \sqrt{1/1} (1 \text{ CsBa})$$

$$\mu = +1 \quad \sqrt{1/2} (1 \text{ BaBa})$$

³D ; n = 6 x 6; l = 1 x 1

m = -2

$\mu = -1$ sqrt[1/2] (1 TITl)

$\mu = 0$ sqrt[1/1] (1 TIPb)

$\mu = +1$ sqrt[1/2] (1 PbPb)

m = -1

$\mu = -1$ sqrt[1/1] (1 TIBi)

$\mu = 0$ sqrt[1/2] (1 TIPo + 1 PbBi)

$\mu = +1$ sqrt[1/1] (1 PbPo)

m = 0

$\mu = -1$ sqrt[1/3] (1 TIAt + 1 BiBi)

$\mu = 0$ sqrt[1/6] (1 TIRn + 1 PbAt + 2 BiPo)

$\mu = +1$ sqrt[1/3] (1 PbRn + 1 PoPo)

m = +1

$\mu = -1$ sqrt[1/1] (1 BiAt)

$\mu = 0$ sqrt[1/2] (1 BiRn + 1 PoAt)

$\mu = +1$ sqrt[1/1] (1 PoRn)

m = +2

$\mu = -1$ sqrt[1/2] (1 AtAt)

$\mu = 0$ sqrt[1/1] (1 AtRn)

$\mu = +1$ sqrt[1/2] (1 RnRn)

³G ; n = 6 x 6; l = 2 x 2

m = -4

$\mu = -1$ sqrt[1/2] (1 YY)

$\mu = 0$ sqrt[1/1] (1 YZr)

$\mu = +1$ sqrt[1/2] (1 ZrZr)

·
·
·

3S ; $n = 7 \times 7$; $l = 0 \times 0$

$m = 0$

$\mu = -1$ $\sqrt{1/2}$ (1 FrFr)

$\mu = 0$ $\sqrt{1/1}$ (1 FrRa)

$\mu = +1$ $\sqrt{1/2}$ (1 RaRa)

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³Fet, A. I. The System of Elements from the Group-theoretic Viewpoint. preprint number 1, (Institute of Chemical Physics, Siberian Branch, Soviet academy of Sciences, Novosibirsk, 1979) p. 12.

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Representation space L(1) corresponding to the group SO(4,2)xSU(2)

	n=1	n=2	n=3	n=4	n=5	n=6	n=7	n=8	n=9		
<i>l</i> = 0	H	Li	Na	K	Rb	Cs	Fr			$\mu = -1/2$	<i>m</i> = 0
	He	Be	Mg	Ca	Sr	Ba	Ra			$\mu = 1/2$	
<i>l</i> = 1		B	Al	Ga	In	Tl				$\mu = -1/2$	<i>m</i> = -1
		C	Si	Ge	Sn	Pb				$\mu = 1/2$	
		N	P	As	Sb	Bi				$\mu = -1/2$	<i>m</i> = 0
		O	S	Se	Te	Po				$\mu = 1/2$	
		F	Cl	Br	I	At				$\mu = -1/2$	<i>m</i> = 1
	Ne	Ar	Kr	Xe	Rn					$\mu = 1/2$	
<i>l</i> = 2		Sc	Y	Lu	Lr					$\mu = -1/2$	<i>m</i> = -2
		Ti	Zr	Hf	Rf					$\mu = 1/2$	
		V	Nb	Ta						$\mu = -1/2$	<i>m</i> = -1
		Cr	Mo	W						$\mu = 1/2$	
		Mn	Tc	Rh						$\mu = -1/2$	<i>m</i> = 0
		Fe	Ru	Os						$\mu = 1/2$	
		Co	Rh	Ir						$\mu = -1/2$	<i>m</i> = 1
		Ni	Pd	Pt						$\mu = 1/2$	
		Cu	Ag	Au						$\mu = -1/2$	<i>m</i> = 2
		Zn	Cd	Hg						$\mu = 1/2$	
<i>l</i> = 3		La	Ac							$\mu = -1/2$	<i>m</i> = -3
		Ce	Th							$\mu = 1/2$	
		Pr	Pa							$\mu = -1/2$	<i>m</i> = -2
		Nd	U							$\mu = 1/2$	
		Pm	Np							$\mu = -1/2$	<i>m</i> = -1
		Sm	Pu							$\mu = 1/2$	
		Eu	Am							$\mu = -1/2$	<i>m</i> = 0
		Gd	Cm							$\mu = 1/2$	
		Tb	Bk							$\mu = -1/2$	<i>m</i> = 1
		Dy	Cf							$\mu = 1/2$	
		Ho	Es							$\mu = -1/2$	<i>m</i> = 2
		Er	Fm							$\mu = 1/2$	
		Tm	Md							$\mu = -1/2$	<i>m</i> = 3
		Yb	No							$\mu = 1/2$	
<i>l</i> = 4										$\mu = -1/2$	<i>m</i> = -4
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = -3
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = -2
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = -1
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = 0
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = 1
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = 2
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = 3
										$\mu = 1/2$	
										$\mu = -1/2$	<i>m</i> = 4
										$\mu = 1/2$	

Figure: 1

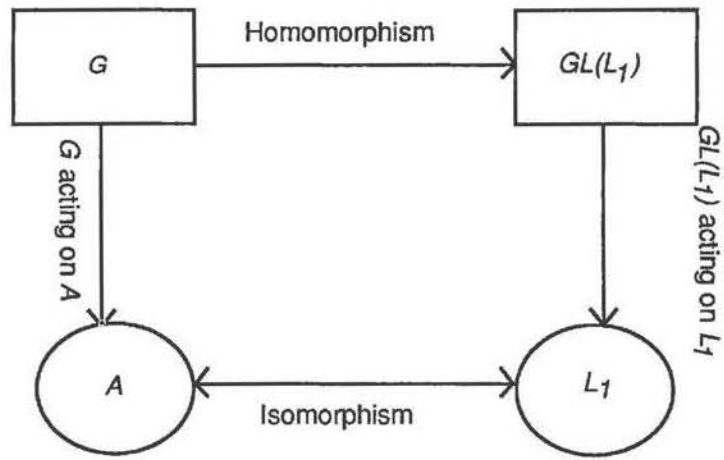


Figure 2:

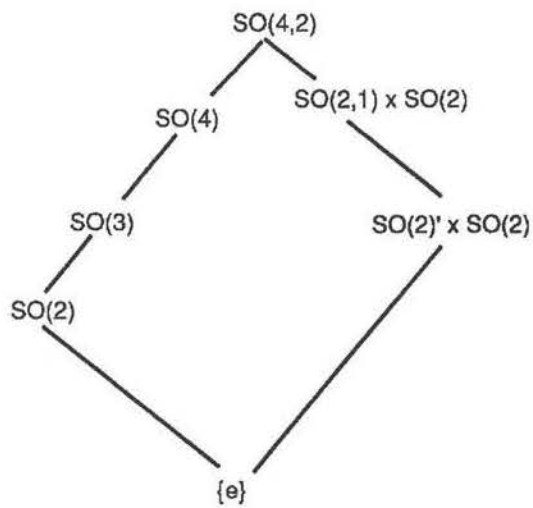


Figure 3:

Multiplets corresponding to the subgroup $SO(4) \times SU(2)$

	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$		
$l=0$	H	Li	Na	K	Rb	Cs	Fr		$\mu=-1/2$	$m=0$
	He	Be	Mg	Ca	Sr	Ba	Ra		$\mu=1/2$	
$l=1$		B	Al	Ga	In	Tl			$\mu=-1/2$	$m=-1$
		C	Si	Ge	Sn	Pb			$\mu=1/2$	
		N	P	As	Sb	Bi			$\mu=-1/2$	$m=0$
		O	S	Se	Te	Po			$\mu=1/2$	
		F	Cl	Br	I	At			$\mu=-1/2$	$m=1$
$l=2$		Ne	Ar	Kr	Xe	Rn			$\mu=1/2$	
			Sc	Y	Lu	Lr			$\mu=-1/2$	$m=-2$
			Ti	Zr	Hf	Ku			$\mu=1/2$	
			V	Nb	Ta				$\mu=-1/2$	$m=-1$
			Cr	Mo	W				$\mu=1/2$	
			Mn	Tc	Re				$\mu=-1/2$	$m=0$
			Fe	Ru	Os				$\mu=1/2$	
			Co	Rh	Ir				$\mu=-1/2$	$m=1$
			Ni	Pd	Pt				$\mu=1/2$	
			Cu	Ag	Au				$\mu=-1/2$	$m=2$
$l=3$			Zn	Cd	Hg				$\mu=1/2$	
				La	Ac				$\mu=-1/2$	$m=-3$
				Ce	Th				$\mu=1/2$	
				Pr	Pa				$\mu=-1/2$	$m=-2$
				Nd	U				$\mu=1/2$	
				Pm	Np				$\mu=-1/2$	$m=-1$
				Sm	Pu				$\mu=1/2$	
				Eu	Am				$\mu=-1/2$	$m=0$
				Gd	Cm				$\mu=1/2$	
				Tb	Bk				$\mu=-1/2$	$m=1$
				Dy	Cf				$\mu=1/2$	
				Ho	Es				$\mu=-1/2$	$m=2$
				Er	Fm				$\mu=1/2$	
				Tm	Md				$\mu=-1/2$	$m=3$
$l=4$				Yb	No				$\mu=1/2$	
									$\mu=-1/2$	$m=-4$
									$\mu=1/2$	
									$\mu=-1/2$	$m=-3$
									$\mu=1/2$	
									$\mu=-1/2$	$m=-2$
									$\mu=1/2$	
									$\mu=-1/2$	$m=-1$
									$\mu=1/2$	
									$\mu=-1/2$	$m=0$
									$\mu=1/2$	
									$\mu=-1/2$	$m=1$
									$\mu=1/2$	
									$\mu=-1/2$	$m=2$
									$\mu=1/2$	
									$\mu=-1/2$	$m=3$
									$\mu=1/2$	
									$\mu=-1/2$	$m=4$
									$\mu=1/2$	

Figure: 4

Multiplets corresponding to the subgroup SO(3)xSU(2)

	<i>n=1</i>	<i>n=2</i>	<i>n=3</i>	<i>n=4</i>	<i>n=5</i>	<i>n=6</i>	<i>n=7</i>		
<i>l = 0</i>	H He	Li Be	Na Mg	K Ca	Rb Sr	Cs Ba	Fr Ra	$\mu = -1/2$ $\mu = 1/2$	<i>m = 0</i>
<i>l = 1</i>		B C N O F Ne	Al Si P S Cl Ar	Ga Ge As Se Br Kr	In Sn Sb Te I Xe	Tl Pb Bi Po At Fr		$\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$	<i>m = -1</i> <i>m = 0</i> <i>m = 1</i>
<i>l = 2</i>			Sc Ti V Cr Mn Fe Co Ni Cu Zn	Y Zr Nb Mo Tc Ru Rh Pd Ag Cd	Lu Hf Ta W Re Os Ir Pt Au Hg	Lr Ku		$\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$	<i>m = -2</i> <i>m = -1</i> <i>m = 0</i> <i>m = 1</i> <i>m = 2</i>
<i>l = 3</i>				La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb	Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No			$\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$ $\mu = -1/2$ $\mu = 1/2$	<i>m = -3</i> <i>m = -2</i> <i>m = -1</i> <i>m = 0</i> <i>m = 1</i> <i>m = 2</i> <i>m = 3</i>

Figure: 5

Multiplets corresponding to the subgroup $SO(2) \times SU(2)$

	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$			
$l = 0$	H	Li	Na	K	Rb	Cs	Fr	$\mu = -1/2$	$m = 0$	
	He	Be	Mg	Ca	Sr	Ba	Ra			$\mu = 1/2$
$l = 1$		B	Al	Ga	In	Tl		$\mu = -1/2$	$m = -1$	
		C	Si	Ge	Sn	Pb				$\mu = 1/2$
		N	P	As	Sb	Bi		$\mu = -1/2$	$m = 0$	
		O	S	Se	Te	Po				$\mu = 1/2$
		F	Cl	Br	I	At		$\mu = -1/2$	$m = 1$	
		Ne	Ar	Kr	Xe	Rn				$\mu = 1/2$
$l = 2$			Sc	Y	Lu	Lr		$\mu = -1/2$	$m = -2$	
			Ti	Zr	Hf	Ku				$\mu = 1/2$
			V	Nb	Ta			$\mu = -1/2$	$m = -1$	
			Cr	Mo	W					$\mu = 1/2$
			Mn	Tc	Rh			$\mu = -1/2$	$m = 0$	
			Fe	Ru	Os					$\mu = 1/2$
			Co	Rh	Ir			$\mu = -1/2$	$m = 1$	
			Ni	Pd	Pt					$\mu = 1/2$
			Cu	Ag	Au			$\mu = -1/2$	$m = 2$	
			Zn	Cd	Hg					$\mu = 1/2$
	$l = 3$			La	Ac				$\mu = -1/2$	$m = -3$
				Ce	Th					
			Pr	Pa				$\mu = -1/2$	$m = -2$	
			Nd	U						$\mu = 1/2$
			Pm	Np				$\mu = -1/2$	$m = -1$	
			Sm	Pu						$\mu = 1/2$
			Eu	Am				$\mu = -1/2$	$m = 0$	
			Gd	Cm						$\mu = 1/2$
			Tb	Bk				$\mu = -1/2$	$m = 1$	
			Dy	Cf						$\mu = 1/2$
			Ho	Es				$\mu = -1/2$	$m = 2$	
			Er	Fm						$\mu = 1/2$
			Tm	Md				$\mu = -1/2$	$m = 3$	
			Yb	No						$\mu = 1/2$

Figure: 6

Decomposition of the representation space L_2
 corresponding to diatomic molecules from the P atoms of row 2
 in $SO(3) \times SU(2)$ symmetry

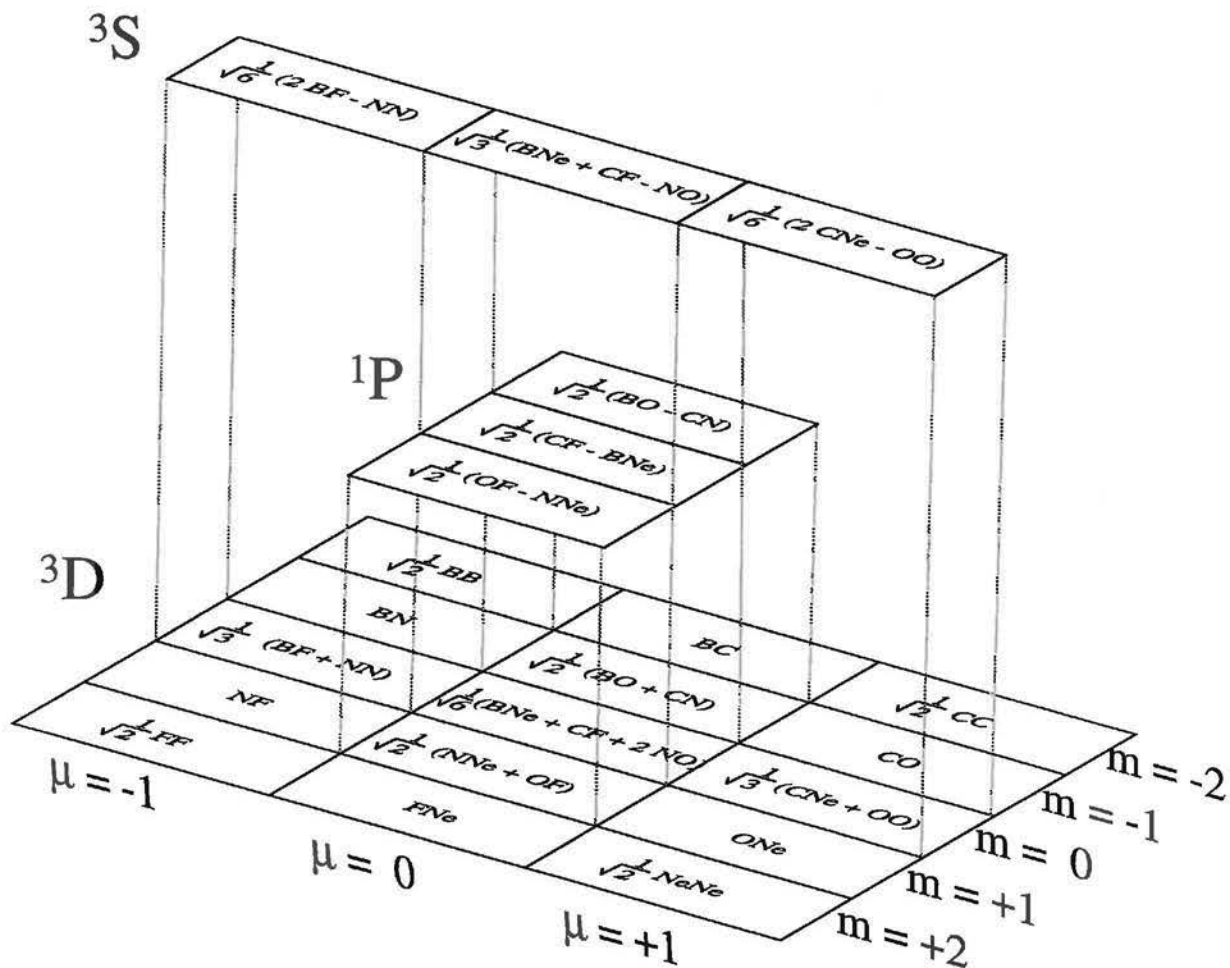
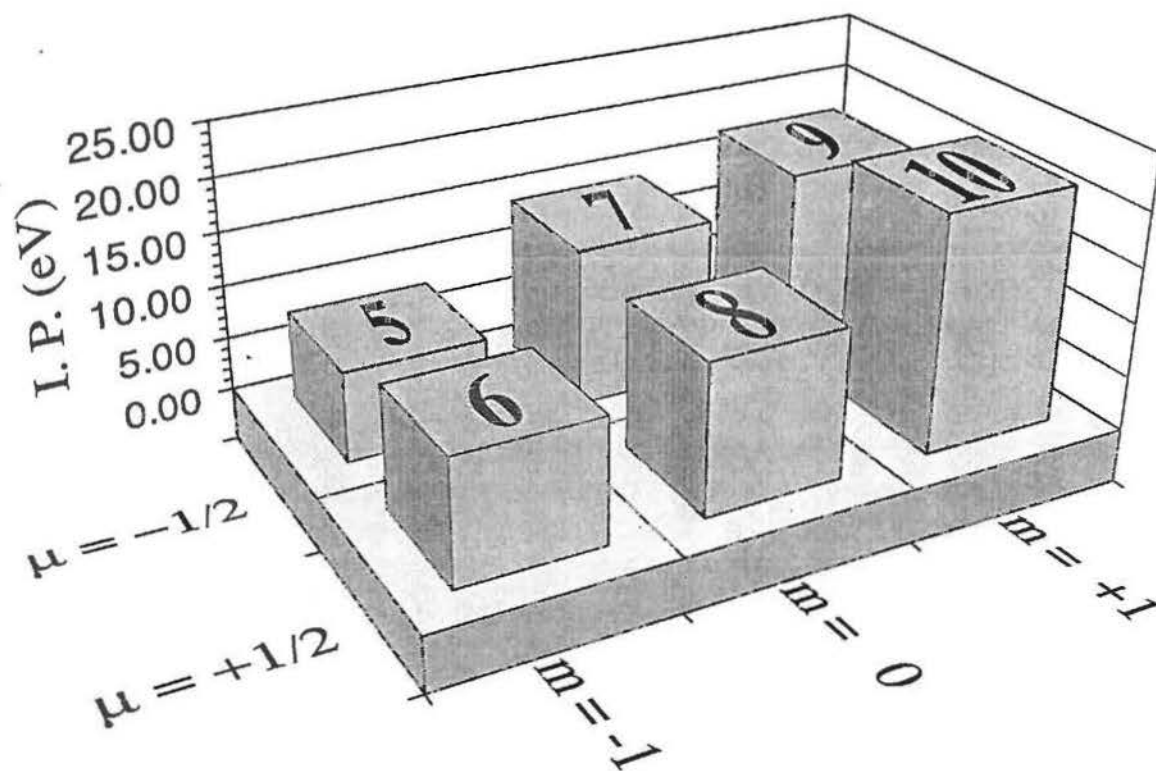


Figure: 7

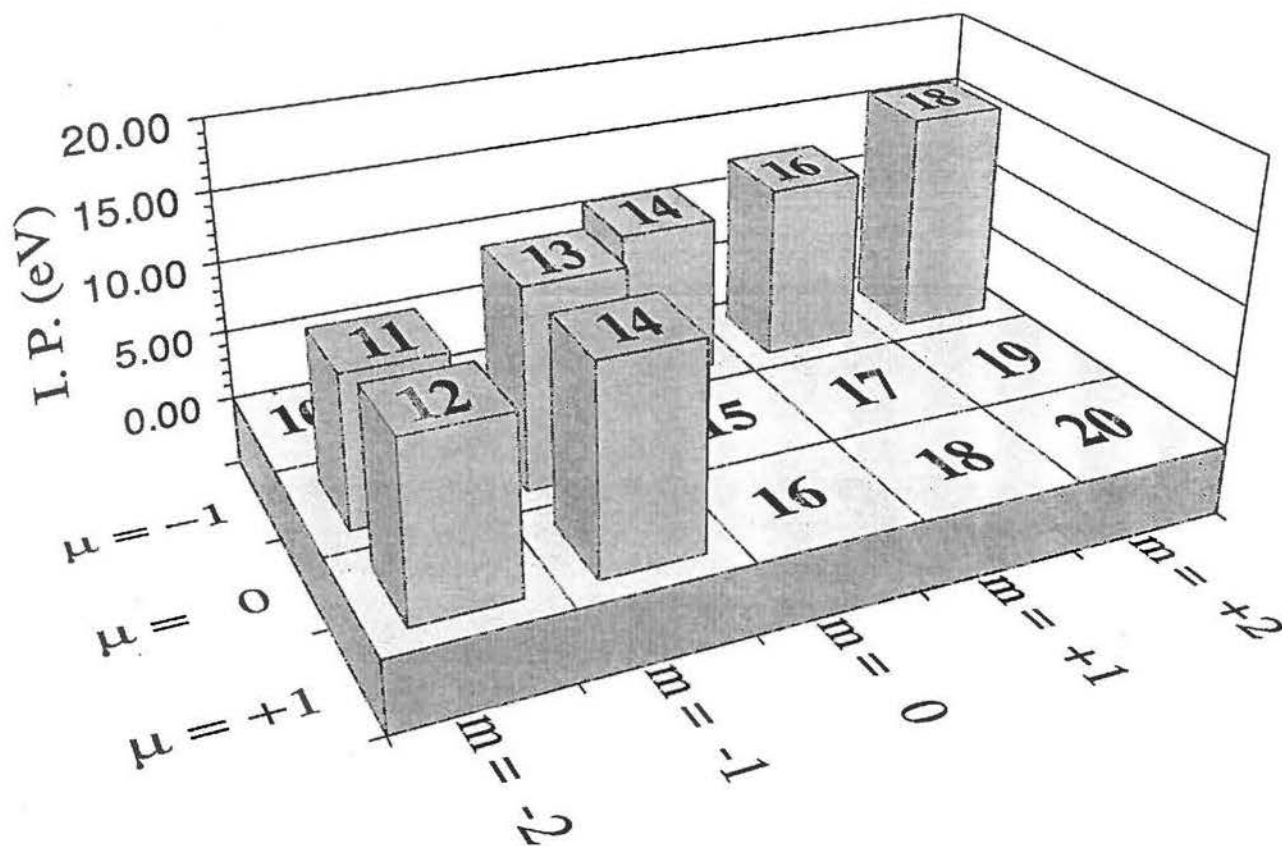
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Atoms 2^2P multiplet
Single Particle Operator

Figure: 8

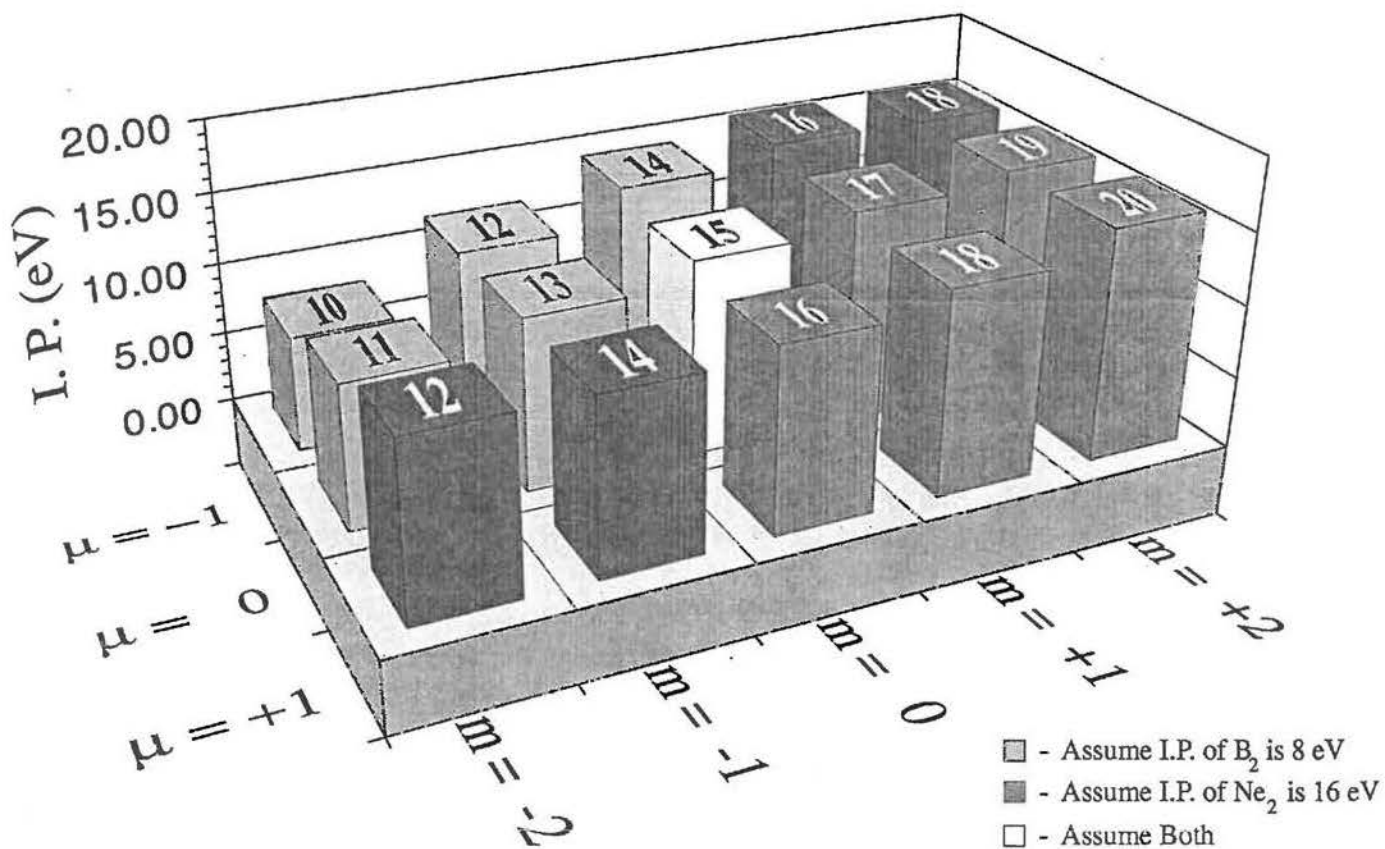
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3D multiplet
Single Particle Operator

Figure: 9

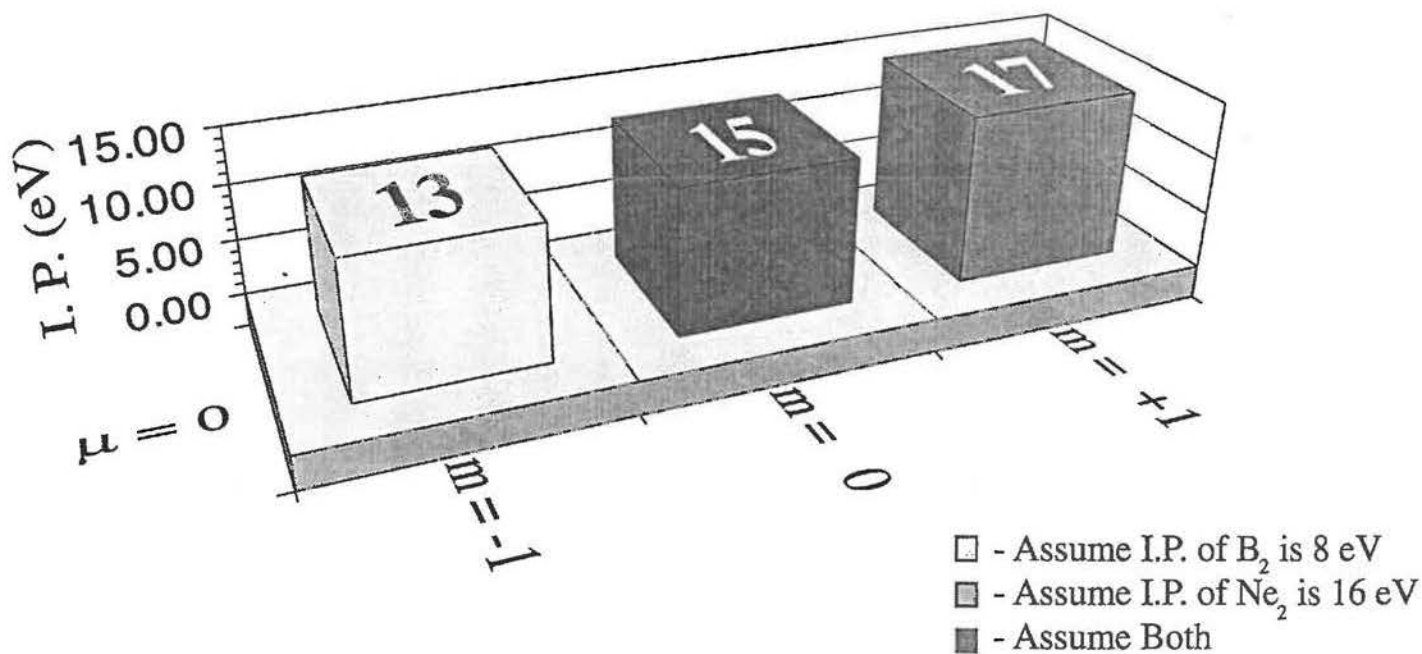
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3D multiplet
 Single Particle Operator on Homonuclear Vectors

Figure: 10

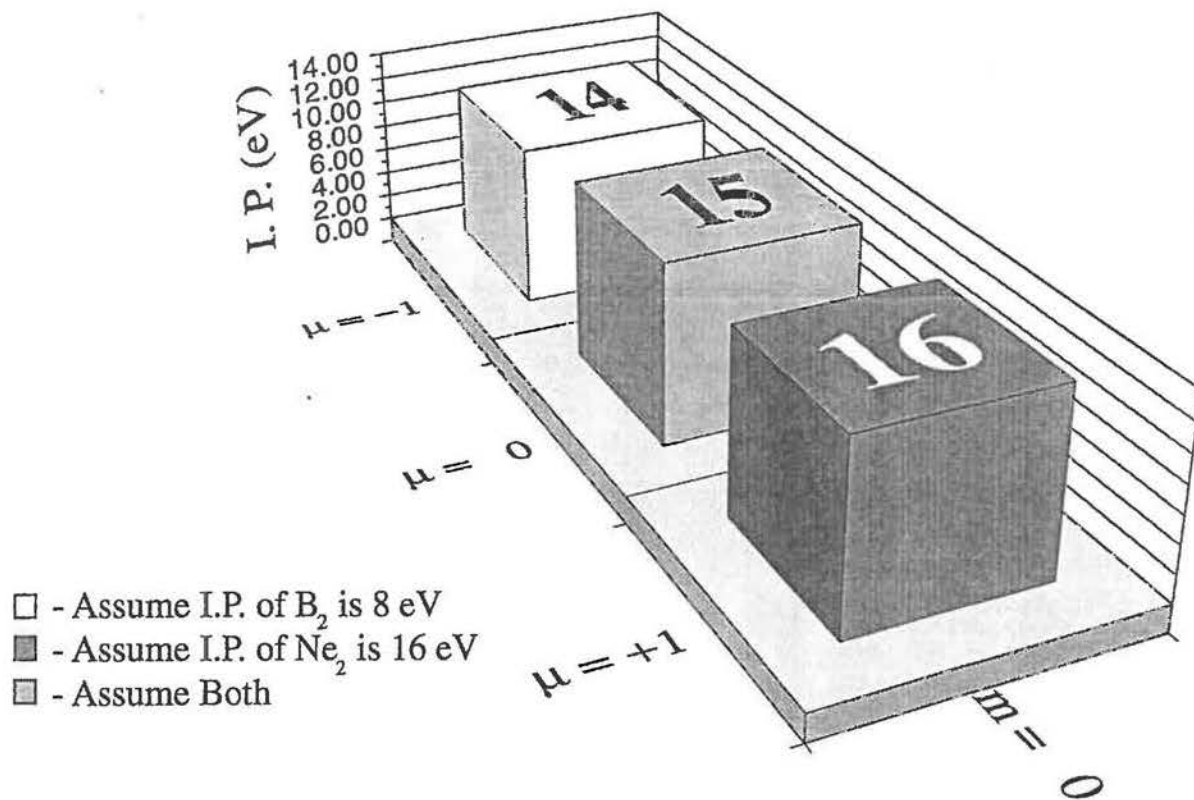
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^1P multiplet
Single Particle Operator on Homonuclear Vectors

Figure: 11

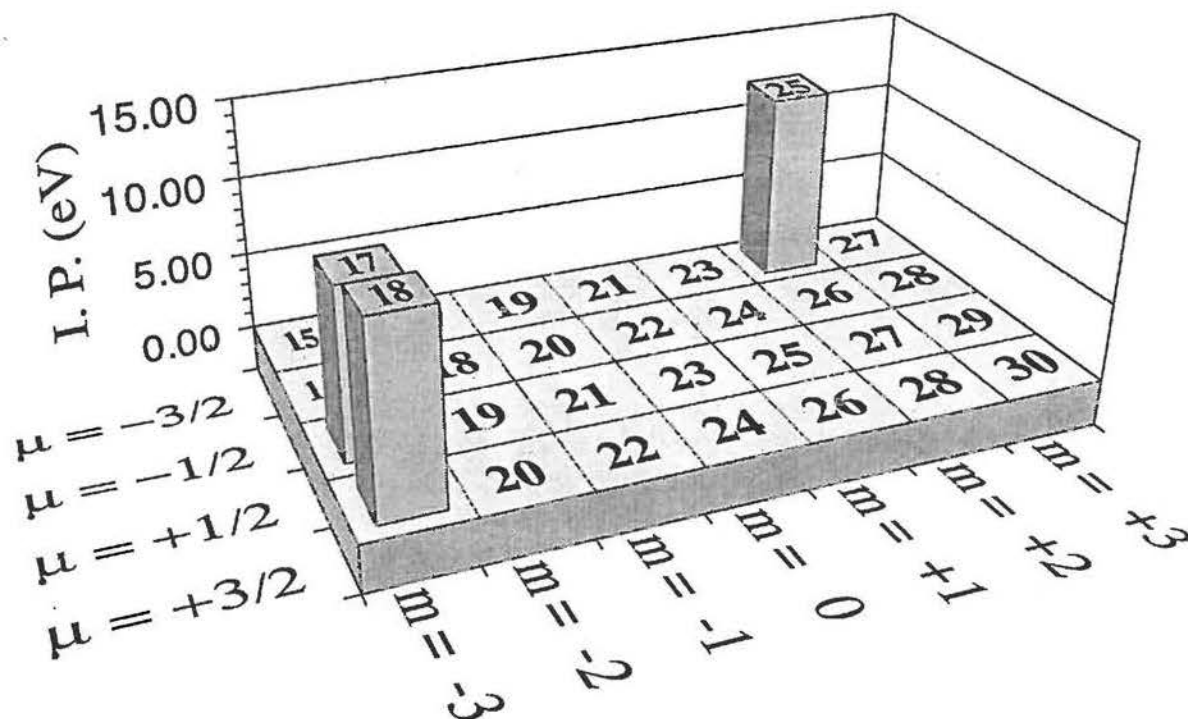
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3S multiplet
Single Particle Operator on Homonuclear Vectors

Figure: 12

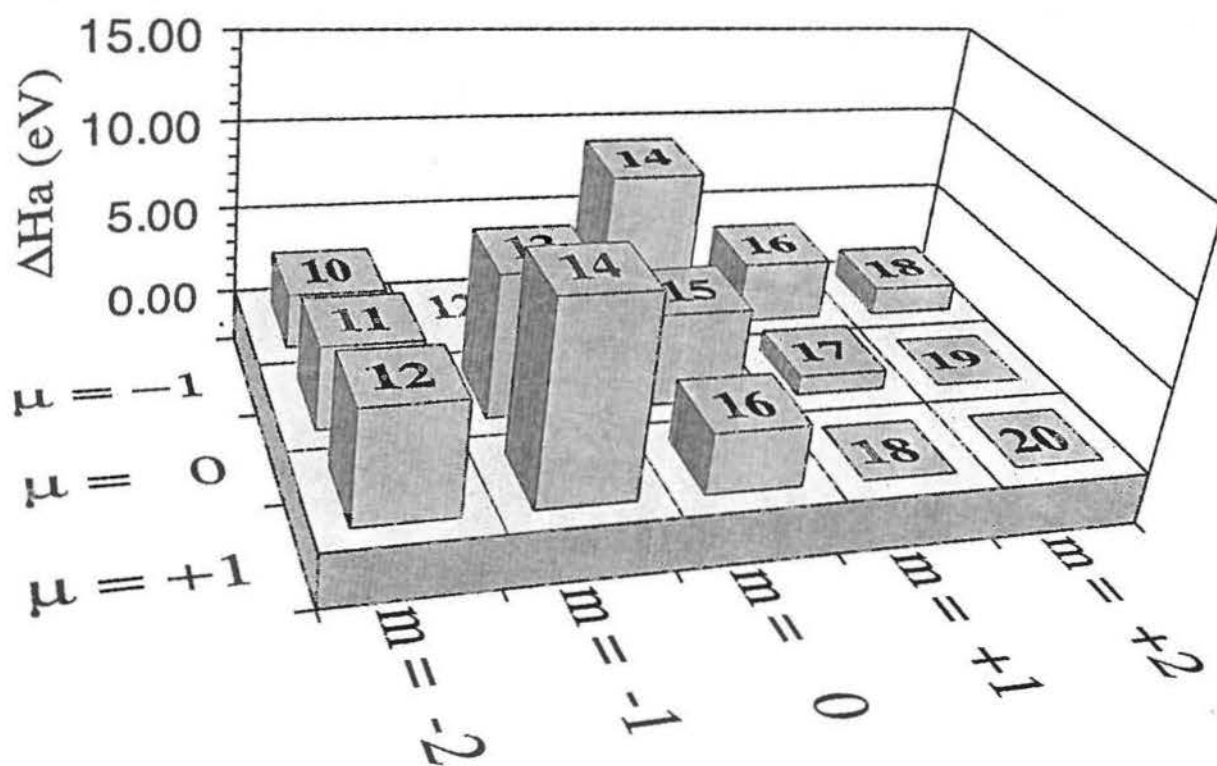
Ionization Potentials for $SO(3) \times SU(2)$ Symmetry



Triatomic Molecules 2^4F multiplet
Single Particle Operator

Figure: 13

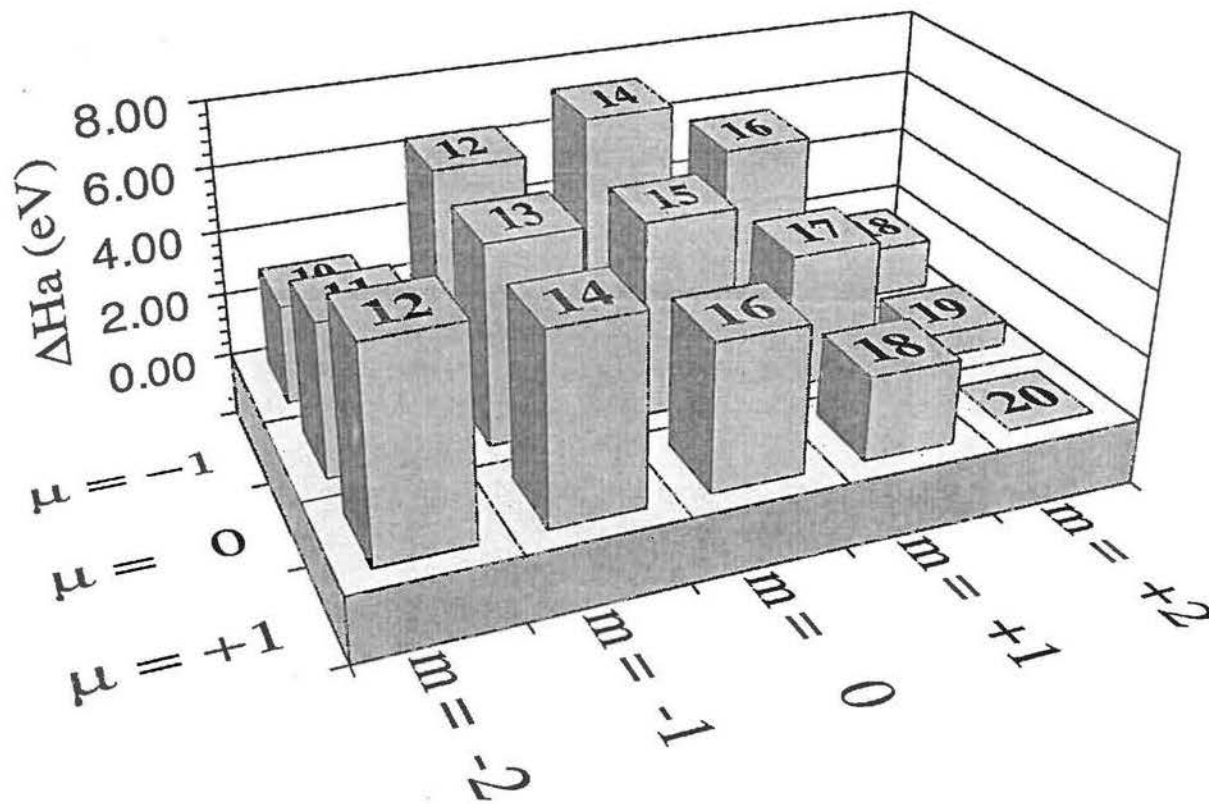
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3D multiplet
Single Particle Operator

Figure: 14

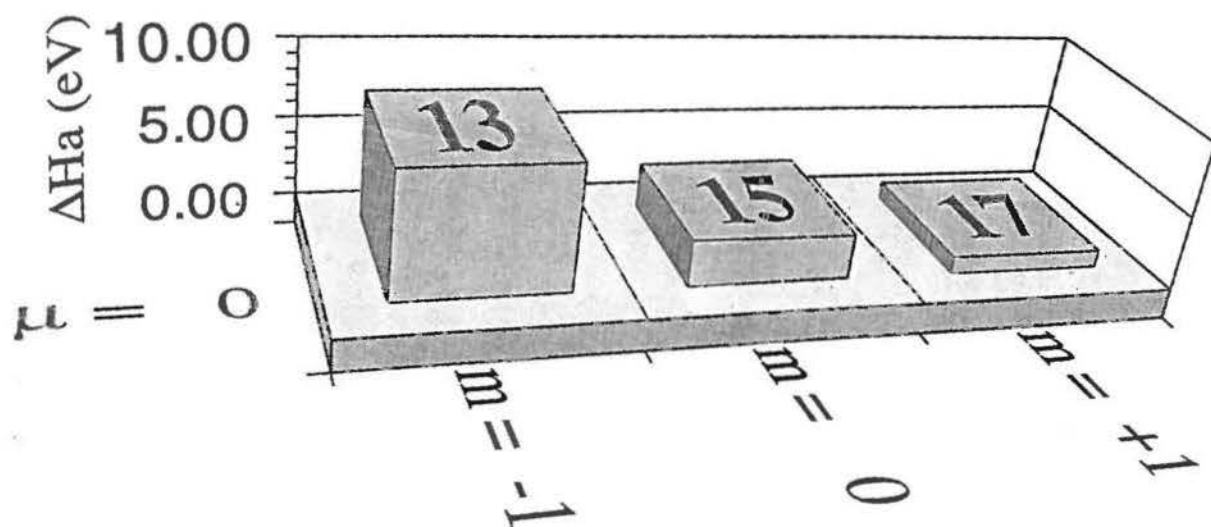
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3D multiplet
Single Particle Operator on Homonuclear Vectors

Figure: 15

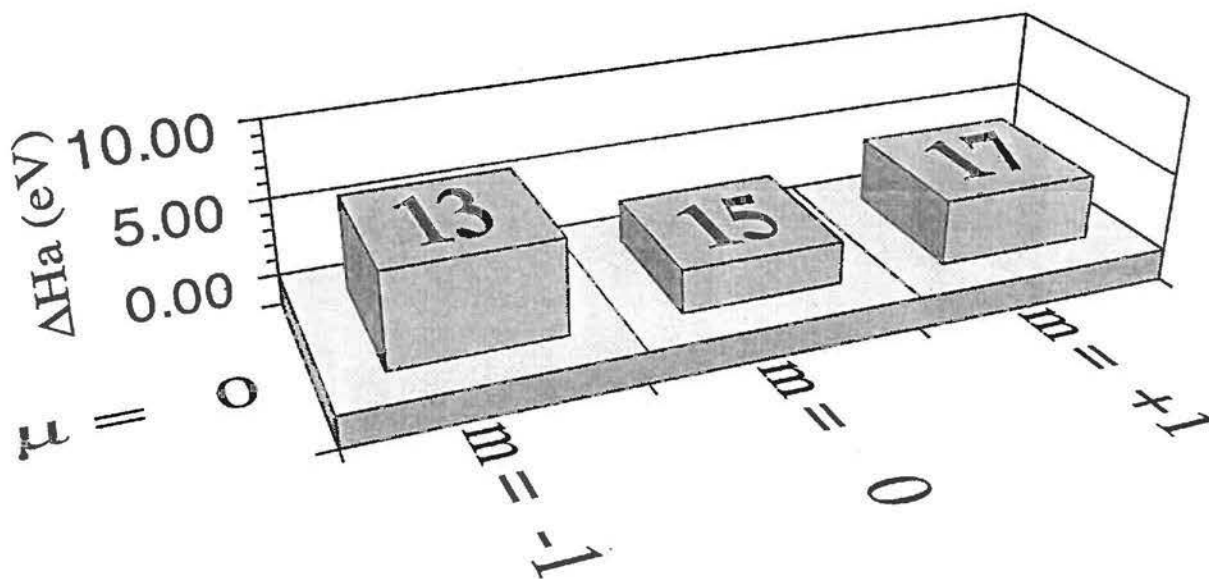
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^1P multiplet
Single Particle Operator

Figure: 16

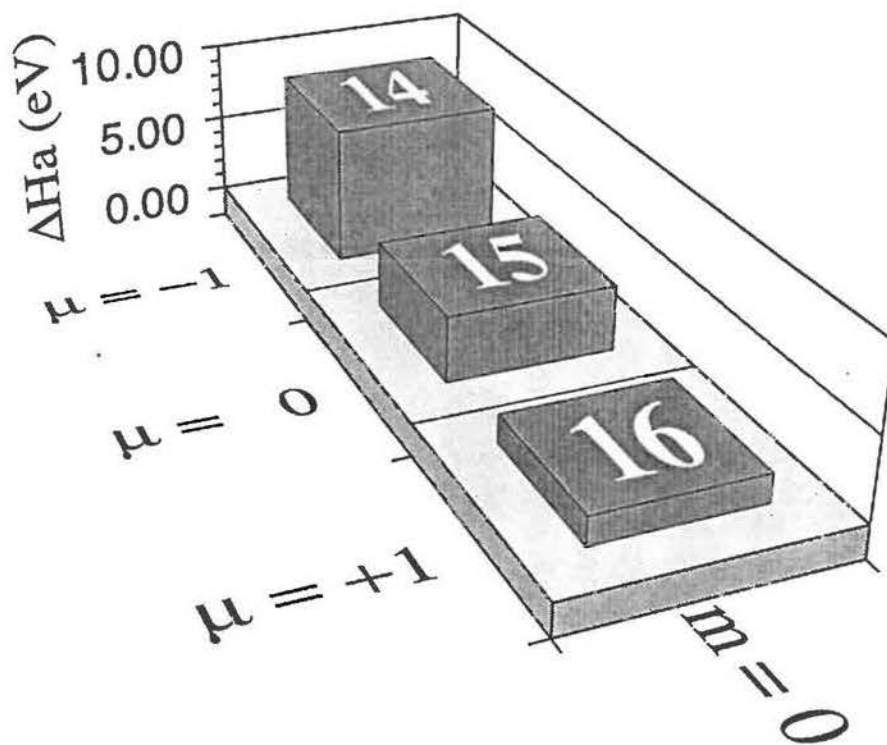
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^1P multiplet
Single Particle Operator on Homonuclear Vectors

Figure: 17

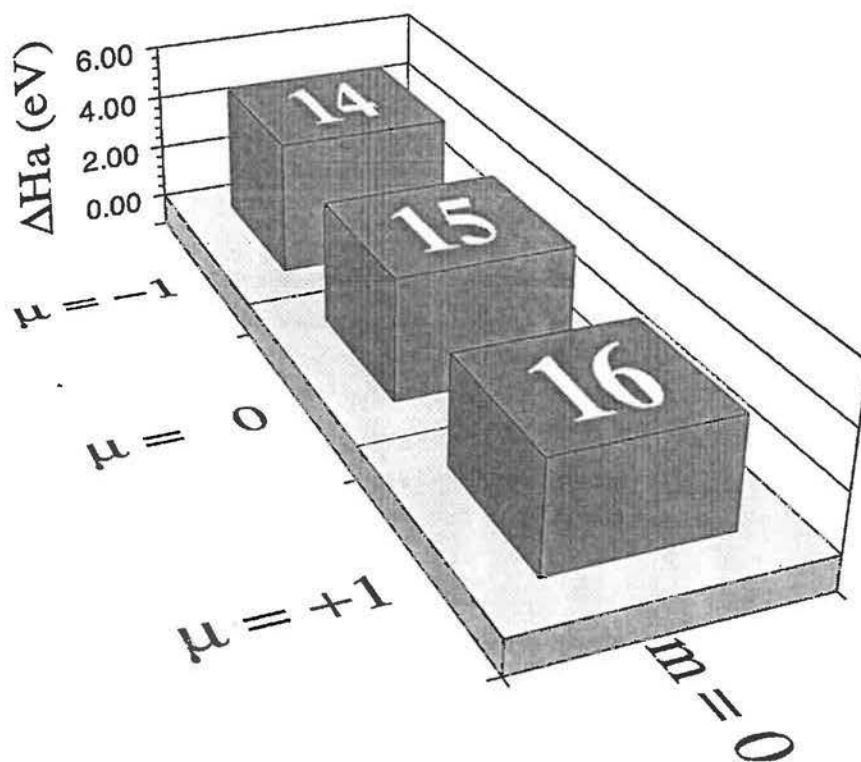
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3S multiplet
Single Particle Operator

Figure: 18

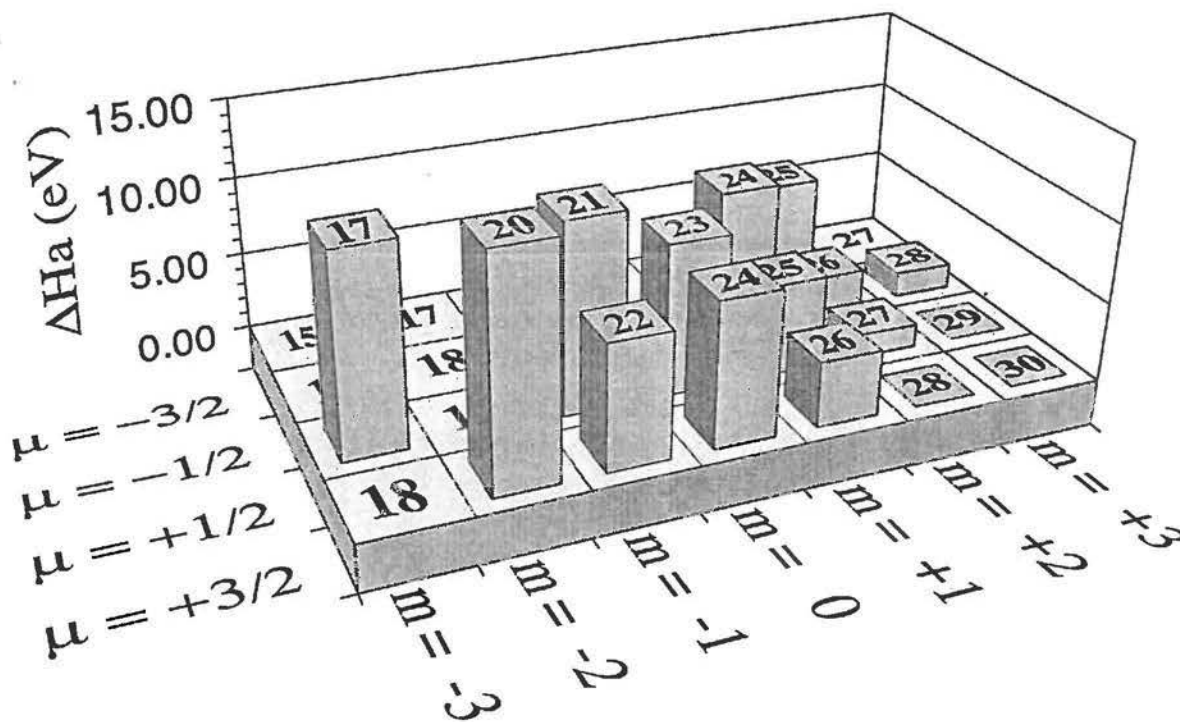
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Diatomic Molecules 2^3S multiplet
Single Particle Operator on Homonuclear Vectors

Figure: 19

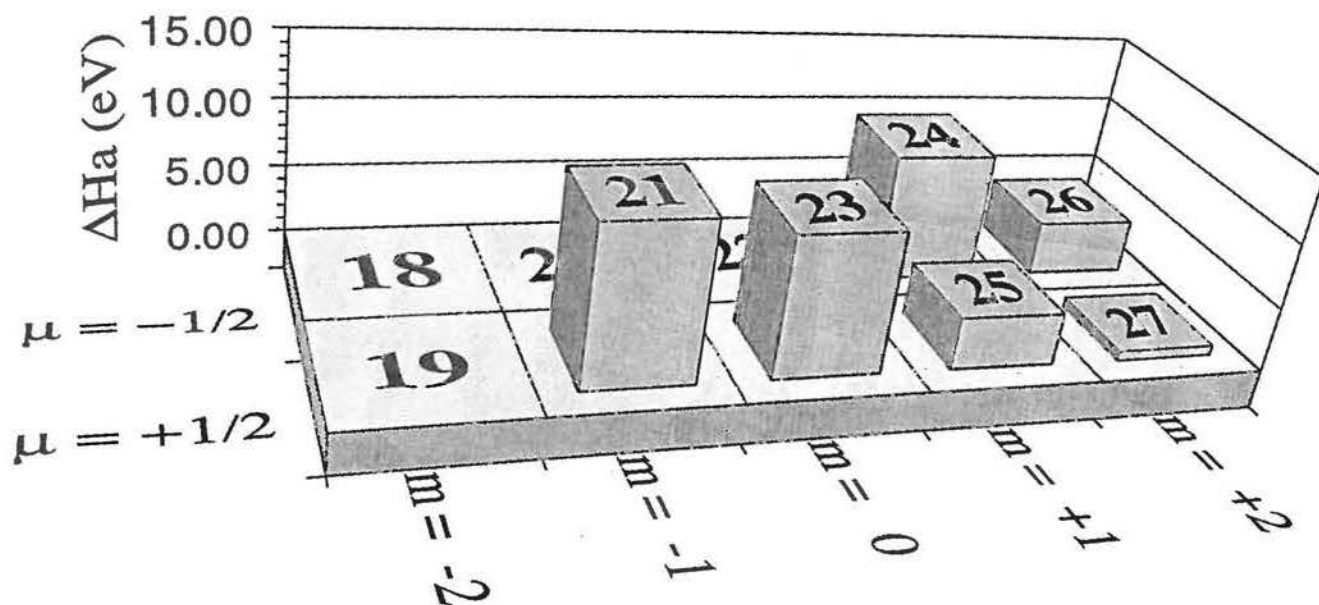
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Triatomic Molecules 2^4F multiplet
Single Particle Operator

Figure: 20

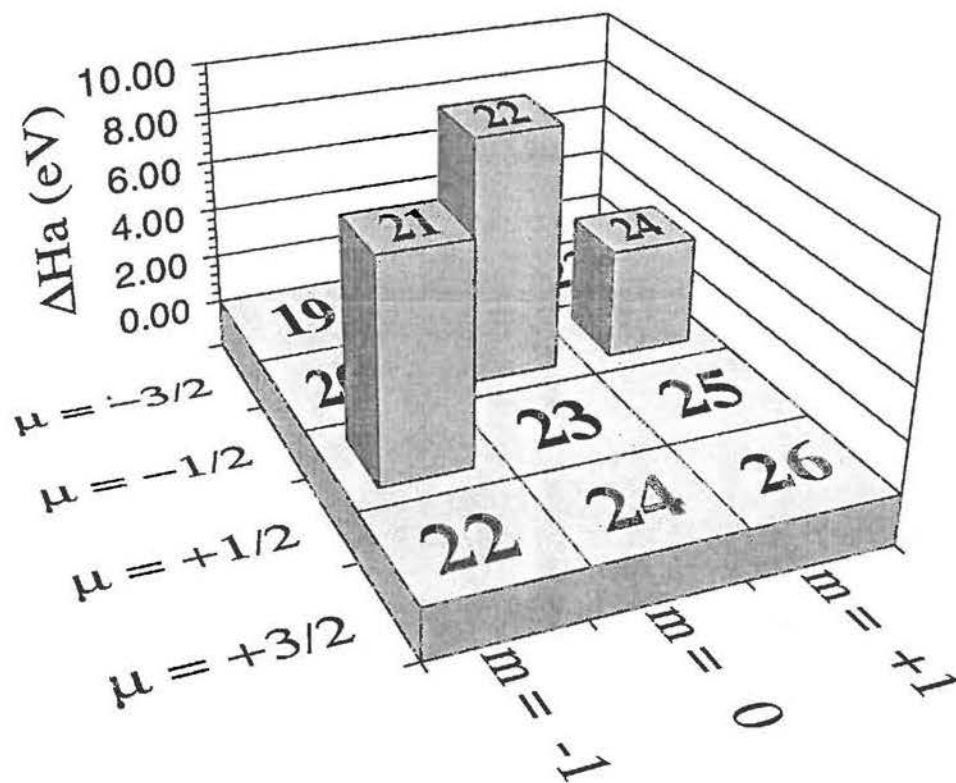
Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Triatomic Molecules 2^2D multiplet
Single Particle Operator

Figure: 21

Heat of Atomization for $SO(3) \times SU(2)$ Symmetry



Triatomic Molecules 2^4P multiplet
Single Particle Operator

Figure: 22

Table 1: Groups ^a	
Group name	Matrices in representation group
U(n)	n x n unitary ($U^H U = I$)
SU(n)	n x n unitary with determinant 1
O(n)	n x n orthogonal ($O^T O = I$)
SO(n)	n x n orthogonal with determinant 1

Captions:

- FIG. 1. The representation space L_1 corresponding to the set of atoms.
- FIG. 2. Diagrammatic relationships between G , A , $GL(L_1)$, and L_1 .
- FIG. 3. The two chains of subgroups of $SO(4,2)$.
- FIG. 4. Multiplets corresponding to the subgroup $SO(4)$.
- FIG. 5. Multiplets corresponding to the subgroup $SO(3)$.
- FIG. 6. Multiplets corresponding to the subgroup $SO(2)$.
- FIG. 7. Periodic system of diatomic molecules formed from B,C,N,O,F,Ne.
- FIG. 8. Ionization potentials for doublet P atoms.
- FIG. 9. Ionization potentials for triplet D diatomic molecules.
- FIG. 10. Ionization potentials for triplet D diatomic molecules using homonuclear identities.
- FIG. 11. Ionization potentials for singlet P diatomic molecules using homonuclear identities.
- FIG. 12. Ionization potentials for triplet S diatomic molecules using homonuclear identities.
- FIG. 13. Ionization potentials for quartet F triatomic molecules.
- FIG. 14. Heat of atomization for triplet D diatomic molecules.
- FIG. 15. Heat of atomization for triplet D diatomic molecules using homonuclear identities.
- FIG. 16. Heat of atomization for singlet P diatomic molecules.
- FIG. 17. Heat of atomization for singlet P diatomic molecules using homonuclear identities.
- FIG. 18. Heat of atomization for triplet S diatomic molecules.
- FIG. 19. Heat of atomization for triplet S diatomic molecules using homonuclear identities.
- FIG. 20. Heat of atomization for quartet F triatomic molecules.
- FIG. 21. Heat of atomization for doublet D triatomic molecules.
- FIG. 22. Heat of atomization for quartet P triatomic molecules.
- TABLE. 1. Different types of groups.